wwPDB EM Map/Model Validation Report (i)

Jun 14, 2016 – 01:57 PM EDT

PDB ID	:	5IY8
EMDB ID:	:	EMD-8133
Title	:	Human holo-PIC in the initial transcribing state
Authors	:	He, Y.; Yan, C.; Fang, J.; Inouye, C.; Tjian, R.; Ivanov, I.; Nogales, E.
Deposited on	:	2016-03-24
Resolution	:	7.90 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

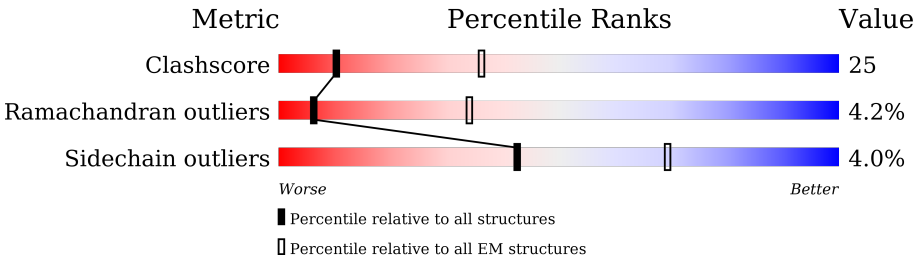
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027790

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 7.90 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 <=5%

Mol	Chain	Length	Quality of chain
1	A	1970	49% 21% • • 26%
2	B	1174	63% 31% 5% ••
3	C	275	72% 24% • •
4	D	142	82% 8% 9%
5	E	210	72% 25% ••
6	F	127	51% 16% • 32%
7	G	172	76% 23% ••
8	H	150	58% 33% 8% •
9	I	125	56% 34% 5% 5%

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Mol	Chain	Length	Quality of chain
10	J	67	63% 25% 9%
11	K	117	78% 21%
12	L	58	45% 29% 21%
13	M	316	69% 24%
14	N	376	21% 8% 70%
15	O	109	68% 23% 9%
16	P	339	41% 12% 45%
17	Q	439	25% 13% 59%
18	R	291	32% 20% 43%
19	S	517	18% 8% 73%
20	T	249	60% 25% 11%
21	U	301	40% 14% 44%
22	V	782	40% 16% 5% 39%
23	W	760	59% 23% 13%
24	0	395	32% 14% 52%
25	1	71	17% 59% 10% 13%
26	2	462	21% 34% 41%
27	3	308	16% 42% 5% 37%
28	X	83	36% 48% 13%
29	Y	83	42% 51% 5%

2 Entry composition

There are 31 unique types of molecules in this entry. The entry contains 62944 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
			Total	C	N	O	S		
1	A	1454	11515	7234	2058	2150	73	0	0

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

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

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

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

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

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

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

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

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

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

- 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	310	Total	C	N	O	S	0	0
			2391	1490	426	457	18		

- 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
			1138	719	208	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 protein called TFIIH basal transcription factor complex helicase XPB subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	475	Total	C	N	O	S	0	0
			3855	2454	663	712	26		

- Molecule 23 is a protein called TFIIH basal transcription factor complex helicase XPD subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	665	Total	C	N	O	S	0	0
			5348	3415	932	975	26		

- Molecule 24 is a protein called General transcription factor IIH subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	0	188	Total	C	N	O	S	0	0
			1479	935	258	276	10		

- Molecule 25 is a protein called General transcription factor IIH subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	1	62	Total	C	N	O	S	0	0
			491	317	77	93	4		

- Molecule 26 is a protein called General transcription factor IIH subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	2	274	Total	C	N	O	S	0	0
			2196	1417	377	392	10		

- Molecule 27 is a protein called General transcription factor IIH subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	3	193	Total	C	N	O	S	0	0
			1526	978	252	284	12		

- Molecule 28 is a DNA chain called SCP-X.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	X	83	Total	C	N	O	P	0	0
			1710	815	307	506	82		

- Molecule 29 is a DNA chain called SCP-Y.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Y	83	Total	C	N	O	P	0	0
			1681	798	300	501	82		

- Molecule 30 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
30	A	2	Total	Mg	0
			2	2	

- Molecule 31 is ZINC ION (three-letter code: ZN) (formula: Zn).

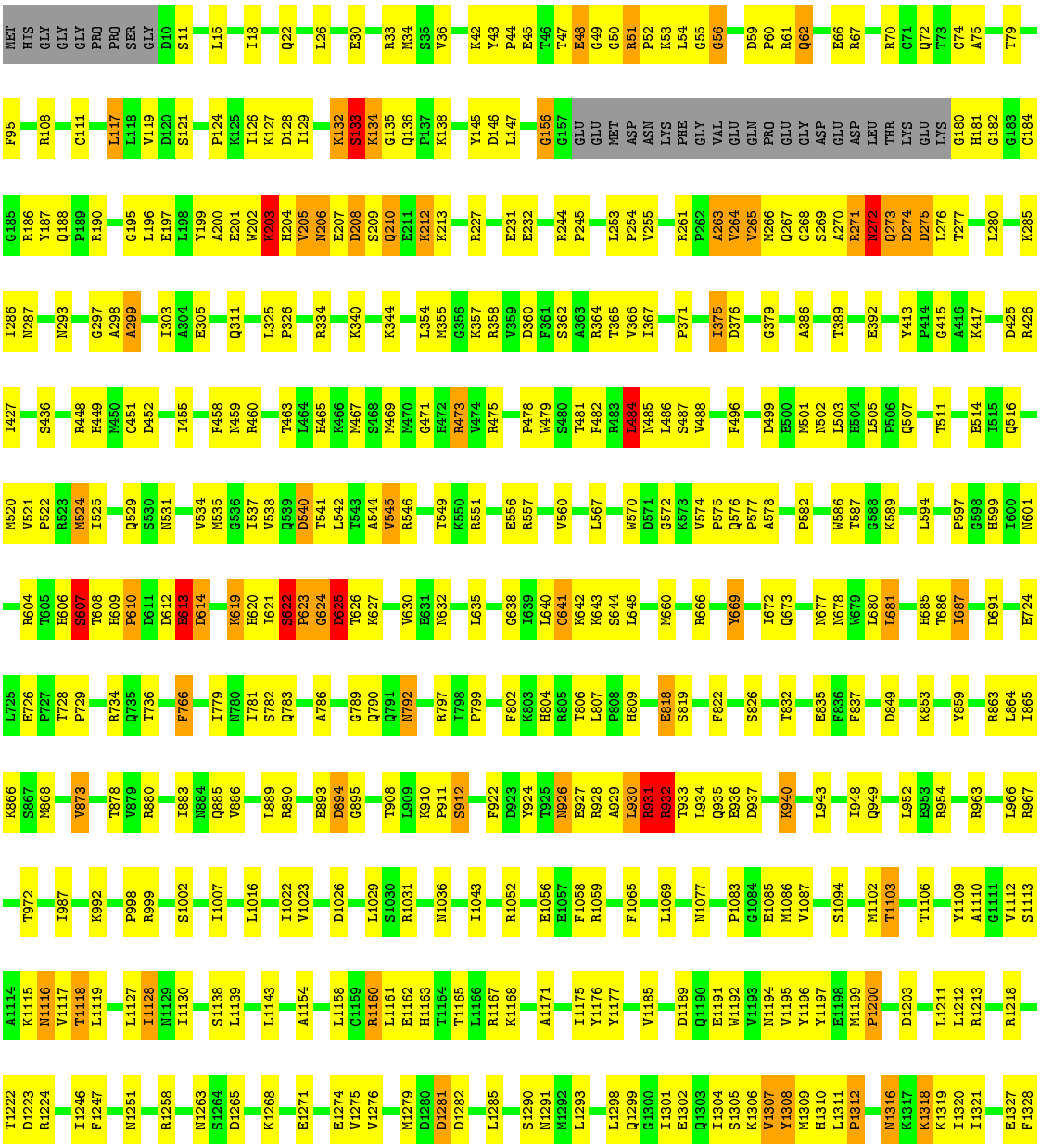
Mol	Chain	Residues	Atoms		AltConf
31	J	1	Total	Zn	0
			1	1	
31	Q	1	Total	Zn	0
			1	1	
31	B	1	Total	Zn	0
			1	1	
31	I	2	Total	Zn	0
			2	2	
31	C	1	Total	Zn	0
			1	1	
31	A	2	Total	Zn	0
			2	2	
31	U	1	Total	Zn	0
			1	1	
31	L	1	Total	Zn	0
			1	1	
31	M	1	Total	Zn	0
			1	1	

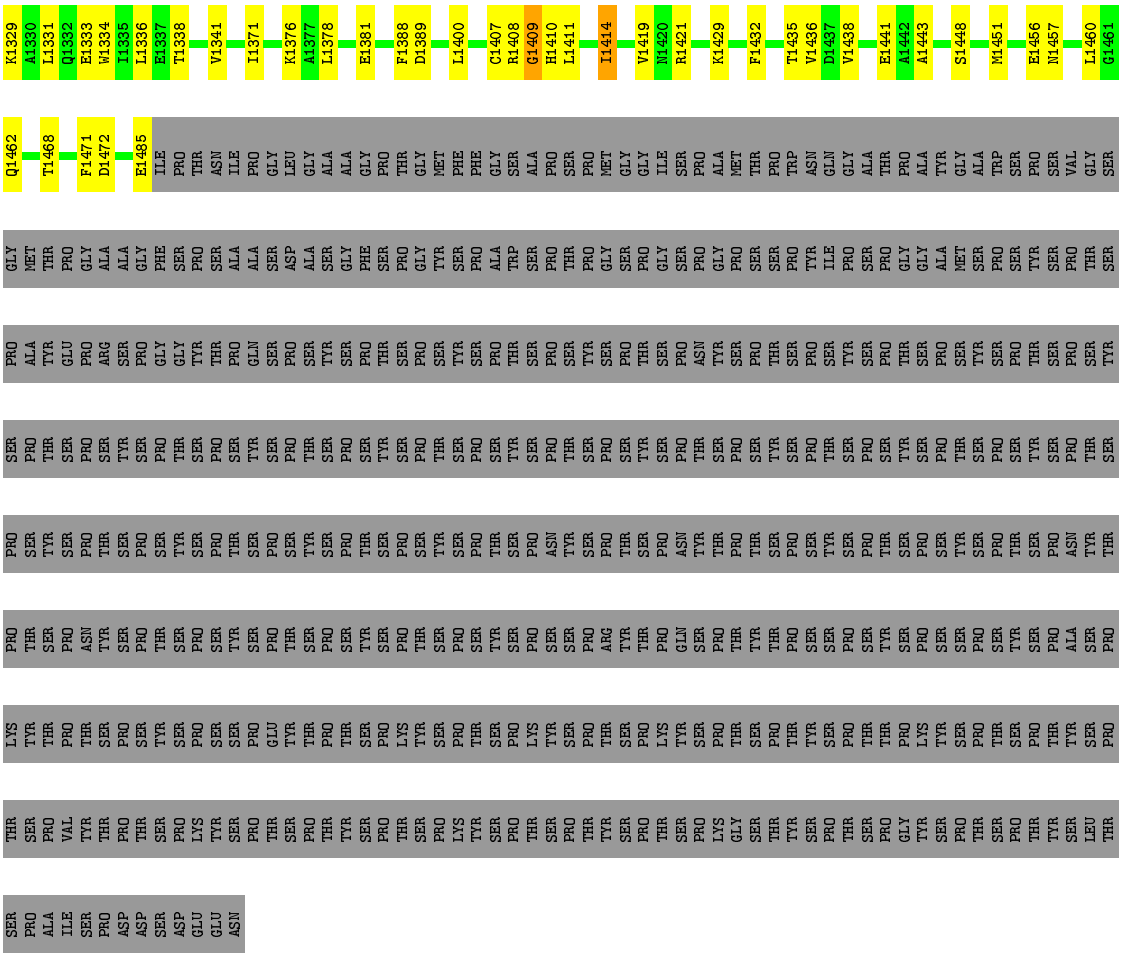
3 Residue-property plots (i)

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

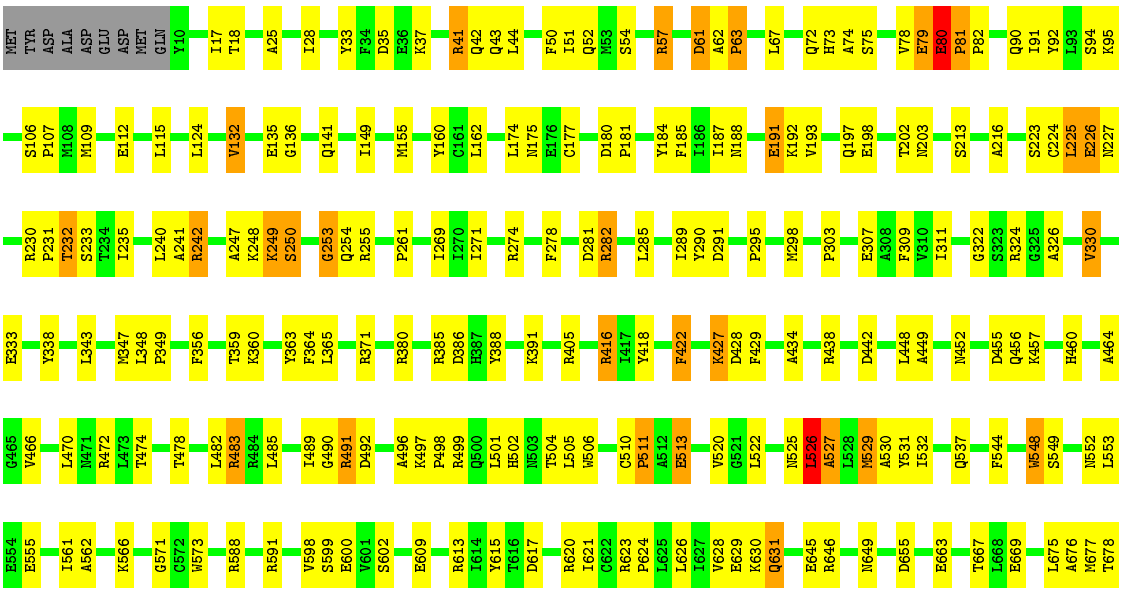
Chain A:

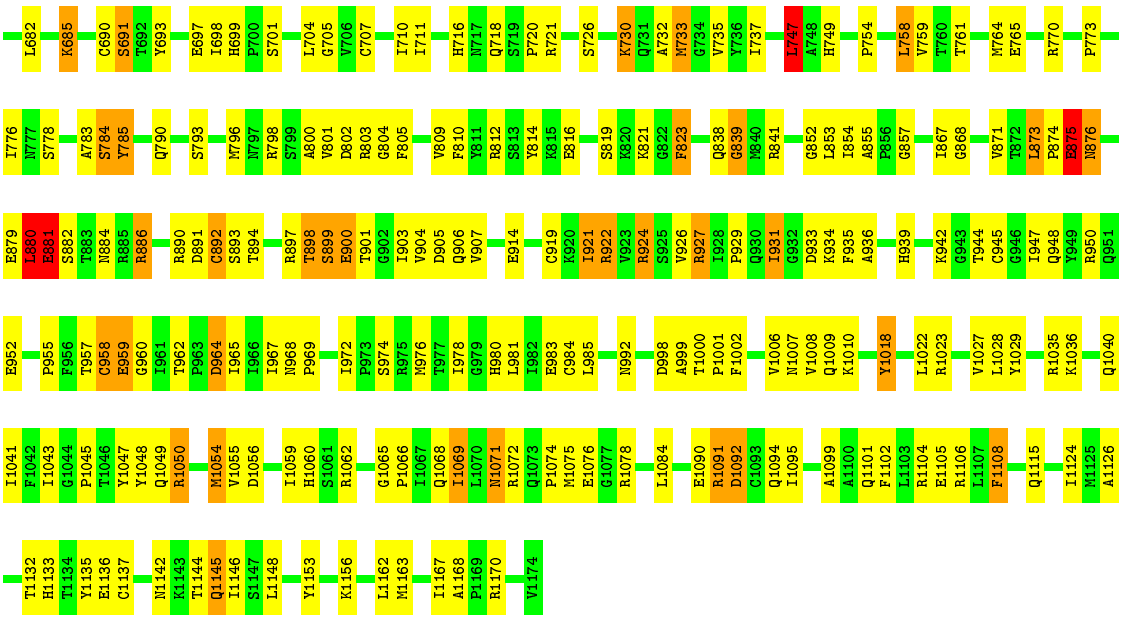




• Molecule 2: DNA-directed RNA polymerase II subunit RPB2

Chain B:



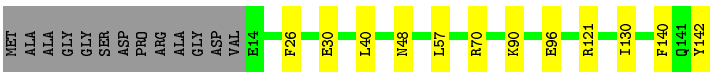


• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

Chain C:

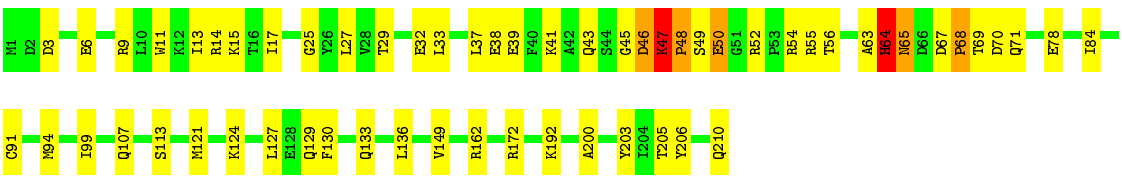
• Molecule 4: DNA-directed RNA polymerase II subunit RPB4

Chain D:



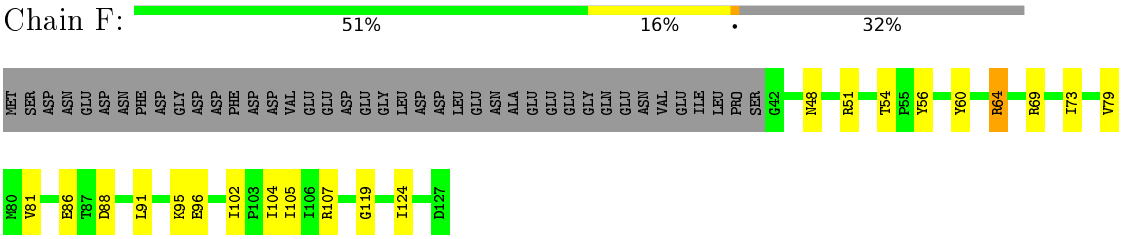
• Molecule 5: DNA-directed RNA polymerase II subunit RPB5

Chain E:



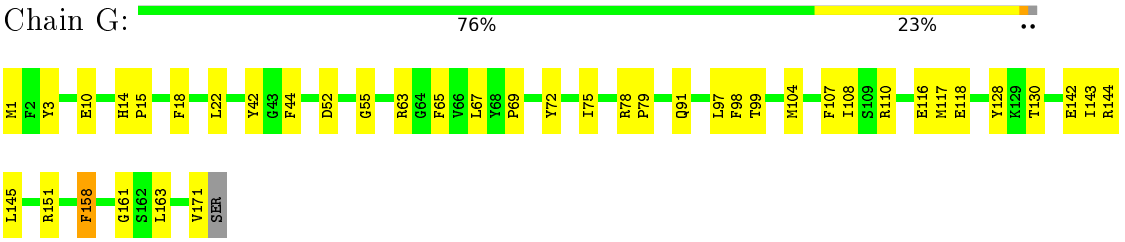
• Molecule 6: DNA-directed RNA polymerase II subunit RPB6

Chain F:



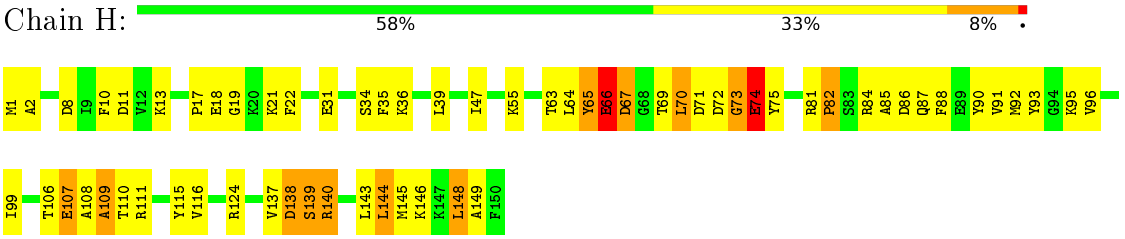
• Molecule 7: DNA-directed RNA polymerase II subunit RPB7

Chain G:



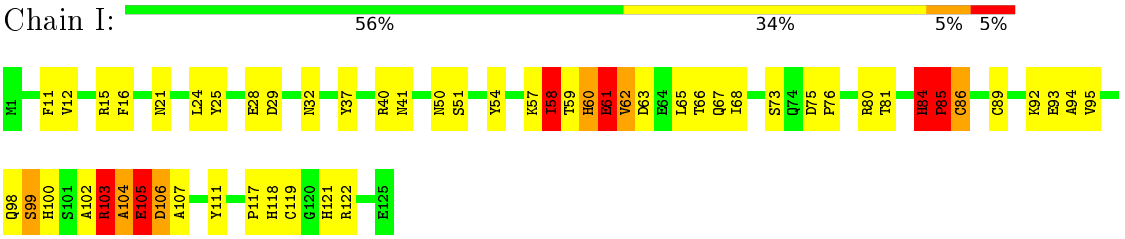
• Molecule 8: DNA-directed RNA polymerase II subunit RPB8

Chain H:



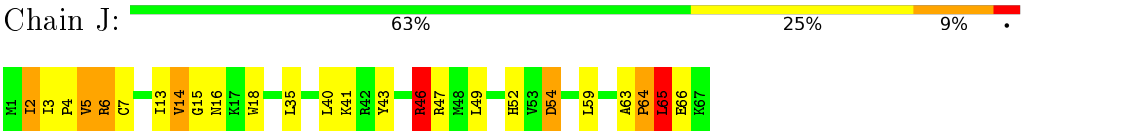
• Molecule 9: DNA-directed RNA polymerase II subunit RPB9

Chain I:



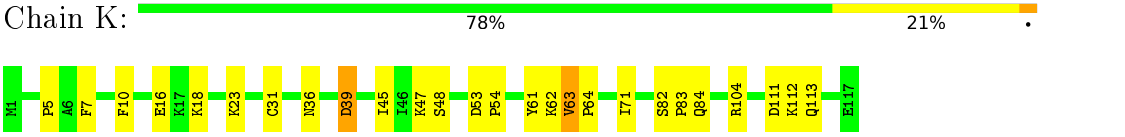
• Molecule 10: DNA-directed RNA polymerase II subunit RPB10

Chain J:



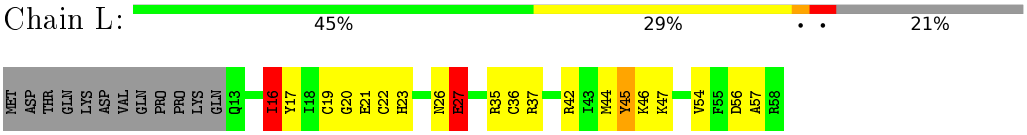
• Molecule 11: DNA-directed RNA polymerase II subunit RPB11-a

Chain K:



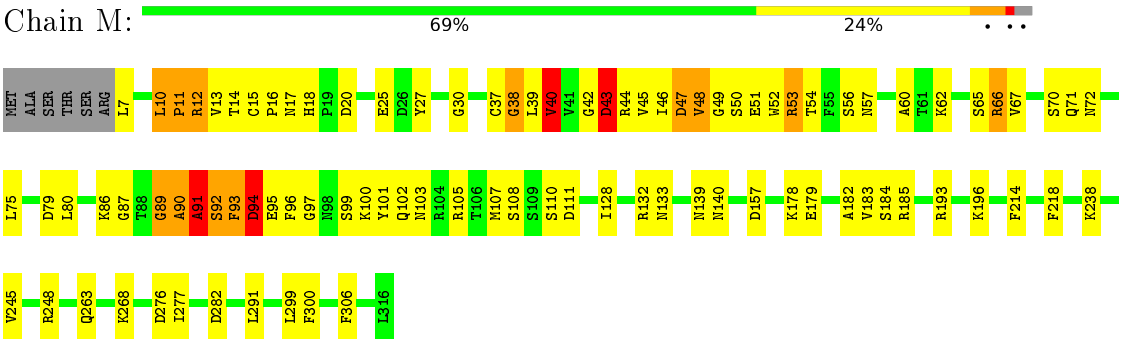
• Molecule 12: DNA-directed RNA polymerase II subunit RPB12

Chain L:



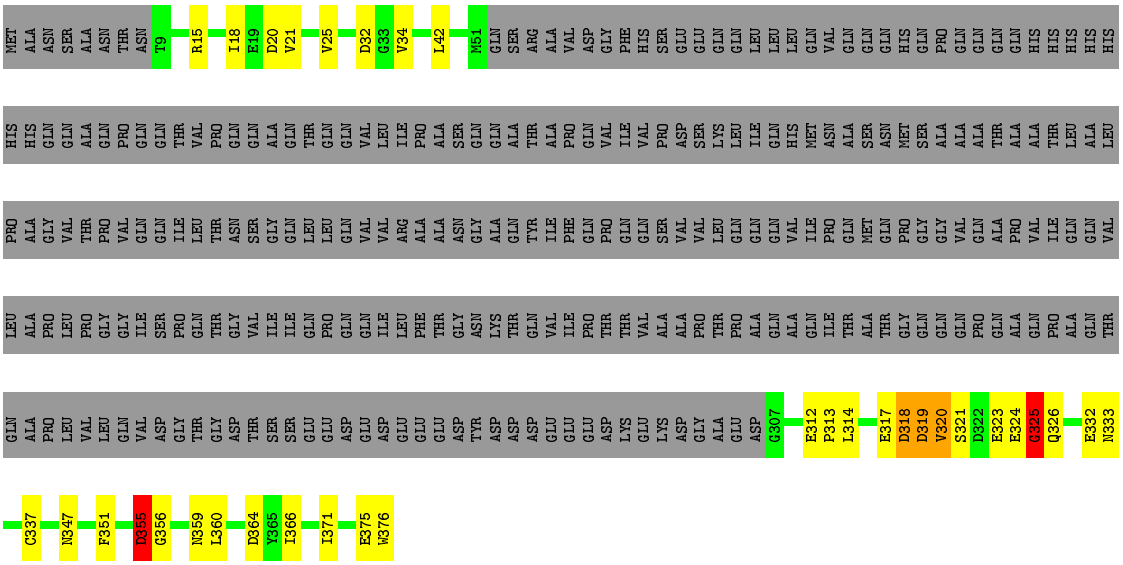
• Molecule 13: Transcription initiation factor IIB

Chain M:



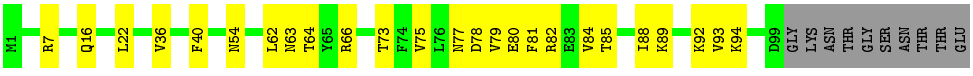
• Molecule 14: Transcription initiation factor IIA subunit 1

Chain N:



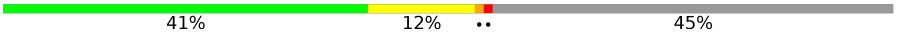
• Molecule 15: Transcription initiation factor IIA subunit 2

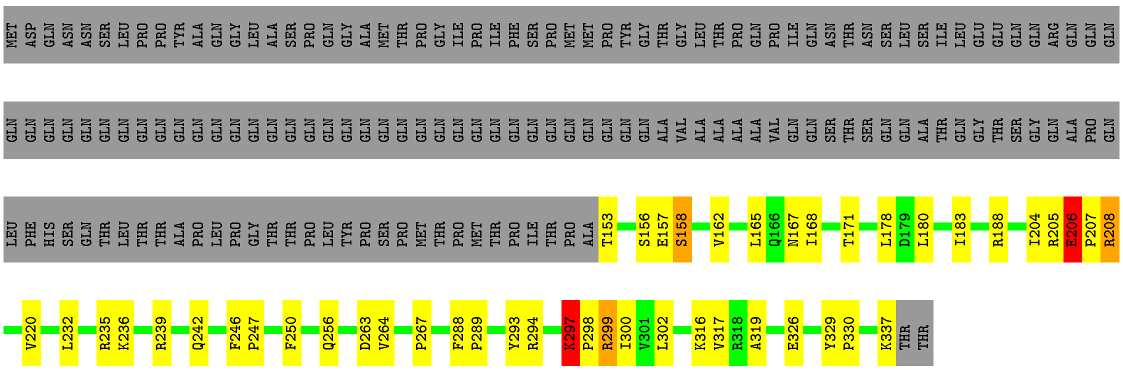
Chain O:



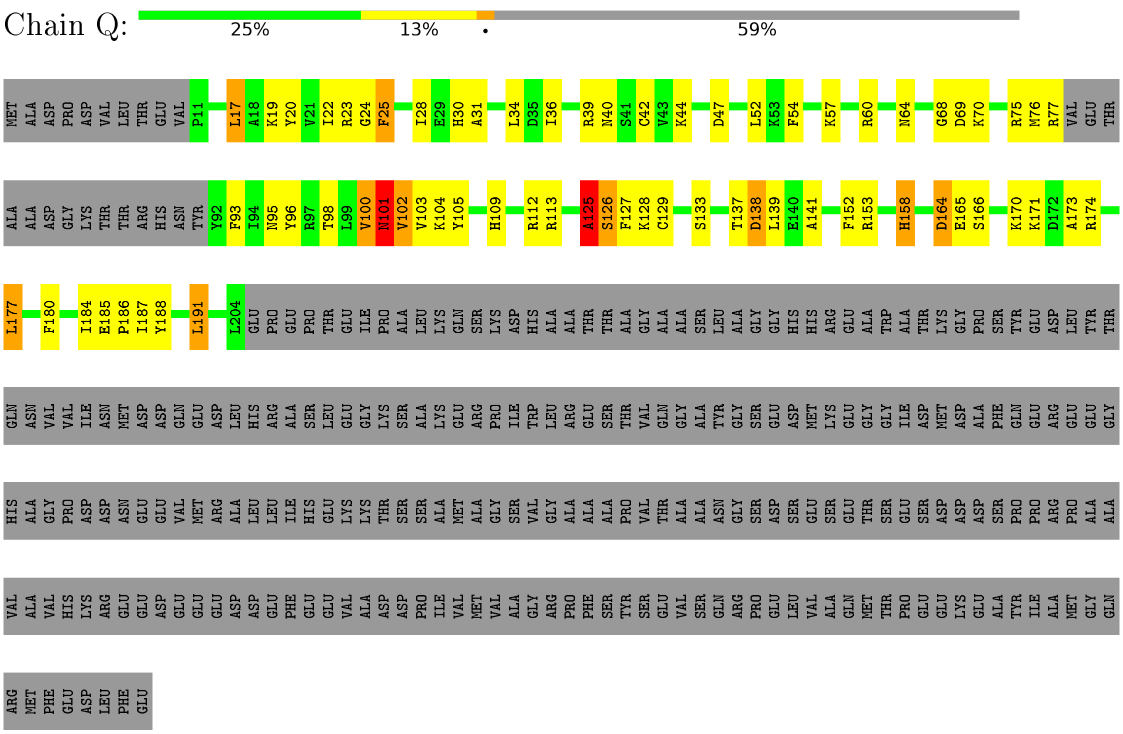
• Molecule 16: TATA-box-binding protein

Chain P:

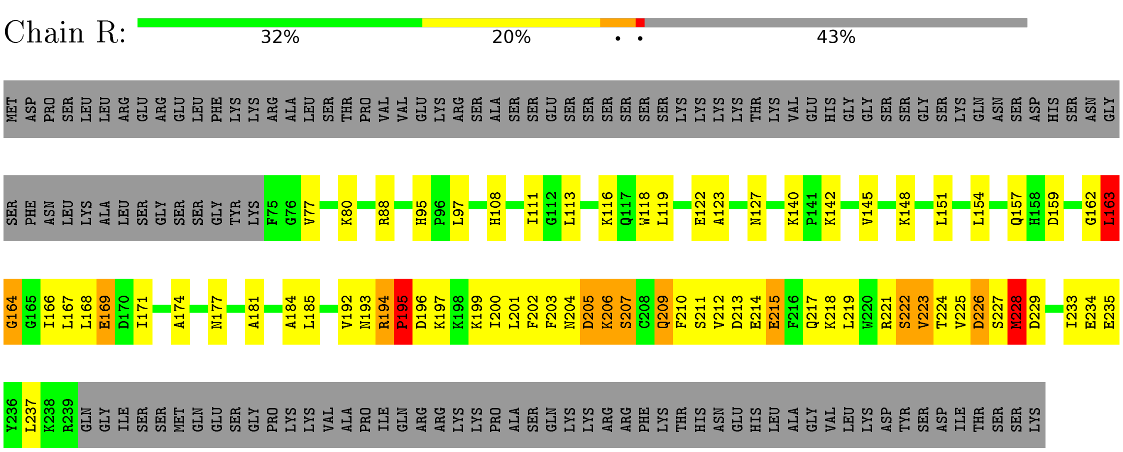




- Molecule 17: General transcription factor IIE subunit 1

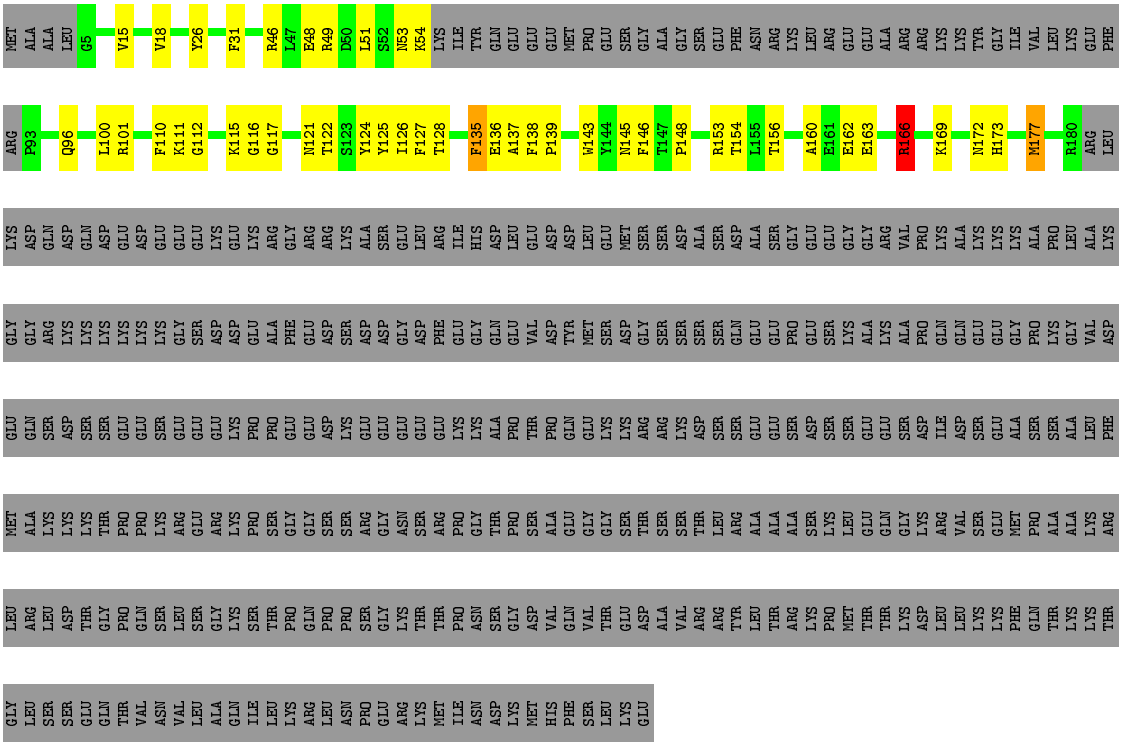


- Molecule 18: Transcription initiation factor IIE subunit beta



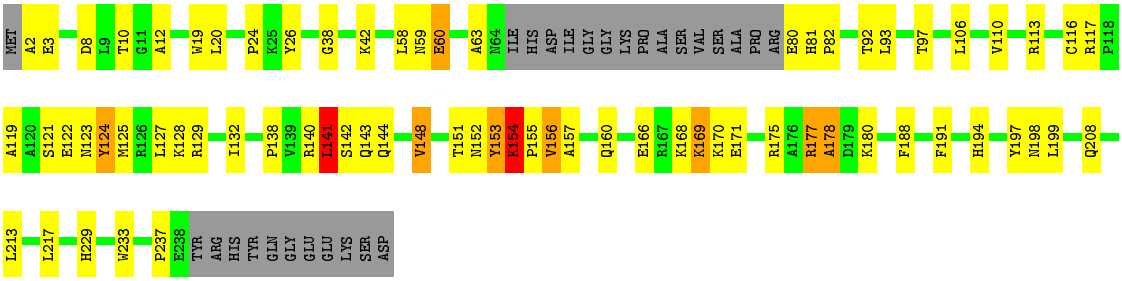
• Molecule 19: General transcription factor IIF subunit 1

Chain S:



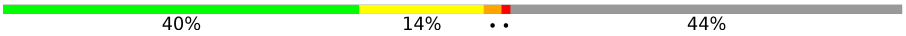
• Molecule 20: General transcription factor IIF subunit 2

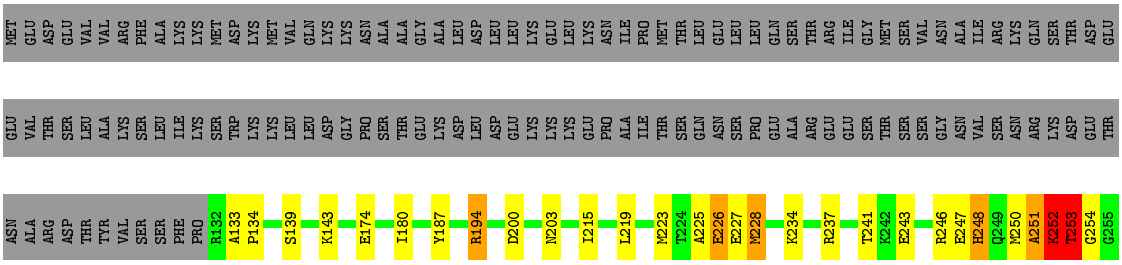
Chain T:



• Molecule 21: Transcription elongation factor A protein 1

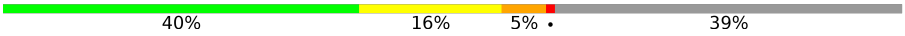
Chain U:

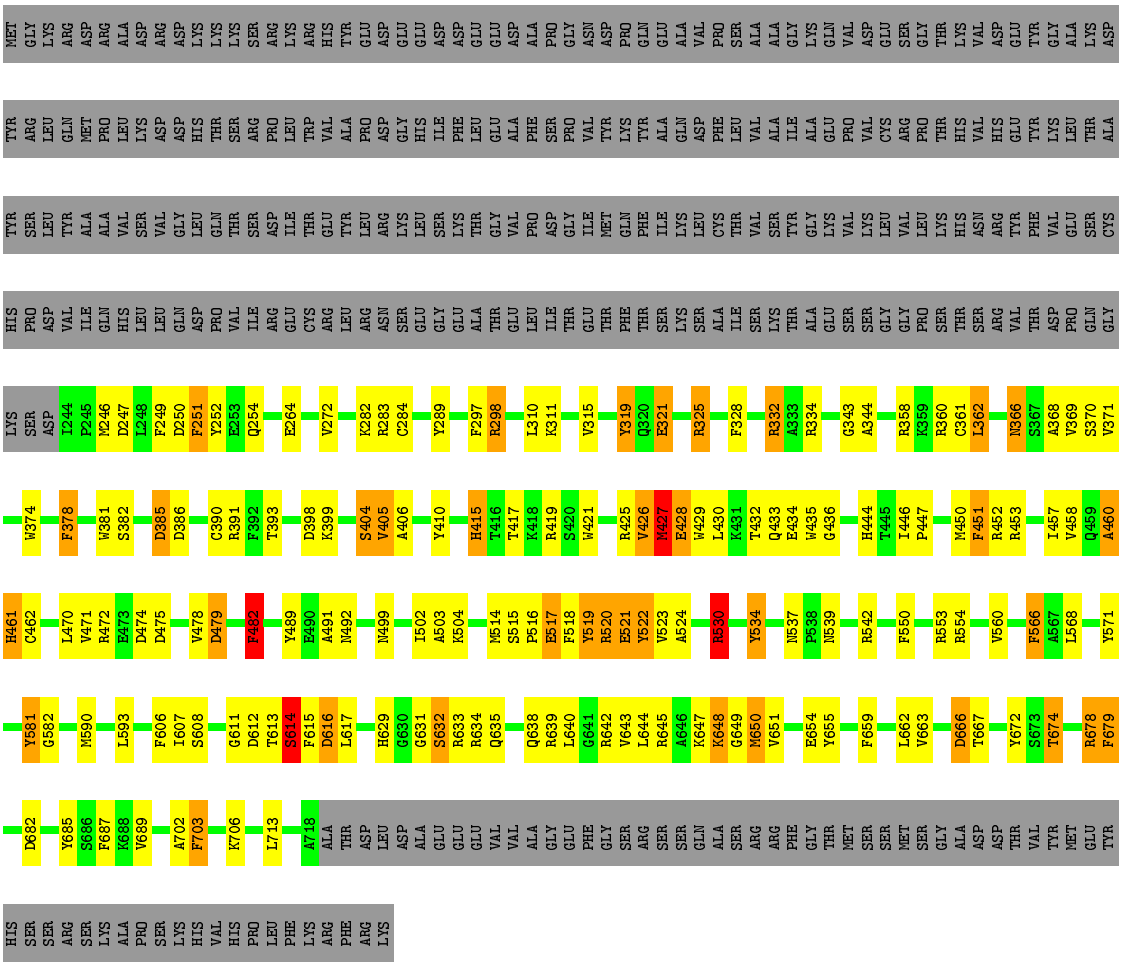




• Molecule 22: TFIIH basal transcription factor complex helicase XPB subunit

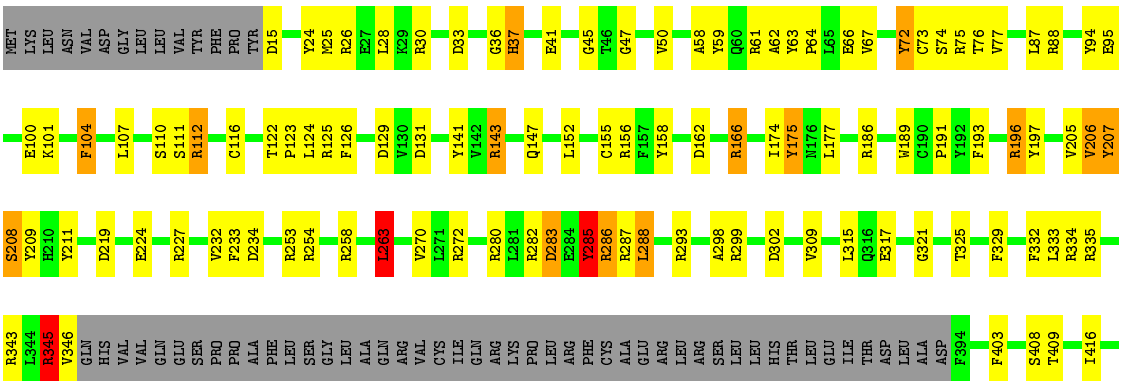
Chain V:

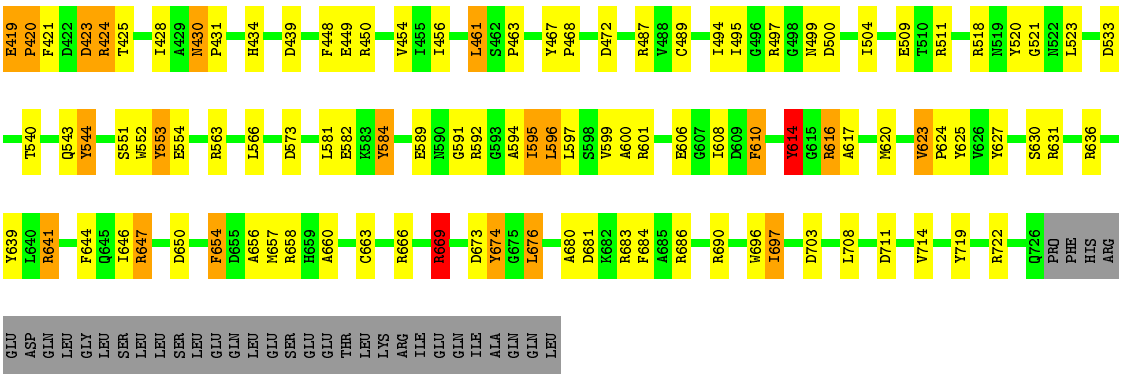




• Molecule 23: TFIIH basal transcription factor complex helicase XPD subunit

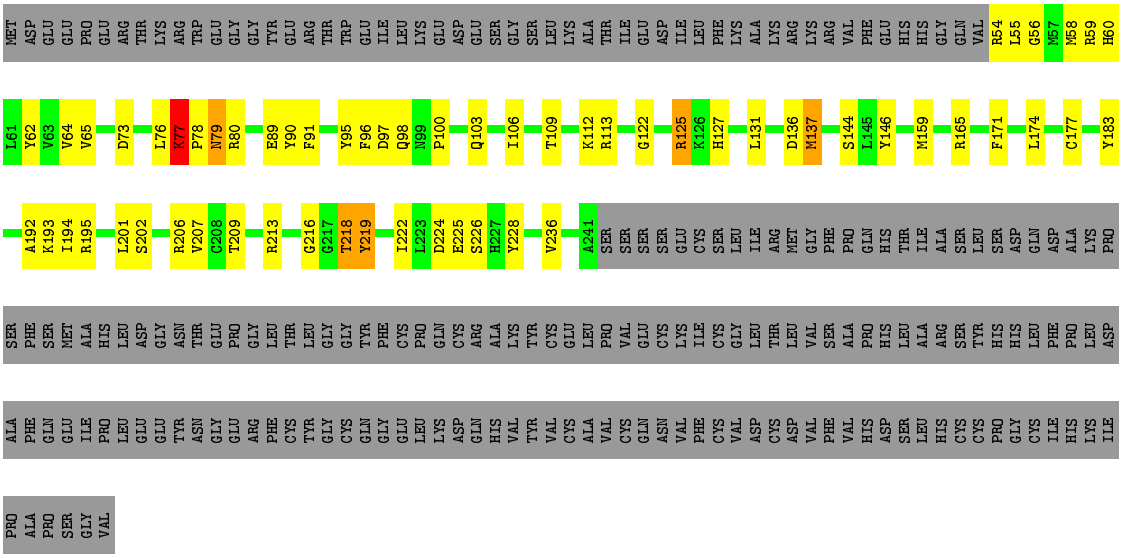
Chain W:





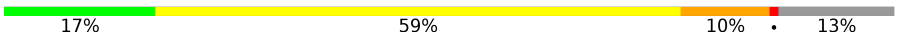
- Molecule 24: General transcription factor IIH subunit 2

