



wwPDB EM Map/Model Validation Report ⓘ

Jun 14, 2016 – 12:26 PM EDT

PDB ID : 5IYA
EMDB ID: : EMD-8135
Title : Human core-PIC in the closed state
Authors : He, Y.; Yan, C.; Fang, J.; Inouye, C.; Tjian, R.; Ivanov, I.; Nogales, E.
Deposited on : 2016-03-24
Resolution : 5.40 Å(reported)
Based on PDB ID : ?

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027790

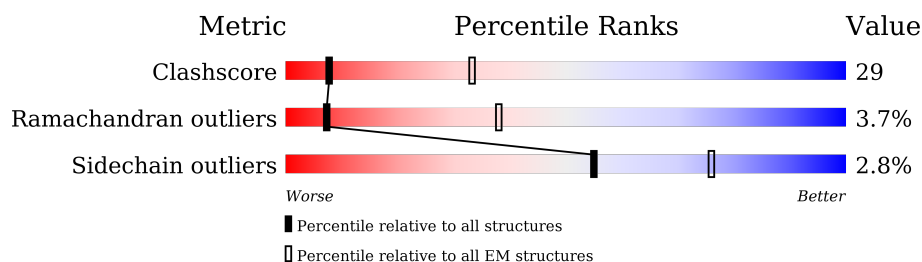
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.40 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	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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

Mol	Chain	Length	Quality of chain
1	A	1970	41% 30% .. 26%
2	B	1174	50% 46% . .
3	C	275	47% 50% .
4	D	142	65% 25% 9%
5	E	210	52% 46% .
6	F	127	35% 31% . 32%
7	G	172	65% 32% ..
8	H	150	44% 47% 7% .
9	I	125	39% 53% 8%

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Mol	Chain	Length	Quality of chain
10	J	67	
11	K	117	
12	L	58	
13	M	316	
14	N	376	
15	O	109	
16	P	339	
17	Q	439	
18	R	291	
19	S	517	
20	T	249	
21	U	301	
22	X	59	
23	Y	59	

2 Entry composition

There are 25 unique types of molecules in this entry. The entry contains 46697 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 DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1454	Total	C	N	O	S	0	0
			11515	7234	2058	2150	73		

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1165	Total	C	N	O	S	0	0
			9317	5878	1637	1738	64		

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	275	Total	C	N	O	S	0	0
			2213	1386	380	440	7		

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	129	Total	C	N	O	S	0	0
			1062	665	179	214	4		

- Molecule 5 is a protein called DNA-directed RNA polymerase II subunit RPB5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	210	Total	C	N	O	S	0	0
			1723	1088	301	325	9		

- Molecule 6 is a protein called DNA-directed RNA polymerase II subunit RPB6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	86	Total	C	N	O	S	0	0
			689	437	120	127	5		

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	171	Total	C	N	O	S	0	0
			1351	875	219	249	8		

- Molecule 8 is a protein called DNA-directed RNA polymerase II subunit RPB8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	150	Total	C	N	O	S	0	0
			1205	764	196	239	6		

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	125	Total	C	N	O	S	0	0
			1013	626	177	198	12		

- Molecule 10 is a protein called DNA-directed RNA polymerase II subunit RPB10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	67	Total	C	N	O	S	0	0
			533	345	90	92	6		

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB11-a.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	117	Total	C	N	O	S	0	0
			937	604	154	177	2		

- Molecule 12 is a protein called DNA-directed RNA polymerase II subunit RPB12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	46	Total	C	N	O	S	0	0
			388	241	75	66	6		

- Molecule 13 is a protein called Transcription initiation factor IIB.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	260	Total	C	N	O	S	0	0
			2018	1265	360	376	17		

- Molecule 14 is a protein called Transcription initiation factor IIA subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	113	Total	C	N	O	S	0	0
			930	585	152	189	4		

- Molecule 15 is a protein called Transcription initiation factor IIA subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	99	Total	C	N	O	S	0	0
			806	510	142	151	3		

- Molecule 16 is a protein called TATA-box-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	185	Total	C	N	O	S	0	0
			1462	946	257	252	7		

- Molecule 17 is a protein called General transcription factor IIE subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	180	Total	C	N	O	S	0	0
			1484	938	262	273	11		

- Molecule 18 is a protein called Transcription initiation factor IIE subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	165	Total	C	N	O	S	0	0
			1357	865	235	253	4		

- Molecule 19 is a protein called General transcription factor IIF subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	138	Total	C	N	O	S	0	0
			1137	719	207	208	3		

- Molecule 20 is a protein called General transcription factor IIF subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	222	Total	C	N	O	S	0	0
			1788	1127	320	338	3		

- Molecule 21 is a protein called Transcription elongation factor A protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	170	Total	C	N	O	S	0	0
			1343	818	247	263	15		

- Molecule 22 is a DNA chain called SCP-X.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	X	59	Total	C	N	O	P	0	0
			1218	575	235	350	58		

- Molecule 23 is a DNA chain called SCP-Y.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Y	59	Total	C	N	O	P	0	0
			1195	568	215	354	58		

- Molecule 24 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
24	B	1	Total	Mg	0
			1	1	
24	A	1	Total	Mg	0
			1	1	

- Molecule 25 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
25	J	1	Total	Zn	0
			1	1	
25	Q	1	Total	Zn	0
			1	1	
25	B	1	Total	Zn	0
			1	1	
25	I	2	Total	Zn	0
			2	2	
25	C	1	Total	Zn	0
			1	1	
25	A	2	Total	Zn	0
			2	2	
25	U	1	Total	Zn	0
			1	1	
25	L	1	Total	Zn	0
			1	1	

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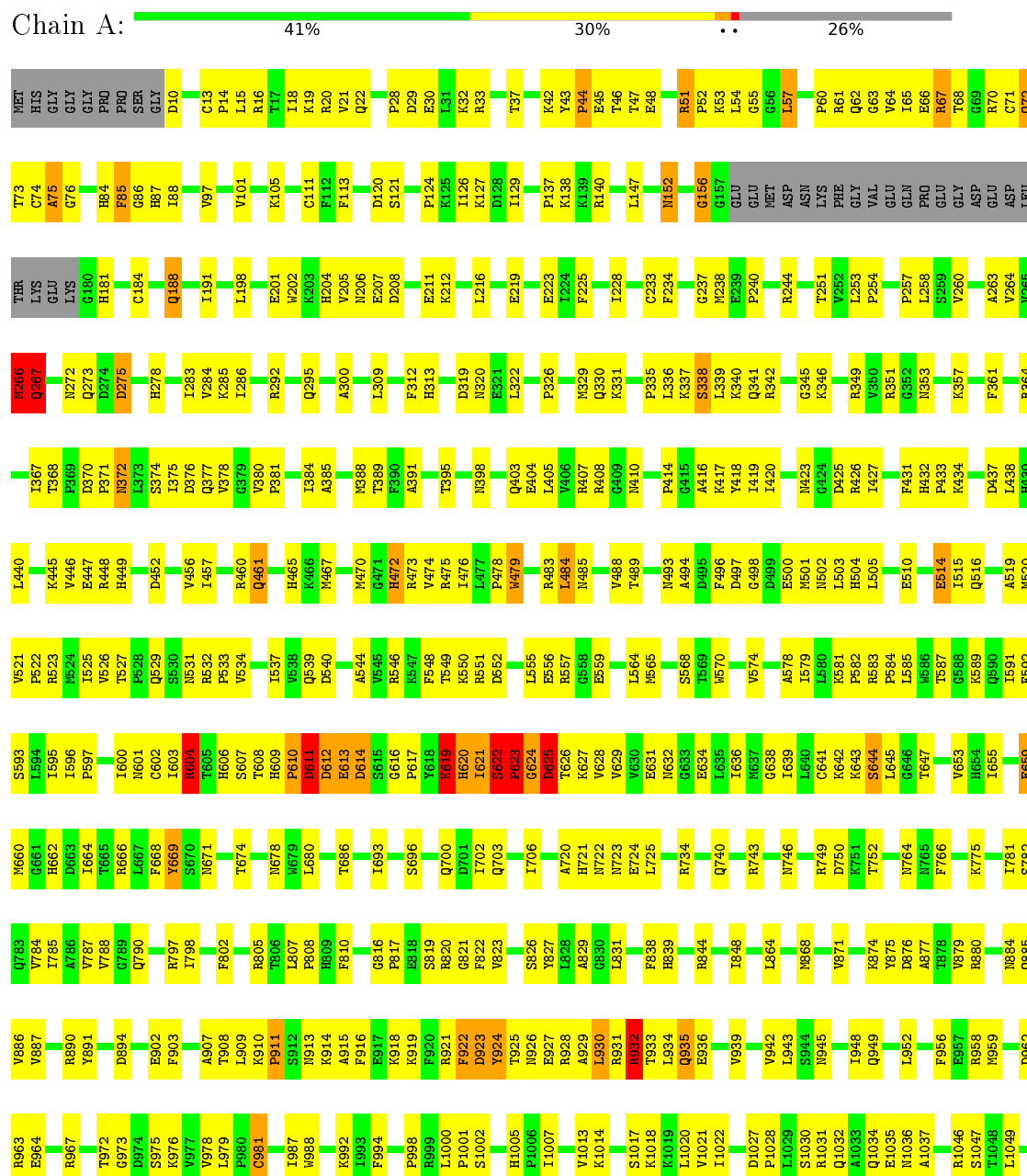
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Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
25	M	1	1	1	0

3 Residue-property plots

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

- Molecule 1: DNA-directed RNA polymerase II subunit RPB1





I152	E79	Met
P153	E80	Tyr
I154	P81	Asp
M155	P82	Ala
L156	R83	Asp
R157	Y84	Glu
	L85	Asp
Y160	L86	Met
C161	K87	Glu
M164	R88	Y10
G165	R89	D11
L166	Q90	E12
	I91	
	Y92	
R169	L93	L21
D170	S94	W22
L171		Q23
C172		E24
E173	T97	A25
L174	R98	C26
M175	W99	W27
E176	I100	I28
	R101	V29
	D102	I30
P181		
G182	P107	E36
G183	M108	K37
Y184	M109	
G189	E112	V40
		R41
		Q42
K192	R116	
V193	N117	S46
L194		
E198	Y120	F50
	S121	I51
A201	A122	Q52
	P123	M53
	L124	S54
V205	Y125	V55
	V126	Q56
A209	D127	R57
K210	I128	
R211	I129	E60
A216	K130	D61
	T131	A62
R222	V132	P63
S223	I133	P64
C224	K134	I65
L225	K135	D66
E226	G136	L67
N227	E137	Q68
S228	I138	A69
S229	Q139	F70
R230	L140	A71
P231	Q141	W72
T232	Q145	H73
		A74
W236	F148	E77
		H78

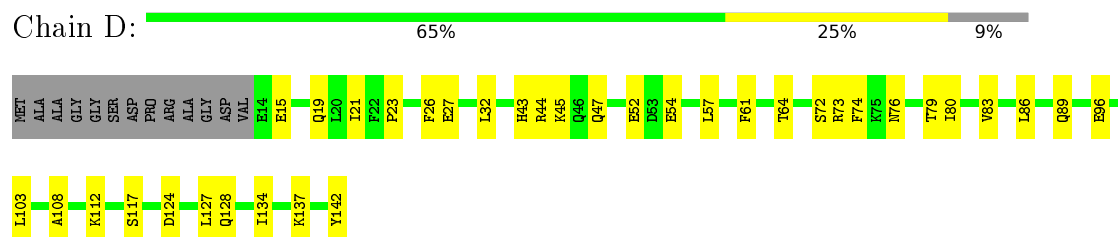
N239	E429	L501	1596	D666	V759	R834	T901	P1074	I1146
L240	N430	H502	1697	E669	T760	E835	G902	M1075	S1147
A241	L431	H505	V598	E670	T761	T836	D905	M1076	L1148
R242	E432	L506	S599	E671	T762	R837	D906	S1079	P1152
G243	L433	V509	E600	T672	T763	G838	T910	D1081	P1153
G244	A434	H509	V601	T673	T764	R840	T911	G1082	L1158
Q245	L435	A512	S602	T674	T765	R841	G915	G1083	M1163
	R438	E513	V603	T675	T766	H842	Y916	L1084	M1167
K248	L439	H519	1604	A676	T767	Y845	T921	F1085	R1170
K249	I440	V520	1607		T768		R922	G1086	
A251	S441	H521	R608	L682	P773	L848	G923	E1090	R1171
G253	D442	L522	E609	Q683	T776	D849	V924	C1093	M1172
Q254	K445	V523	R610	E684	T777	D850	R927	Q1094	S1173
R255	Y446	K524	E611	K695	T778	D851	T928	H1098	V1174
R256	Y446	N525	R612	E697	T779	G852	P929	G1099	
V257	G451	L526	R613	I698	T780	P856	G932	H1098	
A258	V452	A527	V615	T692			D933	G1099	
T259	N453	A530	R620	H695	Y788	V860	R934	A1100	
K264	G454	Y531	1621	C696	T789	G861	T935	Q1101	
P268	D455	S539	C622	I698	T790	G862	A936	A1102	
T269	K457		R623		T791	D863	G945	F1103	
L270	V458	L542	1626	I711	T792	D864	G946	L1103	
L271	H460	E543	1627	P712	T795	V865	R939	R1106	
V272	L472	F544	V628	P713	T796	R866	T942	L1107	
R273	L372	L545	R629	P714	T797	G868	G943	L1108	
R274	L373	E546	R630	P715	T798	K869	T944	A1110	
A275	L374	P547	R631	D716	T799	T870	G945	S1111	
L276	V466	N548	R632	T717	T800		G946	D1112	
G277	S467	S549	R633	P718	T801	L873	T947	P1113	
F278	N471	E550	L634	P719	T802	P874	Q1040	Q1114	
V279	L473	N552	L635	R720	T803	R875	I1041	V1115	
S280	L474	L553		R721	T804	N876	P1045	V1116	
D281	T474	E554	R638	T722	T805	R877	T1046	H1117	
	S477	E556	H639	T723	T806	R878	T1047	V1118	
L284		I556	1640	M728	T807	E879	Y1048	C1119	
L289	H481	I561	L643	G729	T808	L880	Y1049	G1123	
D291	R483	A562	R646	K730	T809	R881	Q1050	I1124	
D294	R485	K566	R649	Y736	T810	R882	L1051	M1125	
P295	L486	F568	R650	T737	T811	R883	K1052	A1126	
E299	J486	S487	R651	T738	T812	R884	H1053		
K300	P488	S652	R652	N739	T813	R885	D1056	N1129	
V301	I489	K573	R653	T740	T814	R886	D1057	T1130	
K302	G490	V574	Q654	R743	T815	R887	K1058	R1131	
P303	R491	G575	D655	T746	T816	R888	S1061	T1132	
E307	C493	I576	A658		T817	R889	R1062	H1133	
A308	L495	L583	S659	L751	T818	R890	R1063	T1134	
F309	L496	R588	G660	Y752	T819	D891	A1063	Y1135	
	K497	R591	V661	Y753	T820	S892	N976	C1136	
Q312	P498	R592	V662	Y754	T821	R893	G979	R1138	
D428	R499	R592	V663	Y755	T822	D894	R980	G1139	
	R499	R592	V664	Y756	T823	R895	T981		
	Q500		1665	L758	T833	R897	T982	N1142	
						T898	Q1068	Q1145	
						E900	R1072		
							Q1073		

• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

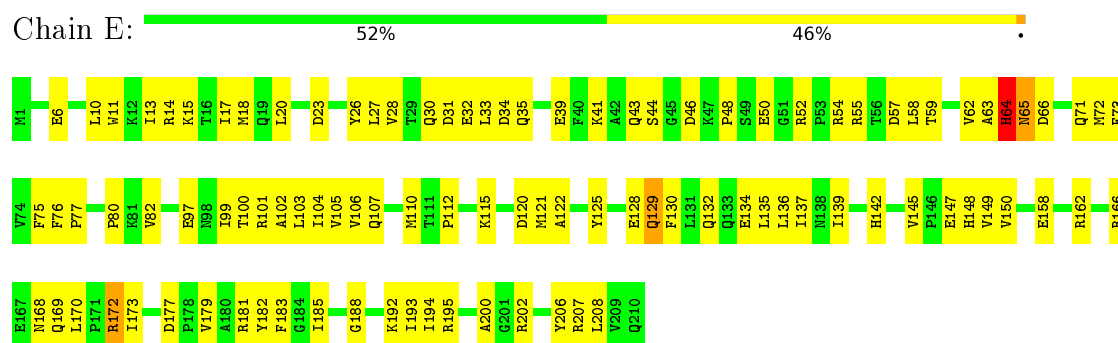
Chain C:  47% 50%

M1	I74	V151	N223	
P2	S76	K152	R228	
Y3	D76	K155		
A4	D77			
N6	I78	E158	Y231	
P7	V79	L159	V232	
T8	D80	R160	V233	
V9	K81	L161	E234	
R10	L82	L162	S235	
I11	T89	A163		
T12	Q90	Y164	S238	
E13	E91	A165	L239	
L14		K166	R240	
T15	C94	K167	P241	
D16				
V19	S98	G170	T244	
K20	V99	K171	A248	
F21	E100	H172	K283	
I22	F101	H173	D258	
I23	V105	M176	Q262	
E24	R106	P177	E266	
N25	C107	T178		
T26	M108	T179		
D27	E109			
V30	D110	A183	D270	
S33	R113	F184		
I34	H114	E185		
R35	V115	Y186		
R36	S117			
V37	L120	D189		
F38	I121	N190		
A40		R193		
P43	S124	H194		
I44	P125	T195		
L45	R126	Y196		
A46	V127	Y197		
I47	I128	K198		
D48	P129	P200		
W49	V130	E201		
V50	N134	E202		
D53	R135	W203		
A54	D136	K205		
N55	M137			
S56	D138	S209		
D61	V143	E210		
E62	E144	L211		
F63	E213	D212		
	D214	E215		
R67	D146	S216		
L68	D147	Q217		
	L148	A218		
I71	I150			

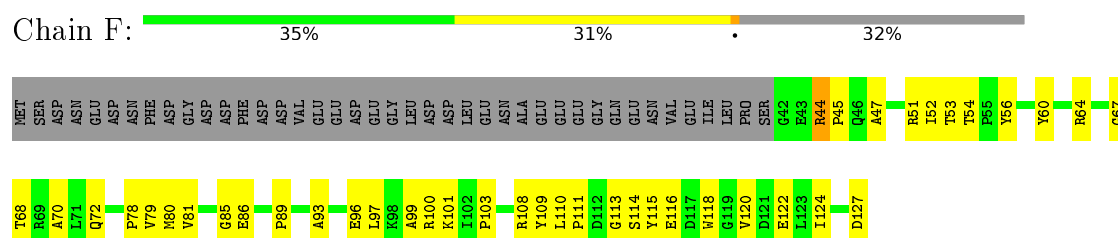
- Molecule 4: DNA-directed RNA polymerase II subunit RPB4



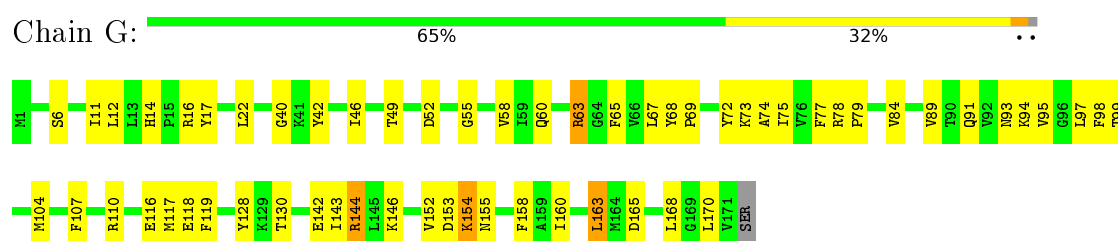
- Molecule 5: DNA-directed RNA polymerase II subunit RPB5



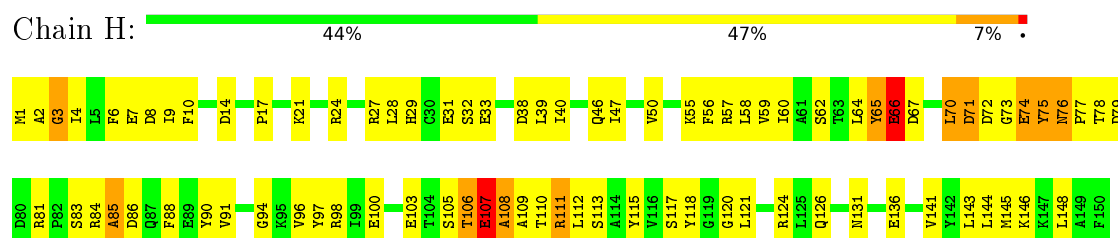
- Molecule 6: DNA-directed RNA polymerase II subunit RPB6



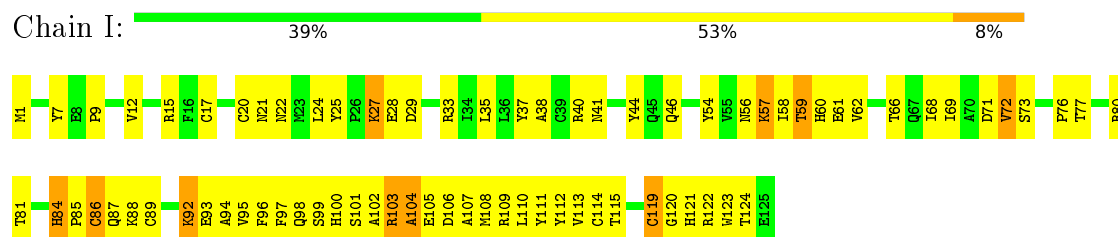
- Molecule 7: DNA-directed RNA polymerase II subunit RPB7



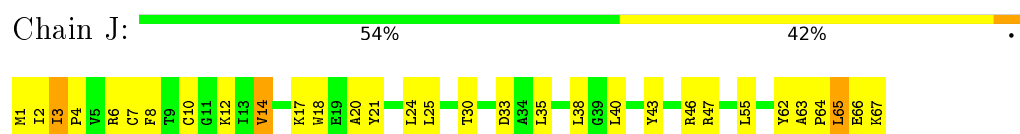
- Molecule 8: DNA-directed RNA polymerase II subunit RPB8



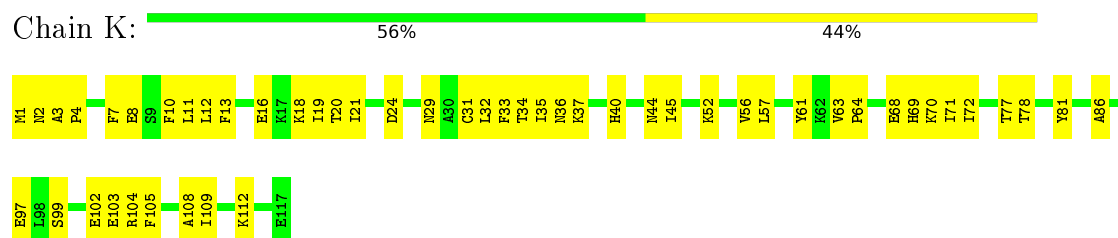
- Molecule 9: DNA-directed RNA polymerase II subunit RPB9



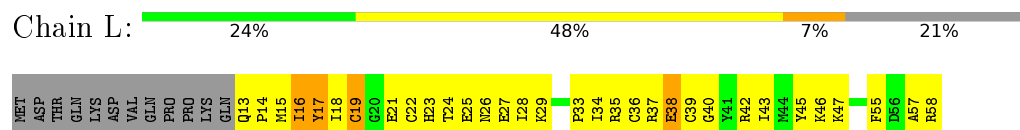
- Molecule 10: DNA-directed RNA polymerase II subunit RPB10



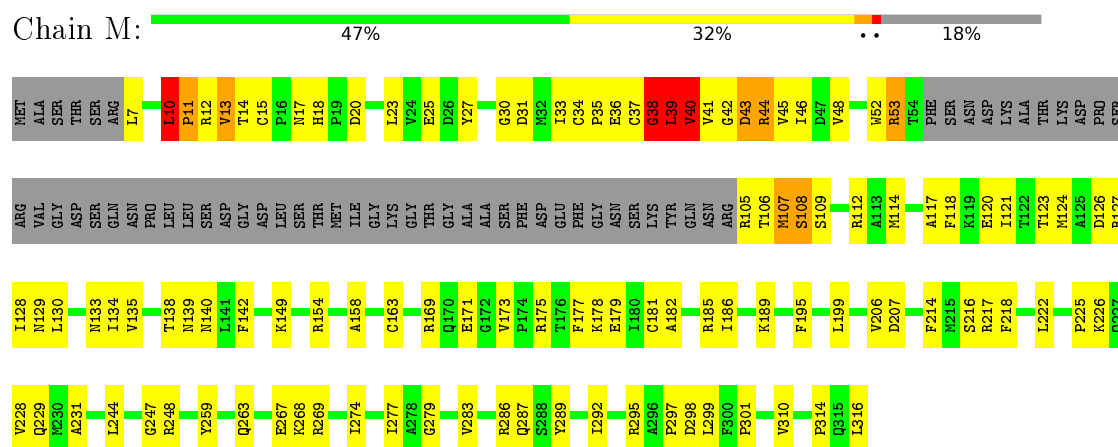
- Molecule 11: DNA-directed RNA polymerase II subunit RPB11-a



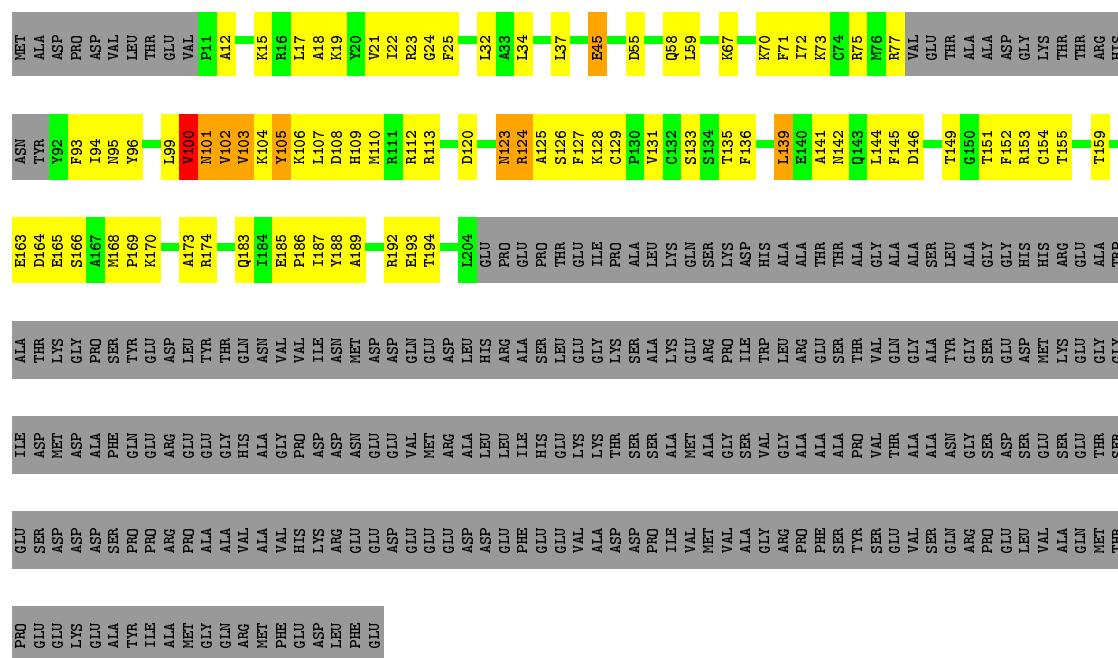
- Molecule 12: DNA-directed RNA polymerase II subunit RPB12



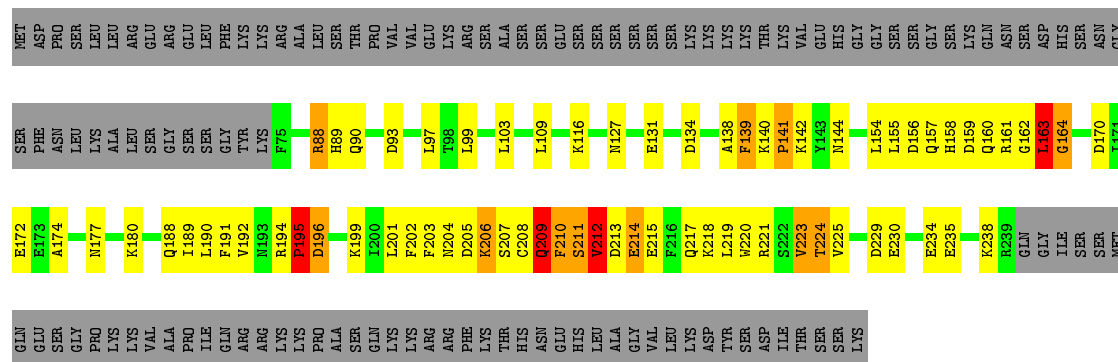
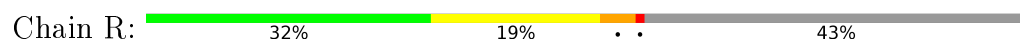
- Molecule 13: Transcription initiation factor IIB



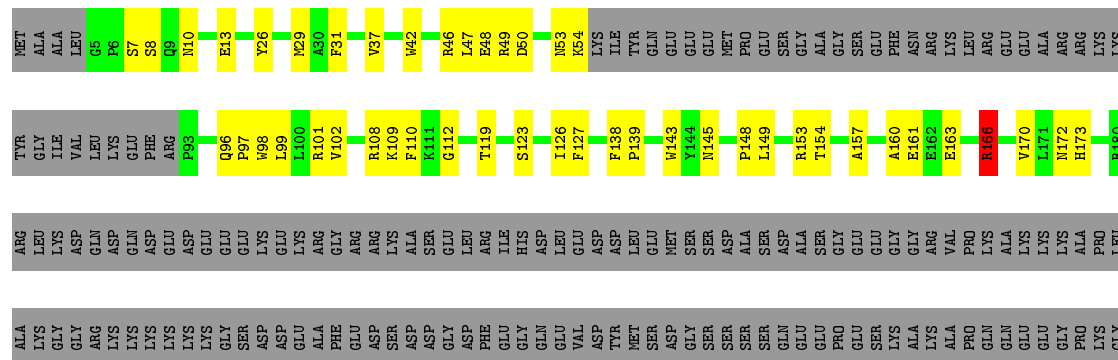
- Molecule 14: Transcription initiation factor IIA subunit 1

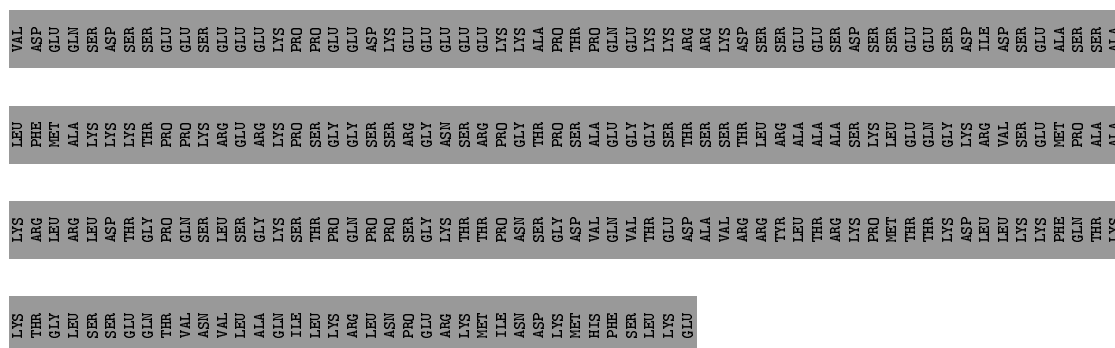


- Molecule 18: Transcription initiation factor IIE subunit beta

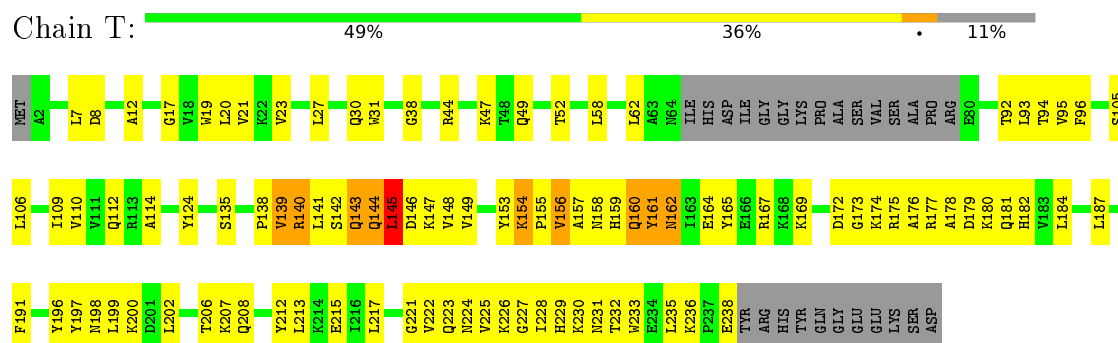


- Molecule 19: General transcription factor IIF subunit 1

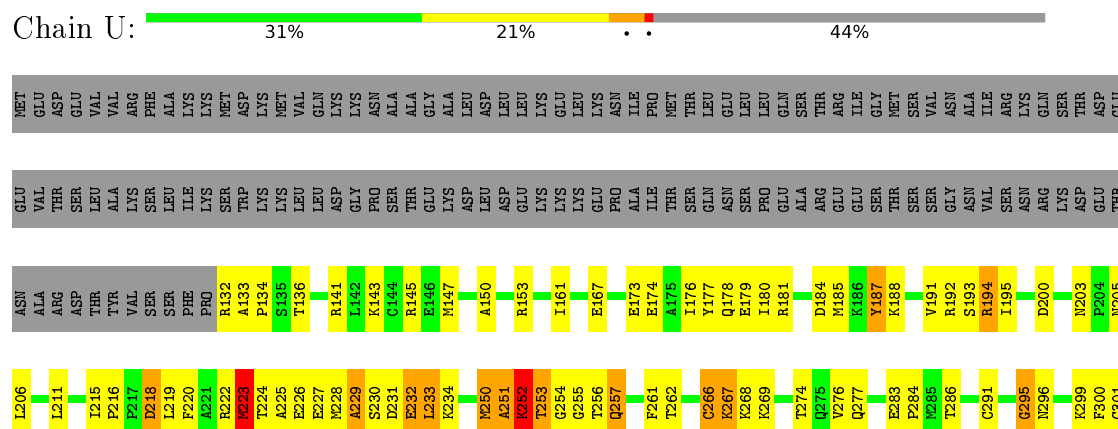




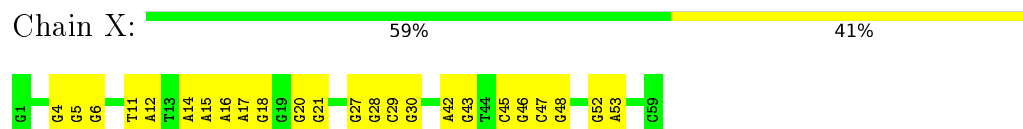
- Molecule 20: General transcription factor IIF subunit 2



