



Full wwPDB/EMDataBank EM Map/Model Validation Report ⓘ

Jan 30, 2018 – 08:15 PM EST

PDB ID : 6B43
EMDB ID: : EMD-7047
Title : CryoEM structure and atomic model of the Kaposi's sarcoma-associated herpesvirus capsid
Authors : Dai, X.H.; Gong, D.Y.; Sun, R.; Zhou, Z.H.
Deposited on : 2017-09-25
Resolution : 4.20 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.

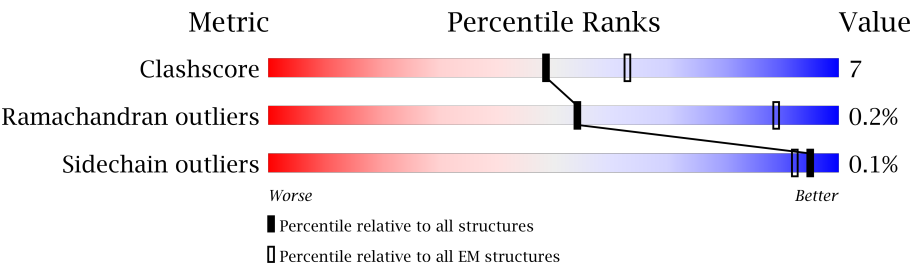
MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030736

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




























Metric	Whole archive (#Entries)	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	4	1376	69% 19% 12%
1	A	1376	80% 18% .
1	B	1376	81% 17% .
1	C	1376	76% 22% .
1	D	1376	77% 21% .
1	E	1376	81% 18% .
1	F	1376	79% 19% .
1	M	1376	79% 19% .
1	N	1376	79% 20% .

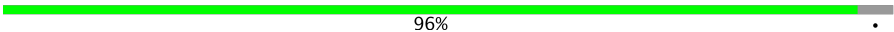








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Mol	Chain	Length	Quality of chain
1	O	1376	
1	S	1376	
1	T	1376	
1	U	1376	
1	V	1376	
1	W	1376	
1	X	1376	
2	0	170	
2	1	170	
2	2	170	
2	3	170	
2	G	170	
2	H	170	
2	I	170	
2	J	170	
2	K	170	
2	L	170	
2	P	170	
2	Q	170	
2	R	170	
2	Y	170	
2	Z	170	
3	5	331	
3	8	331	
3	b	331	

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Mol	Chain	Length	Quality of chain
3	e	331	 96% .
3	h	331	 96% ..
4	6	305	 78% 18% .
4	7	305	 81% 17% .
4	9	305	 77% 19% .
4	a	305	 97% ..
4	c	305	 95% . .
4	d	305	 98% .
4	f	305	 96% . .
4	g	305	 97% . .
4	i	305	 96% .
4	j	305	 97% . .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 214334 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 Major capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1363	Total	C	N	O	S	0	0
			10682	6786	1854	1969	73		
1	B	1355	Total	C	N	O	S	0	0
			10627	6751	1843	1960	73		
1	C	1354	Total	C	N	O	S	0	0
			10621	6748	1842	1959	72		
1	D	1355	Total	C	N	O	S	0	0
			10627	6751	1843	1960	73		
1	E	1363	Total	C	N	O	S	0	0
			10682	6786	1854	1969	73		
1	F	1356	Total	C	N	O	S	0	0
			10638	6757	1847	1961	73		
1	M	1355	Total	C	N	O	S	0	0
			10627	6751	1843	1960	73		
1	N	1363	Total	C	N	O	S	0	0
			10682	6786	1854	1969	73		
1	O	1355	Total	C	N	O	S	0	0
			10627	6751	1843	1960	73		
1	S	1281	Total	C	N	O	S	0	0
			10060	6397	1737	1855	71		
1	T	1360	Total	C	N	O	S	0	0
			10666	6776	1851	1966	73		
1	U	1355	Total	C	N	O	S	0	0
			10627	6751	1843	1960	73		
1	V	1352	Total	C	N	O	S	0	0
			10604	6739	1839	1954	72		
1	W	1354	Total	C	N	O	S	0	0
			10621	6748	1842	1959	72		
1	X	1345	Total	C	N	O	S	0	0
			10548	6701	1829	1946	72		
1	4	1216	Total	C	N	O	S	0	0
			9586	6102	1665	1748	71		

- Molecule 2 is a protein called Small capsomere-interacting protein.

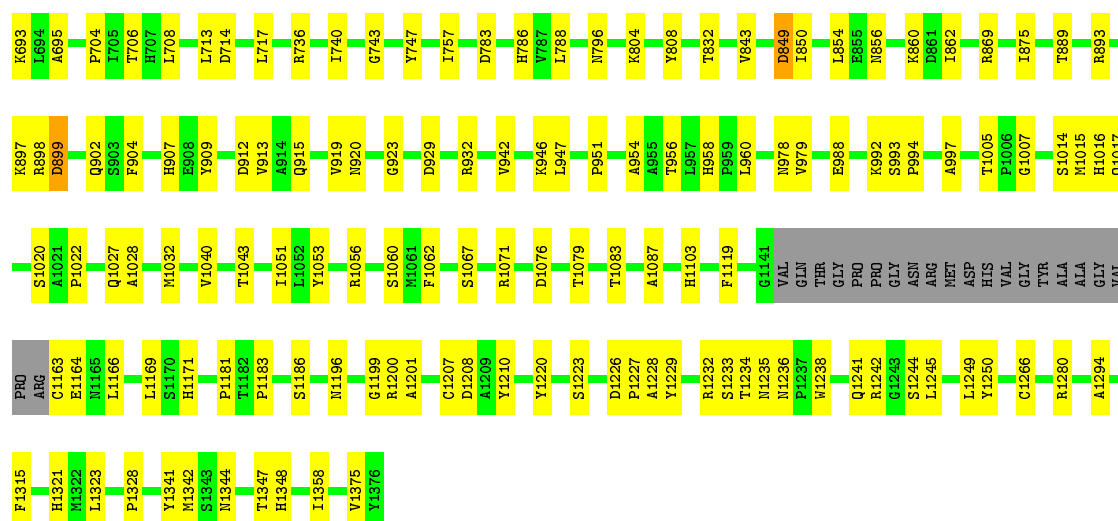
Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	78	Total	C	N	O	S	0	0
			666	418	130	115	3		
2	H	78	Total	C	N	O	S	0	0
			666	418	130	115	3		
2	I	78	Total	C	N	O	S	0	0
			666	418	130	115	3		
2	J	78	Total	C	N	O	S	0	0
			666	418	130	115	3		
2	K	78	Total	C	N	O	S	0	0
			666	418	130	115	3		
2	L	78	Total	C	N	O	S	0	0
			666	418	130	115	3		
2	P	78	Total	C	N	O	S	0	0
			666	418	130	115	3		
2	Q	78	Total	C	N	O	S	0	0
			666	418	130	115	3		
2	R	78	Total	C	N	O	S	0	0
			666	418	130	115	3		
2	Y	78	Total	C	N	O	S	0	0
			666	418	130	115	3		
2	Z	78	Total	C	N	O	S	0	0
			666	418	130	115	3		
2	0	78	Total	C	N	O	S	0	0
			666	418	130	115	3		
2	1	78	Total	C	N	O	S	0	0
			666	418	130	115	3		
2	2	78	Total	C	N	O	S	0	0
			666	418	130	115	3		
2	3	78	Total	C	N	O	S	0	0
			666	418	130	115	3		

- Molecule 3 is a protein called Triplex capsid protein 1.

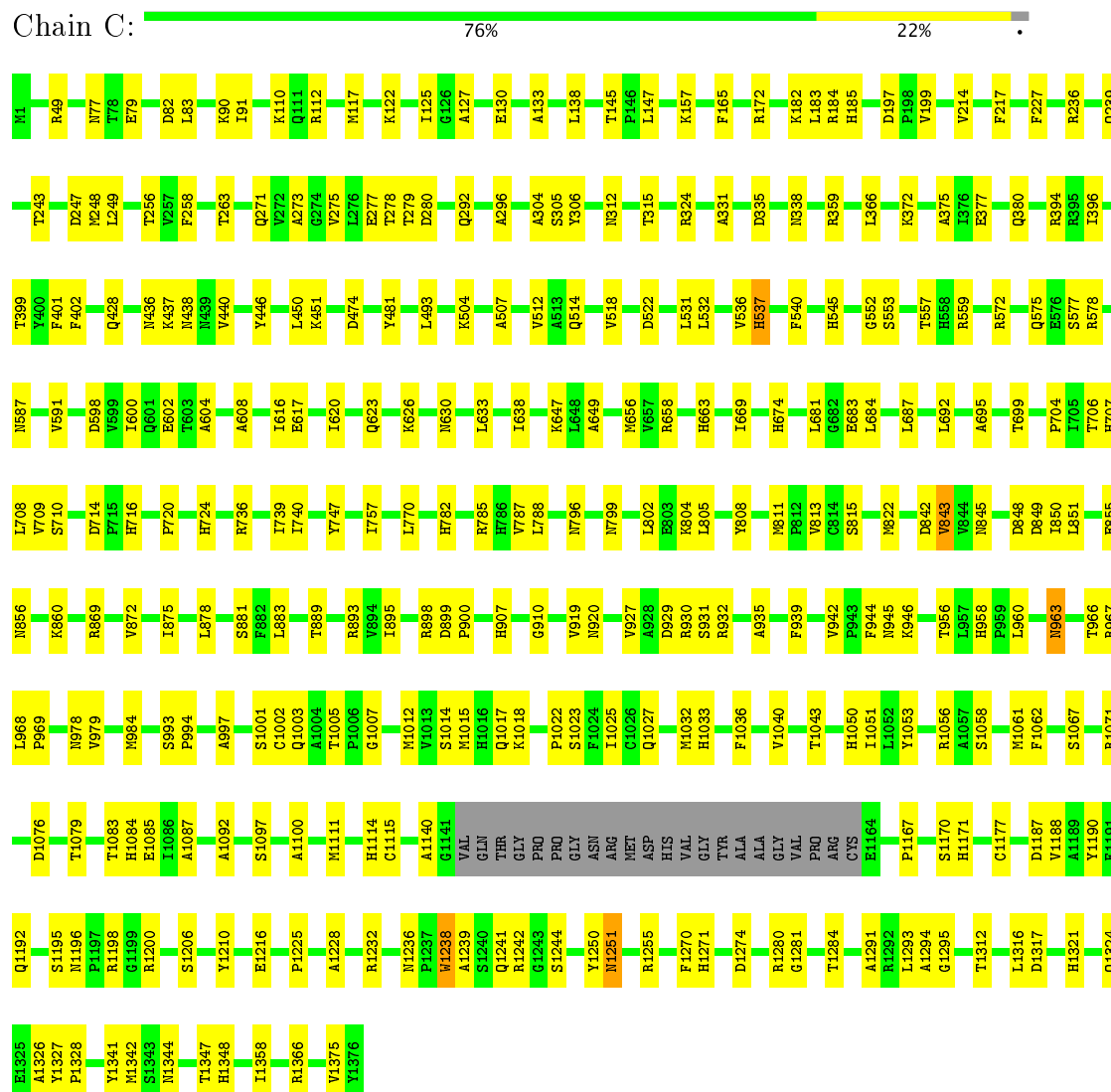
Mol	Chain	Residues	Atoms					AltConf	Trace
3	5	319	Total	C	N	O	S	0	0
			2463	1578	421	449	15		
3	8	321	Total	C	N	O	S	0	0
			2477	1586	424	452	15		
3	b	321	Total	C	N	O	S	0	0
			2477	1586	424	452	15		
3	e	319	Total	C	N	O	S	0	0
			2460	1575	422	448	15		
3	h	321	Total	C	N	O	S	0	0
			2477	1586	424	452	15		

- Molecule 4 is a protein called Triplex capsid protein 2.


Mol	Chain	Residues	Atoms					AltConf	Trace
4	6	294	Total	C	N	O	S	0	0
			2329	1485	397	433	14		
4	7	300	Total	C	N	O	S	0	0
			2364	1505	401	443	15		
4	9	294	Total	C	N	O	S	0	0
			2329	1485	397	433	14		
4	a	300	Total	C	N	O	S	0	0
			2364	1505	401	443	15		
4	c	294	Total	C	N	O	S	0	0
			2329	1485	397	433	14		
4	d	300	Total	C	N	O	S	0	0
			2364	1505	401	443	15		
4	f	294	Total	C	N	O	S	0	0
			2329	1485	397	433	14		
4	g	300	Total	C	N	O	S	0	0
			2364	1505	401	443	15		
4	i	294	Total	C	N	O	S	0	0
			2329	1485	397	433	14		
4	j	300	Total	C	N	O	S	0	0
			2364	1505	401	443	15		

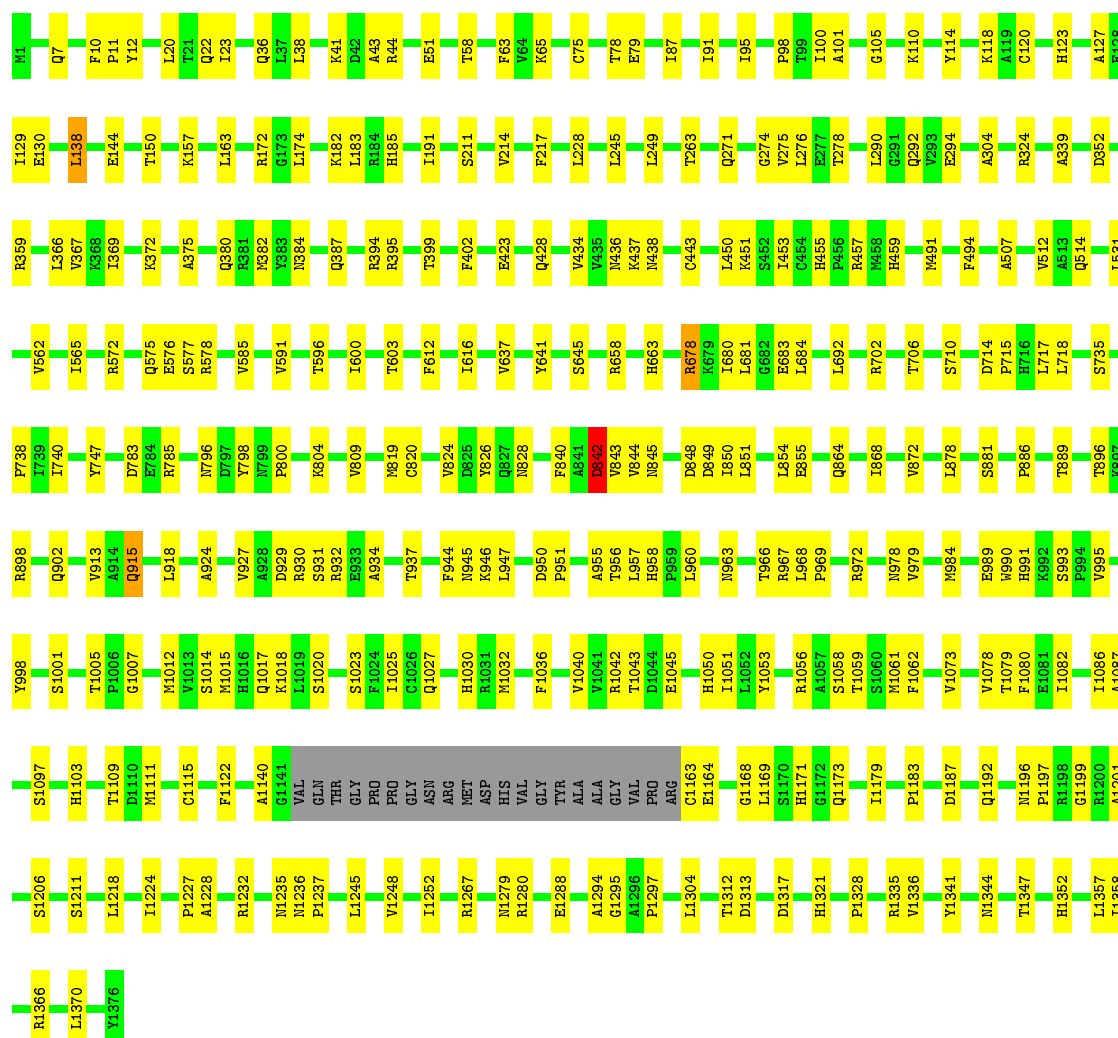


• Molecule 1: Major capsid protein




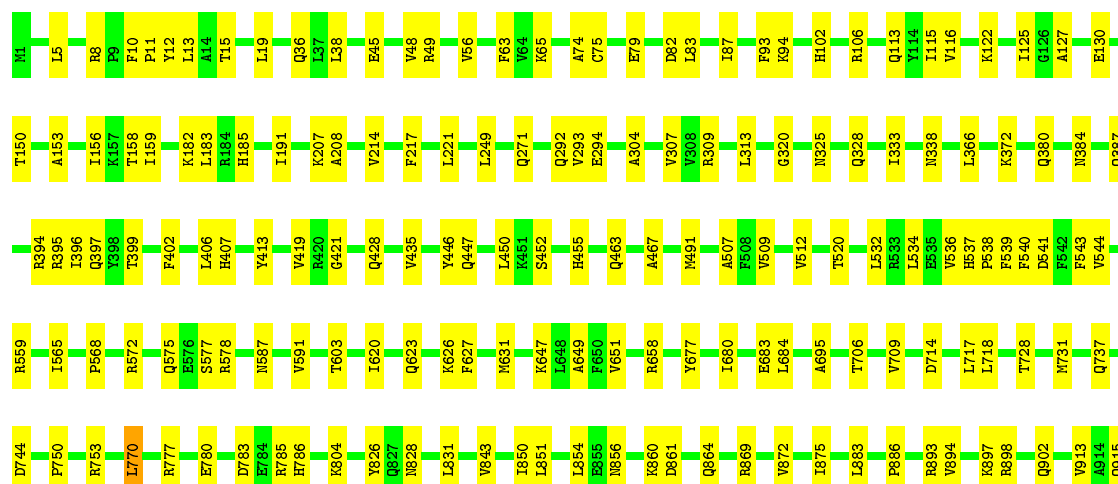
• Molecule 1: Major capsid protein

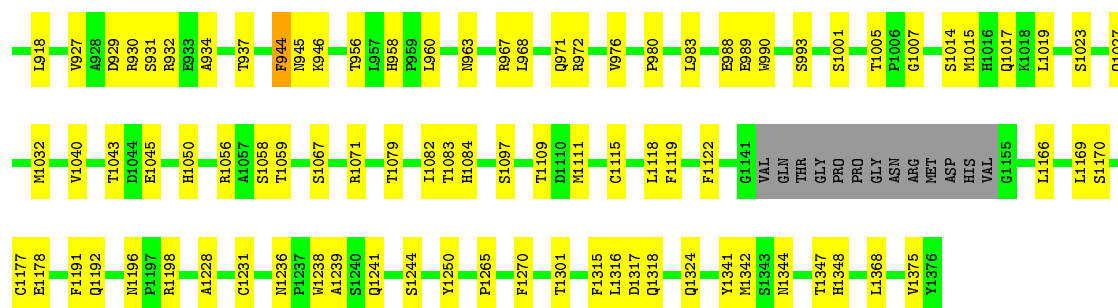
Chain D:  77% 21%



• Molecule 1: Major capsid protein

Chain E:  81% 18%





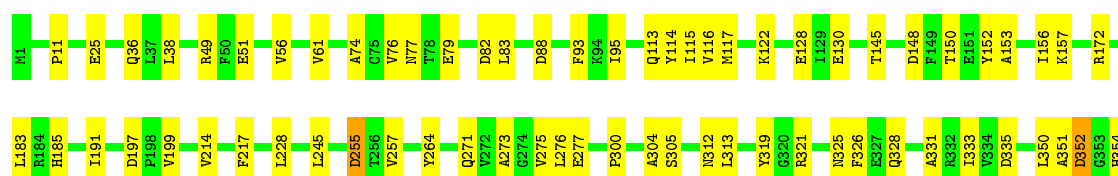
• Molecule 1: Major capsid protein

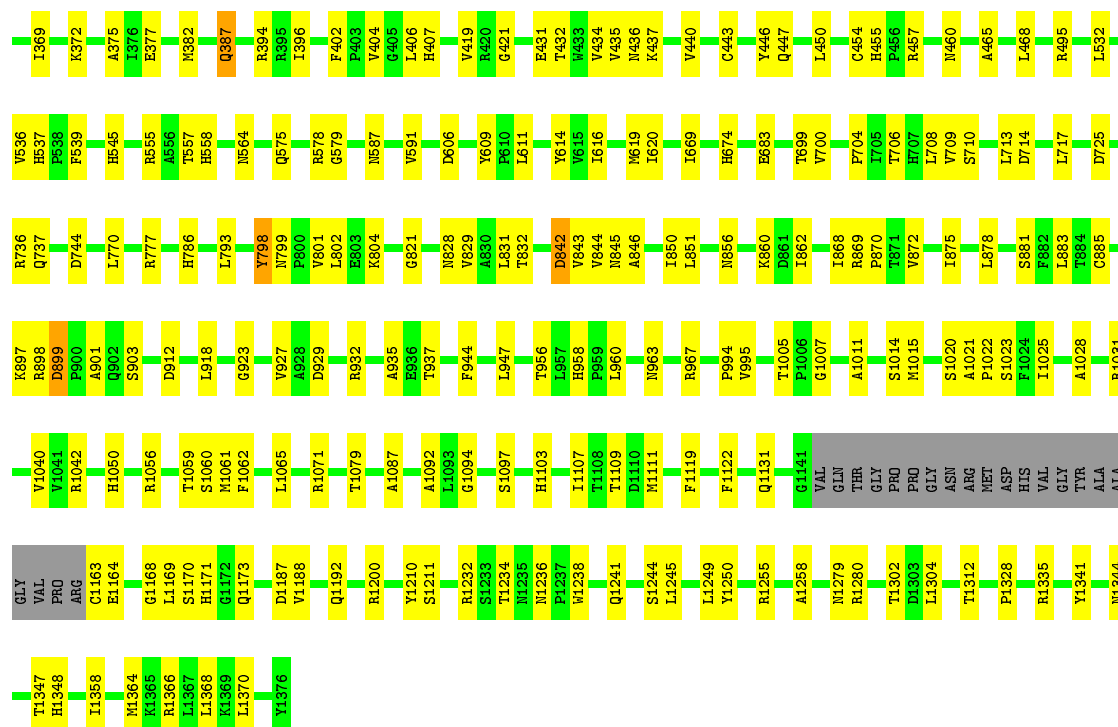
Chain F: 79% 19%



• Molecule 1: Major capsid protein

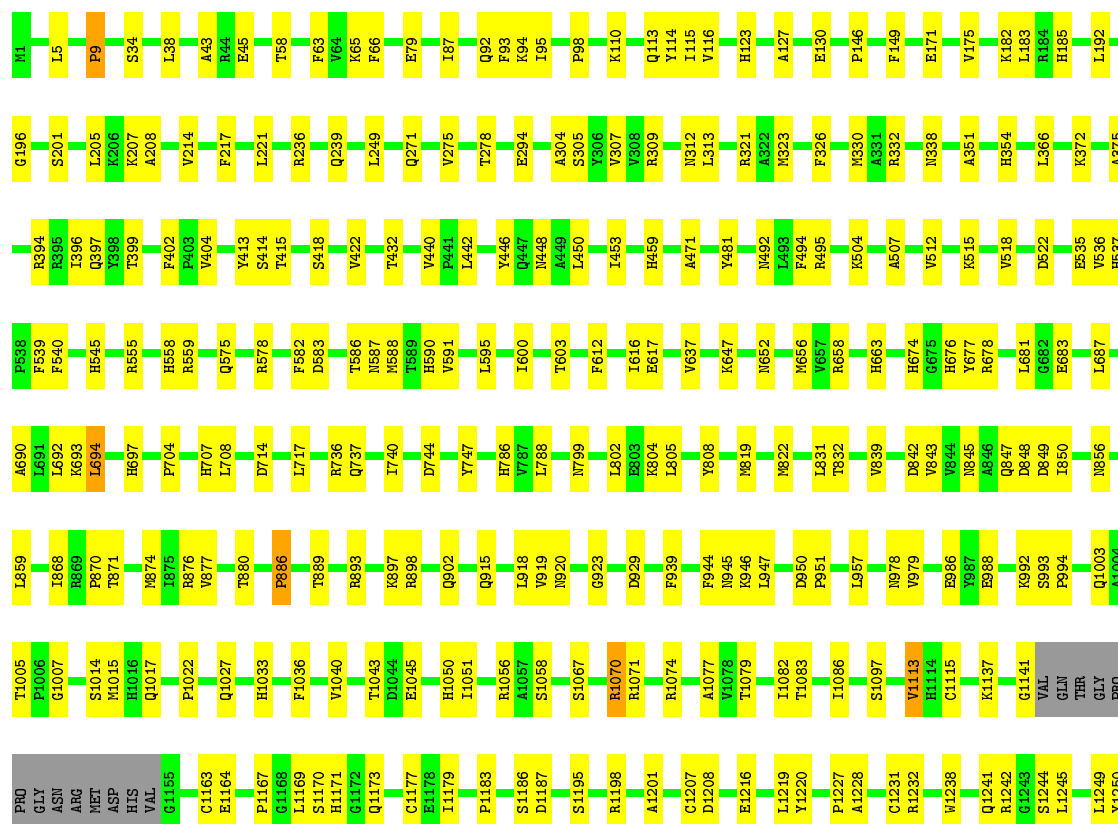
Chain M: 79% 19%

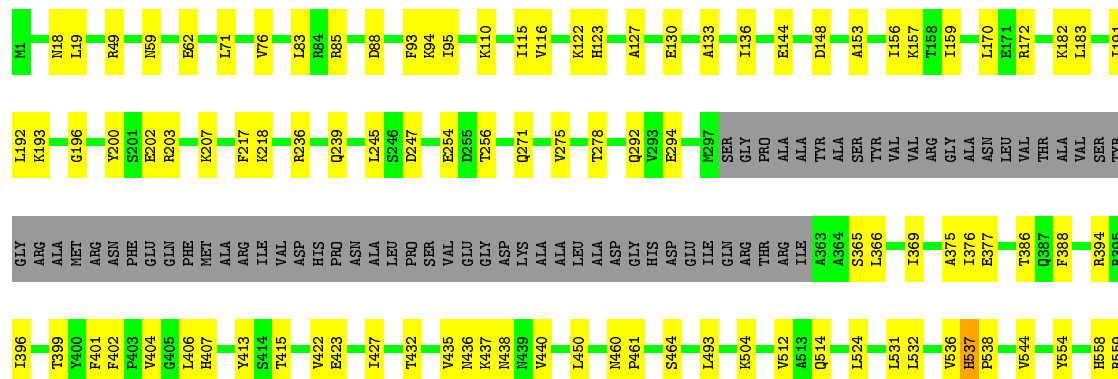


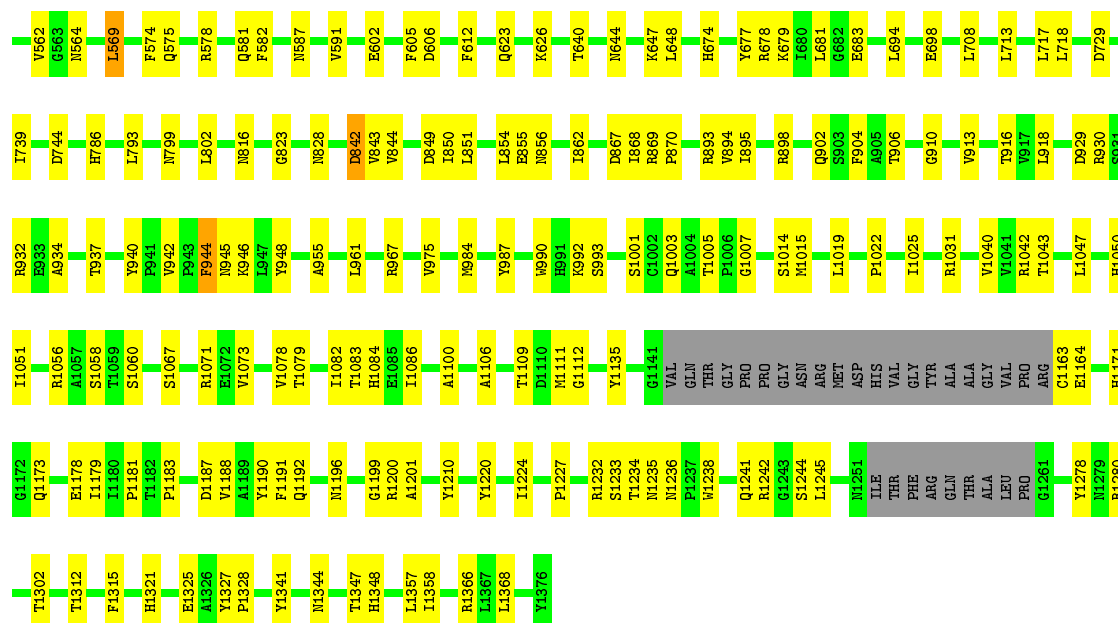


• Molecule 1: Major capsid protein

Chain N: 79% 20%

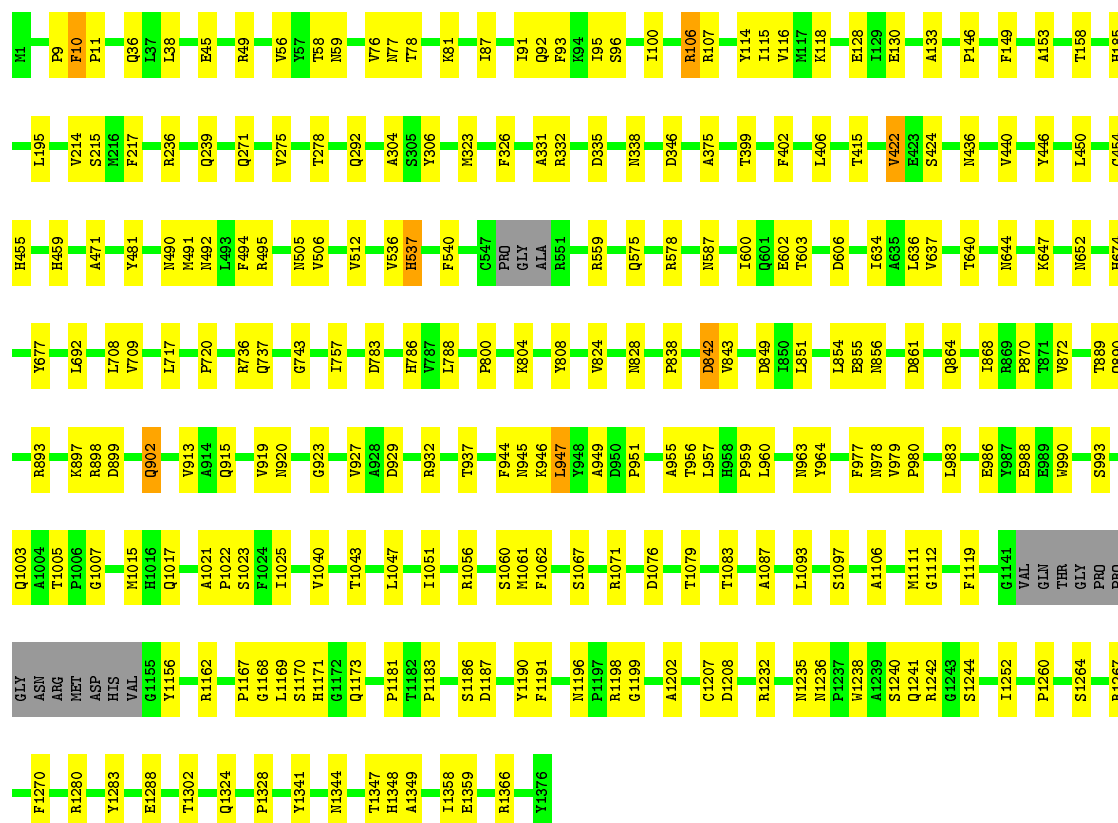






• Molecule 1: Major capsid protein

Chain T: 81% 17%




• Molecule 1: Major capsid protein

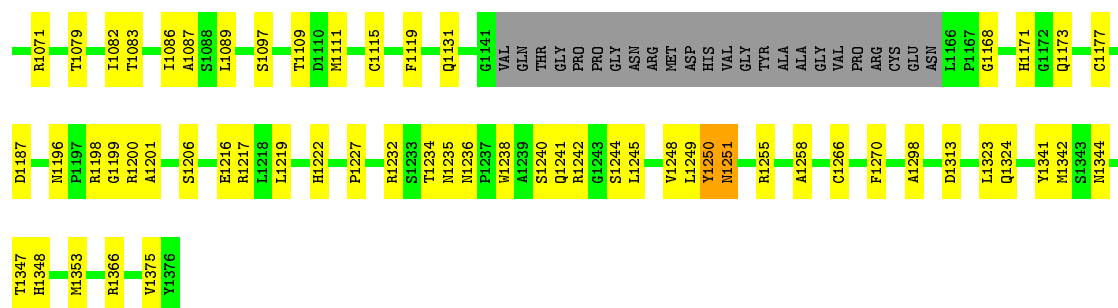
Chain U: 78% 20%

H1	L192	L406	T560	R762	V927	A1057	G1163	F1270
L5	K206	S414	M561	D765	R930	S1058	P1167	R1280
F10	K207	T415	M564	I773	S931	T1059	G1168	R1281
P11	S211	S416	R572	T776	R932	M1061	E1288	E1288
V12	V214	V417	Q575	T776	R933	F1062	S1170	A1284
L13	F217	S418	E576	E780	A934	V1068	H1171	G1295
Q36	R217	R420	S577	D783	R935	R1071	C1177	D1313
L38	A251	V422	R578	E784	T937	T1079	E1178	V1314
R49	V252	Q428	G579	R785	P941	T1082	F1190	F1315
A52	V257	N436	V991	R804	V942	I1085	Q1318	Q1348
L54	Y264	K437	D606	R804	F943	E1085	H1321	H1321
B59	Q271	N438	A618	Y807	N945	I1086	A1326	A1326
A73	V275	V439	M619	Y826	I947	S1088	R1200	H1334
A74	L276	V440	K626	Q627	A948	L1089	A1201	R1335
C75	E277	Y446	Y641	R828	A949	T1091	Y1210	V1336
V76	L290	L450	K647	D842	L957	S1096	L1218	N1344
D82	G291	T453	F650	V844	V979	G1115	I1224	T1347
L83	Q292	C454	V651	R845	E986	T1116	P1225	Q1355
R84	L313	H455	I660	D848	E989	D1117	P1227	Y1376
L87	P300	L468	H663	N856	R991	F1122	A1228	Y1229
I91	V307	Y481	N666	G857	Y1127	Y1127	S1233	S1233
Q92	R309	N491	H674	T858	C1002	Q1128	T1234	T1234
F93	L313	N492	Y677	R860	Q1003	Q1131	N1235	N1235
K94	R332	L493	E683	D861	T1005	K1137	P1237	N1236
I95	N338	Q514	V872	Q864	F1006	G1141	N1238	Y1238
K110	Q113	V518	G701	R876	A1011	VAL	Q1241	Q1241
I115	V343	D522	L708	S881	S1014	GLN	R1242	G1243
V116	L350	L523	V709	P887	M1015	THR	S1244	S1244
K118	V367	L531	L712	T889	P1022	GLY	D1247	D1247
K122	A375	L532	D714	T889	S1023	ASN	Y1250	Y1250
H123	I376	V536	M731	K897	F1024	ARG	N1251	N1251
L138	E377	H537	P538	D899	T1025	MET	I1252	I1252
K143	P389	P539	R736	S903	C1026	ASP	T1253	T1253
T150	R394	F540	P738	L918	Q1027	HIS	F1254	F1254
E151	I395	F543	K741	V919	M1032	VAL	A1258	A1258
I152	I396	R555	N746	N920	T1043	GLY	L1259	L1259
A153	Q397	R555	N746	R921	H1050	ALA	P1260	P1260
K182	T399	R559	N746	F922	S1055	GLY	S1264	S1264
					R1056	VAL	R1267	R1267
						ARG		

• Molecule 1: Major capsid protein

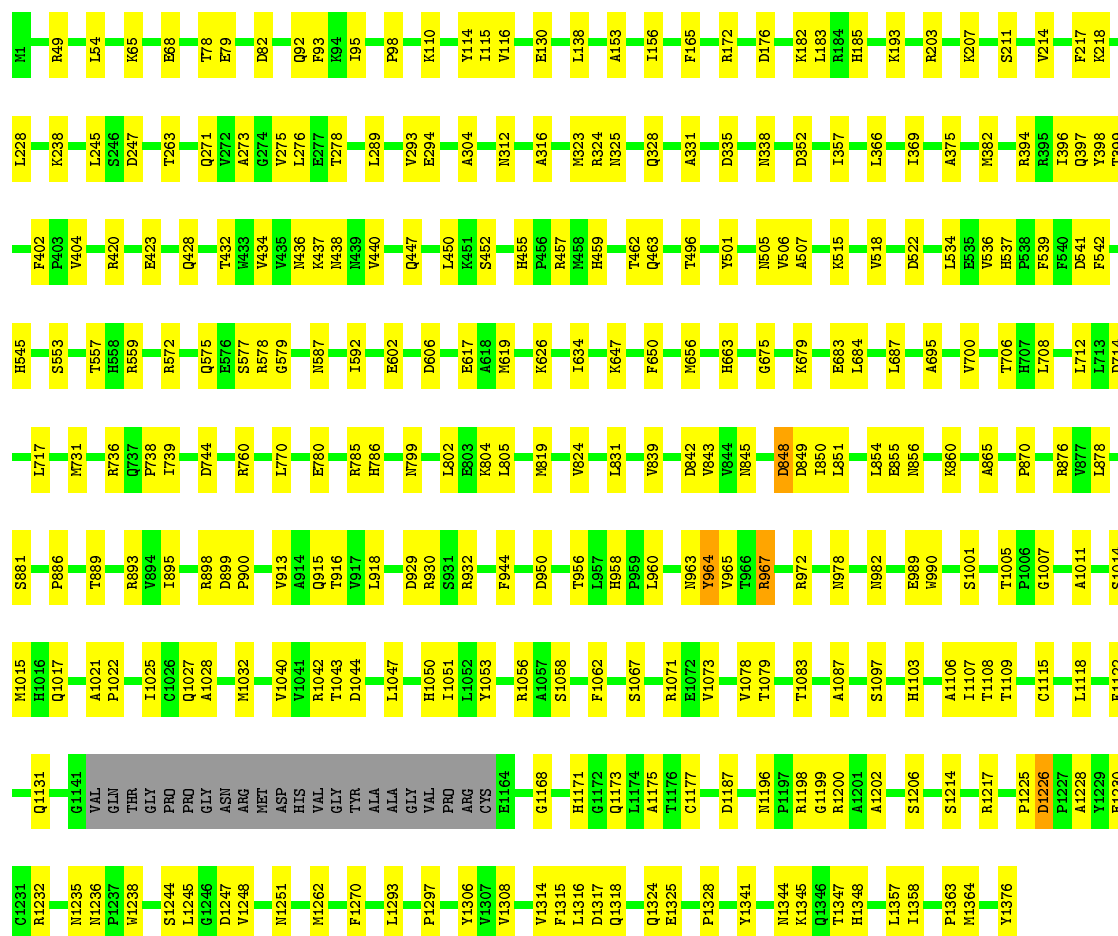
Chain V:  79% 19% •

H1	K182	L376	R578	H786	H958
R8	L183	E377	F582	D797	F959
K41	H185	R394	V685	Y798	L960
R44	D197	I395	I592	L802	N963
R49	P198	Q397	D606	L805	T966
V56	V199	T399	E617	L805	R967
N59	R203	T415	A618	V813	L968
H60	K207	Q428	M619	V813	V979
V61	S211	V434	K647	R828	L983
V76	V214	V435	M656	V829	S993
N77	F217	N436	V657	L830	P994
V78	K218	K437	R658	T832	Y998
E79	H224	N438	H663	D842	T1005
F80	M244	V440	K679	V843	P1006
L83	V252	Q443	I680	D848	G1007
I87	V252	Q447	L684	R850	M1012
R88	T263	L450	L694	E855	V1013
G89	T266	H455	V700	R856	S1014
I91	Q271	P456	T706	Q864	M1015
F93	L276	R457	R707	Q867	Q1017
K94	E277	Q463	L712	V872	K1018
H102	R284	Y481	L713	S881	L1019
R106	N288	N491	L717	K897	S1020
Y114	M297	N492	P720	R898	S1023
V116	A304	F494	R736	D899	F1024
H123	S305	R495	I740	Q915	I1025
A127	L313	Q514	G743	T916	H1030
E130	S318	H525	P720	V917	H1033
E142	M323	T527	R736	R930	F1036
K143	R324	L531	I740	S931	R1042
P146	N338	L532	G743	A934	T1043
F149	R359	H537	Y747	T937	H1050
K157	R361	Q567	N752	Y940	Y1053
F165	I362	P468	T755	F944	C1054
A375	A375	L569	E780	N945	S1055
			D783	R947	R1056
			E784	F1062	S1058
			S577	S1067	T1059
					S1060
					K1061
					F1062
					S1067



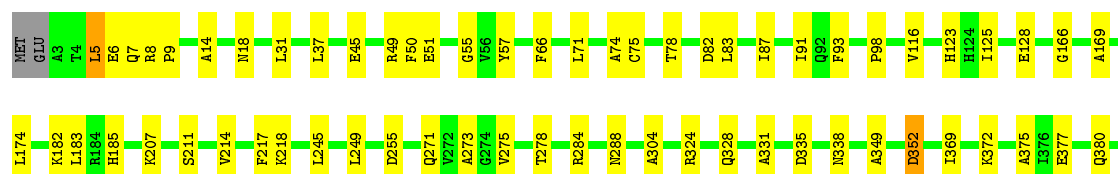
- Molecule 1: Major capsid protein

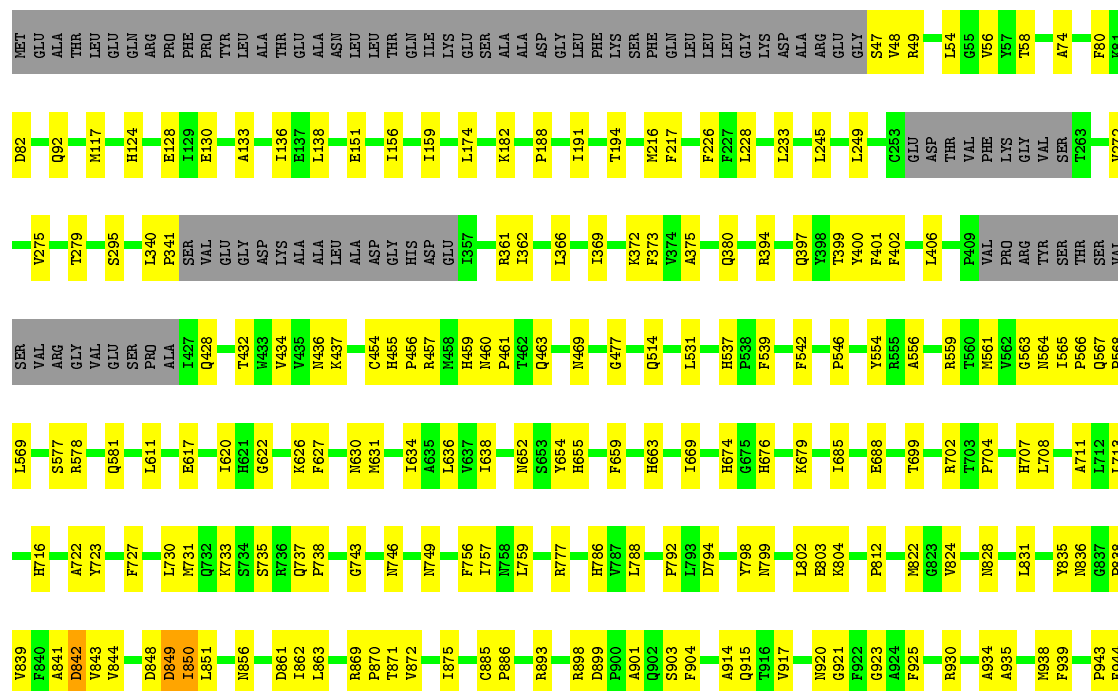
Chain W: 78% 20% .