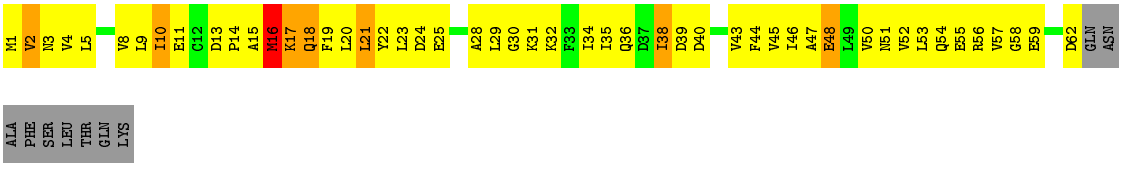
Chain 0:



- Molecule 25: General transcription factor IIH subunit 5

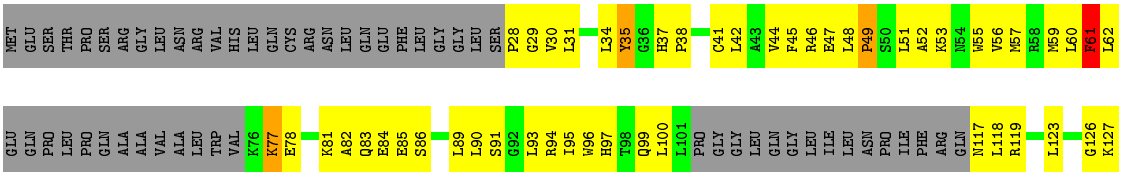
Chain 1:

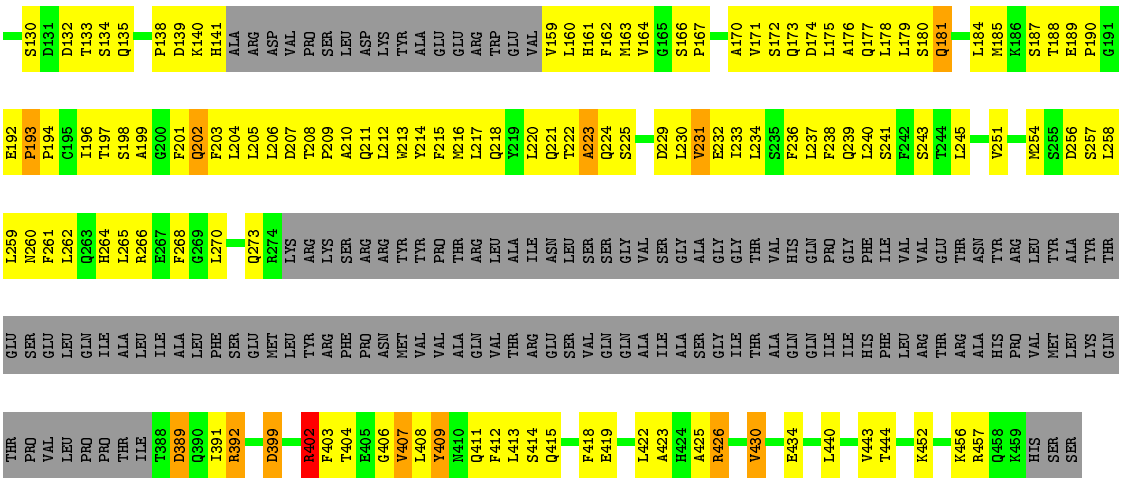




- Molecule 26: General transcription factor IIH subunit 4

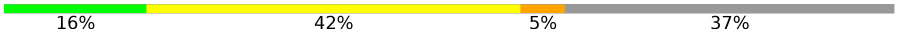
Chain 2:

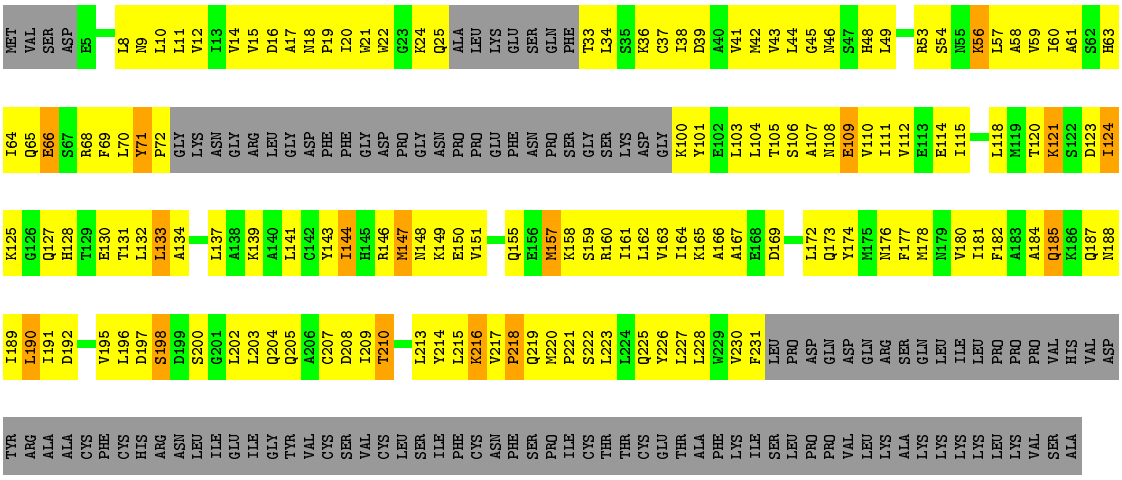




• Molecule 27: General transcription factor IIH subunit 3

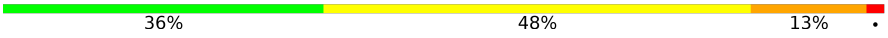
Chain 3:

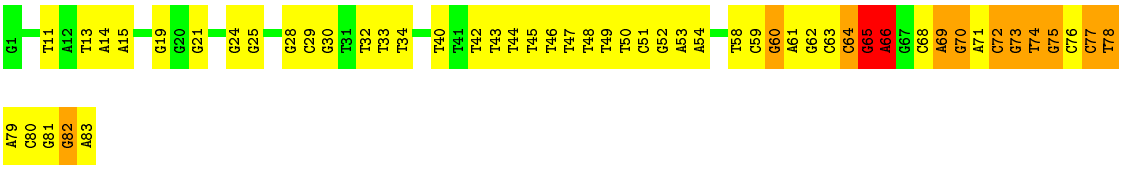




• Molecule 28: SCP-X

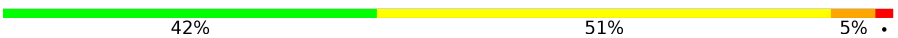
Chain X:

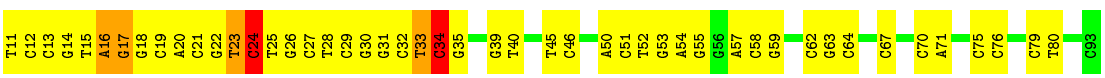




• Molecule 29: SCP-Y

Chain Y:





4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	68858	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 ($e^-/Å^2$)	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	0.62	4/11727 (0.0%)	0.82	17/15833 (0.1%)
10	J	0.74	0/542	0.90	1/730 (0.1%)
11	K	0.49	0/956	0.64	0/1294
12	L	0.53	0/394	0.71	0/524
13	M	0.39	0/2429	0.73	7/3281 (0.2%)
14	N	0.27	0/945	0.68	3/1274 (0.2%)
15	O	0.24	0/816	0.49	0/1105
16	P	0.29	0/1489	0.54	1/2005 (0.0%)
17	Q	0.29	0/1507	0.59	0/2023
18	R	0.49	0/1380	1.05	5/1854 (0.3%)
19	S	0.25	0/1167	0.54	1/1576 (0.1%)
2	B	0.75	9/9503 (0.1%)	0.92	24/12831 (0.2%)
20	T	0.37	2/1817 (0.1%)	0.68	1/2445 (0.0%)
21	U	0.24	0/1358	0.53	0/1820
22	V	1.44	14/3931 (0.4%)	1.91	105/5298 (2.0%)
23	W	1.55	24/5460 (0.4%)	2.06	160/7390 (2.2%)
24	0	1.49	5/1506 (0.3%)	1.95	43/2038 (2.1%)
25	1	0.84	0/496	1.17	1/669 (0.1%)
26	2	0.88	0/2243	1.19	9/3024 (0.3%)
27	3	0.85	0/1548	1.14	3/2090 (0.1%)
28	X	1.24	19/1917 (1.0%)	1.63	49/2962 (1.7%)
29	Y	1.19	18/1880 (1.0%)	1.53	54/2896 (1.9%)
3	C	0.60	0/2259	0.79	5/3073 (0.2%)
4	D	0.24	0/1077	0.44	0/1446
5	E	0.47	0/1753	0.74	2/2368 (0.1%)
6	F	0.64	0/700	0.78	0/946
7	G	0.29	0/1382	0.53	0/1874
8	H	0.44	0/1227	0.73	1/1654 (0.1%)
9	I	0.37	0/1038	1.00	5/1407 (0.4%)
All	All	0.86	95/64447 (0.1%)	1.16	497/87730 (0.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
14	N	0	2
16	P	0	1
17	Q	0	1
18	R	0	6
19	S	0	1
2	B	0	2
20	T	0	2
22	V	0	13
23	W	0	19
25	1	0	1
26	2	0	8
28	X	0	4
29	Y	0	4
7	G	0	1
All	All	0	66

All (95) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	X	59	DC	O3'-P	-13.91	1.44	1.61
28	X	71	DA	P-O5'	-9.90	1.49	1.59
28	X	79	DA	C5'-C4'	8.66	1.60	1.51
28	X	69	DA	C4'-C3'	8.54	1.61	1.53
29	Y	29	DC	C5'-C4'	8.10	1.60	1.51
29	Y	20	DA	P-O5'	8.07	1.67	1.59
23	W	158	TYR	CE1-CZ	8.06	1.49	1.38
29	Y	15	DT	C4'-C3'	7.98	1.61	1.53
28	X	77	DC	C5'-C4'	7.85	1.59	1.51
29	Y	18	DG	O4'-C1'	-7.82	1.32	1.42
22	V	672	TYR	CE1-CZ	7.79	1.48	1.38
20	T	60	GLU	CD-OE1	7.36	1.33	1.25
28	X	81	DG	C5'-C4'	7.20	1.59	1.51
29	Y	30	DG	P-O5'	7.18	1.67	1.59
23	W	104	PHE	CG-CD1	7.11	1.49	1.38
29	Y	17	DG	P-O5'	-7.05	1.52	1.59
22	V	391	ARG	CZ-NH2	-7.03	1.24	1.33
29	Y	14	DG	C2'-C1'	6.87	1.59	1.52
23	W	110	SER	CA-CB	6.77	1.63	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	X	80	DC	C4'-C3'	6.72	1.60	1.53
29	Y	12	DC	C4'-O4'	-6.59	1.38	1.45
22	V	633	ARG	CZ-NH1	-6.57	1.24	1.33
22	V	325	ARG	CZ-NH1	-6.55	1.24	1.33
28	X	75	DG	C5'-C4'	6.55	1.58	1.51
23	W	521	GLY	N-CA	6.44	1.55	1.46
23	W	208	SER	CB-OG	-6.43	1.33	1.42
24	0	122	GLY	N-CA	6.42	1.55	1.46
2	B	191	GLU	CG-CD	6.34	1.61	1.51
29	Y	17	DG	O4'-C1'	-6.32	1.34	1.42
28	X	71	DA	C3'-C2'	6.30	1.59	1.52
23	W	683	ARG	CZ-NH2	-6.29	1.24	1.33
22	V	606	PHE	CG-CD1	6.27	1.48	1.38
22	V	554	ARG	NE-CZ	6.23	1.41	1.33
28	X	75	DG	C4'-O4'	-6.21	1.38	1.45
22	V	453	ARG	CZ-NH2	-6.02	1.25	1.33
20	T	60	GLU	CD-OE2	5.96	1.32	1.25
22	V	319	TYR	CE1-CZ	5.93	1.46	1.38
29	Y	18	DG	C5'-C4'	5.93	1.57	1.51
28	X	72	DC	C2'-C1'	5.91	1.58	1.52
28	X	71	DA	C4'-O4'	-5.90	1.39	1.45
22	V	435	TRP	CD2-CE2	5.86	1.48	1.41
28	X	81	DG	P-O5'	5.82	1.65	1.59
23	W	321	GLY	N-CA	5.81	1.54	1.46
29	Y	29	DC	C4'-C3'	5.76	1.59	1.53
22	V	252	TYR	CE1-CZ	5.75	1.46	1.38
24	0	195	ARG	CZ-NH1	-5.75	1.25	1.33
29	Y	18	DG	C4'-O4'	-5.70	1.39	1.45
23	W	286	ARG	CZ-NH1	-5.67	1.25	1.33
2	B	1048	TYR	CD2-CE2	-5.66	1.30	1.39
28	X	83	DA	P-O5'	5.65	1.65	1.59
2	B	1047	TYR	CD1-CE1	-5.65	1.30	1.39
2	B	919	CYS	CB-SG	-5.63	1.72	1.81
23	W	47	GLY	N-CA	5.55	1.54	1.46
28	X	75	DG	C1'-N9	-5.51	1.39	1.47
23	W	610	PHE	CG-CD1	5.48	1.47	1.38
28	X	76	DC	O3'-P	5.45	1.67	1.61
22	V	332	ARG	CZ-NH2	-5.45	1.25	1.33
29	Y	28	DT	C5'-C4'	5.43	1.57	1.51
2	B	959	GLU	CB-CG	5.42	1.62	1.52
29	Y	29	DC	P-O5'	5.41	1.65	1.59
23	W	606	GLU	CA-CB	5.40	1.65	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	X	81	DG	C1'-N9	-5.39	1.39	1.47
28	X	66	DA	C4'-O4'	-5.38	1.39	1.45
23	W	448	PHE	CE1-CZ	5.38	1.47	1.37
22	V	452	ARG	CZ-NH2	-5.36	1.26	1.33
1	A	669	TYR	CE2-CZ	-5.35	1.31	1.38
29	Y	30	DG	C5'-C4'	5.35	1.57	1.51
23	W	334	ARG	CZ-NH2	-5.35	1.26	1.33
2	B	924	ARG	CZ-NH1	5.34	1.40	1.33
23	W	24	TYR	CE2-CZ	5.32	1.45	1.38
23	W	286	ARG	CZ-NH2	-5.29	1.26	1.33
23	W	674	TYR	CE1-CZ	5.25	1.45	1.38
2	B	927	ARG	CB-CG	-5.23	1.38	1.52
22	V	659	PHE	CG-CD2	5.22	1.46	1.38
29	Y	29	DC	O3'-P	5.20	1.67	1.61
23	W	253	ARG	CZ-NH1	-5.18	1.26	1.33
29	Y	12	DC	C5'-C4'	5.18	1.57	1.51
24	0	95	TYR	CG-CD1	5.17	1.45	1.39
2	B	984	CYS	CB-SG	-5.17	1.73	1.81
28	X	72	DC	C1'-N1	5.15	1.55	1.49
24	0	112	LYS	N-CA	5.13	1.56	1.46
23	W	639	TYR	CZ-OH	-5.12	1.29	1.37
2	B	1048	TYR	CD1-CE1	-5.11	1.31	1.39
24	0	146	TYR	CD2-CE2	5.10	1.47	1.39
29	Y	16	DA	C4'-C3'	5.09	1.58	1.53
23	W	511	ARG	NE-CZ	-5.08	1.26	1.33
1	A	556	GLU	CG-CD	5.07	1.59	1.51
22	V	451	PHE	CG-CD2	5.07	1.46	1.38
23	W	520	TYR	CZ-OH	-5.06	1.29	1.37
23	W	74	SER	CA-CB	-5.05	1.45	1.52
23	W	654	PHE	CG-CD1	5.04	1.46	1.38
1	A	669	TYR	CD2-CE2	-5.04	1.31	1.39
23	W	254	ARG	CZ-NH1	-5.04	1.26	1.33
1	A	458	PHE	CB-CG	-5.01	1.42	1.51
23	W	518	ARG	CZ-NH2	-5.01	1.26	1.33

All (497) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	I	84	HIS	C-N-CD	-25.47	64.58	120.60
18	R	194	ARG	C-N-CD	-24.67	66.32	120.60
24	0	77	LYS	C-N-CD	-21.79	72.67	120.60
27	3	71	TYR	C-N-CD	-20.65	75.17	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	W	335	ARG	NE-CZ-NH1	-19.53	110.53	120.30
29	Y	14	DG	O4'-C1'-N9	19.12	121.39	108.00
23	W	26	ARG	NE-CZ-NH2	18.61	129.60	120.30
28	X	59	DC	P-O3'-C3'	17.75	141.00	119.70
22	V	358	ARG	NE-CZ-NH2	17.63	129.12	120.30
24	0	195	ARG	NE-CZ-NH1	16.95	128.78	120.30
23	W	186	ARG	NE-CZ-NH1	16.37	128.49	120.30
23	W	497	ARG	NE-CZ-NH1	15.99	128.29	120.30
23	W	287	ARG	NE-CZ-NH2	15.55	128.08	120.30
28	X	83	DA	O4'-C1'-N9	15.33	118.73	108.00
23	W	299	ARG	NE-CZ-NH1	15.21	127.91	120.30
22	V	634	ARG	NE-CZ-NH2	14.82	127.71	120.30
24	0	206	ARG	NE-CZ-NH1	14.81	127.71	120.30
3	C	6	GLN	C-N-CD	-14.79	88.07	120.60
23	W	592	ARG	NE-CZ-NH1	14.20	127.40	120.30
23	W	335	ARG	NE-CZ-NH2	14.13	127.36	120.30
22	V	332	ARG	NE-CZ-NH1	13.94	127.27	120.30
23	W	112	ARG	NE-CZ-NH1	13.90	127.25	120.30
29	Y	15	DT	O4'-C1'-N1	13.84	117.69	108.00
23	W	272	ARG	NE-CZ-NH1	13.84	127.22	120.30
23	W	669	ARG	NE-CZ-NH1	13.70	127.15	120.30
28	X	65	DG	O4'-C1'-N9	13.46	117.42	108.00
23	W	75	ARG	NE-CZ-NH1	13.15	126.87	120.30
23	W	343	ARG	NE-CZ-NH2	12.85	126.72	120.30
28	X	66	DA	O4'-C1'-N9	12.82	116.98	108.00
22	V	633	ARG	NE-CZ-NH2	-12.67	113.96	120.30
29	Y	24	DC	O4'-C1'-N1	12.58	116.81	108.00
23	W	467	TYR	CB-CG-CD1	-12.29	113.63	121.00
23	W	627	TYR	CB-CG-CD2	-12.11	113.73	121.00
23	W	423	ASP	CB-CG-OD1	12.08	129.17	118.30
23	W	601	ARG	NE-CZ-NH2	-12.04	114.28	120.30
28	X	65	DG	P-O3'-C3'	12.03	134.14	119.70
23	W	631	ARG	NE-CZ-NH1	11.99	126.30	120.30
23	W	26	ARG	NH1-CZ-NH2	-11.61	106.63	119.40
22	V	452	ARG	NE-CZ-NH1	11.59	126.09	120.30
23	W	487	ARG	NE-CZ-NH1	11.54	126.07	120.30
22	V	283	ARG	NE-CZ-NH2	-11.52	114.54	120.30
23	W	88	ARG	NE-CZ-NH1	11.43	126.02	120.30
23	W	636	ARG	NE-CZ-NH1	11.43	126.01	120.30
23	W	419	GLU	C-N-CD	-11.32	95.69	120.60
23	W	343	ARG	NE-CZ-NH1	-11.21	114.70	120.30
28	X	65	DG	O4'-C1'-C2'	-11.15	96.98	105.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	W	647	ARG	NE-CZ-NH1	11.15	125.87	120.30
2	B	924	ARG	NE-CZ-NH1	-11.06	114.77	120.30
29	Y	11	DT	O4'-C1'-N1	11.00	115.70	108.00
28	X	79	DA	O4'-C4'-C3'	10.89	112.54	106.00
23	W	683	ARG	NE-CZ-NH2	10.86	125.73	120.30
28	X	79	DA	O4'-C1'-N9	10.73	115.52	108.00
23	W	690	ARG	NE-CZ-NH2	10.71	125.65	120.30
23	W	88	ARG	NE-CZ-NH2	-10.41	115.09	120.30
22	V	391	ARG	NE-CZ-NH1	-10.16	115.22	120.30
28	X	75	DG	O4'-C1'-N9	10.12	115.08	108.00
13	M	42	GLY	N-CA-C	10.03	138.18	113.10
22	V	687	PHE	CB-CG-CD2	-9.94	113.84	120.80
22	V	283	ARG	NE-CZ-NH1	9.87	125.23	120.30
22	V	452	ARG	NE-CZ-NH2	-9.82	115.39	120.30
23	W	497	ARG	NE-CZ-NH2	-9.79	115.41	120.30
22	V	553	ARG	NE-CZ-NH2	9.69	125.14	120.30
22	V	520	ARG	CA-C-N	-9.66	95.94	117.20
28	X	73	DG	O4'-C1'-C2'	9.62	113.59	105.90
22	V	334	ARG	CD-NE-CZ	9.54	136.96	123.60
24	0	59	ARG	NE-CZ-NH2	9.54	125.07	120.30
23	W	658	ARG	NE-CZ-NH2	-9.47	115.56	120.30
23	W	227	ARG	NE-CZ-NH1	9.43	125.01	120.30
29	Y	21	DC	O4'-C4'-C3'	9.33	111.60	106.00
22	V	645	ARG	NE-CZ-NH1	9.28	124.94	120.30
22	V	264	GLU	OE1-CD-OE2	-9.15	112.32	123.30
24	0	219	TYR	CB-CG-CD1	-9.15	115.51	121.00
23	W	511	ARG	NE-CZ-NH2	9.14	124.87	120.30
29	Y	17	DG	O4'-C1'-N9	-9.14	101.60	108.00
23	W	627	TYR	CG-CD2-CE2	-9.11	114.01	121.30
23	W	666	ARG	NE-CZ-NH1	9.11	124.85	120.30
23	W	686	ARG	NE-CZ-NH1	9.09	124.84	120.30
23	W	703	ASP	CB-CG-OD2	9.04	126.43	118.30
23	W	286	ARG	NE-CZ-NH2	8.99	124.80	120.30
24	0	206	ARG	NH1-CZ-NH2	-8.89	109.63	119.40
2	B	526	LEU	CB-CG-CD1	-8.86	95.94	111.00
22	V	550	PHE	CB-CG-CD1	-8.86	114.60	120.80
29	Y	21	DC	C2-N1-C1'	-8.78	109.14	118.80
28	X	70	DG	O4'-C1'-N9	8.69	114.09	108.00
28	X	79	DA	C4'-C3'-C2'	-8.58	95.38	103.10
1	A	503	LEU	CA-CB-CG	8.55	134.96	115.30
28	X	66	DA	O4'-C1'-C2'	-8.48	99.12	105.90
23	W	450	ARG	NE-CZ-NH1	8.47	124.53	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	W	654	PHE	CB-CG-CD2	-8.43	114.90	120.80
24	0	213	ARG	NE-CZ-NH1	8.42	124.51	120.30
28	X	79	DA	C1'-O4'-C4'	-8.38	101.72	110.10
22	V	520	ARG	C-N-CA	-8.34	100.84	121.70
22	V	419	ARG	NE-CZ-NH1	8.33	124.47	120.30
22	V	581	TYR	CG-CD1-CE1	-8.32	114.65	121.30
29	Y	21	DC	C1'-O4'-C4'	-8.30	101.80	110.10
1	A	622	SER	C-N-CD	-8.27	102.41	120.60
22	V	685	TYR	CB-CG-CD2	8.23	125.94	121.00
23	W	497	ARG	CD-NE-CZ	8.21	135.09	123.60
29	Y	34	DC	N3-C2-O2	-8.17	116.18	121.90
23	W	332	PHE	CB-CG-CD2	-8.16	115.09	120.80
29	Y	21	DC	C6-N1-C1'	8.15	130.58	120.80
22	V	634	ARG	NE-CZ-NH1	-8.11	116.24	120.30
22	V	520	ARG	O-C-N	8.09	135.65	122.70
22	V	520	ARG	NE-CZ-NH2	8.06	124.33	120.30
18	R	195	PRO	N-CA-C	-8.04	91.18	112.10
13	M	94	ASP	N-CA-C	-8.00	89.39	111.00
13	M	91	ALA	N-CA-C	-7.90	89.67	111.00
22	V	410	TYR	CB-CG-CD1	-7.89	116.27	121.00
23	W	601	ARG	NE-CZ-NH1	7.89	124.25	120.30
23	W	614	TYR	CB-CG-CD2	-7.89	116.27	121.00
22	V	358	ARG	NH1-CZ-NH2	-7.84	110.78	119.40
28	X	61	DA	C5-C6-N1	7.82	121.61	117.70
29	Y	20	DA	O4'-C4'-C3'	-7.82	101.31	106.00
28	X	61	DA	N1-C6-N6	-7.81	113.91	118.60
29	Y	21	DC	O4'-C1'-C2'	7.81	112.15	105.90
22	V	386	ASP	CB-CG-OD2	-7.81	111.28	118.30
2	B	882	SER	N-CA-C	-7.79	89.97	111.00
23	W	126	PHE	CB-CG-CD2	7.78	126.24	120.80
23	W	75	ARG	NE-CZ-NH2	-7.76	116.42	120.30
23	W	448	PHE	CB-CG-CD2	7.75	126.23	120.80
23	W	644	PHE	CB-CG-CD1	7.73	126.21	120.80
23	W	143	ARG	NE-CZ-NH1	7.72	124.16	120.30
23	W	125	ARG	NE-CZ-NH1	7.67	124.14	120.30
29	Y	18	DG	O4'-C4'-C3'	7.67	110.60	106.00
23	W	467	TYR	CB-CG-CD2	7.66	125.60	121.00
23	W	232	VAL	CA-CB-CG1	7.63	122.35	110.90
23	W	520	TYR	CG-CD1-CE1	-7.62	115.21	121.30
2	B	945	CYS	CA-CB-SG	7.61	127.69	114.00
22	V	542	ARG	NE-CZ-NH2	7.61	124.10	120.30
28	X	64	DC	N3-C2-O2	-7.59	116.58	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	W	582	GLU	OE1-CD-OE2	-7.56	114.23	123.30
28	X	65	DG	C4'-C3'-O3'	7.55	128.57	109.70
23	W	553	TYR	CB-CG-CD2	7.53	125.52	121.00
24	0	95	TYR	CB-CG-CD1	-7.53	116.48	121.00
22	V	474	ASP	CB-CG-OD2	7.51	125.06	118.30
24	0	90	TYR	CB-CG-CD2	-7.50	116.50	121.00
29	Y	18	DG	C4'-C3'-C2'	-7.48	96.37	103.10
29	Y	24	DC	C2-N1-C1'	-7.47	110.58	118.80
9	I	61	GLU	N-CA-C	-7.46	90.87	111.00
26	2	402	ARG	NE-CZ-NH1	7.44	124.02	120.30
22	V	522	TYR	CB-CG-CD2	-7.43	116.54	121.00
23	W	193	PHE	CB-CG-CD1	-7.41	115.61	120.80
23	W	272	ARG	NH1-CZ-NH2	-7.38	111.28	119.40
22	V	249	PHE	CB-CG-CD2	7.36	125.95	120.80
23	W	592	ARG	NH1-CZ-NH2	-7.36	111.30	119.40
24	0	73	ASP	CB-CG-OD2	-7.34	111.69	118.30
2	B	747	LEU	CA-CB-CG	-7.32	98.47	115.30
1	A	360	ASP	CB-CG-OD1	-7.31	111.72	118.30
28	X	66	DA	P-O5'-C5'	7.31	132.59	120.90
29	Y	15	DT	O4'-C1'-C2'	-7.30	100.06	105.90
22	V	685	TYR	CB-CG-CD1	-7.29	116.63	121.00
23	W	186	ARG	NE-CZ-NH2	-7.28	116.66	120.30
1	A	681	LEU	CB-CG-CD2	-7.28	98.63	111.00
22	V	554	ARG	NE-CZ-NH1	7.26	123.93	120.30
24	0	236	VAL	CA-CB-CG1	7.24	121.77	110.90
5	E	64	HIS	N-CA-C	7.16	130.34	111.00
13	M	89	GLY	N-CA-C	-7.16	95.21	113.10
24	0	89	GLU	OE1-CD-OE2	-7.14	114.73	123.30
2	B	927	ARG	NE-CZ-NH1	7.06	123.83	120.30
23	W	317	GLU	OE1-CD-OE2	-7.05	114.84	123.30
1	A	271	ARG	N-CA-C	-7.04	92.00	111.00
22	V	703	PHE	CB-CG-CD2	-7.04	115.88	120.80
23	W	166	ARG	CD-NE-CZ	7.01	133.42	123.60
29	Y	27	DC	C2-N1-C1'	-6.99	111.11	118.80
28	X	79	DA	P-O3'-C3'	6.97	128.06	119.70
22	V	639	ARG	NE-CZ-NH2	6.96	123.78	120.30
23	W	280	ARG	NE-CZ-NH1	-6.94	116.83	120.30
28	X	66	DA	P-O3'-C3'	6.94	128.03	119.70
28	X	63	DC	N3-C2-O2	-6.92	117.06	121.90
8	H	74	GLU	N-CA-C	-6.92	92.32	111.00
23	W	614	TYR	CG-CD2-CE2	-6.91	115.77	121.30
23	W	627	TYR	CD1-CG-CD2	6.91	125.50	117.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	V	643	VAL	CA-CB-CG1	6.90	121.25	110.90
22	V	385	ASP	CB-CG-OD1	-6.89	112.10	118.30
24	0	195	ARG	NE-CZ-NH2	-6.87	116.86	120.30
18	R	162	GLY	N-CA-C	6.86	130.26	113.10
28	X	60	DG	N3-C2-N2	-6.86	115.10	119.90
2	B	483	ARG	NE-CZ-NH1	6.86	123.73	120.30
23	W	219	ASP	CB-CG-OD1	6.83	124.45	118.30
23	W	654	PHE	CB-CG-CD1	6.83	125.58	120.80
23	W	332	PHE	CB-CG-CD1	6.82	125.58	120.80
23	W	644	PHE	CB-CG-CD2	-6.82	116.03	120.80
26	2	35	TYR	CA-CB-CG	-6.82	100.45	113.40
28	X	73	DG	O4'-C1'-N9	6.82	112.77	108.00
23	W	125	ARG	CD-NE-CZ	6.81	133.13	123.60
24	0	136	ASP	CB-CG-OD1	6.79	124.42	118.30
22	V	530	ARG	NE-CZ-NH2	-6.78	116.91	120.30
24	0	95	TYR	CD1-CE1-CZ	-6.78	113.70	119.80
28	X	81	DG	C8-N9-C1'	6.76	135.79	127.00
23	W	253	ARG	NE-CZ-NH1	6.75	123.68	120.30
29	Y	23	DT	O4'-C1'-N1	-6.73	103.29	108.00
23	W	345	ARG	CD-NE-CZ	6.72	133.01	123.60
28	X	81	DG	C4-N9-C1'	-6.70	117.79	126.50
29	Y	32	DC	N3-C2-O2	-6.70	117.21	121.90
23	W	566	LEU	CB-CG-CD1	6.69	122.37	111.00
23	W	50	VAL	CA-CB-CG1	6.68	120.92	110.90
22	V	581	TYR	CD1-CE1-CZ	6.66	125.80	119.80
26	2	61	PHE	CB-CA-C	-6.66	97.08	110.40
23	W	26	ARG	NE-CZ-NH1	6.66	123.63	120.30
22	V	334	ARG	NE-CZ-NH1	6.66	123.63	120.30
22	V	655	TYR	CB-CG-CD2	-6.64	117.01	121.00
23	W	196	ARG	NE-CZ-NH1	6.62	123.61	120.30
23	W	30	ARG	CD-NE-CZ	6.61	132.85	123.60
9	I	58	ILE	N-CA-C	-6.60	93.18	111.00
23	W	616	ARG	NE-CZ-NH1	-6.59	117.01	120.30
18	R	169	GLU	OE1-CD-OE2	-6.58	115.40	123.30
29	Y	34	DC	N3-C4-N4	-6.57	113.40	118.00
23	W	299	ARG	NE-CZ-NH2	-6.56	117.02	120.30
24	0	219	TYR	CG-CD1-CE1	-6.55	116.06	121.30
22	V	298	ARG	NE-CZ-NH1	6.54	123.57	120.30
29	Y	29	DC	C5'-C4'-C3'	6.52	125.84	114.10
23	W	302	ASP	CB-CG-OD1	6.52	124.17	118.30
28	X	61	DA	C4-C5-C6	-6.51	113.75	117.00
23	W	674	TYR	CB-CG-CD1	6.49	124.90	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	W	76	THR	CA-CB-OG1	6.49	122.63	109.00
23	W	315	LEU	CB-CG-CD1	6.48	122.02	111.00
26	2	193	PRO	CA-N-CD	-6.48	102.43	111.50
22	V	404	SER	CB-CA-C	6.48	122.41	110.10
22	V	682	ASP	CB-CG-OD1	6.48	124.13	118.30
28	X	78	DT	N1-C1'-C2'	6.46	124.88	112.60
23	W	487	ARG	NH1-CZ-NH2	-6.45	112.31	119.40
29	Y	20	DA	O4'-C1'-C2'	-6.45	100.74	105.90
29	Y	32	DC	O4'-C4'-C3'	6.43	109.86	106.00
29	Y	27	DC	C6-N1-C1'	6.42	128.51	120.80
23	W	189	TRP	NE1-CE2-CD2	-6.42	100.88	107.30
3	C	68	LEU	CB-CG-CD1	-6.41	100.10	111.00
23	W	722	ARG	CD-NE-CZ	6.39	132.55	123.60
29	Y	27	DC	O4'-C1'-N1	6.39	112.47	108.00
2	B	1043	ILE	CG1-CB-CG2	-6.38	97.36	111.40
23	W	125	ARG	NE-CZ-NH2	-6.38	117.11	120.30
29	Y	22	DG	C4'-C3'-C2'	-6.38	97.36	103.10
3	C	137	ASN	N-CA-C	-6.36	93.83	111.00
23	W	683	ARG	CD-NE-CZ	6.36	132.50	123.60
24	0	113	ARG	NE-CZ-NH1	6.36	123.48	120.30
23	W	641	ARG	NE-CZ-NH1	6.35	123.47	120.30
1	A	484	LEU	CB-CG-CD1	6.34	121.79	111.00
2	B	922	ARG	NE-CZ-NH1	-6.34	117.13	120.30
22	V	369	VAL	CA-CB-CG1	6.34	120.41	110.90
22	V	332	ARG	NH1-CZ-NH2	-6.34	112.43	119.40
23	W	669	ARG	NH1-CZ-NH2	-6.33	112.43	119.40
23	W	131	ASP	CB-CG-OD1	-6.33	112.60	118.30
2	B	115	LEU	CB-CG-CD2	-6.33	100.23	111.00
23	W	263	LEU	N-CA-CB	-6.32	97.76	110.40
23	W	639	TYR	CB-CG-CD2	-6.31	117.21	121.00
28	X	83	DA	C4'-C3'-C2'	-6.31	97.42	103.10
29	Y	29	DC	O5'-C5'-C4'	6.30	126.76	111.00
22	V	522	TYR	CB-CG-CD1	6.29	124.78	121.00
24	0	59	ARG	NH1-CZ-NH2	-6.29	112.48	119.40
29	Y	28	DT	O3'-P-O5'	6.29	115.95	104.00
22	V	344	ALA	N-CA-CB	-6.29	101.30	110.10
2	B	924	ARG	NH1-CZ-NH2	6.29	126.31	119.40
29	Y	29	DC	P-O3'-C3'	6.27	127.22	119.70
29	Y	31	DG	N1-C6-O6	-6.27	116.14	119.90
22	V	521	GLU	OE1-CD-OE2	-6.26	115.79	123.30
29	Y	33	DT	C6-C5-C7	-6.24	119.16	122.90
23	W	30	ARG	NE-CZ-NH1	6.23	123.42	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	X	62	DG	N1-C6-O6	-6.22	116.17	119.90
23	W	206	VAL	CA-CB-CG1	6.22	120.23	110.90
24	0	183	TYR	CB-CG-CD1	-6.19	117.28	121.00
3	C	35	ARG	CG-CD-NE	-6.19	98.80	111.80
2	B	730	LYS	CD-CE-NZ	6.17	125.89	111.70
24	0	137	MET	CG-SD-CE	6.15	110.05	100.20
14	N	356	GLY	N-CA-C	6.15	128.47	113.10
23	W	77	VAL	CG1-CB-CG2	-6.12	101.11	110.90
29	Y	28	DT	C3'-C2'-C1'	-6.09	95.19	102.50
22	V	435	TRP	NE1-CE2-CD2	-6.09	101.21	107.30
29	Y	30	DG	N1-C6-O6	-6.09	116.25	119.90
28	X	64	DC	O4'-C4'-C3'	6.08	109.64	106.00
13	M	43	ASP	N-CA-C	-6.07	94.61	111.00
22	V	410	TYR	CZ-CE2-CD2	-6.04	114.36	119.80
1	A	1160	ARG	NE-CZ-NH2	-6.03	117.29	120.30
22	V	360	ARG	CD-NE-CZ	6.01	132.02	123.60
28	X	83	DA	O4'-C1'-C2'	-6.01	101.09	105.90
22	V	472	ARG	NE-CZ-NH1	6.01	123.30	120.30
23	W	673	ASP	CB-CG-OD1	6.00	123.70	118.30
24	0	218	THR	CA-CB-CG2	-5.98	104.03	112.40
28	X	64	DC	N1-C2-O2	5.97	122.48	118.90
23	W	424	ARG	NE-CZ-NH1	5.97	123.29	120.30
23	W	156	ARG	CD-NE-CZ	5.96	131.94	123.60
23	W	552	TRP	CD1-NE1-CE2	5.95	114.36	109.00
22	V	663	VAL	CG1-CB-CG2	-5.95	101.39	110.90
22	V	321	GLU	OE1-CD-OE2	-5.93	116.19	123.30
23	W	472	ASP	CB-CG-OD2	5.91	123.62	118.30
29	Y	11	DT	P-O3'-C3'	5.91	126.79	119.70
22	V	566	PHE	CB-CG-CD1	5.91	124.94	120.80
29	Y	29	DC	N3-C4-C5	5.90	124.26	121.90
23	W	131	ASP	CB-CG-OD2	5.88	123.59	118.30
29	Y	16	DA	O4'-C1'-C2'	5.88	110.60	105.90
22	V	381	TRP	CZ3-CH2-CZ2	-5.87	114.56	121.60
28	X	71	DA	O4'-C1'-N9	5.86	112.10	108.00
29	Y	21	DC	O4'-C1'-N1	-5.86	103.90	108.00
2	B	1050	ARG	NE-CZ-NH2	5.84	123.22	120.30
3	C	49	TRP	CA-CB-CG	5.83	124.78	113.70
28	X	63	DC	O4'-C4'-C3'	5.83	109.50	106.00
22	V	435	TRP	CD1-NE1-CE2	5.81	114.23	109.00
2	B	704	LEU	CB-CG-CD1	-5.80	101.13	111.00
2	B	880	LEU	N-CA-C	5.80	126.66	111.00
23	W	563	ARG	NE-CZ-NH1	5.80	123.20	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	J	46	ARG	NE-CZ-NH1	-5.78	117.41	120.30
22	V	410	TYR	CB-CG-CD2	5.77	124.46	121.00
22	V	425	ARG	NE-CZ-NH1	5.77	123.19	120.30
24	0	90	TYR	CG-CD2-CE2	-5.76	116.69	121.30
29	Y	34	DC	OP2-P-O3'	5.76	117.88	105.20
23	W	650	ASP	CB-CG-OD1	5.76	123.49	118.30
23	W	112	ARG	NH1-CZ-NH2	-5.76	113.06	119.40
23	W	472	ASP	CB-CG-OD1	-5.74	113.13	118.30
24	0	177	CYS	CA-CB-SG	-5.74	103.67	114.00
24	0	171	PHE	CB-CG-CD1	-5.74	116.78	120.80
29	Y	14	DG	C3'-C2'-C1'	-5.72	95.63	102.50
23	W	72	TYR	CB-CG-CD2	-5.72	117.57	121.00
18	R	223	VAL	CA-CB-CG2	5.72	119.48	110.90
22	V	542	ARG	NH1-CZ-NH2	-5.72	113.11	119.40
23	W	641	ARG	CD-NE-CZ	5.71	131.60	123.60
22	V	614	SER	N-CA-C	5.70	126.39	111.00
24	0	91	PHE	CG-CD2-CE2	-5.70	114.53	120.80
28	X	74	DT	C3'-C2'-C1'	-5.69	95.67	102.50
29	Y	24	DC	C6-N1-C1'	5.69	127.62	120.80
24	0	80	ARG	CD-NE-CZ	5.68	131.55	123.60
2	B	1054	MET	CB-CG-SD	5.67	129.42	112.40
24	0	183	TYR	CD1-CE1-CZ	5.67	124.90	119.80
29	Y	16	DA	O4'-C1'-N9	5.65	111.96	108.00
23	W	41	GLU	O-C-N	5.65	131.74	122.70
22	V	419	ARG	CD-NE-CZ	5.65	131.50	123.60
23	W	711	ASP	CB-CG-OD1	5.64	123.38	118.30
1	A	1378	LEU	CB-CG-CD1	-5.64	101.42	111.00
22	V	251	PHE	CB-CG-CD1	-5.63	116.86	120.80
28	X	82	DG	O4'-C1'-N9	-5.63	104.06	108.00
1	A	540	ASP	CB-CG-OD2	-5.63	113.23	118.30
22	V	284	CYS	CA-CB-SG	-5.63	103.86	114.00
22	V	328	PHE	C-N-CA	5.63	134.13	122.30
23	W	345	ARG	NE-CZ-NH2	-5.63	117.48	120.30
23	W	722	ARG	NE-CZ-NH1	-5.62	117.49	120.30
23	W	270	VAL	CA-C-O	5.61	131.89	120.10
24	0	96	PHE	CB-CG-CD1	-5.61	116.87	120.80
23	W	708	LEU	CB-CG-CD2	-5.61	101.46	111.00
22	V	482	PHE	CB-CG-CD1	-5.61	116.87	120.80
23	W	544	TYR	CG-CD2-CE2	-5.60	116.82	121.30
22	V	430	LEU	CB-CG-CD1	5.60	120.52	111.00
23	W	684	PHE	CB-CG-CD1	-5.60	116.88	120.80
24	0	201	LEU	CB-CG-CD1	5.59	120.50	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	0	183	TYR	CG-CD1-CE1	-5.58	116.83	121.30
28	X	65	DG	C8-N9-C4	-5.58	104.17	106.40
24	0	226	SER	N-CA-CB	-5.58	102.13	110.50
22	V	662	LEU	CB-CG-CD2	-5.58	101.52	111.00
23	W	129	ASP	CB-CG-OD1	5.58	123.32	118.30
22	V	640	LEU	CB-CG-CD2	5.57	120.46	111.00
29	Y	14	DG	C4-N9-C1'	-5.56	119.27	126.50
29	Y	14	DG	C8-N9-C1'	5.56	134.23	127.00
22	V	571	TYR	CG-CD2-CE2	-5.56	116.86	121.30
14	N	325	GLY	N-CA-C	5.55	126.99	113.10
23	W	334	ARG	NE-CZ-NH2	-5.55	117.52	120.30
23	W	207	TYR	CA-CB-CG	5.54	123.93	113.40
22	V	325	ARG	NE-CZ-NH1	5.54	123.07	120.30
23	W	141	TYR	CG-CD2-CE2	5.54	125.73	121.30
29	Y	23	DT	N1-C1'-C2'	5.52	123.10	112.60
23	W	177	LEU	CB-CG-CD1	5.52	120.38	111.00
22	V	419	ARG	NH1-CZ-NH2	-5.51	113.33	119.40
22	V	608	SER	O-C-N	-5.51	113.88	122.70
23	W	258	ARG	NE-CZ-NH1	5.51	123.06	120.30
22	V	393	THR	O-C-N	-5.51	113.89	122.70
23	W	616	ARG	NE-CZ-NH2	5.51	123.05	120.30
22	V	634	ARG	CD-NE-CZ	5.50	131.30	123.60
28	X	80	DC	O4'-C4'-C3'	-5.49	102.30	104.50
22	V	679	PHE	CG-CD1-CE1	-5.49	114.76	120.80
9	I	85	PRO	N-CA-C	5.48	126.36	112.10
23	W	625	TYR	CZ-CE2-CD2	-5.48	114.87	119.80
24	0	65	VAL	CA-CB-CG1	5.47	119.11	110.90
22	V	655	TYR	CB-CG-CD1	5.47	124.28	121.00
26	2	61	PHE	CB-CG-CD2	-5.47	116.97	120.80
22	V	362	LEU	CB-CG-CD1	-5.47	101.70	111.00
22	V	289	TYR	CG-CD2-CE2	-5.46	116.93	121.30
1	A	484	LEU	CB-CG-CD2	-5.46	101.71	111.00
23	W	196	ARG	CD-NE-CZ	5.45	131.22	123.60
29	Y	33	DT	N3-C2-O2	-5.44	119.03	122.30
29	Y	17	DG	P-O3'-C3'	5.44	126.23	119.70
22	V	382	SER	N-CA-CB	-5.44	102.34	110.50
22	V	319	TYR	CB-CG-CD1	-5.43	117.74	121.00
23	W	224	GLU	OE1-CD-OE2	-5.43	116.78	123.30
23	W	631	ARG	NH1-CZ-NH2	-5.43	113.42	119.40
9	I	84	HIS	N-CA-C	5.43	125.66	111.00
23	W	595	ILE	CB-CA-C	5.42	122.45	111.60
23	W	253	ARG	NH1-CZ-NH2	-5.42	113.43	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	V	702	ALA	N-CA-CB	-5.42	102.52	110.10
23	W	205	VAL	CA-CB-CG1	5.41	119.01	110.90
23	W	207	TYR	CB-CG-CD2	-5.41	117.76	121.00
22	V	272	VAL	CA-CB-CG2	-5.40	102.80	110.90
22	V	479	ASP	CB-CG-OD2	5.40	123.16	118.30
23	W	285	TYR	CB-CG-CD1	-5.39	117.76	121.00
23	W	162	ASP	CB-CG-OD2	5.39	123.15	118.30
23	W	690	ARG	CD-NE-CZ	5.39	131.15	123.60
28	X	65	DG	C4'-C3'-C2'	-5.39	98.25	103.10
29	Y	29	DC	O4'-C4'-C3'	-5.38	102.35	104.50
23	W	540	THR	O-C-N	-5.38	114.10	122.70
28	X	74	DT	O4'-C1'-N1	5.37	111.76	108.00
22	V	391	ARG	NE-CZ-NH2	5.37	122.98	120.30
22	V	703	PHE	CG-CD1-CE1	-5.37	114.90	120.80
2	B	529	MET	CB-CG-SD	5.36	128.47	112.40
23	W	663	CYS	CA-CB-SG	-5.36	104.36	114.00
24	0	125	ARG	NE-CZ-NH2	-5.35	117.62	120.30
23	W	33	ASP	CB-CG-OD2	5.35	123.12	118.30
23	W	287	ARG	NH1-CZ-NH2	-5.35	113.52	119.40
2	B	162	LEU	CB-CG-CD1	-5.35	101.91	111.00
29	Y	34	DC	C4'-C3'-C2'	-5.35	98.29	103.10
2	B	44	LEU	CB-CG-CD1	-5.34	101.92	111.00
29	Y	29	DC	N3-C2-O2	-5.34	118.16	121.90
13	M	87	GLY	C-N-CA	-5.33	108.37	121.70
22	V	560	VAL	CA-CB-CG2	5.33	118.89	110.90
5	E	63	ALA	N-CA-C	5.32	125.37	111.00
22	V	571	TYR	CB-CG-CD1	-5.32	117.81	121.00
1	A	473	ARG	CG-CD-NE	-5.32	100.64	111.80
29	Y	11	DT	O4'-C4'-C3'	5.32	109.19	106.00
26	2	35	TYR	CB-CA-C	5.31	121.03	110.40
23	W	286	ARG	NH1-CZ-NH2	-5.31	113.56	119.40
24	0	90	TYR	CB-CG-CD1	5.31	124.19	121.00
28	X	61	DA	O4'-C4'-C3'	5.31	109.18	106.00
24	0	58	MET	O-C-N	5.28	131.15	122.70
2	B	964	ASP	CB-CG-OD1	-5.28	113.55	118.30
23	W	280	ARG	NE-CZ-NH2	5.28	122.94	120.30
24	0	213	ARG	NH1-CZ-NH2	-5.27	113.60	119.40
23	W	623	VAL	CG1-CB-CG2	-5.26	102.48	110.90
23	W	449	GLU	OE1-CD-OE2	-5.26	116.99	123.30
28	X	81	DG	C4'-C3'-C2'	-5.25	98.37	103.10
29	Y	34	DC	P-O3'-C3'	-5.25	113.39	119.70
1	A	546	ARG	NE-CZ-NH2	5.25	122.92	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	0	64	VAL	CA-CB-CG1	5.24	118.76	110.90
26	2	389	ASP	CB-CG-OD1	-5.24	113.58	118.30
24	0	207	VAL	CA-CB-CG1	5.24	118.76	110.90
22	V	478	VAL	CA-CB-CG2	-5.22	103.06	110.90
22	V	678	ARG	NE-CZ-NH2	5.22	122.91	120.30
13	M	87	GLY	N-CA-C	5.22	126.14	113.10
29	Y	19	DC	P-O5'-C5'	5.22	129.25	120.90
20	T	154	LYS	N-CA-C	5.22	125.08	111.00
28	X	65	DG	N1-C6-O6	-5.21	116.78	119.90
2	B	162	LEU	CA-CB-CG	5.20	127.26	115.30
22	V	666	ASP	CB-CG-OD1	-5.20	113.62	118.30
24	0	131	LEU	CB-CG-CD1	5.20	119.83	111.00
23	W	686	ARG	NE-CZ-NH2	-5.19	117.70	120.30
2	B	758	LEU	CA-CB-CG	-5.19	103.36	115.30
22	V	325	ARG	CD-NE-CZ	5.18	130.86	123.60
23	W	617	ALA	N-CA-CB	5.18	117.35	110.10
1	A	567	LEU	CA-CB-CG	5.17	127.19	115.30
29	Y	28	DT	C6-N1-C1'	5.17	128.16	120.40
23	W	253	ARG	NE-CZ-NH2	5.17	122.89	120.30
24	0	90	TYR	CZ-CE2-CD2	5.17	124.45	119.80
23	W	468	PRO	CA-N-CD	-5.16	104.27	111.50
22	V	250	ASP	CB-CG-OD1	5.16	122.94	118.30
22	V	434	GLU	OE1-CD-OE2	5.16	129.49	123.30
23	W	461	LEU	CA-CB-CG	5.16	127.17	115.30
16	P	232	LEU	CA-CB-CG	5.16	127.16	115.30
26	2	457	ARG	NE-CZ-NH1	5.16	122.88	120.30
28	X	64	DC	O4'-C1'-C2'	-5.16	101.78	105.90
23	W	24	TYR	CB-CG-CD2	-5.14	117.92	121.00
1	A	502	ASN	N-CA-CB	-5.14	101.35	110.60
23	W	143	ARG	NH1-CZ-NH2	-5.14	113.75	119.40
23	W	439	ASP	CB-CG-OD2	5.13	122.92	118.30
29	Y	31	DG	O4'-C4'-C3'	5.13	109.08	106.00
14	N	326	GLN	N-CA-C	5.12	124.84	111.00
23	W	283	ASP	CB-CG-OD2	5.12	122.91	118.30
22	V	362	LEU	CB-CG-CD2	5.12	119.70	111.00
24	0	62	TYR	CB-CG-CD1	5.12	124.07	121.00
22	V	415	HIS	CG-CD2-NE2	-5.12	99.48	109.20
22	V	332	ARG	CA-CB-CG	5.11	124.65	113.40
2	B	974	SER	N-CA-CB	-5.11	102.83	110.50
19	S	166	ARG	NE-CZ-NH1	5.11	122.86	120.30
23	W	714	VAL	CA-CB-CG2	5.11	118.56	110.90
22	V	679	PHE	CB-CG-CD1	-5.11	117.23	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	V	398	ASP	CB-CG-OD1	5.10	122.89	118.30
23	W	636	ARG	CD-NE-CZ	5.10	130.74	123.60
23	W	600	ALA	N-CA-CB	-5.10	102.97	110.10
1	A	133	SER	N-CA-C	5.09	124.75	111.00
26	2	392	ARG	NE-CZ-NH1	5.08	122.84	120.30
22	V	644	LEU	CB-CG-CD2	-5.08	102.37	111.00
23	W	288	LEU	O-C-N	-5.07	114.59	122.70
22	V	289	TYR	CZ-CE2-CD2	5.07	124.36	119.80
22	V	344	ALA	CB-CA-C	5.07	117.70	110.10
22	V	289	TYR	CB-CG-CD2	-5.06	117.96	121.00
22	V	378	PHE	CB-CG-CD2	-5.06	117.26	120.80
28	X	77	DC	O4'-C1'-N1	-5.06	104.46	108.00
28	X	73	DG	C1'-O4'-C4'	-5.05	105.05	110.10
23	W	94	TYR	CB-CG-CD2	5.05	124.03	121.00
23	W	676	LEU	CB-CG-CD2	5.05	119.59	111.00
22	V	607	ILE	CA-CB-CG1	5.05	120.59	111.00
24	0	228	TYR	CB-CG-CD2	-5.05	117.97	121.00
23	W	599	VAL	CA-CB-CG1	5.04	118.47	110.90
28	X	62	DG	O4'-C4'-C3'	5.04	109.03	106.00
24	0	224	ASP	N-CA-CB	-5.04	101.53	110.60
23	W	463	PRO	N-CA-CB	5.04	109.34	103.30
1	A	375	ILE	CG1-CB-CG2	-5.02	100.35	111.40
23	W	87	LEU	CB-CA-C	5.02	119.74	110.20
27	3	210	THR	CA-CB-CG2	-5.02	105.37	112.40
25	1	16	MET	CG-SD-CE	5.02	108.23	100.20
1	A	641	CYS	CA-CB-SG	-5.02	104.97	114.00
2	B	981	LEU	CA-CB-CG	5.02	126.84	115.30
28	X	68	DC	O4'-C4'-C3'	5.01	109.01	106.00
23	W	61	ARG	NE-CZ-NH1	5.01	122.81	120.30
27	3	218	PRO	N-CA-C	-5.01	99.08	112.10
23	W	66	GLU	C-N-CA	5.00	134.20	121.70