- Molecule 21: Transcription elongation factor A protein 1



- Molecule 22: SCP-X



- Molecule 23: SCP-Y



G35	G49	A50	G53	A54	G55	G56	A57	G58	G59	A60	A61	G62	G63	G64	G65	G66	G67	G68	G69	G70	A71	G74	G75	T78	T79	T80	A81	A83	G84	G85	G86	G89	G90	T91	T92	G93
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4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	34728	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	27500	Depositor
Image detector	Not provided	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	0.27	0/11727	0.59	9/15833 (0.1%)
10	J	0.26	0/542	0.55	0/730
11	K	0.26	0/956	0.52	0/1294
12	L	0.26	0/394	0.61	0/524
13	M	0.26	0/2049	0.74	4/2769 (0.1%)
14	N	0.31	0/945	0.58	1/1274 (0.1%)
15	O	0.26	0/816	0.54	0/1105
16	P	0.31	0/1489	0.65	3/2005 (0.1%)
17	Q	0.29	0/1507	0.60	2/2023 (0.1%)
18	R	0.42	0/1380	0.91	2/1854 (0.1%)
19	S	0.29	0/1166	0.53	1/1575 (0.1%)
2	B	0.29	1/9503 (0.0%)	0.62	6/12831 (0.0%)
20	T	0.26	0/1817	0.58	1/2445 (0.0%)
21	U	0.33	0/1358	0.69	2/1820 (0.1%)
22	X	0.55	0/1369	0.90	0/2114
23	Y	0.55	0/1337	0.93	0/2059
3	C	0.27	0/2259	0.67	2/3073 (0.1%)
4	D	0.28	0/1077	0.51	0/1446
5	E	0.29	0/1753	0.63	2/2368 (0.1%)
6	F	0.25	0/700	0.51	0/946
7	G	0.27	0/1382	0.54	0/1874
8	H	0.27	0/1227	0.61	2/1654 (0.1%)
9	I	0.27	0/1038	0.90	2/1407 (0.1%)
All	All	0.31	1/47791 (0.0%)	0.65	39/65023 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
17	Q	0	1
18	R	0	1
21	U	0	1
3	C	0	1
All	All	0	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1090	GLU	CD-OE1	7.40	1.33	1.25

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	84	HIS	C-N-CD	-24.01	67.78	120.60
18	R	194	ARG	C-N-CD	-22.48	71.14	120.60
13	M	10	LEU	C-N-CD	-20.59	75.30	120.60
3	C	6	GLN	C-N-CD	-20.16	76.26	120.60
2	B	497	LYS	C-N-CD	-20.03	76.53	120.60
1	A	622	SER	C-N-CD	-10.02	98.56	120.60
16	P	239	ARG	NE-CZ-NH1	9.25	124.92	120.30
1	A	1307	VAL	N-CA-C	9.09	135.55	111.00
2	B	242	ARG	N-CA-C	-8.46	88.15	111.00
13	M	38	GLY	N-CA-C	-8.24	92.49	113.10
1	A	1311	LEU	CB-CG-CD1	-8.12	97.20	111.00
16	P	239	ARG	NE-CZ-NH2	-7.93	116.34	120.30
1	A	266	MET	N-CA-C	-7.76	90.05	111.00
20	T	145	LEU	N-CA-C	-7.38	91.06	111.00
5	E	64	HIS	N-CA-C	6.88	129.58	111.00
2	B	133	ILE	N-CA-C	-6.68	92.96	111.00
13	M	37	CYS	C-N-CA	-6.48	108.70	122.30
18	R	195	PRO	N-CA-C	-6.44	95.36	112.10
21	U	232	GLU	N-CA-C	6.42	128.32	111.00
16	P	160	GLY	N-CA-C	6.27	128.78	113.10
13	M	43	ASP	N-CA-C	6.26	127.90	111.00
8	H	74	GLU	N-CA-C	-5.98	94.86	111.00
14	N	319	ASP	N-CA-C	5.92	126.99	111.00
1	A	622	SER	N-CA-C	-5.77	95.41	111.00
2	B	1090	GLU	OE1-CD-OE2	5.76	130.21	123.30
1	A	614	ASP	N-CA-C	5.63	126.19	111.00
17	Q	102	VAL	C-N-CA	-5.59	107.74	121.70
9	I	103	ARG	N-CA-C	-5.56	95.99	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	S	166	ARG	NE-CZ-NH1	5.50	123.05	120.30
21	U	232	GLU	C-N-CA	-5.44	108.11	121.70
17	Q	73	LYS	N-CA-C	-5.39	96.45	111.00
2	B	880	LEU	N-CA-C	5.37	125.50	111.00
1	A	514	GLU	OE1-CD-OE2	-5.35	116.88	123.30
2	B	546	GLU	CA-CB-CG	5.32	125.10	113.40
5	E	62	VAL	C-N-CA	-5.23	108.63	121.70
8	H	85	ALA	N-CA-C	-5.16	97.07	111.00
1	A	625	ASP	C-N-CA	-5.15	108.81	121.70
1	A	604	ARG	C-N-CA	-5.06	109.06	121.70
3	C	137	ASN	N-CA-C	-5.00	97.50	111.00

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	623	PRO	Mainchain
1	A	85	PHE	Peptide
3	C	210	GLU	Mainchain
17	Q	100	VAL	Mainchain
18	R	230	GLU	Mainchain
21	U	250	MET	Mainchain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11515	0	11607	677	0
2	B	9317	0	9307	574	0
3	C	2213	0	2153	138	0
4	D	1062	0	1042	24	0
5	E	1723	0	1745	82	0
6	F	689	0	715	45	0
7	G	1351	0	1358	53	0
8	H	1205	0	1167	108	0
9	I	1013	0	931	81	0
10	J	533	0	553	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	K	937	0	959	46	0
12	L	388	0	393	65	0
13	M	2018	0	2060	136	0
14	N	930	0	888	64	0
15	O	806	0	818	51	0
16	P	1462	0	1548	117	0
17	Q	1484	0	1496	250	0
18	R	1357	0	1375	294	0
19	S	1137	0	1101	38	0
20	T	1788	0	1819	143	0
21	U	1343	0	1338	92	0
22	X	1218	0	661	25	0
23	Y	1195	0	663	30	0
24	A	1	0	0	0	0
24	B	1	0	0	0	0
25	A	2	0	0	0	0
25	B	1	0	0	0	0
25	C	1	0	0	0	0
25	I	2	0	0	0	0
25	J	1	0	0	0	0
25	L	1	0	0	0	0
25	M	1	0	0	0	0
25	Q	1	0	0	0	0
25	U	1	0	0	0	0
All	All	46697	0	45697	2635	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 29.