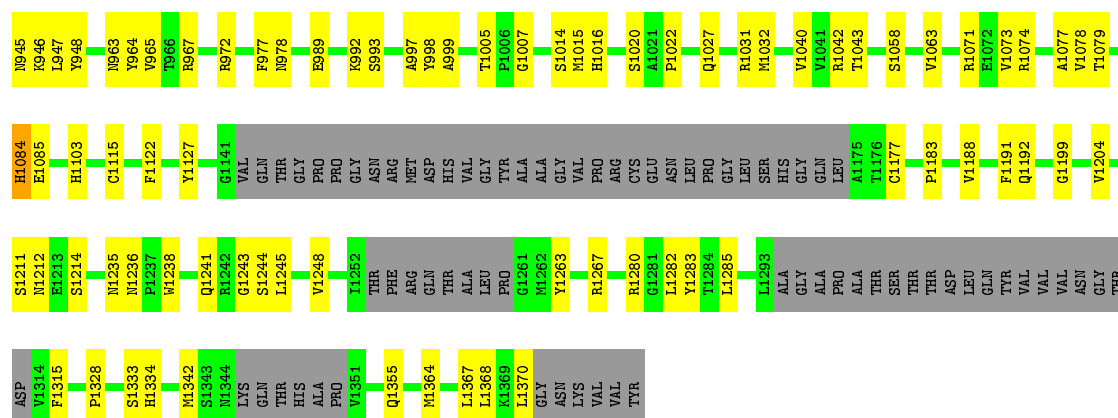


- Molecule 1: Major capsid protein

Chain X: 77% 20% .

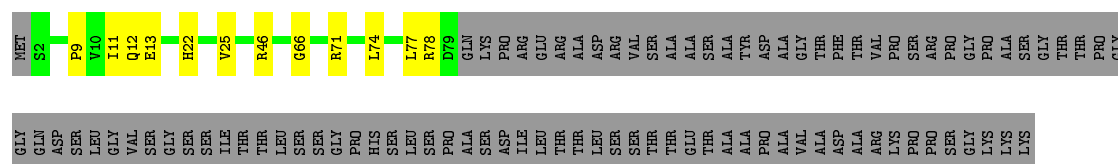






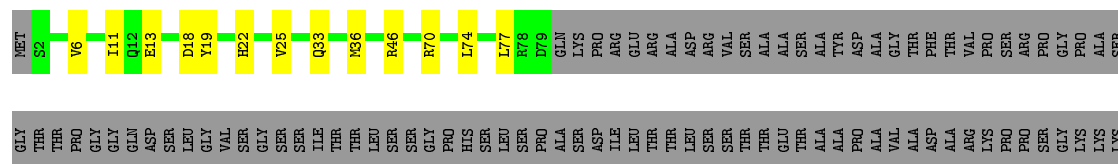
- Molecule 2: Small capsomere-interacting protein

Chain G:



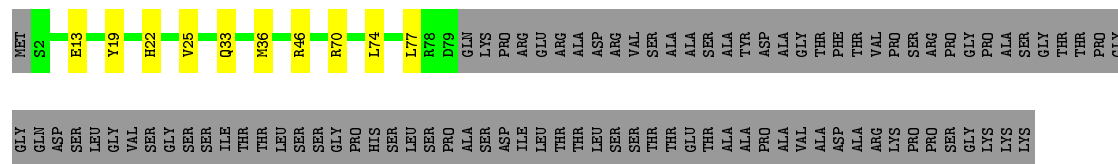
- Molecule 2: Small capsomere-interacting protein

Chain H:



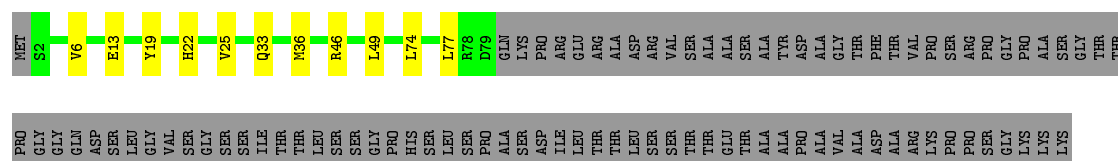
- Molecule 2: Small capsomere-interacting protein

Chain I:

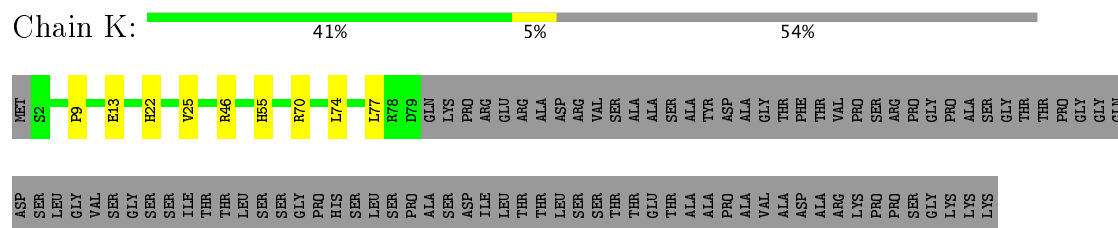


- Molecule 2: Small capsomere-interacting protein

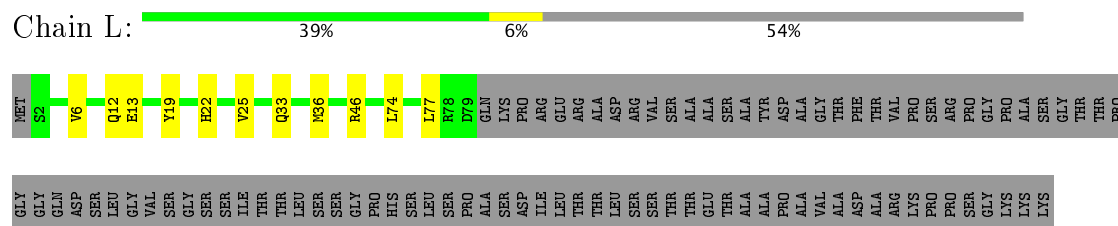
Chain J:



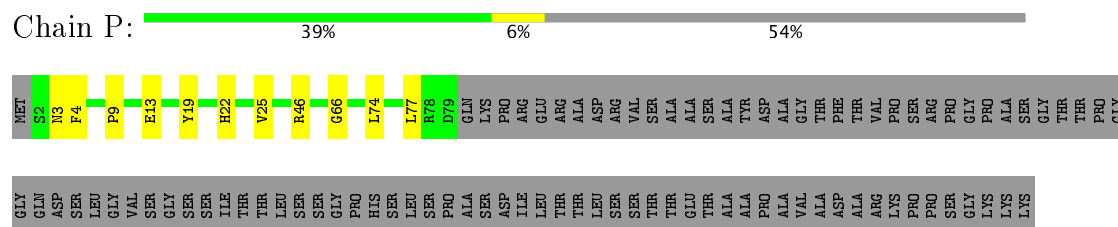
- Molecule 2: Small capsomere-interacting protein



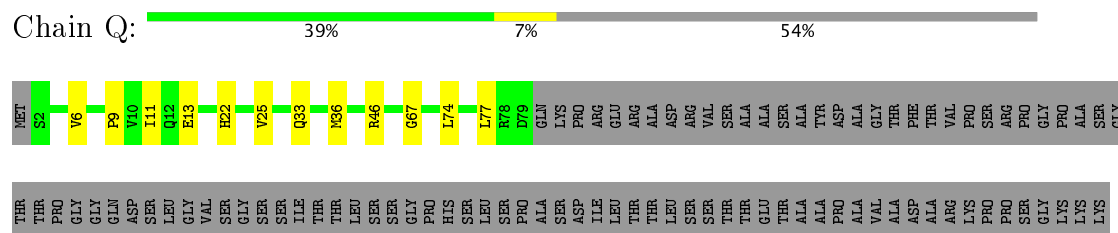
- Molecule 2: Small capsomere-interacting protein



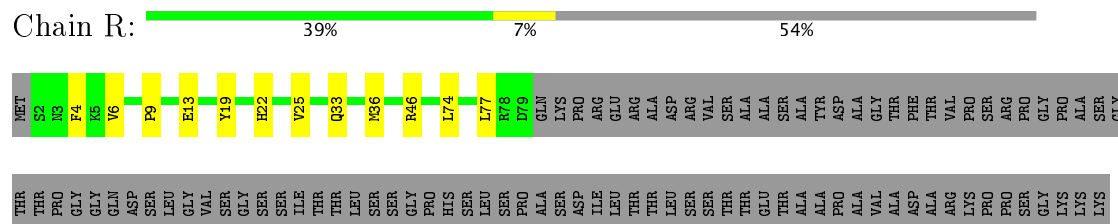
- Molecule 2: Small capsomere-interacting protein



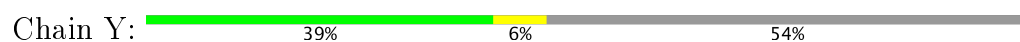
- Molecule 2: Small capsomere-interacting protein



- Molecule 2: Small capsomere-interacting protein



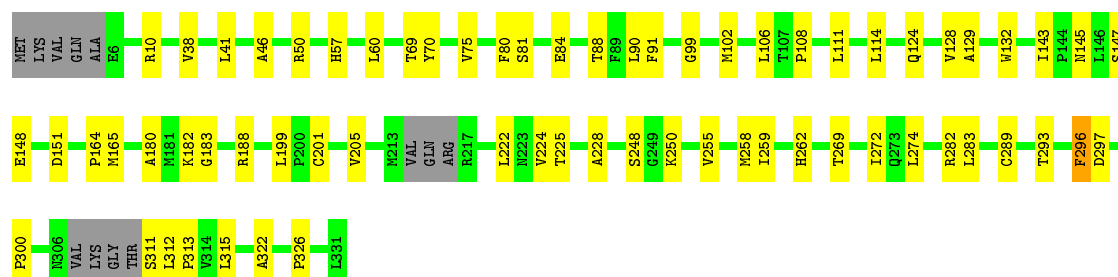
- Molecule 2: Small capsomere-interacting protein



THR THR LYS PRO GLY GLN GLN ASP SER LEU GLY VAL SER GLY SER SER ILE THR THR LEU SER SER GLY PRO HIS SER LEU SER PRO ALA SER ASP ILE LEU THR THR LEU SER SER THR THR GLU THR ALA ALA PRO ALA VAL ALA ASP ALA ARG LYS PRO SER GLY LYS LYS

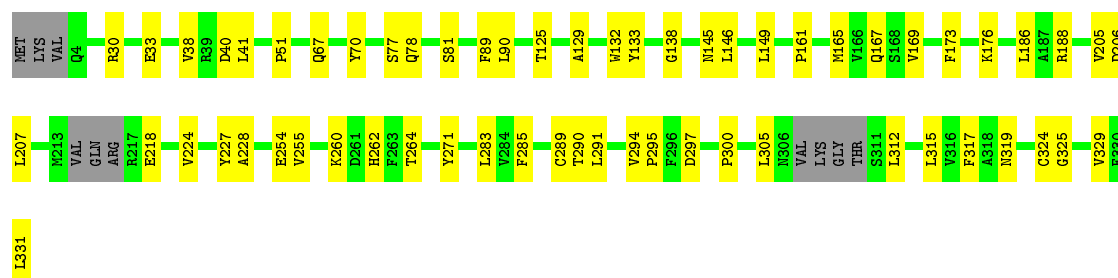
- Molecule 3: Triplex capsid protein 1

Chain 5:  76% 20% .



- Molecule 3: Triplex capsid protein 1

Chain 8:  79% 18% .



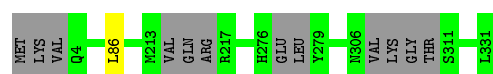
- Molecule 3: Triplex capsid protein 1

Chain b:  97% .



- Molecule 3: Triplex capsid protein 1

Chain e:  96% .

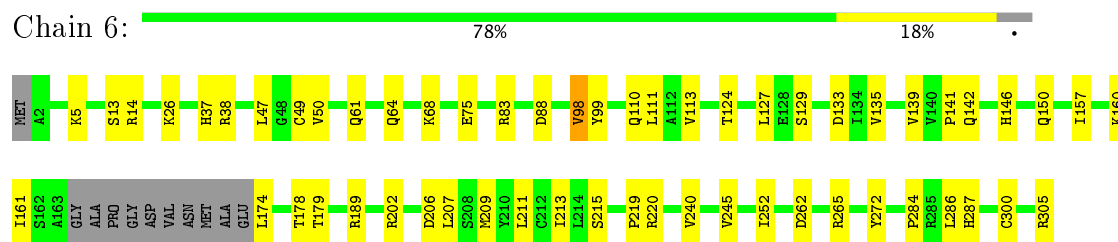


- Molecule 3: Triplex capsid protein 1

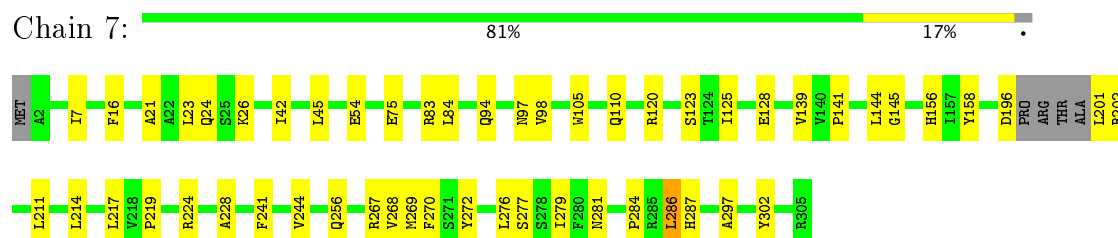
Chain h:  96% . .



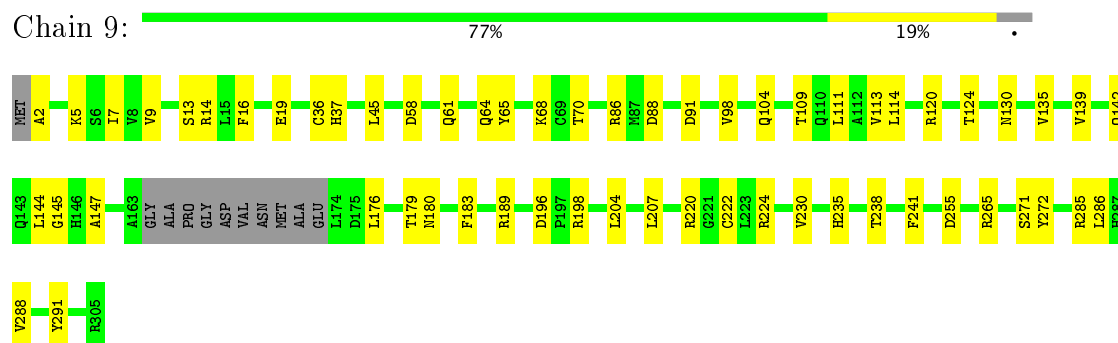
- Molecule 4: Triplex capsid protein 2



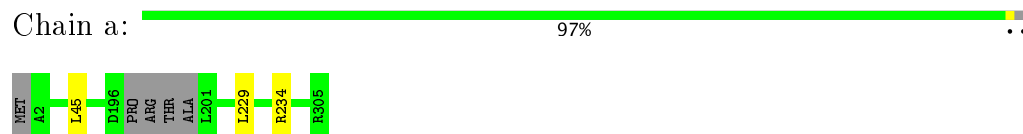
- Molecule 4: Triplex capsid protein 2



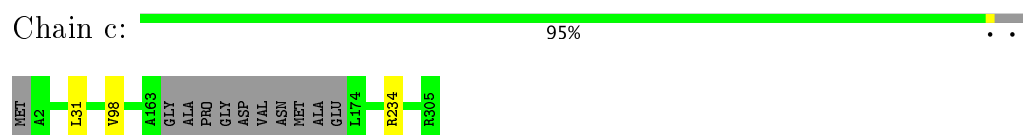
- Molecule 4: Triplex capsid protein 2



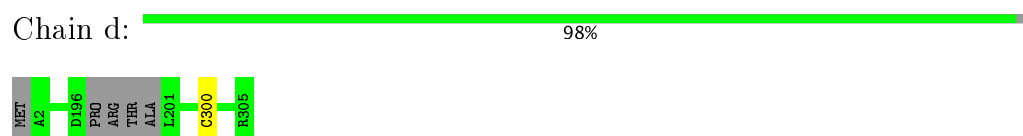
- Molecule 4: Triplex capsid protein 2



- Molecule 4: Triplex capsid protein 2

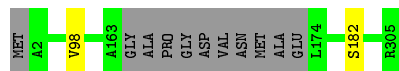


- Molecule 4: Triplex capsid protein 2



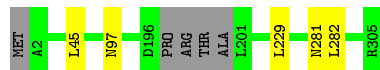
- Molecule 4: Triplex capsid protein 2

Chain f:  96% ..



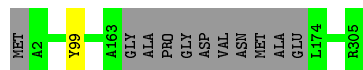
- Molecule 4: Triplex capsid protein 2

Chain g:  97% ..



- Molecule 4: Triplex capsid protein 2

Chain i:  96% .



- Molecule 4: Triplex capsid protein 2

Chain j:  97% ..



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	25315	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 ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	24271	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	4	0.34	0/9812	0.62	3/13326 (0.0%)
1	A	0.42	0/10936	0.64	4/14866 (0.0%)
1	B	0.44	0/10879	0.67	4/14788 (0.0%)
1	C	0.43	0/10873	0.64	7/14780 (0.0%)
1	D	0.43	1/10879 (0.0%)	0.66	4/14788 (0.0%)
1	E	0.45	1/10936 (0.0%)	0.66	3/14866 (0.0%)
1	F	0.44	1/10890 (0.0%)	0.66	4/14802 (0.0%)
1	M	0.44	0/10879	0.66	3/14788 (0.0%)
1	N	0.45	1/10936 (0.0%)	0.67	5/14866 (0.0%)
1	O	0.44	0/10879	0.66	3/14788 (0.0%)
1	S	0.40	0/10298	0.64	3/13995 (0.0%)
1	T	0.42	0/10918	0.65	2/14839 (0.0%)
1	U	0.44	0/10879	0.65	1/14788 (0.0%)
1	V	0.43	0/10856	0.66	5/14757 (0.0%)
1	W	0.43	3/10873 (0.0%)	0.65	7/14780 (0.0%)
1	X	0.40	0/10797	0.64	5/14676 (0.0%)
2	0	0.37	0/682	0.52	0/919
2	1	0.38	0/682	0.52	0/919
2	2	0.37	0/682	0.52	0/919
2	3	0.37	0/682	0.52	0/919
2	G	0.38	0/682	0.52	0/919
2	H	0.37	0/682	0.52	0/919
2	I	0.37	0/682	0.52	0/919
2	J	0.37	0/682	0.52	0/919
2	K	0.38	0/682	0.52	0/919
2	L	0.37	0/682	0.52	0/919
2	P	0.37	0/682	0.52	0/919
2	Q	0.37	0/682	0.52	0/919
2	R	0.38	0/682	0.52	0/919
2	Y	0.37	0/682	0.52	0/919
2	Z	0.37	0/682	0.52	0/919
3	5	0.33	0/2525	0.62	4/3433 (0.1%)
3	8	0.41	0/2539	0.63	1/3452 (0.0%)
3	b	0.41	0/2539	0.63	0/3452

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
3	e	0.40	0/2521	0.62	1/3426 (0.0%)
3	h	0.41	0/2539	0.64	2/3452 (0.1%)
4	6	0.34	0/2375	0.65	0/3234
4	7	0.33	0/2410	0.61	1/3281 (0.0%)
4	9	0.43	0/2375	0.66	0/3234
4	a	0.45	1/2410 (0.0%)	0.65	1/3281 (0.0%)
4	c	0.43	0/2375	0.67	1/3234 (0.0%)
4	d	0.44	0/2410	0.64	0/3281
4	f	0.38	0/2375	0.65	0/3234
4	g	0.41	0/2410	0.66	2/3281 (0.1%)
4	i	0.42	0/2375	0.65	0/3234
4	j	0.43	0/2410	0.66	2/3281 (0.1%)
All	All	0.42	8/219338 (0.0%)	0.65	78/298068 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	4	0	9
1	A	0	4
1	B	0	7
1	C	0	8
1	D	0	10
1	E	0	5
1	F	0	4
1	M	0	6
1	N	0	7
1	O	0	6
1	S	0	6
1	T	0	11
1	U	0	4
1	V	0	6
1	W	0	2
1	X	0	1
3	h	0	1
4	6	0	1
4	7	0	1
4	9	0	2
4	a	0	1
4	c	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
4	d	0	1
4	f	0	2
4	g	0	2
4	i	0	1
4	j	0	2
All	All	0	111

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	454	CYS	C-N	-7.03	1.17	1.34
4	a	234	ARG	CZ-NH2	-6.59	1.24	1.33
1	W	964	TYR	CD1-CE1	-6.35	1.29	1.39
1	N	9	PRO	C-N	-6.01	1.20	1.34
1	E	1192	GLN	C-N	-5.61	1.21	1.34
1	D	1192	GLN	C-N	-5.37	1.21	1.34
1	W	1226	ASP	CB-CG	-5.30	1.40	1.51
1	W	967	ARG	CD-NE	-5.18	1.37	1.46

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1181	PRO	C-N-CA	10.87	148.86	121.70
1	B	1232	ARG	NE-CZ-NH1	9.29	124.94	120.30
1	X	5	LEU	CA-CB-CG	8.38	134.58	115.30
1	B	1232	ARG	NE-CZ-NH2	-8.22	116.19	120.30
1	F	454	CYS	C-N-CA	8.04	141.80	121.70
1	4	1370	LEU	CA-CB-CG	7.74	133.11	115.30
3	h	233	LEU	CA-CB-CG	6.54	130.34	115.30
3	e	86	LEU	CA-CB-CG	6.53	130.32	115.30
1	C	681	LEU	CA-CB-CG	6.51	130.27	115.30
1	O	1316	LEU	CA-CB-CG	6.44	130.11	115.30
1	M	717	LEU	CA-CB-CG	6.39	130.00	115.30
4	g	229	LEU	CA-CB-CG	6.31	129.81	115.30
1	W	1316	LEU	CA-CB-CG	6.24	129.64	115.30
1	X	968	LEU	CA-CB-CG	6.22	129.60	115.30
3	5	222	LEU	CA-CB-CG	6.19	129.54	115.30
4	7	286	LEU	CA-CB-CG	6.05	129.21	115.30
4	a	45	LEU	CA-CB-CG	6.02	129.15	115.30
1	S	569	LEU	CA-CB-CG	-5.93	101.67	115.30
3	5	297	ASP	CB-CG-OD1	5.92	123.63	118.30
3	5	274	LEU	CA-CB-CG	5.87	128.80	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	V	684	LEU	CA-CB-CG	5.79	128.63	115.30
1	D	678	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	E	1316	LEU	CA-CB-CG	5.70	128.40	115.30
1	B	569	LEU	CA-CB-CG	-5.65	102.30	115.30
1	A	276	LEU	CA-CB-CG	5.64	128.27	115.30
1	W	967	ARG	NE-CZ-NH1	5.63	123.12	120.30
1	4	459	HIS	C-N-CA	-5.63	107.63	121.70
4	j	285	ARG	NE-CZ-NH1	-5.62	117.49	120.30
1	X	1316	LEU	CA-CB-CG	5.60	128.19	115.30
1	D	138	LEU	CA-CB-CG	5.58	128.13	115.30
1	T	902	GLN	CA-CB-CG	5.58	125.67	113.40
3	h	297	ASP	CB-CG-OD1	5.57	123.31	118.30
1	N	504	LYS	C-N-CA	5.54	135.56	121.70
1	X	681	LEU	CA-CB-CG	5.53	128.03	115.30
1	W	770	LEU	CA-CB-CG	5.51	127.97	115.30
1	E	1166	LEU	CA-CB-CG	5.50	127.96	115.30
1	S	713	LEU	CA-CB-CG	5.50	127.95	115.30
1	A	1166	LEU	CA-CB-CG	5.49	127.92	115.30
4	j	45	LEU	CA-CB-CG	5.49	127.92	115.30
1	N	957	LEU	CA-CB-CG	-5.46	102.74	115.30
1	W	138	LEU	CA-CB-CG	5.46	127.86	115.30
1	C	968	LEU	CA-CB-CG	5.44	127.81	115.30
1	C	1316	LEU	CA-CB-CG	5.38	127.68	115.30
1	O	1293	LEU	CA-CB-CG	5.37	127.66	115.30
1	W	1226	ASP	CB-CG-OD1	5.37	123.13	118.30
4	g	45	LEU	CA-CB-CG	5.36	127.63	115.30
1	D	968	LEU	CA-CB-CG	5.33	127.57	115.30
1	N	1249	LEU	CA-CB-CG	5.32	127.54	115.30
1	O	1250	TYR	CB-CG-CD2	-5.29	117.83	121.00
1	S	856	ASN	CA-C-N	5.28	126.76	116.20
1	A	1093	LEU	CA-CB-CG	5.23	127.32	115.30
1	V	968	LEU	CA-CB-CG	5.20	127.26	115.30
1	F	687	LEU	CA-CB-CG	5.18	127.22	115.30
1	V	313	LEU	CA-CB-CG	5.17	127.19	115.30
4	c	31	LEU	CA-CB-CG	5.17	127.19	115.30
1	M	1249	LEU	CA-CB-CG	5.16	127.16	115.30
1	C	1238	TRP	CA-CB-CG	-5.13	103.95	113.70
1	E	770	LEU	CA-CB-CG	5.12	127.08	115.30
1	F	1249	LEU	CA-CB-CG	5.11	127.06	115.30
1	X	352	ASP	CB-CG-OD1	5.11	122.90	118.30
1	C	684	LEU	CA-CB-CG	5.10	127.02	115.30
1	4	831	LEU	CA-CB-CG	5.10	127.03	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	138	LEU	CA-CB-CG	5.09	127.01	115.30
1	W	1226	ASP	CB-CG-OD2	5.09	122.88	118.30
1	W	1226	ASP	OD1-CG-OD2	-5.09	113.63	123.30
1	N	694	LEU	CA-CB-CG	5.08	126.99	115.30
1	F	400	TYR	CZ-CE2-CD2	5.07	124.36	119.80
1	A	902	GLN	CA-CB-CG	5.06	124.53	113.40
1	U	276	LEU	CA-CB-CG	5.04	126.89	115.30
3	5	296	PHE	C-N-CA	5.04	134.29	121.70
1	M	276	LEU	CA-CB-CG	5.03	126.88	115.30
1	V	708	LEU	CA-CB-CG	5.03	126.87	115.30
1	D	1317	ASP	C-N-CA	-5.03	109.14	121.70
1	N	459	HIS	C-N-CA	-5.03	109.14	121.70
1	V	1019	LEU	CA-CB-CG	5.03	126.86	115.30
1	T	459	HIS	C-N-CA	-5.02	109.15	121.70
1	C	1293	LEU	CA-CB-CG	5.01	126.82	115.30
3	8	297	ASP	CB-CG-OD1	5.01	122.81	118.30

There are no chirality outliers.

All (111) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	4	1016	HIS	Peptide
1	4	1084	HIS	Peptide
1	4	1334	HIS	Peptide
1	4	735	SER	Peptide
1	4	842	ASP	Peptide
1	4	844	VAL	Peptide
1	4	848	ASP	Peptide
1	4	850	ILE	Peptide
1	4	899	ASP	Peptide
4	6	98	VAL	Peptide
4	7	284	PRO	Peptide
4	9	37	HIS	Peptide
4	9	98	VAL	Peptide
1	A	1109	THR	Peptide
1	A	255	ASP	Peptide
1	A	537	HIS	Peptide
1	A	899	ASP	Peptide
1	B	1315	PHE	Peptide
1	B	422	VAL	Peptide
1	B	651	VAL	Peptide
1	B	849	ASP	Peptide

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Mol	Chain	Res	Type	Group
1	B	899	ASP	Peptide
1	B	913	VAL	Peptide
1	B	946	LYS	Peptide
1	C	1017	GLN	Peptide
1	C	1250	TYR	Peptide
1	C	1255	ARG	Peptide
1	C	292	GLN	Peptide
1	C	537	HIS	Peptide
1	C	900	PRO	Peptide
1	C	944	PHE	Peptide
1	C	963	ASN	Peptide
1	D	138	LEU	Peptide
1	D	144	GLU	Peptide
1	D	292	GLN	Peptide
1	D	457	ARG	Peptide
1	D	459	HIS	Peptide
1	D	596	THR	Peptide
1	D	798	TYR	Peptide
1	D	842	ASP	Peptide
1	D	849	ASP	Peptide
1	D	915	GLN	Peptide
1	E	1017	GLN	Peptide
1	E	292	GLN	Peptide
1	E	320	GLY	Peptide
1	E	651	VAL	Peptide
1	E	944	PHE	Peptide
1	F	1017	GLN	Peptide
1	F	1316	LEU	Peptide
1	F	938	MET	Peptide
1	F	944	PHE	Peptide
1	M	1312	THR	Peptide
1	M	255	ASP	Peptide
1	M	351	ALA	Peptide
1	M	387	GLN	Peptide
1	M	798	TYR	Peptide
1	M	899	ASP	Peptide
1	N	1113	VAL	Peptide
1	N	842	ASP	Peptide
1	N	849	ASP	Peptide
1	N	886	PRO	Peptide
1	N	918	LEU	Peptide
1	N	929	ASP	Peptide

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Mol	Chain	Res	Type	Group
1	N	944	PHE	Peptide
1	O	1042	ARG	Peptide
1	O	1252	ILE	Peptide
1	O	293	VAL	Peptide
1	O	536	VAL	Peptide
1	O	537	HIS	Peptide
1	O	842	ASP	Peptide
1	S	292	GLN	Peptide
1	S	537	HIS	Peptide
1	S	606	ASP	Peptide
1	S	844	VAL	Peptide
1	S	850	ILE	Peptide
1	S	944	PHE	Peptide
1	T	10	PHE	Peptide
1	T	106	ARG	Peptide
1	T	1112	GLY	Peptide
1	T	1181	PRO	Peptide
1	T	292	GLN	Peptide
1	T	422	VAL	Peptide
1	T	537	HIS	Peptide
1	T	842	ASP	Peptide
1	T	849	ASP	Peptide
1	T	899	ASP	Peptide
1	T	944	PHE	Peptide
1	U	292	GLN	Peptide
1	U	537	HIS	Peptide
1	U	59	ASN	Peptide
1	U	651	VAL	Peptide
1	V	1250	TYR	Peptide
1	V	142	GLU	Peptide
1	V	606	ASP	Peptide
1	V	797	ASP	Peptide
1	V	849	ASP	Peptide
1	V	899	ASP	Peptide
1	W	848	ASP	Peptide
1	W	849	ASP	Peptide
1	X	537	HIS	Peptide
4	a	229	LEU	Peptide
4	c	98	VAL	Peptide
4	d	300	CYS	Peptide
4	f	182	SER	Peptide
4	f	98	VAL	Peptide

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Mol	Chain	Res	Type	Group
4	g	282	LEU	Peptide
4	g	97	ASN	Peptide
3	h	296	PHE	Peptide
4	i	99	TYR	Peptide
4	j	281	ASN	Peptide
4	j	59	TYR	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	4	9586	0	9478	157	0
1	A	10682	0	10559	161	0
1	B	10627	0	10502	144	0
1	C	10621	0	10498	188	0
1	D	10627	0	10502	186	0
1	E	10682	0	10558	174	0
1	F	10638	0	10517	166	0
1	M	10627	0	10503	170	0
1	N	10682	0	10558	173	0
1	O	10627	0	10505	164	0
1	S	10060	0	9942	171	0
1	T	10666	0	10542	147	0
1	U	10627	0	10504	190	0
1	V	10604	0	10486	160	0
1	W	10621	0	10499	183	0
1	X	10548	0	10422	178	0
2	0	666	0	647	8	0
2	1	666	0	647	9	0
2	2	666	0	647	5	0
2	3	666	0	647	9	0
2	G	666	0	647	9	0
2	H	666	0	647	9	0
2	I	666	0	647	6	0
2	J	666	0	647	7	0
2	K	666	0	647	6	0
2	L	666	0	647	7	0
2	P	666	0	647	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Q	666	0	647	9	0
2	R	666	0	647	8	0
2	Y	666	0	647	7	0
2	Z	666	0	647	6	0
3	5	2463	0	2453	38	0
3	8	2477	0	2466	36	0
3	b	2477	0	2465	0	0
3	e	2460	0	2448	0	0
3	h	2477	0	2466	0	0
4	6	2329	0	2354	41	0
4	7	2364	0	2379	36	0
4	9	2329	0	2354	34	0
4	a	2364	0	2379	0	0
4	c	2329	0	2354	0	0
4	d	2364	0	2379	0	0
4	f	2329	0	2354	0	0
4	g	2364	0	2379	0	0
4	i	2329	0	2354	0	0
4	j	2364	0	2379	0	0
All	All	214334	0	212243	2709	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 7.