There are no chirality outliers.

All (66) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
25	1	17	LYS	Mainchain
26	2	389	ASP	Sidechain,Mainchain
26	2	399	ASP	Sidechain
26	2	403	PHE	Mainchain,Peptide
26	2	406	GLY	Peptide
26	2	409	TYR	Sidechain

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Mol	Chain	Res	Type	Group
26	2	425	ALA	Mainchain
1	A	1086	MET	Peptide
2	B	416	ARG	Sidechain
2	B	525	ASN	Peptide
7	G	151	ARG	Sidechain
14	N	355	ASP	Peptide
14	N	371	ILE	Peptide
16	P	158	SER	Peptide
17	Q	125	ALA	Peptide
18	R	215	GLU	Mainchain
18	R	221	ARG	Mainchain
18	R	222	SER	Peptide
18	R	228	MET	Peptide
18	R	229	ASP	Sidechain
18	R	235	GLU	Sidechain
19	S	148	PRO	Peptide
20	T	123	ASN	Peptide
20	T	177	ARG	Peptide
22	V	247	ASP	Mainchain
22	V	251	PHE	Sidechain
22	V	319	TYR	Sidechain
22	V	378	PHE	Sidechain
22	V	417	THR	Peptide
22	V	489	TYR	Sidechain
22	V	503	ALA	Peptide
22	V	519	TYR	Sidechain
22	V	530	ARG	Sidechain
22	V	534	TYR	Sidechain
22	V	674	THR	Mainchain
22	V	679	PHE	Sidechain
22	V	703	PHE	Sidechain
23	W	104	PHE	Sidechain
23	W	175	TYR	Sidechain
23	W	197	TYR	Sidechain
23	W	206	VAL	Mainchain
23	W	208	SER	Mainchain
23	W	211	TYR	Sidechain
23	W	282	ARG	Sidechain
23	W	286	ARG	Sidechain
23	W	293	ARG	Sidechain
23	W	409	THR	Peptide
23	W	423	ASP	Peptide

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Mol	Chain	Res	Type	Group
23	W	553	TYR	Sidechain
23	W	614	TYR	Sidechain
23	W	616	ARG	Sidechain
23	W	641	ARG	Sidechain
23	W	669	ARG	Sidechain
23	W	674	TYR	Sidechain
23	W	719	TYR	Sidechain
23	W	72	TYR	Sidechain
28	X	60	DG	Sidechain
28	X	65	DG	Sidechain
28	X	66	DA	Sidechain
28	X	72	DC	Sidechain
29	Y	23	DT	Sidechain
29	Y	24	DC	Sidechain
29	Y	33	DT	Sidechain
29	Y	34	DC	Sidechain

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	534	0
2	B	9317	0	9308	358	0
3	C	2213	0	2153	85	0
4	D	1062	0	1042	10	0
5	E	1723	0	1745	70	0
6	F	689	0	715	19	0
7	G	1351	0	1358	25	0
8	H	1205	0	1168	54	0
9	I	1013	0	930	68	0
10	J	533	0	553	35	0
11	K	937	0	959	21	0
12	L	388	0	393	37	0
13	M	2391	0	2410	133	0
14	N	930	0	888	24	0
15	O	806	0	818	16	0
16	P	1462	0	1549	54	0
17	Q	1484	0	1494	153	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	R	1357	0	1380	190	0
19	S	1138	0	1103	37	0
20	T	1788	0	1819	87	0
21	U	1343	0	1337	62	0
22	V	3855	0	3871	149	0
23	W	5348	0	5372	123	0
24	0	1479	0	1524	40	0
25	1	491	0	507	219	0
26	2	2196	0	2206	568	0
27	3	1526	0	1561	467	0
28	X	1710	0	941	50	0
29	Y	1681	0	932	52	0
30	A	2	0	0	0	0
31	A	2	0	0	0	0
31	B	1	0	0	0	0
31	C	1	0	0	0	0
31	I	2	0	0	0	0
31	J	1	0	0	0	0
31	L	1	0	0	0	0
31	M	1	0	0	0	0
31	Q	1	0	0	0	0
31	U	1	0	0	0	0
All	All	62944	0	61643	3082	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 25.

All (3082) 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)
27:3:59:VAL:HG12	27:3:71:TYR:CD1	1.24	1.67
22:V:516:PRO:CG	25:1:15:ALA:HB3	1.19	1.60
22:V:315:VAL:HG13	23:W:500:ASP:CB	1.21	1.55
24:0:54:ARG:HG3	27:3:182:PHE:CE1	1.42	1.54
27:3:59:VAL:CG1	27:3:71:TYR:HD1	1.16	1.53
26:2:31:LEU:HD11	27:3:33:THR:CB	1.39	1.53
22:V:321:GLU:CG	23:W:499:ASN:HB3	1.39	1.53
22:V:516:PRO:HG3	25:1:15:ALA:CB	1.10	1.51
22:V:315:VAL:CG1	23:W:500:ASP:HB2	1.01	1.49
26:2:31:LEU:HD11	27:3:33:THR:CG2	1.42	1.48
18:R:195:PRO:HG2	18:R:199:LYS:CB	1.01	1.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:195:PRO:CG	18:R:199:LYS:CB	1.86	1.47
16:P:206:GLU:CG	16:P:236:LYS:NZ	1.77	1.47
17:Q:23:ARG:NH2	18:R:206:LYS:CA	1.75	1.46
26:2:117:ASN:ND2	27:3:108:ASN:CB	1.76	1.46
5:E:64:HIS:CD2	5:E:69:THR:H	1.30	1.46
26:2:117:ASN:HD21	27:3:108:ASN:CB	1.27	1.46
1:A:1158:LEU:HD11	1:A:1308:TYR:CD2	1.50	1.45
17:Q:23:ARG:NH2	18:R:206:LYS:CB	1.76	1.44
29:Y:24:DC:H2"	29:Y:25:DT:C7	1.49	1.42
26:2:28:PRO:N	27:3:25:GLN:HA	1.31	1.42
26:2:117:ASN:CG	27:3:108:ASN:HB2	1.39	1.39
1:A:926:ASN:CB	1:A:931:ARG:NH1	1.86	1.39
17:Q:113:ARG:NH2	18:R:218:LYS:HE3	1.34	1.38
22:V:325:ARG:NH2	23:W:499:ASN:HB2	1.05	1.37
26:2:29:GLY:N	27:3:25:GLN:HG3	1.38	1.37
26:2:31:LEU:HD21	27:3:33:THR:N	1.34	1.37
17:Q:20:TYR:CE2	18:R:210:PHE:CB	1.93	1.37
24:0:54:ARG:CG	27:3:182:PHE:HE1	1.35	1.37
22:V:523:VAL:HG11	25:1:20:LEU:CD2	1.50	1.37
1:A:926:ASN:HB3	1:A:931:ARG:NH1	1.04	1.37
17:Q:112:ARG:CD	18:R:237:LEU:HD11	1.54	1.36
9:I:103:ARG:O	9:I:105:GLU:N	1.59	1.36
22:V:321:GLU:OE1	23:W:499:ASN:N	1.57	1.35
26:2:117:ASN:OD1	27:3:108:ASN:ND2	1.57	1.35
1:A:201:GLU:HA	1:A:212:LYS:O	1.24	1.34
5:E:64:HIS:CD2	5:E:69:THR:N	1.95	1.34
26:2:118:LEU:CD2	27:3:39:ASP:OD1	1.75	1.33
22:V:366:ASN:HD21	22:V:613:THR:CG2	1.41	1.33
26:2:30:VAL:HG23	27:3:25:GLN:CB	1.57	1.33
17:Q:23:ARG:NH2	18:R:206:LYS:HB3	1.35	1.32
1:A:1110:ALA:CB	21:U:256:THR:HG21	1.59	1.32
18:R:195:PRO:CG	18:R:199:LYS:HB3	1.50	1.32
26:2:118:LEU:HD22	27:3:39:ASP:OD1	1.16	1.31
22:V:615:PHE:O	22:V:617:LEU:N	1.60	1.31
17:Q:113:ARG:NH2	18:R:218:LYS:CE	1.93	1.31
25:1:1:MET:O	26:2:413:LEU:HG	1.28	1.30
16:P:297:LYS:HB3	16:P:298:PRO:CD	1.47	1.30
16:P:298:PRO:O	16:P:300:ILE:HG12	1.14	1.30
1:A:133:SER:OG	1:A:136:GLN:HB2	1.23	1.30
1:A:263:ALA:O	1:A:264:VAL:CG1	1.80	1.29
17:Q:112:ARG:NE	18:R:237:LEU:HD11	1.45	1.29