All (2635) 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)
17:Q:110:MET:HB2	18:R:218:LYS:CG	1.11	1.56
2:B:239:MET:SD	2:B:256:ILE:HG23	1.45	1.53
17:Q:187:ILE:CD1	18:R:211:SER:CB	1.86	1.51
8:H:65:TYR:CE1	8:H:79:ASP:OD2	1.65	1.50
17:Q:110:MET:CE	18:R:213:ASP:CB	1.89	1.50
1:A:1310:HIS:N	21:U:252:LYS:HD2	1.24	1.48
16:P:209:THR:CG2	16:P:224:ALA:N	1.79	1.45
17:Q:187:ILE:CG1	18:R:211:SER:HB3	1.44	1.45
17:Q:110:MET:CE	18:R:213:ASP:HB3	0.98	1.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:209:THR:HG22	16:P:223:GLY:C	1.31	1.43
17:Q:187:ILE:CG1	18:R:211:SER:CB	1.92	1.43
17:Q:24:GLY:CA	18:R:210:PHE:CD2	1.89	1.43
18:R:155:LEU:CG	18:R:204:ASN:ND2	1.79	1.42
17:Q:23:ARG:NH1	18:R:207:SER:HB3	1.32	1.40
17:Q:187:ILE:HG23	18:R:212:VAL:CA	1.34	1.40
17:Q:110:MET:CB	18:R:218:LYS:CG	2.00	1.40
17:Q:23:ARG:NH2	18:R:206:LYS:CG	1.84	1.39
17:Q:110:MET:HE3	18:R:213:ASP:CB	1.46	1.39
2:B:239:MET:CE	2:B:256:ILE:HD13	1.50	1.39
2:B:132:VAL:CG2	2:B:141:GLN:HG3	1.51	1.38
13:M:178:LYS:O	20:T:154:LYS:CB	1.69	1.38
1:A:922:PHE:CE2	1:A:952:LEU:HD23	1.58	1.37
3:C:200:PRO:HG2	3:C:217:GLN:CG	1.54	1.36
17:Q:187:ILE:CD1	18:R:211:SER:HB3	0.89	1.36
16:P:209:THR:HG22	16:P:224:ALA:N	1.38	1.35
13:M:12:ARG:O	13:M:13:VAL:HG13	1.23	1.33
17:Q:110:MET:CB	18:R:218:LYS:HG3	1.55	1.32
18:R:223:VAL:O	18:R:224:THR:CG2	1.74	1.32
16:P:209:THR:HG22	16:P:223:GLY:CA	1.60	1.32
1:A:924:TYR:CD1	1:A:949:GLN:NE2	1.99	1.30
17:Q:110:MET:CG	18:R:218:LYS:HB2	1.59	1.30
13:M:179:GLU:CA	20:T:154:LYS:HG2	1.62	1.29
1:A:1307:VAL:CG2	1:A:1338:THR:HB	1.62	1.28
17:Q:110:MET:SD	18:R:213:ASP:HB3	1.72	1.28
17:Q:110:MET:HB2	18:R:218:LYS:CB	1.63	1.27
1:A:1310:HIS:HB3	21:U:252:LYS:NZ	1.46	1.27
18:R:195:PRO:HG2	18:R:199:LYS:CB	1.63	1.27
17:Q:70:LYS:HG3	18:R:225:VAL:O	1.09	1.26
17:Q:187:ILE:CG2	18:R:212:VAL:CA	2.08	1.25
17:Q:187:ILE:HD13	18:R:211:SER:CB	1.53	1.24
18:R:155:LEU:HG	18:R:204:ASN:ND2	0.93	1.24
17:Q:23:ARG:NH2	18:R:206:LYS:HG3	0.92	1.24
8:H:65:TYR:CZ	8:H:81:ARG:NH2	2.07	1.22
1:A:621:ILE:O	1:A:623:PRO:HD3	1.35	1.22
2:B:79:GLU:O	2:B:80:GLU:HG2	1.36	1.22
21:U:252:LYS:O	21:U:253:THR:HG23	1.39	1.21
2:B:79:GLU:O	2:B:80:GLU:CG	1.87	1.21
1:A:926:ASN:OD1	1:A:931:ARG:NE	1.74	1.21
12:L:15:MET:O	12:L:16:ILE:HG23	1.35	1.21
1:A:616:GLY:O	1:A:619:LYS:HB2	1.40	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:102:VAL:O	17:Q:103:VAL:C	1.79	1.20
21:U:218:ASP:O	21:U:222:ARG:HB2	1.41	1.19
13:M:179:GLU:HA	20:T:154:LYS:CG	1.71	1.19
18:R:210:PHE:O	18:R:212:VAL:CG1	1.90	1.19
17:Q:105:TYR:HB2	18:R:234:GLU:HG2	1.19	1.18
3:C:200:PRO:CG	3:C:217:GLN:HG3	1.72	1.18
2:B:881:GLU:C	2:B:883:THR:H	1.41	1.18
1:A:621:ILE:O	1:A:623:PRO:CD	1.92	1.18
18:R:202:PHE:O	18:R:203:PHE:CD1	1.97	1.17
8:H:65:TYR:HE1	8:H:79:ASP:OD2	0.91	1.16
17:Q:107:LEU:CA	18:R:218:LYS:HE3	1.75	1.16
17:Q:24:GLY:HA3	18:R:210:PHE:CD2	1.24	1.15
17:Q:105:TYR:HE1	17:Q:109:HIS:NE2	1.43	1.15
18:R:210:PHE:O	18:R:212:VAL:HG13	0.97	1.15
12:L:18:ILE:HD11	12:L:47:LYS:CE	1.75	1.15
2:B:873:LEU:CB	2:B:874:PRO:HD3	1.77	1.14
13:M:34:CYS:H	13:M:39:LEU:CB	1.51	1.14
16:P:297:LYS:HB3	16:P:298:PRO:HD3	1.23	1.14
17:Q:187:ILE:CG2	18:R:212:VAL:HA	1.70	1.14
3:C:136:ASP:HB2	3:C:145:GLN:OE1	1.46	1.14
17:Q:70:LYS:CG	18:R:225:VAL:O	1.94	1.14
18:R:212:VAL:HG23	18:R:213:ASP:N	1.58	1.14
17:Q:102:VAL:HB	17:Q:105:TYR:HB3	1.16	1.13
17:Q:23:ARG:HH11	18:R:207:SER:CB	1.61	1.13
1:A:1310:HIS:H	21:U:252:LYS:CD	1.62	1.13
16:P:209:THR:CG2	16:P:223:GLY:C	2.13	1.13
12:L:15:MET:O	12:L:16:ILE:CG2	1.97	1.13
1:A:1310:HIS:CB	21:U:252:LYS:HZ2	1.63	1.12
17:Q:105:TYR:CE1	17:Q:109:HIS:NE2	2.16	1.12
17:Q:25:PHE:CD2	18:R:215:GLU:CD	2.23	1.12
2:B:239:MET:HE3	2:B:256:ILE:HD13	1.18	1.12
12:L:15:MET:O	12:L:16:ILE:HG12	1.49	1.12
2:B:873:LEU:HB2	2:B:874:PRO:HD3	1.21	1.12
17:Q:109:HIS:HB3	18:R:221:ARG:HG2	1.22	1.12
14:N:318:ASP:HA	16:P:239:ARG:HD2	1.12	1.11
1:A:1307:VAL:HG22	1:A:1338:THR:CB	1.81	1.11
17:Q:112:ARG:CG	18:R:221:ARG:HH22	1.63	1.11
18:R:195:PRO:HG2	18:R:199:LYS:HB2	1.16	1.10
2:B:239:MET:SD	2:B:256:ILE:CG2	2.38	1.10
16:P:206:GLU:HB2	16:P:207:PRO:HD3	1.30	1.10
17:Q:23:ARG:HH21	18:R:206:LYS:CG	1.55	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:92:TYR:CB	20:T:145:LEU:HD22	1.82	1.10
3:C:200:PRO:HB2	3:C:217:GLN:OE1	1.50	1.10
2:B:132:VAL:CG2	2:B:141:GLN:CG	2.30	1.10
16:P:209:THR:HG21	16:P:224:ALA:N	1.63	1.09
17:Q:23:ARG:NH1	18:R:207:SER:CB	2.14	1.09
1:A:922:PHE:CE2	1:A:952:LEU:CD2	2.35	1.09
1:A:924:TYR:CE1	1:A:949:GLN:NE2	2.20	1.09
1:A:1310:HIS:CA	21:U:252:LYS:HD2	1.83	1.09
17:Q:107:LEU:HA	18:R:218:LYS:HE3	1.15	1.09
17:Q:112:ARG:HG2	18:R:221:ARG:HH22	1.07	1.09
20:T:179:ASP:OD1	20:T:182:HIS:HB3	1.53	1.08
1:A:1310:HIS:CB	21:U:252:LYS:NZ	2.14	1.08
17:Q:110:MET:SD	18:R:218:LYS:HD2	1.93	1.08
2:B:876:ASN:O	2:B:879:GLU:HG3	1.54	1.08
16:P:209:THR:HA	16:P:223:GLY:HA3	1.33	1.08
18:R:190:LEU:CD1	18:R:205:ASP:HB2	1.83	1.08
2:B:876:ASN:O	2:B:879:GLU:CG	2.01	1.07
17:Q:187:ILE:HD11	18:R:211:SER:HB3	1.30	1.07
2:B:242:ARG:O	2:B:252:ILE:HG23	1.54	1.07
3:C:136:ASP:C	3:C:138:ASP:H	1.51	1.07
18:R:223:VAL:O	18:R:224:THR:HG23	0.89	1.07
1:A:927:GLU:O	1:A:931:ARG:HG3	1.55	1.07
2:B:79:GLU:O	2:B:80:GLU:CB	2.01	1.07
1:A:932:ARG:HB3	1:A:939:VAL:HG11	1.10	1.06
13:M:34:CYS:N	13:M:39:LEU:HB3	1.68	1.06
21:U:252:LYS:HE3	21:U:252:LYS:HA	1.36	1.06
17:Q:110:MET:HG3	18:R:218:LYS:HB2	1.15	1.06
3:C:200:PRO:CG	3:C:217:GLN:CG	2.32	1.05
17:Q:110:MET:SD	18:R:213:ASP:CB	2.36	1.05
1:A:1310:HIS:N	21:U:252:LYS:CD	2.18	1.05
8:H:75:TYR:O	8:H:77:PRO:HD3	1.53	1.05
1:A:1310:HIS:HB3	21:U:252:LYS:HG2	1.38	1.05
3:C:6:GLN:O	11:K:104:ARG:NH1	1.89	1.05
18:R:212:VAL:HG23	18:R:213:ASP:H	0.94	1.04
13:M:12:ARG:O	13:M:13:VAL:CG1	2.05	1.04
1:A:1304:ILE:HD12	1:A:1307:VAL:CG1	1.86	1.04
1:A:922:PHE:CZ	1:A:952:LEU:HD23	1.93	1.04
2:B:880:LEU:O	2:B:881:GLU:CB	2.03	1.04
16:P:161:ILE:HG21	16:P:263:ASP:O	1.58	1.04
1:A:1304:ILE:HD12	1:A:1307:VAL:HG11	1.38	1.04
17:Q:112:ARG:HB3	18:R:221:ARG:NH2	1.72	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:18:ILE:HD11	12:L:47:LYS:HE3	1.35	1.03
12:L:15:MET:O	12:L:16:ILE:CG1	2.05	1.03
17:Q:110:MET:SD	18:R:213:ASP:CG	2.37	1.03
3:C:5:ASN:C	3:C:7:PRO:HD3	1.74	1.03
16:P:160:GLY:O	16:P:161:ILE:HG12	1.56	1.03
13:M:178:LYS:O	20:T:154:LYS:HB3	0.86	1.03
1:A:932:ARG:CB	1:A:939:VAL:HG11	1.88	1.03
16:P:297:LYS:CB	16:P:298:PRO:CD	2.37	1.03
17:Q:24:GLY:HA2	18:R:210:PHE:CD2	1.88	1.03
1:A:330:GLN:HB3	13:M:107:MET:SD	1.97	1.02
1:A:923:ASP:C	1:A:925:THR:H	1.58	1.02
1:A:1307:VAL:HG22	1:A:1338:THR:HB	1.02	1.02
2:B:132:VAL:HG21	2:B:141:GLN:HG3	1.04	1.02
2:B:499:ARG:O	2:B:500:GLN:O	1.75	1.02
12:L:16:ILE:O	12:L:17:TYR:HB2	1.57	1.02
12:L:18:ILE:HD11	12:L:47:LYS:CD	1.88	1.01
16:P:209:THR:CG2	16:P:224:ALA:H	1.74	1.01
17:Q:110:MET:CB	18:R:218:LYS:CD	2.38	1.00
21:U:232:GLU:O	21:U:233:LEU:HB2	1.58	1.00
1:A:1313:GLN:HG2	1:A:1333:GLU:HG2	1.43	1.00
1:A:923:ASP:O	1:A:925:THR:N	1.94	1.00
17:Q:24:GLY:HA2	18:R:210:PHE:CG	1.96	1.00
1:A:927:GLU:O	1:A:931:ARG:CG	2.09	1.00
1:A:926:ASN:OD1	1:A:931:ARG:CD	2.10	1.00
1:A:622:SER:O	1:A:624:GLY:N	1.95	0.99
2:B:239:MET:CE	2:B:256:ILE:CD1	2.39	0.99
1:A:926:ASN:ND2	1:A:931:ARG:HD2	1.77	0.99
13:M:34:CYS:O	13:M:39:LEU:HB2	1.62	0.99
17:Q:109:HIS:HB3	18:R:221:ARG:CG	1.91	0.99
17:Q:102:VAL:O	17:Q:104:LYS:N	1.96	0.99
2:B:132:VAL:HG21	2:B:141:GLN:CG	1.90	0.99
17:Q:25:PHE:HD2	18:R:215:GLU:CD	1.61	0.99
8:H:85:ALA:O	8:H:144:LEU:CD2	2.10	0.98
13:M:43:ASP:O	13:M:44:ARG:C	1.97	0.98
13:M:34:CYS:H	13:M:39:LEU:HB3	0.83	0.98
18:R:208:CYS:O	18:R:209:GLN:O	1.81	0.98
17:Q:105:TYR:CE1	17:Q:109:HIS:CD2	2.50	0.98
17:Q:110:MET:CB	18:R:218:LYS:CB	2.34	0.98
21:U:218:ASP:O	21:U:222:ARG:CB	2.12	0.98
2:B:132:VAL:HG23	2:B:141:GLN:CG	1.93	0.98
2:B:242:ARG:O	2:B:252:ILE:CG2	2.12	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:132:VAL:HG22	2:B:141:GLN:O	1.63	0.97
3:C:217:GLN:O	3:C:218:ALA:CB	2.12	0.97
1:A:1307:VAL:HG23	1:A:1339:ASP:H	1.30	0.97
8:H:74:GLU:O	8:H:76:ASN:N	1.96	0.97
16:P:297:LYS:HB3	16:P:298:PRO:CD	1.93	0.97
2:B:880:LEU:O	2:B:881:GLU:HB2	1.14	0.97
17:Q:25:PHE:CE2	18:R:215:GLU:HG3	2.00	0.97
3:C:200:PRO:HG2	3:C:217:GLN:HG3	0.98	0.97
8:H:75:TYR:O	8:H:77:PRO:CD	2.12	0.97
1:A:611:ASP:CG	1:A:626:THR:OG1	2.02	0.96
5:E:64:HIS:O	5:E:65:ASN:O	1.83	0.96
18:R:127:ASN:HD21	18:R:140:LYS:CD	1.77	0.96
3:C:6:GLN:CG	3:C:25:ASN:ND2	2.28	0.96
18:R:190:LEU:HD12	18:R:205:ASP:HB2	1.43	0.96
3:C:200:PRO:CB	3:C:217:GLN:OE1	2.13	0.96
8:H:100:GLU:HB2	8:H:113:SER:HB2	1.48	0.96
17:Q:107:LEU:HA	18:R:218:LYS:CE	1.96	0.96
17:Q:109:HIS:O	18:R:221:ARG:HD3	1.65	0.96
2:B:881:GLU:C	2:B:883:THR:N	2.15	0.95
18:R:220:TRP:O	18:R:223:VAL:HG22	1.65	0.95
1:A:551:ARG:HG2	1:A:625:ASP:OD2	1.65	0.95
17:Q:109:HIS:O	18:R:221:ARG:NH1	1.99	0.95
17:Q:110:MET:CB	18:R:218:LYS:HD2	1.94	0.95
17:Q:32:LEU:HD11	18:R:203:PHE:CD2	2.00	0.95
1:A:621:ILE:O	1:A:623:PRO:N	1.99	0.95
17:Q:110:MET:CB	18:R:218:LYS:HB2	1.93	0.95
1:A:932:ARG:HB3	1:A:939:VAL:CG1	1.96	0.95
2:B:240:LEU:HG	2:B:255:ARG:O	1.67	0.95
9:I:99:SER:OG	9:I:105:GLU:HB2	1.67	0.95
2:B:92:TYR:HB3	20:T:145:LEU:CG	1.97	0.95
1:A:426:ARG:HB3	13:M:40:VAL:HG21	1.46	0.94
18:R:210:PHE:O	18:R:211:SER:C	2.04	0.94
18:R:223:VAL:C	18:R:224:THR:HG23	1.88	0.94
8:H:64:LEU:H	8:H:70:LEU:HD21	1.30	0.94
2:B:92:TYR:HB3	20:T:145:LEU:HD22	1.46	0.94
18:R:195:PRO:CG	18:R:199:LYS:CB	2.45	0.94
1:A:1310:HIS:HB3	21:U:252:LYS:HZ2	0.80	0.94
13:M:34:CYS:O	13:M:39:LEU:CD2	2.14	0.93
17:Q:110:MET:HE1	18:R:213:ASP:HB3	1.46	0.93
17:Q:102:VAL:CB	17:Q:105:TYR:HB3	1.98	0.93
17:Q:102:VAL:HB	17:Q:105:TYR:CB	1.97	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:712:PRO:HB3	2:B:999:ALA:HB1	1.51	0.93
12:L:15:MET:O	12:L:16:ILE:CB	2.15	0.93
2:B:132:VAL:HG23	2:B:141:GLN:HG3	1.47	0.93
17:Q:187:ILE:HG21	18:R:212:VAL:O	1.68	0.93
18:R:202:PHE:O	18:R:203:PHE:CG	2.21	0.93
8:H:65:TYR:CE2	8:H:81:ARG:NH2	2.29	0.92
1:A:924:TYR:HD1	1:A:949:GLN:NE2	1.48	0.92
17:Q:187:ILE:HB	18:R:211:SER:OG	1.70	0.92
18:R:155:LEU:CG	18:R:204:ASN:HD21	1.55	0.92
1:A:1313:GLN:C	1:A:1315:ASP:H	1.69	0.92
3:C:200:PRO:HG2	3:C:217:GLN:CD	1.89	0.92
17:Q:110:MET:CG	18:R:218:LYS:CB	2.47	0.92
13:M:178:LYS:C	20:T:154:LYS:CB	2.38	0.92
1:A:551:ARG:HH22	8:H:121:LEU:HA	1.34	0.91
1:A:612:ASP:HB3	1:A:617:PRO:HD3	1.50	0.91
17:Q:109:HIS:C	18:R:221:ARG:HD3	1.89	0.91
17:Q:23:ARG:CZ	18:R:206:LYS:HG3	1.99	0.91
18:R:213:ASP:O	18:R:215:GLU:N	2.03	0.91
17:Q:25:PHE:CD2	18:R:215:GLU:CG	2.53	0.91
17:Q:105:TYR:HE1	17:Q:109:HIS:HE2	0.93	0.91
17:Q:110:MET:HB2	18:R:218:LYS:CD	2.00	0.91
16:P:297:LYS:CB	16:P:298:PRO:HD3	1.98	0.91
17:Q:187:ILE:CB	18:R:211:SER:OG	2.19	0.91
2:B:92:TYR:HB3	20:T:145:LEU:HB2	1.51	0.91
2:B:92:TYR:HB3	20:T:145:LEU:CD2	2.01	0.91
12:L:25:GLU:HB2	12:L:27:GLU:HG2	1.53	0.90
18:R:212:VAL:CG2	18:R:213:ASP:H	1.83	0.90
17:Q:23:ARG:HH11	18:R:207:SER:HB3	0.75	0.90
1:A:922:PHE:HE2	1:A:952:LEU:CD2	1.79	0.90
5:E:64:HIS:O	5:E:65:ASN:C	2.07	0.90
17:Q:107:LEU:N	18:R:218:LYS:HE3	1.87	0.90
2:B:132:VAL:CG2	2:B:141:GLN:O	2.20	0.90
9:I:58:ILE:O	9:I:59:THR:OG1	1.88	0.90
13:M:178:LYS:C	20:T:154:LYS:HB3	1.90	0.90
18:R:162:GLY:C	18:R:164:GLY:H	1.66	0.90
8:H:65:TYR:CZ	8:H:79:ASP:OD2	2.24	0.90
5:E:63:ALA:O	5:E:64:HIS:HB2	1.70	0.89
17:Q:23:ARG:HH22	18:R:206:LYS:HG3	1.34	0.89
13:M:34:CYS:O	13:M:39:LEU:HD23	1.50	0.89
14:N:343:HIS:HB3	14:N:350:LYS:HB2	1.50	0.89
17:Q:113:ARG:NE	18:R:217:GLN:O	2.06	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:112:ARG:HG2	18:R:221:ARG:NH2	1.86	0.89
5:E:6:GLU:OE2	5:E:54:ARG:NH2	2.05	0.89
17:Q:112:ARG:CG	18:R:221:ARG:NH2	2.35	0.89
3:C:45:ILE:HG12	3:C:79:VAL:HB	1.55	0.89
3:C:6:GLN:HG3	3:C:25:ASN:ND2	1.87	0.89
17:Q:25:PHE:CD2	18:R:215:GLU:HG3	2.07	0.89
18:R:195:PRO:HG2	18:R:199:LYS:HB3	1.54	0.89
17:Q:112:ARG:CB	18:R:221:ARG:NH2	2.35	0.89
18:R:210:PHE:CG	18:R:212:VAL:HG11	2.08	0.89
1:A:1310:HIS:CB	21:U:252:LYS:HG2	2.00	0.89
1:A:608:THR:C	1:A:610:PRO:HD2	1.94	0.88
1:A:926:ASN:CG	1:A:931:ARG:HD2	1.93	0.88
17:Q:110:MET:HB3	18:R:218:LYS:HD2	1.55	0.88
20:T:179:ASP:C	20:T:181:GLN:H	1.73	0.88
1:A:923:ASP:C	1:A:925:THR:N	2.24	0.88
18:R:127:ASN:HD21	18:R:140:LYS:CE	1.85	0.88
17:Q:187:ILE:HD13	18:R:211:SER:HB3	0.89	0.88
17:Q:187:ILE:CG1	18:R:211:SER:OG	2.20	0.88
18:R:195:PRO:CG	18:R:199:LYS:HB3	2.03	0.88
8:H:17:PRO:HB3	8:H:27:ARG:HB3	1.53	0.88
17:Q:110:MET:HE1	18:R:213:ASP:CB	2.01	0.88
8:H:65:TYR:CD1	8:H:81:ARG:NE	2.40	0.88
2:B:873:LEU:HB2	2:B:874:PRO:CD	2.03	0.88
18:R:212:VAL:CG2	18:R:213:ASP:N	2.35	0.88
2:B:876:ASN:O	2:B:879:GLU:HG2	1.74	0.87
18:R:210:PHE:C	18:R:212:VAL:HG13	1.93	0.87
12:L:16:ILE:O	12:L:17:TYR:CB	2.22	0.87
17:Q:106:LYS:HG2	18:R:218:LYS:HE2	1.56	0.87
21:U:134:PRO:O	21:U:145:ARG:NH1	2.07	0.87
1:A:1287:CYS:HA	2:B:250:SER:HB2	1.56	0.87
2:B:239:MET:SD	2:B:256:ILE:CD1	2.62	0.87
2:B:881:GLU:O	2:B:883:THR:N	2.07	0.87
2:B:92:TYR:HB3	20:T:145:LEU:CB	2.04	0.87
3:C:136:ASP:C	3:C:138:ASP:N	2.24	0.87
3:C:217:GLN:O	3:C:218:ALA:HB3	1.72	0.87
12:L:18:ILE:HD11	12:L:47:LYS:HD3	1.55	0.87
9:I:103:ARG:HG2	9:I:105:GLU:OE1	1.72	0.87
18:R:158:HIS:CE1	18:R:206:LYS:HE2	2.10	0.87
16:P:209:THR:CG2	16:P:223:GLY:CA	2.50	0.86
1:A:922:PHE:CZ	1:A:952:LEU:CD2	2.56	0.86
3:C:200:PRO:HG3	3:C:217:GLN:HB3	1.57	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:162:GLY:O	18:R:164:GLY:N	2.08	0.86
17:Q:105:TYR:CB	18:R:234:GLU:HG2	2.05	0.86
1:A:1307:VAL:HG23	1:A:1339:ASP:N	1.90	0.86
2:B:239:MET:SD	2:B:256:ILE:HD13	2.16	0.86
17:Q:109:HIS:O	18:R:221:ARG:CD	2.24	0.86
17:Q:24:GLY:CA	18:R:210:PHE:CG	2.52	0.86
17:Q:112:ARG:HB3	18:R:221:ARG:CZ	2.04	0.85
17:Q:110:MET:SD	18:R:213:ASP:OD1	2.34	0.85
17:Q:109:HIS:O	18:R:221:ARG:CZ	2.24	0.85
13:M:106:THR:C	13:M:108:SER:H	1.77	0.85
14:N:327:GLU:HB2	16:P:188:ARG:HH12	1.40	0.85
12:L:16:ILE:CG1	12:L:28:ILE:N	2.38	0.85
17:Q:187:ILE:HG23	18:R:212:VAL:C	1.97	0.85
17:Q:110:MET:CE	18:R:213:ASP:CA	2.53	0.85
20:T:154:LYS:H	20:T:154:LYS:HD2	1.40	0.85
1:A:620:HIS:C	1:A:621:ILE:HG12	1.96	0.85
19:S:102:VAL:HB	19:S:108:ARG:HB3	1.59	0.85
1:A:621:ILE:C	1:A:623:PRO:N	2.26	0.85
2:B:646:ARG:HD3	2:B:651:TYR:H	1.40	0.85
17:Q:187:ILE:CG2	18:R:212:VAL:O	2.25	0.84
21:U:252:LYS:O	21:U:253:THR:CG2	2.23	0.84
17:Q:187:ILE:CG2	18:R:212:VAL:C	2.45	0.84
13:M:179:GLU:HA	20:T:154:LYS:HG2	0.86	0.84
3:C:136:ASP:CB	3:C:145:GLN:OE1	2.26	0.84
5:E:63:ALA:O	5:E:64:HIS:CB	2.26	0.84
12:L:18:ILE:CD1	12:L:47:LYS:HD3	2.07	0.84
2:B:93:LEU:N	20:T:145:LEU:HD23	1.92	0.84
8:H:74:GLU:C	8:H:76:ASN:H	1.80	0.84
10:J:63:ALA:HB3	10:J:64:PRO:HD3	1.59	0.84
2:B:718:GLN:HG2	2:B:720:PRO:HD2	1.57	0.84
1:A:643:LYS:NZ	21:U:301:CYS:O	2.11	0.84
12:L:15:MET:C	12:L:16:ILE:HG12	1.95	0.83
16:P:289:PRO:HB3	23:Y:84:DG:H5'	1.57	0.83
1:A:1310:HIS:HB3	21:U:252:LYS:CG	2.08	0.83
2:B:24:GLU:OE1	2:B:762:ARG:NH1	2.11	0.83
9:I:103:ARG:O	9:I:105:GLU:N	2.11	0.83
1:A:551:ARG:CG	1:A:625:ASP:OD2	2.26	0.83
2:B:490:GLY:O	2:B:491:ARG:C	2.14	0.83
2:B:79:GLU:O	2:B:80:GLU:HB2	1.78	0.83
21:U:252:LYS:HA	21:U:252:LYS:CE	2.09	0.83
3:C:49:TRP:HB3	3:C:164:TYR:HB2	1.59	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:16:ILE:HG13	12:L:28:ILE:N	1.93	0.83
17:Q:110:MET:SD	18:R:218:LYS:CD	2.66	0.83
18:R:190:LEU:HD11	18:R:205:ASP:HB2	1.61	0.83
12:L:19:CYS:HB3	12:L:22:CYS:SG	2.19	0.83
1:A:611:ASP:CG	1:A:626:THR:HG1	1.82	0.82
18:R:210:PHE:CD2	18:R:212:VAL:HG11	2.14	0.82
5:E:147:GLU:HB3	5:E:194:ILE:HB	1.62	0.82
5:E:15:LYS:NZ	5:E:35:GLN:OE1	2.12	0.82
20:T:179:ASP:OD1	20:T:182:HIS:CB	2.27	0.82
13:M:107:MET:H	13:M:107:MET:HE3	1.44	0.82
1:A:426:ARG:HG2	13:M:40:VAL:HG11	1.62	0.82
20:T:175:ARG:HD2	20:T:207:LYS:HB3	1.60	0.82
1:A:549:THR:O	1:A:589:LYS:NZ	2.13	0.82
2:B:499:ARG:HB3	2:B:499:ARG:NH1	1.95	0.82
2:B:499:ARG:O	2:B:500:GLN:C	2.15	0.82
17:Q:110:MET:HB2	18:R:218:LYS:HG3	0.82	0.81
18:R:155:LEU:CD2	18:R:204:ASN:ND2	2.43	0.81
1:A:609:HIS:N	1:A:610:PRO:CD	2.43	0.81
14:N:318:ASP:CA	16:P:239:ARG:HD2	2.04	0.81
18:R:191:PHE:HB3	18:R:202:PHE:CE1	2.15	0.81
17:Q:112:ARG:CB	18:R:221:ARG:HH22	1.90	0.81
1:A:611:ASP:HB3	1:A:617:PRO:HG3	1.63	0.81
1:A:723:ASN:HB2	9:I:109:ARG:HB2	1.61	0.81
1:A:1310:HIS:CA	21:U:252:LYS:CD	2.50	0.81
2:B:79:GLU:C	2:B:80:GLU:HG2	2.00	0.81
1:A:1209:PRO:HB3	9:I:33:ARG:HH12	1.44	0.81
1:A:653:VAL:HG23	1:A:669:TYR:HE2	1.46	0.81
14:N:318:ASP:HA	16:P:239:ARG:CD	2.05	0.81
2:B:227:ASN:O	2:B:405:ARG:NH2	2.14	0.81
2:B:488:PRO:O	2:B:489:ILE:CG1	2.29	0.81
2:B:873:LEU:CB	2:B:874:PRO:CD	2.59	0.81
2:B:289:ILE:HG13	2:B:291:ASP:H	1.43	0.81
2:B:488:PRO:O	2:B:489:ILE:HG12	1.80	0.81
12:L:18:ILE:HA	12:L:25:GLU:HA	1.63	0.81
18:R:127:ASN:ND2	18:R:140:LYS:CD	2.44	0.81
18:R:210:PHE:O	18:R:212:VAL:N	2.13	0.81
21:U:250:MET:O	21:U:251:ALA:HB2	1.80	0.81
10:J:67:LYS:HB2	12:L:23:HIS:HD2	1.47	0.80
1:A:330:GLN:CB	13:M:107:MET:SD	2.68	0.80
16:P:297:LYS:HA	16:P:297:LYS:CE	2.09	0.80
17:Q:25:PHE:HD2	18:R:215:GLU:CG	1.90	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:67:LYS:HG3	12:L:23:HIS:HB3	1.63	0.80
2:B:72:GLN:O	2:B:73:HIS:O	1.99	0.80
8:H:40:ILE:HD12	8:H:124:ARG:HD3	1.61	0.80
16:P:206:GLU:CB	16:P:207:PRO:HD3	2.09	0.80
17:Q:105:TYR:HB2	18:R:234:GLU:CG	2.08	0.80
8:H:106:THR:O	8:H:108:ALA:N	2.12	0.80
17:Q:110:MET:HB3	18:R:218:LYS:CD	2.09	0.80
18:R:163:LEU:O	18:R:164:GLY:O	2.00	0.79
1:A:1313:GLN:C	1:A:1315:ASP:N	2.33	0.79
17:Q:106:LYS:HG2	18:R:218:LYS:HG2	1.64	0.79
10:J:64:PRO:O	10:J:66:GLU:N	2.12	0.79
2:B:623:ARG:NH2	2:B:697:GLU:OE2	2.15	0.79
13:M:43:ASP:O	13:M:45:VAL:N	2.14	0.79
17:Q:110:MET:HE3	18:R:213:ASP:CA	2.12	0.79
17:Q:71:PHE:HA	17:Q:100:VAL:HG22	1.65	0.79
17:Q:110:MET:HE3	18:R:213:ASP:HB3	0.80	0.79
13:M:178:LYS:HG2	20:T:156:VAL:HG12	1.64	0.79
1:A:926:ASN:CG	1:A:931:ARG:CD	2.51	0.79
2:B:216:ALA:HB2	2:B:241:ALA:HB2	1.65	0.79
10:J:17:LYS:HB3	10:J:38:LEU:HD22	1.65	0.78
1:A:1313:GLN:CG	1:A:1333:GLU:HG2	2.13	0.78
17:Q:104:LYS:HZ2	18:R:238:LYS:HD2	1.48	0.78
17:Q:187:ILE:HG12	18:R:211:SER:CB	1.50	0.78
1:A:30:GLU:HA	1:A:33:ARG:HB2	1.65	0.78
18:R:210:PHE:CG	18:R:212:VAL:CG1	2.67	0.78
18:R:195:PRO:CG	18:R:199:LYS:HB2	2.06	0.78
18:R:213:ASP:O	18:R:215:GLU:HB2	1.84	0.78
17:Q:106:LYS:NZ	18:R:219:LEU:HD13	1.99	0.77
20:T:221:GLY:HA2	20:T:236:LYS:HG3	1.67	0.77
18:R:155:LEU:CB	18:R:204:ASN:HD21	1.97	0.77
1:A:921:ARG:O	1:A:1052:ARG:NH1	2.17	0.77
9:I:105:GLU:HG3	9:I:107:ALA:HB3	1.67	0.77
1:A:537:ILE:HB	1:A:645:LEU:HD21	1.67	0.77
18:R:155:LEU:CG	18:R:204:ASN:HD22	1.72	0.77
17:Q:32:LEU:CD1	18:R:203:PHE:CD2	2.67	0.77
1:A:1307:VAL:HG21	1:A:1338:THR:HB	1.64	0.76
17:Q:102:VAL:C	17:Q:104:LYS:N	2.38	0.76
3:C:5:ASN:O	3:C:7:PRO:HD3	1.83	0.76
18:R:162:GLY:C	18:R:164:GLY:N	2.39	0.76
1:A:609:HIS:O	1:A:610:PRO:O	2.04	0.76
2:B:1072:ARG:HH21	2:B:1113:PRO:HG2	1.50	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:130:VAL:O	3:C:134:ASN:ND2	2.19	0.76
8:H:65:TYR:O	8:H:66:GLU:HB2	1.86	0.76
17:Q:187:ILE:HG23	18:R:212:VAL:HA	0.76	0.76
9:I:73:SER:O	9:I:80:ARG:NH2	2.17	0.76
18:R:191:PHE:HB3	18:R:202:PHE:CD1	2.20	0.76
1:A:137:PRO:HB3	1:A:237:GLY:HA3	1.68	0.76
2:B:239:MET:HE1	2:B:256:ILE:HD13	1.63	0.76
19:S:50:ASP:HB3	19:S:97:PRO:HG2	1.66	0.76
1:A:1169:VAL:HG21	1:A:1298:LEU:HD22	1.66	0.76
1:A:884:ASN:ND2	6:F:111:PRO:O	2.18	0.76
8:H:85:ALA:O	8:H:144:LEU:HD23	1.85	0.76
16:P:297:LYS:HB2	16:P:298:PRO:HD2	1.68	0.76
17:Q:107:LEU:N	18:R:218:LYS:CE	2.49	0.75
12:L:40:GLY:O	12:L:42:ARG:NH1	2.19	0.75
17:Q:70:LYS:CG	18:R:225:VAL:HG12	2.16	0.75
21:U:173:GLU:OE2	21:U:187:TYR:OH	2.04	0.75
1:A:1206:ARG:HD3	1:A:1265:ASP:HA	1.69	0.75
1:A:1307:VAL:CG2	1:A:1338:THR:CB	2.50	0.75
2:B:754:PRO:HB2	2:B:773:PRO:HG2	1.69	0.75
17:Q:102:VAL:HB	17:Q:105:TYR:CD2	2.21	0.75
1:A:1208:SER:HB2	1:A:1261:ILE:HG12	1.69	0.75
18:R:210:PHE:HB2	18:R:212:VAL:CG1	2.16	0.75
2:B:133:ILE:CG2	2:B:139:GLN:HE22	2.00	0.74
2:B:817:GLN:HE21	2:B:916:TYR:HB2	1.52	0.74
2:B:92:TYR:C	20:T:145:LEU:HD22	2.06	0.74
2:B:93:LEU:C	20:T:145:LEU:HD23	2.07	0.74
1:A:611:ASP:OD2	1:A:617:PRO:HB3	1.87	0.74
21:U:232:GLU:O	21:U:233:LEU:CB	2.28	0.74
1:A:1310:HIS:CE1	1:A:1334:TRP:HE3	2.06	0.74
1:A:374:SER:OG	1:A:666:ARG:NH2	2.20	0.74
1:A:609:HIS:N	1:A:610:PRO:HD2	2.03	0.74
1:A:700:GLN:OE1	1:A:703:GLN:NE2	2.20	0.74
2:B:134:LYS:HD3	2:B:138:GLU:HB2	1.68	0.74
3:C:100:GLU:OE2	3:C:162:ARG:NH2	2.20	0.74
18:R:154:LEU:HD23	18:R:162:GLY:O	1.86	0.74
20:T:47:LYS:HG2	20:T:52:THR:HG23	1.69	0.74
1:A:539:GLN:HE21	2:B:970:HIS:HB2	1.52	0.74
2:B:239:MET:SD	2:B:256:ILE:HD12	2.27	0.74
2:B:894:THR:HA	13:M:52:TRP:CH2	2.23	0.74
3:C:12:THR:H	3:C:21:PHE:HA	1.52	0.74
2:B:924:ARG:NH1	3:C:62:GLU:OE1	2.19	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:189:LYS:NZ	22:X:12:DA:OP2	2.20	0.74
1:A:1304:ILE:O	1:A:1307:VAL:HB	1.86	0.74
2:B:806:PHE:O	2:B:1050:ARG:NH1	2.21	0.74
18:R:195:PRO:O	18:R:196:ASP:CB	2.34	0.74
1:A:1310:HIS:CB	21:U:252:LYS:HZ3	1.99	0.74
17:Q:107:LEU:CA	18:R:218:LYS:CE	2.61	0.74
1:A:958:ARG:NH1	1:A:962:ASP:OD1	2.21	0.74
17:Q:106:LYS:C	18:R:218:LYS:HE3	2.08	0.74
20:T:231:ASN:HB2	23:Y:68:DC:H5"	1.68	0.74
17:Q:70:LYS:HG3	18:R:225:VAL:C	2.05	0.74
1:A:631:GLU:HG3	1:A:636:ILE:HD11	1.70	0.73
12:L:18:ILE:CD1	12:L:47:LYS:CD	2.66	0.73
17:Q:106:LYS:C	18:R:218:LYS:CE	2.57	0.73
1:A:922:PHE:HZ	1:A:952:LEU:HG	1.53	0.73
17:Q:110:MET:HE1	18:R:213:ASP:CA	2.16	0.73
1:A:611:ASP:O	1:A:612:ASP:HB2	1.87	0.73
13:M:179:GLU:N	20:T:154:LYS:HG2	2.03	0.73
2:B:132:VAL:HG23	2:B:141:GLN:HG2	1.71	0.73
3:C:200:PRO:HG3	3:C:217:GLN:CB	2.19	0.73
1:A:1304:ILE:HD12	1:A:1307:VAL:HG12	1.69	0.73
3:C:101:PHE:HB2	3:C:163:ALA:HB3	1.71	0.73
20:T:139:VAL:O	20:T:140:ARG:CB	2.37	0.73
2:B:759:VAL:HG12	2:B:999:ALA:HB2	1.71	0.73
3:C:200:PRO:HG2	3:C:217:GLN:OE1	1.89	0.73
8:H:110:THR:O	8:H:111:ARG:CB	2.37	0.73
2:B:93:LEU:N	20:T:145:LEU:CD2	2.51	0.73
3:C:200:PRO:CG	3:C:217:GLN:OE1	2.36	0.73
2:B:133:ILE:HG23	2:B:139:GLN:NE2	2.03	0.72
1:A:831:LEU:HB2	2:B:715:ASP:HB2	1.70	0.72
18:R:158:HIS:CE1	18:R:206:LYS:CE	2.71	0.72
2:B:1119:CYS:HB2	2:B:1137:CYS:SG	2.28	0.72
8:H:65:TYR:CE1	8:H:81:ARG:NH2	2.52	0.72
1:A:1310:HIS:CB	21:U:252:LYS:CG	2.65	0.72
2:B:100:GLU:OE2	2:B:116:ARG:NH1	2.22	0.72
12:L:37:ARG:O	12:L:39:CYS:N	2.22	0.72
17:Q:144:LEU:O	17:Q:153:ARG:N	2.23	0.72
19:S:126:ILE:HB	19:S:138:PHE:HB2	1.70	0.72
20:T:179:ASP:C	20:T:181:GLN:N	2.41	0.72
2:B:92:TYR:HB3	20:T:145:LEU:HD13	1.71	0.72
1:A:257:PRO:HD2	1:A:260:VAL:HB	1.71	0.72
2:B:57:ARG:NH1	2:B:60:GLU:OE1	2.23	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:105:GLU:HG3	9:I:107:ALA:CB	2.19	0.72
14:N:26:ARG:NE	14:N:36:GLU:OE1	2.21	0.72
17:Q:32:LEU:HD13	18:R:203:PHE:CE2	2.24	0.72
1:A:616:GLY:O	1:A:619:LYS:CB	2.30	0.72
2:B:252:ILE:HG13	2:B:255:ARG:HD2	1.70	0.72
21:U:218:ASP:HB2	21:U:222:ARG:HH21	1.54	0.72
8:H:111:ARG:NE	8:H:126:GLN:OE1	2.21	0.72
9:I:94:ALA:HA	9:I:114:CYS:HA	1.72	0.72
17:Q:70:LYS:HG3	18:R:225:VAL:HG12	1.71	0.72
2:B:92:TYR:CB	20:T:145:LEU:HB2	2.19	0.72
2:B:109:MET:HE1	2:B:174:LEU:HB3	1.72	0.72
1:A:1163:HIS:HA	1:A:1300:GLY:HA3	1.70	0.72
2:B:205:VAL:O	2:B:371:ARG:NH1	2.23	0.72
2:B:878:ASP:O	2:B:879:GLU:O	2.07	0.72
14:N:311:GLU:HB3	16:P:251:LEU:HD23	1.72	0.72
6:F:56:TYR:O	6:F:108:ARG:NH2	2.22	0.71
16:P:209:THR:O	16:P:210:THR:HB	1.89	0.71
2:B:92:TYR:HB3	20:T:145:LEU:CD1	2.19	0.71
1:A:1211:LEU:HD11	1:A:1258:ARG:HB2	1.71	0.71
1:A:922:PHE:HE2	1:A:952:LEU:HD23	1.27	0.71
12:L:17:TYR:O	12:L:26:ASN:N	2.20	0.71
1:A:1310:HIS:HB2	21:U:252:LYS:HZ3	1.56	0.71
1:A:734:ARG:NH2	9:I:104:ALA:O	2.23	0.71
2:B:1129:ASN:HA	2:B:1135:TYR:HA	1.71	0.71
1:A:1310:HIS:H	21:U:252:LYS:HD2	0.89	0.71
1:A:1303:GLN:HE22	1:A:1342:SER:HB3	1.55	0.71
1:A:608:THR:CB	1:A:610:PRO:HD2	2.19	0.71
1:A:790:GLN:NE2	1:A:820:ARG:O	2.22	0.71
1:A:1457:ASN:OD1	1:A:1462:GLN:NE2	2.22	0.71
1:A:546:ARG:HG3	1:A:639:ILE:HD11	1.72	0.71
9:I:99:SER:OG	9:I:105:GLU:CB	2.37	0.71
16:P:209:THR:CA	16:P:223:GLY:HA3	2.17	0.71
1:A:790:GLN:HA	1:A:822:PHE:HA	1.71	0.71
7:G:110:ARG:NH2	7:G:118:GLU:OE2	2.24	0.71
1:A:582:PRO:HD2	8:H:47:ILE:HD12	1.72	0.71
2:B:743:ARG:O	2:B:922:ARG:NH1	2.24	0.71
2:B:849:ASP:OD2	12:L:29:LYS:NZ	2.23	0.71
14:N:326:GLN:O	15:O:92:LYS:NZ	2.22	0.71
21:U:251:ALA:O	21:U:252:LYS:HB2	1.90	0.71
21:U:286:THR:HG21	21:U:299:LYS:HB3	1.72	0.71
2:B:1067:ILE:HG22	2:B:1068:GLN:H	1.55	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:803:ARG:NH1	10:J:8:PHE:O	2.24	0.70
17:Q:67:LYS:HG3	17:Q:72:ILE:HD11	1.73	0.70
20:T:176:ALA:O	20:T:208:GLN:NE2	2.24	0.70
18:R:154:LEU:CD2	18:R:162:GLY:O	2.39	0.70
15:O:79:VAL:HG21	15:O:93:VAL:HG12	1.73	0.70
13:M:106:THR:C	13:M:108:SER:N	2.44	0.70
16:P:271:GLU:N	16:P:271:GLU:OE1	2.23	0.70
3:C:47:ILE:HA	3:C:165:ALA:HA	1.73	0.70
17:Q:102:VAL:CB	17:Q:105:TYR:HD2	2.04	0.70
2:B:216:ALA:N	2:B:239:MET:O	2.25	0.70
13:M:297:PRO:HB3	13:M:310:VAL:HG21	1.73	0.70
1:A:121:SER:HA	1:A:126:ILE:HG21	1.73	0.70
2:B:983:GLU:OE2	2:B:1047:TYR:N	2.19	0.70
9:I:105:GLU:CG	9:I:107:ALA:HB3	2.22	0.70
3:C:10:ARG:NH2	3:C:24:GLU:OE2	2.23	0.70
14:N:353:LEU:HB2	14:N:370:ALA:HB3	1.74	0.70
1:A:1309:MET:SD	21:U:252:LYS:HD3	2.32	0.69
1:A:266:MET:O	1:A:267:GLN:HB2	1.90	0.69
13:M:286:ARG:HG3	13:M:316:LEU:HG	1.74	0.69
13:M:34:CYS:N	13:M:39:LEU:CB	2.22	0.69
18:R:90:GLN:NE2	18:R:172:GLU:OE2	2.25	0.69
17:Q:25:PHE:HA	18:R:215:GLU:OE1	1.93	0.69
21:U:252:LYS:CA	21:U:252:LYS:HE3	2.18	0.69
1:A:1451:MET:HE1	1:A:1460:LEU:HD22	1.74	0.69
2:B:777:ASN:O	10:J:47:ARG:NH1	2.25	0.69
5:E:80:PRO:HA	5:E:107:GLN:HB2	1.73	0.69
8:H:64:LEU:C	8:H:66:GLU:H	1.94	0.69
8:H:113:SER:OG	8:H:126:GLN:NE2	2.26	0.69
14:N:344:ARG:NH2	23:Y:78:DT:OP1	2.24	0.69
1:A:1310:HIS:HB3	21:U:252:LYS:CE	2.23	0.69
3:C:6:GLN:HG2	3:C:25:ASN:ND2	2.06	0.69
8:H:17:PRO:HG3	8:H:27:ARG:H	1.58	0.69
16:P:209:THR:HG21	16:P:224:ALA:H	1.38	0.69
17:Q:108:ASP:OD2	18:R:234:GLU:OE2	2.10	0.69
20:T:145:LEU:HD11	20:T:148:VAL:HG22	1.75	0.69
2:B:427:LYS:HE3	20:T:164:GLU:HG2	1.74	0.69
17:Q:106:LYS:CG	18:R:218:LYS:HE2	2.22	0.69
19:S:157:ALA:HA	19:S:161:GLU:HB2	1.75	0.69
1:A:1310:HIS:HB2	21:U:252:LYS:NZ	2.06	0.69
1:A:529:GLN:HE22	1:A:1097:GLU:HB3	1.55	0.69
18:R:158:HIS:CE1	18:R:206:LYS:HZ3	2.11	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:307:SER:OG	23:Y:83:DA:OP1	2.09	0.69
2:B:634:LEU:HD23	2:B:661:VAL:HA	1.75	0.69
2:B:133:ILE:CG2	2:B:139:GLN:NE2	2.55	0.68
3:C:136:ASP:O	3:C:138:ASP:N	2.22	0.68
17:Q:113:ARG:CD	18:R:217:GLN:O	2.41	0.68
20:T:179:ASP:O	20:T:181:GLN:N	2.26	0.68
1:A:475:ARG:NH2	11:K:68:GLU:OE2	2.26	0.68
1:A:551:ARG:CD	1:A:625:ASP:OD2	2.41	0.68
2:B:245:GLN:HE21	2:B:252:ILE:HD12	1.58	0.68
5:E:15:LYS:NZ	5:E:33:LEU:O	2.27	0.68
13:M:38:GLY:O	13:M:39:LEU:HB2	1.93	0.68
16:P:209:THR:HG21	16:P:224:ALA:CA	2.23	0.68
2:B:92:TYR:HB2	20:T:145:LEU:HD22	1.71	0.68
2:B:36:GLU:OE1	2:B:652:SER:OG	2.11	0.68
13:M:34:CYS:C	13:M:39:LEU:HB2	2.12	0.68
17:Q:32:LEU:CD1	18:R:203:PHE:CE2	2.76	0.68
2:B:360:LYS:HG3	2:B:553:LEU:HD23	1.74	0.68
6:F:47:ALA:HB1	6:F:51:ARG:HE	1.58	0.68
10:J:3:ILE:HG21	10:J:18:TRP:HB2	1.74	0.68
20:T:8:ASP:HB3	20:T:105:SER:HA	1.75	0.68
1:A:1287:CYS:HA	2:B:250:SER:CB	2.23	0.68
12:L:22:CYS:HB3	12:L:39:CYS:HB2	1.75	0.68
14:N:375:GLU:OE1	15:O:59:ARG:NH2	2.26	0.68
20:T:177:ARG:O	20:T:179:ASP:N	2.26	0.68
2:B:201:ALA:O	2:B:222:ARG:NH2	2.26	0.68
2:B:93:LEU:CA	20:T:145:LEU:HD23	2.23	0.68
1:A:601:ASN:HD21	1:A:632:ASN:H	1.42	0.68
1:A:71:CYS:H	1:A:75:ALA:HA	1.58	0.68
2:B:894:THR:HA	13:M:52:TRP:HH2	1.56	0.68
1:A:67:ARG:HH22	13:M:48:VAL:HG23	1.59	0.68
17:Q:110:MET:CG	18:R:218:LYS:HD2	2.24	0.68
21:U:250:MET:O	21:U:251:ALA:CB	2.41	0.68
1:A:844:ARG:NH2	2:B:500:GLN:O	2.26	0.68
3:C:253:LYS:NZ	11:K:102:GLU:OE1	2.27	0.68
13:M:134:ILE:HG12	13:M:171:GLU:HG3	1.76	0.68
16:P:163:PRO:HA	16:P:262:CYS:HB3	1.75	0.68
1:A:420:ILE:N	1:A:445:LYS:O	2.24	0.68
11:K:44:ASN:OD1	11:K:45:ILE:N	2.27	0.68
2:B:830:GLU:OE2	2:B:870:THR:OG1	2.11	0.68
14:N:353:LEU:N	14:N:370:ALA:O	2.17	0.68
17:Q:109:HIS:O	18:R:221:ARG:NE	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:213:ASP:C	18:R:215:GLU:N	2.45	0.68
1:A:653:VAL:HG23	1:A:669:TYR:CE2	2.27	0.67
2:B:1106:ARG:HA	2:B:1110:ALA:HB3	1.77	0.67
2:B:87:LYS:HB3	2:B:129:THR:HB	1.76	0.67
5:E:170:LEU:HD23	5:E:208:LEU:HB2	1.76	0.67
18:R:158:HIS:CE1	18:R:206:LYS:NZ	2.61	0.67
21:U:206:LEU:HD11	21:U:228:MET:HB3	1.76	0.67
1:A:826:SER:H	1:A:829:ALA:HB3	1.59	0.67
17:Q:105:TYR:CD1	17:Q:109:HIS:CD2	2.83	0.67
17:Q:187:ILE:HD13	18:R:211:SER:HB2	1.68	0.67
18:R:127:ASN:ND2	18:R:140:LYS:HD2	2.08	0.67
1:A:620:HIS:O	1:A:621:ILE:HG12	1.95	0.67
1:A:22:GLN:HB3	2:B:1170:ARG:HG3	1.77	0.67
3:C:53:ASP:HB3	3:C:160:ARG:HB3	1.76	0.67
7:G:99:THR:HG21	7:G:143:ILE:HD11	1.76	0.67
7:G:153:ASP:O	7:G:155:ASN:N	2.27	0.67
7:G:93:ASN:OD1	7:G:94:LYS:N	2.26	0.67
1:A:552:ASP:HB3	8:H:24:ARG:HD3	1.76	0.67
1:A:551:ARG:HD3	1:A:625:ASP:CG	2.15	0.67
1:A:1310:HIS:H	21:U:252:LYS:CE	2.07	0.67
1:A:65:ILE:HD12	1:A:263:ALA:HB3	1.76	0.67
2:B:483:ARG:NH2	2:B:527:ALA:O	2.27	0.67
5:E:64:HIS:C	5:E:65:ASN:O	2.32	0.67
18:R:210:PHE:CB	18:R:212:VAL:CG1	2.73	0.67
1:A:1314:THR:OG1	1:A:1332:GLN:NE2	2.28	0.67
1:A:874:LYS:HG3	1:A:880:ARG:HD2	1.77	0.67
8:H:85:ALA:HB1	8:H:144:LEU:HD22	1.77	0.67
19:S:166:ARG:HH11	19:S:166:ARG:HG3	1.59	0.67
19:S:49:ARG:NH1	19:S:96:GLN:O	2.25	0.67
1:A:1196:TYR:CD2	1:A:1246:ILE:HD11	2.29	0.67
18:R:220:TRP:O	18:R:223:VAL:CG2	2.42	0.67
21:U:180:ILE:HG21	21:U:187:TYR:HB2	1.76	0.67
1:A:43:TYR:HD1	1:A:45:GLU:HG2	1.59	0.67
2:B:133:ILE:HG22	2:B:139:GLN:HE22	1.60	0.67
2:B:63:PRO:HB3	2:B:408:PHE:HZ	1.59	0.67
18:R:89:HIS:CE1	18:R:139:PHE:HE2	2.13	0.67
1:A:1273:GLU:O	1:A:1274:GLU:C	2.32	0.67
8:H:85:ALA:HB3	8:H:144:LEU:HD21	1.76	0.67
17:Q:109:HIS:CB	18:R:221:ARG:HG2	2.13	0.67
8:H:75:TYR:O	8:H:77:PRO:N	2.27	0.67
17:Q:187:ILE:HG12	18:R:211:SER:OG	1.85	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:190:LEU:HD12	18:R:205:ASP:CB	2.22	0.67
1:A:418:TYR:O	1:A:447:GLU:N	2.28	0.66
2:B:501:LEU:HD11	2:B:505:LEU:HD22	1.77	0.66
1:A:885:GLN:NE2	5:E:168:ASN:OD1	2.22	0.66
10:J:21:TYR:HB2	10:J:38:LEU:HD11	1.77	0.66
12:L:25:GLU:CB	12:L:27:GLU:HG2	2.25	0.66
2:B:892:CYS:HA	13:M:52:TRP:HE1	1.58	0.66
1:A:1323:THR:HG23	1:A:1325:ASP:H	1.59	0.66
1:A:642:LYS:HD3	21:U:284:PRO:HD3	1.77	0.66
2:B:842:HIS:HE1	13:M:27:TYR:HB3	1.61	0.66
17:Q:70:LYS:CG	18:R:225:VAL:C	2.63	0.66
8:H:85:ALA:CB	8:H:144:LEU:HD22	2.26	0.66
3:C:50:VAL:HB	12:L:55:PHE:HB2	1.77	0.66
14:N:46:TRP:HZ2	15:O:11:LEU:HD12	1.60	0.66
12:L:34:ILE:HG13	12:L:42:ARG:HD2	1.78	0.66
16:P:179:ASP:OD1	16:P:181:LYS:NZ	2.29	0.66
16:P:293:TYR:HD2	16:P:302:LEU:HD13	1.61	0.66
1:A:619:LYS:O	1:A:620:HIS:HB2	1.94	0.66
3:C:67:ARG:NH1	3:C:150:ILE:O	2.28	0.66
13:M:107:MET:HE3	13:M:107:MET:N	2.10	0.66
1:A:1272:GLU:O	1:A:1274:GLU:N	2.28	0.66
2:B:848:LEU:HD21	2:B:868:GLY:HA3	1.77	0.66
3:C:99:VAL:HG13	3:C:124:SER:HB2	1.77	0.66
10:J:64:PRO:C	10:J:66:GLU:H	1.98	0.66
1:A:426:ARG:CB	13:M:40:VAL:HG21	1.94	0.66
1:A:782:SER:O	1:A:787:VAL:N	2.29	0.66
2:B:1029:TYR:OH	3:C:185:GLU:OE1	2.13	0.66
18:R:191:PHE:CB	18:R:202:PHE:CD1	2.79	0.66
1:A:361:PHE:H	2:B:1063:ALA:HA	1.61	0.66
13:M:124:MET:HA	13:M:127:ARG:NH2	2.11	0.66
3:C:200:PRO:CG	3:C:217:GLN:CB	2.74	0.65
3:C:214:ASP:OD2	3:C:216:SER:OG	2.12	0.65
10:J:63:ALA:N	10:J:64:PRO:CD	2.59	0.65
18:R:140:LYS:NZ	20:T:238:GLU:OE2	2.30	0.65
18:R:191:PHE:CB	18:R:202:PHE:CE1	2.79	0.65
1:A:923:ASP:HB3	1:A:925:THR:OG1	1.96	0.65
2:B:92:TYR:CB	20:T:145:LEU:HD13	2.27	0.65
2:B:935:PHE:HE2	2:B:945:CYS:HB2	1.62	0.65
20:T:164:GLU:OE2	20:T:167:ARG:NH2	2.29	0.65
1:A:1172:ASN:O	1:A:1215:GLU:N	2.19	0.65
1:A:784:VAL:HG23	1:A:785:ILE:HG13	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:5:ASN:C	3:C:7:PRO:CD	2.60	0.65
12:L:18:ILE:CD1	12:L:47:LYS:HE3	2.19	0.65
22:X:17:DA:H2"	22:X:18:DG:C8	2.31	0.65
1:A:275:ASP:HB2	1:A:342:ARG:NH2	2.10	0.65
1:A:551:ARG:HD3	1:A:625:ASP:OD2	1.96	0.65
1:A:1117:VAL:O	1:A:1118:THR:C	2.34	0.65
1:A:1304:ILE:CD1	1:A:1307:VAL:HG11	2.22	0.65
1:A:434:LYS:HB2	1:A:437:ASP:HB3	1.79	0.65
1:A:1290:SER:HB3	2:B:250:SER:O	1.97	0.65
17:Q:23:ARG:NH2	18:R:206:LYS:CB	2.60	0.65
2:B:102:ASP:O	13:M:217:ARG:NE	2.27	0.65
2:B:65:ILE:HG21	2:B:412:LEU:HD11	1.76	0.65
16:P:209:THR:CG2	16:P:224:ALA:CA	2.73	0.65
1:A:1146:GLN:O	1:A:1150:ASP:N	2.27	0.64
1:A:1147:SER:OG	1:A:1351:ASP:OD2	2.15	0.64
2:B:93:LEU:HD12	2:B:123:PRO:O	1.98	0.64
16:P:209:THR:HG22	16:P:223:GLY:HA3	1.71	0.64
1:A:113:PHE:CE1	18:R:229:ASP:N	2.62	0.64
1:A:924:TYR:HD1	1:A:949:GLN:HE22	1.15	0.64
7:G:91:GLN:HB2	7:G:98:PHE:HD2	1.63	0.64
8:H:74:GLU:C	8:H:76:ASN:N	2.40	0.64
11:K:77:THR:OG1	11:K:81:TYR:O	2.14	0.64
1:A:370:ASP:HB2	1:A:483:ARG:HB3	1.80	0.64
2:B:714:PRO:HD2	2:B:1001:PRO:HB3	1.77	0.64
2:B:499:ARG:HB3	2:B:499:ARG:CZ	2.27	0.64
1:A:1253:GLU:HG2	1:A:1254:LYS:HG2	1.79	0.64
1:A:1310:HIS:HE1	1:A:1334:TRP:HA	1.61	0.64
3:C:13:GLU:O	3:C:20:LYS:N	2.30	0.64
17:Q:106:LYS:HG2	18:R:218:LYS:CE	2.27	0.64
19:S:126:ILE:N	19:S:138:PHE:O	2.23	0.64
1:A:1244:ASN:HB3	1:A:1260:ARG:HB2	1.79	0.64
17:Q:105:TYR:CD1	17:Q:109:HIS:NE2	2.66	0.64
3:C:258:ASP:OD2	11:K:18:LYS:NZ	2.31	0.64
9:I:103:ARG:C	9:I:105:GLU:H	2.00	0.64
12:L:15:MET:C	12:L:16:ILE:HG23	2.15	0.64
16:P:160:GLY:C	16:P:161:ILE:HG12	2.17	0.64
11:K:29:ASN:ND2	11:K:78:THR:O	2.30	0.64
18:R:161:ARG:NE	18:R:203:PHE:CE1	2.60	0.64
17:Q:110:MET:HE1	18:R:213:ASP:HA	1.79	0.64
20:T:158:ASN:HB3	20:T:161:TYR:HB3	1.79	0.64
2:B:646:ARG:HD3	2:B:651:TYR:N	2.13	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:874:PRO:O	2:B:876:ASN:N	2.27	0.64
13:M:106:THR:HB	13:M:109:SER:OG	1.96	0.64
20:T:179:ASP:CG	20:T:182:HIS:HB3	2.18	0.64
1:A:1250:ASP:HA	1:A:1255:LEU:HD21	1.78	0.64
1:A:1288:ILE:O	1:A:1292:MET:N	2.27	0.64
8:H:10:PHE:N	8:H:56:PHE:O	2.28	0.64
1:A:1310:HIS:HB3	21:U:252:LYS:CD	2.28	0.63
1:A:629:VAL:HG13	1:A:636:ILE:HB	1.81	0.63
1:A:1036:ASN:HB2	5:E:202:ARG:HB3	1.78	0.63
2:B:1107:LEU:O	2:B:1111:SER:OG	2.15	0.63
16:P:166:GLN:HG3	23:Y:81:DA:H5"	1.80	0.63
17:Q:17:LEU:HD13	17:Q:194:THR:HB	1.80	0.63
2:B:829:PHE:HE1	2:B:869:LYS:HD3	1.63	0.63
9:I:103:ARG:C	9:I:105:GLU:N	2.51	0.63
14:N:368:SER:N	15:O:54:ASN:O	2.25	0.63
2:B:692:THR:HB	9:I:76:PRO:HB2	1.79	0.63
2:B:840:MET:O	2:B:842:HIS:N	2.31	0.63
12:L:26:ASN:HA	12:L:37:ARG:HH12	1.63	0.63
18:R:155:LEU:CB	18:R:204:ASN:ND2	2.59	0.63
1:A:622:SER:C	1:A:624:GLY:N	2.51	0.63
1:A:514:GLU:OE2	2:B:1101:GLN:HB2	1.99	0.63
14:N:333:ASN:HB3	14:N:359:ASN:O	1.99	0.63
1:A:619:LYS:O	1:A:620:HIS:CB	2.46	0.63
5:E:27:LEU:HD12	5:E:64:HIS:CD2	2.33	0.63
11:K:18:LYS:O	11:K:36:ASN:N	2.23	0.63
17:Q:102:VAL:HB	17:Q:105:TYR:HD2	1.62	0.63
1:A:485:ASN:HB3	1:A:488:VAL:HG23	1.79	0.63
1:A:497:ASP:HB2	2:B:942:LYS:HE3	1.80	0.63
1:A:1313:GLN:HG2	1:A:1333:GLU:CG	2.26	0.63
17:Q:109:HIS:HB3	18:R:221:ARG:CD	2.28	0.63
17:Q:25:PHE:HD2	18:R:215:GLU:OE2	1.80	0.63
2:B:1087:GLY:N	2:B:1090:GLU:OE1	2.28	0.62
2:B:765:GLU:O	2:B:768:ARG:NH1	2.31	0.62
13:M:297:PRO:HA	13:M:310:VAL:HG11	1.82	0.62
1:A:191:ILE:HD12	1:A:216:LEU:HD11	1.81	0.62
2:B:779:ILE:HA	2:B:1045:PRO:HA	1.80	0.62
2:B:956:PHE:O	2:B:1029:TYR:N	2.23	0.62
9:I:92:LYS:NZ	9:I:93:GLU:OE2	2.32	0.62
10:J:40:LEU:O	10:J:46:ARG:NE	2.32	0.62
2:B:513:GLU:O	2:B:525:ASN:ND2	2.32	0.62
3:C:129:PRO:HG2	3:C:134:ASN:HD22	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:47:ILE:HG21	3:C:68:LEU:HD23	1.80	0.62
8:H:84:ARG:O	8:H:86:ASP:N	2.31	0.62
17:Q:113:ARG:HB2	18:R:221:ARG:HD2	1.81	0.62
1:A:1208:SER:O	1:A:1260:ARG:NH1	2.31	0.62
1:A:939:VAL:HA	1:A:942:VAL:HG22	1.81	0.62
8:H:85:ALA:O	8:H:144:LEU:HD22	1.99	0.62
9:I:58:ILE:O	9:I:59:THR:CB	2.47	0.62
1:A:43:TYR:CD1	1:A:45:GLU:HG2	2.34	0.62
1:A:1290:SER:CB	2:B:250:SER:O	2.48	0.62
13:M:173:VAL:HB	13:M:175:ARG:HH12	1.64	0.62
17:Q:113:ARG:HE	18:R:217:GLN:HB3	1.64	0.62
3:C:35:ARG:HA	3:C:38:PHE:CD2	2.35	0.62
1:A:1080:ILE:HD13	6:F:54:THR:HG21	1.82	0.62
2:B:322:GLY:HA3	2:B:335:ARG:HB3	1.81	0.62
2:B:838:GLN:OE1	2:B:886:ARG:NH1	2.33	0.62
1:A:948:ILE:HG13	1:A:1007:ILE:HD11	1.81	0.62
2:B:831:LYS:NZ	2:B:845:TYR:O	2.27	0.62
9:I:95:VAL:N	9:I:113:VAL:O	2.24	0.62
2:B:808:SER:OG	2:B:1050:ARG:NH1	2.33	0.62
3:C:56:SER:OG	3:C:158:GLU:N	2.33	0.62
17:Q:102:VAL:O	17:Q:105:TYR:N	2.33	0.62
17:Q:22:ILE:HG22	17:Q:34:LEU:HD13	1.81	0.62
2:B:226:GLU:OE1	2:B:227:ASN:ND2	2.33	0.62
2:B:801:VAL:HA	2:B:805:PHE:HB3	1.81	0.62
3:C:110:ASP:HA	3:C:155:LYS:HD2	1.82	0.62
5:E:107:GLN:HG2	5:E:132:GLN:NE2	2.15	0.62
6:F:78:PRO:HD3	7:G:16:ARG:HA	1.82	0.62
14:N:34:VAL:HG11	15:O:28:ILE:HG22	1.82	0.62
18:R:190:LEU:CD1	18:R:205:ASP:CB	2.72	0.62
1:A:934:LEU:O	1:A:936:GLU:N	2.30	0.61
12:L:16:ILE:HG13	12:L:28:ILE:H	1.64	0.61
17:Q:110:MET:CA	18:R:218:LYS:HG3	2.29	0.61
20:T:31:TRP:HD1	20:T:62:LEU:HD21	1.64	0.61
1:A:1204:VAL:HA	1:A:1207:ILE:HG23	1.81	0.61
2:B:194:LEU:HD11	2:B:466:VAL:HG12	1.81	0.61
5:E:149:VAL:HB	5:E:192:LYS:HB3	1.80	0.61
8:H:9:ILE:O	8:H:33:GLU:HG2	1.99	0.61
1:A:1272:GLU:C	1:A:1274:GLU:H	2.03	0.61
1:A:931:ARG:O	1:A:933:THR:N	2.32	0.61
20:T:177:ARG:NH2	20:T:212:TYR:HB2	2.15	0.61
1:A:621:ILE:HG22	1:A:621:ILE:O	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:87:LYS:O	2:B:129:THR:N	2.23	0.61
3:C:1:MET:HG3	3:C:2:PRO:HD2	1.82	0.61
6:F:100:ARG:HB2	6:F:120:VAL:HG12	1.83	0.61
8:H:96:VAL:HB	8:H:136:GLU:HA	1.83	0.61
8:H:65:TYR:CE1	8:H:81:ARG:NE	2.67	0.61
16:P:297:LYS:HB2	16:P:298:PRO:CD	2.21	0.61
1:A:208:ASP:OD2	1:A:212:LYS:NZ	2.33	0.61
2:B:788:TYR:HB2	2:B:795:ILE:HD11	1.81	0.61
8:H:85:ALA:HB3	8:H:144:LEU:CD2	2.31	0.61
9:I:87:GLN:HE21	9:I:121:HIS:HB3	1.65	0.61
12:L:18:ILE:O	12:L:45:TYR:HB3	2.00	0.61
15:O:59:ARG:O	15:O:80:GLU:N	2.32	0.61
1:A:85:PHE:CD1	1:A:257:PRO:HD3	2.36	0.61
2:B:50:PHE:HA	2:B:54:SER:HB2	1.83	0.61
7:G:58:VAL:HB	7:G:67:LEU:HB3	1.82	0.61
16:P:192:TYR:HB2	16:P:200:VAL:HG22	1.83	0.61
1:A:72:GLN:HE22	1:A:84:HIS:CD2	2.18	0.61
1:A:784:VAL:HA	1:A:827:TYR:HB2	1.83	0.61
1:A:922:PHE:HZ	1:A:952:LEU:CG	2.13	0.61
1:A:1290:SER:OG	2:B:250:SER:O	2.19	0.61
5:E:104:ILE:O	5:E:129:GLN:NE2	2.33	0.61
13:M:34:CYS:O	13:M:39:LEU:CB	2.44	0.61
18:R:142:LYS:HE2	18:R:144:ASN:HB3	1.83	0.61
20:T:20:LEU:O	20:T:114:ALA:N	2.34	0.61
1:A:275:ASP:HA	1:A:278:HIS:ND1	2.16	0.61
1:A:926:ASN:HD21	1:A:931:ARG:HD2	1.62	0.61
5:E:63:ALA:O	5:E:64:HIS:CG	2.54	0.61
13:M:40:VAL:C	13:M:42:GLY:H	2.04	0.61
21:U:251:ALA:O	21:U:252:LYS:CB	2.49	0.61
1:A:1347:LEU:HB3	5:E:137:ILE:HG12	1.82	0.61
1:A:693:ILE:HG13	2:B:1023:ARG:HE	1.63	0.61
2:B:405:ARG:O	2:B:409:LYS:HG3	2.00	0.61
2:B:67:LEU:HD22	2:B:419:ALA:HB1	1.83	0.61
7:G:11:ILE:O	7:G:68:TYR:N	2.25	0.61
1:A:622:SER:C	1:A:624:GLY:H	2.04	0.61
1:A:18:ILE:HG21	2:B:1171:MET:HG3	1.83	0.61
2:B:713:PHE:HB3	2:B:716:HIS:ND1	2.15	0.61
5:E:48:PRO:HD2	5:E:52:ARG:HD2	1.82	0.61
8:H:105:SER:O	8:H:106:THR:CB	2.48	0.61
17:Q:106:LYS:HZ3	18:R:219:LEU:HD13	1.64	0.61
1:A:1248:ASN:ND2	1:A:1254:LYS:O	2.28	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:426:ARG:CG	13:M:40:VAL:HG11	2.30	0.60
1:A:611:ASP:CB	1:A:617:PRO:HG3	2.29	0.60
2:B:37:LYS:HE2	2:B:653:TRP:CD1	2.36	0.60
14:N:341:LYS:HB3	14:N:352:HIS:HB2	1.80	0.60
16:P:161:ILE:O	16:P:161:ILE:HG22	1.99	0.60
17:Q:25:PHE:HE2	18:R:215:GLU:HG3	1.61	0.60
1:A:935:GLN:HA	1:A:1001:PRO:HA	1.81	0.60
2:B:225:LEU:HD13	2:B:228:SER:HB2	1.83	0.60
8:H:103:GLU:HG2	8:H:109:ALA:HB2	1.83	0.60
8:H:31:GLU:HA	8:H:38:ASP:HA	1.82	0.60
12:L:15:MET:HG3	12:L:47:LYS:HB2	1.83	0.60