All (2709) 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)
1:C:736:ARG:HH22	1:C:899:ASP:HA	1.49	0.77
1:F:172:ARG:HH12	1:F:386:THR:HG21	1.49	0.77
1:X:558:HIS:HB3	1:X:898:ARG:HH12	1.50	0.76
1:4:457:ARG:HH12	1:4:463:GLN:HB3	1.50	0.75
1:W:865:ALA:HA	1:W:930:ARG:HH12	1.51	0.75
1:T:855:GLU:HG2	2:Y:70:ARG:HE	1.52	0.73
1:D:387:GLN:HE22	1:M:25:GLU:H	1.35	0.73
1:T:536:VAL:HG13	1:T:1244:SER:HA	1.70	0.73
1:V:1241:GLN:HB3	1:V:1244:SER:HB3	1.71	0.73
1:S:1241:GLN:HB3	1:S:1244:SER:HB3	1.73	0.71
1:E:115:ILE:HB	1:M:36:GLN:HB3	1.73	0.70
1:U:1241:GLN:HB3	1:U:1244:SER:HB3	1.72	0.70
1:M:113:GLN:HB3	1:U:38:LEU:HB2	1.72	0.70
1:C:799:ASN:HD21	1:C:802:LEU:HG	1.55	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:575:GLN:NE2	1:M:1015:MET:SD	2.61	0.70
1:U:389:PRO:HB3	1:V:203:ARG:HH12	1.55	0.70
1:V:443:CYS:SG	1:V:447:GLN:NE2	2.65	0.70
1:D:1199:GLY:HA3	1:D:1235:ASN:H	1.56	0.70
1:M:1241:GLN:HB3	1:M:1244:SER:HB3	1.73	0.69
1:C:1241:GLN:HB3	1:C:1244:SER:HB3	1.74	0.69
1:M:736:ARG:HH12	1:M:899:ASP:HA	1.57	0.69
1:T:1183:PRO:HG2	1:T:1186:SER:HB3	1.74	0.69
1:S:575:GLN:NE2	1:S:1015:MET:SD	2.60	0.69
1:B:602:GLU:HB3	1:B:647:LYS:HE2	1.75	0.69
1:N:591:VAL:HB	1:N:683:GLU:HB2	1.75	0.68
4:9:111:LEU:HB2	4:9:286:LEU:HB2	1.75	0.68
4:9:36:CYS:SG	4:9:86:ARG:NH2	2.67	0.68
1:S:203:ARG:HH21	1:X:395:ARG:HH22	1.41	0.68
3:5:90:LEU:HD11	3:5:165:MET:HG3	1.76	0.68
4:7:286:LEU:HB3	4:7:302:TYR:HD1	1.59	0.68
1:N:575:GLN:NE2	1:N:1015:MET:SD	2.67	0.68
1:V:91:ILE:HD12	1:V:1089:LEU:HD22	1.74	0.68
1:O:963:ASN:O	1:O:967:ARG:N	2.27	0.68
1:D:120:CYS:O	4:9:14:ARG:NH2	2.27	0.68
1:T:575:GLN:NE2	1:T:1015:MET:SD	2.68	0.67
1:U:514:GLN:HG3	1:U:531:LEU:HD21	1.76	0.67
1:B:157:LYS:HD2	1:C:338:ASN:HA	1.76	0.67
1:C:736:ARG:NH2	1:C:899:ASP:OD1	2.27	0.67
1:D:663:HIS:HA	1:E:930:ARG:HD2	1.77	0.67
1:U:736:ARG:HD2	1:U:897:LYS:H	1.59	0.67
1:U:450:LEU:HD21	1:U:1025:ILE:HG13	1.76	0.67
1:A:617:GLU:HG3	1:A:656:MET:HG3	1.76	0.67
1:B:663:HIS:HA	1:C:930:ARG:HD2	1.76	0.67
1:T:1111:MET:SD	1:T:1366:ARG:NH2	2.68	0.67
1:N:886:PRO:O	1:N:920:ASN:ND2	2.27	0.67
1:U:1295:GLY:H	1:U:1321:HIS:HE1	1.42	0.67
1:E:850:ILE:HD12	1:E:875:ILE:HD12	1.78	0.66
1:F:828:ASN:ND2	1:F:937:THR:O	2.28	0.66
1:C:591:VAL:HB	1:C:683:GLU:HB2	1.77	0.66
1:E:399:THR:HG22	1:E:1043:THR:HG22	1.76	0.66
1:V:95:ILE:HB	1:V:114:TYR:HB2	1.76	0.66
1:N:736:ARG:HG3	1:N:737:GLN:HG2	1.78	0.66
1:M:927:VAL:H	1:M:956:THR:HG21	1.61	0.66
1:W:399:THR:HG22	1:W:1043:THR:HG22	1.78	0.66
1:4:1211:SER:HB2	1:4:1214:SER:HB3	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:709:VAL:HG22	1:E:1023:SER:HA	1.78	0.66
1:M:1169:LEU:HD11	1:N:208:ALA:HA	1.78	0.66
1:M:777:ARG:NH2	1:M:885:CYS:O	2.28	0.66
4:9:142:GLN:HE22	4:9:285:ARG:HG2	1.61	0.65
1:U:290:LEU:HB3	1:U:367:VAL:HG21	1.79	0.65
1:U:275:VAL:HG22	1:U:375:ALA:HB3	1.77	0.65
1:X:1111:MET:SD	1:X:1366:ARG:NH2	2.67	0.65
1:E:1170:SER:HA	1:F:211:SER:HB3	1.77	0.65
1:E:532:LEU:O	1:E:1241:GLN:NE2	2.30	0.65
1:E:856:ASN:HA	1:E:860:LYS:HE3	1.78	0.65
1:W:1236:ASN:HB2	1:W:1238:TRP:HE3	1.60	0.65
1:A:290:LEU:HB3	1:A:367:VAL:HG21	1.77	0.65
1:A:558:HIS:HD2	1:A:902:GLN:HE22	1.45	0.65
1:B:1062:PHE:HB2	1:B:1087:ALA:HB3	1.77	0.65
1:C:575:GLN:NE2	1:C:1015:MET:SD	2.70	0.65
1:W:963:ASN:O	1:W:967:ARG:N	2.30	0.65
1:W:965:VAL:O	1:W:972:ARG:NH1	2.29	0.65
4:6:220:ARG:HG2	4:6:265:ARG:HH12	1.62	0.65
1:M:850:ILE:HD12	1:M:875:ILE:HD12	1.78	0.65
1:S:399:THR:HG22	1:S:1043:THR:HG22	1.76	0.65
1:S:828:ASN:ND2	1:S:937:THR:O	2.29	0.65
1:4:757:ILE:HG12	1:4:788:LEU:HD22	1.78	0.65
1:V:606:ASP:OD1	1:V:647:LYS:NZ	2.30	0.65
1:B:575:GLN:NE2	1:B:1015:MET:SD	2.70	0.65
1:O:450:LEU:HD21	1:O:1025:ILE:HG13	1.77	0.65
1:X:1027:GLN:HB3	1:X:1032:MET:HB2	1.78	0.65
1:4:275:VAL:HG22	1:4:375:ALA:HB3	1.77	0.65
1:N:492:ASN:HD22	1:N:495:ARG:HE	1.45	0.65
1:F:575:GLN:NE2	1:F:1015:MET:SD	2.70	0.64
1:E:93:PHE:HB2	1:E:116:VAL:HB	1.78	0.64
1:4:943:PRO:HB3	1:4:977:PHE:HE2	1.63	0.64
1:D:172:ARG:NH1	1:D:382:MET:O	2.30	0.64
1:M:93:PHE:HB2	1:M:116:VAL:HB	1.78	0.64
1:S:855:GLU:HG2	2:3:70:ARG:HE	1.63	0.64
1:A:718:LEU:O	1:A:915:GLN:NE2	2.31	0.64
1:O:93:PHE:HB2	1:O:116:VAL:HB	1.77	0.64
1:X:434:VAL:HG11	1:X:1042:ARG:HH22	1.61	0.64
1:N:1074:ARG:HD2	1:N:1077:ALA:HB3	1.79	0.64
1:N:832:THR:HG22	2:Q:11:ILE:HD11	1.80	0.64
1:U:54:LEU:HB2	1:V:91:ILE:HG12	1.79	0.64
1:4:182:LYS:NZ	1:4:1058:SER:OG	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:477:GLY:HA2	1:4:546:PRO:HG3	1.80	0.64
1:A:701:GLY:HA3	1:A:1131:GLN:HE21	1.62	0.64
1:C:893:ARG:NH1	1:C:984:MET:SD	2.71	0.64
1:S:930:ARG:HD2	1:X:663:HIS:HA	1.80	0.64
1:W:193:LYS:NZ	1:W:247:ASP:OD2	2.30	0.64
1:F:760:ARG:HH22	1:F:886:PRO:HA	1.60	0.64
4:9:5:LYS:HB3	4:9:86:ARG:HB3	1.81	0.63
1:A:777:ARG:NH2	1:A:885:CYS:O	2.31	0.63
1:O:1196:ASN:HD21	1:O:1324:GLN:HG3	1.63	0.63
1:U:701:GLY:HA3	1:U:1131:GLN:HE21	1.63	0.63
1:U:736:ARG:NH2	1:U:899:ASP:OD1	2.30	0.63
1:V:1111:MET:SD	1:V:1366:ARG:NH2	2.70	0.63
1:4:828:ASN:ND2	1:4:938:MET:SD	2.71	0.63
1:A:153:ALA:HB1	1:B:338:ASN:HB3	1.79	0.63
1:V:271:GLN:OE1	1:V:1056:ARG:NH1	2.31	0.63
1:4:743:GLY:HA3	1:4:786:HIS:HE1	1.63	0.63
1:A:514:GLN:HG3	1:A:531:LEU:HD21	1.80	0.63
1:W:92:GLN:HE22	1:W:115:ILE:HG23	1.63	0.63
4:7:26:LYS:HE2	4:7:98:VAL:HB	1.81	0.63
1:A:1111:MET:SD	1:A:1366:ARG:NH2	2.68	0.63
1:C:1312:THR:HG21	1:D:105:GLY:H	1.64	0.63
1:F:394:ARG:HD3	1:F:1315:PHE:HB3	1.79	0.63
1:A:575:GLN:NE2	1:A:1015:MET:SD	2.71	0.63
1:C:855:GLU:HG2	2:H:70:ARG:HE	1.63	0.63
1:F:898:ARG:HD3	1:F:902:GLN:HG3	1.81	0.63
1:M:115:ILE:HB	1:U:36:GLN:HB3	1.81	0.63
1:D:157:LYS:HD2	1:E:338:ASN:HA	1.81	0.63
3:5:91:PHE:HB2	3:5:106:LEU:HB2	1.79	0.63
1:A:1241:GLN:HB3	1:A:1244:SER:HB3	1.81	0.63
1:C:813:VAL:HG21	1:C:1012:MET:HG3	1.81	0.63
1:C:1167:PRO:HD3	1:D:1224:ILE:HD13	1.80	0.63
1:N:93:PHE:HB2	1:N:116:VAL:HB	1.80	0.63
1:T:153:ALA:HB1	1:U:338:ASN:HB3	1.80	0.63
1:W:1293:LEU:HD21	1:W:1297:PRO:HG3	1.81	0.63
1:X:37:LEU:HB2	1:X:50:PHE:HB2	1.81	0.63
1:B:256:THR:HG22	1:B:258:PHE:H	1.64	0.63
1:E:540:PHE:O	1:E:559:ARG:NH1	2.32	0.63
1:A:1228:ALA:HA	1:F:1171:HIS:HE1	1.65	0.62
1:E:915:GLN:HG2	1:E:989:GLU:HG3	1.79	0.62
1:X:611:LEU:HD22	1:X:862:ILE:HG12	1.81	0.62
1:M:856:ASN:HA	1:M:860:LYS:HE3	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:514:GLN:HG3	1:S:531:LEU:HD21	1.80	0.62
1:W:1005:THR:HG22	1:W:1007:GLY:H	1.64	0.62
1:W:714:ASP:O	1:W:804:LYS:NZ	2.31	0.62
1:X:537:HIS:HA	1:X:1238:TRP:HD1	1.63	0.62
1:W:447:GLN:NE2	1:X:521:GLU:OE1	2.32	0.62
4:9:58:ASP:HB3	4:9:196:ASP:HB3	1.81	0.62
1:B:214:VAL:HA	1:B:217:PHE:HD2	1.65	0.62
1:B:893:ARG:NH2	1:B:988:GLU:OE1	2.31	0.62
1:D:1111:MET:SD	1:D:1366:ARG:NH2	2.69	0.62
1:S:415:THR:HG23	1:X:418:SER:HB3	1.81	0.62
2:2:13:GLU:OE1	2:2:46:ARG:NH2	2.31	0.62
1:4:935:ALA:HA	1:4:938:MET:HB2	1.81	0.62
1:E:1005:THR:HG22	1:E:1007:GLY:H	1.64	0.62
1:F:799:ASN:HD21	1:F:802:LEU:HG	1.65	0.62
1:W:325:ASN:ND2	1:W:352:ASP:OD2	2.32	0.62
2:G:71:ARG:HD2	2:H:18:ASP:HA	1.81	0.62
1:U:828:ASN:ND2	1:U:937:THR:O	2.33	0.62
1:V:157:LYS:HD2	1:W:338:ASN:HA	1.80	0.62
1:X:1005:THR:HG22	1:X:1007:GLY:H	1.64	0.62
1:W:663:HIS:HA	1:X:930:ARG:HD2	1.79	0.62
1:4:1267:ARG:NH2	4:7:54:GLU:OE1	2.33	0.62
1:E:828:ASN:ND2	1:E:937:THR:O	2.30	0.62
1:F:714:ASP:O	1:F:804:LYS:NZ	2.32	0.62
1:C:709:VAL:HG22	1:C:1023:SER:HA	1.82	0.62
1:N:708:LEU:HD21	1:N:1022:PRO:HG2	1.81	0.62
1:U:428:GLN:NE2	1:U:577:SER:OG	2.32	0.62
1:V:399:THR:HG22	1:V:1043:THR:HG22	1.81	0.62
2:1:13:GLU:OE1	2:1:46:ARG:NH2	2.30	0.62
1:E:19:LEU:HB2	1:T:59:ASN:HD21	1.65	0.62
2:G:13:GLU:OE1	2:G:46:ARG:NH2	2.30	0.62
2:J:13:GLU:OE1	2:J:46:ARG:NH2	2.31	0.62
1:N:442:LEU:HD13	1:N:1113:VAL:HG23	1.82	0.62
1:S:1163:CYS:SG	1:S:1164:GLU:N	2.72	0.62
1:T:58:THR:HG22	1:U:94:LYS:HB3	1.82	0.62
1:T:946:LYS:NZ	1:T:986:GLU:OE1	2.33	0.62
1:B:275:VAL:HG22	1:B:375:ALA:HB3	1.82	0.62
1:F:760:ARG:HH21	1:F:789:ASP:HB3	1.64	0.62
1:M:275:VAL:HG22	1:M:375:ALA:HB3	1.82	0.62
1:N:399:THR:HG22	1:N:1043:THR:HG22	1.80	0.62
1:O:1295:GLY:H	1:O:1321:HIS:HE1	1.46	0.62
1:V:428:GLN:NE2	1:V:577:SER:OG	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:GLN:OE1	1:A:1056:ARG:NH1	2.33	0.61
1:C:946:LYS:HE2	1:C:993:SER:HA	1.82	0.61
1:N:471:ALA:HA	1:N:1242:ARG:HH12	1.65	0.61
1:B:808:TYR:HB3	1:B:1016:HIS:HE1	1.66	0.61
1:T:275:VAL:HG22	1:T:375:ALA:HB3	1.82	0.61
1:X:271:GLN:OE1	1:X:1056:ARG:NH1	2.33	0.61
1:X:709:VAL:HG22	1:X:1023:SER:HA	1.82	0.61
1:S:144:GLU:OE2	3:5:10:ARG:NH2	2.34	0.61
1:V:1344:ASN:ND2	1:V:1347:THR:OG1	2.28	0.61
1:W:214:VAL:HA	1:W:217:PHE:HD2	1.65	0.61
1:B:1294:ALA:HB1	1:B:1321:HIS:HE1	1.64	0.61
1:N:704:PRO:HG2	1:O:969:PRO:HD2	1.83	0.61
1:U:1236:ASN:HB2	1:U:1238:TRP:HE3	1.65	0.61
1:W:572:ARG:NH2	1:W:1001:SER:O	2.33	0.61
3:8:329:VAL:HG21	4:9:271:SER:HB2	1.82	0.61
1:B:507:ALA:HB1	1:B:978:ASN:HD22	1.66	0.61
1:B:856:ASN:ND2	2:G:66:GLY:O	2.33	0.61
1:U:1005:THR:HG22	1:U:1007:GLY:H	1.65	0.61
1:U:95:ILE:HB	1:U:114:TYR:HB2	1.82	0.61
1:X:617:GLU:HG3	1:X:656:MET:HG3	1.82	0.61
3:5:111:LEU:HA	3:5:114:LEU:HD13	1.82	0.61
1:D:1005:THR:HG22	1:D:1007:GLY:H	1.65	0.61
1:N:687:LEU:HB3	1:N:805:LEU:HD13	1.83	0.61
1:N:58:THR:HG22	1:O:94:LYS:HB3	1.83	0.61
1:T:107:ARG:HG3	4:6:37:HIS:HE1	1.66	0.61
1:E:1027:GLN:HB3	1:E:1032:MET:HB2	1.83	0.61
1:F:1162:ARG:N	1:F:1306:TYR:HH	1.99	0.61
1:M:313:LEU:HD21	1:U:150:THR:HG21	1.83	0.61
1:V:813:VAL:HG21	1:V:1012:MET:HG3	1.83	0.61
1:W:850:ILE:HD12	1:W:870:PRO:HG2	1.82	0.61
2:Z:13:GLU:OE1	2:Z:46:ARG:NH2	2.30	0.61
1:B:919:VAL:HG12	1:B:920:ASN:HB2	1.82	0.61
1:B:1027:GLN:HB3	1:B:1032:MET:HB2	1.83	0.60
1:B:54:LEU:HB2	1:C:91:ILE:HG12	1.81	0.60
1:S:898:ARG:HD3	1:S:902:GLN:HG3	1.83	0.60
1:T:709:VAL:HG22	1:T:1023:SER:HA	1.82	0.60
1:X:83:LEU:HD22	1:X:1085:GLU:HB3	1.83	0.60
1:F:540:PHE:O	1:F:559:ARG:NH1	2.33	0.60
1:M:1211:SER:O	1:M:1279:ASN:ND2	2.35	0.60
1:N:1005:THR:HG22	1:N:1007:GLY:H	1.66	0.60
1:V:1236:ASN:HB2	1:V:1238:TRP:HE3	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1067:SER:HG	1:X:1083:THR:HG1	1.50	0.60
3:8:289:CYS:SG	3:8:290:THR:N	2.74	0.60
1:M:799:ASN:HD21	1:M:802:LEU:HG	1.66	0.60
1:N:537:HIS:HA	1:N:1238:TRP:CD1	2.36	0.60
1:O:828:ASN:ND2	1:O:937:THR:O	2.31	0.60
1:T:1171:HIS:HE1	1:U:1228:ALA:HA	1.66	0.60
1:W:447:GLN:HB3	1:W:1028:ALA:HB1	1.84	0.60
1:X:394:ARG:NH1	1:X:1317:ASP:OD2	2.34	0.60
1:D:36:GLN:HB3	1:N:115:ILE:HB	1.82	0.60
1:O:1005:THR:HG22	1:O:1007:GLY:H	1.66	0.60
1:X:82:ASP:OD1	1:X:82:ASP:N	2.34	0.60
3:5:228:ALA:HB3	3:5:289:CYS:HB3	1.83	0.60
4:7:211:LEU:HA	4:7:214:LEU:HB2	1.83	0.60
1:W:1027:GLN:HB3	1:W:1032:MET:HB2	1.83	0.60
1:X:578:ARG:NH1	1:X:1014:SER:OG	2.34	0.60
1:S:207:LYS:HD3	1:X:1168:GLY:HA2	1.83	0.60
1:B:536:VAL:HG13	1:B:1244:SER:HA	1.84	0.60
1:C:1027:GLN:HB3	1:C:1032:MET:HB2	1.83	0.60
1:D:855:GLU:HG2	2:I:70:ARG:HE	1.67	0.60
1:O:578:ARG:NH1	1:O:1014:SER:O	2.35	0.60
1:S:182:LYS:NZ	1:S:1058:SER:OG	2.35	0.60
1:S:157:LYS:HD2	1:T:338:ASN:HA	1.83	0.60
1:V:93:PHE:HB2	1:V:116:VAL:HB	1.82	0.60
1:W:626:LYS:NZ	1:W:881:SER:O	2.35	0.60
1:W:799:ASN:HD21	1:W:802:LEU:HG	1.65	0.60
1:4:74:ALA:HB1	1:4:182:LYS:HE3	1.82	0.60
1:4:611:LEU:HB3	1:4:862:ILE:HG21	1.84	0.60
3:8:324:CYS:SG	3:8:325:GLY:N	2.75	0.60
1:E:271:GLN:OE1	1:E:1056:ARG:NH1	2.35	0.60
1:M:587:ASN:OD1	1:N:1003:GLN:NE2	2.35	0.60
1:N:850:ILE:HD12	1:N:870:PRO:HG2	1.84	0.60
1:O:575:GLN:NE2	1:O:1015:MET:SD	2.74	0.60
1:O:799:ASN:HD21	1:O:802:LEU:HG	1.65	0.60
1:U:575:GLN:NE2	1:U:1015:MET:SD	2.74	0.60
1:T:1162:ARG:HH22	1:U:206:LYS:HB3	1.66	0.60
1:T:49:ARG:HD3	1:U:87:ILE:HD11	1.84	0.60
4:6:245:VAL:O	4:7:256:GLN:NE2	2.35	0.60
1:A:1201:ALA:HB3	1:A:1227:PRO:HG2	1.84	0.60
1:D:578:ARG:NH1	1:D:1014:SER:O	2.34	0.60
1:F:93:PHE:HB2	1:F:116:VAL:HB	1.84	0.60
1:M:537:HIS:HA	1:M:1238:TRP:HD1	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:964:TYR:HA	1:W:967:ARG:HB2	1.83	0.60
1:X:491:MET:HB2	1:X:783:ASP:HA	1.84	0.60
1:A:512:VAL:HG12	1:A:993:SER:HB3	1.82	0.60
1:E:249:LEU:HD21	1:E:372:LYS:HB2	1.82	0.60
1:O:1241:GLN:HB3	1:O:1244:SER:HB3	1.84	0.60
1:U:271:GLN:OE1	1:U:1056:ARG:NH1	2.31	0.60
1:C:77:ASN:HA	1:C:1061:MET:HB2	1.83	0.60
1:E:572:ARG:NH2	1:E:1001:SER:O	2.35	0.60
1:U:264:TYR:HE1	1:U:300:PRO:HD2	1.67	0.60
1:4:394:ARG:NH1	1:4:1315:PHE:O	2.34	0.59
1:A:711:ALA:HB3	1:A:1016:HIS:HB3	1.84	0.59
1:C:197:ASP:HB3	1:C:199:VAL:HG12	1.84	0.59
1:M:1168:GLY:HA2	1:N:207:LYS:HD3	1.83	0.59
1:W:325:ASN:HB3	1:W:328:GLN:HB3	1.84	0.59
1:W:93:PHE:HB2	1:W:116:VAL:HB	1.83	0.59
1:X:438:ASN:HD22	1:X:1171:HIS:HD2	1.49	0.59
1:C:399:THR:HG22	1:C:1043:THR:HG22	1.84	0.59
1:F:1280:ARG:NH2	1:F:1288:GLU:OE1	2.35	0.59
1:F:683:GLU:O	1:F:687:LEU:N	2.32	0.59
2:K:13:GLU:OE1	2:K:46:ARG:NH2	2.31	0.59
1:4:194:THR:HG21	1:4:216:MET:HB3	1.83	0.59
2:H:13:GLU:OE1	2:H:46:ARG:NH2	2.30	0.59
1:O:450:LEU:HD11	1:O:1025:ILE:HA	1.82	0.59
1:S:1200:ARG:NH1	1:S:1233:SER:O	2.35	0.59
1:V:450:LEU:HD11	1:V:1025:ILE:HG13	1.83	0.59
1:4:1115:CYS:HA	1:4:1177:CYS:H	1.67	0.59
3:5:151:ASP:O	3:5:282:ARG:NH1	2.36	0.59
1:A:850:ILE:HD12	1:A:875:ILE:HD12	1.83	0.59
1:F:658:ARG:HA	1:F:681:LEU:HD11	1.83	0.59
1:M:1163:CYS:SG	1:M:1164:GLU:N	2.74	0.59
1:T:1280:ARG:NH2	1:T:1288:GLU:OE1	2.35	0.59
1:4:456:PRO:O	1:4:460:ASN:N	2.35	0.59
1:4:539:PHE:O	1:4:559:ARG:NH1	2.34	0.59
1:4:963:ASN:O	1:4:967:ARG:N	2.33	0.59
1:B:537:HIS:HA	1:B:1238:TRP:CD1	2.36	0.59
1:O:572:ARG:NH2	1:O:1001:SER:O	2.35	0.59
2:P:13:GLU:OE1	2:P:46:ARG:NH2	2.30	0.59
1:X:214:VAL:HA	1:X:217:PHE:HD2	1.67	0.59
1:4:1241:GLN:HG3	1:4:1243:GLY:H	1.68	0.59
3:8:218:GLU:OE1	4:9:68:LYS:NZ	2.36	0.59
1:W:1187:ASP:OD2	1:W:1232:ARG:NH1	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1169:LEU:HD11	1:B:208:ALA:HA	1.85	0.59
1:A:578:ARG:NH2	1:A:1017:GLN:OE1	2.36	0.59
1:C:536:VAL:HG13	1:C:1244:SER:HA	1.83	0.59
1:D:275:VAL:HG22	1:D:375:ALA:HB3	1.84	0.59
1:F:919:VAL:HG12	1:F:920:ASN:HB2	1.85	0.59
1:4:1342:MET:HG2	1:4:1368:LEU:HB3	1.84	0.59
1:4:886:PRO:HD2	1:4:920:ASN:HD22	1.67	0.59
1:A:91:ILE:HB	1:A:118:LYS:HB2	1.85	0.59
1:B:578:ARG:NH1	1:B:1014:SER:OG	2.36	0.59
1:B:678:ARG:HH22	1:C:608:ALA:HB3	1.67	0.59
1:C:394:ARG:NH1	1:C:1317:ASP:OD2	2.35	0.59
1:E:36:GLN:HB3	1:U:115:ILE:HB	1.85	0.59
1:O:428:GLN:NE2	1:O:577:SER:OG	2.34	0.59
1:V:575:GLN:NE2	1:V:1015:MET:SD	2.76	0.59
1:4:946:LYS:NZ	1:4:977:PHE:O	2.35	0.59
1:A:275:VAL:HG22	1:A:375:ALA:HB3	1.85	0.59
1:C:248:MET:HE1	1:C:1100:ALA:HB2	1.84	0.59
2:L:13:GLU:OE1	2:L:46:ARG:NH2	2.30	0.59
1:M:396:ILE:HD11	1:M:1050:HIS:HE1	1.66	0.59
1:S:537:HIS:HA	1:S:1238:TRP:HD1	1.66	0.59
1:C:704:PRO:HG2	1:D:969:PRO:HD2	1.84	0.59
1:D:575:GLN:HE21	1:D:1015:MET:HG3	1.67	0.59
1:C:157:LYS:NZ	1:D:339:ALA:O	2.35	0.59
1:O:536:VAL:HG22	1:O:1241:GLN:HG2	1.83	0.59
1:O:777:ARG:NH2	1:O:885:CYS:O	2.36	0.58
1:U:1027:GLN:HB3	1:U:1032:MET:HB2	1.84	0.58
1:X:850:ILE:HD11	1:X:872:VAL:HA	1.85	0.58
4:6:179:THR:OG1	4:6:189:ARG:NH1	2.35	0.58
1:E:56:VAL:HG13	1:F:92:GLN:HB3	1.85	0.58
1:E:428:GLN:NE2	1:E:577:SER:OG	2.36	0.58
1:F:893:ARG:NH2	1:F:988:GLU:OE1	2.36	0.58
1:M:714:ASP:O	1:M:804:LYS:NZ	2.35	0.58
1:U:93:PHE:HB2	1:U:116:VAL:HB	1.84	0.58
1:U:422:VAL:HG11	1:U:1355:GLN:HE22	1.68	0.58
1:4:130:GLU:HG2	1:4:1079:THR:HG22	1.85	0.58
1:4:399:THR:HG22	1:4:1043:THR:HG22	1.84	0.58
1:4:652:ASN:ND2	1:4:923:GLY:O	2.33	0.58
1:A:532:LEU:O	1:A:1241:GLN:NE2	2.37	0.58
1:E:384:ASN:O	1:E:387:GLN:NE2	2.36	0.58
1:E:770:LEU:HD11	1:E:883:LEU:HD13	1.85	0.58
1:F:555:ARG:HH21	1:F:907:HIS:HA	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:504:LYS:O	1:S:967:ARG:NH1	2.37	0.58
1:V:1196:ASN:HD21	1:V:1324:GLN:HG3	1.69	0.58
1:W:278:THR:HG22	1:W:1051:ILE:HG12	1.85	0.58
1:4:723:TYR:OH	1:4:921:GLY:O	2.21	0.58
1:4:716:HIS:O	1:4:915:GLN:NE2	2.36	0.58
1:C:757:ILE:HG12	1:C:788:LEU:HD22	1.84	0.58
1:M:56:VAL:HG13	1:N:92:GLN:HB3	1.85	0.58
1:M:611:LEU:HD11	1:M:935:ALA:HB2	1.85	0.58
1:O:555:ARG:HH21	1:O:910:GLY:HA2	1.66	0.58
1:T:77:ASN:HA	1:T:1061:MET:HB2	1.84	0.58
2:Y:13:GLU:OE1	2:Y:46:ARG:NH2	2.31	0.58
1:C:145:THR:HG22	1:C:147:LEU:H	1.68	0.58
1:F:1005:THR:HG22	1:F:1007:GLY:H	1.69	0.58
1:N:95:ILE:HB	1:N:114:TYR:HB2	1.85	0.58
1:N:448:ASN:ND2	1:O:1231:CYS:SG	2.76	0.58
1:S:1328:PRO:HB2	1:S:1358:ILE:HG21	1.85	0.58
1:T:1198:ARG:HB3	1:T:1270:PHE:HE1	1.66	0.58
1:X:1241:GLN:HB3	1:X:1244:SER:HB3	1.84	0.58
1:4:711:ALA:O	1:4:804:LYS:NZ	2.35	0.58
1:B:898:ARG:NH1	1:B:904:PHE:O	2.37	0.58
1:F:75:CYS:SG	1:F:1059:THR:OG1	2.60	0.58
1:M:128:GLU:OE2	1:N:110:LYS:NZ	2.35	0.58
1:O:918:LEU:HB2	1:O:944:PHE:HE2	1.69	0.58
2:Q:13:GLU:OE1	2:Q:46:ARG:NH2	2.30	0.58
1:4:799:ASN:HD21	1:4:802:LEU:HG	1.68	0.58
1:C:263:THR:O	1:C:359:ARG:NH1	2.35	0.58
1:A:338:ASN:HA	1:F:157:LYS:HD2	1.86	0.58
1:S:271:GLN:OE1	1:S:1056:ARG:NH1	2.36	0.58
1:T:491:MET:HB2	1:T:783:ASP:HA	1.83	0.58
1:V:457:ARG:HH22	1:V:463:GLN:HG2	1.67	0.58
1:N:1173:GLN:NE2	1:N:1302:THR:OG1	2.36	0.58
1:S:49:ARG:HD3	1:T:87:ILE:HD11	1.86	0.58
1:U:1062:PHE:HB2	1:U:1087:ALA:HB3	1.85	0.58
1:U:714:ASP:O	1:U:804:LYS:NZ	2.35	0.58
1:4:965:VAL:HG13	1:4:972:ARG:HG2	1.84	0.58
1:A:711:ALA:HB2	1:A:1018:LYS:HD3	1.86	0.58
1:F:856:ASN:OD1	1:F:860:LYS:NZ	2.31	0.58
1:V:1062:PHE:HB2	1:V:1087:ALA:HB3	1.86	0.58
1:V:275:VAL:HG22	1:V:375:ALA:HB3	1.86	0.58
1:4:279:THR:HB	1:4:380:GLN:HE21	1.69	0.58
1:D:163:LEU:HD21	3:8:51:PRO:HG2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1027:GLN:HE22	1:D:1032:MET:HB2	1.67	0.58
1:D:228:LEU:HD22	1:D:1103:HIS:HD2	1.69	0.58
1:E:850:ILE:HD11	1:E:872:VAL:HA	1.86	0.58
1:A:963:ASN:O	1:A:967:ARG:N	2.36	0.57
1:E:958:HIS:HE1	1:E:960:LEU:HB3	1.68	0.57
1:N:5:LEU:HD23	1:N:34:SER:HB2	1.86	0.57
1:O:192:LEU:HD22	1:O:251:ALA:HB1	1.85	0.57
1:U:903:SER:HB2	1:U:1128:GLN:HE22	1.69	0.57
1:W:293:VAL:HG13	1:W:294:GLU:HG3	1.84	0.57
1:B:757:ILE:HG12	1:B:788:LEU:HD22	1.85	0.57
1:C:1198:ARG:NH1	1:C:1200:ARG:O	2.37	0.57
1:D:123:HIS:HB2	1:D:1086:ILE:HB	1.85	0.57
1:M:1005:THR:HG22	1:M:1007:GLY:H	1.69	0.57
1:D:38:LEU:HB2	1:N:113:GLN:HB3	1.86	0.57
1:N:1201:ALA:HB3	1:N:1227:PRO:HG2	1.85	0.57
1:O:197:ASP:HB3	1:O:199:VAL:HG12	1.86	0.57
1:U:1137:LYS:O	1:U:1141:GLY:N	2.36	0.57
1:X:902:GLN:NE2	1:X:1018:LYS:O	2.37	0.57
1:X:893:ARG:NH2	1:X:988:GLU:OE1	2.36	0.57
1:4:581:GLN:NE2	1:4:1031:ARG:O	2.38	0.57
3:5:129:ALA:HA	3:5:132:TRP:HD1	1.69	0.57
1:B:606:ASP:OD1	1:B:647:LYS:NZ	2.33	0.57
1:F:729:ASP:HB2	1:F:793:LEU:HD11	1.86	0.57
1:N:271:GLN:OE1	1:N:1056:ARG:NH1	2.38	0.57
1:O:77:ASN:HA	1:O:1061:MET:HB2	1.87	0.57
1:T:898:ARG:HD3	1:T:902:GLN:HG3	1.86	0.57
1:B:1226:ASP:HB2	1:B:1229:TYR:H	1.69	0.57
1:M:963:ASN:O	1:M:967:ARG:N	2.36	0.57
1:O:1071:ARG:O	1:O:1079:THR:OG1	2.21	0.57
1:T:1071:ARG:O	1:T:1079:THR:OG1	2.23	0.57
1:4:340:LEU:HD12	1:4:341:PRO:HD2	1.87	0.57
1:M:828:ASN:ND2	1:M:937:THR:O	2.31	0.57
2:R:13:GLU:OE1	2:R:46:ARG:NH2	2.30	0.57
3:8:305:LEU:HD12	3:8:312:LEU:HD23	1.85	0.57
1:B:1163:CYS:SG	1:B:1164:GLU:N	2.77	0.57
1:F:929:ASP:OD1	1:F:932:ARG:NH2	2.38	0.57
1:S:365:SER:HB2	1:S:376:ILE:H	1.70	0.57
1:S:532:LEU:O	1:S:1241:GLN:NE2	2.37	0.57
1:V:578:ARG:NH1	1:V:1014:SER:OG	2.37	0.57
1:V:438:ASN:HD22	1:V:1171:HIS:HD2	1.53	0.57
4:6:220:ARG:NH1	4:6:252:ILE:O	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:275:VAL:HG22	1:C:375:ALA:HB3	1.87	0.57
1:T:214:VAL:HA	1:T:217:PHE:HD2	1.69	0.57
1:U:1201:ALA:HB3	1:U:1227:PRO:HG2	1.85	0.57
1:V:77:ASN:HA	1:V:1061:MET:HB2	1.87	0.57
1:O:1198:ARG:NH2	1:O:1219:LEU:O	2.38	0.57
1:X:275:VAL:HG22	1:X:375:ALA:HB3	1.87	0.57
4:7:110:GLN:HG2	4:7:287:HIS:HE1	1.70	0.57
1:E:963:ASN:O	1:E:967:ARG:N	2.32	0.57
1:S:85:ARG:HH21	1:4:138:LEU:HD22	1.69	0.57
1:M:117:MET:HB2	1:U:5:LEU:HD12	1.86	0.57
1:A:717:LEU:HB2	1:A:990:TRP:HZ3	1.70	0.56
1:E:968:LEU:HD11	1:E:971:GLN:HE21	1.69	0.56
1:E:893:ARG:NH2	1:E:988:GLU:OE1	2.37	0.56
1:V:79:GLU:HB3	1:V:305:SER:HA	1.87	0.56
1:X:946:LYS:NZ	1:X:975:VAL:O	2.36	0.56
1:4:839:VAL:HG11	1:4:875:ILE:HD12	1.86	0.56
4:7:217:LEU:HB2	4:7:269:MET:HG3	1.86	0.56
4:9:144:LEU:HD21	4:9:183:PHE:HB2	1.87	0.56
1:E:587:ASN:HB2	1:F:572:ARG:HH22	1.69	0.56
1:S:537:HIS:HA	1:S:1238:TRP:CD1	2.40	0.56
1:T:93:PHE:HB2	1:T:116:VAL:HB	1.87	0.56
1:4:901:ALA:HB3	1:4:1020:SER:HB3	1.86	0.56
1:F:946:LYS:NZ	1:F:986:GLU:OE1	2.38	0.56
1:T:537:HIS:HA	1:T:1238:TRP:CD1	2.40	0.56
1:T:757:ILE:HG12	1:T:788:LEU:HD22	1.87	0.56
1:T:929:ASP:OD1	1:T:932:ARG:NH2	2.38	0.56
1:V:828:ASN:ND2	1:V:937:THR:O	2.37	0.56
1:X:927:VAL:HB	1:X:956:THR:HG21	1.86	0.56
1:D:23:ILE:H	1:M:387:GLN:HE22	1.52	0.56
1:D:572:ARG:NH2	1:D:1001:SER:O	2.38	0.56
1:T:130:GLU:HG2	1:T:1079:THR:HG22	1.86	0.56
1:T:490:ASN:OD1	1:T:495:ARG:NH1	2.38	0.56
1:U:663:HIS:HA	1:V:930:ARG:HD2	1.86	0.56
1:W:575:GLN:NE2	1:W:1015:MET:SD	2.78	0.56
1:X:428:GLN:NE2	1:X:577:SER:OG	2.35	0.56
1:4:849:ASP:HB3	1:4:869:ARG:HB3	1.87	0.56
4:7:141:PRO:O	4:7:145:GLY:N	2.37	0.56
1:E:435:VAL:HG11	1:E:1368:LEU:HD22	1.88	0.56
1:N:249:LEU:HD21	1:N:372:LYS:HB2	1.88	0.56
1:S:581:GLN:NE2	1:S:1031:ARG:O	2.38	0.56
1:S:536:VAL:HG13	1:S:1244:SER:HA	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:88:ASP:OD2	4:6:14:ARG:NH2	2.36	0.56
1:T:91:ILE:HB	1:T:118:LYS:HB2	1.87	0.56
1:U:252:VAL:HG11	1:U:1055:SER:HB3	1.88	0.56
1:U:626:LYS:NZ	1:U:881:SER:O	2.37	0.56
1:V:1201:ALA:HB3	1:V:1227:PRO:HG2	1.86	0.56
1:W:915:GLN:HG2	1:W:989:GLU:HG3	1.88	0.56
4:7:156:HIS:NE2	4:7:201:LEU:O	2.38	0.56
1:A:214:VAL:HA	1:A:217:PHE:HD2	1.70	0.56
1:B:1071:ARG:O	1:B:1079:THR:OG1	2.24	0.56
1:C:782:HIS:HA	1:C:785:ARG:HD2	1.87	0.56
1:D:1252:ILE:HD11	1:D:1267:ARG:HG3	1.87	0.56
1:E:75:CYS:SG	1:E:1059:THR:OG1	2.59	0.56
1:T:236:ARG:NH1	1:T:239:GLN:OE1	2.39	0.56
1:U:1251:ASN:HB3	1:U:1254:PHE:HB3	1.87	0.56
1:V:61:VAL:HG11	1:W:98:PRO:HG3	1.87	0.56
1:X:57:TYR:O	1:4:47:SER:N	2.38	0.56
1:C:739:ILE:HB	1:C:895:ILE:HB	1.87	0.56
1:N:1241:GLN:HB3	1:N:1244:SER:HB3	1.86	0.56
1:X:183:LEU:HD13	1:X:394:ARG:HH21	1.71	0.56
3:8:300:PRO:HB3	3:8:317:PHE:HE1	1.70	0.56
1:B:832:THR:HG22	2:H:11:ILE:HD11	1.87	0.56
1:D:91:ILE:HB	1:D:118:LYS:HB2	1.87	0.56
1:O:929:ASP:OD1	1:O:932:ARG:NH2	2.38	0.56
1:A:1071:ARG:O	1:A:1079:THR:OG1	2.24	0.56
1:M:325:ASN:HB3	1:M:328:GLN:HB3	1.88	0.56
1:N:182:LYS:NZ	1:N:1058:SER:OG	2.37	0.56
1:V:514:GLN:HG3	1:V:531:LEU:HD21	1.87	0.56
1:V:946:LYS:HE2	1:V:993:SER:HA	1.88	0.56
1:W:396:ILE:HD11	1:W:1050:HIS:HE1	1.69	0.56
1:4:1071:ARG:O	1:4:1079:THR:OG1	2.24	0.56
1:4:432:THR:HG22	1:4:1333:SER:HA	1.88	0.56
1:B:717:LEU:HA	1:B:915:GLN:HE22	1.70	0.56
1:D:796:ASN:OD1	1:E:932:ARG:NH1	2.38	0.56
1:S:946:LYS:NZ	1:S:975:VAL:O	2.39	0.56
1:W:182:LYS:NZ	1:W:1058:SER:OG	2.39	0.56
1:B:271:GLN:OE1	1:B:1056:ARG:NH1	2.39	0.56
1:C:514:GLN:HG3	1:C:531:LEU:HD21	1.88	0.56
1:X:74:ALA:HB1	1:X:182:LYS:HE3	1.88	0.56
1:4:1005:THR:HG22	1:4:1007:GLY:H	1.71	0.55
4:6:47:LEU:HB3	4:6:135:VAL:HB	1.88	0.55
4:9:179:THR:OG1	4:9:189:ARG:NH1	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1173:GLN:NE2	1:D:1304:LEU:O	2.38	0.55
1:D:182:LYS:NZ	1:D:1058:SER:OG	2.39	0.55
1:F:406:LEU:HD21	1:F:1191:PHE:HE2	1.72	0.55
2:I:13:GLU:OE1	2:I:46:ARG:NH2	2.31	0.55
1:S:130:GLU:HG2	1:S:1079:THR:HG22	1.87	0.55
1:V:1198:ARG:NH2	1:V:1219:LEU:O	2.39	0.55
1:V:663:HIS:HA	1:W:930:ARG:HD2	1.88	0.55
1:X:447:GLN:HA	1:X:450:LEU:HB2	1.88	0.55
1:B:1207:CYS:SG	1:B:1208:ASP:N	2.79	0.55
1:C:889:THR:HA	1:C:920:ASN:HB3	1.87	0.55
1:F:591:VAL:HB	1:F:683:GLU:HB2	1.89	0.55
1:M:616:ILE:HG23	1:M:620:ILE:HD13	1.87	0.55
1:W:537:HIS:HA	1:W:1238:TRP:HE1	1.70	0.55
4:6:127:LEU:HD13	4:6:133:ASP:HA	1.89	0.55
1:D:947:LEU:HD21	1:D:995:VAL:HG12	1.87	0.55
1:E:182:LYS:NZ	1:E:1058:SER:OG	2.39	0.55
1:E:394:ARG:NH1	1:E:1317:ASP:OD2	2.39	0.55
1:S:1042:ARG:NH2	1:S:1112:GLY:O	2.38	0.55
1:S:460:ASN:HB3	1:S:904:PHE:HB3	1.89	0.55
1:T:492:ASN:HD22	1:T:495:ARG:HE	1.54	0.55
1:X:331:ALA:HA	1:X:335:ASP:HB2	1.87	0.55
1:N:578:ARG:NH1	1:N:1014:SER:O	2.39	0.55
1:S:1173:GLN:NE2	1:S:1302:THR:O	2.39	0.55
1:T:399:THR:HG22	1:T:1043:THR:HG22	1.89	0.55
1:4:626:LYS:O	1:4:630:ASN:ND2	2.39	0.55
1:A:1187:ASP:OD2	1:A:1232:ARG:NH2	2.40	0.55
1:D:399:THR:HG22	1:D:1043:THR:HG22	1.87	0.55
1:E:512:VAL:HG12	1:E:993:SER:HB3	1.88	0.55
1:M:271:GLN:OE1	1:M:1056:ARG:NH1	2.34	0.55
1:N:1264:SER:HB2	1:N:1267:ARG:HB2	1.88	0.55
1:S:591:VAL:HG12	1:S:679:LYS:HG2	1.87	0.55
1:U:1280:ARG:NH2	1:U:1288:GLU:OE1	2.39	0.55
1:V:537:HIS:HB3	1:V:1245:LEU:HB2	1.88	0.55
1:X:93:PHE:HB2	1:X:116:VAL:HB	1.88	0.55
1:A:1254:PHE:HD1	1:A:1267:ARG:HH12	1.55	0.55
1:C:540:PHE:O	1:C:559:ARG:NH1	2.40	0.55
1:D:578:ARG:NH2	1:D:1017:GLN:OE1	2.39	0.55
1:D:428:GLN:NE2	1:D:577:SER:OG	2.39	0.55
1:D:929:ASP:OD1	1:D:932:ARG:NH2	2.40	0.55
1:D:963:ASN:O	1:D:967:ARG:N	2.37	0.55
1:F:271:GLN:OE1	1:F:1056:ARG:NH1	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:471:ALA:HA	1:T:1242:ARG:HH12	1.71	0.55
1:T:736:ARG:HB3	1:T:897:LYS:HB2	1.88	0.55
1:U:606:ASP:OD2	1:U:641:TYR:OH	2.22	0.55
1:X:1051:ILE:HB	1:X:1100:ALA:HB3	1.88	0.55
2:3:13:GLU:OE1	2:3:46:ARG:NH2	2.31	0.55
1:4:434:VAL:HG11	1:4:1042:ARG:HH12	1.72	0.55
1:B:402:PHE:HD2	1:B:1040:VAL:HB	1.70	0.55
1:B:743:GLY:HA3	1:B:786:HIS:HE1	1.72	0.55
1:B:587:ASN:ND2	1:C:1001:SER:O	2.40	0.55
1:C:1111:MET:SD	1:C:1366:ARG:NH2	2.77	0.55
1:C:692:LEU:HD21	1:D:972:ARG:HE	1.70	0.55
1:O:263:THR:HA	1:O:359:ARG:HH12	1.72	0.55
1:S:144:GLU:HB2	1:S:148:ASP:HB2	1.89	0.55
4:6:161:ILE:HG12	4:7:224:ARG:HE	1.72	0.55
1:C:438:ASN:HD22	1:C:1171:HIS:HD2	1.54	0.55
1:D:150:THR:HG21	1:N:313:LEU:HD21	1.89	0.55
1:F:183:LEU:HD13	1:F:394:ARG:HH22	1.72	0.55
1:O:1163:CYS:SG	1:O:1164:GLU:N	2.79	0.55
1:N:587:ASN:HD22	1:O:572:ARG:HH12	1.54	0.55
1:N:494:PHE:HZ	2:Q:6:VAL:HG22	1.71	0.55
1:U:666:ASN:ND2	1:V:867:ASP:OD2	2.39	0.55
1:A:1027:GLN:HB3	1:A:1032:MET:HB2	1.89	0.55
1:D:75:CYS:SG	1:D:1059:THR:OG1	2.64	0.55
1:D:678:ARG:HD3	1:E:647:LYS:HZ1	1.71	0.55
1:F:1250:TYR:HB2	1:F:1270:PHE:HD2	1.70	0.55
1:X:396:ILE:HD11	1:X:1050:HIS:HE1	1.72	0.55
1:X:532:LEU:O	1:X:1241:GLN:NE2	2.40	0.55
1:4:563:GLY:HA3	1:4:1015:MET:HG3	1.88	0.55
4:6:111:LEU:HB2	4:6:286:LEU:HB2	1.89	0.55
1:F:532:LEU:O	1:F:1241:GLN:NE2	2.39	0.55
1:M:1173:GLN:NE2	1:M:1302:THR:OG1	2.40	0.55
1:N:586:THR:HA	1:N:693:LYS:HD2	1.89	0.55
1:N:946:LYS:NZ	1:N:986:GLU:OE1	2.40	0.55
1:T:271:GLN:OE1	1:T:1056:ARG:NH1	2.38	0.55
1:T:893:ARG:NH2	1:T:988:GLU:OE1	2.40	0.55
1:T:92:GLN:HE22	1:T:115:ILE:HG23	1.72	0.55
1:T:828:ASN:ND2	1:T:937:THR:O	2.40	0.55
1:V:592:ILE:HG12	1:V:679:LYS:HB3	1.89	0.55
3:5:164:PRO:HG2	3:5:180:ALA:HB3	1.88	0.54
1:B:578:ARG:NH1	1:B:1014:SER:O	2.40	0.54
1:C:450:LEU:HD11	1:C:1025:ILE:HA	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1073:VAL:HG13	1:D:1078:VAL:HG22	1.89	0.54
1:D:1335:ARG:HH22	1:D:1370:LEU:HD11	1.71	0.54
1:M:842:ASP:OD2	2:P:19:TYR:OH	2.25	0.54
1:U:452:SER:HB3	1:U:1117:ASP:HA	1.89	0.54
1:X:1163:CYS:N	1:X:1303:ASP:OD2	2.40	0.54
1:X:1344:ASN:ND2	1:X:1347:THR:OG1	2.40	0.54
2:0:13:GLU:OE1	2:0:46:ARG:NH2	2.31	0.54
1:B:492:ASN:HD22	1:B:495:ARG:HE	1.53	0.54
1:S:564:ASN:ND2	1:S:990:TRP:O	2.40	0.54
1:F:115:ILE:HB	1:T:36:GLN:HB3	1.90	0.54
1:T:964:TYR:OH	1:T:978:ASN:ND2	2.41	0.54
1:A:587:ASN:HB2	1:B:572:ARG:HH22	1.72	0.54
1:C:273:ALA:O	1:C:1053:TYR:OH	2.24	0.54
1:C:182:LYS:NZ	1:C:1058:SER:OG	2.40	0.54
1:D:1115:CYS:HB2	1:D:1179:ILE:HD11	1.88	0.54
1:F:640:THR:O	1:F:644:ASN:ND2	2.40	0.54
1:M:214:VAL:HA	1:M:217:PHE:HD2	1.71	0.54
1:O:714:ASP:O	1:O:804:LYS:NZ	2.41	0.54
1:S:1067:SER:HG	1:S:1083:THR:HG1	1.55	0.54
1:U:591:VAL:N	1:U:683:GLU:OE1	2.40	0.54
1:4:1282:LEU:HD23	1:4:1285:LEU:HD12	1.88	0.54
1:A:1220:TYR:HD2	1:A:1242:ARG:HH11	1.55	0.54
1:C:1187:ASP:OD2	1:C:1232:ARG:NH2	2.41	0.54
1:M:95:ILE:HB	1:M:114:TYR:HB2	1.89	0.54
1:D:38:LEU:HD12	1:N:113:GLN:HG2	1.88	0.54
1:O:438:ASN:HD22	1:O:1171:HIS:HD2	1.55	0.54
1:S:396:ILE:HD11	1:S:1050:HIS:HE1	1.72	0.54
1:U:536:VAL:HG13	1:U:1244:SER:HA	1.89	0.54
1:U:561:MET:H	1:U:564:ASN:HD22	1.55	0.54
3:5:75:VAL:HG11	3:5:80:PHE:HB2	1.89	0.54
4:9:104:GLN:NE2	4:9:291:TYR:OH	2.41	0.54
1:A:1173:GLN:NE2	1:A:1302:THR:OG1	2.41	0.54
1:A:826:TYR:OH	1:A:920:ASN:O	2.26	0.54
1:C:1196:ASN:HD21	1:C:1324:GLN:HG3	1.73	0.54
1:F:1198:ARG:NH2	1:F:1219:LEU:O	2.41	0.54
1:U:1167:PRO:HG3	1:V:1217:ARG:HB2	1.89	0.54
1:V:8:ARG:NH2	1:W:316:ALA:O	2.40	0.54
1:S:867:ASP:OD2	1:X:666:ASN:ND2	2.41	0.54
1:4:756:PHE:O	1:4:788:LEU:N	2.41	0.54
1:C:518:VAL:HG13	1:C:522:ASP:HB3	1.88	0.54
1:C:929:ASP:OD1	1:C:932:ARG:NH2	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1280:ARG:NH2	1:D:1288:GLU:OE1	2.41	0.54
1:O:959:PRO:HA	1:O:962:ALA:HB3	1.89	0.54
1:S:1220:TYR:HD2	1:S:1242:ARG:HH11	1.56	0.54
1:S:1236:ASN:HB2	1:S:1238:TRP:HE3	1.72	0.54
1:S:192:LEU:O	1:S:196:GLY:N	2.38	0.54
1:T:1167:PRO:HD3	1:U:1224:ILE:HD13	1.90	0.54
1:V:8:ARG:NH1	1:V:49:ARG:O	2.39	0.54
1:V:537:HIS:HA	1:V:1238:TRP:CD1	2.42	0.54
1:V:780:GLU:OE1	1:V:785:ARG:NH1	2.32	0.54
1:4:934:ALA:O	1:4:938:MET:N	2.33	0.54
1:C:620:ILE:HD11	1:C:630:ASN:HD22	1.72	0.54
1:D:963:ASN:HA	1:D:966:THR:HG22	1.90	0.54
1:F:1248:VAL:HG13	1:F:1254:PHE:HD2	1.73	0.54
1:M:578:ARG:NH1	1:M:1014:SER:O	2.39	0.54
1:E:333:ILE:HD11	1:M:11:PRO:HD3	1.89	0.54
1:M:83:LEU:HD21	1:M:122:LYS:HD2	1.90	0.54
1:N:1207:CYS:SG	1:N:1208:ASP:N	2.80	0.54
1:N:717:LEU:HD23	1:N:804:LYS:HD3	1.88	0.54
1:T:1005:THR:HG22	1:T:1007:GLY:H	1.71	0.54
1:U:83:LEU:HD22	1:U:1085:GLU:HB3	1.87	0.54
1:W:1071:ARG:O	1:W:1079:THR:OG1	2.25	0.54
1:W:331:ALA:HA	1:W:335:ASP:HB2	1.90	0.54
1:X:436:ASN:HB3	1:X:440:VAL:H	1.72	0.54
1:D:706:THR:O	1:D:710:SER:OG	2.25	0.54
1:E:507:ALA:HB2	1:E:971:GLN:HE22	1.73	0.54
1:M:725:ASP:HB3	1:M:793:LEU:HD22	1.88	0.54
1:O:1295:GLY:H	1:O:1321:HIS:CE1	2.26	0.54
1:V:1249:LEU:O	1:V:1255:ARG:NH2	2.40	0.54
1:C:278:THR:HG22	1:C:1051:ILE:HG12	1.89	0.54
1:C:899:ASP:OD2	1:C:1018:LYS:NZ	2.32	0.54
1:M:709:VAL:HG22	1:M:1023:SER:HA	1.89	0.54
1:O:736:ARG:HD2	1:O:897:LYS:HB2	1.90	0.54
1:T:1241:GLN:HB3	1:T:1244:SER:HB3	1.89	0.54
1:U:532:LEU:O	1:U:1241:GLN:NE2	2.40	0.54
1:4:1333:SER:HB2	1:4:1355:GLN:HB2	1.89	0.54
1:4:226:PHE:HD2	1:4:1364:MET:HB3	1.72	0.54
1:4:777:ARG:NH2	1:4:885:CYS:O	2.38	0.54
1:A:450:LEU:HD11	1:A:1025:ILE:HA	1.90	0.54
2:G:78:ARG:HH21	2:H:19:TYR:HE1	1.55	0.54
2:Y:12:GLN:HB2	2:3:70:ARG:CZ	2.39	0.53
1:4:133:ALA:HA	1:4:136:ILE:HD12	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1245:LEU:HA	1:D:1248:VAL:HB	1.90	0.53
1:E:15:THR:HG21	1:U:257:VAL:HG13	1.89	0.53
1:N:893:ARG:NH2	1:N:988:GLU:OE1	2.41	0.53
1:S:1067:SER:OG	1:S:1083:THR:OG1	2.26	0.53
1:S:739:ILE:HB	1:S:895:ILE:HB	1.88	0.53
1:S:946:LYS:HE2	1:S:993:SER:HA	1.88	0.53
1:U:153:ALA:HB1	1:V:338:ASN:HB3	1.91	0.53
1:V:963:ASN:O	1:V:967:ARG:N	2.36	0.53
1:4:1236:ASN:HB2	1:4:1238:TRP:HE3	1.73	0.53
1:4:743:GLY:O	1:4:746:ASN:ND2	2.40	0.53
1:C:1344:ASN:ND2	1:C:1347:THR:OG1	2.41	0.53
1:D:211:SER:HG	1:D:1206:SER:HG	1.56	0.53
1:E:929:ASP:OD1	1:E:932:ARG:NH2	2.41	0.53
1:N:448:ASN:HD21	1:N:1113:VAL:HG13	1.73	0.53
1:O:1236:ASN:HB2	1:O:1238:TRP:HE3	1.73	0.53
1:T:195:LEU:HD23	1:T:1283:TYR:HE1	1.74	0.53
1:U:1295:GLY:H	1:U:1321:HIS:CE1	2.26	0.53
1:V:799:ASN:HD21	1:V:802:LEU:HG	1.73	0.53
1:X:537:HIS:HA	1:X:1238:TRP:CD1	2.43	0.53
1:E:1043:THR:HG23	1:E:1265:PRO:HG3	1.91	0.53
1:E:591:VAL:N	1:E:683:GLU:OE1	2.38	0.53
1:M:708:LEU:HD21	1:M:1022:PRO:HG2	1.90	0.53
1:M:897:LYS:HA	1:M:912:ASP:HA	1.90	0.53
1:A:547:CYS:HB2	1:A:550:ALA:HB3	1.90	0.53
1:B:1171:HIS:HE1	1:C:1228:ALA:HA	1.71	0.53
1:D:1187:ASP:OD2	1:D:1232:ARG:NH2	2.42	0.53
1:S:1179:ILE:HG22	1:S:1181:PRO:HD3	1.91	0.53
1:S:893:ARG:HG3	1:S:916:THR:HG22	1.90	0.53
1:S:987:TYR:O	1:S:992:LYS:NZ	2.42	0.53
1:W:932:ARG:HE	1:W:956:THR:HG23	1.73	0.53
1:X:1201:ALA:HB3	1:X:1227:PRO:HG2	1.91	0.53
3:5:81:SER:OG	3:5:84:GLU:OE2	2.27	0.53
1:B:493:LEU:HD13	1:B:942:VAL:HG21	1.90	0.53
1:C:963:ASN:HA	1:C:966:THR:HG22	1.91	0.53
1:D:491:MET:HB2	1:D:783:ASP:HA	1.89	0.53
1:D:819:MET:N	1:D:950:ASP:OD2	2.40	0.53
1:A:206:LYS:HD3	1:F:1162:ARG:HH22	1.72	0.53
1:F:826:TYR:HE2	1:F:886:PRO:HG2	1.73	0.53
1:M:606:ASP:HB3	1:M:609:TYR:HB2	1.91	0.53
1:S:640:THR:O	1:S:644:ASN:ND2	2.40	0.53
1:U:491:MET:HB2	1:U:783:ASP:HA	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:851:LEU:HD23	1:W:854:LEU:HD12	1.89	0.53
1:X:457:ARG:NH1	1:X:462:THR:OG1	2.34	0.53
1:A:1005:THR:HG22	1:A:1007:GLY:H	1.74	0.53
1:A:1062:PHE:HB2	1:A:1087:ALA:HB3	1.89	0.53
1:A:737:GLN:HG2	1:A:897:LYS:HE2	1.89	0.53
1:C:451:LYS:HG2	1:C:1140:ALA:HB1	1.91	0.53
1:D:214:VAL:HA	1:D:217:PHE:HD2	1.73	0.53
1:D:715:PRO:HB3	1:D:800:PRO:HG3	1.89	0.53
1:D:20:LEU:O	1:M:387:GLN:NE2	2.41	0.53
1:O:214:VAL:HA	1:O:217:PHE:HD2	1.72	0.53
1:T:540:PHE:O	1:T:559:ARG:NH1	2.42	0.53
1:T:640:THR:O	1:T:644:ASN:ND2	2.38	0.53
1:W:153:ALA:HB1	1:X:338:ASN:HB3	1.91	0.53
1:X:963:ASN:O	1:X:967:ARG:N	2.42	0.53
1:B:1005:THR:HG22	1:B:1007:GLY:H	1.73	0.53
1:B:1201:ALA:HB3	1:B:1227:PRO:HG2	1.90	0.53
1:B:736:ARG:HD2	1:B:897:LYS:HB2	1.91	0.53
1:D:641:TYR:O	1:D:645:SER:OG	2.26	0.53
1:E:402:PHE:HD2	1:E:1040:VAL:HB	1.73	0.53
1:E:649:ALA:O	1:E:677:TYR:OH	2.26	0.53
1:F:448:ASN:ND2	1:F:1113:VAL:O	2.42	0.53
1:F:38:LEU:HD22	1:F:43:ALA:HA	1.91	0.53
1:M:579:GLY:HA3	1:M:1011:ALA:HA	1.90	0.53
1:O:824:VAL:H	1:O:889:THR:HG21	1.74	0.53
1:U:864:GLN:O	1:U:930:ARG:NH2	2.42	0.53
1:V:617:GLU:HG3	1:V:656:MET:HG3	1.91	0.53
1:W:965:VAL:HG13	1:W:972:ARG:HD3	1.89	0.53
4:7:7:ILE:N	4:7:84:LEU:O	2.38	0.53
1:A:578:ARG:NH1	1:A:1014:SER:O	2.42	0.53
1:D:79:GLU:N	1:D:304:ALA:O	2.42	0.53
1:E:575:GLN:NE2	1:E:1015:MET:SD	2.82	0.53
1:E:48:VAL:HG21	1:F:317:VAL:HA	1.90	0.53
1:M:255:ASP:HB2	1:M:1092:ALA:HB1	1.90	0.53
1:N:540:PHE:O	1:N:559:ARG:NH1	2.42	0.53
1:S:708:LEU:HD21	1:S:1022:PRO:HG2	1.90	0.53
1:X:324:ARG:NE	1:X:352:ASP:OD2	2.42	0.53
1:4:822:MET:H	1:4:944:PHE:HE2	1.56	0.53
1:C:1005:THR:HG22	1:C:1007:GLY:H	1.74	0.53
1:F:406:LEU:O	1:F:428:GLN:NE2	2.42	0.53
1:M:435:VAL:HG11	1:M:1368:LEU:HD22	1.91	0.53
1:M:557:THR:HA	1:M:898:ARG:HH22	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:271:GLN:OE1	1:O:1056:ARG:NH1	2.41	0.53
1:T:56:VAL:HG13	1:U:92:GLN:HB3	1.91	0.53
1:U:399:THR:HG22	1:U:1043:THR:HG22	1.90	0.53
1:V:578:ARG:NH1	1:V:1014:SER:O	2.41	0.53
1:X:1187:ASP:OD2	1:X:1232:ARG:NH2	2.42	0.53
4:7:120:ARG:NH1	4:7:123:SER:OG	2.42	0.53
1:B:540:PHE:O	1:B:559:ARG:NH1	2.42	0.53
1:D:324:ARG:NH2	1:D:352:ASP:OD1	2.42	0.53
1:F:1241:GLN:HB3	1:F:1244:SER:HB3	1.90	0.53
1:O:1187:ASP:OD2	1:O:1232:ARG:NH2	2.42	0.53
1:W:428:GLN:NE2	1:W:577:SER:OG	2.42	0.53
1:X:8:ARG:HH22	1:X:18:ASN:HD21	1.55	0.53
1:X:706:THR:O	1:X:710:SER:OG	2.27	0.53
3:5:225:THR:HG22	3:5:293:THR:HG22	1.91	0.52
4:6:99:TYR:HE2	4:6:139:VAL:H	1.55	0.52
1:C:1071:ARG:O	1:C:1079:THR:OG1	2.27	0.52
1:C:714:ASP:O	1:C:804:LYS:NZ	2.43	0.52
1:D:828:ASN:ND2	1:D:937:THR:O	2.41	0.52
1:E:927:VAL:HB	1:E:956:THR:HG21	1.90	0.52
1:N:307:VAL:HG12	1:N:309:ARG:H	1.75	0.52
1:U:1210:TYR:HE1	1:U:1280:ARG:HG2	1.72	0.52
1:W:958:HIS:CE1	1:W:960:LEU:HB3	2.45	0.52
1:X:1341:TYR:HB2	1:X:1357:LEU:HD11	1.90	0.52
1:A:331:ALA:HA	1:A:335:ASP:HB2	1.90	0.52
1:C:256:THR:HG22	1:C:258:PHE:H	1.74	0.52
1:C:602:GLU:HB3	1:C:647:LYS:HE2	1.91	0.52
1:D:585:VAL:HG11	1:D:1030:HIS:HB3	1.91	0.52
1:D:864:GLN:O	1:D:930:ARG:NH2	2.41	0.52
1:M:744:ASP:H	1:M:786:HIS:HE1	1.56	0.52
1:O:770:LEU:HD11	1:O:883:LEU:HD13	1.91	0.52
1:S:461:PRO:HG2	1:S:906:THR:H	1.74	0.52
1:T:708:LEU:HD21	1:T:1022:PRO:HG2	1.91	0.52
1:T:898:ARG:HE	1:T:913:VAL:HG23	1.75	0.52
1:U:1068:VAL:HG22	1:U:1082:ILE:HG12	1.91	0.52
1:U:1122:PHE:HE1	1:U:1258:ALA:HB2	1.74	0.52
1:C:785:ARG:HG2	1:C:787:VAL:H	1.74	0.52
1:D:450:LEU:HD11	1:D:1025:ILE:HG13	1.90	0.52
1:M:82:ASP:N	1:M:82:ASP:OD1	2.41	0.52
1:N:1263:TYR:OH	1:N:1305:GLN:NE2	2.40	0.52
1:U:572:ARG:NH2	1:U:1001:SER:O	2.41	0.52
1:A:856:ASN:OD1	1:A:860:LYS:NZ	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:611:LEU:HD22	1:B:862:ILE:HG12	1.90	0.52
1:B:958:HIS:CE1	1:B:960:LEU:HB3	2.44	0.52
1:C:849:ASP:HB2	1:C:869:ARG:HH21	1.75	0.52
1:C:130:GLU:OE1	1:D:110:LYS:NZ	2.40	0.52
1:E:958:HIS:CE1	1:E:960:LEU:HB3	2.44	0.52
1:F:588:MET:HB3	1:F:690:ALA:HB2	1.92	0.52
1:N:1071:ARG:O	1:N:1079:THR:OG1	2.25	0.52
1:O:842:ASP:OD2	2:R:19:TYR:OH	2.28	0.52
1:X:799:ASN:HD21	1:X:802:LEU:HG	1.73	0.52
1:A:249:LEU:HD21	1:A:372:LYS:HB2	1.91	0.52
1:E:11:PRO:HB2	1:U:332:ARG:HD2	1.92	0.52
1:O:532:LEU:O	1:O:1241:GLN:NE2	2.42	0.52
1:U:537:HIS:HA	1:U:1238:TRP:HE1	1.74	0.52
1:V:1005:THR:HG22	1:V:1007:GLY:H	1.72	0.52
1:X:1199:GLY:HA2	1:X:1235:ASN:HB3	1.91	0.52
1:4:655:HIS:O	1:4:659:PHE:N	2.42	0.52
1:A:1262:MET:HA	1:A:1306:TYR:HA	1.90	0.52
1:F:849:ASP:HB2	1:F:869:ARG:HH21	1.73	0.52
1:O:742:ILE:HG12	1:O:788:LEU:HD11	1.91	0.52
1:S:95:ILE:HD12	1:S:116:VAL:HG21	1.92	0.52
1:T:1190:TYR:OH	1:T:1196:ASN:O	2.27	0.52
1:V:578:ARG:NH2	1:V:1017:GLN:OE1	2.43	0.52
1:V:1187:ASP:OD2	1:V:1232:ARG:NH2	2.42	0.52
1:W:545:HIS:N	1:W:553:SER:O	2.43	0.52
1:X:49:ARG:HB2	1:4:56:VAL:HB	1.90	0.52
1:D:1197:PRO:O	1:D:1236:ASN:ND2	2.42	0.52
1:E:1071:ARG:O	1:E:1079:THR:OG1	2.25	0.52
1:M:77:ASN:HA	1:M:1061:MET:HB2	1.92	0.52
1:M:172:ARG:NH1	1:M:382:MET:O	2.42	0.52
1:U:842:ASP:OD2	2:0:19:TYR:OH	2.27	0.52
1:W:856:ASN:ND2	2:1:66:GLY:O	2.35	0.52
1:W:420:ARG:NH1	1:X:1353:MET:SD	2.82	0.52
3:5:124:GLN:NE2	3:5:311:SER:O	2.40	0.52
4:7:277:SER:O	4:7:281:ASN:ND2	2.43	0.52
1:D:878:LEU:O	1:D:881:SER:OG	2.28	0.52
1:F:1341:TYR:HA	1:F:1348:HIS:HD2	1.74	0.52
1:F:394:ARG:HB3	1:F:1050:HIS:CD2	2.45	0.52
1:F:850:ILE:HD12	1:F:875:ILE:HD12	1.92	0.52
1:N:1183:PRO:HG2	1:N:1186:SER:HB3	1.91	0.52
1:N:236:ARG:NH1	1:N:239:GLN:OE1	2.43	0.52
1:S:294:GLU:HB2	1:S:366:LEU:HD22	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:455:HIS:HD2	1:T:1119:PHE:HD1	1.56	0.52
1:U:858:THR:HG22	1:U:934:ALA:HB1	1.92	0.52
1:V:396:ILE:HD11	1:V:1050:HIS:HE1	1.75	0.52
1:W:438:ASN:HD22	1:W:1171:HIS:HD2	1.56	0.52
1:W:185:HIS:O	1:W:1097:SER:OG	2.27	0.52
3:8:254:GLU:HG2	4:9:64:GLN:HE21	1.74	0.52
1:A:197:ASP:HB3	1:A:199:VAL:HG12	1.92	0.52
1:B:714:ASP:O	1:B:804:LYS:NZ	2.43	0.52
1:B:387:GLN:OE1	1:C:112:ARG:NH1	2.43	0.52
1:C:699:THR:HA	1:C:704:PRO:HA	1.91	0.52
1:F:558:HIS:CE1	1:F:902:GLN:HE22	2.27	0.52
1:N:130:GLU:HG3	1:O:110:LYS:HD2	1.91	0.52
1:S:193:LYS:NZ	1:S:247:ASP:OD2	2.41	0.52
1:T:402:PHE:HD2	1:T:1040:VAL:HB	1.74	0.52
3:8:78:GLN:NE2	3:8:138:GLY:O	2.43	0.52
1:E:1196:ASN:HD21	1:E:1324:GLN:HG3	1.74	0.52
1:N:127:ALA:HB3	1:N:1082:ILE:HB	1.92	0.52
1:N:1280:ARG:NH2	1:N:1288:GLU:OE1	2.42	0.52
1:O:182:LYS:NZ	1:O:1058:SER:OG	2.42	0.52
1:O:402:PHE:HD2	1:O:1040:VAL:HB	1.74	0.52
1:W:536:VAL:HB	1:W:542:PHE:HE2	1.74	0.52
1:W:839:VAL:O	1:W:876:ARG:NH2	2.43	0.52
1:X:619:MET:SD	1:X:881:SER:OG	2.65	0.52
3:8:300:PRO:HB2	3:8:315:LEU:HD22	1.92	0.51
1:E:185:HIS:O	1:E:1097:SER:OG	2.28	0.51
1:N:536:VAL:HG13	1:N:1244:SER:HA	1.91	0.51
1:O:717:LEU:HB2	1:O:990:TRP:HZ3	1.74	0.51
1:X:578:ARG:NH1	1:X:1014:SER:O	2.43	0.51
1:4:578:ARG:NH1	1:4:1014:SER:O	2.43	0.51
1:4:620:ILE:HG22	1:4:622:GLY:H	1.75	0.51
4:6:215:SER:HB2	4:7:219:PRO:HB3	1.93	0.51
4:6:284:PRO:HA	4:6:305:ARG:HB3	1.93	0.51
1:C:537:HIS:HA	1:C:1238:TRP:CD1	2.45	0.51
1:C:878:LEU:O	1:C:881:SER:OG	2.28	0.51
1:N:889:THR:HA	1:N:920:ASN:HB3	1.92	0.51
1:O:467:ALA:HB2	1:O:1254:PHE:HE2	1.75	0.51
1:O:79:GLU:N	1:O:304:ALA:O	2.44	0.51
1:S:648:LEU:HD13	1:S:677:TYR:HE1	1.74	0.51
1:T:606:ASP:OD1	1:T:647:LYS:NZ	2.36	0.51
1:V:585:VAL:HG11	1:V:1030:HIS:HB3	1.90	0.51
1:V:214:VAL:HA	1:V:217:PHE:HD2	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:720:PRO:HA	1:V:917:VAL:HG13	1.91	0.51
1:W:275:VAL:HG22	1:W:375:ALA:HB3	1.92	0.51
4:6:26:LYS:HA	4:6:98:VAL:HG21	1.92	0.51
1:A:191:ILE:HA	1:A:217:PHE:HE1	1.74	0.51
1:A:854:LEU:HD13	1:A:860:LYS:HG2	1.92	0.51
1:M:1062:PHE:HB2	1:M:1087:ALA:HB3	1.91	0.51
1:O:279:THR:OG1	1:O:280:ASP:N	2.43	0.51
3:8:224:VAL:HG13	3:8:294:VAL:HB	1.93	0.51
1:B:704:PRO:HG2	1:C:969:PRO:HD2	1.92	0.51
1:E:82:ASP:N	1:E:82:ASP:OD1	2.42	0.51
1:M:450:LEU:HD11	1:M:1025:ILE:HG13	1.91	0.51
1:N:1163:CYS:SG	1:N:1164:GLU:N	2.84	0.51
1:M:1170:SER:OG	1:N:1227:PRO:O	2.27	0.51
1:T:1167:PRO:HG2	1:U:1218:LEU:HD23	1.91	0.51
1:U:82:ASP:N	1:U:82:ASP:OD1	2.43	0.51
1:S:200:TYR:HE1	1:X:1105:ALA:HB1	1.75	0.51
1:X:898:ARG:HH21	1:X:913:VAL:HG21	1.75	0.51
1:4:514:GLN:HE21	1:4:531:LEU:HD21	1.75	0.51
4:9:13:SER:OG	4:9:130:ASN:ND2	2.43	0.51
1:A:1003:GLN:NE2	1:F:587:ASN:OD1	2.43	0.51
1:A:1227:PRO:O	1:F:1170:SER:OG	2.28	0.51
1:A:236:ARG:HH21	1:A:239:GLN:HG3	1.76	0.51
1:A:438:ASN:HD22	1:A:1171:HIS:CD2	2.28	0.51
1:C:850:ILE:HD11	1:C:872:VAL:HA	1.92	0.51
1:D:278:THR:HG22	1:D:1051:ILE:HA	1.93	0.51
1:D:395:ARG:HD3	1:D:1045:GLU:HB3	1.93	0.51
1:F:785:ARG:HG2	1:F:787:VAL:H	1.76	0.51
1:M:706:THR:O	1:M:710:SER:OG	2.28	0.51
1:S:587:ASN:OD1	1:T:1003:GLN:NE2	2.44	0.51
1:W:736:ARG:HH22	1:W:900:PRO:HD3	1.75	0.51
1:X:510:PRO:HD2	1:X:976:VAL:HG13	1.92	0.51
4:7:16:PHE:HZ	4:7:128:GLU:HB2	1.74	0.51
1:B:1241:GLN:HB3	1:B:1244:SER:HB3	1.92	0.51
1:F:127:ALA:HB3	1:F:1082:ILE:HB	1.92	0.51
1:F:68:GLU:HA	1:F:362:ILE:HD12	1.93	0.51
1:N:788:LEU:HD21	1:N:919:VAL:HG21	1.92	0.51
1:O:537:HIS:HA	1:O:1238:TRP:HE1	1.74	0.51
1:O:82:ASP:HB2	1:O:85:ARG:HB2	1.93	0.51
1:S:83:LEU:HD21	1:S:122:LYS:HD2	1.91	0.51
1:T:800:PRO:HB2	1:T:804:LYS:HE3	1.91	0.51
1:V:266:THR:HA	1:V:297:MET:HA	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:635:ALA:HB1	1:A:668:SER:HB3	1.92	0.51
1:C:474:ASP:OD1	1:C:552:GLY:N	2.40	0.51