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:0:165:ARG:NH1	24:0:192:ALA:O	1.66	1.29
26:2:118:LEU:HD21	27:3:39:ASP:O	1.23	1.29
22:V:321:GLU:CD	23:W:499:ASN:HB3	1.49	1.29
16:P:206:GLU:HG3	16:P:236:LYS:NZ	1.35	1.28
8:H:85:ALA:O	8:H:87:GLN:N	1.63	1.28
1:A:263:ALA:CB	1:A:272:ASN:O	1.82	1.28
1:A:199:TYR:OH	13:M:93:PHE:CE2	1.79	1.28
17:Q:23:ARG:HH22	18:R:206:LYS:CB	1.34	1.27
26:2:28:PRO:N	27:3:25:GLN:CA	1.97	1.27
12:L:17:TYR:CE1	12:L:46:LYS:HG3	1.70	1.27
22:V:325:ARG:NH2	23:W:499:ASN:CB	1.97	1.26
1:A:1158:LEU:HD21	1:A:1308:TYR:CE2	1.70	1.26
5:E:64:HIS:CE1	5:E:69:THR:O	1.87	1.26
24:0:97:ASP:O	27:3:208:ASP:HB2	1.10	1.26
1:A:926:ASN:HB3	1:A:931:ARG:CZ	1.66	1.25
1:A:263:ALA:HB1	1:A:272:ASN:O	1.13	1.25
26:2:30:VAL:CG2	27:3:25:GLN:HB3	1.66	1.25
1:A:932:ARG:HD2	1:A:943:LEU:CD2	1.66	1.24
17:Q:187:ILE:HD13	18:R:210:PHE:O	1.37	1.24
1:A:425:ASP:OD2	13:M:39:LEU:HD11	1.22	1.24
1:A:551:ARG:HD3	1:A:625:ASP:OD2	1.32	1.24
22:V:674:THR:HG23	26:2:392:ARG:NH2	1.53	1.24
8:H:74:GLU:O	8:H:75:TYR:CD1	1.90	1.23
18:R:195:PRO:CG	18:R:199:LYS:HB2	1.54	1.23
3:C:5:ASN:O	3:C:7:PRO:HD3	1.33	1.23
23:W:59:TYR:CZ	23:W:62:ALA:CB	2.21	1.23
17:Q:20:TYR:CE2	18:R:210:PHE:HB3	1.08	1.22
13:M:94:ASP:OD2	13:M:97:GLY:O	1.55	1.22
1:A:932:ARG:CD	1:A:943:LEU:HD21	1.68	1.22
27:3:58:ALA:N	27:3:71:TYR:OH	1.73	1.21
26:2:31:LEU:CD1	27:3:33:THR:HB	1.69	1.21
23:W:209:TYR:OH	23:W:233:PHE:HA	1.38	1.21
27:3:59:VAL:CG1	27:3:71:TYR:CD1	1.98	1.20
3:C:6:GLN:HB2	11:K:104:ARG:NH1	1.57	1.20
22:V:516:PRO:CG	25:1:15:ALA:CB	1.90	1.20
25:1:59:GLU:OE2	26:2:402:ARG:NH2	1.75	1.20
13:M:47:ASP:O	13:M:49:GLY:N	1.73	1.19
27:3:66:GLU:HA	27:3:132:LEU:HD12	1.22	1.19
16:P:297:LYS:HB3	16:P:298:PRO:HD3	1.19	1.19
17:Q:23:ARG:HH22	18:R:206:LYS:CA	1.45	1.19
2:B:92:TYR:HA	20:T:141:LEU:HD11	1.18	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:366:ASN:ND2	22:V:613:THR:CG2	2.05	1.18
1:A:132:LYS:O	1:A:133:SER:HB2	1.43	1.18
22:V:516:PRO:HB3	25:1:15:ALA:HB1	1.24	1.18
1:A:622:SER:O	1:A:624:GLY:N	1.77	1.18
5:E:46:ASP:O	5:E:48:PRO:HD3	1.42	1.18
26:2:31:LEU:CD1	27:3:33:THR:CG2	2.21	1.18
23:W:59:TYR:CZ	23:W:62:ALA:HB1	1.77	1.17
1:A:608:THR:C	1:A:610:PRO:HD2	1.64	1.17
18:R:151:LEU:CD1	18:R:163:LEU:HD21	1.75	1.17
22:V:428:GLU:O	22:V:433:GLN:HA	1.42	1.17
16:P:298:PRO:O	16:P:300:ILE:CG1	1.93	1.17
17:Q:180:PHE:CZ	18:R:213:ASP:CA	2.26	1.17
25:1:28:ALA:HB1	25:1:31:LYS:HD2	1.27	1.16
26:2:117:ASN:ND2	27:3:108:ASN:HB2	0.85	1.16
17:Q:180:PHE:CZ	18:R:213:ASP:HA	1.79	1.16
25:1:2:VAL:CG1	26:2:456:LYS:HG2	1.74	1.16
17:Q:23:ARG:NH2	18:R:206:LYS:C	1.77	1.16
22:V:325:ARG:HH22	23:W:499:ASN:CB	1.56	1.16
13:M:11:PRO:O	13:M:12:ARG:CG	1.92	1.16
3:C:6:GLN:CB	11:K:104:ARG:HH12	1.58	1.16
21:U:256:THR:OG1	21:U:272:THR:HG21	1.45	1.15
13:M:11:PRO:O	13:M:12:ARG:HG2	1.01	1.15
1:A:199:TYR:OH	13:M:93:PHE:CZ	1.96	1.15
26:2:30:VAL:HB	27:3:25:GLN:O	1.46	1.15
1:A:425:ASP:OD2	13:M:39:LEU:CD1	1.94	1.15
18:R:164:GLY:CA	18:R:203:PHE:CZ	2.30	1.15
27:3:57:LEU:O	27:3:71:TYR:HE2	1.27	1.14
25:1:2:VAL:HG13	26:2:422:LEU:HD11	1.20	1.14
23:W:419:GLU:HB3	23:W:420:PRO:CD	1.76	1.14
24:0:54:ARG:CG	27:3:182:PHE:CE1	2.17	1.13
28:X:15:DA:N6	29:Y:79:DC:H42	1.45	1.13
27:3:59:VAL:HG13	27:3:70:LEU:HB2	1.27	1.13
25:1:1:MET:CG	26:2:413:LEU:HB3	1.76	1.13
1:A:263:ALA:O	1:A:264:VAL:HG13	0.95	1.13
17:Q:105:TYR:CE1	18:R:234:GLU:CD	2.22	1.13
18:R:164:GLY:HA2	18:R:203:PHE:CZ	1.83	1.13
3:C:212:ASP:O	3:C:214:ASP:N	1.82	1.13
22:V:321:GLU:OE1	23:W:499:ASN:CA	1.96	1.12
26:2:160:LEU:HD23	26:2:206:LEU:HD21	1.25	1.12
22:V:321:GLU:OE1	23:W:499:ASN:CB	1.97	1.12
22:V:321:GLU:HG2	23:W:499:ASN:HB3	1.28	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:3:33:THR:HG23	27:3:36:LYS:H	1.13	1.12
1:A:1113:SER:HB3	1:A:1309:MET:SD	1.88	1.12
23:W:59:TYR:CE2	23:W:62:ALA:CB	2.32	1.12
1:A:1158:LEU:HD21	1:A:1308:TYR:HE2	0.97	1.12
27:3:208:ASP:OD1	27:3:209:ILE:N	1.82	1.11
27:3:59:VAL:N	27:3:71:TYR:CE1	2.17	1.11
21:U:257:GLN:NE2	21:U:270:ASN:OD1	1.83	1.11
26:2:42:LEU:HD21	26:2:55:TRP:HB2	1.20	1.11
2:B:90:GLN:NE2	20:T:141:LEU:HA	1.63	1.11
26:2:171:VAL:HG22	26:2:213:TRP:HA	1.27	1.11
1:A:927:GLU:O	1:A:931:ARG:NH2	1.83	1.11
26:2:211:GLN:HG3	26:2:257:SER:HB3	1.29	1.11
25:1:9:LEU:HD13	25:1:48:GLU:HA	1.32	1.11
3:C:133:ARG:HA	3:C:136:ASP:OD2	1.51	1.11
12:L:17:TYR:HE1	12:L:46:LYS:CG	1.63	1.11
16:P:206:GLU:HB3	16:P:207:PRO:HD3	1.33	1.11
25:1:5:LEU:CD2	26:2:408:LEU:HD13	1.80	1.10
25:1:5:LEU:HD11	26:2:408:LEU:HB3	1.17	1.10
16:P:206:GLU:HB3	16:P:207:PRO:CD	1.81	1.10
29:Y:24:DC:C2'	29:Y:25:DT:H71	1.80	1.10
25:1:13:ASP:CG	25:1:14:PRO:HD2	1.72	1.10
16:P:206:GLU:CG	16:P:236:LYS:HZ2	1.44	1.10
1:A:1110:ALA:HB2	21:U:256:THR:HG21	1.23	1.10
26:2:31:LEU:CD1	27:3:33:THR:CB	2.27	1.09
1:A:1290:SER:HB3	2:B:250:SER:HB3	1.32	1.09
25:1:2:VAL:HG11	26:2:456:LYS:CG	1.81	1.09
25:1:18:GLN:HB2	25:1:44:PHE:CE2	1.86	1.09
22:V:516:PRO:CB	25:1:15:ALA:HB1	1.81	1.09
22:V:321:GLU:CD	23:W:499:ASN:CB	2.19	1.09
27:3:49:LEU:HB3	27:3:101:TYR:HB3	1.14	1.09
2:B:91:ILE:HG23	20:T:141:LEU:HD12	1.33	1.09
22:V:315:VAL:CG1	23:W:500:ASP:CB	1.94	1.09
1:A:930:LEU:HB3	1:A:934:LEU:HB2	1.35	1.08
26:2:192:GLU:HG3	26:2:193:PRO:HD2	1.34	1.08
21:U:256:THR:CB	21:U:272:THR:CG2	2.31	1.08
25:1:5:LEU:HD21	26:2:408:LEU:CD1	1.82	1.08
27:3:59:VAL:HB	27:3:71:TYR:CE1	1.88	1.08
16:P:206:GLU:CB	16:P:207:PRO:CD	2.32	1.08
27:3:205:GLN:O	27:3:208:ASP:OD1	1.70	1.08
2:B:225:LEU:C	2:B:227:ASN:H	1.52	1.08
27:3:137:LEU:HB3	27:3:180:VAL:HG11	1.34	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:104:ALA:O	9:I:106:ASP:N	1.86	1.08
29:Y:24:DC:C2'	29:Y:25:DT:C7	2.31	1.08
23:W:419:GLU:CB	23:W:420:PRO:HD2	1.79	1.08
1:A:1158:LEU:CD1	1:A:1308:TYR:HD2	1.66	1.07
16:P:206:GLU:HG2	16:P:236:LYS:HZ3	0.94	1.07
22:V:516:PRO:HG2	22:V:706:LYS:HZ3	1.14	1.07
26:2:159:VAL:HG13	26:2:161:HIS:H	1.16	1.07
2:B:880:LEU:O	2:B:881:GLU:HB2	1.27	1.07
22:V:516:PRO:HG2	22:V:706:LYS:NZ	1.70	1.07
27:3:57:LEU:C	27:3:71:TYR:OH	1.93	1.07
1:A:1158:LEU:CD1	1:A:1308:TYR:CD2	2.37	1.07
1:A:930:LEU:HD22	1:A:934:LEU:HD13	1.07	1.07
21:U:256:THR:O	21:U:272:THR:HG22	1.54	1.07
12:L:17:TYR:HE1	12:L:46:LYS:HG3	0.94	1.07
17:Q:112:ARG:NE	18:R:237:LEU:CD1	2.15	1.06
18:R:225:VAL:HG12	18:R:227:SER:HB2	1.10	1.06
22:V:516:PRO:CG	22:V:706:LYS:HZ3	1.67	1.06
25:1:2:VAL:HG11	26:2:456:LYS:HG2	1.09	1.06
1:A:132:LYS:O	1:A:133:SER:CB	2.04	1.06
22:V:523:VAL:HG11	25:1:20:LEU:HD21	1.11	1.06
24:0:54:ARG:HB2	27:3:209:ILE:HG23	1.36	1.05
27:3:57:LEU:O	27:3:71:TYR:CE2	2.10	1.05
26:2:31:LEU:HD11	27:3:33:THR:HG22	1.37	1.05
24:0:97:ASP:O	27:3:208:ASP:CB	2.02	1.05
25:1:5:LEU:HD12	26:2:409:TYR:O	1.56	1.05
22:V:516:PRO:CG	22:V:706:LYS:NZ	2.18	1.05
26:2:28:PRO:N	27:3:25:GLN:C	2.10	1.05
22:V:321:GLU:CG	23:W:499:ASN:CB	2.35	1.05
22:V:674:THR:HG23	26:2:392:ARG:CZ	1.85	1.05
16:P:297:LYS:CB	16:P:298:PRO:CD	2.35	1.04
25:1:1:MET:CB	26:2:413:LEU:HB3	1.87	1.04
18:R:195:PRO:HG2	18:R:199:LYS:CA	1.85	1.04
1:A:1110:ALA:HB1	21:U:256:THR:HG21	1.38	1.04
21:U:256:THR:HB	21:U:272:THR:CG2	1.87	1.04
18:R:164:GLY:HA3	18:R:203:PHE:HZ	1.23	1.04
17:Q:180:PHE:CE1	18:R:212:VAL:O	2.10	1.04
21:U:227:GLU:O	21:U:228:MET:HB3	1.50	1.04
2:B:92:TYR:CA	20:T:141:LEU:HD11	1.80	1.04
17:Q:180:PHE:CZ	18:R:212:VAL:O	2.10	1.04
26:2:31:LEU:HD11	27:3:33:THR:HB	1.15	1.04
1:A:1112:VAL:O	21:U:252:LYS:HB3	1.57	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:256:THR:OG1	21:U:272:THR:CG2	2.06	1.04
22:V:426:VAL:O	22:V:427:MET:O	1.76	1.04
22:V:612:ASP:OD2	22:V:635:GLN:OE1	1.72	1.03
18:R:154:LEU:HD23	18:R:163:LEU:HD23	1.37	1.03
22:V:516:PRO:CB	25:1:15:ALA:CB	2.36	1.03
25:1:34:ILE:HG12	25:1:50:VAL:HG11	1.39	1.03
5:E:64:HIS:NE2	5:E:69:THR:N	2.05	1.03
17:Q:112:ARG:HD3	18:R:237:LEU:HD11	1.35	1.03
24:0:54:ARG:NE	27:3:182:PHE:CE1	2.26	1.03
26:2:81:LYS:HE3	26:2:93:LEU:HD21	1.40	1.03
1:A:47:THR:HG23	1:A:53:LYS:HG2	1.05	1.02
22:V:523:VAL:HG11	25:1:20:LEU:HD23	1.37	1.02
22:V:366:ASN:HD21	22:V:613:THR:HG22	1.19	1.02
25:1:4:VAL:HG12	26:2:411:GLN:O	1.55	1.02
24:0:54:ARG:CD	27:3:182:PHE:HE1	1.71	1.02
1:A:206:ASN:O	1:A:207:GLU:HB2	1.59	1.02
27:3:59:VAL:HB	27:3:71:TYR:HE1	1.24	1.02
26:2:234:LEU:HD21	26:2:237:LEU:HD12	1.36	1.02
27:3:196:LEU:HD21	27:3:223:LEU:HD23	1.42	1.01
23:W:59:TYR:CE2	23:W:62:ALA:HB3	1.94	1.01
23:W:419:GLU:HB3	23:W:420:PRO:HD2	1.04	1.01
2:B:90:GLN:HE21	20:T:141:LEU:HA	0.85	1.01
1:A:609:HIS:N	1:A:610:PRO:CD	2.24	1.01
1:A:1110:ALA:CB	21:U:256:THR:CG2	2.39	1.00
26:2:28:PRO:CD	27:3:25:GLN:HA	1.90	1.00
26:2:199:ALA:HB3	26:2:202:GLN:HE22	1.22	1.00
22:V:515:SER:HB3	22:V:539:ASN:HD21	1.26	1.00
1:A:1290:SER:CB	2:B:250:SER:HB3	1.89	1.00
17:Q:184:ILE:HD13	18:R:218:LYS:HZ1	1.25	1.00
23:W:209:TYR:OH	23:W:233:PHE:CA	2.09	1.00
3:C:134:ASN:N	3:C:136:ASP:OD1	1.93	1.00
24:0:77:LYS:O	24:0:79:ASN:N	1.93	1.00
27:3:58:ALA:CA	27:3:71:TYR:CZ	2.43	1.00
1:A:535:MET:O	1:A:669:TYR:OH	1.80	0.99
16:P:206:GLU:HG2	16:P:236:LYS:NZ	1.52	0.99
28:X:15:DA:H61	29:Y:79:DC:H42	1.01	0.99
27:3:59:VAL:CB	27:3:71:TYR:CE1	2.44	0.99
16:P:206:GLU:HB2	16:P:207:PRO:HD2	1.45	0.99
29:Y:24:DC:C2	29:Y:25:DT:C4	2.51	0.99
2:B:92:TYR:HD1	20:T:141:LEU:HD21	1.28	0.99
1:A:427:ILE:HG12	13:M:38:GLY:O	1.63	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:63:ALA:HB3	10:J:64:PRO:HD3	1.41	0.98
22:V:315:VAL:HG11	23:W:500:ASP:HB2	1.42	0.98
17:Q:105:TYR:CD1	18:R:234:GLU:OE1	2.16	0.98
1:A:522:PRO:HA	1:A:666:ARG:HE	1.25	0.98
5:E:64:HIS:CE1	5:E:69:THR:C	2.37	0.98
28:X:15:DA:H61	29:Y:79:DC:N4	1.60	0.98
26:2:117:ASN:CG	27:3:108:ASN:CB	2.20	0.98
1:A:930:LEU:HD22	1:A:934:LEU:CD1	1.93	0.98
2:B:880:LEU:O	2:B:881:GLU:CB	2.08	0.98
5:E:64:HIS:NE2	5:E:69:THR:CA	2.27	0.98
18:R:195:PRO:CB	18:R:199:LYS:CB	2.42	0.97
27:3:173:GLN:HA	27:3:176:ASN:HD21	1.28	0.97
26:2:118:LEU:CD2	27:3:39:ASP:O	2.12	0.97
22:V:516:PRO:HA	25:1:15:ALA:O	1.62	0.97
5:E:64:HIS:HE2	5:E:69:THR:CB	1.76	0.97
16:P:206:GLU:CG	16:P:236:LYS:HZ3	1.58	0.97
16:P:297:LYS:HB3	16:P:298:PRO:HD2	1.43	0.97
26:2:196:ILE:HD11	26:2:210:ALA:HB2	1.45	0.97
2:B:958:CYS:SG	2:B:959:GLU:N	2.37	0.97
27:3:165:LYS:HD2	27:3:195:VAL:HG22	1.44	0.97
18:R:164:GLY:HA3	18:R:203:PHE:CZ	1.95	0.97
22:V:523:VAL:CG1	25:1:20:LEU:CD2	2.43	0.97
1:A:930:LEU:CD2	1:A:934:LEU:HD13	1.93	0.97
26:2:176:ALA:HB1	26:2:178:LEU:HD13	1.47	0.96
27:3:148:ASN:HB2	27:3:157:MET:HE2	1.44	0.96
23:W:584:TYR:CD1	23:W:594:ALA:HB2	1.99	0.96
26:2:100:LEU:HD11	26:2:119:ARG:HG3	1.46	0.96
27:3:133:LEU:HD23	27:3:177:PHE:CD1	2.01	0.96
27:3:59:VAL:CB	27:3:71:TYR:CD1	2.48	0.96
23:W:59:TYR:CE1	23:W:62:ALA:HB1	2.01	0.96
13:M:182:ALA:HB1	20:T:152:ASN:OD1	1.66	0.96
23:W:209:TYR:HH	23:W:233:PHE:HA	1.31	0.95
26:2:211:GLN:HA	26:2:261:PHE:CZ	2.02	0.95
25:1:2:VAL:CG1	26:2:422:LEU:HD11	1.96	0.95
1:A:1158:LEU:CD2	1:A:1308:TYR:HE2	1.77	0.95
1:A:926:ASN:HB3	1:A:931:ARG:HH11	1.19	0.95
17:Q:105:TYR:CE1	18:R:234:GLU:OE2	2.17	0.95
25:1:18:GLN:HB2	25:1:44:PHE:HE2	1.26	0.95
2:B:225:LEU:O	2:B:227:ASN:N	2.00	0.95
26:2:118:LEU:HD11	27:3:43:VAL:CG2	1.95	0.95
26:2:35:TYR:CE1	26:2:62:LEU:HG	2.02	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:321:GLU:OE2	23:W:500:ASP:N	2.00	0.94
26:2:117:ASN:N	27:3:104:LEU:HD21	1.83	0.94
25:1:1:MET:HB3	26:2:413:LEU:CG	1.98	0.94
9:I:85:PRO:O	9:I:86:CYS:C	2.04	0.94
1:A:426:ARG:O	13:M:39:LEU:O	1.83	0.94
1:A:133:SER:OG	1:A:136:GLN:CB	2.16	0.94
13:M:94:ASP:O	13:M:96:PHE:N	2.01	0.94
9:I:102:ALA:O	9:I:104:ALA:N	2.00	0.94
21:U:256:THR:CB	21:U:272:THR:HG21	1.93	0.94
23:W:696:TRP:CD1	23:W:697:ILE:HG12	2.03	0.94
1:A:1158:LEU:HD11	1:A:1308:TYR:HD2	0.83	0.94
5:E:45:GLY:O	5:E:46:ASP:O	1.86	0.94
17:Q:113:ARG:HH22	18:R:218:LYS:HE3	1.25	0.94
2:B:645:GLU:OE1	2:B:649:ASN:ND2	2.00	0.94
5:E:64:HIS:HD2	5:E:69:THR:H	1.16	0.94
5:E:64:HIS:HD2	5:E:67:ASP:O	1.50	0.94
25:1:9:LEU:HD22	25:1:51:ASN:HD22	1.33	0.93
26:2:117:ASN:ND2	27:3:42:MET:HE1	1.83	0.93
2:B:91:ILE:CG2	20:T:141:LEU:HD12	1.97	0.93
22:V:515:SER:CB	22:V:539:ASN:HD21	1.80	0.93
27:3:187:GLN:HG3	27:3:189:ILE:HG12	1.51	0.93
21:U:256:THR:CB	21:U:272:THR:HG22	1.96	0.93
26:2:118:LEU:HD23	27:3:42:MET:HB2	1.50	0.93
17:Q:105:TYR:HE1	18:R:234:GLU:OE2	1.49	0.93
22:V:366:ASN:HD21	22:V:613:THR:HG23	1.31	0.93
22:V:631:GLY:O	22:V:632:SER:CB	2.14	0.93
26:2:29:GLY:CA	27:3:25:GLN:HG3	1.98	0.93
1:A:930:LEU:CB	1:A:934:LEU:HB2	1.99	0.93
1:A:1158:LEU:CD2	1:A:1308:TYR:CE2	2.51	0.93
16:P:205:ARG:O	16:P:206:GLU:O	1.86	0.93
8:H:85:ALA:C	8:H:87:GLN:H	1.70	0.93
26:2:177:GLN:HA	26:2:220:LEU:CD2	1.99	0.93
22:V:516:PRO:HB2	22:V:706:LYS:HZ1	1.32	0.93
27:3:190:LEU:HA	27:3:210:THR:HG22	1.50	0.92
26:2:31:LEU:CD2	27:3:33:THR:N	2.30	0.92
2:B:933:ASP:OD2	2:B:1050:ARG:NH2	2.02	0.92
22:V:516:PRO:CB	22:V:706:LYS:HZ1	1.81	0.92
25:1:13:ASP:OD2	25:1:17:LYS:HB3	1.69	0.92
27:3:11:LEU:HD22	27:3:160:ARG:HG2	1.51	0.92
22:V:321:GLU:CD	23:W:499:ASN:CA	2.37	0.92
27:3:165:LYS:HE3	27:3:200:SER:CB	2.00	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1110:ALA:HB2	21:U:256:THR:CG2	1.98	0.92
1:A:1112:VAL:O	21:U:252:LYS:CB	2.17	0.92
2:B:132:VAL:HG21	2:B:141:GLN:HG2	1.50	0.92
17:Q:112:ARG:CD	18:R:237:LEU:CD1	2.48	0.92
18:R:195:PRO:HG2	18:R:199:LYS:HB3	1.07	0.92
27:3:133:LEU:H	27:3:133:LEU:HD13	1.33	0.92
1:A:47:THR:HG23	1:A:53:LYS:CG	1.97	0.92
1:A:199:TYR:OH	13:M:93:PHE:HE2	1.35	0.92
25:1:8:VAL:HG11	25:1:45:VAL:CG1	1.99	0.91
26:2:29:GLY:H	27:3:25:GLN:HG3	1.13	0.91
1:A:355:MET:SD	2:B:1091:ARG:NH1	2.43	0.91
16:P:206:GLU:CB	16:P:207:PRO:HD2	1.98	0.91
18:R:154:LEU:CD2	18:R:163:LEU:HD23	2.00	0.91
5:E:64:HIS:HE1	5:E:69:THR:O	1.46	0.91
25:1:1:MET:HB3	26:2:413:LEU:HB3	1.52	0.91
10:J:64:PRO:C	10:J:66:GLU:H	1.71	0.91
26:2:159:VAL:HG22	26:2:160:LEU:HD12	1.51	0.91
26:2:81:LYS:CE	26:2:93:LEU:HD21	2.00	0.91
3:C:7:PRO:O	3:C:8:THR:OG1	1.87	0.91
22:V:325:ARG:HH21	23:W:499:ASN:HB2	1.32	0.91
24:0:54:ARG:HG3	27:3:182:PHE:CZ	2.05	0.91
27:3:137:LEU:CB	27:3:180:VAL:HG11	2.01	0.91
17:Q:23:ARG:HH21	18:R:206:LYS:CB	1.76	0.91
21:U:227:GLU:O	21:U:228:MET:HE2	1.70	0.91
1:A:197:GLU:OE1	13:M:93:PHE:CD2	2.24	0.91
18:R:195:PRO:CB	18:R:199:LYS:HB3	1.99	0.91
23:W:59:TYR:CE1	23:W:62:ALA:CB	2.52	0.90
1:A:263:ALA:HB1	1:A:272:ASN:C	1.91	0.90
21:U:227:GLU:O	21:U:228:MET:CE	2.19	0.90
23:W:430:ASN:HB3	23:W:431:PRO:HD2	1.54	0.90
27:3:165:LYS:HG3	27:3:203:LEU:HD12	1.52	0.90
27:3:58:ALA:HA	27:3:71:TYR:CE2	2.05	0.90
26:2:29:GLY:N	27:3:25:GLN:CG	2.32	0.90
26:2:81:LYS:HD2	26:2:89:LEU:HD21	1.52	0.90
17:Q:180:PHE:CE1	18:R:213:ASP:HA	2.07	0.90
1:A:609:HIS:N	1:A:610:PRO:HD2	1.83	0.90
3:C:212:ASP:C	3:C:214:ASP:H	1.74	0.89
1:A:1110:ALA:HB1	21:U:256:THR:CG2	2.01	0.89
22:V:315:VAL:HG13	23:W:500:ASP:CA	2.03	0.89
24:0:98:GLN:OE1	27:3:209:ILE:HA	1.70	0.89
17:Q:105:TYR:CD1	18:R:234:GLU:CD	2.45	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:544:ALA:HB2	1:A:680:LEU:HD22	1.53	0.89
25:1:47:ALA:CB	25:1:50:VAL:HB	2.03	0.89
27:3:177:PHE:CE2	27:3:181:ILE:HD11	2.08	0.89
26:2:160:LEU:HB3	26:2:206:LEU:HD11	1.52	0.88
18:R:195:PRO:HG2	18:R:199:LYS:HB2	0.89	0.88
25:1:8:VAL:HG11	25:1:45:VAL:HG13	1.55	0.88
26:2:29:GLY:H	27:3:25:GLN:CG	1.85	0.88
2:B:90:GLN:HE21	20:T:141:LEU:CA	1.80	0.88
18:R:204:ASN:ND2	18:R:205:ASP:N	2.20	0.88
3:C:275:ASN:ND2	11:K:31:CYS:SG	2.46	0.88
26:2:160:LEU:CA	26:2:206:LEU:HD11	2.04	0.88
26:2:117:ASN:CB	27:3:42:MET:CE	2.51	0.88
27:3:71:TYR:CD2	27:3:72:PRO:HD2	2.07	0.88
1:A:156:GLY:HA2	1:A:181:HIS:CG	2.07	0.88
22:V:523:VAL:CG1	25:1:20:LEU:HD23	2.03	0.88
17:Q:20:TYR:HE2	18:R:210:PHE:CB	1.70	0.88
26:2:163:MET:SD	26:2:196:ILE:HG21	2.14	0.88
25:1:4:VAL:HG11	26:2:412:PHE:HD2	1.36	0.88
27:3:177:PHE:CD2	27:3:181:ILE:HD11	2.08	0.88
17:Q:113:ARG:HH21	18:R:218:LYS:HE3	1.10	0.88
3:C:5:ASN:O	3:C:7:PRO:CD	2.20	0.88
23:W:696:TRP:CD1	23:W:697:ILE:CG1	2.57	0.88
26:2:243:SER:CB	26:2:258:LEU:HD22	2.04	0.88
27:3:70:LEU:HD13	27:3:115:ILE:HD11	1.55	0.88
27:3:165:LYS:HE3	27:3:200:SER:HB2	1.56	0.88
1:A:201:GLU:CA	1:A:212:LYS:O	2.19	0.87
17:Q:70:LYS:O	17:Q:102:VAL:HG11	1.74	0.87
26:2:218:GLN:HB3	26:2:264:HIS:HD2	1.38	0.87
27:3:59:VAL:HG11	27:3:71:TYR:HD1	1.39	0.87
1:A:197:GLU:OE1	13:M:93:PHE:CE2	2.28	0.87
1:A:263:ALA:HB1	1:A:272:ASN:HB3	1.56	0.87
13:M:92:SER:O	13:M:93:PHE:O	1.91	0.87
9:I:85:PRO:O	9:I:86:CYS:O	1.93	0.87
26:2:218:GLN:HB3	26:2:264:HIS:CD2	2.08	0.87
27:3:59:VAL:CG1	27:3:70:LEU:HB2	2.03	0.87
2:B:875:GLU:O	2:B:876:ASN:HB2	1.73	0.87
26:2:160:LEU:CD2	26:2:206:LEU:HD21	2.04	0.87
26:2:45:PHE:HB2	26:2:51:LEU:HD13	1.56	0.87
26:2:28:PRO:HD2	27:3:25:GLN:NE2	1.90	0.87
26:2:118:LEU:HD11	27:3:43:VAL:HG22	1.56	0.87
5:E:64:HIS:NE2	5:E:69:THR:C	2.27	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:366:ASN:ND2	22:V:613:THR:HG23	1.86	0.87
25:1:1:MET:HB3	26:2:413:LEU:CB	2.04	0.87
25:1:28:ALA:CB	25:1:31:LYS:HD2	2.04	0.87
26:2:117:ASN:OD1	27:3:108:ASN:CB	2.23	0.87
27:3:58:ALA:C	27:3:71:TYR:CZ	2.48	0.87
2:B:132:VAL:HG23	2:B:141:GLN:HB3	1.56	0.87
3:C:6:GLN:HB2	11:K:104:ARG:HH12	0.72	0.87
17:Q:20:TYR:CE2	18:R:210:PHE:HB2	2.10	0.87
23:W:37:HIS:CE1	23:W:454:VAL:HG13	2.09	0.87
18:R:164:GLY:HA2	18:R:203:PHE:CE2	2.09	0.87
23:W:59:TYR:CG	23:W:62:ALA:HB2	2.10	0.87
26:2:48:LEU:HB3	26:2:49:PRO:HD3	1.57	0.86
27:3:14:VAL:HG21	27:3:163:VAL:HG22	1.57	0.86
13:M:16:PRO:HG2	13:M:39:LEU:HD21	1.54	0.86
18:R:163:LEU:O	18:R:164:GLY:C	2.13	0.86
21:U:251:ALA:O	21:U:253:THR:N	2.07	0.86
26:2:138:PRO:HG3	26:2:189:GLU:HG3	1.57	0.86
27:3:64:ILE:HG13	27:3:123:ASP:HB3	1.57	0.86
1:A:263:ALA:C	1:A:264:VAL:HG13	1.93	0.86
2:B:225:LEU:C	2:B:227:ASN:N	2.27	0.86
8:H:74:GLU:C	8:H:75:TYR:CD1	2.49	0.86
26:2:160:LEU:CB	26:2:206:LEU:HD11	2.04	0.86
17:Q:23:ARG:HH22	18:R:206:LYS:HB3	1.03	0.86
26:2:118:LEU:HD22	27:3:39:ASP:CG	1.94	0.86
27:3:69:PHE:CZ	27:3:139:LYS:HB3	2.10	0.86
17:Q:113:ARG:HH22	18:R:218:LYS:CE	1.79	0.86
26:2:224:GLN:HB2	26:2:268:PHE:CZ	2.09	0.86
17:Q:113:ARG:HH21	18:R:218:LYS:CE	1.70	0.86
26:2:171:VAL:HG22	26:2:213:TRP:CA	2.06	0.86
26:2:211:GLN:HG3	26:2:257:SER:CB	2.05	0.86
27:3:100:LYS:HB3	27:3:103:LEU:HD13	1.58	0.86
26:2:81:LYS:CD	26:2:89:LEU:HD21	2.05	0.86
9:I:61:GLU:O	9:I:63:ASP:N	2.07	0.86
1:A:1457:ASN:OD1	1:A:1462:GLN:NE2	2.09	0.86
8:H:65:TYR:CE2	8:H:70:LEU:HB2	2.10	0.85
21:U:227:GLU:O	21:U:228:MET:CB	2.19	0.85
25:1:1:MET:O	26:2:413:LEU:CG	2.21	0.85
17:Q:101:ASN:C	17:Q:103:VAL:H	1.78	0.85
23:W:59:TYR:CD2	23:W:62:ALA:HB2	2.11	0.85
25:1:2:VAL:HG13	26:2:422:LEU:CD1	2.03	0.85
27:3:124:ILE:HD13	27:3:125:LYS:N	1.91	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:2:118:LEU:CD2	27:3:42:MET:HB2	2.06	0.85
26:2:159:VAL:HG22	26:2:160:LEU:H	1.40	0.85
17:Q:23:ARG:HH21	18:R:206:LYS:CA	1.76	0.85
26:2:81:LYS:CD	26:2:93:LEU:HD21	2.07	0.85
26:2:78:GLU:O	26:2:81:LYS:HG2	1.77	0.85
27:3:190:LEU:HA	27:3:210:THR:CG2	2.05	0.85
25:1:1:MET:SD	26:2:415:GLN:O	2.34	0.85
27:3:59:VAL:HG12	27:3:71:TYR:CG	2.07	0.85
27:3:184:ALA:HA	27:3:187:GLN:HG2	1.57	0.85
27:3:160:ARG:HB3	27:3:190:LEU:HD21	1.57	0.85
21:U:256:THR:O	21:U:272:THR:CG2	2.25	0.85
22:V:631:GLY:O	22:V:632:SER:HB2	1.76	0.85
26:2:221:GLN:HG2	26:2:268:PHE:CZ	2.11	0.84
22:V:612:ASP:OD2	22:V:635:GLN:CD	2.16	0.84
29:Y:24:DC:H2"	29:Y:25:DT:H71	0.87	0.84
18:R:151:LEU:CD1	18:R:163:LEU:CD2	2.54	0.84
25:1:19:PHE:O	25:1:23:LEU:HG	1.75	0.84
27:3:49:LEU:CB	27:3:101:TYR:HB3	2.05	0.84
27:3:49:LEU:HB3	27:3:101:TYR:CB	2.05	0.84
17:Q:105:TYR:HE1	18:R:234:GLU:CD	1.79	0.84
26:2:177:GLN:HA	26:2:220:LEU:HD21	1.56	0.84
26:2:221:GLN:NE2	26:2:230:LEU:HB2	1.93	0.84
25:1:2:VAL:CG1	26:2:422:LEU:CD1	2.55	0.84
1:A:274:ASP:O	1:A:277:THR:N	2.10	0.84
1:A:574:VAL:O	8:H:74:GLU:HA	1.78	0.84
13:M:10:LEU:C	13:M:12:ARG:H	1.78	0.84
18:R:164:GLY:CA	18:R:203:PHE:CE2	2.60	0.84
2:B:492:ASP:O	29:Y:45:DT:C2'	2.25	0.84
26:2:176:ALA:CB	26:2:178:LEU:HD13	2.07	0.84
26:2:118:LEU:CD2	27:3:39:ASP:HA	2.08	0.84
23:W:696:TRP:NE1	23:W:697:ILE:HG12	1.91	0.84
26:2:167:PRO:O	26:2:171:VAL:HG23	1.76	0.84
1:A:79:THR:HG21	13:M:43:ASP:OD1	1.77	0.84
8:H:65:TYR:HE2	8:H:70:LEU:HB2	1.40	0.84
22:V:523:VAL:CG1	25:1:20:LEU:HD21	2.04	0.84
26:2:118:LEU:HD12	26:2:119:ARG:N	1.92	0.84
26:2:159:VAL:HG22	26:2:160:LEU:CD1	2.08	0.84
1:A:264:VAL:HG23	1:A:272:ASN:OD1	1.78	0.84
1:A:621:ILE:O	1:A:623:PRO:N	2.11	0.84
22:V:615:PHE:O	22:V:616:ASP:C	2.17	0.84
5:E:64:HIS:HE2	5:E:69:THR:CA	1.87	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:151:LEU:HD11	18:R:163:LEU:HD21	1.58	0.83
26:2:160:LEU:HD23	26:2:206:LEU:CD2	2.07	0.83
17:Q:52:LEU:HB3	17:Q:54:PHE:HD2	1.43	0.83
26:2:229:ASP:O	26:2:233:ILE:HG12	1.78	0.83
27:3:196:LEU:HD21	27:3:223:LEU:CD2	2.08	0.83
1:A:133:SER:HG	1:A:136:GLN:HB2	1.42	0.83
13:M:10:LEU:O	13:M:12:ARG:N	2.09	0.83
13:M:89:GLY:O	13:M:90:ALA:CB	2.25	0.83
26:2:160:LEU:O	26:2:164:VAL:HG23	1.79	0.83
17:Q:24:GLY:HA3	18:R:210:PHE:CE2	2.13	0.83
26:2:57:MET:HA	26:2:60:LEU:CD1	2.09	0.83
1:A:273:GLN:NE2	13:M:79:ASP:OD2	2.11	0.83
2:B:874:PRO:O	2:B:876:ASN:N	2.10	0.83
9:I:89:CYS:HB3	9:I:119:CYS:SG	2.17	0.83
22:V:516:PRO:CG	25:1:15:ALA:HB1	1.96	0.83
22:V:516:PRO:HG3	25:1:15:ALA:HB2	1.57	0.83
1:A:931:ARG:NE	1:A:931:ARG:HA	1.93	0.83
22:V:315:VAL:HG12	23:W:500:ASP:HB2	1.54	0.83
26:2:259:LEU:HD12	26:2:260:ASN:N	1.94	0.83
1:A:932:ARG:HD2	1:A:943:LEU:HD21	0.84	0.83
9:I:102:ALA:C	9:I:104:ALA:H	1.82	0.83
13:M:178:LYS:C	20:T:154:LYS:HE3	1.98	0.83
25:1:47:ALA:HB2	25:1:50:VAL:HB	1.61	0.82
25:1:52:VAL:HG23	25:1:53:LEU:HD12	1.59	0.82
27:3:12:VAL:HG21	27:3:161:ILE:HG12	1.61	0.82
20:T:141:LEU:O	20:T:143:GLN:OE1	1.96	0.82
25:1:9:LEU:HB2	25:1:51:ASN:HD21	1.43	0.82
26:2:100:LEU:HG	26:2:119:ARG:HE	1.45	0.82
1:A:375:ILE:HG21	1:A:666:ARG:CZ	2.08	0.82
26:2:221:GLN:OE1	26:2:224:GLN:HA	1.80	0.82
25:1:59:GLU:OE1	26:2:402:ARG:NH1	2.13	0.82
27:3:216:LYS:H	27:3:216:LYS:HD2	1.43	0.82
17:Q:68:GLY:O	18:R:226:ASP:HB3	1.79	0.82
26:2:37:HIS:HB3	26:2:38:PRO:HD3	1.61	0.82
27:3:57:LEU:HD23	27:3:58:ALA:N	1.91	0.82
12:L:17:TYR:CE1	12:L:46:LYS:CG	2.47	0.82
17:Q:23:ARG:HH22	18:R:206:LYS:C	1.45	0.82
25:1:52:VAL:CG2	25:1:53:LEU:HD12	2.09	0.81
26:2:175:LEU:HB3	26:2:216:MET:SD	2.20	0.81
26:2:174:ASP:OD1	26:2:179:LEU:HD12	1.80	0.81
9:I:103:ARG:C	9:I:105:GLU:N	2.32	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:427:MET:O	22:V:432:THR:O	1.98	0.81
26:2:117:ASN:OD1	27:3:108:ASN:CG	2.18	0.81
26:2:86:SER:HB3	26:2:140:LYS:HE2	1.60	0.81
26:2:30:VAL:H	27:3:25:GLN:HB3	1.44	0.81
18:R:204:ASN:ND2	18:R:205:ASP:H	1.78	0.81
8:H:65:TYR:CD2	8:H:70:LEU:HD22	2.16	0.81
17:Q:113:ARG:NH2	18:R:218:LYS:CD	2.43	0.81
25:1:9:LEU:CD1	25:1:48:GLU:HA	2.09	0.81
26:2:174:ASP:O	26:2:220:LEU:HD23	1.79	0.81
1:A:1290:SER:HB3	2:B:250:SER:CB	2.11	0.81
23:W:59:TYR:CD1	23:W:62:ALA:HB2	2.16	0.81
5:E:46:ASP:O	5:E:48:PRO:CD	2.27	0.81
5:E:49:SER:O	5:E:50:GLU:O	1.96	0.81
27:3:12:VAL:CG2	27:3:161:ILE:HG12	2.10	0.81
17:Q:184:ILE:HD13	18:R:218:LYS:NZ	1.94	0.81
22:V:516:PRO:CD	22:V:706:LYS:HZ3	1.93	0.81
25:1:50:VAL:HG12	25:1:54:GLN:HG2	1.62	0.81
26:2:31:LEU:CD1	27:3:33:THR:HG22	1.96	0.81
1:A:1113:SER:CB	1:A:1309:MET:SD	2.69	0.81
1:A:1312:PRO:HB3	1:A:1334:TRP:CZ3	2.16	0.81
2:B:226:GLU:OE2	2:B:617:ASP:HB2	1.81	0.81
25:1:34:ILE:HG22	25:1:46:ILE:HD11	1.63	0.80
2:B:566:LYS:HD3	2:B:573:TRP:HE1	1.47	0.80
26:2:256:ASP:O	26:2:259:LEU:HG	1.82	0.80
26:2:42:LEU:HD12	26:2:59:MET:CE	2.11	0.80
2:B:132:VAL:HG21	2:B:141:GLN:CG	2.10	0.80
5:E:64:HIS:CD2	5:E:67:ASP:O	2.34	0.80
17:Q:113:ARG:NH1	18:R:218:LYS:HG3	1.96	0.80
26:2:35:TYR:CD1	26:2:62:LEU:HG	2.16	0.80
27:3:214:TYR:O	27:3:215:LEU:HD23	1.82	0.80
1:A:47:THR:CG2	1:A:53:LYS:HG2	2.01	0.80
27:3:11:LEU:CD2	27:3:160:ARG:HG2	2.12	0.80
1:A:1115:LYS:O	1:A:1116:ASN:O	2.00	0.80
1:A:926:ASN:CB	1:A:931:ARG:HH11	1.78	0.80
16:P:298:PRO:O	16:P:300:ILE:CD1	2.30	0.80
17:Q:113:ARG:HH22	18:R:218:LYS:CD	1.93	0.80
26:2:205:LEU:O	26:2:209:PRO:HD2	1.81	0.80
27:3:121:LYS:O	27:3:124:ILE:HB	1.81	0.80
26:2:93:LEU:HA	26:2:96:TRP:CD1	2.17	0.80
27:3:165:LYS:HE2	27:3:167:ALA:O	1.81	0.80
13:M:7:LEU:HD21	13:M:10:LEU:HD13	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:2:251:VAL:HG11	26:2:254:MET:HG3	1.62	0.79
1:A:1304:ILE:O	1:A:1307:VAL:CG2	2.30	0.79
16:P:297:LYS:CB	16:P:298:PRO:HD2	2.05	0.79
25:1:13:ASP:OD2	25:1:17:LYS:CB	2.31	0.79
26:2:30:VAL:HG23	27:3:25:GLN:HB3	0.80	0.79
22:V:674:THR:CG2	26:2:392:ARG:CZ	2.59	0.79
27:3:64:ILE:HG23	27:3:128:HIS:CD2	2.17	0.79
27:3:14:VAL:CG2	27:3:163:VAL:HG22	2.13	0.79
29:Y:24:DC:H2"	29:Y:25:DT:C5	2.18	0.79
26:2:224:GLN:HB2	26:2:268:PHE:CE2	2.17	0.79
27:3:222:SER:O	27:3:225:GLN:HG2	1.83	0.79
5:E:41:LYS:HG3	5:E:46:ASP:OD2	1.80	0.79
27:3:144:ILE:CD1	27:3:147:MET:HE3	2.13	0.79
28:X:15:DA:N6	29:Y:79:DC:N4	2.24	0.79
25:1:1:MET:HA	26:2:414:SER:H	1.46	0.79
25:1:38:ILE:HA	25:1:44:PHE:HD1	1.48	0.79
26:2:234:LEU:HD23	26:2:234:LEU:O	1.83	0.78
26:2:52:ALA:O	26:2:56:VAL:HG13	1.81	0.78
24:0:54:ARG:NE	27:3:182:PHE:HE1	1.73	0.78
26:2:211:GLN:CG	26:2:257:SER:HB3	2.13	0.78
27:3:58:ALA:HA	27:3:71:TYR:CZ	2.17	0.78
17:Q:69:ASP:HA	18:R:226:ASP:OD1	1.83	0.78
26:2:181:GLN:OE1	26:2:229:ASP:HB2	1.83	0.78
27:3:151:VAL:HG12	27:3:155:GLN:O	1.84	0.78
25:1:34:ILE:CG2	25:1:46:ILE:HD11	2.13	0.78
5:E:55:ARG:NH1	5:E:107:GLN:OE1	2.17	0.78
26:2:189:GLU:HB2	26:2:190:PRO:HD3	1.66	0.78
26:2:34:LEU:O	26:2:38:PRO:HD2	1.84	0.78
26:2:118:LEU:CG	27:3:39:ASP:OD1	2.32	0.78
25:1:1:MET:CB	26:2:413:LEU:CB	2.60	0.78
25:1:1:MET:HB3	26:2:413:LEU:HD23	1.65	0.78
26:2:77:LYS:HD3	26:2:78:GLU:N	1.97	0.78
27:3:208:ASP:OD1	27:3:209:ILE:HG13	1.83	0.78
24:0:55:LEU:HD12	27:3:178:MET:HE3	1.63	0.78
26:2:159:VAL:HG13	26:2:161:HIS:N	1.96	0.78
26:2:203:PHE:CD2	26:2:205:LEU:HD23	2.18	0.78
26:2:207:ASP:O	26:2:211:GLN:HG2	1.84	0.78
26:2:163:MET:CE	26:2:206:LEU:HD12	2.14	0.78
1:A:485:ASN:OD1	1:A:486:LEU:N	2.16	0.78
2:B:490:GLY:O	2:B:491:ARG:HB2	1.84	0.78
22:V:516:PRO:CD	25:1:15:ALA:HB3	2.10	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:2:196:ILE:CD1	26:2:210:ALA:HB2	2.13	0.77
26:2:53:LYS:O	26:2:56:VAL:HG22	1.84	0.77
26:2:42:LEU:HD12	26:2:59:MET:HE3	1.64	0.77
27:3:185:GLN:HE21	27:3:185:GLN:HA	1.48	0.77
17:Q:184:ILE:CD1	18:R:218:LYS:NZ	2.47	0.77
27:3:147:MET:O	27:3:151:VAL:HG23	1.84	0.77
27:3:185:GLN:NE2	27:3:210:THR:HA	2.00	0.77
26:2:208:THR:HG23	26:2:209:PRO:HD3	1.66	0.77
22:V:674:THR:CG2	26:2:392:ARG:NH2	2.43	0.77
25:1:10:ILE:CG2	26:2:407:VAL:HG21	2.15	0.77
26:2:118:LEU:CD1	27:3:39:ASP:OD1	2.31	0.77
25:1:1:MET:HG3	26:2:415:GLN:O	1.84	0.77
26:2:117:ASN:HD21	27:3:108:ASN:HB3	1.47	0.77
25:1:38:ILE:HG22	25:1:44:PHE:CD1	2.18	0.77
26:2:190:PRO:O	26:2:194:PRO:HD2	1.82	0.77
1:A:930:LEU:CD2	1:A:934:LEU:CD1	2.60	0.77
25:1:2:VAL:CG1	26:2:456:LYS:CG	2.53	0.77
22:V:516:PRO:HA	25:1:15:ALA:C	2.03	0.77
26:2:42:LEU:HD21	26:2:55:TRP:CB	2.10	0.77
1:A:926:ASN:CG	1:A:931:ARG:NH1	2.38	0.77
2:B:897:ARG:O	2:B:900:GLU:CG	2.32	0.77
17:Q:112:ARG:CZ	18:R:237:LEU:HD11	2.14	0.77
4:D:48:ASN:HD22	4:D:57:LEU:HG	1.48	0.77
8:H:74:GLU:O	8:H:75:TYR:CE1	2.38	0.77
19:S:49:ARG:NH1	19:S:96:GLN:O	2.18	0.77
26:2:179:LEU:HB3	26:2:184:LEU:HD11	1.65	0.76
1:A:551:ARG:CD	1:A:625:ASP:OD2	2.25	0.76
9:I:103:ARG:O	9:I:105:GLU:CA	2.33	0.76
27:3:58:ALA:C	27:3:71:TYR:CE1	2.58	0.76
26:2:221:GLN:HE22	26:2:230:LEU:HB2	1.47	0.76
1:A:264:VAL:HG23	1:A:272:ASN:CG	2.05	0.76
1:A:270:ALA:O	1:A:272:ASN:N	2.18	0.76
2:B:492:ASP:O	29:Y:45:DT:H2'	1.83	0.76
26:2:208:THR:HG23	26:2:209:PRO:CD	2.16	0.76
26:2:211:GLN:HA	26:2:261:PHE:HZ	1.49	0.76
26:2:218:GLN:NE2	26:2:265:LEU:HA	2.00	0.76
27:3:190:LEU:H	27:3:190:LEU:HD23	1.51	0.76
25:1:1:MET:CE	26:2:440:LEU:HD13	2.16	0.76
25:1:1:MET:HE2	26:2:440:LEU:HD13	1.66	0.76
1:A:298:ALA:HB1	1:A:303:ILE:HD11	1.67	0.76
26:2:177:GLN:CD	26:2:220:LEU:HD22	2.06	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:3:58:ALA:N	27:3:71:TYR:CZ	2.51	0.76
26:2:86:SER:HB3	26:2:140:LYS:CE	2.16	0.76
27:3:172:LEU:HD13	27:3:172:LEU:O	1.86	0.76
26:2:44:VAL:HG13	26:2:45:PHE:CD1	2.20	0.76
2:B:875:GLU:HA	2:B:875:GLU:OE2	1.85	0.76
23:W:298:ALA:HA	23:W:421:PHE:CD2	2.21	0.76
25:1:1:MET:HB3	26:2:413:LEU:CD2	2.15	0.76
2:B:897:ARG:O	2:B:900:GLU:HG3	1.86	0.76
13:M:178:LYS:HB3	20:T:154:LYS:HD3	1.68	0.76
26:2:127:LYS:N	26:2:178:LEU:HD23	2.01	0.76
25:1:1:MET:SD	26:2:413:LEU:HB3	2.25	0.75
1:A:1290:SER:CB	2:B:250:SER:CB	2.62	0.75
18:R:151:LEU:HD13	18:R:163:LEU:HD21	1.64	0.75
24:0:54:ARG:HB2	27:3:209:ILE:CG2	2.14	0.75
26:2:234:LEU:CD2	26:2:237:LEU:HD12	2.14	0.75
13:M:16:PRO:HD2	13:M:39:LEU:CD2	2.16	0.75
28:X:70:DG:N2	29:Y:25:DT:O2	2.19	0.75
27:3:14:VAL:CG2	27:3:163:VAL:HA	2.16	0.75
27:3:11:LEU:HD22	27:3:160:ARG:CG	2.16	0.75
22:V:321:GLU:HG2	23:W:499:ASN:CB	2.07	0.75
1:A:133:SER:O	1:A:134:LYS:C	2.21	0.75
26:2:243:SER:HB3	26:2:258:LEU:HD22	1.69	0.75
27:3:133:LEU:HD23	27:3:177:PHE:HD1	1.49	0.75
26:2:118:LEU:HD22	27:3:39:ASP:HA	1.65	0.75
12:L:27:GLU:HB2	12:L:37:ARG:HH12	1.51	0.75
18:R:151:LEU:HD13	18:R:163:LEU:CD2	2.16	0.75
8:H:65:TYR:CZ	8:H:70:LEU:HD13	2.22	0.75
9:I:84:HIS:CG	9:I:85:PRO:HD3	1.80	0.75
26:2:180:SER:O	26:2:184:LEU:HG	1.87	0.74
27:3:38:ILE:O	27:3:41:VAL:HG12	1.87	0.74
27:3:8:LEU:HD23	27:3:54:SER:HB3	1.68	0.74
2:B:591:ARG:NH1	2:B:663:GLU:OE2	2.18	0.74
20:T:152:ASN:O	20:T:154:LYS:N	2.20	0.74
25:1:24:ASP:OD2	25:1:57:VAL:HG11	1.85	0.74
26:2:35:TYR:CD2	26:2:62:LEU:HB3	2.22	0.74
2:B:92:TYR:HA	20:T:141:LEU:CD1	2.10	0.74
3:C:5:ASN:C	3:C:7:PRO:HD3	2.07	0.74
26:2:117:ASN:CG	27:3:42:MET:CE	2.55	0.74
13:M:94:ASP:HB2	13:M:99:SER:H	1.53	0.74
22:V:444:HIS:O	22:V:447:PRO:HD2	1.86	0.74
23:W:430:ASN:HB3	23:W:431:PRO:CD	2.17	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:1:38:ILE:H	25:1:38:ILE:HD13	1.51	0.74
26:2:100:LEU:CD1	26:2:119:ARG:HG3	2.16	0.74
26:2:132:ASP:O	26:2:135:GLN:HG2	1.88	0.74
2:B:873:LEU:HB3	2:B:874:PRO:HD3	1.68	0.74
25:1:1:MET:HB2	26:2:418:PHE:CB	2.18	0.74
22:V:516:PRO:CB	22:V:706:LYS:NZ	2.48	0.74
23:W:73:CYS:HB2	23:W:209:TYR:CZ	2.22	0.74
26:2:51:LEU:O	26:2:51:LEU:HD23	1.87	0.74
26:2:53:LYS:HE3	26:2:95:ILE:HD11	1.67	0.74
27:3:24:LYS:O	27:3:25:GLN:O	2.06	0.74
27:3:59:VAL:CA	27:3:71:TYR:CE1	2.70	0.74
2:B:490:GLY:O	2:B:491:ARG:CB	2.36	0.74
10:J:64:PRO:C	10:J:66:GLU:N	2.39	0.74
22:V:415:HIS:HA	22:V:421:TRP:CD1	2.22	0.74
26:2:196:ILE:HD11	26:2:210:ALA:CB	2.17	0.74
27:3:33:THR:HG23	27:3:36:LYS:N	1.98	0.74
22:V:516:PRO:HG2	22:V:706:LYS:CE	2.17	0.74
29:Y:63:DG:H3'	29:Y:64:DC:H2'	1.67	0.74
1:A:932:ARG:HG3	1:A:943:LEU:HD11	1.70	0.74
17:Q:187:ILE:CD1	18:R:210:PHE:O	2.29	0.74
26:2:160:LEU:HA	26:2:206:LEU:HD11	1.70	0.73
22:V:523:VAL:HG21	25:1:20:LEU:HG	1.68	0.73
25:1:34:ILE:HD13	25:1:54:GLN:OE1	1.88	0.73
1:A:263:ALA:O	1:A:264:VAL:CB	2.36	0.73
1:A:890:ARG:HH21	1:A:1023:VAL:HG13	1.51	0.73
3:C:56:SER:HG	3:C:158:GLU:H	1.35	0.73
9:I:84:HIS:CG	9:I:85:PRO:CD	2.59	0.73
17:Q:112:ARG:CZ	18:R:237:LEU:CD1	2.66	0.73
2:B:175:ASN:HD21	10:J:64:PRO:HG2	1.52	0.73
14:N:347:ASN:ND2	14:N:375:GLU:OE2	2.21	0.73
18:R:225:VAL:CG1	18:R:227:SER:HB2	2.05	0.73
26:2:237:LEU:O	26:2:240:LEU:HD13	1.88	0.73
27:3:141:LEU:O	27:3:144:ILE:HG22	1.88	0.73
2:B:838:GLN:HB3	2:B:890:ARG:HA	1.70	0.73
26:2:251:VAL:HG11	26:2:254:MET:CG	2.18	0.73
1:A:79:THR:HG21	13:M:43:ASP:CG	2.08	0.73
2:B:793:SER:HA	2:B:944:THR:O	1.89	0.73
22:V:667:THR:HA	25:1:62:ASP:OD1	1.89	0.73
27:3:226:TYR:HA	27:3:230:VAL:HG23	1.71	0.73
2:B:492:ASP:O	29:Y:45:DT:H2"	1.88	0.73
26:2:172:SER:HA	26:2:175:LEU:CD2	2.19	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:3:214:TYR:HE2	27:3:216:LYS:HE2	1.53	0.73
27:3:57:LEU:C	27:3:71:TYR:CE2	2.61	0.73
18:R:163:LEU:O	18:R:164:GLY:O	2.06	0.73
25:1:9:LEU:HD22	25:1:51:ASN:ND2	2.04	0.73
17:Q:188:TYR:HA	17:Q:191:LEU:HD13	1.70	0.73
26:2:199:ALA:HB3	26:2:202:GLN:NE2	2.02	0.73
26:2:218:GLN:HE22	26:2:265:LEU:HA	1.54	0.73
26:2:243:SER:HB2	26:2:258:LEU:HD22	1.71	0.73
27:3:57:LEU:C	27:3:71:TYR:CZ	2.61	0.73
23:W:298:ALA:HA	23:W:421:PHE:HD2	1.52	0.73
25:1:1:MET:HG3	26:2:418:PHE:HB2	1.69	0.72
14:N:320:VAL:HB	16:P:236:LYS:HE3	1.71	0.72
21:U:256:THR:HB	21:U:272:THR:HG22	1.64	0.72
22:V:611:GLY:HA2	22:V:615:PHE:HB3	1.71	0.72
26:2:175:LEU:HD22	26:2:216:MET:SD	2.29	0.72
22:V:689:VAL:HB	26:2:391:ILE:HD11	1.70	0.72
27:3:111:ILE:HG13	27:3:112:VAL:N	2.02	0.72
2:B:132:VAL:CG2	2:B:141:GLN:CG	2.66	0.72
14:N:317:GLU:HG3	16:P:235:ARG:HG2	1.71	0.72
21:U:256:THR:C	21:U:272:THR:HG22	2.09	0.72
23:W:59:TYR:CD2	23:W:62:ALA:CB	2.70	0.72
24:0:76:LEU:O	24:0:77:LYS:O	2.07	0.72
26:2:60:LEU:HD11	26:2:95:ILE:HB	1.71	0.72
1:A:264:VAL:CG2	1:A:272:ASN:ND2	2.51	0.72
1:A:274:ASP:O	1:A:276:LEU:N	2.22	0.72
17:Q:101:ASN:C	17:Q:103:VAL:N	2.43	0.72
26:2:118:LEU:HD22	27:3:39:ASP:CA	2.19	0.72
26:2:134:SER:O	26:2:138:PRO:HD2	1.89	0.72
26:2:41:CYS:O	26:2:44:VAL:HG12	1.88	0.72
1:A:608:THR:CB	1:A:610:PRO:HD2	2.20	0.72
17:Q:23:ARG:HH21	18:R:206:LYS:N	1.86	0.72
25:1:25:GLU:CD	25:1:35:ILE:HG12	2.09	0.72
26:2:117:ASN:HB3	27:3:42:MET:CE	2.18	0.72
22:V:504:LYS:HB3	22:V:654:GLU:O	1.90	0.72
25:1:28:ALA:HB3	25:1:31:LYS:HB2	1.71	0.72
27:3:12:VAL:HG23	27:3:161:ILE:HG23	1.70	0.72
1:A:18:ILE:HB	1:A:1460:LEU:HD21	1.70	0.72
2:B:761:THR:H	2:B:764:MET:HE3	1.54	0.72
1:A:79:THR:CG2	13:M:43:ASP:OD1	2.37	0.72
17:Q:68:GLY:O	18:R:226:ASP:CB	2.38	0.72
26:2:163:MET:HE2	26:2:206:LEU:HD12	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:1:5:LEU:HD21	26:2:408:LEU:HD13	0.87	0.72
26:2:35:TYR:CG	26:2:62:LEU:HD12	2.25	0.72
27:3:69:PHE:CE1	27:3:139:LYS:HD2	2.25	0.72
27:3:217:VAL:HG13	27:3:226:TYR:CZ	2.24	0.72
1:A:1211:LEU:HD11	1:A:1258:ARG:HG3	1.72	0.72
1:A:932:ARG:HG3	1:A:943:LEU:CD1	2.19	0.72
4:D:96:GLU:OE1	4:D:121:ARG:NH1	2.23	0.72
11:K:111:ASP:O	11:K:113:GLN:N	2.19	0.72
26:2:117:ASN:HB2	27:3:104:LEU:HD11	1.71	0.72
2:B:1006:VAL:HG23	2:B:1010:LYS:HB2	1.72	0.72
12:L:19:CYS:SG	12:L:20:GLY:N	2.63	0.72
13:M:16:PRO:CD	13:M:39:LEU:CD2	2.67	0.72
13:M:182:ALA:HB1	20:T:152:ASN:CG	2.09	0.72
25:1:13:ASP:OD1	25:1:14:PRO:HD2	1.89	0.71
25:1:2:VAL:HG12	26:2:422:LEU:HD13	1.72	0.71
27:3:222:SER:HB2	27:3:226:TYR:HE2	1.55	0.71
8:H:65:TYR:CE2	8:H:70:LEU:CB	2.73	0.71
17:Q:19:LYS:O	17:Q:22:ILE:HG13	1.88	0.71
1:A:199:TYR:HH	13:M:93:PHE:HE2	0.99	0.71
17:Q:23:ARG:NH2	18:R:206:LYS:N	2.38	0.71
26:2:118:LEU:CD2	27:3:39:ASP:CA	2.68	0.71
26:2:171:VAL:HG12	26:2:216:MET:SD	2.31	0.71
2:B:73:HIS:O	2:B:75:SER:N	2.22	0.71
5:E:3:ASP:HB2	5:E:50:GLU:OE1	1.90	0.71
27:3:66:GLU:CA	27:3:132:LEU:HD12	2.13	0.71
12:L:35:ARG:HH12	12:L:42:ARG:HH21	1.39	0.71
27:3:148:ASN:CB	27:3:157:MET:HE2	2.20	0.71
27:3:165:LYS:HG3	27:3:203:LEU:CD1	2.20	0.71
1:A:1304:ILE:O	1:A:1307:VAL:HG22	1.90	0.71
1:A:926:ASN:CG	1:A:931:ARG:HH11	1.93	0.71
17:Q:180:PHE:CE1	18:R:212:VAL:C	2.62	0.71
21:U:180:ILE:HG21	21:U:187:TYR:HB2	1.73	0.71
23:W:209:TYR:OH	23:W:234:ASP:N	2.23	0.71
23:W:209:TYR:HE1	23:W:233:PHE:CD1	2.08	0.71
17:Q:20:TYR:HE2	18:R:210:PHE:HB2	1.50	0.71
26:2:30:VAL:H	27:3:25:GLN:CB	2.04	0.71
22:V:516:PRO:CD	22:V:706:LYS:NZ	2.54	0.71
22:V:648:LYS:O	22:V:650:MET:N	2.24	0.71
24:0:54:ARG:CD	27:3:182:PHE:CE1	2.60	0.71
26:2:86:SER:CB	26:2:140:LYS:HE2	2.20	0.71
5:E:64:HIS:NE2	5:E:69:THR:O	2.19	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:79:VAL:HG21	15:O:93:VAL:HG12	1.72	0.71
16:P:206:GLU:HG3	16:P:236:LYS:HZ2	0.61	0.71
18:R:195:PRO:HB2	18:R:199:LYS:CB	2.21	0.71
17:Q:42:CYS:HB3	17:Q:95:ASN:HD21	1.54	0.71
25:1:1:MET:HG2	26:2:413:LEU:HB3	1.71	0.70
3:C:7:PRO:O	3:C:8:THR:CB	2.39	0.70
27:3:177:PHE:CZ	27:3:203:LEU:HD23	2.27	0.70
8:H:66:GLU:O	8:H:67:ASP:HB2	1.89	0.70
22:V:515:SER:HB3	22:V:539:ASN:ND2	2.05	0.70
23:W:589:GLU:O	23:W:594:ALA:HB1	1.91	0.70
27:3:133:LEU:HD22	27:3:134:ALA:H	1.56	0.70
1:A:206:ASN:O	1:A:207:GLU:CB	2.33	0.70
20:T:8:ASP:OD2	20:T:10:THR:OG1	2.08	0.70
27:3:33:THR:HG22	27:3:36:LYS:HB2	1.73	0.70
2:B:812:ARG:HD3	2:B:814:TYR:OH	1.92	0.70
20:T:155:PRO:O	20:T:157:ALA:N	2.17	0.70
26:2:218:GLN:OE1	26:2:265:LEU:HA	1.92	0.70
16:P:267:PRO:HB2	16:P:337:LYS:HD2	1.73	0.70
25:1:29:LEU:HD23	25:1:30:GLY:N	2.06	0.70
25:1:8:VAL:HG11	25:1:45:VAL:HG12	1.74	0.70
26:2:189:GLU:HA	26:2:192:GLU:HG2	1.72	0.70
1:A:263:ALA:CB	1:A:272:ASN:HB3	2.21	0.70
9:I:102:ALA:C	9:I:104:ALA:N	2.38	0.70
17:Q:184:ILE:HG12	18:R:211:SER:HB2	1.74	0.70
14:N:32:ASP:HB3	14:N:34:VAL:HG23	1.73	0.70
23:W:584:TYR:HD1	23:W:594:ALA:HB2	1.51	0.70
24:0:100:PRO:CG	27:3:208:ASP:OD2	2.39	0.70
16:P:206:GLU:HA	16:P:206:GLU:OE2	1.91	0.70
1:A:298:ALA:O	17:Q:60:ARG:NE	2.24	0.70
18:R:201:LEU:HB3	18:R:203:PHE:HE1	1.57	0.70
26:2:31:LEU:CD1	27:3:33:THR:HG21	2.22	0.70
1:A:1158:LEU:HD21	1:A:1308:TYR:CD2	2.25	0.70
1:A:1307:VAL:O	1:A:1308:TYR:HB3	1.91	0.70
2:B:939:HIS:NE2	2:B:983:GLU:OE1	2.24	0.70
1:A:643:LYS:NZ	21:U:299:LYS:O	2.22	0.70
23:W:696:TRP:CD1	23:W:697:ILE:HG13	2.25	0.70
25:1:13:ASP:CG	25:1:14:PRO:CD	2.58	0.69
25:1:18:GLN:CB	25:1:44:PHE:HE2	2.01	0.69
25:1:2:VAL:HG12	26:2:456:LYS:HE2	1.74	0.69
27:3:162:LEU:HA	27:3:192:ASP:OD1	1.92	0.69
1:A:505:LEU:O	2:B:1106:ARG:NH2	2.24	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:24:GLU:HG2	3:C:228:ARG:HG3	1.73	0.69
13:M:10:LEU:C	13:M:12:ARG:N	2.46	0.69
26:2:130:SER:O	26:2:133:THR:HG22	1.92	0.69
26:2:163:MET:O	26:2:167:PRO:HD2	1.91	0.69
9:I:103:ARG:O	9:I:104:ALA:C	2.30	0.69
23:W:59:TYR:CE1	23:W:62:ALA:HB2	2.26	0.69
18:R:195:PRO:HG2	18:R:199:LYS:C	2.12	0.69
2:B:429:PHE:H	20:T:160:GLN:HG2	1.55	0.69
24:0:54:ARG:NE	27:3:182:PHE:CD1	2.60	0.69
26:2:117:ASN:CB	27:3:42:MET:HE3	2.21	0.69
26:2:185:MET:SD	26:2:232:GLU:HB2	2.31	0.69
25:1:1:MET:CG	26:2:415:GLN:O	2.41	0.69
2:B:721:ARG:HG3	2:B:939:HIS:O	1.91	0.69
22:V:516:PRO:HB2	22:V:706:LYS:NZ	2.08	0.69
26:2:118:LEU:HD11	27:3:43:VAL:HG23	1.75	0.69
26:2:163:MET:CE	26:2:206:LEU:HB3	2.23	0.69
26:2:211:GLN:HA	26:2:261:PHE:CE1	2.28	0.69
22:V:674:THR:OG1	26:2:392:ARG:NE	2.25	0.69
27:3:69:PHE:CZ	27:3:139:LYS:HD2	2.27	0.69
1:A:1319:LYS:HE2	1:A:1333:GLU:OE2	1.93	0.69
18:R:127:ASN:HD21	18:R:140:LYS:HD3	1.57	0.69
22:V:522:TYR:HE2	25:1:62:ASP:CG	1.96	0.69
25:1:53:LEU:HD12	25:1:53:LEU:H	1.57	0.69
2:B:92:TYR:HD1	20:T:141:LEU:CD2	2.04	0.69
19:S:115:LYS:HB2	19:S:143:TRP:HB3	1.73	0.69
25:1:34:ILE:HG12	25:1:50:VAL:CG1	2.18	0.69
26:2:140:LYS:HD3	26:2:162:PHE:HE1	1.58	0.69
26:2:81:LYS:HD2	26:2:89:LEU:CD2	2.20	0.69
1:A:138:LYS:NZ	1:A:1441:GLU:OE2	2.25	0.69
17:Q:105:TYR:CE1	18:R:234:GLU:OE1	2.40	0.69
18:R:193:ASN:ND2	18:R:197:LYS:O	2.22	0.69
2:B:92:TYR:CD1	20:T:141:LEU:HD21	2.20	0.69
1:A:156:GLY:HA2	1:A:181:HIS:CD2	2.26	0.69
2:B:905:ASP:OD2	2:B:922:ARG:NH2	2.22	0.69
1:A:269:SER:O	1:A:270:ALA:HB3	1.92	0.69
1:A:608:THR:OG1	1:A:610:PRO:HG2	1.93	0.69
13:M:11:PRO:C	13:M:12:ARG:HG2	2.07	0.69
25:1:4:VAL:CG1	26:2:411:GLN:O	2.39	0.69
27:3:215:LEU:HD12	27:3:230:VAL:CG1	2.23	0.69
13:M:89:GLY:O	13:M:90:ALA:HB2	1.93	0.69
25:1:1:MET:HG2	26:2:413:LEU:C	2.14	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:238:LYS:HD2	13:M:299:LEU:HA	1.75	0.68
22:V:516:PRO:CA	25:1:15:ALA:O	2.40	0.68
25:1:55:GLU:OE2	26:2:402:ARG:HG3	1.93	0.68
26:2:176:ALA:HB1	26:2:178:LEU:CD1	2.23	0.68
26:2:81:LYS:HE3	26:2:93:LEU:CD2	2.20	0.68
27:3:144:ILE:HG12	27:3:147:MET:HE2	1.75	0.68
26:2:48:LEU:CB	26:2:49:PRO:HD3	2.19	0.68
27:3:34:LEU:HD13	27:3:34:LEU:O	1.92	0.68
26:2:117:ASN:HB3	27:3:42:MET:HE3	1.74	0.68
1:A:1291:ASN:OD1	2:B:250:SER:OG	2.09	0.68
13:M:7:LEU:CD2	13:M:10:LEU:HD13	2.23	0.68
26:2:251:VAL:HG12	26:2:254:MET:H	1.58	0.68
27:3:24:LYS:HE2	27:3:220:MET:SD	2.34	0.68
22:V:516:PRO:HB3	25:1:15:ALA:CB	2.04	0.68
25:1:10:ILE:HG21	26:2:407:VAL:HG21	1.76	0.68
1:A:471:GLY:O	1:A:521:VAL:HG23	1.93	0.68
2:B:274:ARG:NH1	2:B:281:ASP:OD1	2.25	0.68
29:Y:24:DC:C2'	29:Y:25:DT:H73	2.23	0.68
27:3:178:MET:HE2	27:3:202:LEU:CD1	2.23	0.68
1:A:263:ALA:CA	1:A:272:ASN:O	2.41	0.68
3:C:272:LEU:HD21	11:K:84:GLN:HG2	1.74	0.68
18:R:202:PHE:O	18:R:203:PHE:CD1	2.46	0.68
18:R:164:GLY:CA	18:R:203:PHE:HZ	1.87	0.68
27:3:114:GLU:O	27:3:118:LEU:HD23	1.92	0.68
1:A:1304:ILE:O	1:A:1307:VAL:N	2.27	0.68
26:2:170:ALA:HB1	26:2:213:TRP:CZ3	2.29	0.68
25:1:1:MET:C	26:2:413:LEU:HG	2.12	0.68
26:2:211:GLN:HB3	26:2:261:PHE:HE1	1.59	0.68
27:3:159:SER:OG	27:3:189:ILE:HD12	1.94	0.68
1:A:202:TRP:H	1:A:212:LYS:HA	1.58	0.68
1:A:487:SER:HB2	1:A:673:GLN:HE22	1.59	0.68
17:Q:113:ARG:CD	18:R:222:SER:CB	2.72	0.68
23:W:584:TYR:CE1	23:W:614:TYR:O	2.46	0.68
26:2:199:ALA:CB	26:2:202:GLN:HE22	2.02	0.68
1:A:1052:ARG:NH1	1:A:1056:GLU:OE1	2.27	0.68
1:A:264:VAL:CG2	1:A:272:ASN:CG	2.63	0.68
17:Q:113:ARG:NH2	18:R:218:LYS:CG	2.57	0.68
8:H:17:PRO:O	8:H:19:GLY:N	2.27	0.67
17:Q:184:ILE:HD11	18:R:218:LYS:HZ2	1.59	0.67
17:Q:184:ILE:HG12	18:R:211:SER:CB	2.24	0.67
26:2:118:LEU:HD13	27:3:39:ASP:OD1	1.92	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:TYR:OH	13:M:93:PHE:HZ	1.69	0.67
1:A:60:PRO:HD2	1:A:62:GLN:HG2	1.75	0.67
25:1:39:ASP:OD1	25:1:43:VAL:HB	1.94	0.67
17:Q:109:HIS:CE1	18:R:233:ILE:HG21	2.30	0.67
27:3:187:GLN:HG3	27:3:189:ILE:CG1	2.24	0.67
27:3:187:GLN:CG	27:3:189:ILE:HG12	2.24	0.67
1:A:201:GLU:CG	1:A:212:LYS:HB3	2.25	0.67
11:K:82:SER:OG	11:K:84:GLN:OE1	2.12	0.67
23:W:73:CYS:C	23:W:209:TYR:CE2	2.67	0.67
23:W:419:GLU:CB	23:W:420:PRO:CD	2.45	0.67
26:2:172:SER:O	26:2:175:LEU:HD23	1.95	0.67
26:2:56:VAL:O	26:2:60:LEU:HG	1.94	0.67
27:3:111:ILE:O	27:3:115:ILE:HD13	1.94	0.67
1:A:67:ARG:NH2	13:M:45:VAL:O	2.28	0.67
5:E:64:HIS:CD2	5:E:68:PRO:HA	2.29	0.67
21:U:226:GLU:HA	21:U:226:GLU:OE2	1.93	0.67
2:B:685:LYS:HD2	2:B:691:SER:HA	1.77	0.67
22:V:325:ARG:HH21	23:W:499:ASN:CB	1.95	0.67
27:3:217:VAL:HG13	27:3:226:TYR:CE2	2.30	0.67
17:Q:101:ASN:O	17:Q:103:VAL:N	2.28	0.67
18:R:195:PRO:HB2	18:R:199:LYS:HB3	1.77	0.67
26:2:56:VAL:HG11	26:2:91:SER:HB2	1.77	0.67
1:A:1154:ALA:HB1	1:A:1310:HIS:HE1	1.59	0.67
1:A:1471:PHE:CE1	6:F:64:ARG:HD3	2.30	0.67
1:A:932:ARG:CG	1:A:943:LEU:HD21	2.25	0.67
16:P:206:GLU:C	16:P:208:ARG:H	1.98	0.67
17:Q:113:ARG:HH12	18:R:218:LYS:HG3	1.60	0.67
27:3:130:GLU:HB2	27:3:173:GLN:NE2	2.09	0.67
2:B:1062:ARG:HH21	2:B:1065:GLY:H	1.41	0.67
3:C:134:ASN:C	3:C:136:ASP:OD1	2.33	0.67
2:B:57:ARG:NH1	2:B:537:GLN:OE1	2.27	0.66
26:2:160:LEU:H	26:2:160:LEU:HD12	1.60	0.66
27:3:207:CYS:SG	27:3:214:TYR:HB2	2.34	0.66
27:3:59:VAL:N	27:3:71:TYR:CD1	2.63	0.66
1:A:1158:LEU:CG	1:A:1308:TYR:CD2	2.78	0.66
1:A:729:PRO:HG2	21:U:250:MET:HB2	1.76	0.66
7:G:10:GLU:HB3	7:G:67:LEU:HD11	1.77	0.66
1:A:426:ARG:HD2	13:M:40:VAL:HG21	1.77	0.66
1:A:609:HIS:N	1:A:610:PRO:HD3	2.07	0.66
3:C:148:ILE:HG13	10:J:5:VAL:HG22	1.77	0.66
18:R:195:PRO:CB	18:R:199:LYS:HB2	2.14	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:X:14:DA:H2"	28:X:15:DA:C8	2.30	0.66
26:2:117:ASN:HD21	27:3:108:ASN:CA	2.05	0.66
27:3:146:ARG:O	27:3:149:LYS:HG2	1.95	0.66
22:V:366:ASN:ND2	22:V:613:THR:HG22	1.93	0.66
25:1:8:VAL:HG12	25:1:9:LEU:N	2.10	0.66
26:2:218:GLN:CG	26:2:268:PHE:HB3	2.26	0.66
1:A:199:TYR:CE2	13:M:93:PHE:HZ	2.14	0.66
5:E:29:THR:HB	5:E:32:GLU:HG3	1.77	0.66
18:R:204:ASN:CG	18:R:205:ASP:H	1.98	0.66
26:2:126:GLY:C	26:2:178:LEU:HD23	2.16	0.66
27:3:178:MET:HE2	27:3:202:LEU:HD12	1.78	0.66
27:3:18:ASN:CG	27:3:20:ILE:HD13	2.15	0.66
27:3:45:GLY:O	27:3:49:LEU:HD23	1.96	0.66
2:B:91:ILE:HG23	20:T:141:LEU:CD1	2.20	0.66
17:Q:180:PHE:CE1	18:R:213:ASP:CA	2.75	0.66
20:T:177:ARG:N	20:T:178:ALA:O	2.27	0.66
22:V:516:PRO:HD2	22:V:706:LYS:HZ3	1.60	0.66
1:A:549:THR:O	1:A:589:LYS:NZ	2.27	0.66
17:Q:141:ALA:HB1	17:Q:152:PHE:HE2	1.60	0.66
25:1:59:GLU:OE2	26:2:402:ARG:CZ	2.41	0.66
26:2:270:LEU:HD23	26:2:270:LEU:O	1.96	0.66
27:3:144:ILE:O	27:3:147:MET:HG3	1.96	0.66
26:2:30:VAL:CB	27:3:25:GLN:O	2.34	0.66
1:A:1309:MET:O	1:A:1309:MET:HG3	1.95	0.66
9:I:65:LEU:O	9:I:122:ARG:NH2	2.29	0.66
26:2:171:VAL:HG13	26:2:216:MET:CB	2.26	0.66
26:2:189:GLU:HA	26:2:192:GLU:CG	2.26	0.66
25:1:35:ILE:HG22	25:1:46:ILE:HD12	1.78	0.65
26:2:218:GLN:CD	26:2:265:LEU:HA	2.17	0.65
27:3:106:SER:O	27:3:110:VAL:HG23	1.97	0.65
1:A:926:ASN:CB	1:A:931:ARG:HH12	2.04	0.65
2:B:132:VAL:HG23	2:B:141:GLN:CB	2.26	0.65
12:L:35:ARG:NH1	12:L:42:ARG:HE	1.94	0.65
25:1:10:ILE:HG22	26:2:407:VAL:HG21	1.79	0.65
25:1:1:MET:SD	26:2:419:GLU:HB2	2.37	0.65
21:U:284:PRO:O	21:U:286:THR:N	2.28	0.65
26:2:270:LEU:HD23	26:2:273:GLN:HE21	1.62	0.65
27:3:137:LEU:HB3	27:3:180:VAL:CG1	2.20	0.65
8:H:72:ASP:O	8:H:73:GLY:O	2.15	0.65
22:V:631:GLY:O	22:V:632:SER:HB3	1.96	0.65
26:2:236:PHE:CZ	26:2:262:LEU:HD22	2.32	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:2:57:MET:HA	26:2:60:LEU:HD11	1.77	0.65
1:A:541:THR:O	1:A:545:VAL:HG23	1.97	0.65
1:A:929:ALA:O	1:A:930:LEU:HB2	1.95	0.65
1:A:930:LEU:HD23	1:A:934:LEU:CA	2.27	0.65
23:W:696:TRP:HD1	23:W:697:ILE:HG13	1.62	0.65
25:1:34:ILE:CG1	25:1:50:VAL:HG11	2.21	0.65
1:A:1022:ILE:HG23	1:A:1023:VAL:HG23	1.77	0.65
1:A:1319:LYS:HG2	1:A:1333:GLU:OE2	1.96	0.65
1:A:42:LYS:HE3	1:A:56:GLY:HA3	1.79	0.65
1:A:358:ARG:HH21	2:B:1076:GLU:HA	1.62	0.65
26:2:118:LEU:HD21	27:3:39:ASP:C	2.12	0.65
26:2:45:PHE:HB2	26:2:51:LEU:CD1	2.26	0.65
26:2:117:ASN:HD22	27:3:42:MET:HE1	1.60	0.65
18:R:202:PHE:C	18:R:203:PHE:CD1	2.70	0.65
27:3:184:ALA:CA	27:3:187:GLN:HG2	2.25	0.65
18:R:195:PRO:O	18:R:196:ASP:HB3	1.95	0.65
3:C:37:VAL:HG13	3:C:41:GLU:HB2	1.79	0.65
4:D:26:PHE:HZ	7:G:42:TYR:HA	1.60	0.65
26:2:192:GLU:HG3	26:2:193:PRO:CD	2.19	0.65
27:3:130:GLU:HB2	27:3:173:GLN:HE22	1.61	0.65
27:3:33:THR:CG2	27:3:36:LYS:HB2	2.26	0.65
27:3:59:VAL:HB	27:3:71:TYR:CD1	2.25	0.65
27:3:17:ALA:CB	27:3:63:HIS:HD2	2.10	0.65
1:A:190:ARG:NH2	28:X:58:DT:OP2	2.29	0.65
2:B:785:TYR:CZ	2:B:955:PRO:HD3	2.32	0.65
8:H:146:LYS:O	8:H:148:LEU:N	2.29	0.65
13:M:86:LYS:NZ	28:X:40:DT:C4	2.64	0.65
26:2:266:ARG:O	26:2:270:LEU:HB2	1.97	0.64
1:A:912:SER:H	1:A:1327:GLU:HB3	1.61	0.64
26:2:160:LEU:HB3	26:2:206:LEU:CD1	2.27	0.64
26:2:181:GLN:HG3	26:2:229:ASP:CG	2.18	0.64