18:R:127:ASN:HD21	18:R:140:LYS:HE2	1.64	0.60
23:Y:59:DG:H2'	23:Y:60:DA:C8	2.36	0.60
1:A:1306:LYS:O	1:A:1307:VAL:HG12	2.00	0.60
1:A:47:THR:O	1:A:48:GLU:CB	2.48	0.60
4:D:103:LEU:HD22	7:G:144:ARG:HH12	1.64	0.60
2:B:91:ILE:HG22	20:T:142:SER:OG	2.02	0.60
8:H:64:LEU:C	8:H:66:GLU:N	2.55	0.60
17:Q:108:ASP:HB2	18:R:234:GLU:OE2	1.99	0.60
1:A:620:HIS:O	1:A:621:ILE:CB	2.47	0.60
1:A:628:VAL:HA	1:A:638:GLY:HA3	1.83	0.60
2:B:600:GLU:O	2:B:620:ARG:NH2	2.30	0.60
2:B:568:PHE:O	2:B:614:ILE:N	2.34	0.60
6:F:96:GLU:O	6:F:100:ARG:N	2.34	0.60
9:I:22:ASN:OD1	9:I:41:ASN:ND2	2.35	0.60
14:N:308:GLN:NE2	14:N:310:GLU:O	2.28	0.60
15:O:86:GLU:HG3	15:O:88:ILE:HD11	1.83	0.60
20:T:224:ASN:HB3	20:T:226:LYS:HG2	1.82	0.60
20:T:228:ILE:HD12	20:T:230:LYS:HD3	1.83	0.60
1:A:1143:LEU:HB3	1:A:1147:SER:HB2	1.83	0.60
16:P:209:THR:HG22	16:P:223:GLY:N	2.08	0.60
12:L:22:CYS:SG	12:L:24:THR:OG1	2.56	0.60
20:T:20:LEU:N	20:T:112:GLN:O	2.28	0.60
1:A:1112:VAL:HA	21:U:254:GLY:HA3	1.83	0.60
2:B:655:ASP:O	2:B:659:SER:N	2.35	0.60
2:B:737:ILE:HD11	2:B:743:ARG:HG3	1.83	0.60
4:D:108:ALA:N	4:D:128:GLN:OE1	2.32	0.60
8:H:98:ARG:HD3	8:H:115:TYR:HD2	1.66	0.60
19:S:47:LEU:HD22	20:T:7:LEU:HD22	1.84	0.60
1:A:47:THR:O	1:A:48:GLU:HB2	2.02	0.60
2:B:117:ASN:HA	2:B:189:GLY:HA3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:162:VAL:HG23	16:P:162:VAL:O	2.02	0.60
18:R:155:LEU:HG	18:R:204:ASN:HD22	0.77	0.60
4:D:26:PHE:HZ	7:G:42:TYR:HA	1.66	0.60
11:K:20:THR:N	11:K:34:THR:O	2.28	0.60
1:A:1212:LEU:HD23	1:A:1259:ILE:HD11	1.83	0.59
14:N:318:ASP:OD1	16:P:239:ARG:HD2	2.01	0.59
17:Q:70:LYS:HB2	18:R:225:VAL:HG12	1.83	0.59
20:T:155:PRO:O	20:T:157:ALA:N	2.27	0.59
1:A:1394:ASN:HB3	1:A:1397:HIS:ND1	2.17	0.59
3:C:146:ASP:O	3:C:148:ILE:N	2.36	0.59
21:U:256:THR:O	21:U:257:GLN:O	2.20	0.59
1:A:593:SER:HB3	1:A:634:GLU:HA	1.84	0.59
2:B:56:GLN:O	2:B:60:GLU:N	2.30	0.59
3:C:106:ARG:NE	3:C:108:ASN:OD1	2.35	0.59
3:C:183:ALA:HB3	3:C:232:ASN:HB3	1.84	0.59
8:H:14:ASP:HB3	8:H:29:HIS:HB2	1.85	0.59
19:S:102:VAL:O	19:S:108:ARG:N	2.35	0.59
1:A:1028:PRO:O	1:A:1032:GLN:N	2.34	0.59
1:A:1310:HIS:CB	21:U:252:LYS:CD	2.81	0.59
1:A:544:ALA:HB2	1:A:680:LEU:HD13	1.83	0.59
17:Q:106:LYS:C	18:R:218:LYS:HE2	2.21	0.59
19:S:126:ILE:O	19:S:138:PHE:N	2.35	0.59
13:M:178:LYS:C	20:T:154:LYS:HB2	2.21	0.59
2:B:240:LEU:HD23	2:B:257:VAL:CG1	2.33	0.59
11:K:21:ILE:HG23	11:K:33:PHE:CE1	2.38	0.59
1:A:816:GLY:O	1:A:819:SER:OG	2.14	0.59
2:B:175:ASN:O	2:B:739:ASN:ND2	2.32	0.59
20:T:222:VAL:HG22	20:T:223:GLN:H	1.67	0.59
1:A:880:ARG:NH1	1:A:884:ASN:O	2.35	0.59
2:B:897:ARG:NH1	2:B:1079:SER:OG	2.35	0.59
2:B:873:LEU:HB3	2:B:874:PRO:HD3	1.80	0.59
2:B:92:TYR:C	20:T:145:LEU:CD2	2.70	0.59
6:F:44:ARG:H	6:F:45:PRO:HD2	1.67	0.59
9:I:119:CYS:SG	9:I:120:GLY:N	2.76	0.59
1:A:686:THR:HG21	2:B:1041:ILE:HG13	1.84	0.59
3:C:217:GLN:O	3:C:218:ALA:HB2	1.99	0.59
6:F:51:ARG:NH1	6:F:122:GLU:OE1	2.34	0.59
9:I:112:TYR:N	9:I:123:TRP:O	2.34	0.59
14:N:21:VAL:HG11	15:O:40:PHE:HD1	1.68	0.59
1:A:1168:LYS:HG3	1:A:1220:HIS:CE1	2.37	0.59
2:B:240:LEU:CG	2:B:255:ARG:O	2.49	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:556:ILE:HD12	2:B:561:ILE:HG21	1.84	0.59
8:H:3:GLY:N	8:H:67:ASP:OD1	2.34	0.59
17:Q:102:VAL:HB	17:Q:105:TYR:CG	2.37	0.59
1:A:1264:SER:O	1:A:1266:GLU:N	2.33	0.59
1:A:611:ASP:O	1:A:612:ASP:CB	2.50	0.59
1:A:479:TRP:N	11:K:2:ASN:O	2.35	0.59
17:Q:131:VAL:HG21	17:Q:159:THR:HG21	1.85	0.59
2:B:1022:LEU:HD12	2:B:1023:ARG:HG2	1.85	0.58
5:E:13:ILE:HG22	5:E:136:LEU:HA	1.85	0.58
13:M:182:ALA:HB2	20:T:154:LYS:HA	1.84	0.58
17:Q:102:VAL:CG2	17:Q:105:TYR:HD2	2.16	0.58
2:B:1115:GLN:HB2	2:B:1148:LEU:HD11	1.84	0.58
2:B:63:PRO:HB3	2:B:408:PHE:CZ	2.38	0.58
2:B:542:LEU:HA	2:B:545:LEU:HD12	1.85	0.58
17:Q:106:LYS:HG2	18:R:218:LYS:CG	2.32	0.58
2:B:1036:LYS:HB2	3:C:194:HIS:HB3	1.85	0.58
2:B:866:ILE:H	2:B:895:PHE:HA	1.67	0.58
20:T:139:VAL:O	20:T:140:ARG:HB2	2.02	0.58
1:A:565:MET:HG2	11:K:61:TYR:C	2.24	0.58
2:B:573:TRP:CZ2	2:B:576:ILE:HG23	2.38	0.58
17:Q:104:LYS:NZ	18:R:238:LYS:HD2	2.18	0.58
2:B:430:ASN:HB2	20:T:159:HIS:HE1	1.67	0.58
1:A:286:ILE:HD13	1:A:313:HIS:CD2	2.38	0.58
1:A:381:PRO:HB3	11:K:2:ASN:HD21	1.68	0.58
1:A:73:THR:OG1	2:B:1130:THR:OG1	2.14	0.58
2:B:548:TRP:CD1	2:B:583:LEU:HD13	2.38	0.58
2:B:88:PHE:CD2	2:B:128:ILE:HG12	2.37	0.58
8:H:85:ALA:CB	8:H:144:LEU:CD2	2.82	0.58
10:J:63:ALA:H	10:J:64:PRO:CD	2.16	0.58
14:N:49:LYS:NZ	15:O:17:GLU:OE1	2.25	0.58
2:B:171:LEU:HD22	2:B:176:GLU:HG2	1.84	0.58
10:J:12:LYS:HE2	10:J:40:LEU:HA	1.86	0.58
12:L:18:ILE:O	12:L:18:ILE:HG22	2.03	0.58
1:A:330:GLN:CG	13:M:107:MET:SD	2.91	0.58
20:T:154:LYS:N	20:T:154:LYS:HD2	2.17	0.58
1:A:1223:ASP:OD2	1:A:1224:ARG:NE	2.36	0.58
1:A:47:THR:HG23	1:A:53:LYS:HA	1.86	0.58
2:B:755:GLN:HB2	2:B:776:ILE:HA	1.85	0.58
2:B:718:GLN:NE2	2:B:975:ARG:O	2.32	0.58
7:G:6:SER:HA	7:G:73:LYS:HA	1.85	0.58
8:H:110:THR:O	8:H:111:ARG:HB3	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:143:LYS:NZ	21:U:147:MET:SD	2.75	0.58
1:A:423:ASN:ND2	1:A:425:ASP:OD2	2.31	0.58
1:A:922:PHE:CZ	1:A:952:LEU:CG	2.87	0.58
2:B:897:ARG:HD2	2:B:1079:SER:HA	1.85	0.58
17:Q:25:PHE:HB3	18:R:215:GLU:OE2	2.04	0.58
1:A:1187:ALA:HA	1:A:1190:GLN:HB2	1.84	0.58
1:A:555:LEU:HD22	1:A:591:ILE:HG13	1.84	0.58
1:A:607:SER:HB2	1:A:641:CYS:SG	2.44	0.58
1:A:797:ARG:HB3	1:A:820:ARG:HB3	1.85	0.58
2:B:936:ALA:HB2	2:B:1051:LEU:HD11	1.86	0.58
9:I:98:GLN:NE2	9:I:108:MET:HG3	2.18	0.58
11:K:11:LEU:O	11:K:37:LYS:NZ	2.36	0.58
16:P:160:GLY:O	16:P:161:ILE:CG1	2.43	0.58
7:G:98:PHE:HZ	17:Q:152:PHE:CE1	2.22	0.58
21:U:200:ASP:OD2	21:U:203:ASN:ND2	2.30	0.58
2:B:224:CYS:HB2	2:B:230:ARG:HA	1.86	0.58
7:G:78:ARG:NH1	7:G:79:PRO:O	2.37	0.58
16:P:209:THR:O	16:P:210:THR:CB	2.51	0.58
17:Q:113:ARG:HE	18:R:217:GLN:C	2.06	0.58
19:S:112:GLY:HA2	19:S:145:ASN:O	2.04	0.58
1:A:1164:THR:N	1:A:1299:GLN:O	2.35	0.57
3:C:77:ASP:HB2	3:C:128:ILE:HG22	1.85	0.57
17:Q:106:LYS:HZ1	18:R:219:LEU:HD13	1.68	0.57
4:D:23:PRO:O	4:D:27:GLU:N	2.35	0.57
5:E:44:SER:OG	5:E:46:ASP:HB2	2.04	0.57
10:J:64:PRO:C	10:J:66:GLU:N	2.55	0.57
16:P:180:LEU:HB3	16:P:200:VAL:HG23	1.86	0.57
17:Q:32:LEU:HD13	18:R:161:ARG:NH2	2.19	0.57
18:R:213:ASP:O	18:R:215:GLU:CB	2.52	0.57
19:S:31:PHE:HB2	20:T:92:THR:HB	1.86	0.57
1:A:44:PRO:HG3	1:A:284:VAL:HB	1.85	0.57
2:B:257:VAL:O	2:B:257:VAL:HG23	2.03	0.57
2:B:552:ASN:OD1	2:B:553:LEU:N	2.37	0.57
14:N:314:LEU:HD11	16:P:238:ALA:HB1	1.86	0.57
1:A:1037:ALA:HA	5:E:200:ALA:HB1	1.86	0.57
2:B:1072:ARG:HE	2:B:1113:PRO:HD2	1.68	0.57
13:M:295:ARG:HG2	13:M:299:LEU:HG	1.86	0.57
20:T:12:ALA:HA	20:T:109:ILE:HD11	1.85	0.57
5:E:110:MET:HB2	5:E:115:LYS:HE3	1.87	0.57
11:K:7:PHE:HA	11:K:10:PHE:CE2	2.39	0.57
17:Q:25:PHE:CD2	18:R:215:GLU:OE2	2.56	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1307:VAL:CG2	1:A:1339:ASP:N	2.65	0.57
2:B:411:LEU:HD12	2:B:440:ILE:HD11	1.86	0.57
3:C:193:ARG:NH2	3:C:218:ALA:O	2.38	0.57
16:P:296:ILE:O	16:P:297:LYS:C	2.42	0.57
1:A:426:ARG:HB3	13:M:40:VAL:CG2	2.28	0.57
1:A:66:GLU:O	1:A:68:THR:N	2.38	0.57
2:B:240:LEU:CD2	2:B:257:VAL:HG11	2.34	0.57
10:J:43:TYR:HA	10:J:46:ARG:HB2	1.86	0.57
14:N:354:LYS:HA	14:N:369:LYS:HA	1.86	0.57
17:Q:23:ARG:CZ	18:R:207:SER:CB	2.76	0.57
16:P:301:VAL:HG11	22:X:14:DA:H5"	1.85	0.57
1:A:21:VAL:HB	1:A:1449:ASP:HB3	1.87	0.57
1:A:642:LYS:HZ3	21:U:283:GLU:HA	1.69	0.57
2:B:1114:TYR:CE1	2:B:1153:TYR:HD2	2.22	0.57
2:B:823:PHE:HD1	13:M:140:ASN:HB3	1.69	0.57
18:R:210:PHE:CB	18:R:212:VAL:HG13	2.34	0.57
21:U:230:SER:O	21:U:231:ASP:HB3	2.05	0.57
5:E:148:HIS:HB2	5:E:183:PHE:CZ	2.40	0.57
17:Q:129:CYS:SG	17:Q:159:THR:OG1	2.62	0.57
18:R:195:PRO:O	18:R:196:ASP:HB3	2.02	0.57
18:R:195:PRO:O	18:R:199:LYS:HD2	2.04	0.57
19:S:8:SER:HB3	20:T:49:GLN:HA	1.86	0.57
1:A:1313:GLN:CB	1:A:1333:GLU:HG2	2.35	0.57
1:A:1313:GLN:HB2	1:A:1333:GLU:HG2	1.85	0.57
1:A:922:PHE:HE2	1:A:952:LEU:HD21	1.68	0.57
2:B:490:GLY:O	2:B:491:ARG:O	2.23	0.57
16:P:293:TYR:HB3	16:P:302:LEU:HB2	1.87	0.57
1:A:202:TRP:HB2	1:A:212:LYS:HE2	1.88	0.56
2:B:488:PRO:O	2:B:489:ILE:HG13	2.04	0.56
3:C:136:ASP:HB2	3:C:145:GLN:CD	2.22	0.56
3:C:205:LYS:HB3	3:C:209:SER:OG	2.05	0.56
12:L:18:ILE:HB	12:L:45:TYR:HD2	1.70	0.56
13:M:173:VAL:O	13:M:175:ARG:NH1	2.38	0.56
15:O:66:ARG:HD3	16:P:185:LEU:HA	1.87	0.56
15:O:66:ARG:NE	16:P:185:LEU:O	2.37	0.56
1:A:275:ASP:HB2	1:A:342:ARG:HH22	1.70	0.56
3:C:115:VAL:O	3:C:150:ILE:N	2.36	0.56
3:C:101:PHE:N	3:C:163:ALA:O	2.27	0.56
17:Q:187:ILE:HG21	18:R:212:VAL:C	2.19	0.56
2:B:239:MET:HE1	2:B:256:ILE:CD1	2.28	0.56
13:M:169:ARG:NH1	13:M:207:ASP:O	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:214:PHE:HB3	13:M:218:PHE:CE2	2.40	0.56
17:Q:128:LYS:NZ	17:Q:133:SER:O	2.37	0.56
8:H:7:GLU:HG3	8:H:59:VAL:HG22	1.87	0.56
2:B:803:ARG:HD3	10:J:8:PHE:HA	1.88	0.56
12:L:33:PRO:HG2	12:L:35:ARG:HG2	1.87	0.56
13:M:279:GLY:HA2	20:T:153:TYR:CE1	2.40	0.56
18:R:155:LEU:CD2	18:R:204:ASN:HD21	2.11	0.56
2:B:92:TYR:CA	20:T:145:LEU:HD22	2.33	0.56
1:A:891:TYR:CZ	1:A:1087:VAL:HG21	2.41	0.56
1:A:1246:ILE:HG23	1:A:1258:ARG:HG3	1.86	0.56
1:A:620:HIS:O	1:A:621:ILE:CG1	2.53	0.56
3:C:48:ASP:HB3	3:C:166:LYS:HD2	1.86	0.56
3:C:6:GLN:CG	3:C:25:ASN:HD22	2.18	0.56
17:Q:70:LYS:CB	18:R:225:VAL:HG12	2.36	0.56
1:A:1196:TYR:HD2	1:A:1246:ILE:HD11	1.68	0.56
1:A:924:TYR:HE1	1:A:949:GLN:NE2	1.93	0.56
4:D:15:GLU:HG2	4:D:23:PRO:HD3	1.87	0.56
10:J:63:ALA:H	10:J:64:PRO:HD2	1.71	0.56
1:A:181:HIS:O	1:A:181:HIS:ND1	2.38	0.56
1:A:357:LYS:O	2:B:1086:PHE:N	2.36	0.56
1:A:375:ILE:HD11	1:A:666:ARG:HE	1.68	0.56
2:B:876:ASN:OD1	2:B:879:GLU:CD	2.43	0.56
12:L:25:GLU:HB2	12:L:27:GLU:CG	2.33	0.56
1:A:740:GLN:O	1:A:743:ARG:HG2	2.05	0.56
2:B:225:LEU:H	2:B:231:PRO:HD2	1.71	0.56
2:B:626:LEU:HD22	2:B:633:LEU:HD11	1.87	0.56
2:B:829:PHE:CE1	2:B:869:LYS:HD3	2.40	0.56
20:T:138:PRO:C	20:T:140:ARG:H	2.09	0.56
1:A:329:MET:HE1	1:A:335:PRO:HA	1.87	0.56
1:A:686:THR:HG21	2:B:1041:ILE:HA	1.88	0.56
8:H:107:GLU:O	8:H:108:ALA:C	2.44	0.56
17:Q:113:ARG:HE	18:R:217:GLN:CA	2.18	0.56
17:Q:104:LYS:HZ1	18:R:238:LYS:HE3	1.70	0.56
19:S:166:ARG:CG	19:S:166:ARG:HH11	2.19	0.56
13:M:179:GLU:HG2	20:T:154:LYS:HE3	1.88	0.56
6:F:79:VAL:HG12	6:F:81:VAL:H	1.71	0.56
7:G:63:ARG:NH2	7:G:65:PHE:O	2.38	0.56
2:B:156:LEU:HB2	2:B:183:GLY:H	1.71	0.56
2:B:591:ARG:HA	2:B:596:ILE:HB	1.88	0.56
2:B:633:LEU:HG	2:B:635:LEU:H	1.71	0.56
3:C:205:LYS:NZ	3:C:213:GLU:OE2	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:63:PHE:O	3:C:67:ARG:HG3	2.06	0.56
1:A:1209:PRO:HB3	9:I:33:ARG:NH1	2.19	0.55
1:A:1307:VAL:O	1:A:1307:VAL:HG22	2.06	0.55
1:A:47:THR:HA	1:A:54:LEU:HG	1.87	0.55
1:A:85:PHE:HD1	1:A:257:PRO:HD3	1.70	0.55
2:B:485:LEU:HB2	2:B:524:LYS:HB2	1.88	0.55
2:B:676:ALA:N	2:B:695:HIS:O	2.33	0.55
2:B:814:TYR:N	2:B:921:ILE:O	2.32	0.55
5:E:30:GLN:O	5:E:34:ASP:N	2.34	0.55
13:M:214:PHE:O	13:M:218:PHE:HD2	1.89	0.55
14:N:318:ASP:OD1	16:P:239:ARG:CD	2.50	0.55
9:I:59:THR:O	9:I:59:THR:HG22	2.05	0.55
17:Q:141:ALA:HB1	17:Q:152:PHE:CE1	2.40	0.55
17:Q:187:ILE:C	18:R:212:VAL:HA	2.26	0.55
1:A:364:ARG:NH1	1:A:461:GLN:OE1	2.39	0.55
1:A:372:ASN:ND2	1:A:372:ASN:O	2.38	0.55
2:B:268:PRO:HB2	2:B:271:ILE:HG12	1.88	0.55
2:B:837:CYS:HB2	2:B:889:LYS:HD2	1.88	0.55
13:M:17:ASN:OD1	13:M:18:HIS:ND1	2.39	0.55
17:Q:102:VAL:HG21	17:Q:105:TYR:HD2	1.71	0.55
4:D:79:THR:HG23	4:D:137:LYS:HG2	1.89	0.55
20:T:217:LEU:HB3	20:T:233:TRP:CE3	2.40	0.55
1:A:408:ARG:NH1	1:A:414:PRO:HB2	2.21	0.55
1:A:43:TYR:CD2	1:A:44:PRO:HD2	2.42	0.55
1:A:922:PHE:N	1:A:922:PHE:CD1	2.74	0.55
5:E:54:ARG:O	5:E:58:LEU:N	2.35	0.55
9:I:68:ILE:HG23	9:I:122:ARG:HD2	1.88	0.55
15:O:67:PHE:HB2	15:O:72:TRP:CE3	2.41	0.55
16:P:288:PHE:CD1	16:P:289:PRO:HD2	2.42	0.55
1:A:1280:ASP:HB3	1:A:1283:VAL:HG22	1.87	0.55
1:A:489:THR:O	1:A:493:ASN:N	2.39	0.55
1:A:516:GLN:HA	1:A:520:MET:HG2	1.89	0.55
1:A:46:THR:HA	1:A:57:LEU:HD13	1.89	0.55
2:B:248:LYS:C	2:B:249:LYS:HG2	2.27	0.55
14:N:360:LEU:HD11	15:O:81:PHE:CD2	2.41	0.55
1:A:1313:GLN:O	1:A:1315:ASP:N	2.39	0.55
1:A:65:ILE:HG22	1:A:66:GLU:H	1.72	0.55
2:B:566:LYS:HA	2:B:576:ILE:HG22	1.89	0.55
2:B:934:LYS:HG2	2:B:1051:LEU:HD12	1.88	0.55
14:N:332:GLU:HB2	15:O:93:VAL:HA	1.88	0.55
16:P:171:THR:HG23	16:P:256:GLN:HG3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:270:LEU:HD22	16:P:291:LEU:HD13	1.89	0.55
18:R:88:ARG:NH1	18:R:97:LEU:HD23	2.22	0.55
19:S:119:THR:HG22	19:S:123:SER:HA	1.89	0.55
20:T:138:PRO:O	20:T:140:ARG:N	2.40	0.55
1:A:910:LYS:HD2	1:A:911:PRO:HD2	1.88	0.55
2:B:829:PHE:HD1	2:B:869:LYS:HB3	1.72	0.55
17:Q:113:ARG:NE	18:R:217:GLN:HB3	2.21	0.55
20:T:31:TRP:CD1	20:T:62:LEU:HD21	2.41	0.55
1:A:1150:ASP:OD2	1:A:1153:ARG:N	2.39	0.55
1:A:21:VAL:HG21	1:A:1427:LEU:HD11	1.88	0.55
1:A:880:ARG:HG2	1:A:886:VAL:HA	1.88	0.55
1:A:935:GLN:O	1:A:1002:SER:N	2.40	0.55
21:U:266:CYS:O	21:U:268:LYS:N	2.32	0.55
1:A:1027:ASP:OD2	5:E:162:ARG:NE	2.25	0.55
1:A:43:TYR:CG	1:A:44:PRO:HD2	2.41	0.55
1:A:426:ARG:NE	1:A:447:GLU:OE2	2.33	0.55
1:A:928:ARG:O	1:A:930:LEU:N	2.40	0.55
2:B:1040:GLN:NE2	3:C:195:THR:OG1	2.40	0.55
2:B:810:PHE:HB2	2:B:927:ARG:HG2	1.89	0.55
6:F:81:VAL:HG12	6:F:101:LYS:HD3	1.88	0.55
7:G:98:PHE:HE2	17:Q:145:PHE:CG	2.25	0.55
19:S:127:PHE:HB2	20:T:19:TRP:HB2	1.88	0.55
20:T:145:LEU:O	20:T:146:ASP:HB3	2.07	0.55
2:B:751:LEU:HD11	2:B:806:PHE:HA	1.89	0.54
5:E:149:VAL:O	5:E:192:LYS:N	2.23	0.54
8:H:84:ARG:C	8:H:86:ASP:N	2.60	0.54
17:Q:24:GLY:HA2	18:R:210:PHE:CD1	2.41	0.54
17:Q:106:LYS:CB	18:R:218:LYS:HE2	2.37	0.54
1:A:613:GLU:HG3	21:U:261:PHE:HD1	1.72	0.54
1:A:1463:LEU:HD21	6:F:64:ARG:HH22	1.71	0.54
1:A:515:ILE:HG23	1:A:519:ALA:HB3	1.89	0.54
1:A:608:THR:HB	1:A:610:PRO:CD	2.36	0.54
2:B:1094:GLN:HA	2:B:1097:HIS:HB2	1.88	0.54
2:B:248:LYS:O	2:B:249:LYS:HG2	2.07	0.54
2:B:552:ASN:HB3	2:B:555:GLU:HB3	1.89	0.54
1:A:1121:VAL:HA	1:A:1124:LEU:HB3	1.89	0.54
1:A:608:THR:HG21	1:A:639:ILE:HG23	1.89	0.54
2:B:953:ASP:HA	3:C:36:ARG:HH12	1.72	0.54
5:E:10:LEU:HB3	5:E:58:LEU:HD11	1.89	0.54
5:E:73:PHE:O	5:E:103:LEU:N	2.28	0.54
10:J:67:LYS:HB2	12:L:23:HIS:CD2	2.35	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:360:LEU:HB2	14:N:365:TYR:HE2	1.72	0.54
16:P:214:PHE:HD2	16:P:218:LYS:HB2	1.73	0.54
17:Q:110:MET:HE3	18:R:213:ASP:C	2.27	0.54
1:A:1146:GLN:HG2	1:A:1150:ASP:HB2	1.88	0.54
1:A:320:ASN:HB2	1:A:336:LEU:HD23	1.90	0.54
1:A:622:SER:O	1:A:624:GLY:CA	2.55	0.54
1:A:926:ASN:OD1	1:A:931:ARG:CG	2.56	0.54
2:B:568:PHE:N	2:B:612:ILE:O	2.33	0.54
2:B:836:THR:HG22	2:B:885:ARG:HB3	1.90	0.54
3:C:125:PRO:O	3:C:127:VAL:N	2.40	0.54
5:E:105:VAL:HG12	5:E:132:GLN:HG3	1.88	0.54
10:J:14:VAL:HG23	10:J:17:LYS:HB2	1.90	0.54
15:O:28:ILE:HB	15:O:32:LEU:HD23	1.88	0.54
1:A:1307:VAL:O	1:A:1307:VAL:HG13	2.08	0.54
2:B:240:LEU:HD23	2:B:257:VAL:CG2	2.37	0.54
3:C:68:LEU:HD12	3:C:71:ILE:HD12	1.90	0.54
1:A:1273:GLU:O	1:A:1273:GLU:HG3	2.07	0.54
1:A:902:GLU:O	1:A:979:LEU:N	2.34	0.54
1:A:936:GLU:HB2	1:A:939:VAL:HG23	1.89	0.54
2:B:512:ALA:HA	2:B:723:THR:HG22	1.89	0.54
8:H:8:ASP:OD1	8:H:9:ILE:N	2.41	0.54
9:I:110:LEU:O	9:I:124:THR:OG1	2.26	0.54
13:M:267:GLU:OE1	13:M:269:ARG:NH2	2.41	0.54
18:R:103:LEU:HB3	18:R:109:LEU:HA	1.90	0.54
2:B:440:ILE:HD12	2:B:440:ILE:H	1.71	0.54
2:B:778:SER:O	2:B:1046:THR:N	2.37	0.54
3:C:23:ILE:HB	3:C:231:TYR:HE2	1.72	0.54
14:N:38:VAL:HG13	15:O:22:LEU:HD22	1.88	0.54
17:Q:23:ARG:CZ	18:R:206:LYS:CG	2.71	0.54
19:S:110:PHE:CD1	19:S:148:PRO:HA	2.42	0.54
20:T:30:GLN:HG2	20:T:62:LEU:HG	1.89	0.54
1:A:927:GLU:O	1:A:931:ARG:CB	2.56	0.54
2:B:573:TRP:CZ3	2:B:575:GLY:HA2	2.43	0.54
16:P:165:LEU:HA	16:P:260:GLY:HA2	1.89	0.54
16:P:297:LYS:HA	16:P:297:LYS:NZ	2.22	0.54
1:A:46:THR:HG23	1:A:57:LEU:HD22	1.88	0.54
1:A:378:VAL:O	1:A:475:ARG:N	2.41	0.54
2:B:1135:TYR:HB2	2:B:1146:ILE:HG13	1.90	0.54
3:C:46:ALA:HB3	3:C:176:TRP:NE1	2.23	0.54
5:E:166:ARG:HB2	5:E:169:GLN:HG3	1.90	0.54
5:E:172:ARG:O	5:E:207:ARG:NE	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:25:GLU:O	12:L:37:ARG:NH2	2.39	0.54
1:A:330:GLN:HG2	13:M:107:MET:SD	2.48	0.54
1:A:43:TYR:OH	1:A:285:LYS:HE2	2.06	0.54
1:A:526:VAL:HA	1:A:533:PRO:HA	1.88	0.54
2:B:1117:HIS:HA	2:B:1147:SER:O	2.07	0.54
2:B:670:GLU:HA	2:B:673:VAL:HG22	1.90	0.54
2:B:868:GLY:HA2	2:B:893:SER:HB2	1.89	0.54
3:C:44:ILE:N	3:C:168:GLY:O	2.31	0.54
3:C:177:ASN:ND2	3:C:179:THR:O	2.41	0.54
11:K:35:ILE:HB	11:K:71:ILE:HG13	1.89	0.54
14:N:32:ASP:OD1	15:O:29:THR:OG1	2.23	0.54
17:Q:102:VAL:CB	17:Q:105:TYR:CD2	2.85	0.54
19:S:48:GLU:O	19:S:99:LEU:N	2.38	0.54
21:U:205:ASN:HB3	21:U:231:ASP:OD2	2.08	0.54
2:B:132:VAL:HG23	2:B:141:GLN:O	2.07	0.53
8:H:6:PHE:HB3	8:H:60:ILE:HB	1.90	0.53
9:I:17:CYS:N	9:I:22:ASN:O	2.35	0.53
15:O:71:VAL:HG22	15:O:98:CYS:HA	1.90	0.53
23:Y:74:DC:H2"	23:Y:75:DC:H6	1.73	0.53
1:A:1005:HIS:CE1	1:A:1007:ILE:HB	2.43	0.53
1:A:871:VAL:HG23	1:A:1088:GLY:HA3	1.90	0.53
2:B:813:SER:HA	2:B:922:ARG:HA	1.88	0.53
18:R:195:PRO:O	18:R:196:ASP:HB2	2.07	0.53
18:R:225:VAL:O	18:R:225:VAL:HG12	2.08	0.53
20:T:30:GLN:NE2	20:T:62:LEU:O	2.28	0.53
21:U:132:ARG:N	21:U:167:GLU:OE2	2.41	0.53
1:A:608:THR:HB	1:A:610:PRO:HD2	1.87	0.53
1:A:875:TYR:HA	1:A:1083:PRO:HB2	1.91	0.53
2:B:752:TYR:HE1	2:B:809:VAL:HG23	1.72	0.53
4:D:112:LYS:HE2	4:D:124:ASP:OD2	2.09	0.53
18:R:210:PHE:CG	18:R:212:VAL:HG13	2.43	0.53
1:A:1307:VAL:HG22	1:A:1338:THR:CA	2.38	0.53
2:B:935:PHE:CE2	2:B:945:CYS:HB2	2.42	0.53
2:B:309:PHE:HE2	9:I:25:TYR:HE2	1.57	0.53
13:M:225:PRO:HG2	13:M:228:VAL:HG23	1.90	0.53
17:Q:34:LEU:HA	17:Q:37:LEU:HD12	1.91	0.53
1:A:579:ILE:O	1:A:584:PRO:HA	2.08	0.53
1:A:602:CYS:HB2	1:A:655:ILE:HD11	1.91	0.53
1:A:910:LYS:O	1:A:963:ARG:NH2	2.37	0.53
2:B:51:ILE:HD12	2:B:160:TYR:CE2	2.44	0.53
3:C:74:ILE:HG13	3:C:76:ASP:H	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:88:PHE:HD1	8:H:146:LYS:HD2	1.73	0.53
16:P:325:PHE:CZ	16:P:329:TYR:HD2	2.26	0.53
17:Q:77:ARG:N	17:Q:93:PHE:O	2.35	0.53
18:R:191:PHE:CB	18:R:202:PHE:HD1	2.22	0.53
2:B:471:ASN:OD1	2:B:473:LEU:HG	2.08	0.53
2:B:956:PHE:HB2	2:B:960:GLY:HA2	1.90	0.53
9:I:84:HIS:HB3	9:I:92:LYS:HB3	1.91	0.53
17:Q:109:HIS:C	18:R:221:ARG:CD	2.70	0.53
1:A:225:PHE:HA	1:A:228:ILE:HG12	1.91	0.53
2:B:591:ARG:NH2	2:B:669:GLU:OE1	2.42	0.53
4:D:26:PHE:CZ	7:G:42:TYR:HA	2.44	0.53
1:A:1123:ARG:NH1	1:A:1126:GLU:OE1	2.40	0.53
1:A:1314:THR:O	1:A:1314:THR:HG22	2.09	0.53
1:A:272:ASN:ND2	1:A:278:HIS:HD2	2.07	0.53
1:A:579:ILE:HB	1:A:585:LEU:HB2	1.91	0.53
2:B:152:ILE:HG23	2:B:154:ILE:HD11	1.90	0.53
2:B:182:GLY:HA2	2:B:184:TYR:CE1	2.44	0.53
2:B:623:ARG:O	2:B:665:ILE:N	2.37	0.53
2:B:71:ALA:HA	2:B:81:PRO:HB3	1.90	0.53
2:B:792:ASP:OD1	2:B:975:ARG:NH2	2.42	0.53
4:D:73:ARG:NH1	4:D:103:LEU:O	2.41	0.53
7:G:119:PHE:HB2	7:G:128:TYR:HE1	1.73	0.53
18:R:213:ASP:O	18:R:215:GLU:CA	2.56	0.53
1:A:1219:LYS:O	1:A:1222:THR:OG1	2.22	0.53
3:C:63:PHE:HE2	10:J:2:ILE:HG21	1.73	0.53
7:G:119:PHE:HB2	7:G:128:TYR:CE1	2.44	0.53
8:H:24:ARG:HG2	8:H:46:GLN:HE22	1.73	0.53
1:A:124:PRO:HA	1:A:127:LYS:HB2	1.91	0.53
1:A:1307:VAL:O	1:A:1338:THR:HG22	2.08	0.53
1:A:152:ASN:O	1:A:152:ASN:ND2	2.41	0.53
2:B:753:TYR:CZ	10:J:4:PRO:HB3	2.44	0.53
1:A:620:HIS:O	1:A:621:ILE:HB	2.09	0.52
2:B:1068:GLN:N	2:B:1073:GLN:O	2.43	0.52
2:B:455:ASP:O	2:B:457:LYS:N	2.37	0.52
3:C:101:PHE:O	3:C:163:ALA:N	2.28	0.52
3:C:19:VAL:HG12	3:C:233:VAL:HB	1.90	0.52
10:J:63:ALA:N	10:J:64:PRO:HD2	2.24	0.52
3:C:14:LEU:HD23	11:K:112:LYS:HE2	1.91	0.52
20:T:94:THR:HG22	20:T:109:ILE:HG23	1.91	0.52
1:A:410:ASN:OD1	1:A:417:LYS:NZ	2.35	0.52
1:A:914:LYS:O	1:A:918:LYS:N	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:240:LEU:HD13	2:B:242:ARG:NE	2.24	0.52
2:B:24:GLU:HA	2:B:27:TRP:HD1	1.74	0.52
8:H:28:LEU:HD11	8:H:50:VAL:HG21	1.91	0.52
8:H:65:TYR:OH	8:H:79:ASP:OD2	2.27	0.52
15:O:9:THR:O	15:O:13:ASN:N	2.30	0.52
16:P:161:ILE:HG13	16:P:329:TYR:CE2	2.44	0.52
18:R:202:PHE:C	18:R:203:PHE:CG	2.83	0.52
19:S:46:ARG:HB2	19:S:101:ARG:HB2	1.91	0.52
1:A:641:CYS:SG	1:A:644:SER:OG	2.52	0.52
1:A:998:PRO:HA	1:A:1059:ARG:NE	2.24	0.52
2:B:1021:HIS:CE1	2:B:1023:ARG:HB2	2.44	0.52
2:B:83:ARG:O	2:B:134:LYS:HA	2.08	0.52
7:G:22:LEU:HD21	7:G:68:TYR:CE2	2.45	0.52
14:N:360:LEU:HD11	15:O:81:PHE:HD2	1.73	0.52
17:Q:71:PHE:HD1	17:Q:72:ILE:HG23	1.74	0.52
20:T:143:GLN:O	20:T:144:GLN:HB2	2.09	0.52
1:A:403:GLN:HG3	1:A:440:LEU:HD21	1.92	0.52
2:B:1026:GLU:N	2:B:1041:ILE:O	2.39	0.52
2:B:566:LYS:NZ	2:B:609:GLU:O	2.43	0.52
8:H:40:ILE:HB	8:H:124:ARG:HG2	1.91	0.52
9:I:66:THR:HA	9:I:122:ARG:NH2	2.25	0.52
18:R:195:PRO:HB2	18:R:199:LYS:HD3	1.90	0.52
21:U:194:ARG:HD2	21:U:220:PHE:CE2	2.44	0.52
1:A:457:ILE:HG21	2:B:1102:PHE:CZ	2.44	0.52
1:A:568:SER:N	1:A:671:ASN:OD1	2.29	0.52
6:F:56:TYR:HE1	6:F:124:ILE:HD12	1.74	0.52
14:N:15:ARG:HA	14:N:18:ILE:HD12	1.91	0.52
18:R:140:LYS:H	18:R:141:PRO:HD2	1.74	0.52
17:Q:106:LYS:CG	18:R:218:LYS:HG2	2.37	0.52
23:Y:62:DC:H1'	23:Y:63:DG:H5'	1.90	0.52
2:B:780:VAL:HG13	2:B:965:ILE:HB	1.90	0.52
13:M:214:PHE:HB3	13:M:218:PHE:HE2	1.75	0.52
18:R:195:PRO:HB2	18:R:199:LYS:CD	2.39	0.52
1:A:1243:LEU:HD11	1:A:1259:ILE:HD12	1.91	0.52
1:A:876:ASP:HA	6:F:52:ILE:HD13	1.92	0.52
2:B:40:VAL:HA	2:B:42:GLN:HE22	1.75	0.52
2:B:613:ARG:HD3	2:B:615:TYR:HE2	1.74	0.52
17:Q:110:MET:SD	18:R:218:LYS:HB2	2.49	0.52
1:A:1416:ARG:NH2	1:A:1434:GLU:OE2	2.43	0.52
1:A:879:VAL:O	1:A:887:VAL:N	2.29	0.52
2:B:544:PHE:O	2:B:548:TRP:N	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:127:ARG:HG3	13:M:127:ARG:HH21	1.74	0.52
13:M:34:CYS:C	13:M:39:LEU:CB	2.74	0.52
17:Q:72:ILE:HD12	17:Q:96:TYR:CD1	2.45	0.52
21:U:230:SER:O	21:U:231:ASP:CB	2.56	0.52
1:A:817:PRO:HB2	1:A:822:PHE:HB3	1.92	0.52
2:B:249:LYS:O	2:B:251:ALA:N	2.42	0.52
2:B:273:PHE:HA	2:B:276:LEU:HD12	1.92	0.52
13:M:23:LEU:HD21	13:M:41:VAL:HG21	1.92	0.52
14:N:25:VAL:HB	15:O:36:VAL:HG22	1.91	0.52
17:Q:18:ALA:HA	17:Q:21:VAL:HG22	1.90	0.52
1:A:1309:MET:SD	21:U:252:LYS:CD	2.98	0.52
1:A:138:LYS:HE3	1:A:1441:GLU:HG3	1.91	0.52
2:B:711:ILE:HD12	2:B:939:HIS:HA	1.90	0.52
2:B:867:ILE:O	2:B:894:THR:N	2.43	0.52
3:C:100:GLU:N	3:C:124:SER:OG	2.43	0.52
1:A:381:PRO:HB3	11:K:2:ASN:ND2	2.25	0.52
1:A:433:PRO:HD3	13:M:35:PRO:O	2.10	0.52
14:N:312:GLU:O	14:N:314:LEU:N	2.37	0.52
1:A:1139:LEU:N	1:A:1338:THR:O	2.42	0.51
1:A:405:LEU:HD23	1:A:448:ARG:HB2	1.92	0.51
1:A:529:GLN:NE2	1:A:1098:PRO:HD3	2.25	0.51
1:A:600:ILE:HD12	1:A:659:GLU:HB2	1.92	0.51
1:A:674:THR:O	1:A:678:ASN:ND2	2.42	0.51
2:B:934:LYS:HE3	2:B:1053:HIS:CG	2.44	0.51
2:B:21:LEU:HD21	2:B:635:LEU:HD23	1.91	0.51
2:B:222:ARG:HB3	2:B:232:THR:O	2.09	0.51
2:B:551:GLU:N	2:B:551:GLU:OE1	2.42	0.51
7:G:12:LEU:HG	7:G:63:ARG:NH1	2.26	0.51
8:H:64:LEU:O	8:H:66:GLU:N	2.33	0.51
8:H:75:TYR:C	8:H:77:PRO:HD3	2.26	0.51
13:M:218:PHE:HD1	13:M:277:ILE:HG22	1.74	0.51
14:N:42:LEU:HD11	15:O:15:LEU:HD12	1.91	0.51
14:N:317:GLU:OE2	16:P:235:ARG:HD2	2.10	0.51
20:T:184:LEU:HA	20:T:187:LEU:HD12	1.92	0.51
1:A:1453:GLY:O	1:A:1457:ASN:ND2	2.44	0.51
2:B:345:LYS:O	2:B:349:PRO:HG3	2.10	0.51
8:H:70:LEU:O	8:H:72:ASP:N	2.38	0.51
9:I:88:LYS:HD2	9:I:121:HIS:CE1	2.45	0.51
1:A:1162:GLU:HG3	1:A:1306:LYS:O	2.10	0.51
1:A:1162:GLU:OE2	1:A:1224:ARG:NH1	2.42	0.51
1:A:611:ASP:HB3	1:A:617:PRO:CG	2.37	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1137:CYS:HB3	2:B:1142:ASN:HB3	1.91	0.51
2:B:842:HIS:ND1	13:M:25:GLU:O	2.43	0.51
8:H:10:PHE:CE1	8:H:32:SER:HB2	2.46	0.51
9:I:86:CYS:HB3	9:I:89:CYS:SG	2.50	0.51
11:K:19:ILE:HA	11:K:35:ILE:HA	1.92	0.51
13:M:231:ALA:HA	13:M:301:PRO:HG3	1.93	0.51
14:N:356:GLY:HA3	14:N:367:PHE:CZ	2.46	0.51
14:N:358:MET:HB2	14:N:365:TYR:HB2	1.92	0.51
15:O:3:TYR:OH	15:O:99:ASP:O	2.24	0.51
17:Q:113:ARG:HE	18:R:217:GLN:CB	2.23	0.51
23:Y:70:DC:H2''	23:Y:71:DA:H8	1.76	0.51
1:A:1175:ILE:HB	9:I:54:TYR:HB3	1.93	0.51
1:A:21:VAL:HG23	1:A:1451:MET:SD	2.51	0.51
2:B:108:MET:SD	2:B:120:TYR:HA	2.51	0.51
2:B:133:ILE:C	2:B:135:GLU:H	2.14	0.51
2:B:258:ALA:HB2	2:B:269:ILE:HG22	1.93	0.51
2:B:331:THR:HG21	2:B:334:LYS:HE2	1.92	0.51
3:C:151:VAL:HG22	3:C:152:LYS:H	1.75	0.51
4:D:72:SER:O	4:D:142:TYR:OH	2.23	0.51
13:M:124:MET:HA	13:M:127:ARG:HH22	1.76	0.51
14:N:312:GLU:HB2	14:N:313:PRO:HD3	1.93	0.51
16:P:207:PRO:HB3	16:P:233:ALA:HB2	1.93	0.51
20:T:206:THR:HG21	20:T:213:LEU:HD13	1.92	0.51
2:B:125:TYR:HE1	2:B:148:PHE:HB2	1.76	0.51
5:E:99:ILE:HD11	5:E:102:ALA:HB2	1.93	0.51
16:P:199:ALA:HB2	16:P:214:PHE:HD1	1.75	0.51
17:Q:146:ASP:HB3	17:Q:149:THR:HG22	1.90	0.51
16:P:167:ASN:HB2	23:Y:80:DT:C4'	2.40	0.51
1:A:1127:LEU:HD21	1:A:1378:LEU:HD11	1.93	0.51
1:A:574:VAL:O	8:H:73:GLY:O	2.29	0.51
1:A:611:ASP:OD2	1:A:617:PRO:CB	2.57	0.51
1:A:696:SER:O	1:A:700:GLN:N	2.36	0.51
1:A:551:ARG:HH12	8:H:120:GLY:C	2.14	0.51
13:M:263:GLN:HA	13:M:268:LYS:HG2	1.92	0.51
18:R:213:ASP:O	18:R:214:GLU:C	2.47	0.51
1:A:1117:VAL:HG12	1:A:1117:VAL:O	2.11	0.51
1:A:1204:VAL:O	1:A:1207:ILE:HG12	2.11	0.51
1:A:1435:THR:OG1	1:A:1436:VAL:N	2.42	0.51
2:B:1079:SER:O	13:M:53:ARG:NH2	2.44	0.51
3:C:20:LYS:HE2	3:C:232:ASN:ND2	2.25	0.51
13:M:40:VAL:C	13:M:42:GLY:N	2.64	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:167:ASN:HB3	16:P:259:VAL:HB	1.92	0.51
16:P:206:GLU:CB	16:P:207:PRO:CD	2.87	0.51
18:R:103:LEU:HD12	18:R:116:LYS:HE3	1.92	0.51
22:X:47:DC:H2"	22:X:48:DG:C8	2.46	0.51
3:C:43:PRO:HA	3:C:169:PHE:HB3	1.91	0.51
5:E:103:LEU:HA	5:E:128:GLU:HB2	1.93	0.51
8:H:17:PRO:CB	8:H:27:ARG:HB3	2.35	0.51
8:H:65:TYR:CE1	8:H:81:ARG:CZ	2.93	0.51
13:M:38:GLY:O	13:M:39:LEU:CB	2.59	0.51
16:P:277:HIS:O	16:P:281:SER:N	2.42	0.51
1:A:456:VAL:HG21	1:A:503:LEU:HD11	1.92	0.51
1:A:987:ILE:HG12	1:A:1068:LEU:HD21	1.91	0.51
2:B:1062:ARG:NH1	2:B:1066:PRO:O	2.43	0.51
2:B:85:LEU:HB3	2:B:131:THR:O	2.10	0.51
3:C:101:PHE:HB3	3:C:120:LEU:HD11	1.92	0.51
1:A:583:ARG:NH2	3:C:223:ASN:OD1	2.34	0.51
4:D:86:LEU:O	4:D:89:GLN:HG2	2.10	0.51
8:H:64:LEU:O	8:H:83:SER:O	2.29	0.51
17:Q:183:GLN:O	17:Q:186:PRO:HD2	2.11	0.51
17:Q:23:ARG:HH21	18:R:206:LYS:HG3	0.69	0.51
21:U:276:VAL:HG22	21:U:277:GLN:H	1.76	0.51
2:B:278:PHE:HZ	2:B:359:THR:HG23	1.76	0.51
2:B:519:ALA:HB1	2:B:523:VAL:HG23	1.93	0.51
8:H:75:TYR:CD2	8:H:77:PRO:HG3	2.45	0.51
1:A:478:PRO:HB3	11:K:4:PRO:CD	2.41	0.51
20:T:27:LEU:HD11	20:T:58:LEU:HD21	1.93	0.51
1:A:564:LEU:HD22	1:A:570:TRP:CE2	2.45	0.50
1:A:909:LEU:HB2	1:A:975:SER:OG	2.11	0.50
2:B:264:LYS:HE3	2:B:326:ALA:HA	1.93	0.50
2:B:425:ARG:HG3	2:B:425:ARG:HH11	1.75	0.50
12:L:38:GLU:O	13:M:226:LYS:NZ	2.43	0.50
19:S:31:PHE:O	20:T:92:THR:N	2.44	0.50
22:X:52:DG:H2"	22:X:53:DA:C8	2.46	0.50
1:A:426:ARG:H	13:M:40:VAL:CG2	2.24	0.50
1:A:722:ASN:HB2	1:A:724:GLU:HG2	1.93	0.50
2:B:797:ASN:ND2	2:B:954:MET:SD	2.85	0.50
2:B:1028:LEU:HD13	2:B:1041:ILE:HB	1.94	0.50
2:B:761:THR:H	2:B:764:MET:HE3	1.76	0.50
5:E:150:VAL:HG12	5:E:185:ILE:HD13	1.93	0.50
5:E:59:THR:HG23	5:E:75:PHE:HA	1.92	0.50
6:F:70:ALA:HB1	6:F:89:PRO:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:721:HIS:HA	9:I:108:MET:O	2.11	0.50
16:P:167:ASN:O	16:P:259:VAL:N	2.41	0.50
16:P:297:LYS:HE2	16:P:297:LYS:HA	1.89	0.50
17:Q:187:ILE:HB	18:R:211:SER:HG	1.69	0.50
1:A:1317:LYS:HB2	21:U:295:GLY:HA3	1.93	0.50
1:A:500:GLU:OE2	2:B:1058:LYS:HB3	2.12	0.50
2:B:568:PHE:CZ	2:B:573:TRP:HD1	2.28	0.50
7:G:11:ILE:HB	7:G:68:TYR:HB2	1.93	0.50
9:I:62:VAL:HA	9:I:103:ARG:NH2	2.26	0.50
13:M:289:TYR:OH	13:M:314:PRO:O	2.17	0.50
1:A:292:ARG:NH1	1:A:295:GLN:OE1	2.45	0.50
2:B:713:PHE:CD1	2:B:1001:PRO:HA	2.46	0.50
2:B:1094:GLN:HG2	2:B:1103:LEU:HB2	1.93	0.50
2:B:884:ASN:OD1	2:B:885:ARG:N	2.44	0.50
2:B:988:LYS:O	2:B:992:ASN:ND2	2.43	0.50
4:D:76:ASN:HB3	4:D:79:THR:HB	1.92	0.50
5:E:54:ARG:HA	5:E:57:ASP:HB2	1.93	0.50
8:H:98:ARG:HB3	8:H:115:TYR:HB2	1.93	0.50
17:Q:108:ASP:CB	18:R:234:GLU:OE2	2.59	0.50
20:T:93:LEU:HB2	20:T:110:VAL:HB	1.93	0.50
2:B:1123:GLY:HA3	2:B:1170:ARG:HB2	1.93	0.50
3:C:11:ILE:HG12	11:K:108:ALA:HB1	1.93	0.50
6:F:44:ARG:HD3	6:F:113:GLY:O	2.12	0.50
3:C:172:GLU:HG2	12:L:58:ARG:HH22	1.77	0.50
13:M:279:GLY:CA	20:T:153:TYR:HE1	2.25	0.50
14:N:333:ASN:HB3	14:N:360:LEU:HA	1.93	0.50
16:P:291:LEU:N	16:P:304:ILE:O	2.31	0.50
20:T:159:HIS:CG	20:T:160:GLN:N	2.79	0.50
1:A:233:CYS:O	1:A:238:MET:N	2.45	0.50
1:A:371:PRO:HD2	2:B:788:TYR:CE1	2.46	0.50
1:A:489:THR:HG23	1:A:494:ALA:HB3	1.92	0.50
1:A:595:ILE:HG22	1:A:668:PHE:CE1	2.46	0.50
2:B:205:VAL:HG21	2:B:368:MET:HG3	1.92	0.50
7:G:12:LEU:HG	7:G:63:ARG:HH11	1.77	0.50
11:K:12:LEU:HD21	11:K:18:LYS:HA	1.92	0.50
13:M:222:LEU:HD22	13:M:269:ARG:HG3	1.94	0.50
17:Q:120:ASP:HB3	17:Q:174:ARG:HG3	1.94	0.50
18:R:163:LEU:C	18:R:164:GLY:O	2.49	0.50
21:U:188:LYS:O	21:U:192:ARG:HG3	2.11	0.50
1:A:432:HIS:CE1	1:A:438:LEU:HB2	2.47	0.50
2:B:1030:ASN:ND2	2:B:1033:THR:OG1	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:65:ASN:OD1	5:E:66:ASP:N	2.44	0.50
18:R:223:VAL:C	18:R:224:THR:CG2	2.60	0.50
1:A:16:ARG:HD2	2:B:1147:SER:HB3	1.93	0.50
1:A:516:GLN:O	1:A:523:ARG:NH1	2.41	0.50
1:A:764:ASN:OD1	1:A:766:PHE:N	2.36	0.50
2:B:1075:MET:HB2	2:B:1082:GLY:HA2	1.94	0.50
2:B:1072:ARG:HD3	2:B:1112:ASP:OD1	2.12	0.50
2:B:157:ARG:HB2	2:B:181:PRO:O	2.12	0.50
2:B:242:ARG:C	2:B:244:GLY:H	2.15	0.50
2:B:240:LEU:CD2	2:B:257:VAL:CG1	2.90	0.50
2:B:591:ARG:HG2	2:B:598:VAL:HG12	1.93	0.50
17:Q:113:ARG:HD3	18:R:217:GLN:O	2.10	0.50
20:T:229:HIS:CD2	22:X:28:DG:H21	2.30	0.50
2:B:10:TYR:CE2	2:B:12:GLU:HB3	2.47	0.49
2:B:36:GLU:OE1	2:B:654:GLN:N	2.34	0.49
4:D:19:GLN:HB2	4:D:21:ILE:HG12	1.93	0.49
7:G:55:GLY:N	7:G:69:PRO:O	2.35	0.49
13:M:118:PHE:HE1	13:M:142:PHE:HB3	1.77	0.49
2:B:1066:PRO:HD3	13:M:30:GLY:HA3	1.94	0.49
1:A:286:ILE:HD13	1:A:313:HIS:HD2	1.77	0.49
1:A:380:VAL:N	1:A:475:ARG:O	2.37	0.49
1:A:510:GLU:HA	6:F:67:GLY:HA3	1.94	0.49
5:E:52:ARG:HG2	5:E:54:ARG:NH1	2.28	0.49
14:N:310:GLU:HB3	14:N:313:PRO:HD2	1.94	0.49
14:N:345:SER:N	14:N:348:LYS:O	2.43	0.49
16:P:293:TYR:CD2	16:P:302:LEU:HD13	2.44	0.49
7:G:93:ASN:HD21	17:Q:151:THR:HA	1.76	0.49
18:R:191:PHE:CB	18:R:202:PHE:HE1	2.23	0.49
18:R:88:ARG:NH2	18:R:93:ASP:HB3	2.27	0.49
20:T:144:GLN:O	20:T:145:LEU:CB	2.60	0.49
1:A:33:ARG:O	2:B:1138:ARG:HG2	2.11	0.49
1:A:389:THR:HG22	1:A:449:HIS:HA	1.95	0.49
2:B:166:LEU:HB3	2:B:170:ASP:HB2	1.94	0.49
5:E:14:ARG:O	5:E:18:MET:HG2	2.12	0.49
10:J:7:CYS:HB3	10:J:10:CYS:SG	2.52	0.49
18:R:177:ASN:HD21	18:R:202:PHE:HE2	1.60	0.49
1:A:1272:GLU:C	1:A:1274:GLU:N	2.66	0.49
2:B:240:LEU:HD23	2:B:257:VAL:HG11	1.95	0.49
2:B:342:VAL:HG13	2:B:346:GLU:HB2	1.94	0.49
6:F:45:PRO:HD3	6:F:115:TYR:CZ	2.48	0.49
9:I:28:GLU:OE2	9:I:33:ARG:NH1	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:88:LYS:HD2	9:I:121:HIS:HE1	1.77	0.49
12:L:19:CYS:HB2	12:L:36:CYS:SG	2.53	0.49
17:Q:106:LYS:O	18:R:218:LYS:HE3	2.12	0.49
20:T:162:ASN:O	20:T:165:TYR:HB3	2.13	0.49
13:M:105:ARG:NH1	23:Y:64:DC:OP1	2.45	0.49
1:A:456:VAL:O	1:A:472:HIS:N	2.35	0.49
1:A:527:THR:N	1:A:532:ARG:O	2.36	0.49
1:A:926:ASN:OD1	1:A:927:GLU:N	2.45	0.49
2:B:1142:ASN:ND2	2:B:1145:GLN:HG2	2.28	0.49
1:A:16:ARG:N	2:B:1148:LEU:O	2.32	0.49
2:B:92:TYR:CG	20:T:145:LEU:HD13	2.48	0.49
3:C:94:CYS:O	3:C:98:SER:N	2.46	0.49
11:K:109:ILE:HA	11:K:112:LYS:NZ	2.27	0.49
2:B:89:GLU:OE2	20:T:140:ARG:NH1	2.46	0.49
1:A:1169:VAL:HG22	1:A:1220:HIS:NE2	2.28	0.49
1:A:1319:LYS:HE3	1:A:1331:LEU:HD23	1.95	0.49
1:A:1309:MET:O	1:A:1336:LEU:HA	2.13	0.49
1:A:97:VAL:HG21	1:A:322:LEU:HD11	1.95	0.49
1:A:364:ARG:HG3	1:A:501:MET:O	2.12	0.49
1:A:581:LYS:HB2	8:H:91:VAL:H	1.78	0.49
13:M:169:ARG:HD3	13:M:207:ASP:H	1.77	0.49
15:O:11:LEU:HG	15:O:40:PHE:HZ	1.77	0.49
1:A:1143:LEU:HB3	1:A:1147:SER:CB	2.42	0.49
1:A:1223:ASP:OD2	1:A:1224:ARG:NH2	2.45	0.49
1:A:1372:GLU:CD	5:E:195:ARG:HH21	2.15	0.49
1:A:525:ILE:O	1:A:534:VAL:N	2.36	0.49
2:B:763:SER:HA	2:B:766:TYR:CD2	2.47	0.49
2:B:89:GLU:HG3	2:B:90:GLN:H	1.77	0.49
3:C:27:ASP:HB3	3:C:30:VAL:HG23	1.95	0.49
11:K:81:TYR:HE2	11:K:86:ALA:HB2	1.78	0.49
1:A:540:ASP:HB3	1:A:680:LEU:HD21	1.94	0.49
1:A:781:ILE:HA	1:A:784:VAL:HG22	1.95	0.49
1:A:802:PHE:HZ	2:B:670:GLU:O	1.96	0.49
7:G:95:VAL:HG11	17:Q:127:PHE:CZ	2.48	0.49
12:L:14:PRO:O	12:L:27:GLU:OE1	2.30	0.49
2:B:915:GLY:HA3	13:M:133:ASN:OD1	2.13	0.49
1:A:432:HIS:HE2	1:A:438:LEU:HD13	1.77	0.49
1:A:821:GLY:HA2	1:A:838:PHE:CD2	2.48	0.49
2:B:798:ARG:O	2:B:801:VAL:HB	2.13	0.49
2:B:835:GLU:OE1	2:B:835:GLU:N	2.46	0.49
2:B:936:ALA:O	2:B:1049:GLN:N	2.29	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:44:ARG:HD2	4:D:47:GLN:OE1	2.12	0.49
8:H:62:SER:HA	8:H:141:VAL:HA	1.93	0.49
11:K:56:VAL:HA	11:K:77:THR:HG22	1.95	0.49
1:A:987:ILE:HG23	1:A:1060:LEU:HD11	1.95	0.49
2:B:418:TYR:OH	2:B:433:LEU:HD23	2.13	0.49
2:B:956:PHE:HD2	2:B:960:GLY:HA2	1.77	0.49
8:H:105:SER:HB2	8:H:108:ALA:HB2	1.93	0.49
20:T:155:PRO:C	20:T:157:ALA:H	2.14	0.49
1:A:1031:ARG:HA	1:A:1034:GLN:HB3	1.94	0.48
1:A:1189:ASP:HA	1:A:1192:TRP:HD1	1.77	0.48
1:A:1310:HIS:CE1	1:A:1334:TRP:HA	2.47	0.48
1:A:903:PHE:HA	1:A:978:VAL:HA	1.95	0.48
2:B:573:TRP:HZ2	2:B:576:ILE:HG23	1.78	0.48
2:B:867:ILE:HB	2:B:894:THR:HB	1.94	0.48
3:C:210:GLU:O	3:C:213:GLU:HB2	2.13	0.48
8:H:105:SER:O	8:H:106:THR:HB	2.12	0.48
13:M:117:ALA:O	13:M:121:ILE:N	2.46	0.48
21:U:218:ASP:O	21:U:222:ARG:HB3	2.10	0.48
1:A:1372:GLU:OE1	5:E:193:ILE:HG21	2.13	0.48
1:A:604:ARG:HA	1:A:604:ARG:HD3	1.58	0.48
3:C:266:GLU:O	3:C:270:ASP:HB2	2.13	0.48
3:C:45:ILE:CG1	3:C:79:VAL:HB	2.36	0.48
5:E:149:VAL:HB	5:E:192:LYS:HE2	1.94	0.48
9:I:57:LYS:HE2	9:I:60:HIS:CE1	2.48	0.48
1:A:1220:HIS:HA	1:A:1223:ASP:HB3	1.93	0.48
1:A:1304:ILE:HG22	1:A:1340:GLY:HA3	1.95	0.48
1:A:642:LYS:NZ	21:U:283:GLU:HA	2.29	0.48
2:B:1003:ASN:ND2	2:B:1007:ASN:OD1	2.42	0.48
2:B:1068:GLN:O	2:B:1072:ARG:N	2.45	0.48
2:B:209:ALA:HB1	2:B:211:LYS:HG3	1.96	0.48
2:B:294:ASP:OD2	2:B:379:ARG:NH2	2.44	0.48
2:B:57:ARG:O	2:B:61:ASP:N	2.46	0.48
2:B:932:GLY:N	2:B:945:CYS:O	2.37	0.48
3:C:134:ASN:OD1	3:C:135:ARG:N	2.46	0.48
5:E:28:VAL:HG13	5:E:32:GLU:OE1	2.13	0.48
9:I:103:ARG:O	9:I:104:ALA:C	2.52	0.48
13:M:295:ARG:NH2	13:M:298:ASP:OD2	2.45	0.48
21:U:225:ALA:HB3	21:U:228:MET:HG2	1.94	0.48
1:A:1117:VAL:O	1:A:1118:THR:O	2.30	0.48
1:A:65:ILE:HD11	1:A:258:LEU:HB2	1.96	0.48
2:B:26:CYS:O	2:B:29:VAL:HB	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:837:CYS:HB3	2:B:840:MET:HE3	1.96	0.48
2:B:848:LEU:HD23	2:B:852:GLY:HA2	1.95	0.48
3:C:105:VAL:HG12	3:C:159:LEU:HB3	1.95	0.48
3:C:262:GLN:O	3:C:266:GLU:HG2	2.14	0.48
13:M:178:LYS:O	20:T:154:LYS:HB2	1.94	0.48
16:P:299:ARG:HA	16:P:299:ARG:HD2	1.47	0.48
17:Q:124:ARG:HG2	17:Q:126:SER:H	1.76	0.48
17:Q:71:PHE:HA	17:Q:100:VAL:CG2	2.40	0.48
1:A:616:GLY:HA2	1:A:619:LYS:HD3	1.96	0.48
2:B:562:ALA:O	2:B:610:ARG:NH2	2.38	0.48
14:N:345:SER:O	14:N:347:ASN:N	2.43	0.48
21:U:145:ARG:NE	21:U:173:GLU:OE1	2.34	0.48
22:X:4:DG:H2"	22:X:5:DG:C8	2.49	0.48
1:A:981:CYS:SG	1:A:1075:LYS:HB3	2.54	0.48
1:A:140:ARG:NH1	1:A:234:PHE:O	2.47	0.48
1:A:156:GLY:HA2	1:A:181:HIS:CE1	2.49	0.48
1:A:14:PRO:HG2	1:A:16:ARG:NH1	2.29	0.48
1:A:426:ARG:N	13:M:40:VAL:CG2	2.77	0.48
1:A:660:MET:HB3	1:A:664:ILE:HB	1.94	0.48
1:A:798:ILE:O	1:A:820:ARG:NE	2.46	0.48
2:B:1163:MET:HA	2:B:1167:ILE:O	2.13	0.48
11:K:40:HIS:CE1	11:K:63:VAL:H	2.31	0.48
17:Q:123:ASN:ND2	17:Q:123:ASN:O	2.45	0.48
19:S:49:ARG:HB3	19:S:96:GLN:HB3	1.96	0.48
22:X:15:DA:H2"	22:X:16:DA:C8	2.49	0.48
1:A:1191:GLU:HG2	9:I:1:MET:SD	2.54	0.48
1:A:345:GLY:O	1:A:351:ARG:HB3	2.13	0.48
4:D:124:ASP:HA	4:D:127:LEU:HB3	1.96	0.48
5:E:39:GLU:O	5:E:43:GLN:N	2.40	0.48
5:E:41:LYS:O	5:E:46:ASP:N	2.42	0.48
6:F:108:ARG:HB2	6:F:116:GLU:HG3	1.96	0.48
7:G:97:LEU:HD13	7:G:128:TYR:CD2	2.48	0.48
12:L:22:CYS:HB3	12:L:39:CYS:CB	2.40	0.48
18:R:170:ASP:OD1	18:R:180:LYS:NZ	2.34	0.48
1:A:253:LEU:HD12	1:A:254:PRO:HD2	1.96	0.48
1:A:817:PRO:HB2	1:A:822:PHE:CB	2.42	0.48
2:B:97:THR:HG22	2:B:107:PRO:HA	1.95	0.48
2:B:133:ILE:HG23	2:B:139:GLN:HE21	1.79	0.48
2:B:675:LEU:HD21	2:B:697:GLU:OE2	2.13	0.48
5:E:106:VAL:HG23	5:E:129:GLN:HE22	1.78	0.48
6:F:86:GLU:N	6:F:86:GLU:OE1	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:38:GLU:HG2	12:L:39:CYS:N	2.27	0.48
17:Q:166:SER:OG	17:Q:170:LYS:HB3	2.13	0.48
19:S:127:PHE:HB2	20:T:19:TRP:CB	2.43	0.48
23:Y:89:DC:H2"	23:Y:90:DC:C5	2.49	0.48
1:A:71:CYS:O	1:A:75:ALA:N	2.47	0.48
1:A:921:ARG:HB2	1:A:956:PHE:CZ	2.48	0.48
2:B:1029:TYR:CE1	2:B:1036:LYS:HG2	2.48	0.48
7:G:14:HIS:HB3	7:G:17:TYR:CD2	2.49	0.48
13:M:244:LEU:HD11	13:M:295:ARG:HD3	1.95	0.48
1:A:426:ARG:H	13:M:40:VAL:HG21	1.79	0.48
16:P:169:VAL:HB	16:P:257:ASN:HB3	1.96	0.48
17:Q:105:TYR:HD1	18:R:234:GLU:OE1	1.97	0.48
22:X:14:DA:H2"	22:X:15:DA:H8	1.79	0.48
1:A:775:LYS:HB3	2:B:974:SER:HB3	1.95	0.48
1:A:927:GLU:O	1:A:931:ARG:HB2	2.14	0.48
2:B:1130:THR:HB	2:B:1134:THR:N	2.28	0.48
2:B:198:GLU:O	2:B:488:PRO:HD3	2.14	0.48
7:G:97:LEU:HD13	7:G:128:TYR:HD2	1.79	0.48
9:I:25:TYR:N	9:I:38:ALA:O	2.40	0.48
15:O:76:LEU:HD13	15:O:95:ILE:HD12	1.95	0.48
14:N:317:GLU:C	16:P:239:ARG:HG3	2.34	0.48
21:U:174:GLU:O	21:U:178:GLN:N	2.42	0.48
1:A:959:MET:HE1	1:A:1047:SER:HA	1.95	0.47
1:A:1430:CYS:HB2	1:A:1435:THR:HA	1.96	0.47
1:A:198:LEU:HB3	1:A:216:LEU:HD12	1.95	0.47
1:A:702:ILE:HG23	1:A:752:THR:HB	1.96	0.47
1:A:913:ASN:OD1	1:A:967:ARG:NH2	2.47	0.47
2:B:10:TYR:HE2	2:B:12:GLU:HB3	1.79	0.47
2:B:438:ARG:HA	2:B:441:SER:HB2	1.96	0.47
3:C:33:SER:O	3:C:37:VAL:HG23	2.14	0.47
6:F:45:PRO:HA	6:F:115:TYR:O	2.14	0.47
10:J:30:THR:HG22	10:J:33:ASP:H	1.78	0.47
12:L:16:ILE:O	12:L:17:TYR:CG	2.67	0.47
17:Q:55:ASP:HB3	17:Q:58:GLN:HB2	1.96	0.47
17:Q:187:ILE:HD11	18:R:211:SER:N	2.29	0.47
2:B:956:PHE:CD2	2:B:960:GLY:HA2	2.49	0.47
2:B:1040:GLN:HG2	3:C:203:TRP:CZ2	2.48	0.47
18:R:192:VAL:HG12	18:R:201:LEU:O	2.14	0.47
17:Q:110:MET:HB3	18:R:218:LYS:CG	2.24	0.47
1:A:101:VAL:O	1:A:105:LYS:HG3	2.14	0.47
1:A:465:HIS:CE1	1:A:467:MET:HB2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:388:TYR:HE1	2:B:502:HIS:HB3	1.80	0.47
3:C:16:ASP:HA	3:C:240:ARG:HG3	1.96	0.47
9:I:105:GLU:HG3	9:I:107:ALA:HB2	1.96	0.47
17:Q:126:SER:HB2	17:Q:136:PHE:O	2.14	0.47
1:A:111:CYS:HA	1:A:188:GLN:NE2	2.29	0.47
1:A:376:ASP:OD2	1:A:473:ARG:NE	2.47	0.47
1:A:478:PRO:HB3	11:K:4:PRO:HD2	1.96	0.47
1:A:592:PHE:CE2	1:A:596:ILE:HD11	2.49	0.47
2:B:242:ARG:HH21	2:B:252:ILE:HD11	1.80	0.47
2:B:780:VAL:HG21	2:B:1048:TYR:CE2	2.50	0.47
3:C:109:GLU:N	3:C:109:GLU:OE1	2.37	0.47
9:I:102:ALA:C	9:I:104:ALA:H	2.16	0.47
2:B:309:PHE:HE2	9:I:25:TYR:CE2	2.32	0.47
15:O:64:THR:OG1	15:O:75:VAL:HB	2.14	0.47
2:B:1028:LEU:HB2	2:B:1041:ILE:HD13	1.95	0.47
2:B:936:ALA:HA	2:B:942:LYS:HA	1.95	0.47
5:E:173:ILE:N	5:E:208:LEU:O	2.41	0.47
7:G:52:ASP:H	7:G:72:TYR:HA	1.79	0.47
16:P:180:LEU:HA	16:P:183:ILE:HD12	1.97	0.47
17:Q:154:CYS:SG	17:Q:155:THR:N	2.88	0.47
1:A:868:MET:HB2	1:A:1092:ALA:HB2	1.95	0.47
1:A:204:HIS:CD2	1:A:207:GLU:HG2	2.50	0.47
2:B:273:PHE:CD1	2:B:284:ILE:HG23	2.49	0.47
2:B:626:LEU:HG	2:B:698:ILE:HD13	1.95	0.47
6:F:99:ALA:O	6:F:100:ARG:HG2	2.14	0.47
6:F:52:ILE:HG21	6:F:110:LEU:HD21	1.97	0.47
18:R:213:ASP:C	18:R:215:GLU:H	2.14	0.47
1:A:597:PRO:HB2	1:A:660:MET:HE3	1.95	0.47
5:E:20:LEU:HD12	5:E:182:TYR:CE1	2.49	0.47
11:K:35:ILE:HB	11:K:71:ILE:CG1	2.44	0.47
18:R:208:CYS:C	18:R:209:GLN:O	2.48	0.47
1:A:391:ALA:HB2	1:A:447:GLU:HG2	1.97	0.47
6:F:80:MET:HG3	6:F:103:PRO:HD3	1.97	0.47
8:H:112:LEU:HB3	8:H:131:ASN:HD21	1.80	0.47
9:I:96:PHE:HD2	9:I:110:LEU:HD22	1.79	0.47
3:C:169:PHE:HZ	11:K:10:PHE:CZ	2.32	0.47
2:B:274:ARG:NH2	2:B:312:GLN:OE1	2.45	0.47
2:B:604:ILE:O	2:B:613:ARG:N	2.44	0.47
3:C:24:GLU:HG2	3:C:228:ARG:HA	1.97	0.47
12:L:25:GLU:O	12:L:37:ARG:NH1	2.47	0.47