1:A:90:LYS:HB3	1:F:53:LEU:HD23	1.93	0.51
1:N:66:PHE:HD1	1:N:175:VAL:HG22	1.76	0.51
1:U:450:LEU:HD11	1:U:1025:ILE:HA	1.91	0.51
1:V:1245:LEU:HA	1:V:1248:VAL:HB	1.92	0.51
1:V:850:ILE:HD11	1:V:872:VAL:HA	1.91	0.51
1:W:450:LEU:HD11	1:W:1025:ILE:HG13	1.93	0.51
1:W:929:ASP:OD1	1:W:932:ARG:NH2	2.43	0.51
1:A:273:ALA:O	1:A:1053:TYR:OH	2.27	0.51
1:C:214:VAL:HA	1:C:217:PHE:HD2	1.76	0.51
1:C:617:GLU:HG3	1:C:656:MET:HG3	1.92	0.51
1:E:127:ALA:HB3	1:E:1082:ILE:HB	1.91	0.51
1:N:1187:ASP:OD2	1:N:1232:ARG:NH2	2.44	0.51
1:O:130:GLU:HG2	1:O:1079:THR:HG22	1.91	0.51
1:V:197:ASP:HB3	1:V:199:VAL:HG12	1.91	0.51
1:V:436:ASN:HB3	1:V:440:VAL:H	1.75	0.51
1:W:606:ASP:OD1	1:W:647:LYS:NZ	2.35	0.51
1:X:687:LEU:HD23	1:X:805:LEU:HD22	1.93	0.51
1:4:539:PHE:HE1	1:4:565:ILE:HD11	1.76	0.51
1:4:836:ASN:HD21	1:4:839:VAL:HB	1.75	0.51
1:A:658:ARG:HA	1:A:681:LEU:HD11	1.92	0.51
1:C:125:ILE:HB	1:C:1084:HIS:HB3	1.93	0.51
1:E:737:GLN:HB3	1:E:897:LYS:H	1.74	0.51
1:N:603:THR:HG22	1:N:647:LYS:HB3	1.93	0.51
1:S:1051:ILE:O	1:S:1100:ALA:N	2.44	0.51
1:T:1196:ASN:HD22	1:T:1202:ALA:H	1.58	0.51
1:W:780:GLU:OE1	1:W:785:ARG:NH1	2.41	0.51
1:X:6:GLU:HG3	1:X:7:GLN:HG3	1.93	0.51
1:4:1074:ARG:HH12	4:6:83:ARG:HG3	1.75	0.51
1:A:210:LYS:NZ	1:A:1207:CYS:O	2.42	0.51
1:O:536:VAL:HB	1:O:542:PHE:HE2	1.76	0.51
1:U:1059:THR:HG22	1:U:1090:HIS:HA	1.93	0.51
1:V:79:GLU:N	1:V:304:ALA:O	2.44	0.51
1:4:737:GLN:NE2	1:4:749:ASN:OD1	2.44	0.50
1:B:932:ARG:HE	1:B:956:THR:HG23	1.77	0.50
2:J:74:LEU:HD23	2:J:77:LEU:HD12	1.94	0.50
1:M:898:ARG:O	1:M:903:SER:OG	2.29	0.50
1:T:1196:ASN:HD21	1:T:1324:GLN:HG3	1.76	0.50
1:U:1200:ARG:NH1	1:U:1233:SER:O	2.44	0.50
1:W:399:THR:HA	1:W:1043:THR:HA	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:397:GLN:NE2	1:4:1263:TYR:OH	2.44	0.50
1:A:67:LEU:HD11	1:A:300:PRO:HG2	1.91	0.50
1:D:902:GLN:NE2	1:D:1018:LYS:O	2.43	0.50
1:D:1196:ASN:HD22	1:D:1201:ALA:HA	1.76	0.50
1:E:5:LEU:HD12	1:U:117:MET:HB2	1.92	0.50
1:N:396:ILE:HD11	1:N:1050:HIS:HE1	1.77	0.50
1:O:537:HIS:HB3	1:O:1245:LEU:HB2	1.93	0.50
1:O:436:ASN:HB3	1:O:440:VAL:H	1.76	0.50
1:O:821:GLY:HA2	1:O:923:GLY:HA2	1.93	0.50
1:X:540:PHE:O	1:X:559:ARG:NH1	2.45	0.50
4:9:176:LEU:O	4:9:180:ASN:ND2	2.43	0.50
1:C:83:LEU:HD13	1:C:1085:GLU:HB3	1.93	0.50
1:D:249:LEU:HD21	1:D:372:LYS:HB2	1.93	0.50
1:E:380:GLN:O	1:E:384:ASN:N	2.45	0.50
1:F:1210:TYR:HE1	1:F:1280:ARG:HG2	1.75	0.50
1:F:855:GLU:HG2	2:K:70:ARG:HE	1.76	0.50
2:R:74:LEU:HD23	2:R:77:LEU:HD12	1.94	0.50
1:F:113:GLN:HB3	1:T:38:LEU:HB2	1.91	0.50
1:E:13:LEU:O	1:T:58:THR:N	2.42	0.50
1:U:1199:GLY:HA2	1:U:1235:ASN:HB3	1.93	0.50
1:W:1199:GLY:HA2	1:W:1235:ASN:HB3	1.94	0.50
1:W:958:HIS:HE1	1:W:960:LEU:HB3	1.77	0.50
1:X:278:THR:HG22	1:X:1051:ILE:HA	1.93	0.50
1:4:47:SER:OG	1:4:48:VAL:N	2.44	0.50
1:A:564:ASN:ND2	1:A:990:TRP:O	2.45	0.50
1:D:826:TYR:HE2	1:D:886:PRO:HG2	1.75	0.50
1:E:770:LEU:HD21	1:E:883:LEU:HD22	1.92	0.50
1:F:75:CYS:HG	1:F:1059:THR:HG1	1.52	0.50
1:S:438:ASN:HD22	1:S:1171:HIS:HD2	1.58	0.50
1:T:636:LEU:HD23	1:T:870:PRO:HA	1.93	0.50
1:U:1168:GLY:HA2	1:V:207:LYS:HD3	1.93	0.50
1:V:277:GLU:HG2	1:V:377:GLU:HB2	1.92	0.50
1:W:183:LEU:HD13	1:W:394:ARG:HH21	1.75	0.50
2:Z:74:LEU:HD23	2:Z:77:LEU:HD12	1.94	0.50
2:1:74:LEU:HD23	2:1:77:LEU:HD12	1.94	0.50
2:2:74:LEU:HD23	2:2:77:LEU:HD12	1.94	0.50
1:4:455:HIS:HE2	1:4:1122:PHE:HB2	1.76	0.50
1:A:434:VAL:HG11	1:A:1042:ARG:HH22	1.77	0.50
1:B:640:THR:O	1:B:644:ASN:ND2	2.45	0.50
1:B:856:ASN:OD1	1:B:860:LYS:NZ	2.41	0.50
1:E:578:ARG:NH1	1:E:1014:SER:OG	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:871:THR:OG1	1:N:874:MET:SD	2.68	0.50
1:S:94:LYS:HG2	1:S:115:ILE:HG12	1.93	0.50
1:T:332:ARG:NH2	1:T:346:ASP:OD1	2.45	0.50
1:T:450:LEU:HD21	1:T:1025:ILE:HG13	1.92	0.50
1:U:397:GLN:HB3	1:U:1318:GLN:HB3	1.92	0.50
1:U:619:MET:SD	1:U:881:SER:OG	2.63	0.50
1:S:423:GLU:OE2	1:X:420:ARG:NH2	2.45	0.50
4:9:114:LEU:HD11	4:9:145:GLY:HA2	1.94	0.50
1:C:481:TYR:OH	1:C:979:VAL:N	2.45	0.50
1:F:1187:ASP:OD2	1:F:1232:ARG:NH2	2.44	0.50
1:M:609:TYR:HE2	1:M:614:TYR:HB2	1.76	0.50
1:N:683:GLU:O	1:N:687:LEU:N	2.38	0.50
1:S:1201:ALA:HB3	1:S:1227:PRO:HG2	1.94	0.50
1:M:319:TYR:OH	1:V:323:MET:SD	2.59	0.50
1:V:855:GLU:HG2	2:0:70:ARG:HE	1.76	0.50
1:V:56:VAL:HG22	1:W:92:GLN:HB3	1.93	0.50
2:Y:74:LEU:HD23	2:Y:77:LEU:HD12	1.94	0.50
3:8:295:PRO:HG3	3:8:319:ASN:HB2	1.94	0.50
1:C:507:ALA:HB1	1:C:978:ASN:HD21	1.76	0.50
1:C:963:ASN:O	1:C:967:ARG:NE	2.39	0.50
1:D:1062:PHE:HB2	1:D:1087:ALA:HB3	1.94	0.50
1:C:1171:HIS:HE1	1:D:1228:ALA:HA	1.76	0.50
1:D:41:LYS:O	1:D:44:ARG:NH1	2.44	0.50
1:M:918:LEU:HB2	1:M:944:PHE:HE2	1.76	0.50
1:T:1173:GLN:NE2	1:T:1302:THR:OG1	2.44	0.50
1:T:9:PRO:HG3	1:T:45:GLU:HB3	1.94	0.50
1:T:743:GLY:HA3	1:T:786:HIS:HE1	1.75	0.50
1:U:537:HIS:HA	1:U:1238:TRP:NE1	2.27	0.50
1:V:397:GLN:HE22	1:V:1298:ALA:HB3	1.76	0.50
1:V:569:LEU:HD13	1:V:1238:TRP:HH2	1.76	0.50
1:W:394:ARG:NH1	1:W:1317:ASP:OD2	2.45	0.50
1:X:773:ILE:O	1:X:776:THR:OG1	2.29	0.50
2:0:74:LEU:HD23	2:0:77:LEU:HD12	1.94	0.50
1:4:699:THR:HG22	1:4:704:PRO:HG3	1.93	0.50
1:4:708:LEU:HD22	1:4:1022:PRO:HG2	1.93	0.50
1:M:228:LEU:HD22	1:M:1103:HIS:HD2	1.77	0.50
1:O:1137:LYS:HA	1:O:1140:ALA:HB3	1.93	0.50
1:S:438:ASN:HD22	1:S:1171:HIS:CD2	2.30	0.50
1:T:1067:SER:OG	1:T:1083:THR:OG1	2.29	0.50
1:T:1207:CYS:SG	1:T:1208:ASP:N	2.84	0.50
1:T:600:ILE:O	1:T:603:THR:OG1	2.28	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:446:TYR:O	1:U:450:LEU:N	2.44	0.50
1:V:525:HIS:HD2	1:V:527:THR:HG22	1.77	0.50
1:V:864:GLN:O	1:V:930:ARG:NH2	2.45	0.50
3:5:269:THR:HA	3:5:272:ILE:HD12	1.94	0.50
3:8:77:SER:N	3:8:173:PHE:O	2.45	0.50
1:A:823:GLY:HA2	1:A:889:THR:HG21	1.94	0.50
1:C:770:LEU:HD11	1:C:883:LEU:HD13	1.94	0.50
1:D:434:VAL:HG11	1:D:1042:ARG:HH22	1.76	0.50
1:E:718:LEU:HD12	1:E:894:VAL:HG21	1.94	0.50
1:M:699:THR:HA	1:M:704:PRO:HA	1.94	0.50
1:N:1033:HIS:NE2	1:N:1036:PHE:O	2.43	0.50
1:N:898:ARG:HB3	1:N:902:GLN:HB2	1.94	0.50
1:O:419:VAL:HG11	1:O:1352:HIS:CD2	2.47	0.50
1:S:842:ASP:OD2	2:Y:19:TYR:OH	2.29	0.50
1:U:1226:ASP:HB2	1:U:1229:TYR:H	1.76	0.50
1:U:406:LEU:HD21	1:U:1191:PHE:HE2	1.77	0.50
1:W:1344:ASN:ND2	1:W:1347:THR:OG1	2.44	0.50
1:X:273:ALA:O	1:X:1053:TYR:OH	2.29	0.50
1:X:708:LEU:HD21	1:X:1022:PRO:HG2	1.93	0.50
1:X:887:PHE:O	1:X:920:ASN:ND2	2.44	0.50
1:4:174:LEU:HD11	1:4:1084:HIS:HE1	1.76	0.49
1:4:731:MET:HG2	1:4:738:PRO:HD2	1.94	0.49
1:A:545:HIS:HE1	1:A:555:ARG:HD2	1.76	0.49
1:B:1067:SER:OG	1:B:1083:THR:OG1	2.29	0.49
1:C:133:ALA:HB2	1:C:1076:ASP:HA	1.94	0.49
1:C:493:LEU:HD13	1:C:942:VAL:HG21	1.93	0.49
1:E:396:ILE:HD11	1:E:1050:HIS:HE1	1.75	0.49
1:D:1169:LEU:HD21	1:E:208:ALA:HA	1.93	0.49
2:G:74:LEU:HD23	2:G:77:LEU:HD12	1.94	0.49
2:K:74:LEU:HD23	2:K:77:LEU:HD12	1.94	0.49
2:L:74:LEU:HD23	2:L:77:LEU:HD12	1.93	0.49
1:N:740:ILE:HB	1:N:747:TYR:HB3	1.94	0.49
1:O:255:ASP:HB3	1:O:1093:LEU:HB3	1.92	0.49
1:T:1047:LEU:HD12	1:T:1106:ALA:HB3	1.93	0.49
1:T:185:HIS:O	1:T:1097:SER:OG	2.30	0.49
1:U:918:LEU:HB2	1:U:944:PHE:CE2	2.47	0.49
1:W:579:GLY:HA3	1:W:1011:ALA:HA	1.94	0.49
1:X:536:VAL:HG13	1:X:1244:SER:HA	1.93	0.49
1:D:714:ASP:O	1:D:804:LYS:NZ	2.44	0.49
1:E:130:GLU:HG2	1:E:1079:THR:HG22	1.94	0.49
1:D:1168:GLY:HA2	1:E:207:LYS:HD3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1344:ASN:ND2	1:F:1347:THR:OG1	2.45	0.49
1:F:757:ILE:HG12	1:F:788:LEU:HD22	1.93	0.49
1:F:842:ASP:OD2	2:L:19:TYR:OH	2.27	0.49
2:H:74:LEU:HD23	2:H:77:LEU:HD12	1.94	0.49
1:D:840:PHE:HE1	2:J:49:LEU:HD11	1.76	0.49
1:M:851:LEU:HD12	1:M:869:ARG:HD2	1.93	0.49
1:N:600:ILE:O	1:N:603:THR:OG1	2.26	0.49
1:T:578:ARG:NH2	1:T:1017:GLN:OE1	2.45	0.49
1:V:1255:ARG:HB2	1:V:1258:ALA:HB2	1.92	0.49
1:W:1062:PHE:HB2	1:W:1087:ALA:HB3	1.94	0.49
2:3:74:LEU:HD23	2:3:77:LEU:HD12	1.94	0.49
4:6:5:LYS:HD3	4:6:88:ASP:HB2	1.93	0.49
1:A:718:LEU:HD12	1:A:894:VAL:HG21	1.93	0.49
1:B:850:ILE:HD12	1:B:875:ILE:HD12	1.93	0.49
1:D:1163:CYS:SG	1:D:1164:GLU:N	2.85	0.49
1:F:146:PRO:HA	1:F:149:PHE:HD2	1.77	0.49
1:F:71:LEU:N	1:F:377:GLU:OE2	2.46	0.49
1:M:619:MET:SD	1:M:881:SER:OG	2.67	0.49
1:N:1115:CYS:HA	1:N:1177:CYS:HB2	1.93	0.49
1:N:839:VAL:HG13	1:N:876:ARG:HG2	1.93	0.49
1:O:504:LYS:HE2	1:O:507:ALA:HB2	1.93	0.49
1:U:414:SER:OG	1:U:416:SER:OG	2.29	0.49
1:V:1251:ASN:ND2	1:V:1270:PHE:O	2.36	0.49
1:V:182:LYS:NZ	1:V:1058:SER:OG	2.46	0.49
1:4:92:GLN:HB3	1:4:117:MET:HG2	1.93	0.49
1:4:898:ARG:O	1:4:903:SER:OG	2.28	0.49
4:6:124:THR:HG22	4:6:135:VAL:HG22	1.94	0.49
1:B:854:LEU:HD13	1:B:860:LYS:HG2	1.93	0.49
1:C:706:THR:O	1:C:710:SER:OG	2.30	0.49
1:E:1115:CYS:HA	1:E:1177:CYS:HB2	1.95	0.49
1:E:491:MET:HB2	1:E:783:ASP:HA	1.94	0.49
1:S:582:PHE:HE1	1:S:694:LEU:HD11	1.78	0.49
1:V:592:ILE:HD11	1:V:680:ILE:HA	1.93	0.49
1:V:831:LEU:HD22	2:1:9:PRO:HG2	1.93	0.49
1:W:49:ARG:HD3	1:X:87:ILE:HD11	1.94	0.49
1:4:945:ASN:HB3	1:4:948:TYR:HD2	1.78	0.49
3:5:128:VAL:HG11	3:5:312:LEU:HD13	1.94	0.49
1:A:1293:LEU:HD21	1:A:1297:PRO:HG3	1.93	0.49
1:A:918:LEU:HB2	1:A:944:PHE:CE2	2.48	0.49
1:B:1169:LEU:O	1:C:1206:SER:OG	2.24	0.49
1:B:600:ILE:O	1:B:604:ALA:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:438:ASN:HD22	1:C:1171:HIS:CD2	2.31	0.49
1:M:183:LEU:HD13	1:M:394:ARG:HH21	1.77	0.49
1:M:1171:HIS:HE1	1:N:1228:ALA:HA	1.76	0.49
1:N:294:GLU:HB2	1:N:366:LEU:HD22	1.92	0.49
1:O:537:HIS:HA	1:O:1238:TRP:NE1	2.27	0.49
2:Q:74:LEU:HD23	2:Q:77:LEU:HD12	1.94	0.49
1:N:831:LEU:HD22	2:Q:9:PRO:HG2	1.94	0.49
1:T:1187:ASP:OD2	1:T:1232:ARG:NH2	2.45	0.49
1:W:447:GLN:HA	1:W:450:LEU:HB2	1.95	0.49
1:W:760:ARG:HH12	1:W:886:PRO:HA	1.77	0.49
3:5:183:GLY:HA2	3:5:322:ALA:H	1.76	0.49
1:C:1210:TYR:HE1	1:C:1280:ARG:HG2	1.76	0.49
1:C:907:HIS:HB2	1:C:910:GLY:H	1.78	0.49
1:F:1071:ARG:O	1:F:1079:THR:OG1	2.30	0.49
1:N:38:LEU:HD11	1:N:43:ALA:HA	1.94	0.49
1:O:624:GLU:HB2	1:O:762:ARG:HH12	1.78	0.49
1:O:684:LEU:HA	1:O:687:LEU:HB2	1.94	0.49
1:W:1328:PRO:HB2	1:W:1358:ILE:HG21	1.94	0.49
1:W:172:ARG:O	1:W:176:ASP:N	2.38	0.49
1:X:850:ILE:HD12	1:X:875:ILE:HD12	1.94	0.49
3:5:147:SER:O	3:5:151:ASP:N	2.43	0.49
1:A:1109:THR:O	1:A:1111:MET:N	2.46	0.49
1:B:491:MET:HB2	1:B:783:ASP:HA	1.95	0.49
1:B:537:HIS:HA	1:B:1238:TRP:HD1	1.78	0.49
1:C:183:LEU:HD13	1:C:394:ARG:HH21	1.77	0.49
1:C:557:THR:HA	1:C:898:ARG:HH22	1.78	0.49
1:D:738:PRO:HB3	1:D:896:THR:HG22	1.94	0.49
1:D:889:THR:HB	1:D:918:LEU:HD11	1.94	0.49
1:E:183:LEU:HD13	1:E:394:ARG:HH21	1.77	0.49
1:F:626:LYS:HZ1	1:F:881:SER:HA	1.78	0.49
1:M:257:VAL:HG12	1:M:350:LEU:HD21	1.95	0.49
1:N:481:TYR:OH	1:N:979:VAL:N	2.46	0.49
1:U:1195:SER:O	1:U:1326:ALA:N	2.43	0.49
1:U:1259:LEU:HD12	1:U:1260:PRO:HD2	1.94	0.49
1:U:418:SER:HB3	1:V:415:THR:HG23	1.94	0.49
1:U:618:ALA:HB2	1:U:922:PHE:HE1	1.77	0.49
1:W:1247:ASP:O	1:W:1251:ASN:ND2	2.46	0.49
1:4:249:LEU:HD21	1:4:372:LYS:HB2	1.95	0.49
3:8:228:ALA:HB3	3:8:289:CYS:HB3	1.94	0.49
1:B:279:THR:HB	1:B:380:GLN:HE21	1.77	0.49
1:E:452:SER:HB2	1:E:1118:LEU:HG	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:536:VAL:HG12	1:E:537:HIS:HD2	1.78	0.49
1:F:934:ALA:O	1:F:937:THR:OG1	2.30	0.49
1:M:1236:ASN:HB2	1:M:1238:TRP:HE3	1.78	0.49
1:M:185:HIS:O	1:M:1097:SER:OG	2.31	0.49
1:N:652:ASN:ND2	1:N:923:GLY:O	2.45	0.49
1:N:418:SER:HB3	1:O:415:THR:HG23	1.95	0.49
1:S:578:ARG:NH1	1:S:1014:SER:OG	2.46	0.49
1:V:717:LEU:HD12	1:V:915:GLN:HE22	1.77	0.49
1:W:541:ASP:N	1:W:557:THR:O	2.46	0.49
1:W:578:ARG:NH1	1:W:1014:SER:O	2.45	0.49
1:X:1239:ALA:O	1:X:1244:SER:OG	2.31	0.49
4:7:196:ASP:HB2	4:7:202:ARG:HH12	1.76	0.49
4:6:213:ILE:HG23	4:7:244:VAL:HG11	1.94	0.49
1:B:695:ALA:HB1	1:B:706:THR:HG22	1.95	0.49
1:C:172:ARG:HG3	1:D:100:ILE:HA	1.95	0.49
1:C:79:GLU:N	1:C:304:ALA:O	2.45	0.49
1:E:463:GLN:HE21	1:E:467:ALA:HB2	1.78	0.49
1:E:539:PHE:O	1:E:559:ARG:N	2.45	0.49
1:M:495:ARG:NH1	2:P:3:ASN:O	2.46	0.49
1:S:729:ASP:HB2	1:S:793:LEU:HD11	1.95	0.49
1:U:918:LEU:HB2	1:U:944:PHE:HE2	1.78	0.49
1:V:658:ARG:NH2	1:W:929:ASP:OD2	2.46	0.49
1:W:684:LEU:HA	1:W:687:LEU:HD13	1.94	0.49
1:W:893:ARG:HG3	1:W:916:THR:HG22	1.94	0.49
1:X:1062:PHE:HB2	1:X:1087:ALA:HB3	1.95	0.49
1:X:770:LEU:HD11	1:X:883:LEU:HD13	1.94	0.49
1:4:361:ARG:NH1	1:4:362:ILE:O	2.46	0.49
1:4:851:LEU:HD22	1:4:863:LEU:HB3	1.94	0.49
3:8:90:LEU:HD11	3:8:165:MET:HG3	1.94	0.49
1:B:1341:TYR:HA	1:B:1348:HIS:HD2	1.78	0.49
1:C:249:LEU:HD21	1:C:372:LYS:HB2	1.95	0.49
1:C:277:GLU:HG2	1:C:377:GLU:HB2	1.94	0.49
1:F:80:PHE:HD2	1:F:83:LEU:HD12	1.77	0.49
1:M:79:GLU:HB3	1:M:305:SER:HA	1.94	0.49
1:N:877:VAL:O	1:N:880:THR:OG1	2.29	0.49
1:W:1225:PRO:HB2	1:W:1230:GLU:HG3	1.94	0.49
1:X:406:LEU:HD21	1:X:1191:PHE:HE2	1.77	0.49
1:4:676:HIS:HA	1:4:679:LYS:HB2	1.94	0.48
4:6:262:ASP:OD2	4:7:158:TYR:OH	2.30	0.48
1:A:1171:HIS:HE1	1:B:1228:ALA:HA	1.78	0.48
1:A:889:THR:HB	1:A:918:LEU:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:342:SER:O	1:B:346:ASP:N	2.45	0.48
1:C:79:GLU:HB3	1:C:305:SER:HA	1.95	0.48
1:E:1250:TYR:HB2	1:E:1270:PHE:HD2	1.76	0.48
1:E:307:VAL:HG12	1:E:309:ARG:H	1.78	0.48
1:E:537:HIS:CE1	1:E:539:PHE:HB2	2.48	0.48
1:M:331:ALA:HA	1:M:335:ASP:HB2	1.94	0.48
1:N:717:LEU:HD11	1:N:808:TYR:HE2	1.78	0.48
1:O:245:LEU:HD22	1:O:369:ILE:HG21	1.95	0.48
2:P:74:LEU:HD23	2:P:77:LEU:HD12	1.94	0.48
1:T:436:ASN:HD22	1:T:440:VAL:HB	1.77	0.48
1:T:824:VAL:H	1:T:889:THR:HG21	1.78	0.48
1:U:927:VAL:HG21	1:U:957:LEU:HD21	1.94	0.48
1:V:1020:SER:N	1:V:1023:SER:OG	2.45	0.48
1:V:276:LEU:HB3	1:V:1053:TYR:HD1	1.78	0.48
1:W:578:ARG:NH2	1:W:1017:GLN:OE1	2.45	0.48
1:W:402:PHE:HD2	1:W:1040:VAL:HB	1.77	0.48
1:S:1224:ILE:HD13	1:X:1167:PRO:HD3	1.95	0.48
4:7:23:LEU:HD11	4:7:125:ILE:HG21	1.95	0.48
3:8:283:LEU:O	4:9:272:TYR:OH	2.32	0.48
1:A:91:ILE:HD11	1:A:1089:LEU:HD11	1.95	0.48
1:D:290:LEU:HD23	1:D:367:VAL:HG21	1.95	0.48
1:E:1301:THR:HG21	1:F:203:ARG:HG2	1.94	0.48
1:E:158:THR:OG1	1:T:45:GLU:OE1	2.31	0.48
1:E:945:ASN:OD1	1:E:946:LYS:N	2.46	0.48
1:M:1210:TYR:HE1	1:M:1280:ARG:HG2	1.78	0.48
1:M:421:GLY:HA3	1:N:413:TYR:HA	1.95	0.48
1:M:564:ASN:HA	1:M:994:PRO:HG2	1.95	0.48
1:O:1134:ASP:O	1:O:1138:MET:N	2.47	0.48
1:O:740:ILE:HB	1:O:747:TYR:HB3	1.94	0.48
1:S:945:ASN:HB3	1:S:948:TYR:H	1.77	0.48
1:T:406:LEU:HD21	1:T:1191:PHE:HE2	1.78	0.48
1:U:277:GLU:HG2	1:U:377:GLU:HB2	1.95	0.48
1:X:447:GLN:HB3	1:X:1028:ALA:HB1	1.95	0.48
1:X:555:ARG:HA	1:X:907:HIS:HE1	1.79	0.48
2:I:74:LEU:HD23	2:I:77:LEU:HD12	1.94	0.48
1:M:878:LEU:O	1:M:881:SER:OG	2.32	0.48
1:N:663:HIS:HA	1:O:930:ARG:HD2	1.95	0.48
1:N:582:PHE:HE1	1:N:694:LEU:HD11	1.77	0.48
1:W:312:ASN:ND2	1:W:323:MET:O	2.46	0.48
1:W:394:ARG:HD3	1:W:1315:PHE:HB3	1.96	0.48
1:X:623:GLN:HB2	1:X:626:LYS:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:727:PHE:HA	1:4:730:LEU:HB3	1.95	0.48
1:C:927:VAL:HB	1:C:956:THR:HG21	1.95	0.48
1:C:504:LYS:HB3	1:C:967:ARG:HH12	1.78	0.48
1:D:276:LEU:HB3	1:D:1053:TYR:HD1	1.79	0.48
1:D:423:GLU:HA	1:D:1352:HIS:HE1	1.78	0.48
1:E:217:PHE:O	1:E:221:LEU:N	2.41	0.48
1:D:22:GLN:NE2	1:N:201:SER:OG	2.44	0.48
1:O:745:GLN:OE1	1:O:786:HIS:ND1	2.46	0.48
1:S:406:LEU:HD21	1:S:1191:PHE:HE2	1.79	0.48
1:T:861:ASP:HA	1:T:864:GLN:HB2	1.95	0.48
1:T:1168:GLY:HA2	1:U:207:LYS:HD3	1.95	0.48
1:W:1109:THR:HG22	1:W:1175:ALA:HB2	1.95	0.48
1:W:1341:TYR:HA	1:W:1348:HIS:CD2	2.48	0.48
4:7:120:ARG:HA	4:7:123:SER:HB3	1.94	0.48
1:A:192:LEU:O	1:A:196:GLY:N	2.45	0.48
1:B:1196:ASN:HD22	1:B:1201:ALA:HA	1.79	0.48
1:C:402:PHE:HB3	1:C:1040:VAL:HB	1.96	0.48
1:C:1236:ASN:HB2	1:C:1238:TRP:HE3	1.78	0.48
1:C:796:ASN:OD1	1:D:932:ARG:NH1	2.46	0.48
1:E:717:LEU:HB2	1:E:990:TRP:HZ3	1.79	0.48
1:F:760:ARG:HB2	1:F:792:PRO:HD3	1.95	0.48
1:F:927:VAL:HB	1:F:956:THR:HG21	1.95	0.48
1:M:153:ALA:HA	1:M:156:ILE:HG22	1.95	0.48
1:O:1344:ASN:ND2	1:O:1347:THR:OG1	2.47	0.48
1:O:436:ASN:OD1	1:O:437:LYS:N	2.47	0.48
1:S:717:LEU:HB2	1:S:990:TRP:HZ3	1.78	0.48
1:V:1071:ARG:O	1:V:1079:THR:OG1	2.31	0.48
1:V:185:HIS:O	1:V:1097:SER:OG	2.32	0.48
1:W:708:LEU:HD21	1:W:1022:PRO:HG2	1.95	0.48
1:V:59:ASN:HD22	1:W:95:ILE:HA	1.76	0.48
1:4:272:VAL:HA	1:4:373:PHE:HB2	1.94	0.48
1:A:1198:ARG:NH1	1:A:1200:ARG:O	2.46	0.48
1:A:808:TYR:OH	1:A:915:GLN:NE2	2.47	0.48
1:B:1341:TYR:HA	1:B:1348:HIS:CD2	2.47	0.48
1:C:1114:HIS:O	1:C:1177:CYS:N	2.43	0.48
1:D:931:SER:HB2	1:D:934:ALA:HB3	1.95	0.48
1:E:8:ARG:NH1	1:F:319:TYR:O	2.46	0.48
1:M:1250:TYR:HA	1:M:1255:ARG:HH21	1.78	0.48
1:N:402:PHE:HD2	1:N:1040:VAL:HB	1.78	0.48
1:N:440:VAL:HG22	1:O:1193:THR:HG21	1.95	0.48
1:O:512:VAL:HG12	1:O:993:SER:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:275:VAL:HG22	1:S:375:ALA:HB3	1.95	0.48
1:U:83:LEU:HD21	1:U:122:LYS:HD2	1.95	0.48
1:U:419:VAL:HG23	1:U:1336:VAL:HG11	1.95	0.48
1:U:708:LEU:HD21	1:U:1022:PRO:HG2	1.94	0.48
1:V:211:SER:OG	1:V:1206:SER:OG	2.30	0.48
1:V:619:MET:SD	1:V:881:SER:OG	2.71	0.48
1:X:45:GLU:O	1:4:58:THR:OG1	2.30	0.48
1:4:1188:VAL:HG12	1:4:1192:GLN:HE22	1.78	0.48
1:4:537:HIS:CE1	1:4:539:PHE:HB2	2.49	0.48
1:B:587:ASN:OD1	1:C:1003:GLN:NE2	2.47	0.48
1:C:428:GLN:NE2	1:C:577:SER:OG	2.34	0.48
1:C:720:PRO:HD3	1:C:808:TYR:CZ	2.49	0.48
1:C:82:ASP:N	1:C:82:ASP:OD1	2.43	0.48
1:E:714:ASP:O	1:E:804:LYS:NZ	2.46	0.48
1:F:245:LEU:HD22	1:F:369:ILE:HG21	1.95	0.48
1:O:658:ARG:HA	1:O:681:LEU:HD11	1.96	0.48
1:O:558:HIS:CD2	1:O:902:GLN:HE22	2.31	0.48
1:T:481:TYR:OH	1:T:979:VAL:N	2.45	0.48
1:U:49:ARG:HD3	1:V:87:ILE:HD11	1.95	0.48
1:V:931:SER:HB2	1:V:934:ALA:HB3	1.95	0.48
1:W:587:ASN:OD1	1:X:1003:GLN:NE2	2.46	0.48
1:X:436:ASN:OD1	1:X:437:LYS:N	2.47	0.48
1:X:929:ASP:OD1	1:X:932:ARG:NH2	2.46	0.48
1:A:851:LEU:HD12	1:A:869:ARG:HD2	1.95	0.48
1:B:76:VAL:HB	1:B:1060:SER:HA	1.96	0.48
1:B:481:TYR:OH	1:B:979:VAL:O	2.25	0.48
1:C:1033:HIS:NE2	1:C:1036:PHE:O	2.45	0.48
1:C:532:LEU:O	1:C:1241:GLN:NE2	2.46	0.48
1:C:919:VAL:HG12	1:C:920:ASN:HB2	1.95	0.48
1:D:845:ASN:N	1:D:848:ASP:OD2	2.45	0.48
1:E:1344:ASN:ND2	1:E:1347:THR:OG1	2.46	0.48
1:F:304:ALA:HB2	1:F:357:ILE:HD11	1.96	0.48
1:E:831:LEU:HD22	2:K:9:PRO:HG2	1.95	0.48
1:M:536:VAL:HG13	1:M:1244:SER:HA	1.95	0.48
1:M:850:ILE:HD11	1:M:872:VAL:HA	1.96	0.48
1:N:518:VAL:HG13	1:N:522:ASP:HB3	1.94	0.48
1:U:123:HIS:N	1:U:1086:ILE:O	2.42	0.48
1:U:438:ASN:HD22	1:U:1171:HIS:HD2	1.61	0.48
1:U:396:ILE:HD11	1:U:1050:HIS:HE1	1.77	0.48
1:V:1067:SER:OG	1:V:1083:THR:OG1	2.32	0.48
1:X:1196:ASN:HD21	1:X:1324:GLN:HG3	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:1027:GLN:HB3	1:4:1032:MET:HB2	1.96	0.48
1:4:1073:VAL:HG13	1:4:1078:VAL:HA	1.96	0.48
1:4:759:LEU:HD22	1:4:792:PRO:HB3	1.95	0.48
1:A:402:PHE:HD2	1:A:1040:VAL:HB	1.79	0.48
1:C:185:HIS:O	1:C:1097:SER:OG	2.32	0.48
1:C:851:LEU:HD12	1:C:869:ARG:HD2	1.96	0.48
1:D:51:GLU:HB3	1:E:87:ILE:HB	1.96	0.48
1:D:718:LEU:H	1:D:915:GLN:HE22	1.62	0.48
1:D:512:VAL:HG12	1:D:993:SER:HB3	1.95	0.48
1:F:578:ARG:NH1	1:F:1014:SER:O	2.44	0.48
1:F:536:VAL:HG13	1:F:1244:SER:HA	1.95	0.48
1:F:217:PHE:O	1:F:221:LEU:N	2.47	0.48
1:M:457:ARG:HH11	1:M:460:ASN:HD21	1.61	0.48
1:N:1198:ARG:NH2	1:N:1219:LEU:O	2.42	0.48
1:N:744:ASP:H	1:N:786:HIS:HE1	1.62	0.48
1:O:191:ILE:HA	1:O:217:PHE:HE1	1.79	0.48
1:S:278:THR:HG22	1:S:1051:ILE:HA	1.96	0.48
1:S:127:ALA:HB3	1:S:1082:ILE:HB	1.96	0.48
1:T:1236:ASN:HB2	1:T:1238:TRP:HE3	1.78	0.48
1:T:95:ILE:HB	1:T:114:TYR:HB2	1.96	0.48
1:W:700:VAL:O	1:W:1131:GLN:NE2	2.47	0.48
1:W:898:ARG:HE	1:W:913:VAL:HG23	1.77	0.48
1:X:463:GLN:HB3	1:X:1248:VAL:HG13	1.95	0.48
1:X:91:ILE:HD11	1:X:1089:LEU:HD22	1.95	0.48
1:4:128:GLU:OE2	1:4:1071:ARG:NH2	2.47	0.48
1:4:567:GLN:HE21	1:4:998:TYR:HA	1.79	0.48
3:8:129:ALA:HA	3:8:132:TRP:HD1	1.79	0.48
3:8:146:LEU:HD23	3:8:149:LEU:HD12	1.95	0.48
1:B:1199:GLY:HA2	1:B:1235:ASN:HB3	1.94	0.48
1:C:436:ASN:OD1	1:C:437:LYS:N	2.47	0.48
1:D:1183:PRO:HG3	1:D:1237:PRO:HD2	1.96	0.48
1:E:49:ARG:HD3	1:F:87:ILE:HD11	1.95	0.48
1:A:831:LEU:HD22	2:G:9:PRO:HG2	1.95	0.48
1:O:537:HIS:HA	1:O:1238:TRP:CD1	2.49	0.48
1:S:955:ALA:HA	1:S:961:LEU:HD22	1.95	0.48
1:U:561:MET:H	1:U:564:ASN:ND2	2.11	0.48
1:V:1199:GLY:HA2	1:V:1235:ASN:HB3	1.96	0.48
1:V:1168:GLY:HA2	1:W:207:LYS:HD3	1.96	0.48
1:X:700:VAL:O	1:X:1131:GLN:NE2	2.47	0.48
1:4:634:ILE:HB	1:4:638:ILE:HD12	1.95	0.47
1:B:508:PHE:O	1:B:978:ASN:ND2	2.38	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1294:ALA:HB3	1:D:1297:PRO:HD3	1.96	0.47
1:D:1171:HIS:HE1	1:E:1228:ALA:HA	1.77	0.47
1:V:224:HIS:HB3	1:V:244:MET:HE3	1.96	0.47
1:V:743:GLY:HA3	1:V:786:HIS:HE1	1.79	0.47
1:X:123:HIS:HB2	1:X:1086:ILE:HB	1.95	0.47
1:X:515:LYS:NZ	1:X:534:LEU:O	2.47	0.47
1:X:856:ASN:HA	1:X:860:LYS:HD2	1.95	0.47
1:C:127:ALA:HB2	1:D:101:ALA:HB2	1.95	0.47
1:D:717:LEU:HA	1:D:990:TRP:HZ3	1.79	0.47
1:E:15:THR:HG22	1:U:350:LEU:HD11	1.96	0.47
1:O:394:ARG:HD3	1:O:1315:PHE:HB3	1.95	0.47
1:T:868:ILE:HG22	1:T:870:PRO:HD3	1.96	0.47
1:E:38:LEU:HB2	1:U:113:GLN:HB3	1.95	0.47
3:5:199:LEU:O	3:5:315:LEU:N	2.45	0.47
4:6:111:LEU:HA	4:6:141:PRO:HA	1.96	0.47
1:B:78:THR:HG22	1:B:304:ALA:HB3	1.96	0.47
1:B:82:ASP:OD1	1:B:82:ASP:N	2.46	0.47
1:C:716:HIS:CE1	1:C:736:ARG:HG3	2.49	0.47
1:D:1294:ALA:HB1	1:D:1321:HIS:HE1	1.80	0.47
1:D:294:GLU:HB2	1:D:366:LEU:HD22	1.95	0.47
1:D:850:ILE:HD11	1:D:872:VAL:HA	1.96	0.47
1:F:6:GLU:OE1	1:F:8:ARG:NH1	2.47	0.47
1:T:1252:ILE:O	1:T:1267:ARG:NH2	2.45	0.47
1:T:306:TYR:OH	1:T:323:MET:O	2.31	0.47
1:V:436:ASN:OD1	1:V:437:LYS:N	2.48	0.47
1:X:380:GLN:NE2	1:X:393:ASN:HD21	2.12	0.47
3:8:40:ASP:O	4:9:2:ALA:N	2.48	0.47
1:C:687:LEU:HB3	1:C:805:LEU:HD13	1.95	0.47
1:D:1341:TYR:HB2	1:D:1357:LEU:HD11	1.95	0.47
1:D:183:LEU:HD13	1:D:394:ARG:HH21	1.80	0.47
1:D:927:VAL:HB	1:D:956:THR:HG21	1.96	0.47
1:E:455:HIS:HD2	1:E:1119:PHE:HD1	1.63	0.47
1:A:1224:ILE:HD13	1:F:1167:PRO:HD3	1.94	0.47
1:M:1122:PHE:HE1	1:M:1258:ALA:HB2	1.79	0.47
1:M:191:ILE:HA	1:M:217:PHE:HE1	1.79	0.47
1:M:49:ARG:HD3	1:N:87:ILE:HD11	1.95	0.47
1:O:406:LEU:HD21	1:O:1191:PHE:HE2	1.79	0.47
1:O:312:ASN:HD21	1:O:326:PHE:HB2	1.80	0.47
1:S:913:VAL:HG11	1:S:990:TRP:CD1	2.50	0.47
1:S:388:PHE:HE2	1:T:100:ILE:H	1.62	0.47
1:T:1170:SER:HA	1:U:211:SER:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:59:ASN:HD22	1:T:96:SER:H	1.62	0.47
1:U:1264:SER:HB2	1:U:1267:ARG:HG3	1.95	0.47
1:X:624:GLU:HB2	1:X:762:ARG:HH12	1.79	0.47
1:4:1212:ASN:HA	1:4:1280:ARG:HH22	1.80	0.47
1:4:245:LEU:HD22	1:4:369:ILE:HG21	1.96	0.47
1:A:1067:SER:OG	1:A:1083:THR:OG1	2.32	0.47
1:A:927:VAL:HB	1:A:956:THR:HG21	1.97	0.47
1:C:994:PRO:HA	1:C:997:ALA:HB3	1.96	0.47
1:M:770:LEU:HD11	1:M:883:LEU:HD13	1.96	0.47
1:N:275:VAL:HG22	1:N:375:ALA:HB3	1.96	0.47
1:T:947:LEU:HG	1:T:947:LEU:H	1.44	0.47
1:U:1344:ASN:ND2	1:U:1347:THR:OG1	2.47	0.47
1:U:606:ASP:OD1	1:U:647:LYS:NZ	2.40	0.47
1:U:780:GLU:OE1	1:U:785:ARG:NH1	2.48	0.47
1:W:617:GLU:HG3	1:W:656:MET:HG3	1.96	0.47
1:X:284:ARG:O	1:X:288:ASN:ND2	2.48	0.47
1:X:493:LEU:HD13	1:X:942:VAL:HG21	1.97	0.47
1:4:652:ASN:HA	1:4:925:PHE:HE2	1.79	0.47
3:5:46:ALA:HB1	3:5:50:ARG:HH12	1.78	0.47
4:6:113:VAL:HG22	4:6:139:VAL:HG12	1.95	0.47
1:D:1027:GLN:NE2	1:D:1032:MET:HB2	2.29	0.47
1:D:402:PHE:HD2	1:D:1040:VAL:HB	1.79	0.47
1:D:637:VAL:HG22	1:D:868:ILE:HD13	1.96	0.47
1:M:899:ASP:O	1:M:901:ALA:N	2.47	0.47
1:S:1051:ILE:HB	1:S:1100:ALA:HB3	1.95	0.47
1:U:887:PHE:O	1:U:920:ASN:ND2	2.43	0.47
1:V:576:GLU:OE1	1:V:998:TYR:OH	2.33	0.47
1:W:404:VAL:HG23	1:W:432:THR:HG23	1.96	0.47
1:W:913:VAL:HG11	1:W:990:TRP:CD1	2.49	0.47
1:A:831:LEU:HD23	2:G:11:ILE:HD12	1.97	0.47
1:A:93:PHE:HB2	1:A:116:VAL:HB	1.95	0.47
1:B:951:PRO:HA	1:B:954:ALA:HB3	1.96	0.47
1:C:1342:MET:HA	1:C:1375:VAL:HG21	1.96	0.47
1:D:958:HIS:CE1	1:D:960:LEU:HB3	2.50	0.47
1:F:512:VAL:HG12	1:F:993:SER:HB3	1.95	0.47
1:M:1302:THR:OG1	1:M:1304:LEU:O	2.31	0.47
1:M:404:VAL:HG23	1:M:432:THR:HG23	1.97	0.47
1:N:588:MET:HB3	1:N:690:ALA:HB2	1.95	0.47
1:O:1062:PHE:HB2	1:O:1087:ALA:HB3	1.95	0.47
1:O:404:VAL:HG23	1:O:432:THR:HG23	1.97	0.47
1:S:1187:ASP:OD2	1:S:1232:ARG:NH2	2.41	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:669:ILE:HD11	1:4:674:HIS:CD2	2.50	0.47
3:5:69:THR:H	3:5:182:LYS:HD2	1.80	0.47
3:8:167:GLN:HB2	3:8:188:ARG:HG3	1.96	0.47
1:B:1344:ASN:ND2	1:B:1347:THR:OG1	2.48	0.47
1:B:306:TYR:OH	1:B:323:MET:O	2.32	0.47
1:B:889:THR:HA	1:B:920:ASN:HB3	1.97	0.47
1:E:125:ILE:HB	1:E:1084:HIS:HB3	1.97	0.47
1:F:609:TYR:HE2	1:F:614:TYR:HB2	1.80	0.47
1:F:889:THR:HA	1:F:920:ASN:HB3	1.97	0.47
1:N:397:GLN:HE22	1:N:1298:ALA:HB3	1.80	0.47
1:N:558:HIS:CE1	1:N:902:GLN:HE22	2.33	0.47
1:O:455:HIS:HE2	1:O:1122:PHE:HB2	1.79	0.47
1:S:62:GLU:O	1:S:172:ARG:NH2	2.46	0.47
1:T:889:THR:HA	1:T:920:ASN:HB3	1.97	0.47
1:U:436:ASN:OD1	1:U:437:LYS:N	2.47	0.47
1:U:856:ASN:OD1	1:U:860:LYS:NZ	2.47	0.47
1:U:92:GLN:NE2	1:U:116:VAL:O	2.47	0.47
1:U:493:LEU:HD13	1:U:942:VAL:HG21	1.97	0.47
1:U:989:GLU:HG2	1:U:991:HIS:H	1.80	0.47
1:V:123:HIS:HB2	1:V:1086:ILE:HB	1.96	0.47
1:V:1342:MET:HA	1:V:1375:VAL:HG21	1.97	0.47
1:V:493:LEU:HB2	1:V:940:TYR:HE2	1.79	0.47
1:V:944:PHE:HE1	1:V:983:LEU:HD22	1.80	0.47
1:W:263:THR:OG1	1:W:1056:ARG:NH1	2.48	0.47
1:W:918:LEU:HD22	1:W:944:PHE:HZ	1.78	0.47
3:5:70:TYR:HE2	3:5:188:ARG:HH22	1.61	0.47
3:5:326:PRO:HA	4:7:110:GLN:HE22	1.80	0.47
1:A:451:LYS:HG2	1:A:1140:ALA:HB1	1.95	0.47
1:E:102:HIS:HE1	1:E:106:ARG:HD2	1.80	0.47
1:E:79:GLU:N	1:E:304:ALA:O	2.48	0.47
1:E:851:LEU:HD12	1:E:869:ARG:HD2	1.95	0.47
1:M:312:ASN:HD21	1:M:326:PHE:HB2	1.79	0.47
1:M:277:GLU:HG2	1:M:377:GLU:HB2	1.96	0.47
1:O:576:GLU:OE1	1:O:998:TYR:OH	2.33	0.47
1:O:9:PRO:HB3	1:O:45:GLU:HB3	1.97	0.47
1:W:1168:GLY:HA2	1:X:207:LYS:HD3	1.97	0.47
1:X:592:ILE:HG23	1:X:596:THR:HG23	1.95	0.47
1:4:457:ARG:HH21	1:4:1248:VAL:HA	1.79	0.47
1:X:57:TYR:HD2	1:4:49:ARG:HD2	1.80	0.47
1:4:461:PRO:HB2	1:4:556:ALA:HB1	1.97	0.47
3:5:88:THR:HB	3:5:108:PRO:HD2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:399:THR:HG22	1:B:1043:THR:HG22	1.97	0.47
1:C:856:ASN:OD1	1:C:860:LYS:NZ	2.46	0.47
1:D:450:LEU:HD11	1:D:1025:ILE:HA	1.97	0.47
1:E:913:VAL:HG11	1:E:990:TRP:CD1	2.50	0.47
1:O:1122:PHE:HE1	1:O:1258:ALA:HB2	1.78	0.47
1:O:1137:LYS:O	1:O:1141:GLY:N	2.37	0.47
1:U:214:VAL:HA	1:U:217:PHE:HD2	1.80	0.47
1:W:271:GLN:OE1	1:W:1056:ARG:NH1	2.48	0.47
1:4:1042:ARG:NE	1:4:1177:CYS:SG	2.85	0.47
1:A:850:ILE:HD11	1:A:872:VAL:HA	1.97	0.47
1:C:49:ARG:HD3	1:D:87:ILE:HD11	1.97	0.47
1:F:450:LEU:HD11	1:F:1025:ILE:HG13	1.97	0.47
1:M:821:GLY:HA2	1:M:923:GLY:HA2	1.97	0.47
1:N:1250:TYR:HB2	1:N:1270:PHE:HD2	1.80	0.47
1:O:918:LEU:HB2	1:O:944:PHE:CE2	2.48	0.47
1:S:461:PRO:HA	1:S:464:SER:HB3	1.97	0.47
1:S:602:GLU:HB3	1:S:647:LYS:HE3	1.97	0.47
1:T:1156:TYR:HE1	1:T:1260:PRO:HB3	1.80	0.47
1:T:587:ASN:HD21	1:U:1003:GLN:HE21	1.63	0.47
1:V:736:ARG:NH1	1:V:897:LYS:O	2.47	0.47
1:V:856:ASN:HB2	2:1:12:GLN:HE21	1.79	0.47
1:W:1107:ILE:HD11	1:W:1364:MET:HE1	1.96	0.47
1:X:1294:ALA:HB3	1:X:1321:HIS:CE1	2.50	0.47
1:X:51:GLU:HB3	1:4:54:LEU:HB3	1.97	0.46
3:5:255:VAL:HA	3:5:258:MET:HB2	1.97	0.46
1:B:1220:TYR:HB3	1:B:1242:ARG:HE	1.80	0.46
1:B:512:VAL:HG11	1:B:992:LYS:HB3	1.98	0.46
1:C:271:GLN:OE1	1:C:1056:ARG:NH1	2.48	0.46
1:E:294:GLU:HB2	1:E:366:LEU:HD22	1.97	0.46
1:E:63:PHE:HE2	1:E:65:LYS:HE2	1.79	0.46
1:E:851:LEU:HD23	1:E:854:LEU:HD21	1.96	0.46
1:F:185:HIS:O	1:F:1097:SER:OG	2.33	0.46
1:N:1137:LYS:O	1:N:1141:GLY:N	2.46	0.46
1:N:79:GLU:HB3	1:N:305:SER:HA	1.96	0.46
1:O:228:LEU:HD22	1:O:1103:HIS:HB2	1.96	0.46
1:O:92:GLN:HE22	1:O:115:ILE:HG23	1.79	0.46
1:S:1199:GLY:HA2	1:S:1235:ASN:HB3	1.95	0.46
1:T:932:ARG:HE	1:T:956:THR:HG23	1.80	0.46
1:U:1115:CYS:HA	1:U:1177:CYS:HB2	1.97	0.46
1:T:1169:LEU:HD12	1:U:211:SER:HB2	1.96	0.46
1:V:700:VAL:O	1:V:1131:GLN:NE2	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:706:THR:HB	1:V:713:LEU:HD13	1.96	0.46
1:W:731:MET:HG2	1:W:738:PRO:HG3	1.97	0.46
1:4:402:PHE:HB3	1:4:1040:VAL:HB	1.97	0.46
1:4:428:GLN:NE2	1:4:577:SER:OG	2.39	0.46
1:4:654:TYR:HE2	1:4:803:GLU:HG2	1.80	0.46
3:5:99:GLY:H	3:5:102:MET:HG3	1.80	0.46
3:8:30:ARG:HH11	3:8:33:GLU:HG2	1.79	0.46
1:A:959:PRO:HA	1:A:962:ALA:HB3	1.96	0.46
1:B:652:ASN:ND2	1:B:923:GLY:O	2.45	0.46
1:C:1195:SER:O	1:C:1326:ALA:N	2.45	0.46
1:D:271:GLN:OE1	1:D:1056:ARG:NH1	2.36	0.46
1:D:989:GLU:HG2	1:D:991:HIS:H	1.79	0.46
1:M:51:GLU:H	1:N:321:ARG:HA	1.80	0.46
1:M:537:HIS:HB3	1:M:1245:LEU:HB2	1.97	0.46
1:S:1005:THR:HG22	1:S:1007:GLY:H	1.80	0.46
1:T:851:LEU:HD23	1:T:854:LEU:HD21	1.97	0.46
1:U:946:LYS:HD3	1:U:986:GLU:HG2	1.96	0.46
1:V:1250:TYR:CZ	1:V:1266:CYS:HB2	2.50	0.46
1:V:481:TYR:OH	1:V:979:VAL:O	2.30	0.46
1:T:856:ASN:ND2	2:Z:12:GLN:HE21	2.13	0.46
1:A:1344:ASN:ND2	1:A:1347:THR:OG1	2.48	0.46
1:C:638:ILE:HG12	1:C:649:ALA:HB3	1.98	0.46
1:E:980:PRO:HD2	1:E:983:LEU:HD12	1.98	0.46
1:F:1236:ASN:HB2	1:F:1238:TRP:HE3	1.80	0.46
1:M:197:ASP:HB3	1:M:199:VAL:HG12	1.96	0.46
1:N:674:HIS:CE1	1:N:678:ARG:HE	2.34	0.46
1:S:436:ASN:HB3	1:S:440:VAL:H	1.79	0.46
1:S:718:LEU:HD12	1:S:894:VAL:HG21	1.97	0.46
1:U:420:ARG:NH1	1:V:1353:MET:SD	2.88	0.46
1:U:52:ALA:H	1:V:89:GLY:HA2	1.79	0.46
1:W:1199:GLY:HA3	1:W:1236:ASN:H	1.80	0.46
1:W:1345:LYS:NZ	1:W:1376:TYR:O	2.49	0.46
1:X:1236:ASN:HB2	1:X:1238:TRP:HE3	1.81	0.46
1:X:717:LEU:HB2	1:X:990:TRP:HZ3	1.81	0.46
1:4:617:GLU:OE2	1:4:723:TYR:OH	2.17	0.46
3:5:300:PRO:HB2	3:5:315:LEU:HD22	1.96	0.46
1:A:1247:ASP:HB3	1:A:1251:ASN:HD21	1.80	0.46
1:A:224:HIS:HB3	1:A:244:MET:HE3	1.96	0.46
1:A:78:THR:HG22	1:A:304:ALA:HB3	1.98	0.46
1:B:83:LEU:HD21	1:B:122:LYS:HD2	1.96	0.46
1:B:578:ARG:NH2	1:B:1017:GLN:OE1	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1190:TYR:OH	1:C:1196:ASN:O	2.32	0.46
1:C:616:ILE:HG21	1:C:633:LEU:HD22	1.95	0.46
1:E:620:ILE:HG23	1:E:626:LYS:HB2	1.97	0.46
1:N:1171:HIS:HE1	1:O:1228:ALA:HA	1.79	0.46
1:S:254:GLU:O	1:S:256:THR:OG1	2.29	0.46
1:T:913:VAL:HG11	1:T:990:TRP:CD1	2.50	0.46
1:U:1178:GLU:OE2	1:U:1250:TYR:OH	2.22	0.46
1:U:537:HIS:HA	1:U:1238:TRP:CD1	2.50	0.46
1:V:829:VAL:O	1:V:832:THR:OG1	2.31	0.46
1:X:567:GLN:HE22	1:X:998:TYR:N	2.13	0.46
1:X:958:HIS:CE1	1:X:960:LEU:HB3	2.50	0.46
3:8:271:TYR:HE2	3:8:331:LEU:HD11	1.79	0.46
1:A:781:ASP:O	1:A:785:ARG:NH1	2.45	0.46
1:B:1020:SER:HB3	1:B:1022:PRO:HD2	1.98	0.46
1:E:731:MET:HB3	1:E:750:PRO:HG3	1.97	0.46
1:S:493:LEU:HD13	1:S:942:VAL:HG21	1.98	0.46
1:W:397:GLN:HB3	1:W:1318:GLN:HB3	1.97	0.46
1:X:66:PHE:HE1	1:X:174:LEU:HD13	1.81	0.46
3:8:70:TYR:OH	3:8:186:LEU:N	2.49	0.46
1:A:419:VAL:HG22	1:A:421:GLY:H	1.80	0.46
1:B:1183:PRO:HG2	1:B:1186:SER:HB3	1.98	0.46
1:C:227:PHE:HE1	1:C:1100:ALA:HB1	1.80	0.46
1:D:1073:VAL:HG22	1:D:1078:VAL:HG13	1.98	0.46
1:E:293:VAL:HG13	1:E:294:GLU:HG3	1.96	0.46
1:M:1071:ARG:O	1:M:1079:THR:OG1	2.31	0.46
1:M:419:VAL:HG22	1:M:421:GLY:H	1.81	0.46
1:N:736:ARG:HB3	1:N:897:LYS:HD3	1.97	0.46
1:S:1047:LEU:HD12	1:S:1106:ALA:HB3	1.96	0.46
1:S:156:ILE:HA	1:S:159:ILE:HG22	1.96	0.46
1:W:537:HIS:HA	1:W:1238:TRP:NE1	2.29	0.46
1:X:245:LEU:HD22	1:X:369:ILE:HG21	1.97	0.46
1:X:739:ILE:HB	1:X:895:ILE:HB	1.98	0.46
1:4:812:PRO:HB2	1:4:999:ALA:HB1	1.98	0.46
1:4:904:PHE:HZ	1:4:1127:TYR:HA	1.80	0.46
4:7:105:TRP:HH2	4:7:139:VAL:HG12	1.81	0.46
1:A:452:SER:HB3	1:A:1118:LEU:H	1.81	0.46
1:A:1328:PRO:HB2	1:A:1358:ILE:HG21	1.97	0.46
1:B:284:ARG:O	1:B:288:ASN:ND2	2.48	0.46
1:E:578:ARG:NH1	1:E:1014:SER:O	2.41	0.46
1:M:455:HIS:HD2	1:M:1119:PHE:HD1	1.62	0.46
1:M:1328:PRO:HB2	1:M:1358:ILE:HG21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:617:GLU:HG3	1:N:656:MET:HG3	1.97	0.46
1:N:714:ASP:O	1:N:804:LYS:NZ	2.45	0.46
1:O:491:MET:HG3	1:O:785:ARG:H	1.81	0.46
1:T:331:ALA:HA	1:T:335:ASP:HB3	1.98	0.46
1:V:1222:HIS:CE1	1:V:1241:GLN:HA	2.50	0.46
1:W:276:LEU:HA	1:W:1053:TYR:HA	1.97	0.46
1:W:1198:ARG:HG2	1:W:1270:PHE:HE1	1.81	0.46
1:W:744:ASP:H	1:W:786:HIS:HE1	1.62	0.46
1:X:249:LEU:HD21	1:X:372:LYS:HB2	1.98	0.46
4:9:204:LEU:HD23	4:9:207:LEU:HD12	1.98	0.46
4:9:70:THR:HG21	4:9:86:ARG:HH12	1.80	0.46
1:A:436:ASN:HB3	1:A:440:VAL:H	1.81	0.46
1:B:1245:LEU:O	1:B:1249:LEU:N	2.48	0.46
1:C:1062:PHE:HB2	1:C:1087:ALA:HB3	1.97	0.46
1:D:958:HIS:HE1	1:D:960:LEU:HB3	1.80	0.46
1:D:692:LEU:HD21	1:E:972:ARG:HH21	1.80	0.46
1:F:76:VAL:HG21	1:F:258:PHE:HD2	1.81	0.46
1:F:394:ARG:HB3	1:F:1050:HIS:HD2	1.81	0.46
1:N:404:VAL:HG23	1:N:432:THR:HG23	1.98	0.46
1:O:326:PHE:O	1:O:330:MET:N	2.48	0.46
1:S:1188:VAL:HG12	1:S:1192:GLN:HE22	1.80	0.46
1:S:623:GLN:HG3	1:S:626:LYS:HD3	1.96	0.46
1:S:744:ASP:H	1:S:786:HIS:HE1	1.62	0.46
1:U:903:SER:O	1:U:1128:GLN:NE2	2.49	0.46
1:V:1033:HIS:NE2	1:V:1036:PHE:O	2.48	0.46
1:V:740:ILE:HB	1:V:747:TYR:HB3	1.96	0.46
1:W:273:ALA:O	1:W:1053:TYR:OH	2.33	0.46
1:X:211:SER:OG	1:X:1206:SER:OG	2.33	0.46
1:X:504:LYS:HB2	1:X:967:ARG:HH12	1.81	0.46
1:4:191:ILE:HA	1:4:217:PHE:HE1	1.81	0.46
4:6:174:LEU:O	4:6:178:THR:OG1	2.32	0.46
4:6:61:GLN:HA	4:6:64:GLN:HB3	1.98	0.46
1:A:436:ASN:OD1	1:A:437:LYS:N	2.49	0.46
1:B:494:PHE:HZ	2:H:6:VAL:HG22	1.80	0.46
1:C:1341:TYR:HA	1:C:1348:HIS:CD2	2.51	0.46
1:D:1109:THR:O	1:D:1111:MET:N	2.49	0.46
1:C:663:HIS:HA	1:D:930:ARG:HD2	1.98	0.46
1:F:493:LEU:HD13	1:F:942:VAL:HG21	1.97	0.46
1:M:1344:ASN:ND2	1:M:1347:THR:OG1	2.49	0.46
1:N:1341:TYR:HA	1:N:1348:HIS:HD2	1.80	0.46
1:N:185:HIS:O	1:N:1097:SER:OG	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:819:MET:N	1:N:950:ASP:OD2	2.46	0.46
1:O:148:ASP:O	1:O:152:TYR:N	2.44	0.46
1:V:434:VAL:HG11	1:V:1042:ARG:HH12	1.81	0.46
1:4:566:PRO:HB2	1:4:568:PRO:HD2	1.98	0.46
1:4:838:PRO:HA	1:4:841:ALA:HB3	1.98	0.46
3:5:148:GLU:HA	3:5:151:ASP:HB2	1.97	0.46
3:8:89:PHE:HZ	3:8:161:PRO:HB3	1.81	0.46
3:8:260:LYS:O	3:8:264:THR:OG1	2.28	0.46
1:A:507:ALA:HB1	1:A:978:ASN:HD22	1.80	0.46
1:A:496:THR:HG21	1:A:982:ASN:HD22	1.81	0.46
1:C:401:PHE:N	1:C:1327:TYR:O	2.48	0.46
1:C:600:ILE:O	1:C:604:ALA:N	2.48	0.46
1:C:1167:PRO:HG2	1:D:1218:LEU:HD23	1.99	0.46
1:D:898:ARG:HE	1:D:913:VAL:HG23	1.80	0.46
1:S:1190:TYR:OH	1:S:1196:ASN:O	2.27	0.46
1:S:407:HIS:CE1	1:S:574:PHE:HB2	2.51	0.46
1:T:128:GLU:HG2	1:U:110:LYS:HG3	1.96	0.46
1:T:737:GLN:H	1:T:897:LYS:HD3	1.81	0.46
1:W:211:SER:OG	1:W:1206:SER:OG	2.33	0.46
1:W:436:ASN:OD1	1:W:437:LYS:N	2.49	0.46
1:W:592:ILE:HG13	1:W:683:GLU:HG2	1.98	0.46
1:A:82:ASP:N	1:A:82:ASP:OD1	2.47	0.45
1:A:913:VAL:HG22	1:A:990:TRP:HE1	1.81	0.45
1:D:174:LEU:HD23	1:D:1086:ILE:HD11	1.99	0.45
1:E:125:ILE:N	1:E:1084:HIS:O	2.49	0.45
1:F:537:HIS:HA	1:F:1238:TRP:CD1	2.51	0.45
1:F:611:LEU:HD22	1:F:862:ILE:HG12	1.96	0.45
1:F:854:LEU:HD13	1:F:860:LYS:HG2	1.97	0.45
1:M:352:ASP:HB2	1:M:354:HIS:CD2	2.51	0.45
1:N:453:ILE:HG12	1:N:1179:ILE:HG21	1.97	0.45
1:O:457:ARG:NH2	1:O:1254:PHE:O	2.50	0.45
1:S:436:ASN:OD1	1:S:437:LYS:N	2.50	0.45
1:S:569:LEU:HD22	1:S:1183:PRO:HB2	1.99	0.45
1:T:1341:TYR:HE1	1:T:1359:GLU:HG2	1.81	0.45
1:T:323:MET:HG3	1:T:326:PHE:HD1	1.81	0.45
1:V:41:LYS:O	1:V:44:ARG:NH1	2.49	0.45
1:V:712:LEU:HD13	1:V:805:LEU:HD21	1.98	0.45
1:W:739:ILE:HB	1:W:895:ILE:HB	1.97	0.45
1:W:845:ASN:N	1:W:848:ASP:OD2	2.49	0.45
1:X:9:PRO:HA	1:X:387:GLN:HG2	1.98	0.45
1:4:228:LEU:HD22	1:4:1103:HIS:HB2	1.96	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:401:PHE:HD2	1:4:1328:PRO:HB3	1.81	0.45
4:9:235:HIS:HB2	4:9:238:THR:HG22	1.98	0.45
1:A:464:SER:HG	1:A:542:PHE:HZ	1.64	0.45
1:A:752:ASN:O	1:A:755:THR:OG1	2.33	0.45
1:B:92:GLN:HE22	1:B:115:ILE:HG23	1.81	0.45
1:C:842:ASP:OD2	2:I:19:TYR:OH	2.29	0.45
1:D:514:GLN:HG3	1:D:531:LEU:HD21	1.98	0.45
1:E:10:PHE:HB2	1:E:12:TYR:CE1	2.52	0.45
1:E:394:ARG:HD3	1:E:1315:PHE:HB3	1.99	0.45
1:F:467:ALA:HB2	1:F:1254:PHE:HE2	1.81	0.45
1:F:994:PRO:HA	1:F:997:ALA:HB3	1.98	0.45
1:N:1017:GLN:HE21	1:N:1027:GLN:HE21	1.62	0.45
1:M:130:GLU:HB2	1:N:110:LYS:HD2	1.96	0.45
1:N:217:PHE:O	1:N:221:LEU:N	2.50	0.45
1:S:934:ALA:O	1:S:937:THR:OG1	2.30	0.45
1:T:602:GLU:HB3	1:T:647:LYS:HE2	1.99	0.45
1:T:720:PRO:HD3	1:T:808:TYR:CZ	2.50	0.45
1:T:652:ASN:ND2	1:T:923:GLY:O	2.39	0.45
1:U:826:TYR:OH	1:U:920:ASN:O	2.33	0.45
1:U:941:PRO:HB3	1:U:957:LEU:HD12	1.98	0.45
1:V:218:LYS:NZ	1:V:1323:LEU:O	2.47	0.45
1:V:263:THR:HA	1:V:359:ARG:HH12	1.81	0.45
1:4:699:THR:HA	1:4:704:PRO:HA	1.99	0.45
3:8:169:VAL:HB	3:8:176:LYS:HB3	1.99	0.45
1:A:78:THR:OG1	1:A:1061:MET:O	2.34	0.45
1:A:743:GLY:HA3	1:A:786:HIS:HE1	1.81	0.45
1:B:79:GLU:N	1:B:304:ALA:O	2.49	0.45
1:D:600:ILE:O	1:D:603:THR:OG1	2.26	0.45
1:E:113:GLN:HB3	1:M:38:LEU:HB2	1.97	0.45
1:E:446:TYR:O	1:E:450:LEU:N	2.50	0.45
1:F:145:THR:HG23	1:F:148:ASP:H	1.81	0.45
1:F:850:ILE:HD11	1:F:872:VAL:HA	1.98	0.45
1:F:980:PRO:HD2	1:F:983:LEU:HD12	1.97	0.45
1:M:74:ALA:O	1:M:1059:THR:OG1	2.33	0.45
1:O:1195:SER:O	1:O:1326:ALA:N	2.49	0.45
1:O:435:VAL:HG11	1:O:1368:LEU:HD22	1.98	0.45
1:O:964:TYR:HA	1:O:967:ARG:HB2	1.97	0.45
1:S:1109:THR:HG22	1:S:1111:MET:H	1.81	0.45
1:S:422:VAL:HG13	1:S:427:ILE:HG21	1.97	0.45
1:X:945:ASN:H	1:X:948:TYR:HB2	1.82	0.45
1:V:495:ARG:HH12	2:1:4:PHE:HB3	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:824:VAL:HG13	1:4:939:PHE:CZ	2.51	0.45
1:B:228:LEU:HD22	1:B:1103:HIS:HB2	1.97	0.45
1:B:958:HIS:HE1	1:B:960:LEU:HB3	1.81	0.45
1:B:994:PRO:HA	1:B:997:ALA:HB3	1.97	0.45
1:C:842:ASP:HB3	1:C:843:VAL:H	1.48	0.45
1:D:129:ILE:HB	1:D:1080:PHE:HB2	1.98	0.45
1:E:918:LEU:HB2	1:E:944:PHE:CE2	2.52	0.45
1:F:582:PHE:HE1	1:F:694:LEU:HD11	1.81	0.45
2:K:22:HIS:HB3	2:K:25:VAL:HG23	1.99	0.45
1:T:634:ILE:HA	1:T:637:VAL:HB	1.99	0.45
1:V:842:ASP:HB3	1:V:843:VAL:H	1.53	0.45
1:W:1044:ASP:HA	1:W:1109:THR:HG21	1.99	0.45
1:W:130:GLU:HG2	1:W:1079:THR:HG22	1.98	0.45
1:X:214:VAL:HG12	1:X:218:LYS:HE2	1.97	0.45
1:X:31:LEU:HD22	1:X:55:GLY:HA2	1.97	0.45
2:2:22:HIS:HB3	2:2:25:VAL:HG23	1.99	0.45
1:D:578:ARG:NH1	1:D:1014:SER:OG	2.49	0.45
1:M:431:GLU:OE1	1:M:1031:ARG:NH1	2.48	0.45
1:S:93:PHE:HB2	1:S:116:VAL:HB	1.99	0.45
1:T:146:PRO:HA	1:T:149:PHE:HD2	1.81	0.45
1:U:709:VAL:HG22	1:U:1023:SER:HA	1.98	0.45
1:U:54:LEU:HD23	1:V:324:ARG:HB2	1.99	0.45
1:W:619:MET:SD	1:W:881:SER:OG	2.65	0.45
1:W:634:ILE:HG22	1:W:650:PHE:HE2	1.80	0.45
1:W:95:ILE:HB	1:W:114:TYR:HB2	1.97	0.45
1:X:78:THR:HA	1:X:304:ALA:HB3	1.99	0.45
2:0:22:HIS:HB3	2:0:25:VAL:HG23	1.99	0.45
2:1:22:HIS:HB3	2:1:25:VAL:HG23	1.99	0.45
3:5:38:VAL:HA	3:5:41:LEU:HD13	1.99	0.45
4:7:214:LEU:HD21	4:7:272:TYR:HB3	1.99	0.45
4:9:61:GLN:O	4:9:65:TYR:N	2.46	0.45
1:F:1074:ARG:HD2	1:F:1077:ALA:HB3	1.99	0.45
1:M:1107:ILE:HD11	1:M:1364:MET:HE1	1.98	0.45
1:M:264:TYR:CE1	1:M:300:PRO:HD2	2.52	0.45
1:N:183:LEU:HD22	1:N:394:ARG:HH22	1.82	0.45
1:S:245:LEU:HD22	1:S:369:ILE:HG21	1.98	0.45
1:V:1341:TYR:HA	1:V:1348:HIS:CD2	2.52	0.45
1:W:1073:VAL:HG13	1:W:1078:VAL:HG22	1.98	0.45
1:W:218:LYS:NZ	1:W:1325:GLU:OE2	2.37	0.45
2:Z:22:HIS:HB3	2:Z:25:VAL:HG23	1.99	0.45
2:3:22:HIS:HB3	2:3:25:VAL:HG23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:839:VAL:HG13	1:4:872:VAL:HG13	1.99	0.45
1:A:76:VAL:HB	1:A:1060:SER:HA	1.99	0.45
1:C:623:GLN:HB2	1:C:626:LYS:HB2	1.98	0.45
1:D:63:PHE:HE2	1:D:65:LYS:HE2	1.81	0.45
1:F:684:LEU:HA	1:F:687:LEU:HB2	1.99	0.45
1:M:76:VAL:HB	1:M:1060:SER:HA	1.99	0.45
1:S:1227:PRO:O	1:X:1170:SER:OG	2.28	0.45
1:S:558:HIS:O	1:S:902:GLN:NE2	2.30	0.45
1:U:1071:ARG:O	1:U:1079:THR:OG1	2.35	0.45
1:U:579:GLY:HA3	1:U:1011:ALA:HA	1.98	0.45
1:X:578:ARG:NH2	1:X:1017:GLN:OE1	2.41	0.45
1:X:1250:TYR:HB2	1:X:1270:PHE:HD2	1.82	0.45
1:X:916:THR:OG1	1:X:984:MET:SD	2.64	0.45
1:4:893:ARG:HH21	1:4:914:ALA:HB3	1.81	0.45
1:A:254:GLU:HG3	1:A:255:ASP:H	1.82	0.45
1:A:307:VAL:HG12	1:A:309:ARG:H	1.82	0.45
1:A:79:GLU:N	1:A:304:ALA:O	2.50	0.45
1:C:578:ARG:NH1	1:C:1014:SER:O	2.45	0.45
1:C:280:ASP:O	1:C:380:GLN:NE2	2.49	0.45
1:E:214:VAL:HA	1:E:217:PHE:HD2	1.82	0.45
1:F:603:THR:HG22	1:F:647:LYS:HB3	1.99	0.45
1:F:744:ASP:H	1:F:786:HIS:HE1	1.64	0.45
1:N:946:LYS:HE2	1:N:993:SER:HA	1.99	0.45
1:N:1170:SER:OG	1:O:1227:PRO:O	2.34	0.45
1:O:826:TYR:HE2	1:O:886:PRO:HG2	1.81	0.45
2:Q:22:HIS:HB3	2:Q:25:VAL:HG23	1.99	0.45
1:S:218:LYS:NZ	1:S:1325:GLU:OE2	2.37	0.45
1:T:717:LEU:HA	1:T:915:GLN:HE22	1.82	0.45
1:U:91:ILE:HD11	1:U:1089:LEU:HD11	1.99	0.45
1:U:481:TYR:OH	1:U:979:VAL:N	2.47	0.45
1:U:1170:SER:OG	1:V:1227:PRO:O	2.27	0.45
1:V:146:PRO:HA	1:V:149:PHE:HD2	1.81	0.45
2:Y:22:HIS:HB3	2:Y:25:VAL:HG23	1.99	0.45
1:4:1204:VAL:O	1:4:1283:TYR:OH	2.28	0.45
1:4:233:LEU:HD11	1:4:1367:LEU:HD21	1.99	0.45
4:9:16:PHE:HB2	4:9:19:GLU:HG2	1.98	0.45
1:A:1195:SER:O	1:A:1326:ALA:N	2.47	0.45
1:A:692:LEU:HA	1:A:692:LEU:HD23	1.80	0.45
1:A:487:GLN:NE2	1:A:744:ASP:O	2.50	0.45
1:C:931:SER:O	1:C:935:ALA:N	2.50	0.45
1:D:245:LEU:HD22	1:D:369:ILE:HG21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:58:THR:HG22	1:E:94:LYS:HB3	1.98	0.45
1:F:437:LYS:HD3	1:F:1107:ILE:HB	1.99	0.45
1:F:323:MET:HG3	1:F:326:PHE:HD1	1.81	0.45
1:F:904:PHE:HZ	1:F:1127:TYR:HA	1.82	0.45
1:M:436:ASN:OD1	1:M:437:LYS:N	2.50	0.45
1:M:465:ALA:HA	1:M:468:LEU:HB3	1.98	0.45
1:M:88:ASP:HB2	1:M:321:ARG:HH22	1.82	0.45
1:N:537:HIS:HB3	1:N:1245:LEU:HB2	1.98	0.45
1:S:136:ILE:HG23	3:5:60:LEU:HD23	1.98	0.45
1:S:401:PHE:N	1:S:1327:TYR:O	2.50	0.45
1:X:945:ASN:OD1	1:X:946:LYS:N	2.49	0.45
1:4:1241:GLN:HB3	1:4:1244:SER:HA	1.98	0.45
4:7:214:LEU:HD11	4:7:272:TYR:CG	2.52	0.45
1:C:658:ARG:NH2	1:D:929:ASP:OD2	2.50	0.45
1:D:443:CYS:N	1:E:1231:CYS:SG	2.90	0.45
1:D:680:ILE:O	1:D:684:LEU:N	2.45	0.45
1:E:1109:THR:O	1:E:1111:MET:N	2.50	0.45
1:E:419:VAL:HG22	1:E:421:GLY:H	1.82	0.45
1:E:534:LEU:HD11	1:E:544:VAL:HG23	1.98	0.45
1:F:1348:HIS:CE1	1:F:1357:LEU:HD22	2.52	0.45
2:I:22:HIS:HB3	2:I:25:VAL:HG23	1.99	0.45