26:2:211:GLN:CB	26:2:261:PHE:HE1	2.11	0.64
1:A:367:ILE:HG13	1:A:496:PHE:HD1	1.62	0.64
1:A:79:THR:CG2	13:M:43:ASP:CG	2.65	0.64
16:P:167:ASN:ND2	29:Y:79:DC:O2	2.26	0.64
25:1:35:ILE:HG22	25:1:46:ILE:CD1	2.27	0.64
27:3:14:VAL:HG22	27:3:163:VAL:HA	1.78	0.64
2:B:1137:CYS:HB3	2:B:1142:ASN:HB3	1.78	0.64
22:V:426:VAL:HG13	22:V:427:MET:H	1.63	0.64
27:3:192:ASP:HB2	27:3:231:PHE:CE1	2.32	0.64
9:I:63:ASP:OD1	9:I:66:THR:OG1	2.16	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:581:LEU:HD21	23:W:608:ILE:HG21	1.78	0.64
26:2:159:VAL:HG11	26:2:161:HIS:HD2	1.62	0.64
26:2:202:GLN:H	26:2:202:GLN:HE21	1.44	0.64
27:3:149:LYS:HG3	27:3:150:GLU:N	2.12	0.64
1:A:608:THR:HB	1:A:610:PRO:CD	2.28	0.64
9:I:84:HIS:CD2	9:I:84:HIS:H	2.13	0.64
12:L:35:ARG:HH12	12:L:42:ARG:HE	1.44	0.64
18:R:225:VAL:HG12	18:R:227:SER:CB	2.06	0.64
26:2:42:LEU:CD2	26:2:55:TRP:HB2	2.13	0.64
1:A:1309:MET:O	1:A:1311:LEU:HD12	1.97	0.64
20:T:20:LEU:HD23	20:T:113:ARG:HG2	1.79	0.64
22:V:366:ASN:ND2	22:V:613:THR:HG21	2.05	0.64
26:2:220:LEU:HD13	26:2:220:LEU:O	1.98	0.64
27:3:70:LEU:HD13	27:3:115:ILE:CD1	2.28	0.64
27:3:64:ILE:HB	27:3:123:ASP:OD2	1.98	0.64
2:B:1062:ARG:HH12	2:B:1075:MET:H	1.45	0.64
2:B:754:PRO:HB2	2:B:773:PRO:HG2	1.78	0.64
2:B:906:GLN:HG2	12:L:45:TYR:OH	1.98	0.64
18:R:154:LEU:CD2	18:R:163:LEU:CD2	2.73	0.64
22:V:321:GLU:CD	23:W:499:ASN:N	2.45	0.64
26:2:163:MET:HE1	26:2:206:LEU:HB3	1.80	0.64
27:3:58:ALA:CA	27:3:71:TYR:OH	2.39	0.64
2:B:501:LEU:HD12	2:B:505:LEU:HD12	1.79	0.64
23:W:59:TYR:CZ	23:W:62:ALA:HB2	2.29	0.64
1:A:640:LEU:HD23	1:A:645:LEU:HD11	1.79	0.64
8:H:137:VAL:HG22	8:H:138:ASP:H	1.63	0.64
17:Q:25:PHE:O	18:R:219:LEU:HD21	1.98	0.64
1:A:51:ARG:H	1:A:52:PRO:HD2	1.61	0.64
1:A:931:ARG:C	1:A:933:THR:H	1.99	0.64
2:B:761:THR:H	2:B:764:MET:CE	2.11	0.64
2:B:823:PHE:HA	13:M:140:ASN:HD21	1.63	0.64
13:M:16:PRO:CD	13:M:39:LEU:HD23	2.27	0.64
22:V:517:GLU:HB2	22:V:713:LEU:HD22	1.79	0.64
18:R:181:ALA:HA	18:R:184:ALA:HB3	1.80	0.63
26:2:100:LEU:HG	26:2:119:ARG:NE	2.13	0.63
26:2:177:GLN:OE1	26:2:220:LEU:HD22	1.98	0.63
27:3:131:THR:O	27:3:133:LEU:HD13	1.97	0.63
27:3:17:ALA:HB1	27:3:63:HIS:HD2	1.63	0.63
17:Q:68:GLY:O	18:R:226:ASP:CG	2.35	0.63
26:2:117:ASN:ND2	27:3:108:ASN:CA	2.57	0.63
27:3:160:ARG:NH2	27:3:190:LEU:HD12	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:VAL:HA	1:A:272:ASN:CB	2.28	0.63
17:Q:113:ARG:HD2	18:R:222:SER:CB	2.28	0.63
25:1:38:ILE:HB	25:1:44:PHE:HE1	1.63	0.63
1:A:1246:ILE:HD11	1:A:1258:ARG:HD2	1.81	0.63
16:P:297:LYS:O	16:P:299:ARG:N	2.26	0.63
26:2:28:PRO:HA	27:3:33:THR:HB	1.81	0.63
26:2:60:LEU:HD11	26:2:95:ILE:CB	2.29	0.63
27:3:18:ASN:CG	27:3:64:ILE:HD11	2.19	0.63
27:3:214:TYR:CE2	27:3:216:LYS:HE2	2.32	0.63
7:G:78:ARG:NH1	7:G:79:PRO:O	2.31	0.63
25:1:2:VAL:HG12	26:2:422:LEU:CD1	2.27	0.63
1:A:108:ARG:NH1	1:A:145:TYR:OH	2.32	0.63
17:Q:180:PHE:CZ	18:R:212:VAL:C	2.71	0.63
16:P:165:LEU:HD23	16:P:168:ILE:HD11	1.80	0.63
25:1:35:ILE:HA	25:1:46:ILE:HG13	1.80	0.63
26:2:140:LYS:HG2	26:2:162:PHE:CE1	2.33	0.63
26:2:258:LEU:HG	26:2:262:LEU:CD2	2.28	0.63
26:2:35:TYR:CZ	26:2:62:LEU:HG	2.34	0.63
2:B:747:LEU:HD11	2:B:810:PHE:CZ	2.34	0.63
26:2:123:LEU:HD23	26:2:123:LEU:O	1.99	0.63
26:2:173:GLN:HG2	26:2:179:LEU:HG	1.81	0.63
27:3:64:ILE:CG1	27:3:123:ASP:HB3	2.29	0.63
27:3:70:LEU:CD1	27:3:115:ILE:HD11	2.27	0.63
1:A:285:LYS:HE3	13:M:80:LEU:HD23	1.80	0.63
26:2:163:MET:HE3	26:2:206:LEU:HD12	1.81	0.62
27:3:134:ALA:HB2	27:3:176:ASN:OD1	1.99	0.62
1:A:930:LEU:HD23	1:A:934:LEU:HA	1.79	0.62
2:B:223:SER:OG	2:B:232:THR:O	2.17	0.62
26:2:89:LEU:HD23	26:2:89:LEU:O	1.99	0.62
26:2:93:LEU:HA	26:2:96:TRP:HD1	1.64	0.62
27:3:165:LYS:HD3	27:3:165:LYS:O	1.98	0.62
3:C:56:SER:OG	3:C:158:GLU:N	2.21	0.62
6:F:48:ASN:ND2	6:F:51:ARG:O	2.26	0.62
22:V:667:THR:HA	25:1:62:ASP:CG	2.19	0.62
1:A:265:VAL:HA	1:A:272:ASN:HB2	1.80	0.62
2:B:588:ARG:NH1	2:B:669:GLU:OE2	2.31	0.62
12:L:16:ILE:HG21	12:L:47:LYS:HD2	1.81	0.62
25:1:38:ILE:HB	25:1:44:PHE:CE1	2.35	0.62
25:1:18:GLN:NE2	25:1:44:PHE:HZ	1.97	0.62
25:1:50:VAL:HA	25:1:53:LEU:HD13	1.82	0.62
1:A:673:GLN:O	1:A:677:ASN:HB2	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:931:ARG:O	1:A:933:THR:N	2.33	0.62
2:B:80:GLU:O	2:B:82:PRO:HD3	1.98	0.62
5:E:64:HIS:CD2	5:E:68:PRO:CA	2.81	0.62
9:I:61:GLU:C	9:I:63:ASP:N	2.52	0.62
13:M:90:ALA:HB2	13:M:100:LYS:HE3	1.80	0.62
18:R:195:PRO:CD	18:R:199:LYS:HB2	2.25	0.62
23:W:584:TYR:CG	23:W:594:ALA:HB2	2.34	0.62
27:3:133:LEU:HD22	27:3:134:ALA:N	2.14	0.62
1:A:924:TYR:O	1:A:926:ASN:ND2	2.32	0.62
2:B:749:HIS:CD2	2:B:810:PHE:CD1	2.88	0.62
13:M:7:LEU:HD21	13:M:10:LEU:CD1	2.29	0.62
19:S:48:GLU:OE1	19:S:101:ARG:NH2	2.33	0.62
23:W:59:TYR:CE2	23:W:62:ALA:HB2	2.22	0.62
25:1:47:ALA:HB1	25:1:50:VAL:HB	1.81	0.62
26:2:181:GLN:CD	26:2:229:ASP:HB2	2.19	0.62
1:A:931:ARG:CZ	1:A:931:ARG:HA	2.29	0.62
15:O:84:VAL:HG23	15:O:85:THR:HG23	1.81	0.62
14:N:318:ASP:OD1	16:P:239:ARG:NH2	2.32	0.62
17:Q:60:ARG:O	17:Q:64:ASN:ND2	2.28	0.62
19:S:166:ARG:HH11	19:S:166:ARG:HG3	1.62	0.62
5:E:84:ILE:HD11	28:X:65:DG:P	2.39	0.62
26:2:189:GLU:O	26:2:193:PRO:HD2	2.00	0.62
1:A:133:SER:O	1:A:135:GLY:N	2.33	0.62
2:B:249:LYS:O	2:B:249:LYS:HG2	1.98	0.62
17:Q:109:HIS:HE1	18:R:233:ILE:HG21	1.64	0.62
13:M:178:LYS:HZ2	20:T:156:VAL:HG11	1.63	0.62
25:1:8:VAL:O	26:2:407:VAL:HG12	1.99	0.62
26:2:46:ARG:CD	26:2:85:GLU:HB2	2.30	0.62
26:2:31:LEU:CG	27:3:33:THR:HB	2.28	0.62
17:Q:113:ARG:CZ	18:R:218:LYS:HG3	2.29	0.62
24:0:100:PRO:HG3	27:3:208:ASP:OD2	1.99	0.62
2:B:998:ASP:OD1	2:B:999:ALA:N	2.32	0.62
8:H:108:ALA:O	8:H:110:THR:N	2.32	0.62
25:1:1:MET:HG2	26:2:414:SER:N	2.15	0.62
26:2:44:VAL:HG13	26:2:45:PHE:HD1	1.59	0.62
27:3:9:ASN:O	27:3:56:LYS:HD3	1.99	0.62
2:B:132:VAL:CG2	2:B:141:GLN:HB3	2.28	0.62
9:I:104:ALA:O	9:I:105:GLU:C	2.37	0.62
26:2:218:GLN:HG2	26:2:268:PHE:HB3	1.82	0.61
27:3:18:ASN:O	27:3:21:TRP:HD1	1.83	0.61
2:B:898:THR:O	2:B:900:GLU:HG3	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:59:TYR:OH	23:W:63:TYR:CE2	2.52	0.61
27:3:190:LEU:H	27:3:190:LEU:CD2	2.11	0.61
2:B:1144:THR:O	2:B:1146:ILE:N	2.33	0.61
15:O:75:VAL:HG22	15:O:94:LYS:HG2	1.81	0.61
25:1:1:MET:HB2	26:2:418:PHE:HB3	1.81	0.61
26:2:60:LEU:CD1	26:2:95:ILE:HB	2.31	0.61
26:2:30:VAL:CG2	27:3:25:GLN:CB	2.48	0.61
1:A:1316:ASN:ND2	1:A:1318:LYS:HE3	2.14	0.61
1:A:1319:LYS:HB3	1:A:1331:LEU:HB3	1.81	0.61
3:C:154:ARG:HD3	10:J:65:LEU:HD11	1.81	0.61
19:S:100:LEU:HD23	19:S:110:PHE:HD2	1.64	0.61
28:X:32:DT:H4'	28:X:33:DT:H5'	1.82	0.61
2:B:42:GLN:HG2	2:B:43:GLN:N	2.15	0.61
2:B:380:ARG:NE	2:B:609:GLU:OE2	2.34	0.61
23:W:584:TYR:HB2	23:W:594:ALA:HB2	1.81	0.61
27:3:184:ALA:HA	27:3:187:GLN:CG	2.29	0.61
1:A:344:LYS:HA	1:A:1435:THR:HG21	1.82	0.61
1:A:199:TYR:CZ	13:M:93:PHE:CZ	2.87	0.61
23:W:37:HIS:CE1	23:W:454:VAL:CG1	2.83	0.61
1:A:1158:LEU:CG	1:A:1308:TYR:CE2	2.83	0.61
1:A:455:ILE:HD13	1:A:520:MET:HE3	1.81	0.61
2:B:78:VAL:O	2:B:78:VAL:HG12	2.00	0.61
13:M:50:SER:O	13:M:53:ARG:HB2	2.01	0.61
18:R:204:ASN:CG	18:R:205:ASP:N	2.53	0.61
26:2:251:VAL:CG1	26:2:254:MET:HG3	2.30	0.61
27:3:100:LYS:HG3	27:3:101:TYR:N	2.16	0.61
1:A:1158:LEU:HD13	1:A:1336:LEU:HD22	1.81	0.61
1:A:685:HIS:HB3	2:B:784:SER:OG	2.01	0.61
1:A:883:ILE:HG13	1:A:885:GLN:HG3	1.82	0.61
1:A:1177:TYR:OH	9:I:28:GLU:OE2	2.14	0.61
24:0:77:LYS:H	24:0:77:LYS:HD2	1.66	0.61
1:A:608:THR:CA	1:A:610:PRO:HD2	2.31	0.61
1:A:1112:VAL:O	21:U:252:LYS:HB2	1.99	0.61
8:H:66:GLU:HA	8:H:66:GLU:OE2	2.00	0.61
2:B:823:PHE:HA	13:M:140:ASN:ND2	2.16	0.61
18:R:163:LEU:HD12	18:R:163:LEU:O	2.01	0.61
22:V:368:ALA:O	22:V:371:VAL:HG22	2.00	0.61
26:2:203:PHE:HD2	26:2:205:LEU:HD23	1.64	0.61
26:2:236:PHE:CE2	26:2:262:LEU:HD13	2.36	0.61
27:3:8:LEU:HA	27:3:54:SER:HB3	1.83	0.61
2:B:529:MET:SD	2:B:623:ARG:HB2	2.41	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:64:PRO:O	10:J:66:GLU:N	2.34	0.61
25:1:13:ASP:OD1	25:1:14:PRO:CD	2.48	0.60
26:2:30:VAL:HG12	26:2:34:LEU:HD23	1.82	0.60
26:2:56:VAL:HG11	26:2:91:SER:CB	2.31	0.60
1:A:379:GLY:HA2	1:A:475:ARG:O	2.01	0.60
7:G:52:ASP:H	7:G:72:TYR:HA	1.64	0.60
16:P:153:THR:N	16:P:326:GLU:OE2	2.34	0.60
26:2:28:PRO:CA	27:3:25:GLN:C	2.69	0.60
1:A:1304:ILE:O	1:A:1307:VAL:HG23	2.00	0.60
1:A:786:ALA:O	1:A:826:SER:HB3	2.00	0.60
25:1:1:MET:HA	26:2:414:SER:N	2.15	0.60
27:3:58:ALA:CA	27:3:71:TYR:CE2	2.76	0.60
1:A:930:LEU:HB3	1:A:934:LEU:CB	2.23	0.60
2:B:968:ASN:OD1	2:B:969:PRO:HD2	2.00	0.60
27:3:143:TYR:O	27:3:146:ARG:HG2	2.01	0.60
1:A:95:PHE:N	1:A:311:GLN:OE1	2.31	0.60
12:L:17:TYR:CD1	12:L:46:LYS:HG3	2.29	0.60
13:M:91:ALA:O	13:M:93:PHE:N	2.35	0.60
26:2:117:ASN:ND2	27:3:42:MET:CE	2.60	0.60
26:2:83:GLN:OE1	26:2:83:GLN:HA	2.01	0.60
27:3:196:LEU:CD2	27:3:223:LEU:HD23	2.25	0.60
27:3:21:TRP:O	27:3:24:LYS:HB2	2.02	0.60
2:B:333:GLU:OE1	19:S:53:ASN:ND2	2.27	0.60
5:E:64:HIS:CG	5:E:68:PRO:HA	2.36	0.60
9:I:65:LEU:HD22	9:I:122:ARG:HG2	1.82	0.60
14:N:21:VAL:HG21	15:O:40:PHE:HD1	1.67	0.60
17:Q:52:LEU:HB3	17:Q:54:PHE:CD2	2.32	0.60
23:W:73:CYS:CB	23:W:209:TYR:CZ	2.84	0.60
25:1:1:MET:HA	26:2:413:LEU:HA	1.83	0.60
24:0:97:ASP:C	27:3:208:ASP:HB2	2.12	0.60
2:B:247:ALA:O	19:S:169:LYS:NZ	2.25	0.60
2:B:73:HIS:C	2:B:75:SER:H	2.04	0.60
1:A:26:LEU:HD23	2:B:1168:ALA:HB2	1.84	0.60
1:A:623:PRO:C	1:A:625:ASP:H	2.04	0.60
2:B:898:THR:O	2:B:900:GLU:N	2.35	0.60
9:I:80:ARG:HD3	9:I:95:VAL:HG12	1.83	0.60
18:R:118:TRP:NE1	18:R:122:GLU:OE1	2.34	0.60
28:X:70:DG:N2	29:Y:25:DT:C2	2.70	0.60
27:3:222:SER:HB2	27:3:226:TYR:CE2	2.37	0.60
2:B:676:ALA:HB2	2:B:693:TYR:CD1	2.36	0.60
2:B:790:GLN:HA	2:B:968:ASN:HD22	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:41:LYS:HG3	5:E:46:ASP:CG	2.22	0.60
18:R:195:PRO:CG	18:R:199:LYS:C	2.69	0.60
23:W:419:GLU:O	23:W:420:PRO:O	2.19	0.60
26:2:173:GLN:CD	26:2:179:LEU:HD21	2.21	0.60
26:2:164:VAL:HG13	26:2:209:PRO:HG2	1.83	0.60
26:2:30:VAL:HG23	27:3:25:GLN:HB2	1.74	0.60
1:A:201:GLU:HG3	1:A:212:LYS:HB3	1.84	0.60
2:B:489:ILE:HG21	2:B:522:LEU:HD13	1.83	0.60
23:W:209:TYR:CE1	23:W:233:PHE:CD1	2.89	0.60
23:W:584:TYR:HB2	23:W:594:ALA:CB	2.32	0.60
29:Y:24:DC:C2	29:Y:25:DT:O4	2.55	0.60
27:3:213:LEU:HD23	27:3:230:VAL:HG12	1.84	0.59
1:A:575:PRO:HG2	1:A:594:LEU:HD11	1.83	0.59
21:U:250:MET:O	21:U:251:ALA:HB2	2.02	0.59
26:2:202:GLN:H	26:2:202:GLN:NE2	2.00	0.59
26:2:196:ILE:HA	26:2:202:GLN:OE1	2.02	0.59
3:C:59:LEU:HD22	3:C:151:VAL:HG23	1.84	0.59
26:2:159:VAL:HG13	26:2:160:LEU:N	2.17	0.59
1:A:1117:VAL:O	1:A:1118:THR:C	2.40	0.59
2:B:718:GLN:HG2	2:B:720:PRO:HD2	1.84	0.59
5:E:64:HIS:CD2	5:E:68:PRO:C	2.70	0.59
13:M:90:ALA:HB2	13:M:100:LYS:CE	2.31	0.59
26:2:206:LEU:HD22	26:2:206:LEU:N	2.17	0.59
27:3:110:VAL:O	27:3:114:GLU:HG2	2.02	0.59
27:3:160:ARG:HB3	27:3:190:LEU:CD2	2.32	0.59
9:I:41:ASN:HA	19:S:177:MET:HE1	1.84	0.59
17:Q:24:GLY:HA2	18:R:209:GLN:HG2	1.84	0.59
18:R:195:PRO:HG3	18:R:199:LYS:HB3	1.72	0.59
22:V:612:ASP:CG	22:V:635:GLN:CD	2.60	0.59
25:1:53:LEU:HD12	25:1:53:LEU:N	2.18	0.59
27:3:14:VAL:HG23	27:3:163:VAL:HA	1.84	0.59
1:A:200:ALA:O	1:A:213:LYS:HA	2.03	0.59
1:A:263:ALA:HB1	1:A:272:ASN:CB	2.32	0.59
13:M:17:ASN:OD1	13:M:18:HIS:ND1	2.35	0.59
23:W:584:TYR:CE2	23:W:614:TYR:HB2	2.37	0.59
28:X:49:DT:H3'	28:X:50:DT:H5"	1.83	0.59
2:B:254:GLN:HG3	2:B:303:PRO:HG2	1.85	0.59
2:B:873:LEU:HB3	2:B:874:PRO:CD	2.31	0.59
7:G:110:ARG:NH2	7:G:118:GLU:OE2	2.36	0.59
9:I:105:GLU:HB3	9:I:107:ALA:CB	2.33	0.59
20:T:129:ARG:HA	20:T:132:ILE:HD12	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:0:55:LEU:HD12	27:3:178:MET:CE	2.31	0.59
1:A:1127:LEU:HD21	1:A:1381:GLU:HB3	1.84	0.59
1:A:540:ASP:CB	2:B:790:GLN:HE21	2.15	0.59
1:A:932:ARG:HB2	1:A:943:LEU:HD11	1.85	0.59
5:E:46:ASP:C	5:E:48:PRO:HD3	2.20	0.59
17:Q:113:ARG:NH2	18:R:218:LYS:HE2	2.11	0.59
17:Q:98:THR:HG22	17:Q:100:VAL:H	1.67	0.59
26:2:160:LEU:HD12	26:2:160:LEU:N	2.18	0.59
26:2:203:PHE:CE2	26:2:205:LEU:HD23	2.38	0.59
26:2:44:VAL:HG13	26:2:45:PHE:N	2.17	0.59
26:2:117:ASN:CG	27:3:108:ASN:ND2	2.50	0.59
1:A:1016:LEU:HD22	1:A:1069:LEU:HD22	1.83	0.59
1:A:199:TYR:CZ	13:M:93:PHE:HZ	2.19	0.59
1:A:540:ASP:HB2	2:B:790:GLN:HE21	1.66	0.59
1:A:926:ASN:OD1	1:A:931:ARG:NH1	2.35	0.59
2:B:841:ARG:NH2	2:B:893:SER:O	2.35	0.59
6:F:88:ASP:OD2	6:F:91:LEU:N	2.35	0.59
7:G:145:LEU:HD13	7:G:161:GLY:HA3	1.84	0.59
12:L:17:TYR:CD1	12:L:46:LYS:HA	2.37	0.59
13:M:218:PHE:HD1	13:M:277:ILE:HG22	1.67	0.59
23:W:37:HIS:ND1	23:W:454:VAL:HG13	2.16	0.59
26:2:217:LEU:HD23	26:2:233:ILE:CD1	2.32	0.59
1:A:998:PRO:HA	1:A:1059:ARG:HG2	1.85	0.59
1:A:354:LEU:O	1:A:357:LYS:HE2	2.02	0.59
1:A:386:ALA:O	1:A:449:HIS:ND1	2.35	0.59
1:A:932:ARG:CD	1:A:943:LEU:CD2	2.50	0.59
2:B:216:ALA:HB2	2:B:241:ALA:HB2	1.84	0.59
25:1:22:TYR:O	25:1:25:GLU:HB3	2.03	0.59
25:1:34:ILE:O	25:1:46:ILE:HG13	2.03	0.59
27:3:173:GLN:CA	27:3:176:ASN:HD21	2.10	0.59
2:B:1040:GLN:HG2	3:C:203:TRP:CZ2	2.38	0.59
17:Q:112:ARG:HD3	18:R:237:LEU:CD1	2.22	0.59
28:X:15:DA:N1	29:Y:79:DC:N3	2.51	0.59
26:2:171:VAL:HG13	26:2:216:MET:HB2	1.83	0.58
27:3:131:THR:CG2	27:3:133:LEU:HD12	2.33	0.58
27:3:215:LEU:CD1	27:3:230:VAL:HG13	2.32	0.58
26:2:30:VAL:CB	27:3:25:GLN:HB3	2.33	0.58
27:3:71:TYR:CG	27:3:72:PRO:HD2	2.19	0.58
1:A:264:VAL:HG23	1:A:272:ASN:ND2	2.18	0.58
2:B:921:ILE:HG13	2:B:921:ILE:O	2.03	0.58
17:Q:25:PHE:CD1	18:R:210:PHE:CZ	2.90	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:2:215:PHE:CD2	26:2:264:HIS:HB2	2.38	0.58
27:3:131:THR:HG23	27:3:133:LEU:CD1	2.33	0.58
18:R:212:VAL:O	18:R:213:ASP:CG	2.41	0.58
23:W:419:GLU:HB3	23:W:420:PRO:HD3	1.82	0.58
25:1:18:GLN:HB2	25:1:44:PHE:CZ	2.37	0.58
26:2:177:GLN:HE22	26:2:220:LEU:HA	1.68	0.58
25:1:2:VAL:HB	26:2:456:LYS:HD3	1.85	0.58
26:2:35:TYR:CB	26:2:62:LEU:HD12	2.33	0.58
27:3:169:ASP:CB	27:3:202:LEU:HD23	2.33	0.58
3:C:6:GLN:O	11:K:104:ARG:NH1	2.35	0.58
27:3:190:LEU:HD23	27:3:190:LEU:N	2.18	0.58
1:A:1307:VAL:O	1:A:1307:VAL:HG12	2.03	0.58
10:J:63:ALA:CB	10:J:64:PRO:HD3	2.18	0.58
16:P:171:THR:HG22	16:P:220:VAL:HG13	1.85	0.58
25:1:38:ILE:CD1	25:1:38:ILE:H	2.16	0.58
25:1:2:VAL:CG1	26:2:456:LYS:CD	2.82	0.58
2:B:1104:ARG:O	2:B:1108:PHE:HB3	2.04	0.58
3:C:85:SER:HB2	3:C:166:LYS:HE3	1.86	0.58
5:E:133:GLN:N	5:E:133:GLN:OE1	2.36	0.58
12:L:17:TYR:HE1	12:L:46:LYS:CD	2.14	0.58
1:A:1191:GLU:O	1:A:1195:VAL:HG23	2.04	0.58
1:A:376:ASP:HB3	1:A:522:PRO:HD3	1.84	0.58
1:A:641:CYS:SG	1:A:643:LYS:N	2.77	0.58
2:B:798:ARG:HD3	2:B:950:ARG:HG2	1.86	0.58
1:A:865:ILE:HG13	1:A:866:LYS:N	2.17	0.58
25:1:34:ILE:HG22	25:1:46:ILE:CD1	2.32	0.58
1:A:927:GLU:O	1:A:929:ALA:N	2.37	0.58
27:3:205:GLN:O	27:3:208:ASP:CG	2.42	0.58
27:3:71:TYR:HD2	27:3:72:PRO:HD2	1.68	0.58
1:A:244:ARG:HD2	1:A:245:PRO:HD2	1.85	0.58
5:E:52:ARG:HG3	5:E:54:ARG:HG3	1.85	0.58
25:1:1:MET:HB3	26:2:413:LEU:HG	1.83	0.58
25:1:59:GLU:CD	26:2:402:ARG:NH1	2.56	0.58
26:2:117:ASN:CG	27:3:42:MET:HE2	2.23	0.58
26:2:236:PHE:CZ	26:2:258:LEU:HD11	2.39	0.58
27:3:14:VAL:HG23	27:3:163:VAL:HG13	1.86	0.58
1:A:1029:LEU:H	5:E:162:ARG:NH1	2.02	0.58
1:A:264:VAL:O	1:A:266:MET:N	2.36	0.58
2:B:1090:GLU:N	2:B:1090:GLU:OE1	2.37	0.58
11:K:63:VAL:HB	11:K:71:ILE:HG22	1.86	0.58
27:3:16:ASP:O	27:3:21:TRP:NE1	2.27	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:2:30:VAL:N	27:3:25:GLN:HB3	2.19	0.57
27:3:59:VAL:CB	27:3:71:TYR:HE1	1.95	0.57
1:A:606:HIS:CG	1:A:607:SER:N	2.72	0.57
2:B:819:SER:HB3	2:B:821:LYS:HG3	1.84	0.57
3:C:60:HIS:NE2	3:C:63:PHE:HB2	2.18	0.57
21:U:257:GLN:HA	21:U:257:GLN:NE2	2.19	0.57
1:A:1102:MET:HG2	21:U:277:GLN:HB2	1.85	0.57
25:1:8:VAL:HG12	25:1:9:LEU:H	1.69	0.57
26:2:82:ALA:HA	26:2:89:LEU:HD11	1.85	0.57
27:3:21:TRP:CD2	27:3:34:LEU:HD23	2.39	0.57
1:A:537:ILE:HG13	1:A:672:ILE:HD13	1.86	0.57
2:B:839:GLY:HA3	2:B:891:ASP:HB3	1.86	0.57
17:Q:25:PHE:CD1	18:R:210:PHE:HZ	2.23	0.57
27:3:216:LYS:H	27:3:216:LYS:CD	2.13	0.57
3:C:154:ARG:HB3	10:J:65:LEU:CD2	2.34	0.57
2:B:812:ARG:HH22	29:Y:52:DT:P	2.26	0.57
1:A:608:THR:CB	1:A:610:PRO:CD	2.83	0.57
2:B:438:ARG:NE	2:B:442:ASP:OD2	2.31	0.57
13:M:16:PRO:CG	13:M:39:LEU:HD21	2.30	0.57
23:W:209:TYR:OH	23:W:233:PHE:C	2.42	0.57
22:V:315:VAL:HG12	23:W:500:ASP:CB	2.17	0.57
24:0:109:THR:HB	24:0:144:SER:H	1.67	0.57
27:3:215:LEU:HD12	27:3:230:VAL:HG13	1.85	0.57
2:B:1029:TYR:CE1	2:B:1036:LYS:HG2	2.39	0.57
2:B:230:ARG:HD2	2:B:405:ARG:HH12	1.69	0.57
2:B:255:ARG:NE	2:B:307:GLU:OE2	2.38	0.57
12:L:27:GLU:OE1	12:L:27:GLU:HA	2.04	0.57
22:V:325:ARG:HH21	23:W:499:ASN:CG	2.08	0.57
23:W:584:TYR:CB	23:W:594:ALA:HB2	2.33	0.57
5:E:84:ILE:HD11	28:X:64:DC:H3'	1.87	0.57
26:2:197:THR:HG21	26:2:239:GLN:CD	2.25	0.57
25:1:1:MET:CG	26:2:418:PHE:HB2	2.35	0.57
1:A:1196:TYR:OH	1:A:1247:PHE:O	2.12	0.57
2:B:290:TYR:CE2	2:B:562:ALA:HA	2.39	0.57
5:E:46:ASP:C	5:E:48:PRO:CD	2.73	0.57
17:Q:113:ARG:CD	18:R:222:SER:HB2	2.34	0.57
27:3:144:ILE:HG12	27:3:147:MET:CE	2.34	0.57
27:3:223:LEU:HD11	27:3:227:LEU:HD11	1.87	0.57
1:A:1281:ASP:O	1:A:1285:LEU:N	2.35	0.57
1:A:789:GLY:HA2	1:A:822:PHE:CE1	2.40	0.57
2:B:690:CYS:SG	2:B:691:SER:N	2.76	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:35:ARG:HH12	12:L:42:ARG:NH2	2.02	0.57
29:Y:39:DG:H2'	29:Y:40:DT:C6	2.40	0.57
27:3:59:VAL:N	27:3:71:TYR:CZ	2.69	0.57
1:A:601:ASN:HD21	1:A:632:ASN:H	1.52	0.57
2:B:223:SER:HB2	2:B:349:PRO:HD2	1.87	0.57
17:Q:105:TYR:CD1	18:R:234:GLU:HB2	2.40	0.57
27:3:187:GLN:NE2	27:3:189:ILE:HG13	2.20	0.57
1:A:1312:PRO:HB3	1:A:1334:TRP:HZ3	1.65	0.57
2:B:1062:ARG:NH1	2:B:1074:PRO:HB3	2.19	0.57
26:2:185:MET:HB2	26:2:229:ASP:OD1	2.04	0.57
27:3:19:PRO:HG2	27:3:123:ASP:O	2.05	0.57
2:B:1069:ILE:HD11	13:M:45:VAL:HG22	1.87	0.57
1:A:1443:ALA:HB2	2:B:1167:ILE:HG23	1.86	0.57
2:B:857:GLY:HA2	2:B:903:ILE:HD11	1.86	0.57
14:N:319:ASP:C	14:N:321:SER:H	2.08	0.57
18:R:214:GLU:OE1	18:R:217:GLN:NE2	2.32	0.57
25:1:9:LEU:CB	25:1:51:ASN:HD21	2.14	0.56
1:A:274:ASP:OD2	1:A:276:LEU:HB3	2.05	0.56
18:R:142:LYS:HD3	18:R:145:VAL:HG23	1.87	0.56
17:Q:184:ILE:CD1	18:R:218:LYS:HZ2	2.16	0.56
25:1:1:MET:CB	26:2:418:PHE:HB2	2.35	0.56
26:2:60:LEU:HD11	26:2:95:ILE:CG2	2.35	0.56
27:3:46:ASN:CG	27:3:104:LEU:HD22	2.25	0.56
16:P:298:PRO:O	16:P:299:ARG:C	2.43	0.56
25:1:52:VAL:HG22	25:1:53:LEU:HD12	1.87	0.56
26:2:117:ASN:HB2	27:3:104:LEU:CD1	2.35	0.56
27:3:195:VAL:HG21	27:3:214:TYR:OH	2.05	0.56
2:B:1040:GLN:CD	2:B:1040:GLN:H	2.08	0.56
2:B:232:THR:OG1	2:B:233:SER:N	2.38	0.56
13:M:60:ALA:HB1	29:Y:54:DA:H2	1.70	0.56
13:M:178:LYS:HB3	20:T:154:LYS:CD	2.35	0.56
21:U:256:THR:HB	21:U:272:THR:CB	2.35	0.56
22:V:428:GLU:OE1	22:V:460:ALA:HA	2.05	0.56
22:V:514:MET:SD	22:V:537:ASN:ND2	2.78	0.56
27:3:178:MET:SD	27:3:181:ILE:HD12	2.46	0.56
27:3:42:MET:SD	27:3:111:ILE:HD13	2.46	0.56
1:A:1128:ILE:HG23	1:A:1414:ILE:HD11	1.87	0.56
1:A:623:PRO:O	1:A:625:ASP:N	2.38	0.56
12:L:16:ILE:HG21	12:L:47:LYS:CD	2.35	0.56
1:A:305:GLU:OE1	13:M:102:GLN:NE2	2.38	0.56
13:M:179:GLU:HG3	20:T:154:LYS:HE2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:1:31:LYS:O	25:1:32:LYS:HB2	2.06	0.56
27:3:144:ILE:HD13	27:3:147:MET:HE3	1.86	0.56
2:B:499:ARG:NH2	2:B:522:LEU:HD11	2.20	0.56
3:C:136:ASP:OD1	3:C:136:ASP:N	2.36	0.56
3:C:5:ASN:ND2	3:C:25:ASN:HD21	2.03	0.56
21:U:243:GLU:CD	21:U:246:ARG:HH12	2.08	0.56
27:3:24:LYS:O	27:3:25:GLN:C	2.44	0.56
1:A:910:LYS:HD2	1:A:911:PRO:HD2	1.86	0.56
2:B:513:GLU:CD	2:B:707:CYS:HB2	2.26	0.56
17:Q:112:ARG:NE	18:R:237:LEU:HD12	2.13	0.56
26:2:130:SER:HB2	26:2:173:GLN:OE1	2.06	0.56
27:3:223:LEU:O	27:3:223:LEU:HD13	2.06	0.56
1:A:608:THR:C	1:A:610:PRO:CD	2.50	0.56
1:A:832:THR:N	1:A:835:GLU:OE1	2.25	0.56
29:Y:24:DC:N1	29:Y:25:DT:C4	2.74	0.56
25:1:1:MET:HB2	26:2:418:PHE:HB2	1.88	0.56
1:A:522:PRO:CA	1:A:666:ARG:HE	2.10	0.56
12:L:35:ARG:NH1	12:L:42:ARG:HH21	2.04	0.56
13:M:89:GLY:O	13:M:90:ALA:HB3	2.01	0.56
17:Q:113:ARG:CZ	18:R:218:LYS:CG	2.84	0.56
25:1:36:GLN:HB3	25:1:45:VAL:HG12	1.88	0.56
1:A:265:VAL:O	1:A:272:ASN:OD1	2.23	0.56
2:B:555:GLU:OE1	19:S:124:TYR:OH	2.18	0.56
3:C:133:ARG:CA	3:C:136:ASP:OD2	2.42	0.56
13:M:183:VAL:HG12	20:T:152:ASN:HD21	1.70	0.56
25:1:10:ILE:C	25:1:10:ILE:HD13	2.26	0.56
26:2:160:LEU:H	26:2:160:LEU:CD1	2.18	0.56
26:2:47:GLU:HG3	26:2:48:LEU:N	2.20	0.56
1:A:1223:ASP:OD1	1:A:1224:ARG:NH1	2.39	0.56
1:A:293:ASN:OD1	1:A:298:ALA:HA	2.06	0.56
26:2:181:GLN:HE21	26:2:181:GLN:HA	1.70	0.56
26:2:423:ALA:HA	26:2:426:ARG:HE	1.70	0.56
1:A:625:ASP:O	1:A:638:GLY:HA2	2.06	0.56
1:A:632:ASN:CA	1:A:992:LYS:HD2	2.36	0.56
5:E:6:GLU:OE2	5:E:9:ARG:NH1	2.39	0.56
11:K:16:GLU:OE1	11:K:36:ASN:ND2	2.39	0.56
19:S:46:ARG:NH2	20:T:2:ALA:O	2.39	0.56
27:3:44:LEU:HD13	27:3:44:LEU:O	2.06	0.55
1:A:1222:THR:HB	21:U:241:THR:HG21	1.88	0.55
1:A:207:GLU:O	1:A:209:SER:N	2.39	0.55
22:V:520:ARG:NE	22:V:521:GLU:OE2	2.29	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:2:206:LEU:H	26:2:206:LEU:HD22	1.71	0.55
27:3:210:THR:O	27:3:210:THR:HG22	2.04	0.55
1:A:265:VAL:C	1:A:272:ASN:OD1	2.44	0.55
1:A:522:PRO:HB3	1:A:666:ARG:CG	2.36	0.55
8:H:65:TYR:CE2	8:H:70:LEU:HD13	2.40	0.55
28:X:47:DT:H3'	28:X:48:DT:H5"	1.88	0.55
28:X:53:DA:H2'	28:X:54:DA:C8	2.40	0.55
1:A:121:SER:HA	1:A:126:ILE:HG21	1.87	0.55
1:A:936:GLU:HA	1:A:1002:SER:HB2	1.89	0.55
10:J:63:ALA:N	10:J:64:PRO:CD	2.69	0.55
17:Q:153:ARG:HH11	17:Q:158:HIS:HB3	1.72	0.55
18:R:154:LEU:HD23	18:R:163:LEU:CD2	2.24	0.55
21:U:256:THR:CA	21:U:272:THR:HG22	2.36	0.55
2:B:529:MET:HG2	2:B:530:ALA:N	2.22	0.55
8:H:106:THR:O	8:H:108:ALA:N	2.37	0.55
8:H:64:LEU:H	8:H:70:LEU:HD21	1.71	0.55
26:2:259:LEU:C	26:2:259:LEU:HD12	2.27	0.55
23:W:209:TYR:HH	23:W:233:PHE:CA	2.09	0.55
25:1:52:VAL:HG23	25:1:53:LEU:N	2.21	0.55
26:2:28:PRO:HD2	27:3:25:GLN:CD	2.26	0.55
1:A:61:ARG:HB3	1:A:72:GLN:HE21	1.71	0.55
8:H:74:GLU:C	8:H:75:TYR:HD1	2.07	0.55
22:V:504:LYS:HD2	22:V:654:GLU:O	2.07	0.55
26:2:53:LYS:CE	26:2:95:ILE:HD11	2.35	0.55
1:A:1143:LEU:HD11	1:A:1336:LEU:HG	1.88	0.55
1:A:624:GLY:O	1:A:626:THR:N	2.35	0.55
2:B:360:LYS:HG3	2:B:553:LEU:HD23	1.88	0.55
5:E:84:ILE:HG23	28:X:64:DC:OP1	2.05	0.55
2:B:1094:GLN:NE2	2:B:1102:PHE:HD2	2.04	0.55
3:C:70:LEU:HD23	10:J:5:VAL:O	2.07	0.55
19:S:31:PHE:HB2	20:T:92:THR:HB	1.89	0.55
21:U:291:CYS:SG	21:U:293:GLU:HB2	2.46	0.55
1:A:1109:TYR:HE2	1:A:1113:SER:H	1.55	0.55
1:A:522:PRO:HB3	1:A:666:ARG:HG3	1.89	0.55
5:E:94:MET:HB2	5:E:99:ILE:HD11	1.88	0.55
2:B:1076:GLU:HB2	13:M:54:THR:OG1	2.06	0.55
16:P:205:ARG:O	16:P:206:GLU:C	2.42	0.55
20:T:58:LEU:HD23	20:T:63:ALA:HB2	1.87	0.55
25:1:34:ILE:HG23	25:1:50:VAL:HG11	1.89	0.55
26:2:123:LEU:CD2	26:2:178:LEU:HD11	2.37	0.55
26:2:208:THR:O	26:2:212:LEU:HG	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:3:223:LEU:HD13	27:3:227:LEU:HG	1.89	0.55
9:I:61:GLU:O	9:I:62:VAL:C	2.46	0.55
13:M:52:TRP:O	13:M:52:TRP:CD1	2.60	0.55
16:P:239:ARG:NH1	16:P:242:GLN:OE1	2.40	0.55
17:Q:102:VAL:HG23	17:Q:102:VAL:O	2.06	0.55
22:V:638:GLN:O	22:V:642:ARG:HG2	2.07	0.55
24:0:54:ARG:CG	27:3:182:PHE:CZ	2.80	0.54
24:0:77:LYS:HD2	24:0:77:LYS:N	2.21	0.54
26:2:123:LEU:HD21	26:2:178:LEU:CD1	2.38	0.54
26:2:177:GLN:NE2	26:2:220:LEU:HA	2.22	0.54
24:0:54:ARG:CB	27:3:209:ILE:HG23	2.25	0.54
2:B:914:GLU:N	2:B:914:GLU:OE1	2.40	0.54
16:P:256:GLN:O	16:P:316:LYS:NZ	2.32	0.54
22:V:516:PRO:HD2	22:V:706:LYS:NZ	2.22	0.54
24:0:54:ARG:C	27:3:209:ILE:HD11	2.25	0.54
22:V:667:THR:HA	25:1:62:ASP:OD2	2.07	0.54
25:1:3:ASN:CB	26:2:412:PHE:O	2.54	0.54
20:T:82:PRO:HG2	20:T:117:ARG:HB2	1.89	0.54
1:A:1161:LEU:HD23	1:A:1307:VAL:CG1	2.38	0.54
4:D:90:LYS:HE3	4:D:130:ILE:HD11	1.88	0.54
5:E:15:LYS:NZ	5:E:33:LEU:O	2.31	0.54
5:E:64:HIS:NE2	5:E:69:THR:OG1	1.98	0.54
24:0:77:LYS:C	24:0:79:ASN:H	2.03	0.54
26:2:118:LEU:CD2	27:3:39:ASP:C	2.72	0.54
27:3:64:ILE:HG23	27:3:128:HIS:CG	2.42	0.54
1:A:261:ARG:C	1:A:263:ALA:H	2.11	0.54
1:A:415:GLY:C	1:A:449:HIS:HD2	2.11	0.54
17:Q:113:ARG:HD2	18:R:222:SER:HB3	1.90	0.54
25:1:29:LEU:HD23	25:1:29:LEU:C	2.27	0.54
27:3:133:LEU:H	27:3:133:LEU:CD1	2.10	0.54
1:A:932:ARG:CG	1:A:943:LEU:HD11	2.36	0.54
20:T:142:SER:O	20:T:144:GLN:HG3	2.08	0.54
13:M:193:ARG:NH1	29:Y:75:DC:OP1	2.41	0.54
25:1:25:GLU:HG2	25:1:32:LYS:HA	1.89	0.54
26:2:214:TYR:CD2	26:2:261:PHE:CD2	2.95	0.54
27:3:100:LYS:O	27:3:103:LEU:HB2	2.08	0.54
1:A:299:ALA:HA	17:Q:60:ARG:NH2	2.23	0.54
26:2:222:THR:HG23	26:2:222:THR:O	2.07	0.54
26:2:211:GLN:HB3	26:2:261:PHE:CE1	2.40	0.54
1:A:156:GLY:HA2	1:A:181:HIS:ND1	2.23	0.54
2:B:78:VAL:O	2:B:79:GLU:C	2.45	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:GLY:HA3	17:Q:57:LYS:HB3	1.90	0.54
26:2:159:VAL:CG1	26:2:161:HIS:H	2.06	0.54
26:2:199:ALA:HB1	26:2:201:PHE:CD2	2.43	0.54
26:2:220:LEU:HD13	26:2:220:LEU:C	2.29	0.54
1:A:1163:HIS:ND1	1:A:1302:GLU:O	2.41	0.54
13:M:103:ASN:HB3	13:M:105:ARG:HH22	1.72	0.54
14:N:15:ARG:HA	14:N:18:ILE:HD12	1.90	0.54
19:S:46:ARG:HB2	19:S:101:ARG:HB2	1.89	0.54
26:2:37:HIS:HB3	26:2:38:PRO:CD	2.35	0.54
26:2:81:LYS:HG3	26:2:82:ALA:N	2.21	0.54
27:3:169:ASP:CG	27:3:202:LEU:HD23	2.28	0.54
1:A:389:THR:HG21	1:A:417:LYS:HD2	1.90	0.54
1:A:521:VAL:HB	1:A:522:PRO:HD3	1.90	0.54
2:B:109:MET:HG3	2:B:174:LEU:HD11	1.89	0.54
5:E:67:ASP:O	5:E:69:THR:N	2.41	0.54
6:F:56:TYR:CE1	6:F:124:ILE:HB	2.43	0.54
19:S:172:ASN:OD1	19:S:173:HIS:N	2.37	0.54
2:B:733:MET:HE1	2:B:1054:MET:SD	2.47	0.54
3:C:134:ASN:CA	3:C:136:ASP:OD1	2.56	0.54
3:C:147:ASP:O	10:J:16:ASN:HB3	2.08	0.54
12:L:27:GLU:HB2	12:L:37:ARG:NH1	2.22	0.54
2:B:248:LYS:HA	19:S:169:LYS:HG2	1.89	0.54
23:W:428:ILE:HA	23:W:430:ASN:ND2	2.23	0.54
26:2:86:SER:O	26:2:90:LEU:HD13	2.08	0.53
3:C:82:LEU:HD23	3:C:167:LYS:HB2	1.90	0.53
26:2:118:LEU:HD12	26:2:118:LEU:C	2.29	0.53
26:2:159:VAL:HG22	26:2:160:LEU:N	2.16	0.53
1:A:34:MET:SD	2:B:1124:ILE:HG21	2.48	0.53
1:A:729:PRO:CG	21:U:250:MET:HB2	2.38	0.53
26:2:138:PRO:O	26:2:139:ASP:HB2	2.08	0.53
1:A:802:PHE:CE1	2:B:504:THR:HG22	2.43	0.53
1:A:894:ASP:OD1	1:A:895:GLY:N	2.40	0.53
2:B:132:VAL:CG2	2:B:141:GLN:CB	2.86	0.53
3:C:30:VAL:HG22	11:K:45:ILE:HD11	1.90	0.53
3:C:47:ILE:H	3:C:47:ILE:HD12	1.73	0.53
6:F:102:ILE:HG22	6:F:104:ILE:HG12	1.89	0.53
18:R:195:PRO:HB2	18:R:199:LYS:CG	2.38	0.53
26:2:211:GLN:HE21	26:2:257:SER:CB	2.21	0.53
26:2:30:VAL:O	26:2:34:LEU:HD23	2.09	0.53
27:3:105:THR:HG23	27:3:106:SER:N	2.23	0.53
27:3:15:VAL:O	27:3:15:VAL:HG23	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:3:191:ILE:N	27:3:210:THR:HG21	2.24	0.53
1:A:930:LEU:HD23	1:A:934:LEU:CB	2.39	0.53
13:M:90:ALA:CB	13:M:100:LYS:HE3	2.37	0.53
13:M:179:GLU:N	20:T:154:LYS:HE3	2.22	0.53
24:0:77:LYS:C	24:0:79:ASN:N	2.56	0.53
26:2:117:ASN:CG	27:3:108:ASN:CG	2.65	0.53
27:3:144:ILE:HD11	27:3:147:MET:HE3	1.89	0.53
1:A:929:ALA:O	1:A:930:LEU:CB	2.57	0.53
6:F:88:ASP:CG	6:F:91:LEU:H	2.12	0.53
17:Q:180:PHE:CZ	18:R:213:ASP:N	2.76	0.53
19:S:26:TYR:CD2	19:S:138:PHE:HB3	2.44	0.53
22:V:523:VAL:CB	25:1:20:LEU:HD23	2.38	0.53
26:2:141:HIS:HA	26:2:162:PHE:CE2	2.43	0.53
26:2:62:LEU:HD13	26:2:62:LEU:C	2.28	0.53
27:3:106:SER:O	27:3:109:GLU:HG3	2.08	0.53
27:3:160:ARG:NH2	27:3:192:ASP:HB3	2.23	0.53
1:A:1309:MET:O	1:A:1311:LEU:CD1	2.56	0.53
1:A:582:PRO:HD2	8:H:47:ILE:HD12	1.91	0.53
2:B:1078:ARG:NH1	29:Y:50:DA:O3'	2.41	0.53
2:B:490:GLY:O	2:B:491:ARG:CG	2.56	0.53
6:F:69:ARG:HG3	6:F:102:ILE:HD12	1.91	0.53
17:Q:125:ALA:HB1	17:Q:138:ASP:HB3	1.91	0.53
26:2:160:LEU:CG	26:2:206:LEU:HD21	2.39	0.53
27:3:10:LEU:HD21	27:3:143:TYR:CE2	2.44	0.53
1:A:1319:LYS:CG	1:A:1333:GLU:CD	2.77	0.53
1:A:467:MET:SD	1:A:524:MET:HB3	2.49	0.53
2:B:1163:MET:HA	2:B:1168:ALA:H	1.73	0.53
18:R:80:LYS:HD3	20:T:188:PHE:HE2	1.74	0.53
19:S:51:LEU:HD21	19:S:54:LYS:HD3	1.90	0.53
27:3:204:GLN:HG2	27:3:214:TYR:CZ	2.44	0.53
1:A:859:TYR:OH	1:A:863:ARG:NH2	2.41	0.53
2:B:91:ILE:HD11	2:B:124:LEU:HD21	1.89	0.53
14:N:359:ASN:ND2	14:N:364:ASP:OD1	2.38	0.53
14:N:332:GLU:HB2	15:O:92:LYS:O	2.09	0.53
1:A:542:LEU:HD21	1:A:642:LYS:HB2	1.91	0.53
5:E:14:ARG:O	5:E:17:ILE:HG13	2.09	0.53
8:H:108:ALA:O	8:H:109:ALA:C	2.47	0.53
8:H:115:TYR:CE1	8:H:124:ARG:HG3	2.43	0.53
14:N:314:LEU:HD21	16:P:250:PHE:HB2	1.90	0.53
20:T:93:LEU:HB2	20:T:110:VAL:HB	1.91	0.53
26:2:241:SER:O	26:2:245:LEU:HD23	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:2:42:LEU:HD12	26:2:59:MET:HE1	1.90	0.53
27:3:44:LEU:HD13	27:3:44:LEU:C	2.30	0.53
1:A:48:GLU:O	1:A:50:GLY:N	2.41	0.52
3:C:6:GLN:O	3:C:7:PRO:C	2.45	0.52
9:I:119:CYS:HB3	9:I:121:HIS:HB2	1.90	0.52
9:I:84:HIS:N	9:I:84:HIS:CD2	2.77	0.52
19:S:115:LYS:NZ	19:S:117:GLY:O	2.28	0.52
25:1:18:GLN:CD	25:1:44:PHE:HZ	2.12	0.52
1:A:930:LEU:CD2	1:A:934:LEU:HB2	2.40	0.52
8:H:74:GLU:O	8:H:75:TYR:CG	2.57	0.52
17:Q:75:ARG:HH21	17:Q:95:ASN:HD22	1.57	0.52
26:2:138:PRO:HG3	26:2:189:GLU:CG	2.35	0.52
27:3:10:LEU:HD21	27:3:143:TYR:CD2	2.44	0.52
27:3:172:LEU:HD13	27:3:172:LEU:C	2.29	0.52
1:A:263:ALA:O	1:A:264:VAL:CG2	2.58	0.52
1:A:255:VAL:HG13	1:A:280:LEU:HD21	1.91	0.52
2:B:852:GLY:O	2:B:868:GLY:N	2.30	0.52
6:F:73:ILE:HD11	6:F:96:GLU:OE2	2.08	0.52
9:I:61:GLU:O	9:I:63:ASP:HB2	2.10	0.52
13:M:13:VAL:HG12	13:M:20:ASP:HB3	1.90	0.52
21:U:279:ARG:NH1	21:U:280:SER:O	2.43	0.52
27:3:22:TRP:O	27:3:25:GLN:NE2	2.40	0.52
1:A:1316:ASN:ND2	1:A:1318:LYS:CE	2.72	0.52
13:M:178:LYS:HG2	20:T:156:VAL:HG12	1.92	0.52
25:1:35:ILE:HG13	25:1:35:ILE:O	2.08	0.52
1:A:253:LEU:HD12	1:A:254:PRO:HD2	1.90	0.52
2:B:1022:LEU:HD11	2:B:1023:ARG:NH1	2.24	0.52
2:B:931:ILE:HD11	2:B:947:ILE:HA	1.92	0.52
13:M:178:LYS:HB3	20:T:154:LYS:CE	2.40	0.52
17:Q:25:PHE:HD1	18:R:210:PHE:CZ	2.27	0.52
20:T:191:PHE:HZ	20:T:237:PRO:HG3	1.74	0.52
26:2:192:GLU:CG	26:2:193:PRO:HD2	2.23	0.52
27:3:70:LEU:HD22	27:3:114:GLU:HB3	1.91	0.52
27:3:18:ASN:O	27:3:21:TRP:CD1	2.63	0.52
1:A:484:LEU:HD12	1:A:484:LEU:O	2.08	0.52
1:A:364:ARG:HB2	2:B:1084:LEU:HD11	1.91	0.52
20:T:208:GLN:HE21	20:T:213:LEU:HB2	1.74	0.52
22:V:611:GLY:HA2	22:V:615:PHE:CB	2.38	0.52
1:A:926:ASN:CB	1:A:931:ARG:CZ	2.61	0.52
1:A:931:ARG:C	1:A:933:THR:N	2.62	0.52
2:B:529:MET:HG3	2:B:624:PRO:HD2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:212:ASP:C	3:C:214:ASP:N	2.43	0.52
3:C:267:ILE:HG13	3:C:272:LEU:HB3	1.92	0.52
5:E:149:VAL:HG23	5:E:192:LYS:HB3	1.92	0.52
5:E:64:HIS:CB	5:E:68:PRO:HA	2.39	0.52
17:Q:105:TYR:HD1	18:R:234:GLU:HB2	1.75	0.52
26:2:193:PRO:HB2	26:2:194:PRO:HD3	1.92	0.52
27:3:222:SER:HB3	27:3:225:GLN:HG2	1.92	0.52
1:A:890:ARG:NH2	1:A:1023:VAL:HG13	2.23	0.52
1:A:263:ALA:O	1:A:264:VAL:HG22	2.10	0.52
1:A:621:ILE:HG22	1:A:621:ILE:O	2.10	0.52
2:B:322:GLY:O	2:B:326:ALA:N	2.34	0.52
2:B:483:ARG:NH1	2:B:527:ALA:O	2.43	0.52
6:F:79:VAL:HG12	6:F:81:VAL:H	1.74	0.52
9:I:84:HIS:ND1	9:I:85:PRO:HD3	2.20	0.52
18:R:212:VAL:O	18:R:213:ASP:OD2	2.28	0.52
27:3:10:LEU:HD22	27:3:147:MET:HG2	1.92	0.52
27:3:57:LEU:HD23	27:3:58:ALA:C	2.31	0.52
1:A:469:MET:HE3	2:B:1094:GLN:HG2	1.90	0.52
2:B:552:ASN:OD1	2:B:553:LEU:N	2.43	0.52
12:L:35:ARG:HH12	12:L:42:ARG:NE	2.07	0.52
24:0:77:LYS:HG2	24:0:225:GLU:OE2	2.09	0.52
27:3:226:TYR:O	27:3:230:VAL:HB	2.10	0.52
3:C:7:PRO:HA	3:C:25:ASN:O	2.09	0.52
17:Q:25:PHE:HA	18:R:219:LEU:HD13	1.90	0.52
20:T:12:ALA:HB2	20:T:106:LEU:HD13	1.90	0.52
27:3:133:LEU:N	27:3:133:LEU:HD13	2.14	0.51
27:3:141:LEU:HG	27:3:187:GLN:HE22	1.75	0.51
9:I:24:LEU:HB3	9:I:37:TYR:HB3	1.92	0.51
13:M:94:ASP:O	13:M:97:GLY:N	2.42	0.51
14:N:366:ILE:O	15:O:54:ASN:ND2	2.44	0.51
17:Q:141:ALA:HB1	17:Q:152:PHE:CE2	2.44	0.51
20:T:177:ARG:N	20:T:178:ALA:HB3	2.24	0.51
26:2:257:SER:O	26:2:261:PHE:HD1	1.93	0.51
26:2:30:VAL:H	27:3:25:GLN:CG	2.23	0.51
27:3:64:ILE:HG21	27:3:128:HIS:CB	2.40	0.51
27:3:147:MET:HE3	27:3:157:MET:SD	2.51	0.51
1:A:972:THR:HA	1:A:1320:ILE:HG21	1.91	0.51
1:A:604:ARG:HG3	1:A:606:HIS:CE1	2.45	0.51
1:A:678:ASN:O	1:A:681:LEU:HB3	2.10	0.51
1:A:790:GLN:NE2	1:A:797:ARG:HG2	2.25	0.51
2:B:1040:GLN:N	2:B:1040:GLN:CD	2.63	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:326:ALA:HB2	2:B:338:TYR:HE2	1.76	0.51
2:B:363:TYR:CD2	2:B:553:LEU:HD21	2.45	0.51
2:B:72:GLN:HE22	2:B:80:GLU:H	1.58	0.51
7:G:91:GLN:HB3	7:G:98:PHE:HD2	1.75	0.51
22:V:689:VAL:CB	26:2:391:ILE:HD11	2.39	0.51
25:1:4:VAL:HG11	26:2:412:PHE:CD2	2.29	0.51
27:3:42:MET:CG	27:3:111:ILE:HD11	2.40	0.51
2:B:50:PHE:O	2:B:54:SER:HB2	2.11	0.51
2:B:976:MET:O	2:B:978:ILE:N	2.41	0.51
20:T:166:GLU:HA	20:T:169:LYS:HE3	1.93	0.51
28:X:65:DG:H2"	28:X:66:DA:O4'	2.10	0.51
25:1:8:VAL:CG1	25:1:45:VAL:HG13	2.35	0.51
26:2:160:LEU:HB3	26:2:206:LEU:HD21	1.93	0.51
27:3:100:LYS:HG3	27:3:101:TYR:H	1.74	0.51
27:3:14:VAL:HG23	27:3:14:VAL:O	2.09	0.51
26:2:31:LEU:HD13	27:3:33:THR:HG22	1.86	0.51
1:A:126:ILE:HD13	1:A:129:ILE:HD12	1.92	0.51
2:B:1072:ARG:O	2:B:1072:ARG:HG3	2.10	0.51
2:B:386:ASP:OD2	2:B:502:HIS:HB2	2.09	0.51
2:B:553:LEU:HB2	2:B:573:TRP:HZ3	1.75	0.51
2:B:675:LEU:HD11	2:B:697:GLU:OE2	2.09	0.51
2:B:891:ASP:OD1	2:B:892:CYS:N	2.44	0.51
11:K:7:PHE:HA	11:K:10:PHE:CE2	2.46	0.51
6:F:86:GLU:OE2	6:F:95:LYS:NZ	2.42	0.51
23:W:209:TYR:CZ	23:W:233:PHE:HA	2.39	0.51
29:Y:24:DC:C1'	29:Y:25:DT:C5	2.93	0.51
27:3:100:LYS:HB3	27:3:103:LEU:CD1	2.37	0.51
27:3:121:LYS:HD3	27:3:121:LYS:N	2.25	0.51
2:B:226:GLU:OE2	2:B:617:ASP:CB	2.57	0.51
2:B:499:ARG:CZ	2:B:522:LEU:HD11	2.41	0.51
2:B:62:ALA:N	2:B:63:PRO:HD3	2.25	0.51
2:B:907:VAL:HG13	2:B:921:ILE:HG22	1.93	0.51
3:C:154:ARG:HH11	10:J:65:LEU:HD11	1.75	0.51
5:E:172:ARG:HD3	5:E:210:GLN:HG2	1.92	0.51
5:E:52:ARG:NH2	5:E:54:ARG:HD3	2.26	0.51
17:Q:109:HIS:CE1	18:R:233:ILE:CG2	2.93	0.51
23:W:73:CYS:O	23:W:209:TYR:CE2	2.64	0.51
23:W:584:TYR:HB2	23:W:591:GLY:HA3	1.92	0.51
27:3:131:THR:HG23	27:3:133:LEU:HD12	1.92	0.51
27:3:165:LYS:HE3	27:3:200:SER:OG	2.09	0.51
2:B:992:ASN:ND2	2:B:1018:TYR:CD2	2.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:95:LYS:HB2	8:H:139:SER:HA	1.92	0.51
20:T:177:ARG:H	20:T:178:ALA:HB3	1.76	0.51
21:U:227:GLU:O	21:U:228:MET:HE3	2.04	0.51
16:P:294:ARG:NH1	28:X:14:DA:OP1	2.28	0.51
26:2:179:LEU:CB	26:2:184:LEU:HD11	2.40	0.51
26:2:236:PHE:CZ	26:2:262:LEU:CD2	2.94	0.51
26:2:46:ARG:HD3	26:2:85:GLU:HB2	1.93	0.51
27:3:165:LYS:HD3	27:3:165:LYS:C	2.31	0.51
2:B:716:HIS:CE1	2:B:1007:ASN:HD21	2.29	0.51
2:B:749:HIS:CD2	2:B:810:PHE:HD1	2.27	0.51
2:B:1101:GLN:HE22	6:F:64:ARG:HG2	1.76	0.51
10:J:66:GLU:HG3	12:L:23:HIS:CG	2.46	0.51
17:Q:180:PHE:HE1	18:R:212:VAL:C	2.12	0.51
17:Q:17:LEU:HD21	17:Q:191:LEU:HB3	1.93	0.51
17:Q:25:PHE:CD2	18:R:219:LEU:CD1	2.94	0.51
29:Y:45:DT:H5"	29:Y:46:DC:H5"	1.92	0.51
26:2:236:PHE:CE1	26:2:261:PHE:CB	2.94	0.51
26:2:57:MET:HA	26:2:60:LEU:CG	2.41	0.51
27:3:12:VAL:HG12	27:3:58:ALA:HB3	1.92	0.51
1:A:375:ILE:HG21	1:A:666:ARG:NH1	2.26	0.51
1:A:621:ILE:C	1:A:623:PRO:N	2.64	0.51
2:B:1060:HIS:HB2	2:B:1078:ARG:HE	1.75	0.51
3:C:60:HIS:CD2	3:C:63:PHE:HB2	2.45	0.51
9:I:61:GLU:C	9:I:63:ASP:H	2.13	0.51
10:J:52:HIS:HE1	10:J:54:ASP:HA	1.75	0.51
26:2:215:PHE:CE2	26:2:264:HIS:HB2	2.46	0.51
26:2:35:TYR:N	26:2:35:TYR:CD1	2.79	0.51
26:2:51:LEU:CD2	26:2:55:TRP:CD1	2.94	0.51
1:A:1161:LEU:HD23	1:A:1307:VAL:HG11	1.93	0.51
1:A:201:GLU:HG3	1:A:212:LYS:CB	2.41	0.51
2:B:240:LEU:O	2:B:253:GLY:HA2	2.11	0.51
13:M:128:ILE:HG23	13:M:183:VAL:HG11	1.93	0.51
19:S:26:TYR:CD1	20:T:97:THR:HG22	2.46	0.51
28:X:19:DG:N2	29:Y:76:DC:O2	2.44	0.51
26:2:199:ALA:HB1	26:2:201:PHE:CE2	2.47	0.50
1:A:1407:CYS:SG	1:A:1408:ARG:N	2.84	0.50
12:L:17:TYR:CE1	12:L:46:LYS:CB	2.94	0.50
19:S:26:TYR:HD1	20:T:97:THR:HG22	1.77	0.50
28:X:42:DT:H2"	28:X:43:DT:H5"	1.92	0.50
27:3:165:LYS:HZ1	27:3:200:SER:H	1.59	0.50
1:A:1167:ARG:HA	1:A:1293:LEU:HD22	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1316:ASN:CG	1:A:1318:LYS:HE2	2.31	0.50
1:A:261:ARG:HD2	1:A:277:THR:OG1	2.12	0.50
1:A:893:GLU:HG2	5:E:203:TYR:CD1	2.47	0.50
2:B:309:PHE:CZ	9:I:40:ARG:HB2	2.46	0.50
13:M:10:LEU:N	13:M:11:PRO:CD	2.74	0.50
19:S:15:VAL:HA	20:T:42:LYS:HG2	1.93	0.50
28:X:44:DT:H3'	28:X:45:DT:H5"	1.91	0.50
29:Y:62:DC:H1'	29:Y:63:DG:H4'	1.93	0.50
26:2:236:PHE:CE2	26:2:262:LEU:CD1	2.94	0.50
1:A:1212:LEU:HB2	1:A:1285:LEU:HD21	1.92	0.50
10:J:5:VAL:HG12	10:J:6:ARG:HG3	1.93	0.50
14:N:323:GLU:HG2	14:N:325:GLY:HA3	1.94	0.50
21:U:286:THR:HG21	21:U:299:LYS:HD2	1.93	0.50
23:W:430:ASN:CB	23:W:431:PRO:CD	2.85	0.50
26:2:30:VAL:CG1	26:2:34:LEU:HD23	2.40	0.50
25:1:1:MET:HE3	26:2:415:GLN:N	2.26	0.50
26:2:93:LEU:CD2	26:2:96:TRP:HE1	2.25	0.50
2:B:939:HIS:NE2	2:B:980:HIS:HA	2.26	0.50
9:I:65:LEU:CA	9:I:122:ARG:HE	2.23	0.50
9:I:85:PRO:C	9:I:86:CYS:O	2.49	0.50
3:C:49:TRP:CZ3	12:L:54:VAL:HG21	2.46	0.50
26:2:223:ALA:O	26:2:224:GLN:HB3	2.12	0.50
26:2:231:VAL:O	26:2:234:LEU:HB3	2.11	0.50
1:A:334:ARG:NH2	13:M:66:ARG:O	2.44	0.50
15:O:64:THR:HG22	15:O:75:VAL:HB	1.92	0.50
17:Q:188:TYR:HD1	17:Q:191:LEU:HD22	1.77	0.50
17:Q:25:PHE:O	18:R:219:LEU:CD2	2.59	0.50
20:T:217:LEU:HB3	20:T:233:TRP:CE3	2.46	0.50
25:1:2:VAL:HG23	25:1:2:VAL:O	2.11	0.50
26:2:29:GLY:H	27:3:25:GLN:CD	2.15	0.50
27:3:108:ASN:O	27:3:111:ILE:HG12	2.12	0.50
27:3:187:GLN:O	27:3:188:ASN:HB2	2.12	0.50
27:3:58:ALA:C	27:3:71:TYR:OH	2.50	0.50
1:A:11:SER:O	2:B:1135:TYR:OH	2.27	0.50
2:B:867:ILE:O	2:B:893:SER:HB2	2.11	0.50
3:C:116:THR:HB	3:C:146:ASP:HB2	1.93	0.50
2:B:906:GLN:HB3	12:L:45:TYR:HE1	1.75	0.50
2:B:92:TYR:CD1	20:T:141:LEU:CD2	2.90	0.50
26:2:214:TYR:CB	26:2:261:PHE:CE2	2.95	0.50
25:1:1:MET:HA	26:2:413:LEU:CA	2.42	0.50
25:1:2:VAL:HG12	26:2:456:LYS:HG2	1.79	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:VAL:O	1:A:481:THR:HB	2.12	0.50
1:A:622:SER:C	1:A:624:GLY:N	2.58	0.50
1:A:673:GLN:O	1:A:677:ASN:CB	2.60	0.50
2:B:1092:ASP:HA	2:B:1095:ILE:HD12	1.94	0.50
13:M:276:ASP:HA	20:T:153:TYR:CE1	2.47	0.50
18:R:195:PRO:O	18:R:196:ASP:CB	2.59	0.50
28:X:29:DC:H2"	28:X:30:DG:H5'	1.94	0.50
26:2:163:MET:HE2	26:2:206:LEU:CD1	2.39	0.50
26:2:188:THR:HG23	26:2:189:GLU:N	2.27	0.50
26:2:81:LYS:CE	26:2:89:LEU:HD21	2.42	0.50
27:3:12:VAL:CG2	27:3:161:ILE:HA	2.42	0.50
2:B:295:PRO:HB2	9:I:11:PHE:HD2	1.77	0.50
2:B:483:ARG:HG3	2:B:526:LEU:HB3	1.94	0.50
17:Q:95:ASN:OD1	17:Q:96:TYR:N	2.45	0.50
22:V:667:THR:CA	25:1:62:ASP:OD1	2.59	0.50
23:W:209:TYR:HH	23:W:234:ASP:H	1.58	0.50
26:2:140:LYS:CG	26:2:162:PHE:CE1	2.94	0.50
26:2:181:GLN:HE22	26:2:220:LEU:HD12	1.76	0.50
25:1:45:VAL:CG2	26:2:409:TYR:CE2	2.95	0.50
26:2:35:TYR:CD1	26:2:62:LEU:CD1	2.95	0.50
27:3:64:ILE:CG2	27:3:128:HIS:HB3	2.42	0.50
27:3:12:VAL:O	27:3:12:VAL:HG23	2.10	0.50
27:3:60:ILE:HG22	27:3:61:ALA:N	2.26	0.50
2:B:455:ASP:O	2:B:457:LYS:N	2.40	0.50
2:B:855:ALA:HB2	12:L:46:LYS:HE2	1.93	0.50
13:M:178:LYS:HB3	20:T:154:LYS:HE3	1.93	0.50
13:M:86:LYS:NZ	28:X:40:DT:N3	2.60	0.50
17:Q:153:ARG:HD3	17:Q:158:HIS:HB3	1.94	0.50
23:W:325:THR:HG22	23:W:329:PHE:CE2	2.47	0.50
27:3:12:VAL:HG22	27:3:161:ILE:HA	1.94	0.49
28:X:13:DT:H2"	28:X:14:DA:H8	1.77	0.49
25:1:1:MET:HE1	26:2:440:LEU:HD13	1.91	0.49
26:2:77:LYS:CD	26:2:78:GLU:HG3	2.41	0.49
27:3:202:LEU:HD22	27:3:202:LEU:N	2.27	0.49
27:3:217:VAL:CG1	27:3:226:TYR:CE2	2.95	0.49
1:A:205:VAL:O	1:A:205:VAL:HG23	2.12	0.49
1:A:30:GLU:CD	1:A:33:ARG:HH21	2.16	0.49
1:A:604:ARG:HG3	1:A:606:HIS:HE1	1.76	0.49
17:Q:23:ARG:HD3	18:R:207:SER:O	2.12	0.49
23:W:116:CYS:SG	23:W:191:PRO:HD2	2.51	0.49
28:X:52:DG:H2"	28:X:53:DA:O4'	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:3:216:LYS:O	27:3:216:LYS:HG2	2.11	0.49
27:3:59:VAL:HG13	27:3:59:VAL:O	2.12	0.49
1:A:269:SER:O	1:A:270:ALA:CB	2.58	0.49
7:G:97:LEU:HB3	7:G:108:ILE:HB	1.93	0.49
22:V:315:VAL:CG1	23:W:500:ASP:HB3	2.26	0.49
26:2:199:ALA:CB	26:2:201:PHE:CE2	2.95	0.49
26:2:245:LEU:HD22	26:2:245:LEU:N	2.27	0.49
27:3:24:LYS:HE2	27:3:196:LEU:HB3	1.93	0.49
27:3:223:LEU:C	27:3:223:LEU:HD13	2.33	0.49
1:A:1158:LEU:HD11	1:A:1308:TYR:CG	2.32	0.49
1:A:1162:GLU:OE2	1:A:1308:TYR:CZ	2.65	0.49
1:A:362:SER:OG	2:B:1084:LEU:HB2	2.11	0.49
1:A:1471:PHE:HE1	6:F:64:ARG:HD3	1.77	0.49
13:M:245:VAL:HG12	13:M:291:LEU:HD23	1.92	0.49
18:R:225:VAL:O	18:R:225:VAL:HG12	2.13	0.49
23:W:494:ILE:HD11	23:W:680:ALA:HB2	1.93	0.49
28:X:45:DT:H4'	28:X:45:DT:OP1	2.12	0.49
29:Y:24:DC:C2'	29:Y:25:DT:C5	2.88	0.49
25:1:34:ILE:HG21	25:1:54:GLN:CD	2.32	0.49
26:2:426:ARG:HD2	26:2:444:THR:CG2	2.43	0.49
26:2:57:MET:HA	26:2:60:LEU:HG	1.93	0.49
27:3:53:ARG:HA	27:3:101:TYR:HE1	1.78	0.49
27:3:137:LEU:CD1	27:3:177:PHE:CE1	2.95	0.49
27:3:220:MET:N	27:3:221:PRO:HD2	2.28	0.49
22:V:321:GLU:CD	23:W:499:ASN:C	2.71	0.49
24:0:55:LEU:N	27:3:209:ILE:HD11	2.28	0.49
26:2:236:PHE:CZ	26:2:258:LEU:CD1	2.95	0.49
26:2:29:GLY:CA	27:3:25:GLN:CG	2.82	0.49
27:3:166:ALA:O	27:3:198:SER:HB2	2.13	0.49
27:3:215:LEU:HD12	27:3:230:VAL:CG2	2.42	0.49
1:A:560:VAL:HG21	1:A:586:TRP:CE3	2.48	0.49
3:C:49:TRP:O	3:C:163:ALA:HA	2.12	0.49
5:E:64:HIS:ND1	5:E:70:ASP:O	2.46	0.49
26:2:203:PHE:CE2	26:2:205:LEU:CD2	2.96	0.49
26:2:28:PRO:HA	27:3:33:THR:CB	2.41	0.49
27:3:107:ALA:O	27:3:111:ILE:HG23	2.11	0.49
27:3:195:VAL:HG23	27:3:214:TYR:CE1	2.48	0.49
27:3:174:TYR:HD1	27:3:202:LEU:HD11	1.78	0.49
1:A:1158:LEU:CD2	1:A:1308:TYR:CD2	2.90	0.49
1:A:358:ARG:NH2	2:B:1076:GLU:HA	2.25	0.49
7:G:158:PHE:N	7:G:158:PHE:CD1	2.80	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:175:ARG:HE	28:X:21:DG:P	2.36	0.49
18:R:80:LYS:HB2	20:T:188:PHE:CE2	2.47	0.49
23:W:624:PRO:O	23:W:656:ALA:HB1	2.12	0.49
26:2:181:GLN:HE21	26:2:181:GLN:CA	2.23	0.49
27:3:10:LEU:CD2	27:3:143:TYR:HE2	2.25	0.49
27:3:177:PHE:CZ	27:3:203:LEU:CD2	2.95	0.49
27:3:21:TRP:HA	27:3:24:LYS:CG	2.41	0.49
1:A:1307:VAL:O	1:A:1308:TYR:CB	2.51	0.49
1:A:459:ASN:O	1:A:501:MET:HE2	2.13	0.49
1:A:524:MET:SD	1:A:524:MET:N	2.82	0.49
2:B:677:MET:HG3	2:B:678:THR:HG23	1.95	0.49
3:C:169:PHE:CE1	3:C:171:LYS:HB3	2.48	0.49
22:V:516:PRO:HG2	22:V:706:LYS:HE2	1.91	0.49
25:1:1:MET:CE	26:2:415:GLN:C	2.80	0.49
26:2:77:LYS:HD3	26:2:78:GLU:HG3	1.94	0.49
1:A:1319:LYS:HG2	1:A:1333:GLU:CD	2.33	0.49
1:A:686:THR:OG1	1:A:687:ILE:N	2.46	0.49
2:B:474:THR:HG23	2:B:732:ALA:O	2.13	0.49
2:B:871:VAL:HG13	2:B:890:ARG:HB2	1.95	0.49
7:G:1:MET:N	7:G:78:ARG:O	2.45	0.49
17:Q:23:ARG:CZ	18:R:207:SER:O	2.48	0.49
22:V:321:GLU:HG3	23:W:499:ASN:HB3	1.70	0.49
28:X:46:DT:H2'	28:X:47:DT:C5	2.48	0.49
26:2:189:GLU:CA	26:2:192:GLU:HG2	2.41	0.49
26:2:208:THR:HG23	26:2:209:PRO:HD2	1.91	0.49
26:2:42:LEU:HD22	26:2:52:ALA:HA	1.95	0.49
27:3:10:LEU:CD2	27:3:143:TYR:CE2	2.95	0.49
27:3:160:ARG:HE	27:3:190:LEU:HG	1.78	0.49
24:0:54:ARG:CB	27:3:209:ILE:CG2	2.87	0.49
2:B:935:PHE:CE1	2:B:1050:ARG:HG3	2.48	0.49
2:B:1132:THR:HG23	2:B:1133:HIS:ND1	2.27	0.49
2:B:72:GLN:HE22	2:B:80:GLU:N	2.11	0.49
2:B:874:PRO:C	2:B:876:ASN:H	2.08	0.49
3:C:135:ARG:O	3:C:136:ASP:O	2.31	0.49
5:E:64:HIS:HD2	5:E:67:ASP:C	2.15	0.49
4:D:30:GLU:O	7:G:3:TYR:HA	2.13	0.49
29:Y:24:DC:C2	29:Y:25:DT:N3	2.81	0.49
2:B:812:ARG:NH2	29:Y:52:DT:OP1	2.38	0.49
26:2:159:VAL:N	26:2:162:PHE:HB3	2.28	0.48
26:2:166:SER:HB3	26:2:167:PRO:CD	2.43	0.48
26:2:251:VAL:HG11	26:2:254:MET:SD	2.53	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:2:89:LEU:HD23	26:2:93:LEU:HG	1.94	0.48
27:3:216:LYS:N	27:3:216:LYS:HD2	2.22	0.48
1:A:201:GLU:HG2	1:A:212:LYS:HB3	1.93	0.48
2:B:1124:ILE:HG22	2:B:1126:ALA:H	1.78	0.48
2:B:566:LYS:HD3	2:B:573:TRP:NE1	2.23	0.48
12:L:19:CYS:HB3	12:L:22:CYS:SG	2.53	0.48
16:P:293:TYR:HD2	16:P:302:LEU:HD13	1.78	0.48
17:Q:44:LYS:HG3	17:Q:47:ASP:H	1.76	0.48
26:2:133:THR:HG23	26:2:134:SER:N	2.29	0.48
26:2:198:SER:OG	26:2:238:PHE:HE2	1.96	0.48
26:2:60:LEU:CD1	26:2:95:ILE:CG2	2.91	0.48
1:A:1138:SER:OG	1:A:1139:LEU:N	2.46	0.48
1:A:261:ARG:HB2	1:A:274:ASP:HB3	1.95	0.48
2:B:873:LEU:CB	2:B:874:PRO:HD3	2.41	0.48
17:Q:188:TYR:CE1	18:R:210:PHE:HB2	2.48	0.48
24:0:209:THR:HA	24:0:219:TYR:CD1	2.48	0.48
25:1:45:VAL:HG21	26:2:409:TYR:CE2	2.48	0.48
26:2:90:LEU:CD2	26:2:140:LYS:HD3	2.42	0.48
1:A:522:PRO:HA	1:A:666:ARG:NE	2.09	0.48
2:B:513:GLU:HG3	2:B:726:SER:HB3	1.94	0.48
2:B:80:GLU:O	2:B:82:PRO:CD	2.61	0.48
5:E:48:PRO:O	5:E:52:ARG:NH1	2.45	0.48
10:J:6:ARG:HA	10:J:13:ILE:HA	1.95	0.48
11:K:47:LYS:HD2	11:K:61:TYR:HD1	1.78	0.48
23:W:73:CYS:HB2	23:W:209:TYR:CE1	2.48	0.48
23:W:596:LEU:HG	23:W:597:LEU:N	2.27	0.48
28:X:50:DT:OP1	28:X:50:DT:H4'	2.13	0.48
25:1:3:ASN:HB2	26:2:412:PHE:O	2.12	0.48
26:2:176:ALA:O	26:2:177:GLN:HB2	2.12	0.48
27:3:34:LEU:HD13	27:3:34:LEU:C	2.33	0.48
1:A:1162:GLU:HA	1:A:1307:VAL:HB	1.96	0.48
1:A:1319:LYS:HD3	1:A:1319:LYS:HA	1.69	0.48
1:A:455:ILE:HD13	1:A:520:MET:CE	2.43	0.48
2:B:747:LEU:HD11	2:B:810:PHE:HZ	1.79	0.48
2:B:798:ARG:O	2:B:801:VAL:HG22	2.14	0.48
9:I:57:LYS:O	9:I:58:ILE:HG12	2.13	0.48
2:B:464:ALA:HB1	13:M:62:LYS:NZ	2.28	0.48
19:S:124:TYR:HB3	20:T:20:LEU:HD11	1.95	0.48
26:2:234:LEU:C	26:2:234:LEU:HD23	2.34	0.48
2:B:1060:HIS:CE1	2:B:1078:ARG:HG3	2.48	0.48
2:B:489:ILE:HG13	2:B:490:GLY:H	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:873:LEU:CB	2:B:874:PRO:CD	2.90	0.48
18:R:167:LEU:HD22	18:R:200:ILE:HB	1.96	0.48
2:B:324:ARG:NH1	19:S:162:GLU:OE2	2.46	0.48
23:W:285:TYR:CE1	23:W:403:PHE:CZ	3.01	0.48
25:1:38:ILE:CG2	25:1:44:PHE:CE1	2.96	0.48
26:2:35:TYR:CE2	26:2:62:LEU:CB	2.96	0.48
27:3:21:TRP:CG	27:3:34:LEU:HD23	2.48	0.48
1:A:632:ASN:HA	1:A:992:LYS:HD2	1.96	0.48
2:B:418:TYR:CD1	2:B:434:ALA:HB2	2.48	0.48
2:B:626:LEU:HG	2:B:698:ILE:HG22	1.95	0.48
2:B:929:PRO:HB3	2:B:935:PHE:HZ	1.78	0.48
17:Q:184:ILE:HD11	18:R:218:LYS:NZ	2.19	0.48
23:W:37:HIS:NE2	23:W:454:VAL:CG1	2.76	0.48
25:1:34:ILE:HG22	25:1:46:ILE:CG1	2.44	0.48
26:2:178:LEU:HD12	26:2:178:LEU:N	2.28	0.48
1:A:53:LYS:HE3	1:A:59:ASP:HB3	1.95	0.48
2:B:1101:GLN:NE2	6:F:64:ARG:CG	2.77	0.48
2:B:124:LEU:HD23	2:B:149:ILE:HD11	1.95	0.48
2:B:726:SER:O	2:B:730:LYS:HE2	2.14	0.48
2:B:796:MET:O	2:B:948:GLN:HA	2.14	0.48
3:C:154:ARG:HB3	10:J:65:LEU:CD1	2.43	0.48
17:Q:164:ASP:O	17:Q:166:SER:N	2.45	0.48
2:B:356:PHE:O	19:S:116:GLY:HA2	2.13	0.48
22:V:504:LYS:CB	22:V:654:GLU:O	2.59	0.48
23:W:73:CYS:HB3	23:W:209:TYR:CG	2.48	0.48
26:2:211:GLN:HE21	26:2:257:SER:HB3	1.78	0.48
1:A:1276:VAL:HG12	1:A:1279:MET:HB2	1.93	0.48
1:A:202:TRP:O	1:A:203:LYS:O	2.32	0.48