14:N:332:GLU:HB3	15:O:92:LYS:HE2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:161:TYR:O	20:T:164:GLU:HB3	2.15	0.47
2:B:1036:LYS:HB2	3:C:194:HIS:CB	2.43	0.47
12:L:26:ASN:HA	12:L:37:ARG:NH1	2.26	0.47
18:R:210:PHE:O	18:R:212:VAL:CB	2.61	0.47
19:S:42:TRP:CD1	19:S:102:VAL:HG11	2.50	0.47
19:S:10:ASN:O	20:T:47:LYS:HB2	2.15	0.47
21:U:184:ASP:O	21:U:188:LYS:HG3	2.15	0.47
16:P:167:ASN:ND2	23:Y:79:DT:H1'	2.30	0.47
1:A:1307:VAL:CG2	1:A:1338:THR:CA	2.93	0.47
1:A:1468:THR:O	6:F:64:ARG:NH2	2.42	0.47
1:A:609:HIS:N	1:A:610:PRO:HD3	2.29	0.47
2:B:46:SER:HB2	2:B:395:LEU:HD23	1.95	0.47
2:B:499:ARG:HH11	2:B:499:ARG:HB3	1.75	0.47
2:B:539:SER:HA	2:B:542:LEU:HB3	1.97	0.47
2:B:685:LYS:HA	2:B:688:ALA:HB2	1.97	0.47
6:F:108:ARG:HB2	6:F:116:GLU:CG	2.45	0.47
8:H:65:TYR:CE1	8:H:79:ASP:CG	2.71	0.47
15:O:4:GLN:OE1	15:O:4:GLN:N	2.43	0.47
1:A:601:ASN:ND2	1:A:632:ASN:H	2.09	0.46
3:C:8:THR:H	3:C:25:ASN:HB3	1.79	0.46
5:E:188:GLY:HA2	5:E:208:LEU:HD21	1.97	0.46
12:L:18:ILE:N	12:L:45:TYR:O	2.47	0.46
13:M:39:LEU:CD1	13:M:41:VAL:HG13	2.45	0.46
13:M:48:VAL:O	13:M:52:TRP:N	2.48	0.46
17:Q:188:TYR:CD2	17:Q:192:ARG:HB2	2.49	0.46
17:Q:104:LYS:NZ	18:R:238:LYS:CE	2.78	0.46
1:A:922:PHE:CE2	1:A:952:LEU:HD21	2.39	0.46
2:B:255:ARG:HG2	2:B:307:GLU:OE2	2.15	0.46
2:B:551:GLU:HB3	2:B:556:ILE:HD13	1.96	0.46
10:J:67:LYS:NZ	12:L:23:HIS:O	2.47	0.46
11:K:99:SER:O	11:K:103:GLU:HG3	2.15	0.46
17:Q:25:PHE:CB	18:R:215:GLU:OE2	2.63	0.46
1:A:1290:SER:OG	2:B:250:SER:C	2.53	0.46
1:A:1371:ILE:HD11	1:A:1406:THR:HG22	1.98	0.46
1:A:452:ASP:HA	1:A:474:VAL:HG23	1.97	0.46
1:A:60:PRO:HG2	1:A:62:GLN:HB3	1.97	0.46
2:B:1061:SER:HA	2:B:1084:LEU:HD11	1.96	0.46
1:A:74:CYS:HA	2:B:1129:ASN:O	2.15	0.46
2:B:1132:THR:HG23	2:B:1133:HIS:CD2	2.50	0.46
2:B:455:ASP:C	2:B:457:LYS:H	2.18	0.46
9:I:12:VAL:HG11	9:I:15:ARG:NH2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:10:LEU:H	13:M:11:PRO:HD3	1.34	0.46
13:M:15:CYS:HB2	13:M:18:HIS:O	2.16	0.46
17:Q:106:LYS:HG2	18:R:218:LYS:CD	2.45	0.46
21:U:291:CYS:N	21:U:296:ASN:O	2.36	0.46
23:Y:66:DC:H2"	23:Y:67:DC:C6	2.50	0.46
2:B:1114:TYR:CD1	2:B:1153:TYR:HB2	2.50	0.46
2:B:386:ASP:HB3	2:B:502:HIS:HD2	1.80	0.46
3:C:53:ASP:N	3:C:160:ARG:O	2.48	0.46
1:A:662:HIS:NE2	6:F:127:ASP:OD2	2.28	0.46
8:H:50:VAL:HG13	8:H:56:PHE:CZ	2.51	0.46
2:B:172:CYS:HB2	10:J:62:TYR:CG	2.51	0.46
14:N:32:ASP:HB3	14:N:34:VAL:HG23	1.98	0.46
14:N:349:TRP:HH2	16:P:191:GLU:OE2	1.98	0.46
17:Q:104:LYS:HZ2	18:R:238:LYS:CD	2.25	0.46
7:G:95:VAL:HG11	17:Q:127:PHE:HZ	1.79	0.46
18:R:140:LYS:HB2	18:R:141:PRO:HD3	1.96	0.46
17:Q:105:TYR:HA	18:R:234:GLU:CD	2.35	0.46
22:X:12:DA:N6	23:Y:82:DT:H3	2.14	0.46
1:A:18:ILE:HD11	1:A:1460:LEU:CD2	2.46	0.46
1:A:619:LYS:O	1:A:620:HIS:CG	2.69	0.46
1:A:76:GLY:HA3	2:B:1131:ARG:NH2	2.31	0.46
2:B:249:LYS:HE3	2:B:249:LYS:HB3	1.41	0.46
2:B:752:TYR:HE1	2:B:809:VAL:CG2	2.29	0.46
6:F:56:TYR:HD1	6:F:124:ILE:HB	1.81	0.46
3:C:4:ALA:HB1	11:K:97:GLU:OE1	2.14	0.46
13:M:118:PHE:CE1	13:M:142:PHE:HB3	2.51	0.46
16:P:289:PRO:HB2	23:Y:83:DA:H4'	1.97	0.46
19:S:26:TYR:HB2	19:S:139:PRO:O	2.16	0.46
20:T:228:ILE:HA	22:X:30:DG:H5"	1.97	0.46
1:A:994:PHE:CZ	1:A:1064:ALA:HA	2.50	0.46
1:A:520:MET:HB3	1:A:522:PRO:HD2	1.97	0.46
2:B:1130:THR:N	2:B:1134:THR:O	2.48	0.46
3:C:14:LEU:HB3	3:C:19:VAL:HG23	1.98	0.46
5:E:71:GLN:O	5:E:100:THR:OG1	2.25	0.46
8:H:110:THR:O	8:H:111:ARG:HB2	2.13	0.46
10:J:35:LEU:HB3	10:J:46:ARG:HD2	1.98	0.46
14:N:343:HIS:O	14:N:350:LYS:N	2.36	0.46
16:P:268:ILE:HD13	16:P:332:LEU:HG	1.98	0.46
17:Q:110:MET:O	17:Q:113:ARG:HB3	2.16	0.46
23:Y:89:DC:H2"	23:Y:90:DC:C6	2.51	0.46
1:A:1274:GLU:HG3	1:A:1276:VAL:HG23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:LYS:HE3	2:B:1073:GLN:HG2	1.98	0.46
1:A:384:ILE:O	1:A:388:MET:N	2.43	0.46
1:A:432:HIS:NE2	1:A:438:LEU:HD13	2.31	0.46
1:A:788:VAL:HB	1:A:823:VAL:HB	1.98	0.46
1:A:848:ILE:HD13	2:B:499:ARG:HG3	1.97	0.46
2:B:1066:PRO:HB2	2:B:1075:MET:HG3	1.98	0.46
2:B:242:ARG:O	2:B:244:GLY:N	2.49	0.46
2:B:425:ARG:HD3	2:B:427:LYS:HD2	1.98	0.46
3:C:54:ALA:HB3	3:C:160:ARG:HB2	1.97	0.46
5:E:122:ALA:HB3	5:E:125:TYR:HB3	1.98	0.46
13:M:279:GLY:HA2	20:T:153:TYR:HE1	1.81	0.46
17:Q:185:GLU:O	17:Q:189:ALA:N	2.48	0.46
19:S:109:LYS:HD2	19:S:149:LEU:HD23	1.97	0.46
1:A:408:ARG:HH11	1:A:414:PRO:HB2	1.79	0.46
1:A:364:ARG:HB2	1:A:502:ASN:OD1	2.16	0.46
1:A:527:THR:HG22	1:A:532:ARG:O	2.16	0.46
1:A:611:ASP:CB	1:A:626:THR:OG1	2.64	0.46
1:A:63:GLY:HA3	1:A:258:LEU:HD23	1.98	0.46
2:B:573:TRP:CH2	2:B:575:GLY:HA2	2.51	0.46
6:F:116:GLU:HG3	6:F:118:TRP:HE1	1.81	0.46
2:B:910:THR:HB	12:L:43:ILE:HD13	1.98	0.46
16:P:209:THR:HG21	16:P:224:ALA:CB	2.46	0.46
18:R:190:LEU:O	18:R:203:PHE:N	2.49	0.46
20:T:172:ASP:OD1	20:T:173:GLY:N	2.48	0.46
1:A:1274:GLU:O	1:A:1276:VAL:N	2.49	0.46
2:B:1093:CYS:O	2:B:1097:HIS:N	2.49	0.46
2:B:240:LEU:HD13	2:B:242:ARG:HD3	1.97	0.46
2:B:26:CYS:O	2:B:30:ILE:HG13	2.15	0.46
2:B:63:PRO:HG2	2:B:64:PRO:HD3	1.97	0.46
3:C:117:SER:HB2	3:C:130:VAL:HG11	1.98	0.46
8:H:107:GLU:HA	8:H:107:GLU:OE1	2.15	0.46
1:A:557:ARG:HD2	8:H:75:TYR:CE2	2.49	0.46
9:I:73:SER:HB2	9:I:115:THR:OG1	2.15	0.46
9:I:81:THR:HG22	9:I:94:ALA:O	2.16	0.46
12:L:17:TYR:O	12:L:25:GLU:HA	2.15	0.46
13:M:268:LYS:O	13:M:269:ARG:NH1	2.37	0.46
20:T:30:GLN:O	20:T:62:LEU:HD11	2.16	0.46
1:A:1310:HIS:CG	21:U:252:LYS:HG2	2.50	0.46
1:A:1030:SER:O	1:A:1034:GLN:N	2.41	0.46
2:B:1062:ARG:NH2	2:B:1074:PRO:HB3	2.31	0.46
2:B:29:VAL:HG22	2:B:643:LEU:HD11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:451:GLY:HA2	2:B:467:SER:HB3	1.97	0.46
2:B:520:VAL:C	2:B:522:LEU:H	2.20	0.46
1:A:930:LEU:HD11	8:H:107:GLU:OE2	2.16	0.46
8:H:117:SER:HA	8:H:121:LEU:O	2.16	0.46
9:I:56:ASN:CG	9:I:57:LYS:H	2.20	0.46
12:L:25:GLU:CG	12:L:27:GLU:HG2	2.46	0.46
13:M:185:ARG:HA	20:T:158:ASN:HB2	1.98	0.46
20:T:198:ASN:HD21	20:T:200:LYS:HZ3	1.64	0.46
20:T:197:TYR:HB2	20:T:202:LEU:HD21	1.98	0.46
20:T:177:ARG:HH21	20:T:212:TYR:HB2	1.81	0.46
22:X:42:DA:H2"	22:X:43:DG:H8	1.81	0.46
1:A:721:HIS:O	9:I:109:ARG:HA	2.16	0.45
2:B:876:ASN:OD1	2:B:879:GLU:OE2	2.34	0.45
1:A:1036:ASN:OD1	1:A:1037:ALA:N	2.49	0.45
1:A:909:LEU:HD13	1:A:973:GLY:HA2	1.98	0.45
2:B:89:GLU:HB3	2:B:127:ASP:HB3	1.98	0.45
2:B:175:ASN:HA	10:J:62:TYR:CD2	2.51	0.45
2:B:295:PRO:O	2:B:299:GLU:HG2	2.16	0.45
2:B:834:ARG:HA	2:B:840:MET:SD	2.55	0.45
2:B:939:HIS:CD2	2:B:980:HIS:HA	2.50	0.45
3:C:212:ASP:O	3:C:213:GLU:C	2.50	0.45
5:E:72:MET:HG3	5:E:101:ARG:HB2	1.97	0.45
7:G:165:ASP:HB2	7:G:168:LEU:HD11	1.98	0.45
8:H:2:ALA:O	8:H:4:ILE:N	2.50	0.45
17:Q:12:ALA:O	17:Q:15:LYS:HB2	2.15	0.45
20:T:146:ASP:OD2	20:T:147:LYS:HG2	2.16	0.45
1:A:1085:GLU:OE1	6:F:60:TYR:OH	2.28	0.45
1:A:452:ASP:CG	1:A:476:ILE:HG12	2.36	0.45
1:A:51:ARG:H	1:A:52:PRO:HD2	1.81	0.45
1:A:75:ALA:C	2:B:1131:ARG:HH21	2.19	0.45
2:B:93:LEU:H	20:T:145:LEU:HB3	1.81	0.45
8:H:10:PHE:CE2	8:H:58:LEU:HD13	2.52	0.45
9:I:25:TYR:HD2	9:I:40:ARG:HG3	1.81	0.45
17:Q:18:ALA:O	17:Q:22:ILE:HG23	2.15	0.45
20:T:139:VAL:O	20:T:140:ARG:HB3	2.11	0.45
21:U:136:THR:OG1	21:U:141:ARG:NH1	2.49	0.45
1:A:1137:PRO:HA	1:A:1360:ASN:HD21	1.80	0.45
1:A:385:ALA:HB2	1:A:476:ILE:HD12	1.98	0.45
1:A:478:PRO:HB2	1:A:479:TRP:CE3	2.52	0.45
2:B:125:TYR:HE2	20:T:148:VAL:O	1.99	0.45
3:C:11:ILE:HA	3:C:21:PHE:CB	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:116:GLU:O	7:G:130:THR:HA	2.16	0.45
13:M:39:LEU:HD12	13:M:41:VAL:HG13	1.99	0.45
20:T:198:ASN:OD1	20:T:199:LEU:N	2.50	0.45
21:U:133:ALA:HB2	21:U:167:GLU:HG3	1.98	0.45
23:Y:53:DG:H2"	23:Y:54:DA:C8	2.51	0.45
1:A:1301:ILE:O	1:A:1304:ILE:HG12	2.16	0.45
1:A:956:PHE:HA	1:A:959:MET:HB2	1.99	0.45
2:B:1029:TYR:CD1	2:B:1036:LYS:HG2	2.51	0.45
2:B:128:ILE:HB	2:B:145:GLN:HB2	1.99	0.45
2:B:369:VAL:O	2:B:373:LEU:N	2.41	0.45
2:B:384:ASP:OD2	2:B:387:HIS:N	2.49	0.45
2:B:631:GLN:O	2:B:683:GLN:HG2	2.16	0.45
2:B:845:TYR:OH	2:B:891:ASP:OD1	2.33	0.45
11:K:64:PRO:HD2	11:K:70:LYS:O	2.16	0.45
13:M:123:THR:O	13:M:127:ARG:NH2	2.50	0.45
16:P:209:THR:CG2	16:P:223:GLY:HA3	2.36	0.45
16:P:264:VAL:HG23	16:P:266:PHE:H	1.81	0.45
16:P:297:LYS:CA	16:P:297:LYS:CE	2.89	0.45
17:Q:70:LYS:HB2	18:R:225:VAL:CG1	2.47	0.45
1:A:431:PHE:HD2	13:M:33:ILE:HG21	1.82	0.45
1:A:514:GLU:OE1	2:B:1099:ALA:HB1	2.17	0.45
2:B:201:ALA:HA	2:B:392:ARG:HG2	1.98	0.45
2:B:68:GLN:HA	2:B:83:ARG:HA	1.98	0.45
2:B:881:GLU:HA	2:B:883:THR:OG1	2.16	0.45
6:F:44:ARG:HB3	6:F:114:SER:HA	1.97	0.45
8:H:98:ARG:HD3	8:H:115:TYR:CD2	2.48	0.45
8:H:57:ARG:O	8:H:145:MET:HA	2.17	0.45
18:R:202:PHE:O	18:R:203:PHE:CE1	2.64	0.45
21:U:299:LYS:HB2	21:U:301:CYS:O	2.17	0.45
1:A:1178:ASP:OD1	1:A:1184:THR:HA	2.16	0.45
1:A:548:PHE:HE2	1:A:592:PHE:HB2	1.81	0.45
1:A:84:HIS:N	1:A:257:PRO:HB3	2.32	0.45
2:B:795:ILE:HG12	2:B:947:ILE:HG22	1.99	0.45
7:G:107:PHE:O	7:G:160:ILE:HG13	2.17	0.45
7:G:46:ILE:HD11	7:G:77:PHE:HB2	1.99	0.45
2:B:281:ASP:CG	9:I:22:ASN:HD22	2.20	0.45
10:J:3:ILE:HD13	10:J:18:TRP:CB	2.47	0.45
13:M:177:PHE:O	13:M:181:CYS:N	2.38	0.45
14:N:25:VAL:HG11	15:O:36:VAL:HG13	1.99	0.45
16:P:329:TYR:N	16:P:330:PRO:HD2	2.32	0.45
1:A:1310:HIS:NE2	1:A:1334:TRP:HE3	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:193:VAL:HG11	2:B:481:HIS:CD2	2.52	0.45
2:B:640:ILE:HA	2:B:643:LEU:HD12	1.98	0.45
5:E:134:GLU:CD	5:E:181:ARG:HH12	2.20	0.45
7:G:60:GLN:HB2	7:G:63:ARG:NE	2.32	0.45
18:R:156:ASP:O	18:R:158:HIS:N	2.50	0.45
19:S:172:ASN:OD1	19:S:173:HIS:N	2.50	0.45
20:T:23:VAL:HG21	20:T:31:TRP:CZ3	2.52	0.45
1:A:1479:LYS:HD3	6:F:103:PRO:HA	1.99	0.45
2:B:780:VAL:HG21	2:B:1048:TYR:HE2	1.80	0.45
2:B:66:ASP:HB3	2:B:85:LEU:HD13	1.99	0.45
2:B:738:THR:OG1	10:J:62:TYR:OH	2.23	0.45
12:L:18:ILE:O	12:L:19:CYS:C	2.54	0.45
17:Q:145:PHE:HA	17:Q:152:PHE:HA	1.98	0.45
20:T:95:VAL:O	20:T:106:LEU:HD12	2.17	0.45
1:A:909:LEU:HD22	1:A:1328:PHE:CZ	2.51	0.45
1:A:926:ASN:OD1	1:A:931:ARG:HG3	2.17	0.45
1:A:902:GLU:N	1:A:979:LEU:O	2.48	0.45
2:B:939:HIS:HE2	2:B:983:GLU:HB2	1.82	0.45
11:K:105:PHE:O	11:K:109:ILE:HG12	2.16	0.45
18:R:155:LEU:HD11	18:R:203:PHE:HA	1.98	0.45
19:S:29:MET:HB2	20:T:96:PHE:CD1	2.52	0.45
20:T:138:PRO:O	20:T:141:LEU:HG	2.17	0.45
22:X:11:DT:H2"	22:X:12:DA:C8	2.52	0.45
1:A:1241:ASP:O	1:A:1262:MET:HG3	2.17	0.44
1:A:1361:ASP:OD2	1:A:1364:GLU:HG2	2.16	0.44
1:A:404:GLU:OE1	1:A:407:ARG:HD2	2.17	0.44
1:A:579:ILE:HD12	1:A:585:LEU:HD12	1.99	0.44
1:A:972:THR:O	1:A:1317:LYS:HD3	2.17	0.44
2:B:254:GLN:NE2	2:B:300:MET:SD	2.74	0.44
2:B:626:LEU:HA	2:B:662:VAL:HG12	1.98	0.44
3:C:37:VAL:HG12	3:C:248:ALA:HB1	1.99	0.44
3:C:6:GLN:HG2	3:C:25:ASN:HD21	1.77	0.44
4:D:83:VAL:HG13	4:D:134:ILE:HG12	1.99	0.44
12:L:13:GLN:O	12:L:29:LYS:HD3	2.17	0.44
20:T:145:LEU:HD11	20:T:148:VAL:CG2	2.46	0.44
20:T:165:TYR:O	20:T:169:LYS:HG2	2.17	0.44
22:X:14:DA:H2"	22:X:15:DA:C8	2.52	0.44
1:A:1022:ILE:HG12	1:A:1034:GLN:OE1	2.17	0.44
1:A:47:THR:C	1:A:48:GLU:HG2	2.38	0.44
1:A:556:GLU:HG3	1:A:559:GLU:H	1.82	0.44
1:A:894:ASP:OD1	1:A:1396:ARG:NH2	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1117:HIS:CE1	2:B:1148:LEU:HD13	2.52	0.44
2:B:385:ARG:HD2	2:B:497:LYS:HE3	1.99	0.44
2:B:862:GLY:O	2:B:898:THR:HA	2.18	0.44
3:C:189:ASP:OD2	3:C:212:ASP:HB3	2.17	0.44
2:B:856:PRO:HD3	12:L:46:LYS:HD3	1.99	0.44
1:A:431:PHE:HB2	13:M:33:ILE:HG21	1.99	0.44
16:P:212:LEU:O	16:P:219:MET:HA	2.18	0.44
17:Q:187:ILE:O	18:R:212:VAL:HG12	2.17	0.44
17:Q:23:ARG:CZ	18:R:207:SER:H	2.30	0.44
17:Q:187:ILE:HG21	18:R:212:VAL:CA	2.20	0.44
20:T:199:LEU:HD13	20:T:233:TRP:NE1	2.32	0.44
21:U:229:ALA:HB1	21:U:234:LYS:HB3	1.99	0.44
20:T:227:GLY:C	22:X:30:DG:H5''	2.38	0.44
1:A:395:THR:OG1	1:A:398:ASN:OD1	2.31	0.44
1:A:361:PHE:N	2:B:1062:ARG:O	2.50	0.44
2:B:240:LEU:HD22	2:B:242:ARG:NH1	2.33	0.44
2:B:629:GLU:N	2:B:632:LYS:O	2.42	0.44
2:B:21:LEU:HD23	2:B:633:LEU:HD23	2.00	0.44
2:B:674:MET:HB2	9:I:77:THR:HG22	1.98	0.44
5:E:26:TYR:HD1	5:E:65:ASN:H	1.63	0.44
8:H:76:ASN:OD1	8:H:78:THR:OG1	2.33	0.44
21:U:177:TYR:CE1	21:U:181:ARG:HA	2.52	0.44
16:P:309:LYS:HD2	23:Y:82:DT:H3'	2.00	0.44
2:B:93:LEU:HD23	2:B:160:TYR:CE2	2.52	0.44
2:B:905:ASP:OD2	2:B:922:ARG:NE	2.44	0.44
2:B:99:TRP:HB2	13:M:129:ASN:ND2	2.32	0.44
3:C:200:PRO:CG	3:C:217:GLN:CD	2.68	0.44
5:E:192:LYS:HA	5:E:206:TYR:HD1	1.82	0.44
8:H:71:ASP:OD1	8:H:71:ASP:N	2.50	0.44
12:L:15:MET:HA	12:L:27:GLU:OE1	2.16	0.44
14:N:29:PHE:CE1	15:O:36:VAL:HG21	2.52	0.44
17:Q:135:THR:HG23	17:Q:164:ASP:OD1	2.18	0.44
17:Q:55:ASP:O	17:Q:59:LEU:N	2.42	0.44
21:U:223:MET:HB3	21:U:224:THR:H	1.58	0.44
1:A:578:ALA:N	1:A:585:LEU:O	2.51	0.44
1:A:926:ASN:ND2	1:A:931:ARG:CD	2.64	0.44
1:A:931:ARG:C	1:A:933:THR:H	2.19	0.44
2:B:1056:ASP:OD1	2:B:1056:ASP:N	2.51	0.44
2:B:83:ARG:HB3	2:B:133:ILE:O	2.17	0.44
2:B:134:LYS:HG3	2:B:136:GLY:H	1.83	0.44
2:B:627:ILE:HA	2:B:695:HIS:CD2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:888:THR:O	2:B:890:ARG:HG2	2.17	0.44
2:B:888:THR:O	2:B:890:ARG:N	2.50	0.44
5:E:104:ILE:HG23	5:E:129:GLN:NE2	2.32	0.44
5:E:71:GLN:NE2	5:E:97:GLU:HG3	2.32	0.44
6:F:53:THR:HB	6:F:108:ARG:HH11	1.83	0.44
7:G:60:GLN:HB2	7:G:63:ARG:HE	1.82	0.44
8:H:94:GLY:HA3	8:H:118:TYR:HA	1.98	0.44
20:T:223:GLN:HB3	20:T:233:TRP:CE3	2.52	0.44
1:A:1031:ARG:O	1:A:1035:GLU:N	2.42	0.44
1:A:283:ILE:HA	1:A:286:ILE:HG12	2.00	0.44
2:B:11:ASP:HB2	2:B:638:ARG:HD3	2.00	0.44
9:I:17:CYS:O	9:I:21:ASN:N	2.46	0.44
9:I:96:PHE:HA	9:I:111:TYR:O	2.18	0.44
13:M:11:PRO:HB2	13:M:12:ARG:H	1.60	0.44
13:M:138:THR:HG23	13:M:163:CYS:HB3	1.99	0.44
15:O:64:THR:HG22	16:P:188:ARG:HB3	2.00	0.44
16:P:294:ARG:HH21	16:P:294:ARG:HG3	1.82	0.44
18:R:154:LEU:HD21	18:R:162:GLY:O	2.15	0.44
19:S:143:TRP:NE1	19:S:145:ASN:OD1	2.37	0.44
1:A:607:SER:O	21:U:301:CYS:HA	2.17	0.44
1:A:1199:MET:O	1:A:1201:ASP:N	2.51	0.44
2:B:169:ARG:HA	2:B:172:CYS:SG	2.57	0.44
2:B:655:ASP:HA	2:B:658:ALA:HB3	2.00	0.44
3:C:101:PHE:HA	3:C:121:ILE:O	2.18	0.44
4:D:44:ARG:HB2	4:D:61:PHE:CZ	2.53	0.44
7:G:84:VAL:HG12	7:G:144:ARG:HD3	1.98	0.44
8:H:39:LEU:HA	8:H:124:ARG:O	2.17	0.44
8:H:75:TYR:CG	8:H:75:TYR:O	2.70	0.44
14:N:337:CYS:O	15:O:97:ALA:HA	2.17	0.44
16:P:174:LEU:O	16:P:249:LYS:N	2.51	0.44
20:T:17:GLY:HA2	20:T:109:ILE:O	2.17	0.44
20:T:223:GLN:HB3	20:T:233:TRP:CD2	2.52	0.44
21:U:225:ALA:CB	21:U:228:MET:HG2	2.48	0.44
23:Y:49:DG:H2'	23:Y:50:DA:C8	2.53	0.44
1:A:1313:GLN:OE1	1:A:1335:ILE:HD13	2.18	0.44
1:A:349:ARG:O	1:A:353:ASN:HB2	2.17	0.44
2:B:663:GLU:OE2	2:B:695:HIS:NE2	2.50	0.44
10:J:63:ALA:CB	10:J:64:PRO:HD3	2.32	0.44
16:P:167:ASN:HB2	23:Y:80:DT:H4'	2.00	0.44
1:A:129:ILE:CD1	1:A:140:ARG:HA	2.48	0.44
1:A:64:VAL:HB	1:A:70:ARG:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:875:TYR:HE1	1:A:1470:CYS:SG	2.40	0.44
2:B:37:LYS:HE2	2:B:653:TRP:HD1	1.80	0.44
3:C:241:PRO:HA	3:C:244:ILE:HD12	2.00	0.44
3:C:74:ILE:HG22	3:C:129:PRO:O	2.17	0.44
6:F:68:THR:O	6:F:72:GLN:HG3	2.17	0.44
9:I:97:PHE:HD1	9:I:98:GLN:O	2.00	0.44
9:I:97:PHE:O	9:I:111:TYR:N	2.47	0.44
18:R:160:GLN:C	18:R:162:GLY:H	2.21	0.44
19:S:47:LEU:HG	19:S:98:TRP:CE3	2.53	0.44
20:T:225:VAL:HG23	20:T:227:GLY:H	1.83	0.44
21:U:176:ILE:HG22	21:U:187:TYR:CD2	2.53	0.44
1:A:1014:LYS:O	1:A:1018:LYS:HG3	2.18	0.43
1:A:367:ILE:HD13	1:A:494:ALA:HB1	1.99	0.43
1:A:43:TYR:O	1:A:45:GLU:N	2.51	0.43
2:B:1030:ASN:OD1	2:B:1031:GLY:N	2.51	0.43
2:B:198:GLU:OE1	2:B:487:SER:OG	2.33	0.43
2:B:280:SER:HB3	9:I:21:ASN:HB2	1.99	0.43
2:B:318:LEU:HD13	2:B:336:ILE:HG23	1.99	0.43
2:B:746:THR:O	2:B:812:ARG:HA	2.18	0.43
5:E:192:LYS:HG3	5:E:206:TYR:CE1	2.53	0.43
15:O:48:LEU:HD23	15:O:52:VAL:HG21	2.00	0.43
14:N:327:GLU:OE1	16:P:188:ARG:NH1	2.51	0.43
17:Q:45:GLU:OE1	17:Q:94:ILE:N	2.43	0.43
18:R:127:ASN:ND2	18:R:140:LYS:HD3	2.31	0.43
21:U:150:ALA:HA	21:U:153:ARG:NH1	2.33	0.43
20:T:229:HIS:ND1	22:X:29:DC:O4'	2.51	0.43
23:Y:55:DG:H2''	23:Y:56:DG:C8	2.53	0.43
1:A:908:THR:C	1:A:910:LYS:H	2.21	0.43
2:B:249:LYS:C	2:B:251:ALA:H	2.21	0.43
2:B:309:PHE:CD2	9:I:40:ARG:HD2	2.54	0.43
2:B:845:TYR:CE2	2:B:865:VAL:HG11	2.53	0.43
1:A:1369:LEU:HD23	5:E:139:ILE:HB	2.00	0.43
6:F:51:ARG:HD3	6:F:118:TRP:CZ2	2.53	0.43
7:G:49:THR:H	7:G:74:ALA:HA	1.82	0.43
8:H:50:VAL:HG13	8:H:56:PHE:HZ	1.83	0.43
13:M:178:LYS:O	20:T:154:LYS:CG	2.57	0.43
19:S:46:ARG:N	19:S:101:ARG:O	2.38	0.43
20:T:196:TYR:HD1	20:T:232:THR:HG21	1.83	0.43
20:T:198:ASN:HD21	20:T:200:LYS:HE2	1.83	0.43
21:U:216:PRO:HD2	21:U:219:LEU:HD23	1.99	0.43
22:X:16:DA:H2''	22:X:17:DA:N7	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:431:LEU:O	2:B:435:ILE:HG12	2.17	0.43
2:B:602:SER:O	2:B:614:ILE:HG23	2.19	0.43
2:B:979:GLY:HA2	2:B:982:ILE:HD12	2.00	0.43
8:H:56:PHE:CE1	8:H:148:LEU:HA	2.54	0.43
8:H:1:MET:HA	8:H:66:GLU:OE2	2.17	0.43
1:A:331:LYS:HE2	13:M:107:MET:HG3	1.99	0.43
14:N:363:ARG:NH2	15:O:86:GLU:OE2	2.51	0.43
17:Q:123:ASN:O	17:Q:125:ALA:N	2.50	0.43
18:R:163:LEU:O	18:R:164:GLY:C	2.56	0.43
20:T:141:LEU:HD13	20:T:143:GLN:NE2	2.32	0.43
21:U:266:CYS:O	21:U:267:LYS:HG2	2.18	0.43
1:A:1184:THR:HG22	1:A:1190:GLN:HA	2.00	0.43
1:A:137:PRO:HB3	1:A:237:GLY:CA	2.45	0.43
1:A:20:ARG:HE	2:B:1174:VAL:C	2.22	0.43
1:A:219:GLU:O	1:A:223:GLU:HG2	2.18	0.43
1:A:367:ILE:CD1	1:A:494:ALA:HB1	2.47	0.43
1:A:457:ILE:CG2	1:A:504:HIS:HB2	2.48	0.43
2:B:891:ASP:OD1	2:B:893:SER:OG	2.36	0.43
2:B:970:HIS:C	2:B:973:PRO:HD2	2.39	0.43
11:K:109:ILE:HA	11:K:112:LYS:HZ3	1.83	0.43
13:M:179:GLU:HG2	20:T:154:LYS:CE	2.48	0.43
15:O:57:ASN:OD1	15:O:58:PHE:N	2.51	0.43
16:P:174:LEU:HD22	16:P:248:ALA:HB1	2.00	0.43
1:A:1151:ALA:HB2	1:A:1334:TRP:CZ2	2.53	0.43
1:A:1167:ARG:HA	1:A:1293:LEU:HD22	2.01	0.43
1:A:1345:ARG:O	1:A:1349:GLU:HG2	2.19	0.43
1:A:28:PRO:HB3	1:A:251:THR:OG1	2.18	0.43
1:A:312:PHE:HE2	1:A:326:PRO:HB2	1.82	0.43
1:A:456:VAL:HG12	1:A:505:LEU:HD13	2.00	0.43
1:A:910:LYS:HB3	1:A:963:ARG:HH12	1.83	0.43
2:B:161:CYS:O	2:B:164:ASN:ND2	2.51	0.43
2:B:682:LEU:HD23	2:B:682:LEU:HA	1.82	0.43
2:B:68:GLN:HG3	2:B:82:PRO:O	2.19	0.43
4:D:96:GLU:OE2	4:D:117:SER:OG	2.22	0.43
17:Q:32:LEU:HD11	18:R:203:PHE:HD2	1.68	0.43
20:T:191:PHE:CD2	20:T:235:LEU:HG	2.54	0.43
1:A:1013:VAL:HG22	1:A:1049:LEU:HD23	2.00	0.43
1:A:391:ALA:HA	1:A:446:VAL:O	2.19	0.43
1:A:907:ALA:H	1:A:975:SER:HB3	1.82	0.43
2:B:360:LYS:HA	2:B:363:TYR:HD2	1.82	0.43
2:B:454:GLY:HA3	2:B:459:ALA:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:112:PRO:HA	5:E:115:LYS:HD2	2.00	0.43
5:E:76:PHE:HA	5:E:77:PRO:HD2	1.82	0.43
15:O:20:ASP:OD1	15:O:24:GLN:NE2	2.52	0.43
15:O:60:GLY:O	15:O:76:LEU:HD23	2.18	0.43
16:P:297:LYS:HE2	16:P:297:LYS:CA	2.48	0.43
18:R:210:PHE:CB	18:R:212:VAL:HG11	2.46	0.43
13:M:182:ALA:HB2	20:T:154:LYS:HG3	2.01	0.43
21:U:276:VAL:HG13	21:U:277:GLN:HG3	2.00	0.43
1:A:1018:LYS:O	1:A:1021:VAL:HG23	2.18	0.43
1:A:1301:ILE:HD13	1:A:1342:SER:OG	2.19	0.43
1:A:264:VAL:O	1:A:266:MET:HG3	2.19	0.43
2:B:442:ASP:HA	2:B:445:LYS:HD2	1.99	0.43
2:B:736:TYR:CD2	2:B:737:ILE:HG12	2.54	0.43
3:C:173:HIS:HB3	3:C:176:TRP:CE3	2.53	0.43
2:B:1036:LYS:HG3	3:C:186:TYR:OH	2.18	0.43
3:C:235:SER:HB2	3:C:241:PRO:HG3	1.99	0.43
4:D:74:PHE:CD2	4:D:80:ILE:HG12	2.54	0.43
7:G:94:LYS:O	7:G:110:ARG:HD2	2.18	0.43
10:J:21:TYR:CZ	10:J:25:LEU:HD21	2.54	0.43
14:N:332:GLU:HB3	15:O:92:LYS:CE	2.49	0.43
14:N:46:TRP:CZ2	15:O:11:LEU:HD12	2.48	0.43
15:O:64:THR:HG21	16:P:188:ARG:CZ	2.49	0.43
16:P:303:LEU:O	16:P:310:VAL:HA	2.18	0.43
17:Q:19:LYS:O	17:Q:22:ILE:HG13	2.19	0.43
17:Q:34:LEU:HD23	17:Q:37:LEU:HD12	2.00	0.43
21:U:262:THR:HA	21:U:269:LYS:HG2	2.00	0.43
1:A:1027:ASP:OD1	1:A:1027:ASP:N	2.52	0.43
1:A:1365:ILE:O	1:A:1370:GLY:N	2.46	0.43
1:A:19:LYS:N	2:B:1173:SER:HA	2.34	0.43
1:A:877:ALA:O	1:A:890:ARG:HA	2.19	0.43
1:A:967:ARG:HG3	1:A:967:ARG:HH11	1.84	0.43
2:B:240:LEU:HD23	2:B:257:VAL:HG21	2.00	0.43
2:B:588:ARG:O	2:B:592:ARG:N	2.41	0.43
2:B:654:GLN:O	2:B:658:ALA:N	2.39	0.43
8:H:106:THR:C	8:H:108:ALA:N	2.71	0.43
8:H:90:TYR:O	8:H:144:LEU:HA	2.18	0.43
1:A:1209:PRO:CB	9:I:33:ARG:HH12	2.23	0.43
2:B:777:ASN:O	10:J:47:ARG:HD2	2.19	0.43
13:M:169:ARG:HD3	13:M:206:VAL:HB	2.00	0.43
14:N:337:CYS:SG	14:N:353:LEU:HD13	2.58	0.43
15:O:60:GLY:HA3	15:O:79:VAL:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:209:THR:HG21	16:P:224:ALA:HB2	2.00	0.43
17:Q:22:ILE:HG21	17:Q:34:LEU:HB3	2.00	0.43
17:Q:104:LYS:NZ	18:R:238:LYS:HE3	2.34	0.43
19:S:53:ASN:HB2	19:S:96:GLN:OE1	2.19	0.43
20:T:21:VAL:HA	20:T:114:ALA:O	2.18	0.43
21:U:184:ASP:OD1	21:U:185:MET:N	2.52	0.43
1:A:945:ASN:HB3	1:A:948:ILE:HG22	2.00	0.43
1:A:805:ARG:NH2	2:B:671:GLU:O	2.52	0.43
2:B:79:GLU:OE2	2:B:79:GLU:HA	2.18	0.43
2:B:874:PRO:C	2:B:876:ASN:H	2.17	0.43
3:C:11:ILE:HA	3:C:21:PHE:HB2	2.01	0.43
10:J:20:ALA:O	10:J:24:LEU:HG	2.19	0.43
16:P:165:LEU:HD13	16:P:318:ARG:HG3	2.00	0.43
19:S:127:PHE:CB	20:T:19:TRP:HB2	2.48	0.43
1:A:460:ARG:HA	1:A:501:MET:SD	2.59	0.43
1:A:18:ILE:HD13	2:B:1171:MET:HB2	2.00	0.43
1:A:1372:GLU:HG3	5:E:148:HIS:HE1	1.84	0.43
10:J:1:MET:SD	10:J:55:LEU:N	2.81	0.43
13:M:14:THR:N	13:M:20:ASP:HB3	2.34	0.43
13:M:18:HIS:NE2	13:M:36:GLU:OE2	2.52	0.43
16:P:161:ILE:HG13	16:P:329:TYR:HE2	1.83	0.43
1:A:875:TYR:HA	1:A:1083:PRO:CB	2.49	0.42
1:A:1166:LEU:HD12	1:A:1296:MET:SD	2.59	0.42
1:A:1317:LYS:HE2	21:U:295:GLY:HA3	2.00	0.42
1:A:368:THR:O	1:A:483:ARG:HA	2.19	0.42
1:A:807:LEU:HB2	1:A:810:PHE:CD2	2.54	0.42
1:A:601:ASN:HB2	1:A:988:TRP:CZ3	2.54	0.42
2:B:23:GLN:N	2:B:23:GLN:OE1	2.51	0.42
2:B:72:GLN:C	2:B:73:HIS:O	2.57	0.42
2:B:805:PHE:O	2:B:929:PRO:HG2	2.19	0.42
2:B:838:GLN:HE21	2:B:890:ARG:HD3	1.84	0.42
3:C:151:VAL:HG22	3:C:152:LYS:N	2.34	0.42
5:E:58:LEU:HB3	5:E:76:PHE:CD2	2.54	0.42
1:A:874:LYS:HD2	6:F:111:PRO:HB3	2.01	0.42
8:H:66:GLU:O	8:H:67:ASP:OD1	2.36	0.42
3:C:9:VAL:HG11	11:K:105:PHE:HA	1.99	0.42
20:T:212:TYR:O	20:T:215:GLU:HB2	2.19	0.42
23:Y:58:DC:H2'	23:Y:59:DG:H5'	2.00	0.42
1:A:1175:ILE:HG12	1:A:1212:LEU:HD13	1.99	0.42
1:A:1470:CYS:O	6:F:109:TYR:HD2	2.02	0.42
1:A:364:ARG:NH2	1:A:500:GLU:O	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1030:ASN:HB3	2:B:1034:GLY:N	2.34	0.42
2:B:1102:PHE:O	2:B:1106:ARG:HG2	2.19	0.42
2:B:1130:THR:HB	2:B:1134:THR:H	1.84	0.42
2:B:860:VAL:HG12	2:B:902:GLY:C	2.38	0.42
5:E:82:VAL:HG23	5:E:106:VAL:HG13	2.00	0.42
1:A:880:ARG:HH12	5:E:169:GLN:CD	2.22	0.42
8:H:9:ILE:HA	8:H:57:ARG:HA	2.01	0.42
13:M:12:ARG:C	13:M:13:VAL:HG13	2.20	0.42
18:R:195:PRO:HG3	18:R:199:LYS:HB3	1.98	0.42
20:T:200:LYS:NZ	23:Y:68:DC:OP1	2.51	0.42
1:A:319:ASP:O	1:A:322:LEU:HG	2.19	0.42
1:A:64:VAL:HG21	1:A:68:THR:HG23	2.00	0.42
1:A:826:SER:OG	1:A:829:ALA:N	2.47	0.42
1:A:88:ILE:HD13	1:A:284:VAL:HG22	2.01	0.42
2:B:65:ILE:CG2	2:B:412:LEU:HD11	2.44	0.42
2:B:53:MET:O	2:B:57:ARG:N	2.50	0.42
2:B:757:PRO:HD3	2:B:769:PHE:CE2	2.54	0.42
1:A:540:ASP:OD2	2:B:968:ASN:ND2	2.53	0.42
6:F:45:PRO:HB3	6:F:115:TYR:CE1	2.54	0.42
8:H:75:TYR:O	8:H:76:ASN:C	2.57	0.42
10:J:20:ALA:O	10:J:24:LEU:N	2.45	0.42
11:K:13:PHE:HB2	11:K:16:GLU:HG3	2.01	0.42
17:Q:187:ILE:HD11	18:R:211:SER:CB	2.09	0.42
1:A:609:HIS:HB2	21:U:300:PHE:CZ	2.54	0.42
2:B:1028:LEU:HD13	2:B:1041:ILE:HD13	2.02	0.42
2:B:69:ALA:N	2:B:82:PRO:O	2.46	0.42
2:B:728:MET:HE2	2:B:942:LYS:HE2	2.01	0.42
2:B:94:SER:O	2:B:122:ALA:HB1	2.19	0.42
3:C:40:ALA:HB1	3:C:171:LYS:HB2	2.00	0.42
9:I:98:GLN:HB2	9:I:100:HIS:CE1	2.55	0.42
10:J:35:LEU:HB3	10:J:46:ARG:CD	2.49	0.42
12:L:17:TYR:HB2	12:L:26:ASN:HB3	2.02	0.42
16:P:261:SER:HB3	23:Y:81:DA:H4'	2.02	0.42
16:P:284:GLU:HB3	16:P:287:LEU:HB3	2.01	0.42
1:A:1310:HIS:CE1	1:A:1334:TRP:CE3	2.96	0.42
1:A:484:LEU:HD21	1:A:496:PHE:HE1	1.83	0.42
1:A:775:LYS:CB	2:B:974:SER:HB3	2.50	0.42
1:A:909:LEU:HD22	1:A:1328:PHE:CE2	2.55	0.42
1:A:10:ASP:N	2:B:1132:THR:HA	2.34	0.42
2:B:527:ALA:HB3	2:B:530:ALA:HB2	2.00	0.42
2:B:862:GLY:N	2:B:900:GLU:O	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:55:ARG:HH11	5:E:107:GLN:HE22	1.68	0.42
5:E:130:PHE:HB3	5:E:135:LEU:HD11	2.01	0.42
8:H:24:ARG:HG2	8:H:46:GLN:NE2	2.33	0.42
9:I:37:TYR:N	9:I:46:GLN:O	2.35	0.42
11:K:24:ASP:H	11:K:31:CYS:HA	1.84	0.42
11:K:37:LYS:HA	11:K:69:HIS:HB3	2.01	0.42
11:K:57:LEU:H	11:K:77:THR:HA	1.84	0.42
13:M:158:ALA:HA	13:M:186:ILE:HG13	2.01	0.42
14:N:329:PHE:HB3	14:N:331:THR:HG23	2.01	0.42
17:Q:106:LYS:O	18:R:218:LYS:CE	2.66	0.42
19:S:13:GLU:HG3	20:T:44:ARG:HA	2.00	0.42
1:A:903:PHE:CZ	1:A:976:LYS:HB3	2.55	0.42
2:B:1116:VAL:HG11	2:B:1125:MET:SD	2.59	0.42
2:B:240:LEU:HD13	2:B:242:ARG:CD	2.50	0.42
2:B:896:LEU:HD21	2:B:900:GLU:HB2	2.00	0.42
2:B:972:ILE:O	2:B:976:MET:N	2.51	0.42
3:C:75:SER:N	3:C:238:SER:O	2.42	0.42
3:C:61:ASP:N	3:C:61:ASP:OD1	2.52	0.42
13:M:135:VAL:HG12	13:M:139:ASN:ND2	2.34	0.42
13:M:214:PHE:HA	13:M:217:ARG:NH1	2.34	0.42
16:P:227:GLU:HG2	16:P:228:GLU:H	1.85	0.42
1:A:611:ASP:CG	1:A:617:PRO:HG3	2.40	0.42
1:A:606:HIS:HB3	1:A:627:LYS:HA	2.01	0.42
1:A:908:THR:O	1:A:963:ARG:NH1	2.53	0.42
1:A:931:ARG:C	1:A:933:THR:N	2.73	0.42
1:A:939:VAL:O	1:A:943:LEU:HG	2.19	0.42
2:B:1015:LEU:HD21	2:B:1024:GLY:HA2	2.01	0.42
3:C:5:ASN:O	3:C:7:PRO:CD	2.62	0.42
4:D:32:LEU:HD11	7:G:75:ILE:HG22	2.02	0.42
5:E:177:ASP:OD2	5:E:179:VAL:HB	2.19	0.42
7:G:55:GLY:HA3	7:G:69:PRO:HB2	2.00	0.42
14:N:38:VAL:CG1	15:O:22:LEU:HD22	2.49	0.42
17:Q:112:ARG:HB3	18:R:221:ARG:NH1	2.31	0.42
1:A:1151:ALA:C	1:A:1155:LYS:HZ3	2.22	0.42
1:A:1217:ASP:OD2	1:A:1220:HIS:N	2.53	0.42
1:A:72:GLN:HG2	1:A:74:CYS:H	1.83	0.42
1:A:1460:LEU:O	2:B:1152:PRO:HD3	2.20	0.42
2:B:411:LEU:HD12	2:B:440:ILE:CD1	2.49	0.42
2:B:442:ASP:OD1	2:B:445:LYS:HD2	2.19	0.42
1:A:371:PRO:HD2	2:B:788:TYR:CD1	2.53	0.42
7:G:158:PHE:CZ	17:Q:139:LEU:HA	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:99:LEU:O	17:Q:101:ASN:ND2	2.52	0.42
20:T:174:LYS:HE3	22:X:20:DG:H1'	2.02	0.42
21:U:218:ASP:C	21:U:218:ASP:OD1	2.58	0.42
21:U:215:ILE:HG22	21:U:220:PHE:HB2	2.01	0.42
1:A:1096:GLY:O	1:A:1100:THR:HG23	2.20	0.42
1:A:1302:GLU:O	1:A:1303:GLN:HB3	2.20	0.42
1:A:13:CYS:HB2	2:B:1135:TYR:CE2	2.55	0.42
1:A:71:CYS:N	1:A:75:ALA:HA	2.31	0.42
2:B:487:SER:C	2:B:489:ILE:H	2.24	0.42
2:B:800:ALA:O	2:B:805:PHE:HB2	2.20	0.42
2:B:837:CYS:SG	2:B:838:GLN:N	2.93	0.42
2:B:849:ASP:HB3	2:B:851:ASP:OD1	2.20	0.42
2:B:934:LYS:HA	2:B:944:THR:HG22	2.01	0.42
3:C:81:LYS:HG3	3:C:82:LEU:HD12	2.01	0.42
5:E:31:ASP:O	5:E:35:GLN:N	2.53	0.42
8:H:75:TYR:CE2	8:H:77:PRO:CG	3.03	0.42
9:I:57:LYS:HE2	9:I:60:HIS:NE2	2.35	0.42
9:I:61:GLU:O	9:I:103:ARG:NH1	2.53	0.42
12:L:21:GLU:OE1	12:L:21:GLU:N	2.53	0.42
15:O:42:LYS:HE3	15:O:42:LYS:HB3	1.75	0.42
16:P:168:ILE:HG13	16:P:226:SER:C	2.40	0.42
16:P:209:THR:HG22	16:P:224:ALA:H	1.47	0.42
17:Q:187:ILE:O	18:R:212:VAL:HA	2.19	0.42
21:U:191:VAL:O	21:U:195:ILE:N	2.46	0.42
1:A:1454:VAL:HG11	1:A:1466:ALA:HB3	2.02	0.42
1:A:606:HIS:HB3	1:A:628:VAL:H	1.85	0.42
1:A:632:ASN:OD1	1:A:992:LYS:NZ	2.52	0.42
2:B:1080:ARG:HG2	13:M:53:ARG:CZ	2.50	0.42
2:B:497:LYS:H	2:B:498:PRO:HD3	1.04	0.42
5:E:158:GLU:OE2	5:E:162:ARG:NH2	2.53	0.42
8:H:75:TYR:CE2	8:H:77:PRO:HG3	2.55	0.42
16:P:231:ARG:O	16:P:235:ARG:HG3	2.20	0.42
22:X:27:DG:H2''	22:X:28:DG:C8	2.55	0.42
1:A:1171:ALA:O	9:I:57:LYS:HD3	2.20	0.41
1:A:419:ILE:O	1:A:426:ARG:HA	2.19	0.41
2:B:109:MET:HB3	2:B:112:GLU:HB2	2.02	0.41
2:B:374:LEU:O	2:B:378:GLY:N	2.51	0.41
2:B:67:LEU:CD2	2:B:419:ALA:HB1	2.48	0.41
2:B:499:ARG:C	2:B:500:GLN:O	2.53	0.41
2:B:552:ASN:O	2:B:556:ILE:HG12	2.19	0.41
3:C:6:GLN:HG3	3:C:25:ASN:CG	2.37	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:52:GLU:O	4:D:54:GLU:N	2.52	0.41
8:H:88:PHE:CD1	8:H:146:LYS:HD2	2.52	0.41
9:I:7:TYR:CZ	9:I:9:PRO:HG3	2.55	0.41
3:C:6:GLN:HB2	11:K:104:ARG:HH12	1.85	0.41
13:M:283:VAL:O	13:M:287:GLN:HG2	2.20	0.41
15:O:18:SER:O	15:O:22:LEU:HG	2.20	0.41
18:R:131:GLU:HB3	18:R:138:ALA:HB3	2.01	0.41
18:R:188:GLN:HG3	18:R:189:ILE:HG13	2.01	0.41
19:S:37:VAL:HG11	19:S:42:TRP:CZ2	2.55	0.41
21:U:286:THR:CG2	21:U:299:LYS:HB3	2.47	0.41
1:A:1304:ILE:O	1:A:1306:LYS:N	2.54	0.41
1:A:204:HIS:O	1:A:206:ASN:N	2.43	0.41
1:A:275:ASP:OD1	1:A:275:ASP:N	2.52	0.41
1:A:427:ILE:HG23	13:M:38:GLY:CA	2.50	0.41
1:A:378:VAL:N	1:A:473:ARG:O	2.52	0.41
1:A:963:ARG:HG2	1:A:967:ARG:NH1	2.35	0.41
2:B:473:LEU:HD22	2:B:1052:LYS:HD3	2.02	0.41
2:B:798:ARG:N	2:B:949:TYR:O	2.48	0.41
3:C:20:LYS:HA	3:C:232:ASN:HA	2.00	0.41
7:G:63:ARG:HH22	7:G:67:LEU:N	2.18	0.41
11:K:1:MET:SD	11:K:3:ALA:HB3	2.59	0.41
16:P:227:GLU:HG2	16:P:228:GLU:N	2.35	0.41
18:R:155:LEU:HB3	18:R:204:ASN:HD21	1.80	0.41
22:X:45:DC:H2"	22:X:46:DG:C8	2.56	0.41
23:Y:85:DG:C2	23:Y:86:DC:C2	3.09	0.41
1:A:1167:ARG:HE	1:A:1293:LEU:HB3	1.86	0.41
1:A:349:ARG:HB3	2:B:1158:LEU:HD12	2.02	0.41
1:A:611:ASP:OD2	1:A:617:PRO:HG3	2.19	0.41
2:B:109:MET:CE	2:B:174:LEU:HB3	2.48	0.41
2:B:453:TRP:HB3	2:B:463:ARG:CB	2.49	0.41
2:B:531:TYR:HD2	2:B:622:CYS:SG	2.44	0.41
2:B:836:THR:C	2:B:886:ARG:HA	2.41	0.41
7:G:40:GLY:HA2	7:G:152:VAL:HG11	2.03	0.41
7:G:154:LYS:HG3	7:G:155:ASN:H	1.86	0.41
7:G:146:LYS:HD3	7:G:165:ASP:OD2	2.21	0.41
7:G:79:PRO:HG3	7:G:104:MET:SD	2.60	0.41
8:H:105:SER:HB2	8:H:108:ALA:CB	2.50	0.41
9:I:102:ALA:C	9:I:104:ALA:N	2.72	0.41
13:M:154:ARG:HD3	13:M:154:ARG:HA	1.88	0.41
15:O:62:LEU:HA	15:O:76:LEU:HG	2.02	0.41
17:Q:113:ARG:HB2	18:R:221:ARG:CD	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:23:VAL:HG13	20:T:27:LEU:HD23	2.01	0.41
1:A:1207:ILE:HD12	1:A:1260:ARG:CB	2.51	0.41
1:A:1456:GLU:HG2	1:A:1457:ASN:N	2.35	0.41
1:A:202:TRP:O	1:A:211:GLU:HA	2.21	0.41
1:A:419:ILE:HA	1:A:446:VAL:HA	2.02	0.41
1:A:504:HIS:HB3	2:B:1106:ARG:NH2	2.35	0.41
2:B:166:LEU:HB3	2:B:170:ASP:CB	2.50	0.41
2:B:258:ALA:HB2	2:B:269:ILE:CG2	2.49	0.41
2:B:302:LYS:HB3	2:B:303:PRO:HD3	2.02	0.41
2:B:505:LEU:HG	2:B:509:VAL:HB	2.03	0.41
2:B:720:PRO:HG2	2:B:721:ARG:NH1	2.35	0.41
2:B:865:VAL:HA	2:B:895:PHE:HB3	2.02	0.41
5:E:41:LYS:HA	5:E:46:ASP:HB3	2.02	0.41
7:G:142:GLU:O	7:G:170:LEU:HA	2.20	0.41
9:I:101:SER:HB2	9:I:102:ALA:H	1.59	0.41
1:A:1173:THR:HB	9:I:56:ASN:CB	2.49	0.41
14:N:25:VAL:HG12	15:O:39:GLN:HB3	2.02	0.41
20:T:177:ARG:NH1	22:X:20:DG:OP2	2.54	0.41
21:U:161:ILE:HG21	21:U:211:LEU:HB3	2.01	0.41
21:U:193:SER:OG	21:U:194:ARG:NH1	2.53	0.41
1:A:1355:VAL:HA	5:E:142:HIS:HA	2.02	0.41
1:A:374:SER:HB3	1:A:377:GLN:HG3	2.02	0.41
1:A:478:PRO:HB3	11:K:4:PRO:HD3	2.02	0.41
1:A:546:ARG:CG	1:A:639:ILE:HD11	2.47	0.41
2:B:1040:GLN:NE2	3:C:197:TYR:H	2.18	0.41
2:B:1126:ALA:HB3	2:B:1137:CYS:SG	2.61	0.41
2:B:799:SER:O	2:B:802:ASP:HB2	2.21	0.41
2:B:833:THR:O	2:B:840:MET:HE3	2.20	0.41
6:F:53:THR:HB	6:F:108:ARG:NH1	2.36	0.41
7:G:117:MET:HE1	7:G:163:LEU:HD22	2.03	0.41
13:M:216:SER:HA	13:M:229:GLN:NE2	2.35	0.41
14:N:10:VAL:HB	14:N:11:PRO:HD3	2.02	0.41
1:A:375:ILE:HG12	1:A:666:ARG:HB2	2.03	0.41
1:A:37:THR:OG1	1:A:86:GLY:HA3	2.20	0.41
2:B:1130:THR:C	2:B:1132:THR:H	2.21	0.41
2:B:669:GLU:O	2:B:673:VAL:HG13	2.21	0.41
3:C:190:ASN:ND2	3:C:195:THR:O	2.50	0.41
9:I:69:ILE:O	9:I:72:VAL:HG22	2.21	0.41
12:L:38:GLU:HG2	12:L:39:CYS:H	1.86	0.41
17:Q:21:VAL:O	17:Q:25:PHE:HD1	2.04	0.41
18:R:208:CYS:O	18:R:209:GLN:C	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:174:LYS:HB3	22:X:20:DG:H4'	2.02	0.41
20:T:202:LEU:HD11	20:T:233:TRP:HB2	2.03	0.41
13:M:248:ARG:NH2	23:Y:85:DG:OP2	2.51	0.41
1:A:201:GLU:HA	1:A:212:LYS:O	2.21	0.41
1:A:61:ARG:O	1:A:72:GLN:HB3	2.19	0.41
1:A:916:PHE:CD1	1:A:963:ARG:HD2	2.55	0.41
2:B:764:MET:HG2	2:B:767:LEU:HD12	2.01	0.41
2:B:790:GLN:HA	2:B:968:ASN:HD22	1.86	0.41
3:C:1:MET:SD	11:K:52:LYS:HE3	2.61	0.41
4:D:23:PRO:HG2	4:D:26:PHE:HB2	2.03	0.41
1:A:1080:ILE:CD1	6:F:54:THR:HG21	2.50	0.41
6:F:93:ALA:O	6:F:97:LEU:N	2.52	0.41
8:H:39:LEU:HD12	8:H:124:ARG:O	2.21	0.41
13:M:118:PHE:HA	13:M:121:ILE:HB	2.03	0.41
13:M:279:GLY:CA	20:T:153:TYR:CE1	3.01	0.41
14:N:315:ASN:C	14:N:317:GLU:H	2.23	0.41
16:P:180:LEU:HD12	16:P:183:ILE:HD12	2.02	0.41
17:Q:75:ARG:N	17:Q:95:ASN:O	2.41	0.41
20:T:227:GLY:O	22:X:30:DG:H5''	2.21	0.41
22:X:6:DG:N2	23:Y:89:DC:O2	2.54	0.41
1:A:1000:LEU:HD12	1:A:1001:PRO:HD2	2.02	0.41
1:A:120:ASP:OD1	1:A:121:SER:N	2.51	0.41
2:B:22:TRP:HD1	2:B:24:GLU:HB2	1.86	0.41
2:B:194:LEU:HD13	2:B:467:SER:HB2	2.03	0.41
2:B:63:PRO:HB2	2:B:88:PHE:CD1	2.56	0.41
2:B:471:ASN:HD22	2:B:730:LYS:HE3	1.85	0.41
3:C:190:ASN:ND2	3:C:193:ARG:HA	2.36	0.41
3:C:199:LYS:NZ	3:C:201:GLU:OE1	2.46	0.41
4:D:45:LYS:HD2	4:D:45:LYS:HA	1.74	0.41
1:A:1175:ILE:H	9:I:54:TYR:HB3	1.86	0.41
14:N:39:LEU:HD12	14:N:42:LEU:HD23	2.01	0.41
15:O:19:LEU:HD23	15:O:22:LEU:HD12	2.03	0.41
14:N:314:LEU:HD12	16:P:248:ALA:O	2.21	0.41
18:R:140:LYS:N	18:R:141:PRO:HD2	2.35	0.41
1:A:1306:LYS:HB2	1:A:1306:LYS:HE3	1.57	0.41
1:A:1479:LYS:HB3	6:F:103:PRO:HB3	2.02	0.41
1:A:266:MET:O	1:A:267:GLN:CB	2.60	0.41
1:A:702:ILE:O	1:A:706:ILE:HG12	2.21	0.41
2:B:1137:CYS:HB3	2:B:1142:ASN:CB	2.51	0.41
2:B:236:TRP:HB2	2:B:259:THR:HB	2.03	0.41
2:B:821:LYS:N	2:B:825:GLN:O	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:92:TYR:O	2:B:125:TYR:N	2.30	0.41
13:M:218:PHE:CD1	13:M:277:ILE:HG22	2.55	0.41
17:Q:170:LYS:HG3	17:Q:173:ALA:H	1.86	0.41
20:T:198:ASN:O	20:T:202:LEU:HG	2.21	0.41
1:A:1053:ARG:NE	1:A:1057:GLU:OE1	2.53	0.41
1:A:338:SER:O	1:A:342:ARG:HG3	2.21	0.41
1:A:42:LYS:HD3	1:A:55:GLY:H	1.86	0.41
1:A:608:THR:OG1	1:A:610:PRO:HD2	2.20	0.41
1:A:65:ILE:HG22	1:A:66:GLU:N	2.34	0.41
2:B:68:GLN:OE1	2:B:135:GLU:HG3	2.21	0.41
2:B:198:GLU:CD	2:B:524:LYS:HZ2	2.23	0.41
9:I:29:ASP:O	9:I:33:ARG:N	2.53	0.41
11:K:32:LEU:HD21	11:K:72:ILE:HB	2.03	0.41
14:N:39:LEU:O	14:N:42:LEU:HB3	2.21	0.41
15:O:70:ASN:HB3	15:O:99:ASP:HB3	2.02	0.41
16:P:193:ASN:HA	16:P:194:PRO:HD2	1.92	0.41
16:P:200:VAL:HG12	16:P:213:ILE:HD13	2.02	0.41
19:S:54:LYS:HE2	19:S:54:LYS:HB2	1.84	0.41
21:U:232:GLU:OE1	21:U:232:GLU:HA	2.20	0.41
1:A:1165:THR:O	1:A:1169:VAL:HG23	2.21	0.41
1:A:470:MET:SD	1:A:521:VAL:HG23	2.61	0.41
1:A:549:THR:OG1	1:A:639:ILE:HG13	2.20	0.41
1:A:63:GLY:HA2	1:A:71:CYS:SG	2.61	0.41
1:A:720:ALA:HB2	1:A:725:LEU:HD13	2.02	0.41
1:A:915:ALA:O	1:A:919:LYS:N	2.45	0.41
2:B:192:LYS:HB3	2:B:192:LYS:HE3	1.87	0.41
2:B:602:SER:OG	2:B:620:ARG:NH1	2.54	0.41
5:E:142:HIS:HB3	5:E:145:VAL:HG23	2.02	0.41
5:E:17:ILE:O	5:E:20:LEU:HB3	2.21	0.41
9:I:24:LEU:HD11	9:I:44:TYR:HE2	1.86	0.41
9:I:84:HIS:CD2	9:I:84:HIS:H	2.39	0.41
10:J:3:ILE:HD13	10:J:18:TRP:HB2	2.02	0.41
13:M:128:ILE:HG13	13:M:130:LEU:HG	2.02	0.41
13:M:259:TYR:HD1	13:M:274:ILE:HD12	1.86	0.41
16:P:240:VAL:O	16:P:244:LEU:HG	2.20	0.41
17:Q:129:CYS:HB2	17:Q:154:CYS:HB2	2.02	0.41
17:Q:23:ARG:CZ	18:R:207:SER:N	2.84	0.41
19:S:49:ARG:HD2	19:S:96:GLN:HB2	2.03	0.41
23:Y:91:DT:H2"	23:Y:92:DT:C6	2.56	0.41
1:A:1017:SER:HA	1:A:1020:LEU:HG	2.03	0.40
1:A:1054:MET:O	1:A:1059:ARG:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1218:ARG:HA	1:A:1221:MET:HG2	2.03	0.40
1:A:33:ARG:HB3	2:B:1139:GLY:HA2	2.02	0.40
1:A:420:ILE:O	1:A:445:LYS:N	2.39	0.40
1:A:432:HIS:CG	1:A:433:PRO:HD2	2.56	0.40
1:A:452:ASP:OD1	1:A:476:ILE:HG12	2.21	0.40
1:A:620:HIS:C	1:A:621:ILE:CG1	2.69	0.40
1:A:864:LEU:HD22	1:A:1095:LEU:HD23	2.02	0.40
1:A:922:PHE:CZ	1:A:952:LEU:HG	2.42	0.40
1:A:15:LEU:HA	2:B:1148:LEU:HB3	2.02	0.40
2:B:1123:GLY:HA3	2:B:1171:MET:H	1.85	0.40
2:B:481:HIS:HA	2:B:484:ARG:NH1	2.36	0.40
2:B:761:THR:H	2:B:764:MET:CE	2.33	0.40
3:C:47:ILE:HG22	12:L:57:ALA:HB2	2.03	0.40
4:D:64:THR:HG21	7:G:46:ILE:HG23	2.02	0.40
5:E:11:TRP:CZ2	5:E:15:LYS:HE3	2.56	0.40
5:E:120:ASP:O	5:E:122:ALA:N	2.54	0.40
7:G:11:ILE:N	7:G:68:TYR:O	2.49	0.40
9:I:80:ARG:HE	9:I:115:THR:HG21	1.85	0.40
11:K:81:TYR:CE2	11:K:86:ALA:HB2	2.55	0.40
16:P:281:SER:HG	16:P:293:TYR:HD1	1.68	0.40
17:Q:37:LEU:HD13	17:Q:71:PHE:CE1	2.55	0.40
19:S:48:GLU:OE1	19:S:101:ARG:NH2	2.55	0.40
20:T:154:LYS:HA	20:T:155:PRO:HD3	1.97	0.40
20:T:231:ASN:CB	23:Y:68:DC:H5"	2.44	0.40
1:A:746:ASN:HA	1:A:749:ARG:HE	1.86	0.40
2:B:607:ILE:HG21	9:I:72:VAL:N	2.36	0.40
2:B:88:PHE:CE2	2:B:128:ILE:HG12	2.56	0.40
7:G:163:LEU:HD23	7:G:163:LEU:O	2.21	0.40
7:G:89:VAL:HA	7:G:99:THR:HA	2.03	0.40
8:H:97:TYR:CZ	8:H:115:TYR:HB3	2.56	0.40
1:A:1173:THR:HB	9:I:56:ASN:HB3	2.02	0.40
12:L:34:ILE:HD12	12:L:42:ARG:HB3	2.03	0.40
13:M:178:LYS:C	20:T:154:LYS:CG	2.87	0.40
13:M:195:PHE:CZ	13:M:199:LEU:HD11	2.56	0.40
14:N:332:GLU:HA	15:O:92:LYS:O	2.21	0.40
21:U:191:VAL:O	21:U:195:ILE:HG13	2.22	0.40
1:A:962:ASP:OD2	1:A:1046:ARG:HD2	2.21	0.40
1:A:1173:THR:HA	1:A:1214:VAL:HA	2.03	0.40
1:A:340:LYS:HG3	1:A:1436:VAL:HG21	2.03	0.40
1:A:240:PRO:HB3	1:A:244:ARG:HH11	1.87	0.40
1:A:312:PHE:CE2	1:A:326:PRO:HB2	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:LEU:HG	1:A:313:HIS:CD2	2.57	0.40
1:A:337:LYS:O	1:A:341:GLN:HB3	2.21	0.40
1:A:404:GLU:OE1	1:A:407:ARG:NH1	2.45	0.40
1:A:550:LYS:HG2	1:A:552:ASP:H	1.86	0.40
1:A:587:THR:O	1:A:591:ILE:HG12	2.21	0.40
1:A:808:PRO:HG2	2:B:675:LEU:HD23	2.03	0.40
1:A:32:LYS:HG2	1:A:87:HIS:NE2	2.36	0.40
2:B:474:THR:H	2:B:477:SER:HB2	1.85	0.40
2:B:875:GLU:HA	2:B:875:GLU:OE1	2.21	0.40
3:C:19:VAL:CG1	3:C:233:VAL:HB	2.51	0.40
5:E:82:VAL:HG21	5:E:106:VAL:HG22	2.03	0.40
6:F:110:LEU:N	6:F:114:SER:O	2.55	0.40
6:F:44:ARG:H	6:F:45:PRO:CD	2.34	0.40
11:K:35:ILE:N	11:K:35:ILE:HD12	2.36	0.40
13:M:289:TYR:HA	13:M:292:ILE:HG12	2.03	0.40
16:P:203:ARG:HG3	16:P:203:ARG:HH21	1.87	0.40
1:A:336:LEU:HG	1:A:338:SER:H	1.86	0.40
1:A:420:ILE:HB	1:A:445:LYS:HB2	2.03	0.40
1:A:416:ALA:HA	1:A:448:ARG:HA	2.03	0.40
1:A:790:GLN:OE1	1:A:822:PHE:HB2	2.22	0.40
1:A:802:PHE:CZ	1:A:808:PRO:HB3	2.57	0.40
2:B:1080:ARG:HG2	13:M:53:ARG:NH1	2.36	0.40
2:B:249:LYS:C	2:B:251:ALA:N	2.75	0.40
2:B:834:ARG:HD2	2:B:840:MET:SD	2.61	0.40
2:B:874:PRO:HB3	2:B:877:GLU:HB3	2.04	0.40
3:C:7:PRO:O	3:C:8:THR:C	2.59	0.40
5:E:172:ARG:NE	5:E:208:LEU:HD22	2.36	0.40
8:H:111:ARG:HG3	8:H:126:GLN:HE22	1.85	0.40
8:H:91:VAL:HA	8:H:143:LEU:O	2.21	0.40
9:I:27:LYS:O	9:I:35:LEU:HD12	2.22	0.40
17:Q:124:ARG:HD3	17:Q:168:MET:SD	2.61	0.40
22:X:20:DG:H1'	22:X:21:DG:H5'	2.02	0.40
1:A:18:ILE:CD1	2:B:1171:MET:HB2	2.51	0.40
2:B:1068:GLN:HA	13:M:46:ILE:HG21	2.03	0.40
2:B:225:LEU:O	2:B:230:ARG:HG2	2.20	0.40
5:E:192:LYS:HG3	5:E:206:TYR:HE1	1.87	0.40
6:F:99:ALA:HB1	6:F:101:LYS:HG3	2.01	0.40
8:H:111:ARG:HG3	8:H:126:GLN:OE1	2.22	0.40
9:I:27:LYS:HE3	9:I:38:ALA:HB2	2.03	0.40
15:O:64:THR:CG2	16:P:188:ARG:HB3	2.52	0.40
16:P:207:PRO:HB3	16:P:233:ALA:CB	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:211:ALA:HA	16:P:220:VAL:O	2.21	0.40
17:Q:187:ILE:CD1	18:R:211:SER:CA	2.80	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1450/1970 (74%)	1297 (89%)	100 (7%)	53 (4%)	4	38
2	B	1163/1174 (99%)	1044 (90%)	82 (7%)	37 (3%)	5	41
3	C	273/275 (99%)	244 (89%)	17 (6%)	12 (4%)	3	33
4	D	127/142 (89%)	118 (93%)	8 (6%)	1 (1%)	24	69
5	E	208/210 (99%)	198 (95%)	7 (3%)	3 (1%)	14	58
6	F	84/127 (66%)	78 (93%)	4 (5%)	2 (2%)	7	47
7	G	169/172 (98%)	158 (94%)	10 (6%)	1 (1%)	30	74
8	H	148/150 (99%)	121 (82%)	15 (10%)	12 (8%)	1	18
9	I	123/125 (98%)	102 (83%)	12 (10%)	9 (7%)	1	21
10	J	65/67 (97%)	53 (82%)	8 (12%)	4 (6%)	2	25
11	K	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
12	L	44/58 (76%)	36 (82%)	4 (9%)	4 (9%)	1	16
13	M	256/316 (81%)	235 (92%)	11 (4%)	10 (4%)	4	36
14	N	109/376 (29%)	99 (91%)	6 (6%)	4 (4%)	4	38
15	O	97/109 (89%)	90 (93%)	7 (7%)	0	100	100
16	P	183/339 (54%)	167 (91%)	12 (7%)	4 (2%)	8	49
17	Q	176/439 (40%)	159 (90%)	11 (6%)	6 (3%)	5	40
18	R	163/291 (56%)	129 (79%)	20 (12%)	14 (9%)	1	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	S	134/517 (26%)	123 (92%)	7 (5%)	4 (3%)	5	42
20	T	218/249 (88%)	191 (88%)	17 (8%)	10 (5%)	3	32
21	U	168/301 (56%)	135 (80%)	20 (12%)	13 (8%)	1	20
All	All	5473/7524 (73%)	4889 (89%)	381 (7%)	203 (4%)	7	38