1:N:1195:SER:O	1:N:1326:ALA:N	2.50	0.45
1:O:700:VAL:O	1:O:1131:GLN:NE2	2.50	0.45
1:O:1341:TYR:HB2	1:O:1357:LEU:HD11	1.99	0.45
1:O:945:ASN:O	1:O:949:ALA:N	2.50	0.45
1:U:945:ASN:O	1:U:949:ALA:N	2.50	0.45
1:X:166:GLY:HA2	1:X:169:ALA:HB3	1.99	0.45
1:S:202:GLU:HA	1:X:387:GLN:HE22	1.82	0.45
2:Z:70:ARG:NH2	2:0:12:GLN:HB2	2.32	0.44
2:3:33:GLN:NE2	2:3:36:MET:O	2.46	0.44
1:4:566:PRO:HD2	1:4:569:LEU:HD12	1.97	0.44
4:6:49:CYS:SG	4:6:50:VAL:N	2.90	0.44
1:A:1044:ASP:HA	1:A:1109:THR:HB	1.99	0.44
1:A:95:ILE:HB	1:A:114:TYR:HB2	1.99	0.44
1:D:290:LEU:HD23	1:D:367:VAL:HG11	1.99	0.44
1:E:695:ALA:HB1	1:E:706:THR:HG22	1.98	0.44
1:E:74:ALA:HB1	1:E:182:LYS:HE3	1.98	0.44
1:F:1115:CYS:HA	1:F:1177:CYS:HB2	1.99	0.44
1:F:1181:PRO:HG3	1:F:1245:LEU:HD22	1.98	0.44
1:F:188:PRO:HD2	1:F:191:ILE:HD12	1.99	0.44
1:F:540:PHE:HA	1:F:558:HIS:HA	1.97	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:22:HIS:HB3	2:G:25:VAL:HG23	1.99	0.44
1:M:611:LEU:HD22	1:M:862:ILE:HG12	1.99	0.44
1:O:481:TYR:OH	1:O:979:VAL:N	2.50	0.44
1:S:183:LEU:HD13	1:S:394:ARG:HH21	1.82	0.44
1:T:454:CYS:HA	1:T:1021:ALA:HB1	1.99	0.44
1:T:512:VAL:HG12	1:T:993:SER:HB3	1.99	0.44
1:W:79:GLU:N	1:W:304:ALA:O	2.48	0.44
1:4:850:ILE:HD12	1:4:870:PRO:HG2	1.99	0.44
3:5:205:VAL:HG21	3:5:262:HIS:HE1	1.82	0.44
4:9:124:THR:HG22	4:9:135:VAL:HG22	1.98	0.44
1:C:1067:SER:OG	1:C:1083:THR:OG1	2.33	0.44
1:C:1200:ARG:NH1	1:C:1225:PRO:O	2.48	0.44
1:C:587:ASN:HD22	1:D:572:ARG:HH12	1.65	0.44
1:C:598:ASP:O	1:C:602:GLU:N	2.42	0.44
1:D:562:VAL:HG13	1:D:565:ILE:HD12	1.99	0.44
1:D:945:ASN:OD1	1:D:946:LYS:N	2.50	0.44
1:E:946:LYS:HE2	1:E:993:SER:HA	1.99	0.44
1:N:79:GLU:N	1:N:304:ALA:O	2.50	0.44
1:N:992:LYS:HB2	1:N:994:PRO:HD2	1.99	0.44
2:R:22:HIS:HB3	2:R:25:VAL:HG23	1.99	0.44
1:V:183:LEU:HD13	1:V:394:ARG:HH21	1.81	0.44
1:U:59:ASN:ND2	1:V:96:SER:O	2.50	0.44
1:V:567:GLN:NE2	1:V:994:PRO:O	2.50	0.44
1:W:1196:ASN:HD22	1:W:1202:ALA:H	1.65	0.44
1:W:324:ARG:HH22	1:W:352:ASP:HB2	1.83	0.44
1:X:1341:TYR:HA	1:X:1348:HIS:CD2	2.53	0.44
1:X:947:LEU:HD21	1:X:995:VAL:HG12	1.98	0.44
1:A:236:ARG:HE	1:A:239:GLN:HB2	1.83	0.44
1:A:946:LYS:HE2	1:A:993:SER:HA	1.98	0.44
1:B:276:LEU:HA	1:B:1053:TYR:HA	1.99	0.44
1:D:7:GLN:HE21	1:D:36:GLN:HG2	1.82	0.44
1:M:455:HIS:HD2	1:M:1119:PHE:CD1	2.36	0.44
1:M:264:TYR:HE1	1:M:300:PRO:HD2	1.82	0.44
1:N:1045:GLU:OE1	1:N:1300:SER:OG	2.32	0.44
1:N:658:ARG:HA	1:N:681:LEU:HD11	1.98	0.44
1:S:1341:TYR:HA	1:S:1348:HIS:CD2	2.52	0.44
1:S:236:ARG:HH21	1:S:239:GLN:HG3	1.81	0.44
1:T:76:VAL:HB	1:T:1060:SER:HA	1.99	0.44
1:U:945:ASN:OD1	1:U:946:LYS:N	2.51	0.44
1:V:1344:ASN:HD21	1:V:1347:THR:HG1	1.62	0.44
1:V:842:ASP:OD2	2:1:19:TYR:OH	2.25	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:898:ARG:NH1	1:V:904:PHE:O	2.51	0.44
1:X:75:CYS:SG	1:X:1059:THR:OG1	2.63	0.44
1:X:865:ALA:HA	1:X:930:ARG:HH22	1.83	0.44
1:4:989:GLU:HB3	1:4:992:LYS:HD3	1.99	0.44
3:5:283:LEU:O	4:6:272:TYR:OH	2.35	0.44
4:7:97:ASN:HD22	4:7:105:TRP:HE1	1.64	0.44
4:9:113:VAL:HG22	4:9:139:VAL:HG12	2.00	0.44
4:9:7:ILE:HD11	4:9:86:ARG:HH11	1.83	0.44
1:A:76:VAL:O	1:A:1061:MET:N	2.42	0.44
1:B:447:GLN:HB2	1:B:1028:ALA:HB1	1.99	0.44
1:B:1200:ARG:HG3	1:B:1234:THR:HG23	1.98	0.44
1:C:172:ARG:HB3	1:D:100:ILE:HG23	1.98	0.44
1:D:185:HIS:O	1:D:1097:SER:OG	2.36	0.44
1:F:324:ARG:HH21	1:F:352:ASP:HB3	1.82	0.44
1:F:380:GLN:O	1:F:384:ASN:N	2.36	0.44
1:O:1033:HIS:NE2	1:O:1036:PHE:O	2.51	0.44
1:O:723:TYR:HE1	1:O:921:GLY:H	1.64	0.44
1:S:823:GLY:N	1:S:940:TYR:O	2.50	0.44
1:V:455:HIS:HD2	1:V:1119:PHE:HD1	1.66	0.44
1:V:361:ARG:NH1	1:V:362:ILE:O	2.51	0.44
1:W:675:GLY:O	1:W:679:LYS:N	2.43	0.44
1:4:537:HIS:HB3	1:4:1245:LEU:HD12	2.00	0.44
1:4:561:MET:H	1:4:564:ASN:HD22	1.66	0.44
1:4:627:PHE:O	1:4:631:MET:N	2.51	0.44
4:6:110:GLN:HG2	4:6:142:GLN:HE21	1.82	0.44
3:8:145:ASN:O	3:8:149:LEU:N	2.44	0.44
1:C:1294:ALA:HB1	1:C:1321:HIS:CE1	2.53	0.44
1:D:453:ILE:HD13	1:D:1036:PHE:HZ	1.83	0.44
1:D:191:ILE:HA	1:D:217:PHE:HE1	1.83	0.44
1:E:603:THR:HG22	1:E:647:LYS:HB3	1.99	0.44
1:F:1195:SER:O	1:F:1326:ALA:N	2.50	0.44
1:F:699:THR:HA	1:F:704:PRO:HA	1.98	0.44
2:H:22:HIS:HB3	2:H:25:VAL:HG23	1.99	0.44
1:O:1074:ARG:HG2	1:O:1076:ASP:H	1.82	0.44
1:N:1170:SER:HA	1:O:211:SER:HB3	1.99	0.44
1:O:856:ASN:HD21	2:Q:67:GLY:HA3	1.82	0.44
1:S:435:VAL:HG11	1:S:1368:LEU:HD22	1.99	0.44
1:S:524:LEU:O	1:S:1233:SER:N	2.49	0.44
1:S:605:PHE:HZ	1:S:816:ASN:HD22	1.64	0.44
1:T:838:PRO:HB2	1:T:872:VAL:HG11	1.99	0.44
1:M:333:ILE:HD11	1:U:11:PRO:HD3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:848:ASP:H	1:V:872:VAL:HG23	1.82	0.44
1:W:153:ALA:HA	1:W:156:ILE:HG22	1.99	0.44
4:6:75:GLU:OE1	4:6:83:ARG:NE	2.50	0.44
1:C:850:ILE:HD12	1:C:875:ILE:HD12	2.00	0.44
1:D:38:LEU:HD13	1:D:43:ALA:HA	2.00	0.44
1:E:150:THR:HG21	1:U:313:LEU:HD21	1.98	0.44
1:F:1226:ASP:HB2	1:F:1229:TYR:H	1.82	0.44
1:N:507:ALA:HB1	1:N:978:ASN:HD21	1.82	0.44
1:O:994:PRO:HA	1:O:997:ALA:HB3	1.99	0.44
2:Q:33:GLN:NE2	2:Q:36:MET:O	2.46	0.44
1:S:674:HIS:O	1:S:678:ARG:N	2.40	0.44
1:W:304:ALA:HB2	1:W:357:ILE:HD11	1.98	0.44
1:W:65:LYS:HB2	1:W:68:GLU:HB2	2.00	0.44
3:5:57:HIS:HA	3:5:60:LEU:HD13	2.00	0.44
1:A:945:ASN:OD1	1:A:946:LYS:N	2.50	0.44
1:B:130:GLU:HG3	1:C:110:LYS:HD2	1.99	0.44
1:C:1294:ALA:HB1	1:C:1321:HIS:HE1	1.82	0.44
1:D:394:ARG:HB2	1:D:1050:HIS:NE2	2.33	0.44
1:D:576:GLU:OE1	1:D:998:TYR:OH	2.36	0.44
1:E:541:ASP:HB2	1:E:559:ARG:HG3	1.99	0.44
1:F:402:PHE:HD2	1:F:1040:VAL:HB	1.83	0.44
1:F:402:PHE:O	1:F:1040:VAL:N	2.45	0.44
1:F:541:ASP:HB2	1:F:559:ARG:HG3	2.00	0.44
1:M:454:CYS:HA	1:M:1021:ALA:HB1	1.99	0.44
1:O:518:VAL:HG13	1:O:522:ASP:HB3	2.00	0.44
1:T:78:THR:HG22	1:T:304:ALA:HB3	2.00	0.44
1:U:578:ARG:NH1	1:U:1014:SER:O	2.46	0.44
1:W:238:LYS:HG2	1:W:289:LEU:HD22	2.00	0.44
1:W:294:GLU:HB2	1:W:366:LEU:HD22	2.00	0.44
1:X:507:ALA:HB2	1:X:968:LEU:HD11	1.99	0.44
4:6:240:VAL:HG21	4:7:268:VAL:HG21	2.00	0.44
4:9:230:VAL:HG11	4:9:241:PHE:HD2	1.82	0.44
1:A:1166:LEU:O	1:B:207:LYS:NZ	2.48	0.44
1:B:1328:PRO:HB2	1:B:1358:ILE:HG21	2.00	0.44
1:B:740:ILE:HB	1:B:747:TYR:HB3	1.99	0.44
1:C:83:LEU:HD11	1:C:122:LYS:HD2	2.00	0.44
1:D:1344:ASN:ND2	1:D:1347:THR:OG1	2.51	0.44
1:F:1201:ALA:HB3	1:F:1227:PRO:HG2	2.00	0.44
2:P:22:HIS:HB3	2:P:25:VAL:HG23	1.99	0.44
1:S:386:THR:HG21	1:T:100:ILE:HG13	1.99	0.44
1:S:438:ASN:ND2	1:T:215:SER:OG	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:115:ILE:HG22	1:U:5:LEU:HD11	2.00	0.44
1:U:807:TYR:O	1:U:948:TYR:OH	2.31	0.44
1:W:1196:ASN:HD21	1:W:1324:GLN:HG3	1.82	0.44
1:W:856:ASN:OD1	1:W:860:LYS:NZ	2.36	0.44
1:X:185:HIS:O	1:X:1097:SER:OG	2.35	0.44
4:7:94:GLN:HE21	4:7:297:ALA:HB1	1.83	0.44
1:C:1018:LYS:HB2	1:C:1023:SER:HB3	1.99	0.44
1:C:958:HIS:CE1	1:C:960:LEU:HB3	2.53	0.44
1:E:406:LEU:HD21	1:E:1191:PHE:HE2	1.82	0.44
1:F:91:ILE:HD11	1:F:1089:LEU:HD21	2.00	0.44
1:F:448:ASN:HD22	1:F:1113:VAL:HG12	1.82	0.44
1:F:851:LEU:HD12	1:F:869:ARG:HD2	1.99	0.44
1:M:669:ILE:HD13	1:M:674:HIS:HB2	2.00	0.44
1:N:312:ASN:ND2	1:N:323:MET:HB2	2.32	0.44
1:O:1198:ARG:HA	1:O:1239:ALA:HB3	2.00	0.44
1:O:1271:HIS:ND1	1:O:1274:ASP:OD2	2.51	0.44
1:T:1199:GLY:HA2	1:T:1235:ASN:HB3	1.99	0.44
1:T:1341:TYR:HA	1:T:1348:HIS:CD2	2.53	0.44
1:U:872:VAL:HG12	1:U:876:ARG:HG3	1.99	0.44
1:W:537:HIS:HB3	1:W:1245:LEU:HB2	2.00	0.44
1:X:1328:PRO:HB2	1:X:1358:ILE:HG21	2.00	0.44
1:X:736:ARG:HH21	1:X:900:PRO:HG3	1.81	0.44
2:0:33:GLN:NE2	2:0:36:MET:O	2.46	0.43
1:4:80:PHE:HB3	1:4:1063:VAL:H	1.83	0.43
1:4:188:PRO:HD2	1:4:191:ILE:HD12	2.00	0.43
1:4:704:PRO:HD2	1:4:707:HIS:CE1	2.53	0.43
1:C:279:THR:OG1	1:C:280:ASP:N	2.50	0.43
1:D:591:VAL:HB	1:D:683:GLU:HB2	1.99	0.43
1:E:1241:GLN:HB3	1:E:1244:SER:HB3	1.98	0.43
2:L:22:HIS:HB3	2:L:25:VAL:HG23	1.99	0.43
1:M:434:VAL:HG11	1:M:1042:ARG:HH22	1.83	0.43
1:M:1187:ASP:OD2	1:M:1232:ARG:NH2	2.50	0.43
1:N:446:TYR:O	1:N:450:LEU:N	2.51	0.43
1:O:361:ARG:NH1	1:O:362:ILE:O	2.51	0.43
1:S:153:ALA:HA	1:S:156:ILE:HG22	1.99	0.43
1:S:538:PRO:O	1:S:559:ARG:NH1	2.51	0.43
1:S:868:ILE:HG22	1:S:870:PRO:HD3	1.99	0.43
1:T:116:VAL:HG11	1:T:1093:LEU:HD12	2.00	0.43
1:U:1313:ASP:OD1	1:V:106:ARG:NH1	2.51	0.43
1:U:524:LEU:O	1:U:1233:SER:N	2.40	0.43
1:X:125:ILE:HD12	1:X:1084:HIS:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:57:TYR:CD2	1:4:49:ARG:HD2	2.53	0.43
1:4:964:TYR:OH	1:4:978:ASN:ND2	2.51	0.43
1:A:947:LEU:HD23	1:A:996:ALA:HB2	2.00	0.43
1:B:897:LYS:HA	1:B:912:ASP:HA	2.00	0.43
1:E:931:SER:HB2	1:E:934:ALA:HB3	1.99	0.43
1:F:537:HIS:HA	1:F:1238:TRP:NE1	2.33	0.43
1:O:1190:TYR:HD1	1:O:1229:TYR:HE2	1.66	0.43
1:O:558:HIS:HD2	1:O:560:THR:HA	1.84	0.43
1:S:562:VAL:HA	1:S:1019:LEU:HD11	1.98	0.43
1:T:1344:ASN:ND2	1:T:1347:THR:OG1	2.52	0.43
1:T:415:THR:HB	1:T:1349:ALA:HB1	2.01	0.43
1:U:578:ARG:NH1	1:U:1014:SER:OG	2.51	0.43
1:W:1047:LEU:HD12	1:W:1106:ALA:HB3	1.99	0.43
1:W:1262:MET:HA	1:W:1306:TYR:HA	2.00	0.43
1:4:454:CYS:O	1:4:1127:TYR:OH	2.24	0.43
3:8:38:VAL:HG13	3:8:41:LEU:HD13	2.01	0.43
1:A:861:ASP:O	1:A:931:SER:OG	2.35	0.43
1:C:90:LYS:HG3	1:C:117:MET:HE3	2.00	0.43
1:C:945:ASN:OD1	1:C:946:LYS:N	2.51	0.43
1:E:1067:SER:OG	1:E:1083:THR:OG1	2.36	0.43
1:F:380:GLN:HB3	1:F:384:ASN:ND2	2.33	0.43
1:M:245:LEU:HD22	1:M:369:ILE:HG21	2.00	0.43
1:S:1312:THR:O	1:T:106:ARG:NH1	2.44	0.43
1:S:591:VAL:N	1:S:683:GLU:OE1	2.50	0.43
1:S:744:ASP:H	1:S:786:HIS:CE1	2.35	0.43
1:U:1294:ALA:HB1	1:U:1321:HIS:CE1	2.53	0.43
1:V:752:ASN:O	1:V:755:THR:OG1	2.31	0.43
1:W:1196:ASN:ND2	1:W:1202:ALA:H	2.17	0.43
1:W:245:LEU:HD22	1:W:369:ILE:HD13	1.99	0.43
1:X:591:VAL:HG12	1:X:679:LYS:HG2	1.99	0.43
1:W:855:GLU:HG2	2:1:70:ARG:HG3	2.01	0.43
1:4:436:ASN:OD1	1:4:437:LYS:N	2.51	0.43
1:A:431:GLU:OE1	1:A:1031:ARG:NH1	2.51	0.43
1:F:306:TYR:OH	1:F:323:MET:O	2.32	0.43
1:F:92:GLN:HE22	1:F:115:ILE:HG23	1.82	0.43
2:I:33:GLN:NE2	2:I:36:MET:O	2.46	0.43
1:M:447:GLN:HB3	1:M:1028:ALA:HB1	2.00	0.43
1:N:123:HIS:N	1:N:1086:ILE:O	2.51	0.43
1:N:637:VAL:HG22	1:N:868:ILE:HD13	1.99	0.43
1:S:450:LEU:HD11	1:S:1025:ILE:HA	2.00	0.43
1:V:1313:ASP:OD2	1:W:203:ARG:NH2	2.40	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:54:LEU:HB2	1:X:91:ILE:HG13	2.00	0.43
1:W:744:ASP:H	1:W:786:HIS:CE1	2.36	0.43
1:X:5:LEU:HD22	1:X:14:ALA:HB1	2.01	0.43
1:X:893:ARG:HA	1:X:916:THR:HG22	2.00	0.43
1:4:514:GLN:HG3	1:4:531:LEU:HD11	1.99	0.43
1:4:993:SER:O	1:4:997:ALA:N	2.50	0.43
4:6:287:HIS:N	4:6:300:CYS:SG	2.87	0.43
4:7:267:ARG:HA	4:7:270:PHE:HD2	1.84	0.43
4:9:109:THR:HG22	4:9:288:VAL:HB	1.99	0.43
1:A:1073:VAL:HG13	1:A:1078:VAL:HG22	2.01	0.43
1:A:442:LEU:HB2	1:A:1113:VAL:HG21	2.01	0.43
1:B:907:HIS:HB3	1:B:909:TYR:H	1.83	0.43
1:D:491:MET:HG3	1:D:785:ARG:H	1.83	0.43
1:C:165:PHE:HE1	1:D:98:PRO:HA	1.84	0.43
1:E:534:LEU:HD13	1:E:543:PHE:HA	2.00	0.43
1:E:627:PHE:O	1:E:631:MET:N	2.51	0.43
1:M:79:GLU:N	1:M:304:ALA:O	2.51	0.43
1:O:1341:TYR:HA	1:O:1348:HIS:CD2	2.53	0.43
1:S:799:ASN:HD21	1:S:802:LEU:HG	1.84	0.43
1:S:916:THR:OG1	1:S:984:MET:SD	2.71	0.43
1:U:406:LEU:HD21	1:U:1191:PHE:CE2	2.53	0.43
1:U:540:PHE:O	1:U:559:ARG:NH1	2.51	0.43
1:W:1067:SER:OG	1:W:1083:THR:OG1	2.36	0.43
1:W:501:TYR:OH	1:W:978:ASN:O	2.31	0.43
1:4:757:ILE:HA	1:4:788:LEU:HB3	1.99	0.43
1:B:529:HIS:CE1	1:B:1223:SER:HB3	2.54	0.43
1:C:708:LEU:HD21	1:C:1022:PRO:HG2	1.98	0.43
1:D:451:LYS:HG2	1:D:1140:ALA:HB1	2.01	0.43
1:A:95:ILE:HA	1:F:59:ASN:HD22	1.83	0.43
2:J:22:HIS:HB3	2:J:25:VAL:HG23	1.99	0.43
2:L:33:GLN:NE2	2:L:36:MET:O	2.46	0.43
1:M:145:THR:HG23	1:M:148:ASP:H	1.84	0.43
1:M:929:ASP:OD1	1:M:932:ARG:NH2	2.52	0.43
1:N:192:LEU:O	1:N:196:GLY:N	2.51	0.43
1:O:368:LYS:HG3	1:O:373:PHE:HE1	1.84	0.43
1:O:422:VAL:HG13	1:O:427:ILE:HG21	2.00	0.43
1:S:123:HIS:HB2	1:S:1086:ILE:HB	2.01	0.43
1:S:929:ASP:OD1	1:S:932:ARG:NH2	2.52	0.43
1:S:918:LEU:HB2	1:S:944:PHE:CZ	2.53	0.43
1:T:422:VAL:O	1:T:424:SER:N	2.51	0.43
1:T:959:PRO:O	1:T:963:ASN:N	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:701:GLY:HA3	1:U:1131:GLN:NE2	2.33	0.43
1:W:878:LEU:O	1:W:881:SER:OG	2.36	0.43
1:X:918:LEU:HB2	1:X:944:PHE:CE2	2.53	0.43
1:4:1077:ALA:HB3	4:6:83:ARG:HH22	1.84	0.43
1:4:707:HIS:HA	1:4:713:LEU:HD22	1.99	0.43
4:6:13:SER:HG	4:6:129:SER:HG	1.62	0.43
1:A:1025:ILE:HG22	1:A:1029:LYS:HE2	1.99	0.43
1:D:10:PHE:HB2	1:D:12:TYR:CE1	2.54	0.43
1:D:436:ASN:OD1	1:D:437:LYS:N	2.49	0.43
1:D:927:VAL:HG21	1:D:957:LEU:HD11	2.00	0.43
1:E:1198:ARG:HG2	1:E:1239:ALA:HB1	2.01	0.43
1:F:1188:VAL:HG12	1:F:1192:GLN:HE22	1.82	0.43
1:M:831:LEU:HD22	2:P:9:PRO:HG2	2.00	0.43
1:M:947:LEU:HD21	1:M:995:VAL:HG12	2.00	0.43
1:O:124:HIS:ND1	1:O:1085:GLU:HG2	2.33	0.43
1:S:1200:ARG:HG3	1:S:1234:THR:HG23	1.99	0.43
1:S:404:VAL:HG23	1:S:432:THR:HG23	2.00	0.43
1:S:76:VAL:HB	1:S:1060:SER:HA	1.99	0.43
1:T:960:LEU:O	1:T:964:TYR:N	2.51	0.43
1:U:342:SER:OG	1:U:343:VAL:N	2.51	0.43
1:X:380:GLN:HE21	1:X:393:ASN:HD21	1.67	0.43
1:4:1183:PRO:HD2	1:4:1236:ASN:HD22	1.84	0.43
1:4:1199:GLY:HA2	1:4:1235:ASN:HB3	2.01	0.43
1:4:722:ALA:H	1:4:917:VAL:HG13	1.83	0.43
1:A:215:SER:OG	4:9:222:CYS:SG	136.92	0.43
1:A:992:LYS:HB2	1:A:994:PRO:HD2	2.00	0.43
1:B:197:ASP:HB3	1:B:199:VAL:HG12	2.00	0.43
1:C:1216:GLU:OE2	1:C:1242:ARG:NH2	2.52	0.43
1:D:658:ARG:HA	1:D:681:LEU:HD11	2.00	0.43
1:D:951:PRO:O	1:D:955:ALA:N	2.52	0.43
1:E:898:ARG:HE	1:E:913:VAL:HG23	1.83	0.43
1:F:404:VAL:HG23	1:F:432:THR:HG23	2.01	0.43
1:M:1109:THR:HG22	1:M:1111:MET:H	1.84	0.43
1:M:700:VAL:O	1:M:1131:GLN:NE2	2.52	0.43
1:M:495:ARG:HH22	2:P:4:PHE:HB3	1.82	0.43
1:M:713:LEU:HA	1:M:801:VAL:HG22	2.01	0.43
1:N:512:VAL:HG12	1:N:993:SER:HB3	2.00	0.43
1:O:1366:ARG:HD2	1:O:1368:LEU:HD21	2.00	0.43
1:S:236:ARG:HE	1:S:239:GLN:HB2	1.82	0.43
1:S:71:LEU:N	1:S:377:GLU:OE2	2.52	0.43
1:T:949:ALA:HB1	1:T:977:PHE:HD2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:1247:ASP:OD1	1:U:1251:ASN:ND2	2.52	0.43
1:U:845:ASN:N	1:U:848:ASP:OD2	2.47	0.43
1:V:532:LEU:O	1:V:1241:GLN:NE2	2.52	0.43
1:W:695:ALA:HB1	1:W:706:THR:HG22	2.01	0.43
1:W:496:THR:HG21	1:W:982:ASN:HD22	1.82	0.43
1:4:708:LEU:HD21	1:4:1020:SER:HB2	2.00	0.43
4:7:21:ALA:HA	4:7:24:GLN:HB2	2.00	0.43
1:B:1342:MET:HA	1:B:1375:VAL:HG21	2.00	0.43
1:B:560:THR:HG23	1:B:902:GLN:HE22	1.83	0.43
1:D:263:THR:HA	1:D:359:ARG:HH12	1.84	0.43
1:E:520:THR:HG22	1:E:568:PRO:HA	2.00	0.43
1:F:824:VAL:HG13	1:F:938:MET:HB3	2.01	0.43
1:F:926:ALA:HB2	1:F:953:VAL:HG22	2.00	0.43
1:O:75:CYS:SG	1:O:1059:THR:OG1	2.70	0.43
1:T:278:THR:HG22	1:T:1051:ILE:HG12	2.01	0.43
1:U:856:ASN:HB2	2:0:12:GLN:HE21	1.83	0.43
1:X:474:ASP:OD1	1:X:552:GLY:N	2.52	0.43
1:4:851:LEU:H	1:4:869:ARG:HE	1.67	0.43
1:C:306:TYR:HA	1:C:324:ARG:HH12	1.82	0.43
1:D:438:ASN:HD22	1:D:1171:HIS:HD2	1.67	0.43
1:F:1199:GLY:HA2	1:F:1235:ASN:HB3	2.00	0.43
1:F:26:SER:HB3	1:F:31:LEU:HB2	2.01	0.43
1:F:744:ASP:H	1:F:786:HIS:CE1	2.37	0.43
1:M:402:PHE:HD2	1:M:1040:VAL:HB	1.83	0.43
1:N:678:ARG:HH22	1:O:608:ALA:HB3	1.83	0.43
1:O:71:LEU:N	1:O:377:GLU:OE2	2.52	0.43
1:O:898:ARG:HD2	1:O:903:SER:HA	2.01	0.43
1:S:578:ARG:NH1	1:S:1014:SER:O	2.39	0.43
1:U:762:ARG:HB2	1:U:765:ASP:HB2	2.00	0.43
1:W:1115:CYS:HA	1:W:1177:CYS:H	1.84	0.43
1:W:1308:VAL:HG21	1:W:1314:VAL:HG21	2.00	0.43
1:W:228:LEU:HD22	1:W:1103:HIS:HD2	1.84	0.43
1:W:82:ASP:N	1:W:82:ASP:OD1	2.51	0.43
3:5:201:CYS:HB2	3:5:313:PRO:HG2	2.01	0.42
4:9:220:ARG:HG2	4:9:265:ARG:HH12	1.83	0.42
1:A:77:ASN:HA	1:A:1061:MET:HB2	2.00	0.42
1:A:1271:HIS:ND1	1:A:1274:ASP:OD2	2.50	0.42
1:A:545:HIS:CE1	1:A:555:ARG:HD2	2.52	0.42
1:C:1271:HIS:HB3	1:C:1274:ASP:HB2	2.00	0.42
1:E:620:ILE:HG22	1:E:623:GLN:H	1.84	0.42
1:E:777:ARG:NH2	1:E:886:PRO:O	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1200:ARG:HG3	1:F:1234:THR:HG23	2.01	0.42
1:X:831:LEU:HD23	2:3:11:ILE:HD12	2.01	0.42
1:4:295:SER:HA	1:4:366:LEU:HD13	1.99	0.42
1:4:702:ARG:NH1	1:4:733:LYS:O	2.52	0.42
4:7:141:PRO:HG2	4:7:144:LEU:HD12	2.02	0.42
1:A:1348:HIS:CE1	1:A:1357:LEU:HD22	2.54	0.42
1:B:849:ASP:HB2	1:B:869:ARG:HH21	1.85	0.42
1:C:436:ASN:HB3	1:C:440:VAL:H	1.83	0.42
1:C:1170:SER:OG	1:D:1227:PRO:O	2.37	0.42
1:E:826:TYR:HE2	1:E:886:PRO:HG2	1.83	0.42
1:F:1022:PRO:HD3	1:F:1136:ILE:HD11	2.00	0.42
1:N:583:ASP:OD1	1:N:590:HIS:NE2	2.48	0.42
1:N:704:PRO:HD2	1:N:707:HIS:CE1	2.54	0.42
1:O:822:MET:SD	1:O:939:PHE:HB3	2.59	0.42
1:N:494:PHE:CZ	2:Q:6:VAL:HG22	2.53	0.42
1:T:133:ALA:HB2	1:T:1076:ASP:HA	2.01	0.42
1:U:560:THR:HG22	1:U:561:MET:HG3	2.01	0.42
1:U:674:HIS:HA	1:U:677:TYR:HD2	1.84	0.42
1:W:505:ASN:OD1	1:W:506:VAL:N	2.52	0.42
1:W:824:VAL:H	1:W:889:THR:HG21	1.84	0.42
1:X:255:ASP:HB3	1:X:1093:LEU:H	1.85	0.42
1:X:811:MET:O	1:X:815:SER:OG	2.32	0.42
1:X:963:ASN:HA	1:X:966:THR:HG22	2.01	0.42
3:5:143:ILE:HG22	3:5:145:ASN:H	1.85	0.42
3:8:285:PHE:HB2	3:8:331:LEU:HD13	2.01	0.42
4:9:144:LEU:HA	4:9:147:ALA:HB3	2.01	0.42
1:A:505:ASN:OD1	1:A:506:VAL:N	2.52	0.42
1:A:720:PRO:HD3	1:A:808:TYR:CZ	2.55	0.42
1:B:455:HIS:HA	1:B:1119:PHE:HE1	1.84	0.42
1:E:728:THR:HG21	1:E:753:ARG:HD3	2.01	0.42
1:F:1198:ARG:NH1	1:F:1201:ALA:O	2.52	0.42
1:F:494:PHE:HZ	2:L:6:VAL:HG22	1.83	0.42
1:M:350:LEU:HD12	1:U:13:LEU:HB3	2.00	0.42
1:M:402:PHE:O	1:M:1040:VAL:N	2.52	0.42
1:M:918:LEU:HB2	1:M:944:PHE:CE2	2.54	0.42
1:S:1278:TYR:HE2	1:S:1321:HIS:HB3	1.85	0.42
1:S:402:PHE:O	1:S:1040:VAL:N	2.51	0.42
1:S:849:ASP:HB3	1:S:869:ARG:HB3	2.00	0.42
1:U:118:LYS:NZ	1:U:1091:THR:O	2.52	0.42
1:U:454:CYS:O	1:U:1127:TYR:OH	2.27	0.42
1:U:518:VAL:HG13	1:U:522:ASP:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:543:PHE:CZ	1:U:555:ARG:HD3	2.54	0.42
1:U:74:ALA:HB1	1:U:182:LYS:HE3	2.01	0.42
1:V:76:VAL:HB	1:V:1060:SER:HA	2.00	0.42
1:W:507:ALA:HB1	1:W:978:ASN:HD21	1.84	0.42
1:X:71:LEU:N	1:X:377:GLU:OE2	2.53	0.42
1:X:613:CYS:HB3	1:X:637:VAL:HG11	2.00	0.42
1:X:777:ARG:HH12	1:X:882:PHE:HZ	1.67	0.42
1:X:720:PRO:HD2	1:X:807:TYR:HD2	1.84	0.42
1:4:835:TYR:OH	1:4:856:ASN:O	2.38	0.42
1:A:438:ASN:HB2	1:A:1171:HIS:HD2	1.85	0.42
1:A:856:ASN:HB2	2:G:12:GLN:HE21	1.84	0.42
1:B:524:LEU:O	1:B:1233:SER:N	2.41	0.42
1:B:586:THR:HA	1:B:693:LYS:HD2	2.00	0.42
1:C:331:ALA:HA	1:C:335:ASP:HB2	2.01	0.42
1:D:1328:PRO:HB2	1:D:1358:ILE:HG21	2.01	0.42
1:D:455:HIS:HE2	1:D:1122:PHE:HB2	1.84	0.42
1:D:842:ASP:O	1:D:844:VAL:N	2.53	0.42
1:E:1342:MET:HA	1:E:1375:VAL:HG21	2.00	0.42
1:F:448:ASN:ND2	1:F:1113:VAL:HG12	2.34	0.42
1:F:133:ALA:N	1:F:1076:ASP:O	2.52	0.42
1:M:1366:ARG:HD2	1:M:1368:LEU:HD21	2.01	0.42
1:N:414:SER:OG	1:N:415:THR:N	2.52	0.42
1:O:850:ILE:HD11	1:O:872:VAL:HA	2.01	0.42
1:S:394:ARG:HD3	1:S:1315:PHE:HB3	2.01	0.42
1:S:851:LEU:HD22	1:S:854:LEU:HD11	2.02	0.42
1:T:1062:PHE:HB2	1:T:1087:ALA:HB3	2.01	0.42
1:U:192:LEU:HD22	1:U:251:ALA:HB1	2.02	0.42
1:U:650:PHE:HD2	1:U:660:ILE:HD11	1.85	0.42
1:V:1115:CYS:HA	1:V:1177:CYS:HB2	2.02	0.42
1:W:463:GLN:HB3	1:W:1248:VAL:HG13	2.01	0.42
3:8:125:THR:O	3:8:129:ALA:N	2.47	0.42
3:8:205:VAL:HG21	3:8:262:HIS:CE1	2.55	0.42
1:B:218:LYS:HZ3	1:B:1323:LEU:HD13	1.84	0.42
1:C:1328:PRO:HB2	1:C:1358:ILE:HG21	2.01	0.42
1:C:545:HIS:N	1:C:553:SER:O	2.40	0.42
1:E:102:HIS:CE1	1:E:106:ARG:HD2	2.55	0.42
1:F:541:ASP:N	1:F:557:THR:O	2.49	0.42
1:N:63:PHE:HZ	1:N:171:GLU:HG3	1.83	0.42
1:M:51:GLU:HB3	1:N:87:ILE:HB	2.01	0.42
1:O:842:ASP:O	1:O:844:VAL:N	2.52	0.42
1:O:831:LEU:HD22	2:R:9:PRO:HG2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:110:LYS:HZ3	1:X:128:GLU:HB3	1.82	0.42
1:S:1344:ASN:ND2	1:S:1347:THR:OG1	2.52	0.42
1:S:612:PHE:HD1	1:S:862:ILE:HG22	1.84	0.42
1:S:698:GLU:OE2	1:S:1135:TYR:OH	2.32	0.42
1:U:773:ILE:O	1:U:776:THR:OG1	2.36	0.42
1:W:457:ARG:HH22	1:W:463:GLN:HB2	1.85	0.42
1:W:539:PHE:O	1:W:559:ARG:N	2.45	0.42
1:X:1339:ASP:O	1:X:1343:SER:N	2.49	0.42
1:X:829:VAL:O	1:X:832:THR:OG1	2.31	0.42
1:X:987:TYR:O	1:X:992:LYS:NZ	2.49	0.42
1:4:402:PHE:O	1:4:1040:VAL:N	2.52	0.42
4:6:146:HIS:O	4:6:150:GLN:N	2.40	0.42
1:T:107:ARG:HA	4:6:37:HIS:CE1	2.54	0.42
1:A:1115:CYS:HA	1:A:1177:CYS:HB2	2.01	0.42
1:A:1116:GLN:HE21	1:A:1262:MET:HG3	1.84	0.42
1:A:70:ALA:HB3	1:A:377:GLU:HG2	1.99	0.42
1:A:457:ARG:HH22	1:A:463:GLN:HB2	1.84	0.42
1:A:591:VAL:HG12	1:A:679:LYS:HG2	2.02	0.42
1:A:898:ARG:HD3	1:A:902:GLN:HG3	2.01	0.42
1:B:472:PHE:HB3	1:B:475:PRO:HG3	2.02	0.42
1:E:717:LEU:HB2	1:E:990:TRP:CZ3	2.53	0.42
1:E:658:ARG:NH2	1:F:929:ASP:OD2	2.52	0.42
1:M:842:ASP:O	1:M:844:VAL:N	2.52	0.42
1:N:278:THR:HG22	1:N:1051:ILE:HG12	2.02	0.42
1:N:539:PHE:O	1:N:559:ARG:N	2.46	0.42
1:N:717:LEU:HD12	1:N:915:GLN:HE22	1.85	0.42
1:U:394:ARG:HD3	1:U:1315:PHE:HB3	2.00	0.42
1:V:709:VAL:HG13	1:V:1023:SER:HA	2.00	0.42
1:W:819:MET:N	1:W:950:ASP:OD2	2.46	0.42
1:X:958:HIS:HE1	1:X:960:LEU:HB3	1.84	0.42
4:6:160:LYS:NZ	4:7:228:ALA:O	2.43	0.42
1:B:422:VAL:O	1:B:424:SER:N	2.53	0.42
1:F:129:ILE:HD11	1:F:1082:ILE:HD11	2.01	0.42
1:F:687:LEU:HD23	1:F:805:LEU:HB3	2.02	0.42
1:N:674:HIS:HA	1:N:677:TYR:HD2	1.85	0.42
1:N:9:PRO:HB3	1:N:45:GLU:HB3	2.02	0.42
1:S:133:ALA:HA	1:S:136:ILE:HD12	2.00	0.42
1:S:413:TYR:HA	1:X:421:GLY:HA3	2.01	0.42
1:T:505:ASN:OD1	1:T:506:VAL:N	2.53	0.42
1:U:1334:HIS:HB2	1:U:1355:GLN:HG2	2.02	0.42
1:U:539:PHE:O	1:U:559:ARG:N	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:328:GLN:HG2	1:X:349:ALA:HB1	2.02	0.42
1:B:191:ILE:HA	1:B:217:PHE:HE1	1.85	0.42
1:A:165:PHE:HE1	1:B:98:PRO:HA	1.85	0.42
1:C:1188:VAL:HG12	1:C:1192:GLN:HE22	1.83	0.42
1:E:1169:LEU:O	1:F:1206:SER:OG	2.31	0.42
1:E:861:ASP:HA	1:E:864:GLN:HB2	2.02	0.42
1:F:856:ASN:ND2	2:L:12:GLN:HE21	2.17	0.42
1:N:697:HIS:HB2	1:O:509:VAL:HG21	2.02	0.42
1:S:18:ASN:OD1	1:S:19:LEU:N	2.53	0.42
1:T:78:THR:OG1	1:T:1061:MET:O	2.32	0.42
1:T:980:PRO:HD2	1:T:983:LEU:HD12	2.02	0.42
1:T:1170:SER:OG	1:U:1227:PRO:O	2.31	0.42
1:V:1200:ARG:HG3	1:V:1234:THR:HG23	2.02	0.42
1:W:452:SER:HB3	1:W:1118:LEU:H	1.85	0.42
1:4:685:ILE:HA	1:4:688:GLU:HG2	2.01	0.42
4:6:209:MET:HG2	4:7:241:PHE:HE2	1.85	0.42
3:8:227:TYR:HD2	3:8:255:VAL:HG11	1.85	0.42
4:9:224:ARG:NH2	4:9:255:ASP:O	2.53	0.42
1:A:1169:LEU:HD12	1:B:211:SER:HB2	2.01	0.42
1:C:623:GLN:OE1	1:C:724:HIS:NE2	2.40	0.42
1:D:130:GLU:HG2	1:D:1079:THR:HG22	2.01	0.42
1:D:820:CYS:O	1:D:924:ALA:N	2.53	0.42
1:E:538:PRO:HD3	1:E:1238:TRP:NE1	2.35	0.42
1:E:509:VAL:HG22	1:E:976:VAL:HG13	2.02	0.42
1:F:537:HIS:HA	1:F:1238:TRP:HE1	1.85	0.42
1:N:214:VAL:HA	1:N:217:PHE:CD2	2.55	0.42
1:O:102:HIS:CE1	1:O:106:ARG:HD2	2.55	0.42
1:N:1169:LEU:HD12	1:O:211:SER:HB2	2.02	0.42
1:O:777:ARG:HG2	1:O:782:HIS:CE1	2.55	0.42
1:S:537:HIS:HB3	1:S:1245:LEU:HB2	2.02	0.42
1:U:861:ASP:HB3	1:U:931:SER:HB2	2.01	0.42
1:W:1341:TYR:HB2	1:W:1357:LEU:HD11	2.00	0.42
1:W:455:HIS:CE1	1:W:1122:PHE:HB2	2.55	0.42
1:W:78:THR:HG22	1:W:304:ALA:HB3	2.01	0.42
1:X:1163:CYS:SG	1:X:1164:GLU:N	2.93	0.42
1:B:278:THR:HG22	1:B:1051:ILE:HG12	2.01	0.42
1:C:236:ARG:HD2	1:C:239:GLN:HB3	2.02	0.42
1:C:811:MET:O	1:C:815:SER:OG	2.36	0.42
1:E:780:GLU:HB3	1:E:785:ARG:HH12	1.85	0.42
1:N:744:ASP:H	1:N:786:HIS:CE1	2.38	0.42
1:S:945:ASN:OD1	1:S:946:LYS:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:890:GLN:HB2	1:T:919:VAL:HB	2.01	0.42
1:U:1250:TYR:HB2	1:U:1270:PHE:HD2	1.83	0.42
1:U:455:HIS:HE2	1:U:1122:PHE:HB2	1.85	0.42
1:V:1109:THR:HG23	1:V:1173:GLN:HB3	2.02	0.42
1:V:80:PHE:HE2	1:V:83:LEU:HD12	1.84	0.42
1:W:438:ASN:HD22	1:W:1171:HIS:CD2	2.34	0.42
1:X:1044:ASP:HA	1:X:1109:THR:HB	2.02	0.42
2:Y:33:GLN:NE2	2:Y:36:MET:O	2.46	0.42
1:4:1073:VAL:HG22	1:4:1079:THR:H	1.84	0.41
3:5:224:VAL:HB	3:5:296:PHE:HB2	2.02	0.41
4:9:88:ASP:HB2	4:9:91:ASP:HB2	2.01	0.41
1:A:401:PHE:N	1:A:1327:TYR:O	2.43	0.41
1:A:649:ALA:O	1:A:677:TYR:OH	2.30	0.41
1:C:591:VAL:N	1:C:683:GLU:OE1	2.52	0.41
1:C:845:ASN:N	1:C:848:ASP:OD2	2.51	0.41
1:D:1295:GLY:H	1:D:1321:HIS:HE1	1.67	0.41
1:E:10:PHE:HB2	1:E:12:TYR:HE1	1.85	0.41
1:E:455:HIS:CE1	1:E:1122:PHE:HB2	2.54	0.41
1:E:538:PRO:HB2	1:E:565:ILE:HG12	2.02	0.41
1:E:918:LEU:HD13	1:E:944:PHE:HZ	1.84	0.41
1:F:177:THR:O	1:F:181:VAL:N	2.48	0.41
1:F:511:ASP:H	1:F:987:TYR:HH	1.67	0.41
1:F:958:HIS:CE1	1:F:960:LEU:HB3	2.55	0.41
2:H:33:GLN:NE2	2:H:36:MET:O	2.46	0.41
1:M:1188:VAL:HG12	1:M:1192:GLN:HE22	1.84	0.41
1:M:273:ALA:HB3	1:M:372:LYS:HB3	2.01	0.41
1:O:1116:GLN:HE21	1:O:1121:ILE:HD11	1.84	0.41
1:O:1225:PRO:HB2	1:O:1230:GLU:HA	2.01	0.41
1:O:76:VAL:O	1:O:1061:MET:N	2.50	0.41
1:S:402:PHE:HD2	1:S:1040:VAL:HB	1.85	0.41
1:S:623:GLN:HB2	1:S:626:LYS:HB2	2.02	0.41
1:U:138:LEU:HD21	1:U:151:GLU:HG3	2.02	0.41
1:U:826:TYR:HA	1:U:829:VAL:HG23	2.02	0.41
1:V:102:HIS:HE1	1:V:106:ARG:HD2	1.84	0.41
1:W:1214:SER:HA	1:W:1217:ARG:HD3	2.01	0.41
1:W:434:VAL:HG11	1:W:1042:ARG:HH22	1.85	0.41
1:X:582:PHE:HE1	1:X:694:LEU:HD11	1.85	0.41
1:4:124:HIS:HA	1:4:1085:GLU:HG2	2.00	0.41
1:A:92:GLN:HE22	1:A:115:ILE:HG23	1.84	0.41
1:A:851:LEU:HD23	1:A:851:LEU:HA	1.88	0.41
1:B:133:ALA:HB2	1:B:1076:ASP:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:11:PRO:HB2	1:N:332:ARG:HG2	2.01	0.41
1:F:718:LEU:HD12	1:F:894:VAL:HG21	2.02	0.41
1:M:591:VAL:N	1:M:683:GLU:OE1	2.52	0.41
1:O:1294:ALA:HB1	1:O:1321:HIS:HE1	1.85	0.41
1:O:394:ARG:HB2	1:O:1050:HIS:NE2	2.35	0.41
1:S:1210:TYR:HE1	1:S:1280:ARG:HG2	1.84	0.41
1:S:170:LEU:HD11	1:S:1084:HIS:HB2	2.01	0.41
1:S:512:VAL:HG12	1:S:993:SER:HB3	2.01	0.41
1:U:468:LEU:HD13	1:U:1243:GLY:HA3	2.02	0.41
1:V:963:ASN:HA	1:V:966:THR:HG22	2.02	0.41
1:W:1200:ARG:HG2	1:W:1226:ASP:OD2	2.20	0.41
1:X:946:LYS:HE2	1:X:993:SER:HA	2.02	0.41
3:5:111:LEU:HD12	3:5:114:LEU:HD22	2.02	0.41
4:7:75:GLU:HB3	4:7:83:ARG:HD3	2.03	0.41
1:A:181:VAL:HG22	1:A:184:ARG:HD2	2.01	0.41
1:C:256:THR:HA	1:C:1092:ALA:HB2	2.02	0.41
1:D:95:ILE:HB	1:D:114:TYR:HB2	2.01	0.41
1:D:191:ILE:HA	1:D:217:PHE:CE1	2.55	0.41
1:E:1178:GLU:OE2	1:E:1265:PRO:HD2	2.20	0.41
1:E:538:PRO:HA	1:E:559:ARG:NH1	2.35	0.41
1:M:446:TYR:O	1:M:450:LEU:N	2.53	0.41
1:N:1067:SER:OG	1:N:1083:THR:OG1	2.35	0.41
1:N:1167:PRO:HD3	1:O:1224:ILE:HD13	2.01	0.41
1:N:205:LEU:HD13	1:N:1282:LEU:HD22	2.01	0.41
1:N:63:PHE:HE2	1:N:65:LYS:HE2	1.85	0.41
1:N:692:LEU:HA	1:N:692:LEU:HD23	1.84	0.41
1:N:845:ASN:N	1:N:848:ASP:OD2	2.47	0.41
1:O:1067:SER:OG	1:O:1083:THR:OG1	2.38	0.41
1:O:1198:ARG:NH1	1:O:1200:ARG:O	2.54	0.41
1:O:1251:ASN:ND2	1:O:1271:HIS:HA	2.35	0.41
1:O:759:LEU:HD22	1:O:792:PRO:HB3	2.03	0.41
1:S:1071:ARG:HH22	4:6:38:ARG:N	2.18	0.41
1:T:1264:SER:HB2	1:T:1267:ARG:HB2	2.01	0.41
1:U:76:VAL:HB	1:U:1060:SER:HA	2.02	0.41
1:U:396:ILE:HD11	1:U:1050:HIS:CE1	2.55	0.41
1:V:1216:GLU:OE2	1:V:1242:ARG:NH2	2.53	0.41
1:V:284:ARG:O	1:V:288:ASN:ND2	2.54	0.41
1:V:582:PHE:HE1	1:V:694:LEU:HD11	1.85	0.41
1:W:736:ARG:HH22	1:W:899:ASP:HA	1.84	0.41
1:4:461:PRO:HB2	1:4:542:PHE:HE1	1.86	0.41
4:6:219:PRO:HA	4:6:265:ARG:HH11	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:8:228:ALA:HB2	3:8:291:LEU:HD11	2.02	0.41
1:A:1334:HIS:CD2	1:A:1335:ARG:H	2.38	0.41
1:A:1170:SER:OG	1:B:1227:PRO:O	2.32	0.41
1:C:396:ILE:HD11	1:C:1050:HIS:HE1	1.85	0.41
1:D:402:PHE:O	1:D:1040:VAL:N	2.48	0.41
1:D:957:LEU:HA	1:D:957:LEU:HD23	1.87	0.41
1:M:845:ASN:HB3	1:M:846:ALA:H	1.66	0.41
1:M:737:GLN:HB3	1:M:897:LYS:HE2	2.01	0.41
1:N:799:ASN:HD21	1:N:802:LEU:HG	1.86	0.41
1:S:191:ILE:HA	1:S:217:PHE:HE1	1.84	0.41
1:S:851:LEU:HD23	1:S:854:LEU:HD21	2.02	0.41
1:U:1200:ARG:HG3	1:U:1234:THR:HG23	2.01	0.41
1:V:252:VAL:HG11	1:V:1055:SER:HB3	2.02	0.41
1:X:831:LEU:HD22	2:3:9:PRO:HG2	2.03	0.41
1:A:454:CYS:O	1:A:1127:TYR:OH	2.31	0.41
1:A:509:VAL:HG22	1:A:976:VAL:HG13	2.03	0.41
1:B:1236:ASN:HB2	1:B:1238:TRP:HE3	1.86	0.41
1:B:457:ARG:HH22	1:B:463:GLN:HB3	1.84	0.41
1:B:796:ASN:OD1	1:C:932:ARG:NH1	2.54	0.41
1:D:78:THR:OG1	1:D:1061:MET:O	2.30	0.41
1:D:740:ILE:HB	1:D:747:TYR:HB3	2.02	0.41
1:E:1341:TYR:HA	1:E:1348:HIS:CD2	2.56	0.41
2:J:33:GLN:NE2	2:J:36:MET:O	2.46	0.41
1:M:1020:SER:O	1:M:1023:SER:OG	2.35	0.41
1:M:1335:ARG:HH22	1:M:1370:LEU:HD11	1.86	0.41
1:M:402:PHE:HZ	1:M:432:THR:HG1	1.68	0.41
1:M:868:ILE:HG22	1:M:870:PRO:HD3	2.02	0.41
1:M:958:HIS:CE1	1:M:960:LEU:HB3	2.56	0.41
1:N:422:VAL:H	1:N:422:VAL:HG23	1.62	0.41
1:O:736:ARG:HA	1:O:736:ARG:HD3	1.86	0.41
1:T:1199:GLY:H	1:T:1240:SER:HG	1.68	0.41
1:U:1210:TYR:CE1	1:U:1280:ARG:HG2	2.55	0.41
1:U:712:LEU:HD23	1:U:712:LEU:HA	1.88	0.41
1:U:73:ALA:O	1:U:1057:ALA:N	2.45	0.41
1:X:245:LEU:HD22	1:X:369:ILE:HD13	2.01	0.41
2:2:33:GLN:NE2	2:2:36:MET:O	2.46	0.41
1:A:608:ALA:HA	1:A:928:ALA:HB2	2.02	0.41
1:C:1115:CYS:HA	1:C:1177:CYS:HB2	2.03	0.41
1:C:1251:ASN:HD21	1:C:1270:PHE:C	2.24	0.41
1:D:1312:THR:OG1	1:D:1313:ASP:N	2.53	0.41
1:D:290:LEU:HB3	1:D:367:VAL:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:826:TYR:CE2	1:E:886:PRO:HG2	2.55	0.41
1:F:946:LYS:HE2	1:F:993:SER:HA	2.01	0.41
1:M:532:LEU:O	1:M:1241:GLN:NE2	2.53	0.41
1:O:1109:THR:O	1:O:1111:MET:N	2.50	0.41
1:O:145:THR:HG23	1:O:148:ASP:H	1.84	0.41
1:E:45:GLU:OE1	1:T:158:THR:OG1	2.37	0.41
1:T:927:VAL:HG21	1:T:957:LEU:HD21	2.02	0.41
1:V:1341:TYR:HA	1:V:1348:HIS:HD2	1.86	0.41
1:V:684:LEU:HD23	1:V:802:LEU:HD22	2.03	0.41
1:W:172:ARG:NH1	1:W:382:MET:O	2.54	0.41
4:9:120:ARG:O	4:9:124:THR:N	2.38	0.41
1:A:211:SER:HG	1:A:1206:SER:HG	1.59	0.41
1:A:1190:TYR:HD1	1:A:1229:TYR:HE2	1.68	0.41
1:B:436:ASN:HD21	1:B:442:LEU:HG	1.86	0.41
1:C:296:ALA:H	1:C:366:LEU:HD13	1.85	0.41
1:D:1020:SER:N	1:D:1023:SER:OG	2.54	0.41
1:D:1336:VAL:HG22	1:E:413:TYR:CD2	2.56	0.41
1:E:406:LEU:HB3	1:E:407:HIS:H	1.72	0.41
1:F:675:GLY:O	1:F:679:LYS:HG2	2.20	0.41
1:M:255:ASP:OD2	1:M:1094:GLY:N	2.41	0.41
1:M:537:HIS:HA	1:M:1238:TRP:CD1	2.50	0.41
1:O:493:LEU:HB2	1:O:940:TYR:HE2	1.85	0.41
2:R:33:GLN:NE2	2:R:36:MET:O	2.46	0.41
1:U:307:VAL:HG12	1:U:309:ARG:H	1.85	0.41
1:V:945:ASN:OD1	1:V:946:LYS:N	2.54	0.41
1:X:75:CYS:HG	1:X:1059:THR:HG1	1.57	0.41
1:X:842:ASP:O	1:X:844:VAL:N	2.54	0.41
3:8:206:ASP:OD1	3:8:207:LEU:N	2.52	0.41
1:N:1070:ARG:HD3	3:8:67:GLN:HE22	1.85	0.41
1:B:512:VAL:HG12	1:B:993:SER:HB3	2.02	0.41
1:B:706:THR:HB	1:B:713:LEU:HD13	2.03	0.41
1:C:572:ARG:HH21	1:C:1002:CYS:HA	1.84	0.41
1:D:612:PHE:O	1:D:616:ILE:HD12	2.19	0.41
1:E:395:ARG:HD3	1:E:1045:GLU:HB3	2.02	0.41
1:E:83:LEU:HD21	1:E:122:LYS:HD2	2.02	0.41
1:E:153:ALA:HA	1:E:156:ILE:HG22	2.03	0.41
1:E:538:PRO:HA	1:E:559:ARG:HH11	1.85	0.41
1:M:545:HIS:ND1	1:M:555:ARG:HG2	2.36	0.41
1:N:351:ALA:HB1	1:N:354:HIS:HB2	2.03	0.41
1:N:545:HIS:CD2	1:N:555:ARG:HD3	2.55	0.41
1:O:123:HIS:HB2	1:O:1086:ILE:HB	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:76:VAL:HB	1:O:1060:SER:HA	2.03	0.41
1:T:1328:PRO:HB2	1:T:1358:ILE:HG21	2.03	0.41
1:V:130:GLU:HG3	1:W:110:LYS:HD2	2.03	0.41
1:W:1198:ARG:HH12	1:W:1200:ARG:HB2	1.85	0.41
1:V:1171:HIS:HE1	1:W:1228:ALA:HA	1.85	0.41
1:W:602:GLU:C	1:W:647:LYS:HZ3	2.24	0.41
1:4:861:ASP:O	1:4:930:ARG:NH2	2.54	0.41
3:8:81:SER:N	3:8:133:TYR:OH	2.54	0.41
1:D:127:ALA:HB3	1:D:1082:ILE:HB	2.03	0.41
1:E:1236:ASN:HB2	1:E:1238:TRP:HE3	1.85	0.41
1:E:313:LEU:HD21	1:M:150:THR:HG21	2.03	0.41
1:F:368:LYS:HG2	1:F:373:PHE:CE1	2.55	0.41
1:F:422:VAL:HG13	1:F:427:ILE:HD13	2.02	0.41
1:F:620:ILE:HG22	1:F:622:GLY:H	1.86	0.41
1:F:731:MET:HG3	1:F:747:TYR:HE2	1.85	0.41
1:M:157:LYS:HD2	1:N:338:ASN:HA	2.02	0.41
1:M:829:VAL:O	1:M:832:THR:OG1	2.30	0.41
1:N:612:PHE:O	1:N:616:ILE:HD12	2.20	0.41
1:O:83:LEU:HD22	1:O:1085:GLU:HB3	2.03	0.41
1:O:1251:ASN:HB3	1:O:1252:ILE:H	1.67	0.41
1:O:515:LYS:NZ	1:O:534:LEU:O	2.44	0.41
1:S:1178:GLU:HB3	1:S:1179:ILE:H	1.68	0.41
1:S:1341:TYR:HB2	1:S:1357:LEU:HD11	2.03	0.41
1:T:692:LEU:HA	1:T:692:LEU:HD23	1.79	0.41
1:U:1190:TYR:OH	1:U:1196:ASN:O	2.31	0.41
1:V:491:MET:HB2	1:V:783:ASP:HA	2.02	0.41
1:W:536:VAL:HG13	1:W:1244:SER:HA	2.01	0.41
1:V:165:PHE:HE1	1:W:98:PRO:HA	1.86	0.41
1:S:1003:GLN:NE2	1:X:587:ASN:OD1	2.53	0.41
1:X:839:VAL:O	2:3:57:TYR:OH	2.27	0.41
1:4:406:LEU:HD21	1:4:1191:PHE:HE2	1.85	0.41
1:4:636:LEU:HD21	1:4:871:THR:H	1.86	0.41
3:5:225:THR:OG1	3:5:248:SER:O	2.31	0.41
4:7:276:LEU:HD12	4:7:279:ILE:HD11	2.03	0.41
1:A:780:GLU:HB3	1:A:785:ARG:HH12	1.86	0.41
1:B:680:ILE:O	1:B:684:LEU:N	2.54	0.41
1:C:184:ARG:HG2	1:C:1291:ALA:HA	2.03	0.41
1:D:12:TYR:HD2	1:N:94:LYS:HD2	1.86	0.41
1:D:274:GLY:H	1:D:1056:ARG:HB2	1.86	0.41
1:D:809:VAL:HG13	1:D:1012:MET:HB2	2.03	0.41
1:D:918:LEU:HB2	1:D:944:PHE:CE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:457:ARG:HH22	1:O:1254:PHE:HB3	1.85	0.41
1:W:1108:THR:O	1:W:1173:GLN:N	2.51	0.41
1:W:436:ASN:HB3	1:W:440:VAL:H	1.86	0.41
1:X:394:ARG:HB2	1:X:1050:HIS:NE2	2.35	0.41
1:X:569:LEU:HD23	1:X:569:LEU:HA	1.87	0.41
1:4:156:ILE:HA	1:4:159:ILE:HG22	2.02	0.41
3:5:250:LYS:HA	4:6:68:LYS:HG2	2.03	0.41
1:A:185:HIS:O	1:A:1097:SER:OG	2.39	0.41
1:A:889:THR:HA	1:A:920:ASN:HB3	2.03	0.41
1:B:307:VAL:HB	1:B:309:ARG:HH11	1.86	0.41
1:B:558:HIS:CE1	1:B:902:GLN:HG3	2.56	0.41
1:B:598:ASP:O	1:B:602:GLU:N	2.41	0.41
1:B:627:PHE:HE2	1:B:663:HIS:HB2	1.87	0.41
1:B:708:LEU:HD21	1:B:1022:PRO:HG2	2.02	0.41
1:B:717:LEU:HA	1:B:915:GLN:NE2	2.35	0.41
1:D:494:PHE:HZ	2:J:6:VAL:HG22	1.86	0.41
1:E:538:PRO:HD3	1:E:1238:TRP:HE1	1.85	0.41
1:E:397:GLN:HB3	1:E:1318:GLN:HB3	2.03	0.41
1:M:61:VAL:HG11	1:N:98:PRO:HG3	2.02	0.41
1:M:793:LEU:HD12	1:M:798:TYR:HE1	1.86	0.41
1:N:146:PRO:HA	1:N:149:PHE:HD2	1.86	0.41
1:N:595:LEU:HD23	1:N:676:HIS:HE1	1.86	0.41
1:S:85:ARG:HH22	1:4:151:GLU:HB3	1.85	0.41
1:T:494:PHE:HZ	2:Z:6:VAL:HG22	1.86	0.41
1:U:436:ASN:HB3	1:U:440:VAL:H	1.86	0.41
1:U:889:THR:HB	1:U:918:LEU:HD11	2.03	0.41
1:V:1109:THR:O	1:V:1111:MET:N	2.54	0.41
1:V:1198:ARG:HB3	1:V:1240:SER:HG	1.86	0.41
1:W:736:ARG:NH2	1:W:899:ASP:OD1	2.54	0.41
1:X:1011:ALA:O	1:X:1015:MET:N	2.54	0.41
1:X:780:GLU:OE1	1:X:785:ARG:NH1	2.39	0.41
1:4:627:PHE:HE2	1:4:663:HIS:HB2	1.85	0.40
4:6:207:LEU:O	4:6:211:LEU:N	2.38	0.40
1:B:1250:TYR:CD2	1:B:1266:CYS:HB2	2.55	0.40
1:C:736:ARG:NH1	1:C:898:ARG:O	2.38	0.40
1:E:539:PHE:HE1	1:E:1019:LEU:HD22	1.85	0.40
1:E:898:ARG:HD3	1:E:902:GLN:HG3	2.03	0.40
1:F:226:PHE:HE2	1:F:1364:MET:HB3	1.86	0.40
1:M:1065:LEU:HA	1:M:1065:LEU:HD23	1.93	0.40
1:M:557:THR:HA	1:M:898:ARG:NH2	2.36	0.40
1:N:1043:THR:HG23	1:N:1265:PRO:HG3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:326:PHE:O	1:N:330:MET:N	2.54	0.40
1:O:1280:ARG:NH2	1:O:1288:GLU:OE1	2.54	0.40
1:S:898:ARG:NH1	1:S:910:GLY:O	2.53	0.40
1:T:446:TYR:O	1:T:450:LEU:N	2.54	0.40
1:T:951:PRO:O	1:T:955:ALA:N	2.50	0.40
1:U:252:VAL:HG13	1:U:1096:SER:HA	2.03	0.40
1:V:127:ALA:HB3	1:V:1082:ILE:HB	2.03	0.40
1:V:455:HIS:ND1	1:V:457:ARG:HG2	2.36	0.40
1:W:165:PHE:HE1	1:X:98:PRO:HA	1.86	0.40
1:W:518:VAL:HG13	1:W:522:ASP:HB3	2.03	0.40
1:W:712:LEU:HD22	1:W:805:LEU:HD23	2.01	0.40
1:4:469:ASN:HA	1:4:554:TYR:HE2	1.86	0.40
4:6:202:ARG:O	4:6:206:ASP:N	2.53	0.40
1:A:612:PHE:O	1:A:616:ILE:HD12	2.21	0.40
1:B:1210:TYR:HE1	1:B:1280:ARG:HG2	1.86	0.40
1:B:540:PHE:HE1	1:B:558:HIS:HD2	1.68	0.40
1:B:675:GLY:O	1:B:679:LYS:HG2	2.22	0.40
1:B:1171:HIS:CE1	1:C:1228:ALA:HA	2.54	0.40
1:C:740:ILE:HB	1:C:747:TYR:HB3	2.03	0.40
1:E:191:ILE:HA	1:E:217:PHE:HE1	1.87	0.40
1:E:394:ARG:HB2	1:E:1050:HIS:NE2	2.35	0.40
1:F:627:PHE:HE2	1:F:663:HIS:HB2	1.86	0.40
1:A:608:ALA:HB3	1:F:678:ARG:HH12	1.86	0.40
1:M:1341:TYR:HA	1:M:1348:HIS:HD2	1.87	0.40
1:M:406:LEU:HB3	1:M:407:HIS:H	1.79	0.40
1:N:847:GLN:HG2	1:N:871:THR:HG21	2.03	0.40
1:N:950:ASP:HA	1:N:951:PRO:HD3	1.92	0.40
1:O:279:THR:HB	1:O:380:GLN:HE21	1.86	0.40
1:O:562:VAL:HA	1:O:1019:LEU:HD11	2.04	0.40
1:N:856:ASN:ND2	2:P:66:GLY:O	2.55	0.40
1:S:681:LEU:HD23	1:S:681:LEU:HA	1.92	0.40
1:U:1058:SER:OG	1:U:1059:THR:N	2.54	0.40
1:U:932:ARG:O	1:U:936:GLU:N	2.54	0.40
1:U:10:PHE:HE1	1:V:318:SER:HA	1.86	0.40
1:W:854:LEU:HA	1:W:854:LEU:HD23	1.87	0.40
1:X:402:PHE:O	1:X:1040:VAL:N	2.47	0.40
1:W:831:LEU:HD22	2:2:9:PRO:HG2	2.03	0.40
1:4:794:ASP:H	1:4:798:TYR:HE1	1.68	0.40
4:7:7:ILE:HB	4:7:84:LEU:HB2	2.03	0.40
4:9:9:VAL:HG21	4:9:45:LEU:HD21	2.01	0.40
1:A:294:GLU:HB2	1:A:366:LEU:HD22	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:697:HIS:CE1	1:B:509:VAL:HG11	2.56	0.40
1:B:53:LEU:HD23	1:C:90:LYS:HB3	2.03	0.40
1:B:592:ILE:HG13	1:B:683:GLU:HG2	2.03	0.40
1:B:736:ARG:NH2	1:B:899:ASP:OD1	2.29	0.40
1:C:1281:GLY:O	1:C:1284:THR:OG1	2.26	0.40
1:C:1295:GLY:H	1:C:1321:HIS:CE1	2.38	0.40
1:C:704:PRO:HD2	1:C:707:HIS:ND1	2.37	0.40
1:D:824:VAL:H	1:D:889:THR:HG21	1.85	0.40
1:E:744:ASP:H	1:E:786:HIS:HE1	1.69	0.40
1:M:1341:TYR:HA	1:M:1348:HIS:CD2	2.56	0.40
1:N:822:MET:SD	1:N:939:PHE:HB3	2.61	0.40
1:O:191:ILE:HA	1:O:217:PHE:CE1	2.57	0.40
1:S:1366:ARG:HD2	1:S:1368:LEU:HD21	2.04	0.40
1:U:731:MET:HG2	1:U:738:PRO:HG2	2.04	0.40
1:W:459:HIS:NE2	1:W:1021:ALA:HB2	2.37	0.40
1:W:398:TYR:CZ	1:W:1363:PRO:HG3	2.56	0.40
3:5:255:VAL:O	3:5:259:ILE:N	2.42	0.40
1:A:868:ILE:HG22	1:A:870:PRO:HD3	2.03	0.40
1:B:929:ASP:OD1	1:B:932:ARG:NH2	2.55	0.40
1:C:1198:ARG:HA	1:C:1239:ALA:HB3	2.03	0.40
1:C:243:THR:O	1:C:247:ASP:N	2.49	0.40
1:C:446:TYR:O	1:C:450:LEU:N	2.55	0.40
1:C:512:VAL:HG12	1:C:993:SER:HB3	2.04	0.40
1:D:842:ASP:OD2	2:J:19:TYR:OH	2.39	0.40
1:D:979:VAL:HG11	1:D:984:MET:HB2	2.03	0.40
1:E:156:ILE:HA	1:E:159:ILE:HG22	2.03	0.40
1:E:325:ASN:HB3	1:E:328:GLN:HB3	2.04	0.40
1:E:680:ILE:O	1:E:684:LEU:N	2.50	0.40
1:E:883:LEU:HD11	2:K:55:HIS:HA	2.02	0.40
1:M:148:ASP:O	1:M:152:TYR:N	2.48	0.40
1:M:436:ASN:HB3	1:M:440:VAL:H	1.86	0.40
1:N:515:LYS:NZ	1:N:535:GLU:HG3	2.37	0.40
1:O:494:PHE:HZ	2:R:6:VAL:HG22	1.87	0.40
1:T:81:LYS:HA	1:T:81:LYS:HD3	1.89	0.40
1:W:515:LYS:NZ	1:W:534:LEU:O	2.51	0.40
1:4:400:TYR:N	1:4:1042:ARG:O	2.49	0.40
1:4:82:ASP:OD1	1:4:82:ASP:N	2.51	0.40
4:6:157:ILE:HG22	4:6:161:ILE:HD11	2.04	0.40
4:7:42:ILE:HG13	4:7:45:LEU:HD21	2.03	0.40
1:B:1166:LEU:HD13	1:B:1169:LEU:HD23	2.04	0.40
1:C:312:ASN:O	1:C:315:THR:OG1	2.30	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:669:ILE:HD13	1:C:674:HIS:HB2	2.04	0.40
1:C:695:ALA:HB1	1:C:706:THR:HG22	2.03	0.40
1:C:822:MET:SD	1:C:939:PHE:HB3	2.61	0.40
1:D:1211:SER:H	1:D:1279:ASN:HD21	1.69	0.40
1:D:380:GLN:HB3	1:D:384:ASN:ND2	2.37	0.40
1:D:702:ARG:NH1	1:D:735:SER:OG	2.54	0.40
1:D:851:LEU:HD23	1:D:854:LEU:HD11	2.03	0.40
1:D:507:ALA:HB1	1:D:978:ASN:HD22	1.87	0.40
1:E:447:GLN:NE2	1:F:521:GLU:OE1	2.53	0.40
1:F:457:ARG:HG3	1:F:1122:PHE:CD2	2.56	0.40
1:M:1200:ARG:HG3	1:M:1234:THR:HG23	2.04	0.40
1:M:539:PHE:HB3	1:M:558:HIS:CE1	2.56	0.40
1:N:1216:GLU:HG3	1:N:1220:TYR:HD2	1.86	0.40
1:M:443:CYS:N	1:N:1231:CYS:SG	2.95	0.40
1:N:859:LEU:HD23	1:N:859:LEU:HA	1.84	0.40
1:O:188:PRO:HD2	1:O:191:ILE:HD12	2.04	0.40
1:O:301:ALA:HB2	1:O:360:THR:HB	2.03	0.40
1:O:63:PHE:HE2	1:O:65:LYS:HE2	1.87	0.40
1:O:492:ASN:ND2	2:R:4:PHE:O	2.54	0.40
1:S:1001:SER:O	1:X:587:ASN:ND2	2.55	0.40
1:S:1073:VAL:HG13	1:S:1078:VAL:HG22	2.02	0.40
1:S:544:VAL:HG22	1:S:554:TYR:HE1	1.87	0.40
1:T:674:HIS:HA	1:T:677:TYR:HD2	1.86	0.40
1:U:741:LYS:HG2	1:U:746:ASN:ND2	2.37	0.40
1:V:394:ARG:HB2	1:V:1050:HIS:NE2	2.37	0.40
1:V:958:HIS:CE1	1:V:960:LEU:HB3	2.57	0.40
1:W:457:ARG:NH1	1:W:462:THR:OG1	2.48	0.40
1:W:717:LEU:HB2	1:W:990:TRP:CZ3	2.56	0.40
1:X:545:HIS:N	1:X:553:SER:O	2.51	0.40
1:X:824:VAL:HG13	1:X:939:PHE:HE1	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	4	1200/1376 (87%)	1061 (88%)	136 (11%)	3 (0%)	44	81
1	A	1359/1376 (99%)	1204 (89%)	155 (11%)	0	100	100
1	B	1351/1376 (98%)	1192 (88%)	158 (12%)	1 (0%)	55	88
1	C	1350/1376 (98%)	1200 (89%)	148 (11%)	2 (0%)	55	88
1	D	1351/1376 (98%)	1186 (88%)	163 (12%)	2 (0%)	55	88
1	E	1359/1376 (99%)	1203 (88%)	155 (11%)	1 (0%)	55	88
1	F	1352/1376 (98%)	1197 (88%)	149 (11%)	6 (0%)	38	76
1	M	1351/1376 (98%)	1185 (88%)	163 (12%)	3 (0%)	51	84
1	N	1359/1376 (99%)	1189 (88%)	168 (12%)	2 (0%)	55	88
1	O	1351/1376 (98%)	1191 (88%)	155 (12%)	5 (0%)	38	76
1	S	1273/1376 (92%)	1126 (88%)	145 (11%)	2 (0%)	51	84
1	T	1354/1376 (98%)	1195 (88%)	154 (11%)	5 (0%)	38	76
1	U	1351/1376 (98%)	1199 (89%)	150 (11%)	2 (0%)	55	88
1	V	1348/1376 (98%)	1200 (89%)	146 (11%)	2 (0%)	55	88
1	W	1350/1376 (98%)	1211 (90%)	136 (10%)	3 (0%)	51	84
1	X	1339/1376 (97%)	1198 (90%)	140 (10%)	1 (0%)	55	88
2	0	76/170 (45%)	73 (96%)	3 (4%)	0	100	100
2	1	76/170 (45%)	73 (96%)	3 (4%)	0	100	100
2	2	76/170 (45%)	73 (96%)	3 (4%)	0	100	100
2	3	76/170 (45%)	73 (96%)	3 (4%)	0	100	100
2	G	76/170 (45%)	73 (96%)	3 (4%)	0	100	100
2	H	76/170 (45%)	73 (96%)	3 (4%)	0	100	100
2	I	76/170 (45%)	73 (96%)	3 (4%)	0	100	100
2	J	76/170 (45%)	73 (96%)	3 (4%)	0	100	100
2	K	76/170 (45%)	73 (96%)	3 (4%)	0	100	100
2	L	76/170 (45%)	73 (96%)	3 (4%)	0	100	100
2	P	76/170 (45%)	73 (96%)	3 (4%)	0	100	100
2	Q	76/170 (45%)	73 (96%)	3 (4%)	0	100	100
2	R	76/170 (45%)	73 (96%)	3 (4%)	0	100	100
2	Y	76/170 (45%)	73 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	Z	76/170 (45%)	73 (96%)	3 (4%)	0	100	100
3	5	313/331 (95%)	279 (89%)	34 (11%)	0	100	100
3	8	315/331 (95%)	293 (93%)	22 (7%)	0	100	100
3	b	315/331 (95%)	288 (91%)	27 (9%)	0	100	100
3	e	311/331 (94%)	288 (93%)	23 (7%)	0	100	100
3	h	315/331 (95%)	288 (91%)	26 (8%)	1 (0%)	44	81
4	6	290/305 (95%)	263 (91%)	27 (9%)	0	100	100
4	7	296/305 (97%)	261 (88%)	35 (12%)	0	100	100
4	9	290/305 (95%)	264 (91%)	26 (9%)	0	100	100
4	a	296/305 (97%)	270 (91%)	26 (9%)	0	100	100
4	c	290/305 (95%)	265 (91%)	25 (9%)	0	100	100
4	d	296/305 (97%)	277 (94%)	19 (6%)	0	100	100
4	f	290/305 (95%)	263 (91%)	27 (9%)	0	100	100
4	g	296/305 (97%)	269 (91%)	27 (9%)	0	100	100
4	i	290/305 (95%)	264 (91%)	26 (9%)	0	100	100
4	j	296/305 (97%)	272 (92%)	24 (8%)	0	100	100
All	All	27037/29271 (92%)	24136 (89%)	2860 (11%)	41 (0%)	54	84