1:A:578:ALA:HB3	1:A:587:THR:HG23	1.96	0.48
2:B:1000:THR:HG23	2:B:1001:PRO:HD2	1.96	0.48
2:B:213:SER:HA	2:B:242:ARG:HD2	1.96	0.48
2:B:598:VAL:C	2:B:600:GLU:H	2.16	0.48
5:E:13:ILE:HG22	5:E:136:LEU:HA	1.94	0.48
13:M:30:GLY:HA2	13:M:44:ARG:HG2	1.96	0.48
18:R:119:LEU:HA	18:R:123:ALA:HB3	1.95	0.48
22:V:370:SER:O	22:V:374:TRP:HD1	1.96	0.48
25:1:21:LEU:HD23	25:1:21:LEU:N	2.29	0.48
26:2:211:GLN:CA	26:2:261:PHE:CE1	2.95	0.48
1:A:187:TYR:HB2	1:A:205:VAL:HG21	1.95	0.48
2:B:964:ASP:OD1	2:B:964:ASP:N	2.47	0.48
18:R:195:PRO:HB2	18:R:199:LYS:HG3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:81:HIS:HB3	20:T:116:CYS:SG	2.54	0.48
23:W:73:CYS:CB	23:W:209:TYR:CE1	2.97	0.48
29:Y:52:DT:H2"	29:Y:53:DG:O4'	2.13	0.48
24:0:165:ARG:HB2	24:0:193:LYS:O	2.14	0.48
25:1:53:LEU:CD1	25:1:53:LEU:H	2.26	0.48
26:2:218:GLN:HG2	26:2:268:PHE:CB	2.44	0.48
26:2:236:PHE:CD1	26:2:261:PHE:HB3	2.49	0.48
27:3:124:ILE:O	27:3:127:GLN:HB2	2.14	0.48
27:3:226:TYR:CA	27:3:230:VAL:HG23	2.42	0.48
1:A:1263:ASN:HB2	1:A:1268:LYS:HD2	1.96	0.48
1:A:932:ARG:CB	1:A:943:LEU:HD11	2.43	0.48
2:B:94:SER:OG	2:B:95:LYS:N	2.47	0.48
9:I:105:GLU:HB3	9:I:107:ALA:HB2	1.94	0.48
10:J:63:ALA:CB	10:J:64:PRO:CD	2.90	0.48
16:P:156:SER:O	16:P:158:SER:N	2.47	0.48
25:1:38:ILE:HG22	25:1:44:PHE:CE1	2.48	0.47
26:2:170:ALA:CB	26:2:213:TRP:CZ3	2.95	0.47
27:3:34:LEU:HD22	27:3:37:CYS:SG	2.54	0.47
27:3:10:LEU:CD1	27:3:56:LYS:HG2	2.44	0.47
1:A:265:VAL:HG23	1:A:266:MET:H	1.79	0.47
2:B:810:PHE:CD2	2:B:927:ARG:NH2	2.81	0.47
3:C:148:ILE:HG12	3:C:149:LEU:N	2.28	0.47
21:U:248:HIS:O	21:U:252:LYS:NZ	2.47	0.47
28:X:82:DG:N2	29:Y:13:DC:C2	2.81	0.47
29:Y:24:DC:O2	29:Y:25:DT:N3	2.47	0.47
25:1:43:VAL:HG12	25:1:44:PHE:N	2.28	0.47
26:2:203:PHE:CD2	26:2:204:LEU:N	2.82	0.47
27:3:165:LYS:NZ	27:3:200:SER:H	2.12	0.47
1:A:375:ILE:HD12	1:A:375:ILE:HG23	1.54	0.47
1:A:790:GLN:CD	1:A:797:ARG:HG2	2.34	0.47
5:E:71:GLN:HE21	5:E:99:ILE:HG22	1.79	0.47
8:H:65:TYR:CG	8:H:70:LEU:HD22	2.49	0.47
8:H:85:ALA:C	8:H:87:GLN:N	2.38	0.47
10:J:40:LEU:HD11	10:J:49:LEU:HD13	1.97	0.47
17:Q:105:TYR:CD1	18:R:234:GLU:CB	2.97	0.47
22:V:361:CYS:HB3	22:V:405:VAL:HG21	1.96	0.47
27:3:10:LEU:HA	27:3:56:LYS:HG2	1.96	0.47
1:A:623:PRO:C	1:A:625:ASP:N	2.68	0.47
2:B:184:TYR:HE2	2:B:191:GLU:HG2	1.79	0.47
2:B:875:GLU:O	2:B:876:ASN:CB	2.49	0.47
2:B:947:ILE:HG12	2:B:948:GLN:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:169:PHE:HE1	3:C:171:LYS:HB3	1.78	0.47
20:T:229:HIS:CD2	28:X:28:DG:H21	2.33	0.47
26:2:205:LEU:N	26:2:205:LEU:HD22	2.30	0.47
26:2:236:PHE:HE2	26:2:262:LEU:CD1	2.27	0.47
1:A:807:LEU:HB3	1:A:809:HIS:HD2	1.78	0.47
2:B:348:LEU:HD13	2:B:364:PHE:HD2	1.79	0.47
3:C:184:PHE:HD1	3:C:231:TYR:CE1	2.33	0.47
10:J:43:TYR:HA	10:J:46:ARG:HB2	1.95	0.47
1:A:426:ARG:HB3	13:M:40:VAL:HG22	1.94	0.47
14:N:360:LEU:HD11	15:O:81:PHE:HD2	1.79	0.47
20:T:80:GLU:O	20:T:119:ALA:HB2	2.14	0.47
23:W:73:CYS:HB3	23:W:209:TYR:CD1	2.50	0.47
27:3:160:ARG:HB2	27:3:190:LEU:HG	1.96	0.47
27:3:216:LYS:O	27:3:218:PRO:HD3	2.14	0.47
1:A:878:THR:HG1	1:A:880:ARG:HE	1.63	0.47
1:A:880:ARG:HG2	1:A:886:VAL:HA	1.97	0.47
2:B:177:CYS:HB3	2:B:180:ASP:HB2	1.95	0.47
17:Q:184:ILE:HD11	18:R:213:ASP:OD1	2.14	0.47
25:1:50:VAL:CG1	25:1:54:GLN:HG2	2.41	0.47
1:A:1065:PHE:CE2	1:A:1069:LEU:HD11	2.49	0.47
1:A:275:ASP:OD1	1:A:276:LEU:N	2.47	0.47
3:C:69:GLY:HA3	12:L:57:ALA:HB1	1.95	0.47
15:O:77:ASN:OD1	15:O:78:ASP:N	2.48	0.47
18:R:151:LEU:HB3	18:R:154:LEU:HB3	1.97	0.47
26:2:100:LEU:HD11	26:2:119:ARG:CG	2.31	0.47
27:3:12:VAL:CG2	27:3:161:ILE:HG23	2.43	0.47
27:3:34:LEU:HD13	27:3:38:ILE:HG12	1.95	0.47
26:2:118:LEU:HD21	27:3:39:ASP:OD1	1.95	0.47
27:3:70:LEU:HD22	27:3:114:GLU:CB	2.44	0.47
1:A:1319:LYS:O	1:A:1321:ILE:HG23	2.15	0.47
1:A:1472:ASP:HB2	6:F:107:ARG:HB3	1.97	0.47
1:A:274:ASP:O	1:A:275:ASP:C	2.53	0.47
1:A:608:THR:HB	1:A:610:PRO:HD2	1.92	0.47
2:B:950:ARG:HB2	2:B:952:GLU:OE1	2.15	0.47
2:B:957:THR:O	2:B:960:GLY:N	2.36	0.47
5:E:129:GLN:OE1	5:E:130:PHE:N	2.47	0.47
8:H:65:TYR:CE2	8:H:70:LEU:HD22	2.49	0.47
3:C:86:ARG:HH22	11:K:10:PHE:HE1	1.62	0.47
13:M:16:PRO:HD2	13:M:39:LEU:HD22	1.96	0.47
19:S:122:THR:HA	20:T:24:PRO:HA	1.96	0.47
24:0:77:LYS:HA	24:0:77:LYS:HE3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:2:221:GLN:CD	26:2:230:LEU:HB2	2.34	0.47
1:A:1320:ILE:HD12	1:A:1329:LYS:O	2.14	0.47
3:C:262:GLN:HG3	11:K:18:LYS:HG2	1.95	0.47
3:C:75:SER:HB3	3:C:79:VAL:HB	1.96	0.47
25:1:38:ILE:CG2	25:1:44:PHE:CD1	2.94	0.47
25:1:9:LEU:HD12	25:1:9:LEU:N	2.30	0.47
25:1:59:GLU:CD	26:2:402:ARG:HH12	2.13	0.47
26:2:89:LEU:CD2	26:2:93:LEU:HG	2.44	0.47
8:H:90:TYR:HB3	8:H:145:MET:HB3	1.96	0.47
8:H:93:TYR:HE1	8:H:140:ARG:HA	1.79	0.47
13:M:300:PHE:HD2	13:M:306:PHE:HE1	1.62	0.47
26:2:51:LEU:HD21	26:2:55:TRP:CD1	2.50	0.47
27:3:137:LEU:HD11	27:3:177:PHE:CE1	2.50	0.47
1:A:889:LEU:HD21	5:E:206:TYR:HE1	1.80	0.47
1:A:926:ASN:OD1	1:A:932:ARG:HG2	2.15	0.47
2:B:1091:ARG:O	2:B:1095:ILE:HG13	2.14	0.47
2:B:628:VAL:HG21	2:B:682:LEU:HD11	1.97	0.47
2:B:972:ILE:O	2:B:976:MET:N	2.48	0.47
10:J:66:GLU:HG3	12:L:23:HIS:CE1	2.49	0.47
13:M:75:LEU:HD22	13:M:139:ASN:OD1	2.14	0.47
16:P:206:GLU:C	16:P:208:ARG:N	2.67	0.47
26:2:46:ARG:CD	26:2:85:GLU:CB	2.93	0.47
26:2:85:GLU:O	26:2:89:LEU:HB2	2.14	0.47
27:3:56:LYS:HD3	27:3:56:LYS:N	2.30	0.47
27:3:64:ILE:HG21	27:3:128:HIS:HB3	1.97	0.47
1:A:1163:HIS:H	1:A:1307:VAL:HG21	1.80	0.47
1:A:367:ILE:HA	1:A:482:PHE:O	2.15	0.47
1:A:837:PHE:HB2	2:B:506:TRP:HZ3	1.79	0.47
1:A:966:LEU:HD13	1:A:1043:ILE:HD11	1.96	0.47
2:B:81:PRO:HD2	2:B:135:GLU:HG3	1.97	0.47
3:C:35:ARG:HG2	3:C:36:ARG:N	2.30	0.47
13:M:16:PRO:HG2	13:M:39:LEU:CD2	2.38	0.47
14:N:25:VAL:HG11	15:O:36:VAL:HG13	1.97	0.47
23:W:143:ARG:HH11	23:W:143:ARG:HG2	1.80	0.47
23:W:657:MET:O	23:W:660:ALA:HB3	2.15	0.47
25:1:38:ILE:HA	25:1:44:PHE:CD1	2.37	0.46
25:1:38:ILE:O	25:1:38:ILE:HG12	2.15	0.46
26:2:201:PHE:CD1	26:2:202:GLN:N	2.83	0.46
26:2:93:LEU:CA	26:2:96:TRP:CD1	2.94	0.46
2:B:470:LEU:HD11	2:B:478:THR:HG23	1.96	0.46
9:I:98:GLN:O	9:I:100:HIS:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:173:ALA:O	17:Q:177:LEU:HD23	2.15	0.46
21:U:223:MET:O	21:U:226:GLU:O	2.33	0.46
25:1:38:ILE:CB	25:1:44:PHE:CE1	2.98	0.46
25:1:53:LEU:O	25:1:57:VAL:HG12	2.15	0.46
26:2:211:GLN:CB	26:2:261:PHE:CE1	2.95	0.46
22:V:689:VAL:CG2	26:2:391:ILE:CD1	2.92	0.46
26:2:84:GLU:OE1	26:2:84:GLU:HA	2.15	0.46
1:A:1408:ARG:O	1:A:1410:HIS:N	2.48	0.46
2:B:1062:ARG:HH12	2:B:1075:MET:N	2.11	0.46
3:C:157:GLN:CG	10:J:65:LEU:HB3	2.45	0.46
9:I:58:ILE:C	9:I:60:HIS:H	2.19	0.46
10:J:63:ALA:N	10:J:64:PRO:HD2	2.30	0.46
13:M:16:PRO:CG	13:M:39:LEU:CD2	2.93	0.46
20:T:125:MET:O	20:T:129:ARG:N	2.41	0.46
25:1:10:ILE:HG12	25:1:43:VAL:CG1	2.45	0.46
25:1:4:VAL:HG12	26:2:411:GLN:C	2.30	0.46
27:3:131:THR:HG23	27:3:133:LEU:HD13	1.95	0.46
27:3:177:PHE:O	27:3:181:ILE:HG13	2.15	0.46
1:A:1130:ILE:HG21	1:A:1411:LEU:HD13	1.98	0.46
1:A:156:GLY:HA2	1:A:181:HIS:CE1	2.50	0.46
1:A:525:ILE:HG12	1:A:666:ARG:NH2	2.30	0.46
2:B:422:PHE:HD1	2:B:428:ASP:H	1.62	0.46
2:B:73:HIS:C	2:B:75:SER:N	2.67	0.46
13:M:214:PHE:HB3	13:M:218:PHE:CE2	2.49	0.46
20:T:198:ASN:OD1	20:T:199:LEU:N	2.49	0.46
25:1:40:ASP:HB2	25:1:43:VAL:H	1.81	0.46
26:2:96:TRP:CH2	26:2:97:HIS:CE1	3.03	0.46
1:A:608:THR:CB	1:A:610:PRO:HG2	2.45	0.46
1:A:818:GLU:CD	1:A:818:GLU:H	2.19	0.46
3:C:5:ASN:C	3:C:7:PRO:CD	2.77	0.46
1:A:1185:VAL:HG21	9:I:51:SER:OG	2.16	0.46
3:C:154:ARG:HB3	10:J:65:LEU:HD22	1.96	0.46
16:P:298:PRO:O	16:P:300:ILE:N	2.48	0.46
21:U:215:ILE:HG23	21:U:219:LEU:HD23	1.97	0.46
26:2:240:LEU:HD12	26:2:240:LEU:N	2.30	0.46
26:2:35:TYR:CD1	26:2:62:LEU:CG	2.92	0.46
27:3:10:LEU:HB2	27:3:56:LYS:HE3	1.97	0.46
1:A:261:ARG:HB2	1:A:274:ASP:CB	2.45	0.46
1:A:451:CYS:SG	1:A:452:ASP:N	2.88	0.46
2:B:960:GLY:O	2:B:962:THR:N	2.48	0.46
3:C:76:ASP:OD1	3:C:243:THR:HG21	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1171:ALA:O	9:I:59:THR:HG23	2.15	0.46
18:R:116:LYS:HA	18:R:119:LEU:HD12	1.98	0.46
19:S:135:PHE:HD1	19:S:135:PHE:HA	1.66	0.46
22:V:613:THR:O	22:V:614:SER:HB2	2.14	0.46
23:W:581:LEU:HD13	23:W:581:LEU:C	2.36	0.46
29:Y:16:DA:H2'	29:Y:17:DG:C8	2.50	0.46
27:3:196:LEU:HB3	27:3:220:MET:SD	2.56	0.46
1:A:1130:ILE:HD13	1:A:1411:LEU:HD22	1.96	0.46
1:A:963:ARG:O	1:A:967:ARG:HG3	2.16	0.46
2:B:676:ALA:HB2	2:B:693:TYR:CG	2.50	0.46
4:D:40:LEU:HD13	7:G:75:ILE:HD11	1.97	0.46
7:G:55:GLY:HA3	7:G:69:PRO:HG2	1.97	0.46
2:B:282:ARG:HD2	9:I:21:ASN:HD21	1.80	0.46
10:J:3:ILE:HD13	10:J:18:TRP:CD2	2.50	0.46
11:K:39:ASP:N	11:K:39:ASP:OD1	2.37	0.46
23:W:37:HIS:CG	23:W:454:VAL:HG13	2.50	0.46
25:1:2:VAL:HG12	26:2:456:LYS:CE	2.44	0.46
26:2:214:TYR:CE1	26:2:233:ILE:HG23	2.51	0.46
27:3:69:PHE:HE1	27:3:139:LYS:HD2	1.77	0.46
27:3:15:VAL:HG12	27:3:164:ILE:HD12	1.97	0.46
1:A:557:ARG:HH11	1:A:557:ARG:HB3	1.79	0.46
2:B:526:LEU:HA	2:B:526:LEU:HD12	1.48	0.46
2:B:964:ASP:O	2:B:965:ILE:HG13	2.14	0.46
3:C:149:LEU:HD21	3:C:152:LYS:HG3	1.98	0.46
4:D:70:ARG:NE	7:G:142:GLU:OE2	2.43	0.46
22:V:325:ARG:HH22	23:W:499:ASN:HB2	0.64	0.46
28:X:73:DG:C2	28:X:74:DT:C2	3.04	0.46
25:1:13:ASP:OD2	25:1:17:LYS:HB2	2.13	0.46
26:2:171:VAL:HG13	26:2:216:MET:HB3	1.98	0.46
26:2:81:LYS:CG	26:2:82:ALA:N	2.79	0.46
26:2:96:TRP:CZ2	26:2:97:HIS:NE2	2.83	0.46
27:3:10:LEU:N	27:3:56:LYS:HE3	2.31	0.46
27:3:25:GLN:NE2	27:3:25:GLN:HA	2.31	0.46
1:A:117:LEU:HB2	1:A:232:GLU:HG2	1.96	0.46
1:A:49:GLY:O	1:A:52:PRO:HD2	2.16	0.46
1:A:619:LYS:HA	1:A:619:LYS:HD3	1.47	0.46
1:A:868:MET:HE1	1:A:1400:LEU:HG	1.97	0.46
2:B:1066:PRO:HB2	2:B:1075:MET:HG3	1.97	0.46
2:B:223:SER:OG	2:B:233:SER:HB2	2.15	0.46
2:B:380:ARG:HE	2:B:609:GLU:CD	2.19	0.46
5:E:41:LYS:HG3	5:E:46:ASP:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:29:ASP:OD2	9:I:32:ASN:ND2	2.37	0.46
19:S:127:PHE:HB2	20:T:19:TRP:HB2	1.98	0.46
22:V:519:TYR:CE2	25:1:20:LEU:HG	2.51	0.46
23:W:623:VAL:HG23	23:W:681:ASP:HB2	1.98	0.46
26:2:187:SER:OG	26:2:190:PRO:HD2	2.16	0.46
26:2:171:VAL:CG2	26:2:213:TRP:HA	2.19	0.46
2:B:180:ASP:OD1	2:B:181:PRO:HD2	2.16	0.46
13:M:183:VAL:HG12	20:T:152:ASN:ND2	2.31	0.46
17:Q:185:GLU:HB3	17:Q:186:PRO:HD3	1.97	0.46
18:R:80:LYS:HG2	18:R:108:HIS:HE1	1.81	0.46
25:1:57:VAL:HG13	25:1:58:GLY:N	2.31	0.46
27:3:64:ILE:CG2	27:3:128:HIS:CG	2.99	0.46
1:A:1026:ASP:O	1:A:1031:ARG:NH2	2.49	0.46
1:A:1158:LEU:O	1:A:1162:GLU:HG3	2.16	0.46
1:A:1319:LYS:HG3	1:A:1333:GLU:CD	2.36	0.46
2:B:1101:GLN:HE22	6:F:64:ARG:CG	2.29	0.46
8:H:85:ALA:HB1	8:H:88:PHE:CZ	2.51	0.46
1:A:734:ARG:HH12	9:I:104:ALA:HB1	1.81	0.46
15:O:80:GLU:HG3	15:O:89:LYS:HG2	1.98	0.46
17:Q:104:LYS:HE3	17:Q:105:TYR:CZ	2.50	0.46
17:Q:170:LYS:O	17:Q:174:ARG:N	2.47	0.46
29:Y:25:DT:H2"	29:Y:26:DG:C8	2.51	0.46
25:1:54:GLN:O	25:1:57:VAL:HG12	2.16	0.45
27:3:8:LEU:HD23	27:3:54:SER:CB	2.42	0.45
1:A:1163:HIS:H	1:A:1307:VAL:CG2	2.29	0.45
1:A:42:LYS:NZ	1:A:43:TYR:O	2.49	0.45
1:A:621:ILE:O	1:A:623:PRO:CD	2.64	0.45
1:A:365:THR:HG22	2:B:1059:ILE:HG22	1.97	0.45
1:A:511:THR:HG21	2:B:1105:GLU:OE2	2.16	0.45
2:B:422:PHE:CD1	2:B:427:LYS:HA	2.50	0.45
23:W:420:PRO:O	23:W:421:PHE:CG	2.68	0.45
28:X:77:DC:H2"	28:X:78:DT:H72	1.98	0.45
26:2:117:ASN:HB2	27:3:104:LEU:CG	2.47	0.45
26:2:90:LEU:HD21	26:2:140:LYS:HD3	1.98	0.45
26:2:217:LEU:CD2	26:2:233:ILE:HD11	2.45	0.45
1:A:1408:ARG:HH22	1:A:1421:ARG:HB2	1.81	0.45
1:A:48:GLU:O	1:A:49:GLY:C	2.53	0.45
13:M:157:ASP:OD2	13:M:185:ARG:NH2	2.49	0.45
17:Q:112:ARG:NH2	18:R:237:LEU:O	2.50	0.45
17:Q:113:ARG:NH2	18:R:218:LYS:HG3	2.29	0.45
18:R:123:ALA:O	18:R:127:ASN:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:180:PHE:CE1	18:R:213:ASP:N	2.84	0.45
21:U:251:ALA:C	21:U:253:THR:N	2.69	0.45
22:V:517:GLU:CB	22:V:713:LEU:HD22	2.46	0.45
27:3:64:ILE:CG2	27:3:128:HIS:CB	2.94	0.45
1:A:119:VAL:HG21	1:A:147:LEU:HD21	1.97	0.45
1:A:465:HIS:CE1	1:A:467:MET:HB2	2.52	0.45
1:A:873:VAL:HG22	1:A:1083:PRO:HA	1.99	0.45
2:B:1001:PRO:HB2	2:B:1002:PHE:CE1	2.51	0.45
2:B:809:VAL:HG23	2:B:924:ARG:HG3	1.99	0.45
8:H:8:ASP:HB3	8:H:10:PHE:CE1	2.52	0.45
1:A:804:HIS:NE2	9:I:100:HIS:HA	2.31	0.45
10:J:3:ILE:HG13	10:J:52:HIS:CD2	2.51	0.45
21:U:256:THR:HB	21:U:272:THR:HB	1.99	0.45
29:Y:54:DA:H3'	29:Y:55:DG:H5"	1.97	0.45
26:2:203:PHE:CG	26:2:204:LEU:N	2.85	0.45
27:3:190:LEU:HA	27:3:210:THR:HG21	1.91	0.45
27:3:33:THR:HG22	27:3:36:LYS:CB	2.44	0.45
1:A:111:CYS:SG	1:A:188:GLN:NE2	2.90	0.45
1:A:196:LEU:HG	1:A:325:LEU:HD21	1.98	0.45
1:A:529:GLN:HG3	1:A:1094:SER:HB3	1.98	0.45
1:A:610:PRO:HB3	1:A:626:THR:CG2	2.47	0.45
2:B:573:TRP:O	2:B:573:TRP:HE3	2.00	0.45
9:I:73:SER:HA	9:I:95:VAL:HG21	1.97	0.45
17:Q:187:ILE:HG21	18:R:210:PHE:O	2.16	0.45
17:Q:36:ILE:HG23	17:Q:39:ARG:NH2	2.32	0.45
25:1:2:VAL:HG11	26:2:456:LYS:CB	2.44	0.45
1:A:948:ILE:HG23	1:A:1007:ILE:HD11	1.99	0.45
1:A:1451:MET:CE	1:A:1456:GLU:HB3	2.47	0.45
1:A:516:GLN:HA	1:A:520:MET:CE	2.46	0.45
2:B:1062:ARG:HH21	2:B:1065:GLY:N	2.10	0.45
2:B:109:MET:O	2:B:112:GLU:N	2.50	0.45
4:D:140:PHE:CZ	4:D:142:TYR:HB3	2.52	0.45
5:E:84:ILE:CD1	28:X:65:DG:OP1	2.64	0.45
5:E:91:CYS:HA	5:E:94:MET:HG2	1.98	0.45
8:H:85:ALA:CB	8:H:88:PHE:CE2	2.99	0.45
8:H:88:PHE:CE1	8:H:146:LYS:HD2	2.51	0.45
16:P:204:ILE:HD12	16:P:206:GLU:HB2	1.98	0.45
26:2:189:GLU:CB	26:2:190:PRO:HD3	2.43	0.45
27:3:121:LYS:H	27:3:121:LYS:HD3	1.80	0.45
1:A:1163:HIS:N	1:A:1307:VAL:HG21	2.31	0.45
1:A:1119:LEU:HD13	1:A:1388:PHE:CG	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:496:ALA:HB3	2:B:498:PRO:HD2	1.99	0.45
7:G:107:PHE:CZ	17:Q:127:PHE:HZ	2.34	0.45
9:I:75:ASP:HA	9:I:76:PRO:HD3	1.87	0.45
3:C:275:ASN:ND2	11:K:23:LYS:HA	2.31	0.45
2:B:1068:GLN:HB3	13:M:51:GLU:HB3	1.99	0.45
14:N:333:ASN:HB3	14:N:359:ASN:O	2.16	0.45
16:P:263:ASP:OD1	16:P:264:VAL:N	2.49	0.45
21:U:194:ARG:HD3	21:U:194:ARG:HA	1.61	0.45
26:2:130:SER:HB2	26:2:179:LEU:HD23	1.98	0.45
26:2:203:PHE:CD2	26:2:205:LEU:CD2	2.95	0.45
26:2:30:VAL:CG1	26:2:34:LEU:CD2	2.94	0.45
26:2:35:TYR:HB2	26:2:62:LEU:HD12	1.99	0.45
27:3:42:MET:CG	27:3:111:ILE:CD1	2.95	0.45
1:A:1189:ASP:O	1:A:1192:TRP:N	2.48	0.45
1:A:271:ARG:O	1:A:272:ASN:OD1	2.34	0.45
1:A:516:GLN:HA	1:A:520:MET:HE2	1.97	0.45
1:A:576:GLN:HG3	1:A:577:PRO:HD2	1.97	0.45
2:B:41:ARG:HA	2:B:41:ARG:HD2	1.36	0.45
2:B:531:TYR:CD2	2:B:532:ILE:N	2.85	0.45
19:S:166:ARG:CG	19:S:166:ARG:HH11	2.28	0.45
22:V:461:HIS:CE1	22:V:462:CYS:HG	2.34	0.45
28:X:48:DT:OP1	28:X:48:DT:H4'	2.16	0.45
27:3:219:GLN:HA	27:3:219:GLN:OE1	2.17	0.45
1:A:1468:THR:HA	6:F:60:TYR:HB3	1.98	0.45
1:A:522:PRO:HG3	1:A:666:ARG:HG3	1.99	0.45
1:A:893:GLU:O	5:E:200:ALA:HB2	2.17	0.45
1:A:931:ARG:O	1:A:933:THR:HG23	2.16	0.45
2:B:91:ILE:HD11	2:B:124:LEU:HD11	1.98	0.45
5:E:52:ARG:NH2	5:E:54:ARG:HH11	2.15	0.45
9:I:11:PHE:HE1	9:I:54:TYR:HA	1.81	0.45
9:I:84:HIS:HB3	9:I:92:LYS:HB3	1.99	0.45
11:K:5:PRO:HB2	11:K:7:PHE:CE2	2.52	0.45
13:M:7:LEU:CG	13:M:10:LEU:HD13	2.46	0.45
14:N:313:PRO:HD2	16:P:250:PHE:HB3	1.98	0.45
9:I:41:ASN:HB2	19:S:153:ARG:HD2	1.99	0.45
28:X:65:DG:C6	28:X:66:DA:C2	3.05	0.45
29:Y:34:DC:H1'	29:Y:35:DG:OP2	2.16	0.45
26:2:217:LEU:CD2	26:2:233:ILE:CD1	2.95	0.45
26:2:51:LEU:C	26:2:51:LEU:HD23	2.37	0.45
1:A:267:GLN:O	1:A:268:GLY:C	2.55	0.45
12:L:26:ASN:OD1	12:L:36:CYS:HA	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:312:GLU:C	14:N:314:LEU:H	2.20	0.45
15:O:7:ARG:HB3	15:O:16:GLN:NE2	2.32	0.45
23:W:37:HIS:NE2	23:W:454:VAL:HG11	2.32	0.45
26:2:35:TYR:CD2	26:2:62:LEU:CB	2.95	0.45
27:3:148:ASN:ND2	27:3:157:MET:HG3	2.32	0.45
1:A:1139:LEU:HB3	1:A:1338:THR:OG1	2.16	0.45
1:A:26:LEU:HD12	1:A:26:LEU:O	2.17	0.45
1:A:540:ASP:CB	2:B:790:GLN:NE2	2.79	0.45
7:G:63:ARG:C	7:G:65:PHE:H	2.20	0.45
18:R:171:ILE:HG12	18:R:177:ASN:H	1.82	0.45
29:Y:58:DC:H1'	29:Y:59:DG:C4	2.51	0.45
26:2:123:LEU:CD2	26:2:178:LEU:CD1	2.95	0.44
26:2:140:LYS:HD3	26:2:162:PHE:CE1	2.47	0.44
24:0:100:PRO:HG2	27:3:208:ASP:OD2	2.17	0.44
27:3:71:TYR:O	27:3:71:TYR:CG	2.70	0.44
1:A:1103:THR:HG21	1:A:1119:LEU:HG	1.99	0.44
1:A:1103:THR:HG23	1:A:1106:THR:OG1	2.17	0.44
1:A:1128:ILE:HD12	1:A:1414:ILE:HD11	1.98	0.44
1:A:208:ASP:OD1	1:A:209:SER:N	2.38	0.44
1:A:599:HIS:O	1:A:992:LYS:NZ	2.50	0.44
2:B:289:ILE:HG12	2:B:291:ASP:H	1.82	0.44
5:E:84:ILE:CD1	28:X:65:DG:P	3.04	0.44
7:G:44:PHE:HE2	7:G:104:MET:HB2	1.83	0.44
23:W:37:HIS:CD2	23:W:454:VAL:CG1	3.00	0.44
26:2:28:PRO:CD	27:3:25:GLN:NE2	2.72	0.44
1:A:1029:LEU:H	5:E:162:ARG:HH12	1.66	0.44
1:A:1199:MET:SD	1:A:1200:PRO:HD2	2.56	0.44
1:A:1435:THR:OG1	1:A:1436:VAL:N	2.49	0.44
1:A:624:GLY:C	1:A:626:THR:H	2.20	0.44
2:B:598:VAL:O	2:B:600:GLU:N	2.49	0.44
5:E:11:TRP:CE3	5:E:37:LEU:HD13	2.51	0.44
8:H:71:ASP:N	8:H:71:ASP:OD1	2.48	0.44
10:J:3:ILE:HG22	10:J:15:GLY:HA2	1.99	0.44
1:A:197:GLU:CD	13:M:93:PHE:CE2	2.90	0.44
17:Q:128:LYS:HG3	17:Q:129:CYS:N	2.32	0.44
17:Q:188:TYR:CE2	18:R:211:SER:HB3	2.52	0.44
17:Q:25:PHE:CE1	18:R:210:PHE:CZ	3.05	0.44
20:T:121:SER:OG	20:T:122:GLU:N	2.50	0.44
22:V:370:SER:O	22:V:374:TRP:CD1	2.71	0.44
24:0:106:ILE:HD11	24:0:127:HIS:HB3	2.00	0.44
24:0:165:ARG:HD3	24:0:194:ILE:HG12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:2:258:LEU:HG	26:2:262:LEU:HD21	1.99	0.44
1:A:1112:VAL:HG12	21:U:254:GLY:HA2	2.00	0.44
1:A:1310:HIS:O	21:U:252:LYS:HD3	2.16	0.44
1:A:426:ARG:HB3	13:M:40:VAL:CG2	2.48	0.44
2:B:1055:VAL:HG13	2:B:1056:ASP:N	2.33	0.44
3:C:85:SER:CB	3:C:166:LYS:HE3	2.46	0.44
9:I:105:GLU:HB3	9:I:107:ALA:HB3	1.98	0.44
18:R:157:GLN:HG3	18:R:159:ASP:H	1.82	0.44
21:U:134:PRO:HG2	21:U:174:GLU:HG2	1.99	0.44
26:2:159:VAL:HG22	26:2:160:LEU:HD13	1.95	0.44
27:3:65:GLN:O	27:3:132:LEU:HD11	2.18	0.44
1:A:1117:VAL:O	1:A:1118:THR:O	2.35	0.44
1:A:1371:ILE:HD13	1:A:1409:GLY:O	2.17	0.44
1:A:415:GLY:O	1:A:449:HIS:HD2	2.00	0.44
8:H:96:VAL:HG22	8:H:116:VAL:HG13	2.00	0.44
9:I:25:TYR:HD2	9:I:40:ARG:HG3	1.82	0.44
16:P:317:VAL:HG12	16:P:319:ALA:H	1.82	0.44
17:Q:188:TYR:CE1	18:R:210:PHE:CG	3.04	0.44
19:S:18:VAL:HG22	19:S:137:ALA:HB3	1.98	0.44
21:U:243:GLU:O	21:U:247:GLU:N	2.46	0.44
27:3:228:LEU:HD23	27:3:228:LEU:O	2.18	0.44
1:A:1429:LYS:HB2	1:A:1438:VAL:HG21	2.00	0.44
1:A:340:LYS:HG3	1:A:1436:VAL:HG21	1.99	0.44
1:A:263:ALA:C	1:A:264:VAL:HG22	2.37	0.44
1:A:672:ILE:HD13	1:A:672:ILE:HG21	1.74	0.44
11:K:53:ASP:OD1	11:K:54:PRO:HD2	2.18	0.44
12:L:56:ASP:N	12:L:56:ASP:OD1	2.46	0.44
19:S:128:THR:HG22	19:S:136:GLU:HB3	1.98	0.44
22:V:444:HIS:O	22:V:447:PRO:CD	2.61	0.44
22:V:647:LYS:O	22:V:648:LYS:O	2.35	0.44
23:W:73:CYS:CB	23:W:209:TYR:CE2	3.01	0.44
25:1:21:LEU:O	25:1:24:ASP:HB3	2.17	0.44
26:2:159:VAL:HG12	26:2:161:HIS:HB2	1.99	0.44
26:2:204:LEU:HD23	26:2:254:MET:HE2	1.98	0.44
27:3:33:THR:CG2	27:3:36:LYS:H	2.04	0.44
2:B:899:SER:O	2:B:901:THR:N	2.51	0.44
2:B:926:VAL:O	2:B:926:VAL:HG23	2.17	0.44
2:B:934:LYS:HE2	2:B:942:LYS:HD2	1.98	0.44
5:E:3:ASP:O	5:E:6:GLU:HB2	2.18	0.44
9:I:84:HIS:HB2	9:I:85:PRO:HD3	0.96	0.44
13:M:60:ALA:HB1	29:Y:54:DA:C2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:148:LYS:HD3	18:R:174:ALA:HB2	2.00	0.44
13:M:178:LYS:NZ	20:T:156:VAL:HG11	2.31	0.44
20:T:194:HIS:N	20:T:197:TYR:OH	2.50	0.44
21:U:260:LEU:HB3	21:U:261:PHE:H	1.61	0.44
26:2:164:VAL:HG13	26:2:209:PRO:CG	2.45	0.44
26:2:206:LEU:CD2	26:2:206:LEU:H	2.31	0.44
25:1:1:MET:SD	26:2:419:GLU:N	2.90	0.44
27:3:124:ILE:HG23	27:3:124:ILE:O	2.18	0.44
27:3:160:ARG:HB2	27:3:160:ARG:HE	1.58	0.44
27:3:160:ARG:CB	27:3:190:LEU:CD2	2.95	0.44
1:A:1407:CYS:SG	1:A:1408:ARG:HG2	2.58	0.44
1:A:186:ARG:HH11	1:A:208:ASP:HB2	1.82	0.44
2:B:783:ALA:HB2	2:B:1041:ILE:CG2	2.48	0.44
3:C:31:ALA:HB1	3:C:184:PHE:HE1	1.81	0.44
14:N:42:LEU:HB2	15:O:22:LEU:HD11	1.99	0.44
25:1:11:GLU:HG2	26:2:404:THR:OG1	2.17	0.44
25:1:34:ILE:CG2	25:1:50:VAL:HG11	2.48	0.44
25:1:21:LEU:HB3	25:1:54:GLN:NE2	2.33	0.44
26:2:189:GLU:HB2	26:2:190:PRO:CD	2.43	0.44
26:2:221:GLN:HG2	26:2:268:PHE:HZ	1.75	0.44
26:2:35:TYR:CD1	26:2:62:LEU:HD12	2.52	0.44
27:3:144:ILE:HD13	27:3:144:ILE:O	2.17	0.44
27:3:60:ILE:HG23	27:3:68:ARG:O	2.17	0.44
1:A:271:ARG:O	1:A:272:ASN:CB	2.64	0.44
7:G:116:GLU:O	7:G:130:THR:HA	2.16	0.44
7:G:18:PHE:HA	7:G:22:LEU:HD13	2.00	0.44
9:I:92:LYS:HG3	9:I:93:GLU:HG2	1.99	0.44
13:M:37:CYS:SG	13:M:38:GLY:N	2.91	0.44
17:Q:68:GLY:C	18:R:226:ASP:CG	2.76	0.44
18:R:88:ARG:NH1	18:R:97:LEU:HD11	2.33	0.44
2:B:333:GLU:CD	19:S:53:ASN:HD21	2.17	0.44
20:T:128:LYS:O	20:T:132:ILE:N	2.44	0.44
26:2:214:TYR:OH	26:2:265:LEU:HD13	2.18	0.44
2:B:1072:ARG:HD3	2:B:1153:TYR:CD2	2.53	0.44
3:C:59:LEU:HA	3:C:59:LEU:HD12	1.73	0.44
22:V:282:LYS:HE3	22:V:482:PHE:CD1	2.53	0.44
23:W:73:CYS:HB3	23:W:209:TYR:CD2	2.52	0.44
28:X:51:DC:H2'	28:X:52:DG:C4	2.53	0.44
25:1:13:ASP:CB	25:1:14:PRO:HD2	2.46	0.43
26:2:236:PHE:HZ	26:2:258:LEU:HD11	1.83	0.43
26:2:60:LEU:CD1	26:2:95:ILE:CB	2.95	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:2:117:ASN:CA	27:3:104:LEU:HD21	2.47	0.43
1:A:865:ILE:HD12	2:B:1092:ASP:OD1	2.17	0.43
1:A:931:ARG:CA	1:A:931:ARG:NE	2.74	0.43
1:A:926:ASN:CA	1:A:931:ARG:NH1	2.73	0.43
2:B:17:ILE:HG23	2:B:18:THR:HG23	2.00	0.43
2:B:271:ILE:HD12	2:B:311:ILE:HD11	2.00	0.43
5:E:41:LYS:HG3	5:E:46:ASP:CB	2.48	0.43
13:M:25:GLU:OE1	13:M:44:ARG:NH2	2.36	0.43
13:M:91:ALA:O	13:M:92:SER:C	2.55	0.43
16:P:288:PHE:CD1	16:P:289:PRO:HD2	2.54	0.43
17:Q:100:VAL:O	17:Q:103:VAL:HG23	2.18	0.43
17:Q:69:ASP:HA	18:R:226:ASP:CG	2.37	0.43
24:0:60:HIS:CE1	24:0:159:MET:SD	3.11	0.43
25:1:3:ASN:HB3	26:2:412:PHE:O	2.18	0.43
26:2:166:SER:HB3	26:2:167:PRO:HD3	2.00	0.43
26:2:117:ASN:ND2	27:3:104:LEU:O	2.52	0.43
1:A:614:ASP:OD2	21:U:267:LYS:HG3	2.17	0.43
2:B:106:SER:HB2	2:B:107:PRO:HD2	2.00	0.43
1:A:514:GLU:OE1	2:B:1099:ALA:HB1	2.18	0.43
2:B:529:MET:HE2	2:B:624:PRO:O	2.18	0.43
2:B:759:VAL:CG1	2:B:999:ALA:HB2	2.48	0.43
3:C:71:ILE:HG22	3:C:148:ILE:HG21	2.00	0.43
10:J:35:LEU:HD13	10:J:46:ARG:HG2	2.00	0.43
16:P:329:TYR:N	16:P:330:PRO:HD2	2.34	0.43
22:V:519:TYR:HA	22:V:522:TYR:HB3	2.00	0.43
13:M:57:ASN:HA	29:Y:51:DC:N4	2.33	0.43
26:2:56:VAL:HG23	26:2:57:MET:N	2.31	0.43
27:3:178:MET:O	27:3:182:PHE:HD2	2.01	0.43
27:3:178:MET:CE	27:3:202:LEU:CD1	2.95	0.43
1:A:779:ILE:O	1:A:783:GLN:HG3	2.19	0.43
2:B:1029:TYR:CD1	2:B:1029:TYR:N	2.85	0.43
2:B:936:ALA:O	2:B:1049:GLN:N	2.42	0.43
9:I:58:ILE:O	9:I:59:THR:OG1	2.36	0.43
17:Q:113:ARG:CD	18:R:222:SER:HB3	2.46	0.43
22:V:446:ILE:HD12	22:V:451:PHE:HB3	1.99	0.43
25:1:4:VAL:HG22	25:1:5:LEU:N	2.33	0.43
26:2:127:LYS:CA	26:2:178:LEU:HD23	2.48	0.43
26:2:218:GLN:HE22	26:2:265:LEU:CA	2.28	0.43
26:2:224:GLN:N	26:2:268:PHE:HZ	2.16	0.43
26:2:94:ARG:HD2	26:2:95:ILE:CD1	2.47	0.43
26:2:61:PHE:CE1	26:2:99:GLN:NE2	2.85	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:2:117:ASN:ND2	27:3:108:ASN:N	2.65	0.43
27:3:33:THR:CG2	27:3:36:LYS:CB	2.95	0.43
1:A:1162:GLU:OE2	1:A:1308:TYR:CE2	2.71	0.43
1:A:866:LYS:HG2	1:A:1432:PHE:CD1	2.54	0.43
2:B:1028:LEU:C	2:B:1029:TYR:HD1	2.21	0.43
3:C:71:ILE:CG2	3:C:148:ILE:HG21	2.48	0.43
3:C:24:GLU:HG2	3:C:228:ARG:CG	2.46	0.43
6:F:102:ILE:CG2	6:F:104:ILE:HG12	2.49	0.43
8:H:10:PHE:CE2	8:H:39:LEU:HD13	2.54	0.43
8:H:34:SER:O	8:H:36:LYS:HG3	2.19	0.43
9:I:65:LEU:HA	9:I:122:ARG:HE	1.83	0.43
14:N:319:ASP:C	14:N:321:SER:N	2.72	0.43
15:O:80:GLU:OE2	15:O:82:ARG:NE	2.44	0.43
17:Q:126:SER:O	17:Q:164:ASP:HB2	2.18	0.43
20:T:138:PRO:HG2	20:T:140:ARG:HH22	1.83	0.43
21:U:139:SER:O	21:U:143:LYS:HG2	2.19	0.43
28:X:77:DC:C2'	28:X:78:DT:H72	2.48	0.43
22:V:666:ASP:CB	25:1:17:LYS:HZ3	2.30	0.43
26:2:214:TYR:HB3	26:2:261:PHE:CE2	2.54	0.43
26:2:223:ALA:H	26:2:268:PHE:HE1	1.64	0.43
26:2:243:SER:HB3	26:2:258:LEU:CD2	2.45	0.43
26:2:270:LEU:HA	26:2:273:GLN:HG3	2.00	0.43
27:3:121:LYS:CD	27:3:121:LYS:H	2.32	0.43
27:3:178:MET:HA	27:3:181:ILE:HD12	2.00	0.43
1:A:924:TYR:CE2	1:A:949:GLN:HG2	2.54	0.43
1:A:987:ILE:HD13	1:A:1058:PHE:CD2	2.53	0.43
2:B:1115:GLN:HB2	2:B:1148:LEU:HD11	2.00	0.43
1:A:1290:SER:HB2	2:B:250:SER:CB	2.47	0.43
2:B:783:ALA:HB2	2:B:1041:ILE:HG21	2.01	0.43
3:C:6:GLN:HA	3:C:7:PRO:HD2	1.78	0.43
10:J:4:PRO:O	10:J:14:VAL:HG12	2.18	0.43
1:A:199:TYR:HE2	13:M:93:PHE:HZ	1.64	0.43
21:U:200:ASP:OD2	21:U:203:ASN:N	2.52	0.43
22:V:524:ALA:HB2	25:1:23:LEU:HD13	1.99	0.43
23:W:107:LEU:HB2	23:W:175:TYR:CZ	2.54	0.43
25:1:25:GLU:OE2	25:1:35:ILE:HG12	2.18	0.43
26:2:215:PHE:CE2	26:2:264:HIS:ND1	2.86	0.43
26:2:409:TYR:CD2	26:2:443:VAL:HG22	2.54	0.43
27:3:165:LYS:HZ1	27:3:200:SER:N	2.16	0.43
2:B:758:LEU:HA	2:B:758:LEU:HD23	1.68	0.43
2:B:967:ILE:HD12	2:B:968:ASN:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:134:ASN:H	3:C:136:ASP:CG	2.16	0.43
4:D:26:PHE:CE2	7:G:78:ARG:HG2	2.53	0.43
8:H:11:ASP:HB2	8:H:55:LYS:HG2	2.00	0.43
13:M:27:TYR:HD1	13:M:46:ILE:HG21	1.84	0.43
1:A:326:PRO:HD3	13:M:92:SER:OG	2.18	0.43
14:N:376:TRP:HD1	15:O:62:LEU:O	2.01	0.43
19:S:100:LEU:HD23	19:S:110:PHE:CD2	2.50	0.43
20:T:229:HIS:HD2	28:X:28:DG:H21	1.65	0.43
22:V:405:VAL:HG12	22:V:406:ALA:H	1.83	0.43
22:V:514:MET:SD	22:V:537:ASN:CG	2.97	0.43
25:1:50:VAL:HG12	25:1:50:VAL:O	2.18	0.43
25:1:8:VAL:CG1	25:1:9:LEU:N	2.80	0.43
26:2:236:PHE:CE1	26:2:239:GLN:NE2	2.87	0.43
27:3:184:ALA:O	27:3:187:GLN:HG2	2.19	0.43
1:A:15:LEU:HD12	2:B:1148:LEU:O	2.19	0.43
2:B:765:GLU:OE1	2:B:770:ARG:NE	2.49	0.43
16:P:178:LEU:HB3	16:P:183:ILE:HD11	2.00	0.43
20:T:82:PRO:HD2	20:T:117:ARG:O	2.19	0.43
22:V:519:TYR:HB3	25:1:16:MET:HG3	2.00	0.43
23:W:263:LEU:C	23:W:263:LEU:HD23	2.39	0.43
23:W:28:LEU:HD13	23:W:28:LEU:C	2.38	0.43
26:2:117:ASN:HB3	27:3:42:MET:HE2	2.00	0.43
1:A:505:LEU:HD23	1:A:507:GLN:HE22	1.84	0.43
2:B:51:ILE:HD13	2:B:51:ILE:HA	1.75	0.43
2:B:90:GLN:NE2	20:T:141:LEU:CA	2.56	0.43
5:E:47:LYS:HA	5:E:47:LYS:HD3	1.63	0.43
17:Q:137:THR:OG1	17:Q:139:LEU:HG	2.18	0.43
1:A:1128:ILE:HA	1:A:1128:ILE:HD13	1.80	0.43
1:A:156:GLY:O	1:A:180:GLY:HA2	2.19	0.43
2:B:52:GLN:HB2	2:B:160:TYR:OH	2.19	0.43
9:I:50:ASN:OD1	9:I:51:SER:N	2.51	0.43
9:I:60:HIS:C	9:I:62:VAL:N	2.71	0.43
17:Q:113:ARG:HD3	18:R:222:SER:HB2	1.99	0.43
21:U:133:ALA:HA	21:U:134:PRO:HD3	1.89	0.43
22:V:615:PHE:O	22:V:615:PHE:CG	2.70	0.43
26:2:117:ASN:HD21	27:3:108:ASN:N	2.16	0.43
27:3:42:MET:HE1	27:3:108:ASN:HB2	2.00	0.43
1:A:274:ASP:C	1:A:276:LEU:N	2.72	0.43
1:A:609:HIS:O	1:A:610:PRO:O	2.36	0.43
2:B:1162:LEU:O	2:B:1167:ILE:HB	2.18	0.43
2:B:132:VAL:CG2	2:B:141:GLN:HG3	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:422:PHE:CD1	2:B:422:PHE:C	2.91	0.43
13:M:184:SER:OG	13:M:185:ARG:N	2.52	0.43
1:A:264:VAL:HB	13:M:52:TRP:CE3	2.53	0.43
16:P:297:LYS:C	16:P:299:ARG:N	2.71	0.43
18:R:151:LEU:HD12	18:R:163:LEU:HD21	1.86	0.43
20:T:59:ASN:OD1	20:T:60:GLU:N	2.52	0.43
23:W:584:TYR:CB	23:W:591:GLY:HA3	2.48	0.43
26:2:118:LEU:HD22	27:3:39:ASP:CB	2.50	0.42
26:2:34:LEU:HD22	26:2:34:LEU:N	2.33	0.42
27:3:141:LEU:HA	27:3:144:ILE:HG22	2.01	0.42
1:A:1175:ILE:HG23	1:A:1285:LEU:HD23	2.01	0.42
1:A:231:GLU:OE1	1:A:231:GLU:N	2.41	0.42
1:A:937:ASP:O	1:A:940:LYS:HD2	2.19	0.42
2:B:25:ALA:HA	2:B:28:ILE:HD12	2.01	0.42
8:H:65:TYR:N	8:H:65:TYR:CD1	2.87	0.42
2:B:285:LEU:HD22	9:I:16:PHE:HZ	1.84	0.42
14:N:347:ASN:HB3	16:P:208:ARG:HH11	1.84	0.42
20:T:26:TYR:CE2	20:T:127:LEU:HD21	2.54	0.42
26:2:138:PRO:HD3	26:2:189:GLU:CD	2.40	0.42
27:3:111:ILE:HG13	27:3:112:VAL:H	1.83	0.42
1:A:199:TYR:CE2	13:M:93:PHE:CZ	3.02	0.42
1:A:212:LYS:HE2	1:A:212:LYS:H	1.84	0.42
3:C:73:LEU:O	3:C:238:SER:HB3	2.20	0.42
5:E:56:THR:N	5:E:78:GLU:OE2	2.52	0.42
16:P:297:LYS:HA	16:P:297:LYS:HD2	1.76	0.42
18:R:166:ILE:HG22	18:R:168:LEU:H	1.84	0.42
23:W:416:ILE:HA	23:W:434:HIS:O	2.19	0.42
29:Y:70:DC:H2"	29:Y:71:DA:C8	2.54	0.42
22:V:514:MET:HB3	25:1:16:MET:SD	2.59	0.42
26:2:117:ASN:CB	27:3:42:MET:HE1	2.47	0.42
26:2:57:MET:CA	26:2:60:LEU:HG	2.49	0.42
26:2:117:ASN:CG	27:3:42:MET:HE1	2.23	0.42
1:A:1154:ALA:HB1	1:A:1310:HIS:CE1	2.46	0.42
1:A:1301:ILE:HG13	1:A:1302:GLU:HG2	2.01	0.42
1:A:1304:ILE:C	1:A:1307:VAL:HG22	2.32	0.42
1:A:666:ARG:HD3	1:A:666:ARG:HA	1.79	0.42
1:A:766:PHE:CD1	1:A:781:ILE:HD11	2.54	0.42
1:A:799:PRO:O	1:A:806:THR:HG22	2.19	0.42
1:A:954:ARG:HD3	1:A:954:ARG:HA	1.84	0.42
2:B:230:ARG:HB2	2:B:405:ARG:CZ	2.50	0.42
4:D:48:ASN:ND2	4:D:57:LEU:HG	2.24	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:25:GLY:O	5:E:65:ASN:HA	2.19	0.42
10:J:66:GLU:HG3	12:L:23:HIS:ND1	2.34	0.42
12:L:26:ASN:ND2	12:L:44:MET:SD	2.92	0.42
13:M:178:LYS:HD3	20:T:154:LYS:HD3	2.00	0.42
13:M:245:VAL:HB	13:M:248:ARG:HB2	2.01	0.42
21:U:226:GLU:HB3	21:U:227:GLU:H	1.57	0.42
26:2:203:PHE:HD2	26:2:205:LEU:H	1.65	0.42
27:3:124:ILE:HD13	27:3:124:ILE:C	2.38	0.42
27:3:128:HIS:NE2	27:3:130:GLU:CG	2.82	0.42
27:3:137:LEU:HD12	27:3:177:PHE:CE1	2.54	0.42
1:A:1251:ASN:HB3	21:U:234:LYS:HE2	2.01	0.42
2:B:1027:VAL:HG12	2:B:1029:TYR:HE1	1.84	0.42
2:B:906:GLN:HB3	12:L:45:TYR:CE1	2.53	0.42
5:E:121:MET:HG2	5:E:127:LEU:HD13	2.00	0.42
6:F:105:ILE:HG22	6:F:119:GLY:HA2	2.00	0.42
7:G:108:ILE:HG21	7:G:163:LEU:HG	2.01	0.42
7:G:117:MET:HG2	7:G:128:TYR:HB3	2.00	0.42
21:U:250:MET:O	21:U:251:ALA:CB	2.68	0.42
1:A:1389:ASP:O	21:U:297:ARG:NH2	2.53	0.42
26:2:133:THR:CG2	26:2:134:SER:N	2.83	0.42
26:2:140:LYS:CD	26:2:162:PHE:HE1	2.29	0.42
27:3:42:MET:SD	27:3:111:ILE:CD1	3.07	0.42
27:3:14:VAL:CG2	27:3:163:VAL:HG13	2.48	0.42
27:3:160:ARG:CZ	27:3:190:LEU:CD1	2.97	0.42
27:3:9:ASN:OD1	27:3:158:LYS:HB3	2.19	0.42
1:A:392:GLU:OE1	1:A:448:ARG:NE	2.45	0.42
1:A:612:ASP:O	1:A:613:GLU:C	2.57	0.42
1:A:922:PHE:HA	1:A:1052:ARG:HD3	2.01	0.42
2:B:1029:TYR:CD1	2:B:1036:LYS:HG2	2.54	0.42
2:B:510:CYS:SG	2:B:511:PRO:HD2	2.60	0.42
9:I:105:GLU:HA	9:I:105:GLU:OE1	2.18	0.42
12:L:17:TYR:HD1	12:L:46:LYS:HA	1.83	0.42
13:M:214:PHE:HB3	13:M:218:PHE:HE2	1.84	0.42
13:M:263:GLN:HA	13:M:268:LYS:HG2	2.01	0.42
20:T:155:PRO:C	20:T:157:ALA:N	2.73	0.42
22:V:516:PRO:CA	25:1:15:ALA:C	2.82	0.42
26:2:188:THR:CG2	26:2:189:GLU:N	2.83	0.42
26:2:236:PHE:CE1	26:2:261:PHE:HB3	2.54	0.42
2:B:192:LYS:HE2	2:B:449:ALA:O	2.20	0.42
2:B:198:GLU:OE2	2:B:391:LYS:HD3	2.20	0.42
3:C:225:LYS:O	3:C:227:GLU:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:74:ILE:O	3:C:128:ILE:HG13	2.19	0.42
8:H:108:ALA:C	8:H:110:THR:N	2.72	0.42
8:H:81:ARG:HA	8:H:82:PRO:HD3	1.83	0.42
10:J:64:PRO:HG3	12:L:21:GLU:OE2	2.19	0.42
13:M:179:GLU:HA	20:T:154:LYS:HZ1	1.85	0.42
18:R:113:LEU:HA	18:R:116:LYS:HE3	2.01	0.42
13:M:178:LYS:HG2	20:T:156:VAL:CG1	2.48	0.42
26:2:77:LYS:HD3	26:2:78:GLU:CG	2.50	0.42
1:A:376:ASP:HB3	1:A:521:VAL:HB	2.00	0.42
1:A:43:TYR:O	1:A:45:GLU:N	2.49	0.42
1:A:455:ILE:HG12	1:A:473:ARG:HG2	2.02	0.42
1:A:620:HIS:O	1:A:621:ILE:C	2.54	0.42
2:B:155:MET:HB2	2:B:185:PHE:CE1	2.54	0.42
2:B:613:ARG:HD3	2:B:615:TYR:OH	2.19	0.42
2:B:72:GLN:NE2	2:B:80:GLU:N	2.67	0.42
3:C:67:ARG:NH1	3:C:150:ILE:HA	2.35	0.42
1:A:999:ARG:CZ	8:H:99:ILE:HG21	2.49	0.42
9:I:66:THR:O	9:I:68:ILE:HG22	2.20	0.42
13:M:46:ILE:O	13:M:46:ILE:HG13	2.19	0.42
19:S:51:LEU:HG	19:S:54:LYS:HB2	2.00	0.42
13:M:196:LYS:NZ	28:X:13:DT:OP1	2.41	0.42
29:Y:24:DC:C6	29:Y:25:DT:H73	2.55	0.42
29:Y:57:DA:H5"	29:Y:58:DC:H2'	2.02	0.42
26:2:35:TYR:CG	26:2:62:LEU:CD1	2.99	0.42
27:3:147:MET:CE	27:3:157:MET:SD	3.07	0.42
27:3:144:ILE:HG13	27:3:159:SER:OG	2.20	0.42
27:3:197:ASP:O	27:3:198:SER:HB3	2.20	0.42
27:3:202:LEU:N	27:3:202:LEU:CD2	2.83	0.42
27:3:217:VAL:HG12	27:3:218:PRO:O	2.20	0.42
1:A:486:LEU:HA	1:A:486:LEU:HD12	1.79	0.42
2:B:1124:ILE:HD11	2:B:1170:ARG:HD3	2.00	0.42
8:H:13:LYS:HE2	8:H:31:GLU:HB2	2.02	0.42
9:I:99:SER:OG	9:I:100:HIS:N	2.52	0.42
10:J:6:ARG:HG2	10:J:13:ILE:HG22	2.01	0.42
17:Q:54:PHE:CD1	18:R:194:ARG:HG2	2.55	0.42
18:R:213:ASP:C	18:R:215:GLU:N	2.72	0.42
20:T:124:TYR:O	20:T:127:LEU:HB3	2.19	0.42
22:V:518:PHE:CD1	22:V:713:LEU:HD13	2.55	0.42
28:X:77:DC:H2"	28:X:78:DT:C7	2.49	0.42
26:2:159:VAL:HG11	26:2:161:HIS:CD2	2.49	0.42
26:2:160:LEU:CD1	26:2:160:LEU:N	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:689:VAL:CG2	26:2:391:ILE:HD13	2.50	0.42
27:3:133:LEU:CD2	27:3:134:ALA:N	2.82	0.42
27:3:215:LEU:HD23	27:3:215:LEU:HA	1.89	0.42
27:3:8:LEU:CD2	27:3:54:SER:HB3	2.45	0.42
1:A:1218:ARG:HG2	21:U:237:ARG:NH2	2.34	0.42
1:A:575:PRO:CG	1:A:594:LEU:HD11	2.48	0.42
2:B:588:ARG:NH2	2:B:663:GLU:OE1	2.51	0.42
2:B:623:ARG:NH2	2:B:675:LEU:HD21	2.35	0.42
2:B:730:LYS:HB2	2:B:730:LYS:HE3	1.92	0.42
3:C:45:ILE:HD11	3:C:82:LEU:HD22	2.00	0.42
2:B:464:ALA:HB1	13:M:62:LYS:HZ3	1.83	0.42
13:M:65:SER:O	13:M:67:VAL:N	2.53	0.42
17:Q:112:ARG:CG	18:R:237:LEU:HD11	2.37	0.42
20:T:168:LYS:C	20:T:170:LYS:H	2.22	0.42
28:X:33:DT:H2"	28:X:34:DT:C5	2.54	0.42
25:1:1:MET:HG2	26:2:413:LEU:CB	2.47	0.42
26:2:118:LEU:HD23	27:3:42:MET:CB	2.35	0.42
26:2:202:GLN:HE21	26:2:202:GLN:N	2.15	0.42
1:A:203:LYS:CE	1:A:203:LYS:HA	2.47	0.42
1:A:203:LYS:NZ	1:A:203:LYS:HA	2.35	0.42
1:A:672:ILE:HG23	1:A:673:GLN:N	2.35	0.42
1:A:728:THR:HG23	1:A:736:THR:HG23	2.02	0.42
1:A:792:ASN:N	1:A:792:ASN:OD1	2.53	0.42
1:A:924:TYR:OH	1:A:952:LEU:HD12	2.19	0.42
2:B:203:ASN:O	2:B:571:GLY:HA3	2.20	0.42
3:C:60:HIS:CE1	3:C:63:PHE:HB2	2.54	0.42
9:I:84:HIS:HB3	9:I:92:LYS:CB	2.49	0.42
17:Q:28:ILE:HA	17:Q:31:ALA:HB3	2.02	0.42
28:X:69:DA:C2	29:Y:26:DG:N2	2.88	0.42
25:1:1:MET:N	26:2:418:PHE:CB	2.83	0.41
27:3:105:THR:CG2	27:3:106:SER:N	2.82	0.41
1:A:22:GLN:OE1	1:A:1448:SER:OG	2.32	0.41
1:A:48:GLU:OE1	1:A:48:GLU:N	2.53	0.41
1:A:930:LEU:HD23	1:A:934:LEU:HB2	2.00	0.41
2:B:343:LEU:O	2:B:347:MET:HB3	2.20	0.41
8:H:69:THR:HG22	8:H:140:ARG:NH1	2.35	0.41
17:Q:30:HIS:O	17:Q:34:LEU:HB2	2.20	0.41
18:R:181:ALA:O	18:R:185:LEU:N	2.52	0.41
22:V:315:VAL:HG13	23:W:500:ASP:HB2	0.42	0.41
28:X:43:DT:H2'	28:X:44:DT:C6	2.55	0.41
29:Y:70:DC:H2"	29:Y:71:DA:H8	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:2:171:VAL:CG1	26:2:216:MET:SD	3.06	0.41
27:3:100:LYS:HE2	27:3:100:LYS:HB2	1.89	0.41
1:A:244:ARG:HA	1:A:245:PRO:HD3	1.87	0.41
1:A:612:ASP:O	1:A:613:GLU:O	2.38	0.41
1:A:630:VAL:HG12	1:A:635:LEU:CD1	2.51	0.41
1:A:779:ILE:O	1:A:782:SER:HB2	2.20	0.41
2:B:187:ILE:HG22	2:B:188:ASN:OD1	2.20	0.41
2:B:202:THR:OG1	2:B:226:GLU:OE1	2.38	0.41
2:B:710:ILE:HD13	2:B:710:ILE:HA	1.87	0.41
17:Q:113:ARG:HD2	18:R:222:SER:CA	2.49	0.41
20:T:191:PHE:CZ	20:T:237:PRO:HG3	2.54	0.41
23:W:15:ASP:HA	23:W:100:GLU:OE2	2.21	0.41
23:W:25:MET:SD	23:W:58:ALA:HB2	2.59	0.41
20:T:229:HIS:CD2	29:Y:67:DC:H1'	2.55	0.41
26:2:223:ALA:C	26:2:225:SER:H	2.24	0.41
26:2:47:GLU:HG3	26:2:48:LEU:H	1.83	0.41
27:3:69:PHE:HZ	27:3:139:LYS:HD2	1.80	0.41
1:A:413:TYR:OH	1:A:451:CYS:HA	2.21	0.41
2:B:1008:VAL:HG13	2:B:1009:GLN:N	2.35	0.41
2:B:235:ILE:CD1	2:B:261:PRO:HD3	2.50	0.41
2:B:35:ASP:OD2	2:B:646:ARG:NH2	2.50	0.41
2:B:602:SER:OG	2:B:620:ARG:NH1	2.54	0.41
7:G:14:HIS:HA	7:G:15:PRO:HD3	1.94	0.41
13:M:15:CYS:HA	13:M:16:PRO:HD3	1.75	0.41
17:Q:113:ARG:HH21	18:R:218:LYS:HE2	1.67	0.41
19:S:111:LYS:O	19:S:146:PHE:HA	2.20	0.41
20:T:93:LEU:HD11	20:T:113:ARG:HD2	2.01	0.41
22:V:519:TYR:CE2	22:V:523:VAL:HG21	2.54	0.41
26:2:42:LEU:HA	26:2:42:LEU:HD23	1.78	0.41
27:3:69:PHE:HZ	27:3:139:LYS:HB3	1.73	0.41
27:3:14:VAL:HG22	27:3:162:LEU:O	2.21	0.41
27:3:18:ASN:ND2	27:3:64:ILE:HD11	2.35	0.41
1:A:1319:LYS:HG3	1:A:1333:GLU:OE1	2.20	0.41
2:B:1022:LEU:CD1	2:B:1023:ARG:HG3	2.50	0.41
2:B:629:GLU:O	2:B:631:GLN:N	2.53	0.41
8:H:1:MET:CE	8:H:85:ALA:HB2	2.51	0.41
9:I:81:THR:HG22	9:I:94:ALA:O	2.19	0.41
10:J:2:ILE:HD12	10:J:2:ILE:HA	1.82	0.41
13:M:27:TYR:CD1	13:M:46:ILE:HG21	2.56	0.41
22:V:523:VAL:HG21	25:1:20:LEU:CG	2.43	0.41
29:Y:24:DC:O2	29:Y:25:DT:C4	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:Y:50:DA:H2"	29:Y:51:DC:O5'	2.20	0.41
26:2:176:ALA:HB3	26:2:178:LEU:HD13	1.97	0.41
26:2:206:LEU:CD2	26:2:206:LEU:N	2.84	0.41
27:3:11:LEU:CD1	27:3:48:HIS:NE2	2.82	0.41
27:3:41:VAL:HG13	27:3:42:MET:N	2.34	0.41
1:A:375:ILE:HG13	1:A:666:ARG:NH1	2.36	0.41
1:A:460:ARG:NH2	1:A:499:ASP:HB3	2.35	0.41
1:A:570:TRP:CZ3	1:A:572:GLY:HA2	2.56	0.41
1:A:641:CYS:SG	1:A:642:LYS:N	2.93	0.41
2:B:1071:ASN:O	2:B:1072:ARG:HG2	2.19	0.41
2:B:347:MET:CE	2:B:365:LEU:HD13	2.51	0.41
2:B:470:LEU:HD23	2:B:472:ARG:HH11	1.86	0.41
2:B:721:ARG:NE	2:B:721:ARG:HA	2.34	0.41
2:B:816:GLU:OE1	2:B:894:THR:OG1	2.31	0.41
18:R:77:VAL:HG21	18:R:111:ILE:HD11	2.02	0.41
20:T:166:GLU:HA	20:T:169:LYS:CE	2.50	0.41
22:V:325:ARG:NH2	23:W:499:ASN:CG	2.62	0.41
23:W:420:PRO:O	23:W:431:PRO:HB3	2.20	0.41
25:1:18:GLN:CD	25:1:44:PHE:CZ	2.92	0.41
25:1:43:VAL:CG1	25:1:44:PHE:N	2.83	0.41
26:2:221:GLN:O	26:2:268:PHE:CE1	2.74	0.41
25:1:4:VAL:CG1	26:2:412:PHE:HD2	2.20	0.41
26:2:93:LEU:HD23	26:2:96:TRP:HE1	1.85	0.41
27:3:64:ILE:CB	27:3:123:ASP:HB3	2.50	0.41
27:3:159:SER:HG	27:3:189:ILE:HD12	1.85	0.41
1:A:286:ILE:HG13	1:A:287:ASN:N	2.36	0.41
1:A:597:PRO:HB2	1:A:660:MET:HG3	2.01	0.41
1:A:734:ARG:HH22	9:I:104:ALA:HB1	1.86	0.41
2:B:1101:GLN:NE2	6:F:64:ARG:HG3	2.36	0.41
2:B:552:ASN:O	2:B:555:GLU:HG2	2.20	0.41
2:B:838:GLN:OE1	2:B:886:ARG:NH1	2.53	0.41
7:G:144:ARG:HE	7:G:171:VAL:HG11	1.86	0.41
8:H:92:MET:CE	8:H:143:LEU:HD23	2.51	0.41
9:I:65:LEU:CB	9:I:122:ARG:HE	2.33	0.41
13:M:11:PRO:HD2	13:M:13:VAL:HG22	2.01	0.41
13:M:179:GLU:HA	20:T:154:LYS:NZ	2.36	0.41
1:A:425:ASP:CG	13:M:39:LEU:CD1	2.82	0.41
13:M:47:ASP:C	13:M:49:GLY:N	2.59	0.41
14:N:324:GLU:OE1	16:P:188:ARG:NH1	2.40	0.41
17:Q:180:PHE:HZ	18:R:213:ASP:N	2.15	0.41
17:Q:184:ILE:HG12	18:R:211:SER:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:3:125:LYS:C	27:3:127:GLN:H	2.24	0.41
26:2:118:LEU:HD21	27:3:42:MET:HB2	1.99	0.41
1:A:117:LEU:H	1:A:232:GLU:CD	2.24	0.41
1:A:1191:GLU:HA	1:A:1194:ASN:ND2	2.35	0.41
1:A:1191:GLU:O	1:A:1194:ASN:ND2	2.54	0.41
1:A:1320:ILE:HD11	1:A:1328:PHE:HB3	2.03	0.41
1:A:375:ILE:HA	1:A:375:ILE:HD13	1.69	0.41
1:A:478:PRO:O	1:A:479:TRP:HB2	2.19	0.41
1:A:932:ARG:HG3	1:A:943:LEU:CD2	2.50	0.41
2:B:1022:LEU:HD11	2:B:1023:ARG:CZ	2.51	0.41
2:B:285:LEU:HD21	2:B:298:MET:HE2	2.02	0.41
2:B:802:ASP:C	2:B:804:GLY:H	2.24	0.41
3:C:38:PHE:HE1	3:C:245:VAL:HA	1.86	0.41
1:A:79:THR:HG23	13:M:43:ASP:CG	2.40	0.41
18:R:88:ARG:HH21	18:R:95:HIS:HB3	1.85	0.41
22:V:390:CYS:SG	22:V:399:LYS:HE3	2.61	0.41
28:X:11:DT:H6	28:X:11:DT:H2'	1.71	0.41
20:T:229:HIS:NE2	28:X:28:DG:N3	2.60	0.41
25:1:52:VAL:CG2	25:1:53:LEU:N	2.83	0.41
26:2:170:ALA:C	26:2:213:TRP:CZ3	2.94	0.41
27:3:109:GLU:HG3	27:3:110:VAL:N	2.35	0.41
27:3:146:ARG:HG3	27:3:147:MET:N	2.35	0.41
27:3:59:VAL:CA	27:3:71:TYR:CD1	3.03	0.41
1:A:128:ASP:O	1:A:132:LYS:HB2	2.21	0.41
2:B:1142:ASN:ND2	2:B:1145:GLN:HG2	2.36	0.41
2:B:544:PHE:HD1	2:B:544:PHE:HA	1.78	0.41
5:E:45:GLY:O	5:E:48:PRO:HD3	2.21	0.41
8:H:85:ALA:CB	8:H:88:PHE:CZ	3.04	0.41
9:I:66:THR:O	9:I:68:ILE:N	2.47	0.41
19:S:125:TYR:CD1	19:S:139:PRO:HA	2.56	0.41
26:2:211:GLN:CD	26:2:261:PHE:CE1	2.94	0.41
27:3:191:ILE:H	27:3:210:THR:HG21	1.85	0.41
27:3:222:SER:HB3	27:3:225:GLN:CG	2.51	0.41
1:A:1376:LYS:HD2	1:A:1376:LYS:HA	1.80	0.41
1:A:209:SER:O	1:A:210:GLN:HG2	2.21	0.41
1:A:482:PHE:HE2	1:A:501:MET:O	2.03	0.41
2:B:1001:PRO:HB2	2:B:1002:PHE:CD1	2.55	0.41
2:B:33:TYR:CE1	2:B:37:LYS:HG3	2.55	0.41
2:B:193:VAL:HG21	2:B:482:LEU:HD23	2.02	0.41
2:B:800:ALA:O	2:B:805:PHE:HB2	2.20	0.41
2:B:897:ARG:O	2:B:900:GLU:HG2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:721:ARG:CG	2:B:939:HIS:O	2.66	0.41
3:C:25:ASN:HA	3:C:227:GLU:OE1	2.21	0.41
3:C:47:ILE:N	3:C:47:ILE:HD12	2.34	0.41
5:E:39:GLU:O	5:E:43:GLN:N	2.51	0.41
20:T:175:ARG:HB3	20:T:208:GLN:HA	2.02	0.41
22:V:315:VAL:CG1	23:W:500:ASP:CG	2.80	0.41
22:V:321:GLU:OE1	23:W:499:ASN:HB3	1.73	0.41
29:Y:80:DT:H2'	29:Y:80:DT:H6	1.72	0.41
22:V:518:PHE:HB2	25:1:16:MET:SD	2.61	0.41
25:1:52:VAL:O	25:1:56:ARG:HG2	2.21	0.41
26:2:174:ASP:OD2	26:2:213:TRP:CZ3	2.74	0.41
26:2:236:PHE:CD1	26:2:239:GLN:CD	2.95	0.41
27:3:9:ASN:C	27:3:56:LYS:HE3	2.41	0.41
1:A:1194:ASN:O	1:A:1197:TYR:HD2	2.04	0.41
1:A:202:TRP:H	1:A:212:LYS:CA	2.29	0.41
1:A:522:PRO:CG	1:A:666:ARG:HG3	2.50	0.41
1:A:36:VAL:HG11	1:A:72:GLN:HE22	1.85	0.41
2:B:51:ILE:HB	2:B:160:TYR:CE2	2.56	0.41
3:C:133:ARG:HA	3:C:136:ASP:CG	2.33	0.41
8:H:107:GLU:HA	8:H:107:GLU:OE1	2.21	0.41
11:K:82:SER:HA	11:K:83:PRO:HD3	1.85	0.41
12:L:35:ARG:HH12	12:L:42:ARG:CZ	2.34	0.41
13:M:16:PRO:HD3	13:M:39:LEU:HD23	2.00	0.41
23:W:428:ILE:HA	23:W:430:ASN:HD21	1.85	0.41
25:1:39:ASP:OD2	26:2:434:GLU:OE2	2.39	0.41
26:2:78:GLU:HB3	26:2:81:LYS:HZ2	1.85	0.41
27:3:141:LEU:C	27:3:144:ILE:HG22	2.41	0.41
27:3:222:SER:HB3	27:3:225:GLN:OE1	2.21	0.41
1:A:124:PRO:HA	1:A:127:LYS:HE3	2.02	0.41
1:A:685:HIS:ND1	1:A:686:THR:N	2.69	0.41
2:B:778:SER:O	2:B:1045:PRO:HA	2.21	0.41
2:B:776:ILE:HD13	2:B:776:ILE:HG21	1.73	0.41
2:B:931:ILE:CD1	2:B:947:ILE:HA	2.51	0.41
3:C:7:PRO:HA	3:C:25:ASN:HB3	2.03	0.41
17:Q:128:LYS:HE3	17:Q:133:SER:HA	2.03	0.41
22:V:366:ASN:HD22	22:V:613:THR:CG2	2.20	0.41
26:2:123:LEU:HD23	26:2:123:LEU:C	2.42	0.40
26:2:236:PHE:HZ	26:2:258:LEU:CD1	2.34	0.40
26:2:93:LEU:CA	26:2:96:TRP:HD1	2.31	0.40
27:3:114:GLU:OE1	27:3:114:GLU:HA	2.21	0.40
27:3:18:ASN:OD1	27:3:19:PRO:HD2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:818:GLU:HG2	1:A:819:SER:N	2.36	0.40
7:G:99:THR:HG21	7:G:143:ILE:HD11	2.03	0.40
9:I:12:VAL:HG11	9:I:15:ARG:HH21	1.85	0.40
3:C:154:ARG:CD	10:J:65:LEU:HD11	2.49	0.40
13:M:57:ASN:OD1	13:M:57:ASN:N	2.54	0.40
20:T:3:GLU:CD	20:T:3:GLU:H	2.24	0.40
22:V:297:PHE:CG	22:V:298:ARG:N	2.89	0.40
25:1:10:ILE:HG23	25:1:10:ILE:O	2.21	0.40
26:2:236:PHE:HZ	26:2:262:LEU:CD2	2.35	0.40
27:3:17:ALA:CB	27:3:63:HIS:CD2	2.99	0.40
27:3:187:GLN:CG	27:3:189:ILE:CG1	2.94	0.40
1:A:1419:VAL:HG11	1:A:1432:PHE:CE2	2.57	0.40
1:A:51:ARG:H	1:A:52:PRO:CD	2.33	0.40
1:A:522:PRO:O	1:A:525:ILE:HG13	2.21	0.40
2:B:699:HIS:CE1	2:B:701:SER:OG	2.74	0.40
3:C:19:VAL:HB	3:C:241:PRO:HB2	2.02	0.40
8:H:115:TYR:HE1	8:H:124:ARG:HG3	1.85	0.40
13:M:52:TRP:C	13:M:52:TRP:CD1	2.92	0.40
22:V:450:MET:HG3	28:X:75:DG:H3'	2.04	0.40
22:V:678:ARG:NH1	26:2:392:ARG:HH12	2.19	0.40
25:1:20:LEU:O	25:1:24:ASP:N	2.48	0.40
26:2:196:ILE:HG13	26:2:197:THR:N	2.36	0.40
26:2:93:LEU:O	26:2:96:TRP:CD1	2.74	0.40
27:3:42:MET:HG2	27:3:111:ILE:CD1	2.52	0.40
27:3:60:ILE:CG2	27:3:61:ALA:N	2.84	0.40
1:A:937:ASP:HB2	1:A:1002:SER:O	2.22	0.40
1:A:133:SER:O	1:A:136:GLN:N	2.37	0.40
1:A:48:GLU:C	1:A:50:GLY:N	2.73	0.40
1:A:540:ASP:O	1:A:544:ALA:N	2.41	0.40
1:A:626:THR:OG1	1:A:627:LYS:N	2.54	0.40
1:A:837:PHE:HB2	2:B:506:TRP:CZ3	2.56	0.40
2:B:1060:HIS:CD2	2:B:1078:ARG:HD2	2.56	0.40
2:B:254:GLN:HG3	2:B:303:PRO:CG	2.50	0.40
2:B:290:TYR:HE2	2:B:562:ALA:HA	1.83	0.40
2:B:363:TYR:CG	2:B:553:LEU:HD21	2.56	0.40
2:B:520:VAL:O	2:B:520:VAL:HG13	2.20	0.40
2:B:854:ILE:HD12	2:B:904:VAL:HG21	2.02	0.40
3:C:47:ILE:HB	3:C:69:GLY:HA2	2.04	0.40
11:K:62:LYS:O	11:K:64:PRO:HD3	2.21	0.40
12:L:17:TYR:O	12:L:26:ASN:HB2	2.22	0.40
13:M:107:MET:HG3	13:M:108:SER:H	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:70:SER:C	13:M:72:ASN:H	2.25	0.40
14:N:337:CYS:HB2	14:N:355:ASP:O	2.22	0.40
16:P:246:PHE:HA	16:P:247:PRO:HD3	1.95	0.40
17:Q:23:ARG:CD	18:R:207:SER:O	2.70	0.40
19:S:126:ILE:O	19:S:138:PHE:N	2.50	0.40
13:M:178:LYS:O	20:T:154:LYS:HE3	2.21	0.40
22:V:516:PRO:HB3	25:1:15:ALA:O	2.22	0.40
22:V:593:LEU:HD11	22:V:615:PHE:CZ	2.56	0.40
23:W:233:PHE:HB2	23:W:456:ILE:HG22	2.02	0.40
28:X:24:DG:H2'	28:X:25:DG:C8	2.56	0.40
26:2:100:LEU:CG	26:2:119:ARG:HE	2.22	0.40
26:2:181:GLN:NE2	26:2:181:GLN:HA	2.35	0.40
26:2:34:LEU:N	26:2:34:LEU:CD2	2.84	0.40
26:2:94:ARG:HD2	26:2:95:ILE:HD13	2.02	0.40
1:A:1158:LEU:HG	1:A:1308:TYR:CE2	2.57	0.40
1:A:386:ALA:O	1:A:449:HIS:CE1	2.74	0.40
2:B:197:GLN:NE2	2:B:466:VAL:HG22	2.36	0.40
2:B:278:PHE:HZ	2:B:359:THR:HG22	1.85	0.40
2:B:385:ARG:HH11	2:B:497:LYS:HE3	1.87	0.40
2:B:854:ILE:H	2:B:854:ILE:HG12	1.63	0.40
2:B:873:LEU:H	2:B:874:PRO:HD2	1.86	0.40
2:B:985:LEU:HA	2:B:985:LEU:HD12	1.93	0.40
5:E:64:HIS:HB3	5:E:68:PRO:HA	2.04	0.40
8:H:91:VAL:HG13	8:H:144:LEU:HD12	2.04	0.40
17:Q:28:ILE:HD12	18:R:192:VAL:HG12	2.03	0.40
19:S:112:GLY:HA2	19:S:145:ASN:O	2.22	0.40
26:2:399:ASP:OD1	26:2:402:ARG:NH1	2.55	0.40
1:A:1176:TYR:HE2	1:A:1213:ARG:NH1	2.20	0.40
1:A:1421:ARG:HA	1:A:1421:ARG:HD3	2.01	0.40
1:A:930:LEU:CD2	1:A:934:LEU:CB	2.98	0.40
2:B:548:TRP:O	2:B:549:SER:OG	2.35	0.40
2:B:759:VAL:HG13	2:B:999:ALA:HB2	2.03	0.40
3:C:189:ASP:N	3:C:189:ASP:OD1	2.53	0.40
8:H:2:ALA:HB1	8:H:63:THR:HG23	2.03	0.40
1:A:197:GLU:CD	13:M:93:PHE:CD2	2.93	0.40
15:O:66:ARG:N	15:O:73:THR:O	2.54	0.40
17:Q:77:ARG:HB3	17:Q:93:PHE:HB3	2.03	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%)	1266 (87%)	119 (8%)	65 (4%)	3 33
2	B	1163/1174 (99%)	1004 (86%)	109 (9%)	50 (4%)	3 34
3	C	273/275 (99%)	241 (88%)	22 (8%)	10 (4%)	4 38
4	D	127/142 (89%)	120 (94%)	7 (6%)	0	100 100
5	E	208/210 (99%)	191 (92%)	8 (4%)	9 (4%)	3 34
6	F	84/127 (66%)	80 (95%)	4 (5%)	0	100 100
7	G	169/172 (98%)	161 (95%)	8 (5%)	0	100 100
8	H	148/150 (99%)	116 (78%)	14 (10%)	18 (12%)	0 8
9	I	123/125 (98%)	91 (74%)	20 (16%)	12 (10%)	1 14
10	J	65/67 (97%)	54 (83%)	5 (8%)	6 (9%)	1 17
11	K	115/117 (98%)	106 (92%)	8 (7%)	1 (1%)	21 67
12	L	44/58 (76%)	32 (73%)	9 (20%)	3 (7%)	1 23
13	M	308/316 (98%)	262 (85%)	28 (9%)	18 (6%)	2 27
14	N	109/376 (29%)	97 (89%)	9 (8%)	3 (3%)	6 44
15	O	97/109 (89%)	96 (99%)	1 (1%)	0	100 100
16	P	183/339 (54%)	170 (93%)	7 (4%)	6 (3%)	5 40
17	Q	176/439 (40%)	159 (90%)	7 (4%)	10 (6%)	2 28
18	R	163/291 (56%)	141 (86%)	14 (9%)	8 (5%)	3 31
19	S	134/517 (26%)	119 (89%)	11 (8%)	4 (3%)	5 42
20	T	218/249 (88%)	187 (86%)	19 (9%)	12 (6%)	2 29
21	U	168/301 (56%)	143 (85%)	17 (10%)	8 (5%)	3 32
22	V	473/782 (60%)	400 (85%)	45 (10%)	28 (6%)	2 27
23	W	661/760 (87%)	571 (86%)	67 (10%)	23 (4%)	4 39
24	0	186/395 (47%)	168 (90%)	13 (7%)	5 (3%)	6 45
25	1	60/71 (84%)	53 (88%)	5 (8%)	2 (3%)	5 40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
26	2	264/462 (57%)	246 (93%)	14 (5%)	4 (2%)	13 57
27	3	187/308 (61%)	176 (94%)	9 (5%)	2 (1%)	17 63
All	All	7356/10302 (71%)	6450 (88%)	599 (8%)	307 (4%)	6 34