All (203) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	67	ARG
1	A	205	VAL
1	A	531	ASN
1	A	610	PRO
1	A	619	LYS
1	A	621	ILE
1	A	622	SER
1	A	623	PRO
1	A	911	PRO
1	A	924	TYR
1	A	929	ALA
1	A	932	ARG
1	A	1273	GLU
1	A	1303	GLN
2	B	61	ASP
2	B	73	HIS
2	B	80	GLU
2	B	232	THR
2	B	250	SER
2	B	491	ARG
2	B	498	PRO
2	B	500	GLN
2	B	549	SER
2	B	841	ARG
2	B	879	GLU
3	C	7	PRO
3	C	89	THR
3	C	126	ARG
3	C	147	ASP
3	C	218	ALA
5	E	64	HIS
5	E	65	ASN
7	G	154	LYS

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Mol	Chain	Res	Type
8	H	75	TYR
8	H	108	ALA
8	H	111	ARG
9	I	59	THR
9	I	85	PRO
9	I	86	CYS
9	I	104	ALA
9	I	106	ASP
12	L	16	ILE
12	L	38	GLU
13	M	11	PRO
13	M	13	VAL
13	M	40	VAL
13	M	44	ARG
16	P	160	GLY
16	P	161	ILE
18	R	134	ASP
18	R	163	LEU
18	R	195	PRO
18	R	196	ASP
18	R	209	GLN
18	R	211	SER
18	R	214	GLU
18	R	224	THR
20	T	139	VAL
20	T	140	ARG
20	T	156	VAL
21	U	223	MET
21	U	257	GLN
1	A	44	PRO
1	A	267	GLN
1	A	273	GLN
1	A	346	LYS
1	A	612	ASP
1	A	620	HIS
1	A	624	GLY
1	A	930	LEU
1	A	935	GLN
1	A	1101	GLN
1	A	1118	THR
1	A	1264	SER
1	A	1275	VAL