All (41) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	1251	ASN
1	O	144	GLU
1	T	10	PHE
1	V	1251	ASN
1	B	843	VAL
1	D	843	VAL
1	E	843	VAL
1	F	843	VAL
1	M	843	VAL
1	O	294	GLU
1	O	843	VAL
1	O	1251	ASN
1	S	843	VAL
1	T	843	VAL
1	T	945	ASN

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Mol	Chain	Res	Type
1	U	843	VAL
1	V	843	VAL
1	W	423	GLU
1	W	843	VAL
1	X	843	VAL
1	D	842	ASP
1	F	294	GLU
1	F	423	GLU
1	M	352	ASP
1	O	279	THR
1	U	1252	ILE
1	C	843	VAL
1	F	945	ASN
1	M	842	ASP
1	N	843	VAL
1	N	945	ASN
1	W	842	ASP
1	4	842	ASP
1	4	843	VAL
1	F	842	ASP
1	S	842	ASP
1	T	842	ASP
1	4	849	ASP
1	T	11	PRO
3	h	297	ASP
1	F	738	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	4	1039/1166 (89%)	1038 (100%)	1 (0%)	94	97
1	A	1155/1166 (99%)	1155 (100%)	0	100	100
1	B	1151/1166 (99%)	1150 (100%)	1 (0%)	94	97
1	C	1150/1166 (99%)	1150 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	1151/1166 (99%)	1151 (100%)	0	100	100
1	E	1155/1166 (99%)	1155 (100%)	0	100	100
1	F	1152/1166 (99%)	1151 (100%)	1 (0%)	94	97
1	M	1151/1166 (99%)	1151 (100%)	0	100	100
1	N	1155/1166 (99%)	1153 (100%)	2 (0%)	94	97
1	O	1151/1166 (99%)	1149 (100%)	2 (0%)	94	97
1	S	1094/1166 (94%)	1094 (100%)	0	100	100
1	T	1154/1166 (99%)	1153 (100%)	1 (0%)	94	97
1	U	1151/1166 (99%)	1149 (100%)	2 (0%)	94	97
1	V	1148/1166 (98%)	1146 (100%)	2 (0%)	94	97
1	W	1150/1166 (99%)	1150 (100%)	0	100	100
1	X	1143/1166 (98%)	1143 (100%)	0	100	100
2	0	70/141 (50%)	70 (100%)	0	100	100
2	1	70/141 (50%)	70 (100%)	0	100	100
2	2	70/141 (50%)	70 (100%)	0	100	100
2	3	70/141 (50%)	70 (100%)	0	100	100
2	G	70/141 (50%)	70 (100%)	0	100	100
2	H	70/141 (50%)	70 (100%)	0	100	100
2	I	70/141 (50%)	70 (100%)	0	100	100
2	J	70/141 (50%)	70 (100%)	0	100	100
2	K	70/141 (50%)	70 (100%)	0	100	100
2	L	70/141 (50%)	70 (100%)	0	100	100
2	P	70/141 (50%)	70 (100%)	0	100	100
2	Q	70/141 (50%)	70 (100%)	0	100	100
2	R	70/141 (50%)	70 (100%)	0	100	100
2	Y	70/141 (50%)	70 (100%)	0	100	100
2	Z	70/141 (50%)	70 (100%)	0	100	100
3	5	271/281 (96%)	271 (100%)	0	100	100
3	8	272/281 (97%)	272 (100%)	0	100	100
3	b	272/281 (97%)	272 (100%)	0	100	100
3	e	270/281 (96%)	270 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	h	272/281 (97%)	272 (100%)	0	100	100
4	6	267/274 (97%)	267 (100%)	0	100	100
4	7	270/274 (98%)	270 (100%)	0	100	100
4	9	267/274 (97%)	266 (100%)	1 (0%)	93	96
4	a	270/274 (98%)	270 (100%)	0	100	100
4	c	267/274 (97%)	266 (100%)	1 (0%)	93	96
4	d	270/274 (98%)	270 (100%)	0	100	100
4	f	267/274 (97%)	267 (100%)	0	100	100
4	g	270/274 (98%)	269 (100%)	1 (0%)	93	96
4	i	267/274 (97%)	267 (100%)	0	100	100
4	j	270/274 (98%)	270 (100%)	0	100	100
All	All	23342/24916 (94%)	23327 (100%)	15 (0%)	95	97