All (307) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	70	ARG
1	A	133	SER
1	A	203	LYS
1	A	208	ASP
1	A	264	VAL
1	A	265	VAL
1	A	272	ASN
1	A	275	ASP
1	A	531	ASN
1	A	607	SER
1	A	610	PRO
1	A	622	SER
1	A	623	PRO
1	A	931	ARG
1	A	932	ARG
1	A	1087	VAL
1	A	1116	ASN
1	A	1200	PRO
1	A	1307	VAL
2	B	74	ALA
2	B	226	GLU
2	B	231	PRO
2	B	452	ASN
2	B	460	HIS
2	B	491	ARG
2	B	513	GLU
2	B	526	LEU
2	B	876	ASN
2	B	881	GLU
2	B	898	THR
2	B	1108	PHE
3	C	6	GLN
3	C	7	PRO
3	C	8	THR

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Mol	Chain	Res	Type
3	C	136	ASP
3	C	137	ASN
3	C	213	GLU
5	E	46	ASP
5	E	47	LYS
5	E	50	GLU
5	E	64	HIS
5	E	65	ASN
5	E	68	PRO
8	H	18	GLU
8	H	67	ASP
8	H	73	GLY
8	H	74	GLU
8	H	86	ASP
9	I	85	PRO
9	I	86	CYS
9	I	99	SER
9	I	104	ALA
9	I	105	GLU
9	I	106	ASP
10	J	2	ILE
11	K	112	LYS
13	M	48	VAL
13	M	90	ALA
13	M	92	SER
13	M	93	PHE
13	M	94	ASP
13	M	95	GLU
14	N	355	ASP
16	P	206	GLU
16	P	297	LYS
16	P	299	ARG
17	Q	102	VAL
17	Q	126	SER
18	R	195	PRO
18	R	226	ASP
18	R	228	MET
19	S	160	ALA
20	T	124	TYR
20	T	151	THR
20	T	153	TYR
20	T	156	VAL