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Mol	Chain	Res	Type
1	A	1282	ASP
1	A	1435	THR
2	B	257	VAL
2	B	428	ASP
2	B	460	HIS
2	B	649	ASN
2	B	791	GLU
2	B	875	GLU
2	B	881	GLU
2	B	882	SER
2	B	883	THR
2	B	889	LYS
3	C	91	GLU
3	C	143	VAL
4	D	57	LEU
5	E	121	MET
8	H	3	GLY
8	H	21	LYS
8	H	66	GLU
8	H	107	GLU
9	I	57	LYS
10	J	14	VAL
10	J	65	LEU
12	L	17	TYR
17	Q	103	VAL
17	Q	169	PRO
18	R	157	GLN
18	R	164	GLY
20	T	145	LEU
20	T	178	ALA
20	T	180	LYS
21	U	227	GLU
21	U	233	LEU
21	U	251	ALA
21	U	252	LYS
21	U	253	THR
21	U	267	LYS
1	A	156	GLY
1	A	338	SER
1	A	611	ASP
1	A	1200	PRO
1	A	1274	GLU

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Mol	Chain	Res	Type
1	A	1305	SER
1	A	1313	GLN
1	A	1314	THR
1	A	1417	HIS
2	B	229	SER
2	B	456	GLN
2	B	497	LYS
2	B	651	TYR
2	B	863	ASP
2	B	898	THR
2	B	1129	ASN
2	B	1132	THR
3	C	144	GLU
8	H	65	TYR
8	H	106	THR
9	I	92	LYS
9	I	119	CYS
13	M	10	LEU
14	N	346	LYS
17	Q	163	GLU
18	R	139	PHE
18	R	212	VAL
19	S	170	VAL
20	T	124	TYR
20	T	144	GLN
21	U	226	GLU
1	A	72	GLN
1	A	184	CYS
1	A	266	MET
1	A	461	GLN
1	A	479	TRP
1	A	981	CYS
2	B	74	ALA
2	B	256	ILE
2	B	495	LEU
2	B	873	LEU
2	B	1136	GLU
3	C	137	ASN
6	F	85	GLY
8	H	70	LEU
8	H	76	ASN
9	I	20	CYS