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	947	LEU
1	F	947	LEU
1	N	947	LEU
1	N	1070	ARG
1	O	1251	ASN
1	O	1255	ARG
1	T	947	LEU
1	U	84	ARG
1	U	143	LYS
1	V	143	LYS
1	V	947	LEU
1	4	947	LEU
4	9	198	ARG
4	c	234	ARG
4	g	281	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (354) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	GLN
1	A	224	HIS

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Mol	Chain	Res	Type
1	A	380	GLN
1	A	438	ASN
1	A	545	HIS
1	A	587	ASN
1	A	746	ASN
1	A	786	HIS
1	A	902	GLN
1	A	1003	GLN
1	A	1030	HIS
1	A	1103	HIS
1	A	1116	GLN
1	A	1131	GLN
1	A	1173	GLN
1	A	1222	HIS
1	A	1241	GLN
1	A	1251	ASN
1	A	1268	GLN
1	A	1334	HIS
1	A	1344	ASN
1	B	92	GLN
1	B	113	GLN
1	B	224	HIS
1	B	288	ASN
1	B	312	ASN
1	B	380	GLN
1	B	567	GLN
1	B	587	ASN
1	B	674	HIS
1	B	724	HIS
1	B	752	ASN
1	B	915	GLN
1	B	1003	GLN
1	B	1133	HIS
1	B	1171	HIS
1	B	1241	GLN
1	B	1344	ASN
1	C	113	GLN
1	C	224	HIS
1	C	463	GLN
1	C	498	HIS
1	C	630	ASN
1	C	746	ASN