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Mol	Chain	Res	Type
10	J	3	ILE
13	M	149	LYS
14	N	355	ASP
16	P	210	THR
17	Q	124	ARG
17	Q	165	GLU
18	R	141	PRO
20	T	38	GLY
20	T	135	SER
1	A	75	ALA
1	A	300	ALA
1	A	1106	THR
1	A	1266	GLU
1	A	1342	SER
3	C	151	VAL
8	H	71	ASP
10	J	6	ARG
13	M	39	LEU
13	M	108	SER
16	P	297	LYS
18	R	174	ALA
19	S	153	ARG
19	S	154	THR
19	S	160	ALA
21	U	229	ALA
21	U	266	CYS
21	U	295	GLY
1	A	1265	ASP
1	A	1281	ASP
2	B	737	ILE
6	F	44	ARG
12	L	19	CYS
13	M	247	GLY
14	N	312	GLU
13	M	38	GLY
1	A	51	ARG
1	A	498	GLY
2	B	493	GLY
21	U	255	GLY
3	C	6	GLN
3	C	78	ILE
17	Q	100	VAL

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Mol	Chain	Res	Type
2	B	1008	VAL
14	N	313	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	A	1279/1748 (73%)	1243 (97%)	36 (3%)	51	79
2	B	1020/1028 (99%)	994 (98%)	26 (2%)	55	81
3	C	252/252 (100%)	247 (98%)	5 (2%)	63	85
4	D	119/126 (94%)	118 (99%)	1 (1%)	86	94
5	E	192/192 (100%)	187 (97%)	5 (3%)	54	80
6	F	74/111 (67%)	74 (100%)	0	100	100
7	G	152/153 (99%)	149 (98%)	3 (2%)	63	85
8	H	131/131 (100%)	128 (98%)	3 (2%)	58	83
9	I	112/112 (100%)	109 (97%)	3 (3%)	52	79
10	J	56/56 (100%)	55 (98%)	1 (2%)	66	87
11	K	106/106 (100%)	105 (99%)	1 (1%)	84	93
12	L	43/55 (78%)	43 (100%)	0	100	100
13	M	222/268 (83%)	211 (95%)	11 (5%)	30	66
14	N	105/324 (32%)	104 (99%)	1 (1%)	82	92
15	O	90/98 (92%)	89 (99%)	1 (1%)	80	91
16	P	159/293 (54%)	154 (97%)	5 (3%)	47	77
17	Q	164/373 (44%)	157 (96%)	7 (4%)	35	70
18	R	150/261 (58%)	140 (93%)	10 (7%)	20	58
19	S	121/448 (27%)	118 (98%)	3 (2%)	55	81
20	T	196/218 (90%)	189 (96%)	7 (4%)	42	74
21	U	148/266 (56%)	141 (95%)	7 (5%)	32	68
All	All	4891/6619 (74%)	4755 (97%)	136 (3%)	55	79

All (136) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	ASP
1	A	57	LEU
1	A	147	LEU
1	A	152	ASN
1	A	188	GLN
1	A	266	MET
1	A	267	GLN
1	A	275	ASP
1	A	339	LEU
1	A	372	ASN
1	A	472	HIS
1	A	484	LEU
1	A	603	ILE
1	A	604	ARG
1	A	611	ASP
1	A	613	GLU
1	A	614	ASP
1	A	619	LYS
1	A	625	ASP
1	A	644	SER
1	A	647	THR
1	A	659	GLU
1	A	669	TYR
1	A	750	ASP
1	A	839	HIS
1	A	922	PHE
1	A	923	ASP
1	A	932	ARG
1	A	964	GLU
1	A	1152	GLU
1	A	1272	GLU
1	A	1289	GLU
1	A	1306	LYS
1	A	1311	LEU
1	A	1313	GLN
1	A	1386	ILE
2	B	26	CYS
2	B	54	SER
2	B	73	HIS
2	B	77	GLU
2	B	97	THR
2	B	125	TYR

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Mol	Chain	Res	Type
2	B	131	THR
2	B	132	VAL
2	B	169	ARG
2	B	242	ARG
2	B	249	LYS
2	B	250	SER
2	B	256	ILE
2	B	407	MET
2	B	442	ASP
2	B	446	TYR
2	B	499	ARG
2	B	546	GLU
2	B	588	ARG
2	B	604	ILE
2	B	664	TYR
2	B	666	ASP
2	B	814	TYR
2	B	880	LEU
2	B	881	GLU
2	B	1080	ARG
3	C	35	ARG
3	C	61	ASP
3	C	113	ARG
3	C	215	GLU
3	C	217	GLN
4	D	43	HIS
5	E	23	ASP
5	E	50	GLU
5	E	64	HIS
5	E	129	GLN
5	E	172	ARG
7	G	63	ARG
7	G	144	ARG
7	G	163	LEU
8	H	55	LYS
8	H	66	GLU
8	H	107	GLU
9	I	27	LYS
9	I	71	ASP
9	I	72	VAL
10	J	65	LEU
11	K	8	GLU

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Mol	Chain	Res	Type
13	M	7	LEU
13	M	10	LEU
13	M	31	ASP
13	M	39	LEU
13	M	40	VAL
13	M	53	ARG
13	M	107	MET
13	M	112	ARG
13	M	114	MET
13	M	120	GLU
13	M	126	ASP
14	N	319	ASP
15	O	10	THR
16	P	208	ARG
16	P	239	ARG
16	P	271	GLU
16	P	297	LYS
16	P	299	ARG
17	Q	45	GLU
17	Q	101	ASN
17	Q	105	TYR
17	Q	123	ASN
17	Q	139	LEU
17	Q	142	ASN
17	Q	193	GLU
18	R	88	ARG
18	R	99	LEU
18	R	159	ASP
18	R	163	LEU
18	R	206	LYS
18	R	209	GLN
18	R	210	PHE
18	R	212	VAL
18	R	223	VAL
18	R	235	GLU
19	S	7	SER
19	S	163	GLU
19	S	166	ARG
20	T	143	GLN
20	T	145	LEU
20	T	149	VAL
20	T	154	LYS

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Mol	Chain	Res	Type
20	T	160	GLN
20	T	161	TYR
20	T	162	ASN
21	U	179	GLU
21	U	187	TYR
21	U	194	ARG
21	U	218	ASP
21	U	223	MET
21	U	252	LYS
21	U	274	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	516	GLN
1	A	529	GLN
1	A	539	GLN
1	A	700	GLN
1	A	703	GLN
1	A	1310	HIS
1	A	1332	GLN
2	B	98	HIS
2	B	227	ASN
2	B	245	GLN
2	B	452	ASN
2	B	817	GLN
2	B	970	HIS
2	B	1003	ASN
2	B	1007	ASN
2	B	1040	GLN
2	B	1101	GLN
2	B	1117	HIS
2	B	1160	GLN
3	C	5	ASN
3	C	6	GLN
3	C	25	ASN
3	C	137	ASN
5	E	64	HIS
5	E	71	GLN
5	E	129	GLN
5	E	132	GLN
9	I	87	GLN

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Mol	Chain	Res	Type
9	I	98	GLN
9	I	121	HIS
12	L	23	HIS
16	P	229	GLN
18	R	177	ASN
18	R	204	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 13 ligands modelled in this entry, 13 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.