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Mol	Chain	Res	Type
1	C	978	ASN
1	C	1003	GLN
1	C	1171	HIS
1	C	1196	ASN
1	C	1241	GLN
1	C	1321	HIS
1	C	1334	HIS
1	C	1344	ASN
1	D	22	GLN
1	D	224	HIS
1	D	384	ASN
1	D	387	GLN
1	D	428	GLN
1	D	438	ASN
1	D	498	HIS
1	D	567	GLN
1	D	575	GLN
1	D	746	ASN
1	D	816	ASN
1	D	1027	GLN
1	D	1103	HIS
1	D	1171	HIS
1	D	1196	ASN
1	D	1279	ASN
1	D	1334	HIS
1	E	102	HIS
1	E	224	HIS
1	E	354	HIS
1	E	428	GLN
1	E	448	ASN
1	E	463	GLN
1	E	697	HIS
1	E	716	HIS
1	E	752	ASN
1	E	786	HIS
1	E	902	GLN
1	E	971	GLN
1	E	1003	GLN
1	E	1171	HIS
1	E	1241	GLN
1	E	1251	ASN
1	E	1348	HIS

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Mol	Chain	Res	Type
1	F	92	GLN
1	F	224	HIS
1	F	312	ASN
1	F	448	ASN
1	F	459	HIS
1	F	587	ASN
1	F	674	HIS
1	F	786	HIS
1	F	902	GLN
1	F	945	ASN
1	F	1171	HIS
1	F	1241	GLN
1	F	1279	ASN
1	F	1344	ASN
2	G	12	GLN
2	J	22	HIS
2	K	12	GLN
2	K	73	HIS
2	L	12	GLN
1	M	224	HIS
1	M	312	ASN
1	M	354	HIS
1	M	380	GLN
1	M	460	ASN
1	M	498	HIS
1	M	558	HIS
1	M	587	ASN
1	M	674	HIS
1	M	978	ASN
1	M	1033	HIS
1	M	1103	HIS
1	M	1131	GLN
1	M	1171	HIS
1	M	1241	GLN
1	N	113	GLN
1	N	224	HIS
1	N	312	ASN
1	N	397	GLN
1	N	448	ASN
1	N	492	ASN
1	N	545	HIS
1	N	587	ASN

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Mol	Chain	Res	Type
1	N	674	HIS
1	N	856	ASN
1	N	902	GLN
1	N	907	HIS
1	N	915	GLN
1	N	978	ASN
1	N	1003	GLN
1	N	1017	GLN
1	N	1133	HIS
1	N	1171	HIS
1	N	1173	GLN
1	O	92	GLN
1	O	113	GLN
1	O	224	HIS
1	O	312	ASN
1	O	428	GLN
1	O	438	ASN
1	O	558	HIS
1	O	567	GLN
1	O	716	HIS
1	O	724	HIS
1	O	782	HIS
1	O	816	ASN
1	O	978	ASN
1	O	1003	GLN
1	O	1196	ASN
1	O	1241	GLN
1	O	1251	ASN
1	O	1318	GLN
1	O	1321	HIS
2	P	12	GLN
2	P	73	HIS
1	S	224	HIS
1	S	438	ASN
1	S	447	GLN
1	S	558	HIS
1	S	587	ASN
1	S	782	HIS
1	S	816	ASN
1	S	907	HIS
1	S	1003	GLN
1	S	1268	GLN

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Mol	Chain	Res	Type
1	S	1279	ASN
1	S	1334	HIS
1	S	1344	ASN
1	T	59	ASN
1	T	92	GLN
1	T	224	HIS
1	T	537	HIS
1	T	567	GLN
1	T	587	ASN
1	T	724	HIS
1	T	786	HIS
1	T	978	ASN
1	T	1003	GLN
1	T	1171	HIS
1	T	1196	ASN
1	T	1344	ASN
1	U	92	GLN
1	U	113	GLN
1	U	124	HIS
1	U	312	ASN
1	U	384	ASN
1	U	428	GLN
1	U	438	ASN
1	U	545	HIS
1	U	564	ASN
1	U	666	ASN
1	U	716	HIS
1	U	746	ASN
1	U	818	HIS
1	U	970	ASN
1	U	978	ASN
1	U	1003	GLN
1	U	1128	GLN
1	U	1131	GLN
1	U	1133	HIS
1	U	1241	GLN
1	U	1256	GLN
1	U	1321	HIS
1	U	1334	HIS
1	U	1344	ASN
1	U	1355	GLN
1	V	59	ASN

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Mol	Chain	Res	Type
1	V	102	HIS
1	V	224	HIS
1	V	288	ASN
1	V	312	ASN
1	V	397	GLN
1	V	428	GLN
1	V	438	ASN
1	V	525	HIS
1	V	746	ASN
1	V	786	HIS
1	V	818	HIS
1	V	978	ASN
1	V	1003	GLN
1	V	1171	HIS
1	V	1196	ASN
1	V	1222	HIS
1	V	1241	GLN
1	V	1334	HIS
1	W	92	GLN
1	W	102	HIS
1	W	113	GLN
1	W	123	HIS
1	W	224	HIS
1	W	428	GLN
1	W	438	ASN
1	W	463	GLN
1	W	498	HIS
1	W	558	HIS
1	W	587	ASN
1	W	724	HIS
1	W	746	ASN
1	W	786	HIS
1	W	818	HIS
1	W	902	GLN
1	W	970	ASN
1	W	978	ASN
1	W	1003	GLN
1	W	1033	HIS
1	W	1103	HIS
1	W	1131	GLN
1	W	1196	ASN
1	W	1251	ASN

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Mol	Chain	Res	Type
1	W	1344	ASN
1	X	18	ASN
1	X	113	GLN
1	X	224	HIS
1	X	288	ASN
1	X	312	ASN
1	X	354	HIS
1	X	380	GLN
1	X	387	GLN
1	X	428	GLN
1	X	438	ASN
1	X	499	GLN
1	X	567	GLN
1	X	587	ASN
1	X	630	ASN
1	X	666	ASN
1	X	907	HIS
1	X	1003	GLN
1	X	1050	HIS
1	X	1084	HIS
1	X	1131	GLN
1	X	1268	GLN
1	X	1318	GLN
1	X	1321	HIS
1	X	1334	HIS
1	X	1344	ASN
2	Y	47	HIS
2	Z	12	GLN
2	0	12	GLN
2	1	12	GLN
2	1	55	HIS
2	1	73	HIS
2	2	73	HIS
2	3	55	HIS
1	4	380	GLN
1	4	397	GLN
1	4	498	HIS
1	4	514	GLN
1	4	567	GLN
1	4	581	GLN
1	4	590	HIS
1	4	630	ASN

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Mol	Chain	Res	Type
1	4	674	HIS
1	4	689	GLN
1	4	786	HIS
1	4	907	HIS
1	4	920	ASN
1	4	978	ASN
1	4	1033	HIS
1	4	1084	HIS
3	5	262	HIS
4	6	37	HIS
4	6	110	GLN
4	6	146	HIS
4	7	94	GLN
4	7	150	GLN
3	8	262	HIS
3	8	299	HIS
4	9	37	HIS
4	9	41	ASN
4	9	104	GLN
4	9	130	ASN
4	9	150	GLN
4	a	146	HIS
3	b	262	HIS
4	c	40	GLN
4	c	110	GLN
4	c	130	ASN
4	c	146	HIS
4	c	150	GLN
4	c	151	GLN
4	c	281	ASN
4	d	41	ASN
4	d	104	GLN
4	d	146	HIS
4	d	156	HIS
4	d	232	HIS
3	e	98	ASN
3	e	262	HIS
4	f	37	HIS
4	f	40	GLN
4	f	104	GLN
4	f	110	GLN
4	f	130	ASN

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Mol	Chain	Res	Type
4	f	150	GLN
4	f	151	GLN
4	f	281	ASN
4	g	37	HIS
4	g	150	GLN
4	g	156	HIS
4	g	256	GLN
4	g	281	ASN
4	i	40	GLN
4	i	104	GLN
4	i	110	GLN
4	i	130	ASN
4	i	146	HIS
4	i	150	GLN
4	i	281	ASN
4	j	150	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	F	1
1	N	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	N	9:PRO	C	10:PHE	N	1.20
1	F	454:CYS	C	455:HIS	N	1.17