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Mol	Chain	Res	Type
20	T	180	LYS
21	U	228	MET
21	U	251	ALA
21	U	252	LYS
21	U	253	THR
21	U	258	THR
21	U	285	MET
21	U	300	PHE
22	V	385	ASP
22	V	427	MET
22	V	461	HIS
22	V	491	ALA
22	V	499	ASN
22	V	614	SER
22	V	616	ASP
22	V	632	SER
22	V	648	LYS
22	V	649	GLY
23	W	67	VAL
23	W	420	PRO
23	W	424	ARG
23	W	430	ASN
23	W	504	ILE
23	W	573	ASP
23	W	595	ILE
23	W	630	SER
24	0	77	LYS
24	0	78	PRO
25	1	48	GLU
26	2	49	PRO
27	3	120	THR
1	A	51	ARG
1	A	66	GLU
1	A	263	ALA
1	A	613	GLU
1	A	624	GLY
1	A	625	ASP
1	A	912	SER
1	A	926	ASN
1	A	928	ARG
1	A	935	GLN
1	A	1305	SER

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Mol	Chain	Res	Type
1	A	1409	GLY
2	B	79	GLU
2	B	249	LYS
2	B	456	GLN
2	B	599	SER
2	B	705	GLY
2	B	875	GLU
2	B	879	GLU
2	B	899	SER
2	B	1145	GLN
3	C	143	VAL
3	C	272	LEU
5	E	124	LYS
8	H	109	ALA
8	H	111	ARG
8	H	139	SER
9	I	62	VAL
9	I	103	ARG
10	J	41	LYS
10	J	65	LEU
12	L	16	ILE
12	L	27	GLU
13	M	12	ARG
13	M	53	ARG
13	M	66	ARG
13	M	91	ALA
13	M	110	SER
14	N	320	VAL
16	P	157	GLU
16	P	208	ARG
17	Q	101	ASN
17	Q	125	ALA
17	Q	158	HIS
18	R	163	LEU
18	R	164	GLY
18	R	223	VAL
18	R	224	THR
20	T	169	LYS
20	T	178	ALA
22	V	254	GLN
22	V	404	SER
22	V	460	ALA

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Mol	Chain	Res	Type
23	W	124	LEU
23	W	408	SER
23	W	646	ILE
26	2	223	ALA
26	2	231	VAL
1	A	54	LEU
1	A	134	LYS
1	A	156	GLY
1	A	195	GLY
1	A	274	ASP
1	A	614	ASP
1	A	724	GLU
1	A	1085	GLU
1	A	1265	ASP
1	A	1274	GLU
1	A	1299	GLN
1	A	1316	ASN
2	B	63	PRO
2	B	242	ARG
2	B	548	TRP
2	B	630	LYS
2	B	691	SER
2	B	839	GLY
2	B	873	LEU
2	B	892	CYS
2	B	1136	GLU
8	H	21	LYS
8	H	35	PHE
8	H	66	GLU
8	H	70	LEU
8	H	138	ASP
8	H	140	ARG
8	H	148	LEU
9	I	118	HIS
13	M	14	THR
13	M	101	TYR
14	N	325	GLY
17	Q	40	ASN
17	Q	100	VAL
17	Q	164	ASP
17	Q	165	GLU
19	S	156	THR

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Mol	Chain	Res	Type
22	V	343	GLY
23	W	147	GLN
23	W	155	CYS
23	W	509	GLU
27	3	198	SER
1	A	44	PRO
1	A	62	GLN
1	A	75	ALA
1	A	184	CYS
1	A	205	VAL
1	A	206	ASN
1	A	210	GLN
1	A	726	GLU
1	A	894	ASP
1	A	930	LEU
1	A	1103	THR
1	A	1118	THR
2	B	80	GLU
2	B	427	LYS
2	B	527	ALA
2	B	823	PHE
3	C	217	GLN
5	E	27	LEU
8	H	22	PHE
8	H	149	ALA
12	L	45	TYR
13	M	40	VAL
13	M	56	SER
13	M	71	GLN
17	Q	25	PHE
18	R	207	SER
19	S	154	THR
20	T	141	LEU
20	T	154	LYS
21	U	225	ALA
22	V	310	LEU
22	V	428	GLU
22	V	436	GLY
22	V	475	ASP
22	V	502	ILE
22	V	629	HIS
1	A	56	GLY

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Mol	Chain	Res	Type
1	A	1271	GLU
2	B	232	THR
2	B	511	PRO
2	B	631	GLN
2	B	803	ARG
2	B	886	ARG
2	B	900	GLU
9	I	67	GLN
10	J	5	VAL
16	P	162	VAL
20	T	148	VAL
22	V	470	LEU
22	V	650	MET
23	W	152	LEU
23	W	551	SER
24	0	79	ASN
26	2	430	VAL
1	A	132	LYS
1	A	299	ALA
1	A	1414	ILE
2	B	61	ASP
2	B	685	LYS
2	B	884	ASN
2	B	1069	ILE
9	I	58	ILE
10	J	6	ARG
13	M	11	PRO
19	S	121	ASN
20	T	171	GLU
22	V	582	GLY
23	W	36	GLY
23	W	111	SER
23	W	345	ARG
23	W	697	ILE
1	A	1275	VAL
9	I	117	PRO
22	V	311	LYS
22	V	651	VAL
23	W	174	ILE
1	A	182	GLY
2	B	136	GLY
2	B	330	VAL

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Mol	Chain	Res	Type
2	B	561	ILE
22	V	426	VAL
22	V	457	ILE
23	W	495	ILE
24	0	216	GLY
1	A	1312	PRO
2	B	253	GLY
5	E	48	PRO
8	H	82	PRO
10	J	64	PRO
22	V	405	VAL
25	1	2	VAL
2	B	81	PRO
2	B	931	ILE
3	C	151	VAL
20	T	38	GLY
1	A	55	GLY
1	A	371	PRO
13	M	38	GLY
23	W	45	GLY
24	0	56	GLY

5.3.2 Protein sidechains (i)

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%)	1228 (96%)	51 (4%)	38 71
2	B	1020/1028 (99%)	980 (96%)	40 (4%)	39 72
3	C	252/252 (100%)	244 (97%)	8 (3%)	46 76
4	D	119/126 (94%)	119 (100%)	0	100 100
5	E	192/192 (100%)	187 (97%)	5 (3%)	54 80
6	F	74/111 (67%)	72 (97%)	2 (3%)	52 79
7	G	152/153 (99%)	151 (99%)	1 (1%)	88 94
8	H	131/131 (100%)	125 (95%)	6 (5%)	33 68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
9	I	112/112 (100%)	106 (95%)	6 (5%)	27 64
10	J	56/56 (100%)	49 (88%)	7 (12%)	6 30
11	K	106/106 (100%)	103 (97%)	3 (3%)	51 78
12	L	43/55 (78%)	41 (95%)	2 (5%)	32 68
13	M	263/268 (98%)	254 (97%)	9 (3%)	44 75
14	N	105/324 (32%)	101 (96%)	4 (4%)	40 73
15	O	90/98 (92%)	88 (98%)	2 (2%)	60 83
16	P	159/293 (54%)	156 (98%)	3 (2%)	65 86
17	Q	164/373 (44%)	157 (96%)	7 (4%)	35 70
18	R	150/261 (58%)	144 (96%)	6 (4%)	38 71
19	S	121/448 (27%)	117 (97%)	4 (3%)	45 76
20	T	196/218 (90%)	193 (98%)	3 (2%)	72 88
21	U	148/266 (56%)	141 (95%)	7 (5%)	32 68
22	V	422/688 (61%)	403 (96%)	19 (4%)	34 69
23	W	577/664 (87%)	543 (94%)	34 (6%)	24 61
24	0	171/352 (49%)	163 (95%)	8 (5%)	32 68
25	1	56/64 (88%)	51 (91%)	5 (9%)	12 44
26	2	238/399 (60%)	229 (96%)	9 (4%)	40 73
27	3	171/272 (63%)	159 (93%)	12 (7%)	19 56
All	All	6567/9058 (72%)	6304 (96%)	263 (4%)	42 71

All (263) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	GLU
1	A	74	CYS
1	A	117	LEU
1	A	146	ASP
1	A	203	LYS
1	A	204	HIS
1	A	212	LYS
1	A	227	ARG
1	A	272	ASN
1	A	273	GLN
1	A	436	SER

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Mol	Chain	Res	Type
1	A	463	THR
1	A	484	LEU
1	A	488	VAL
1	A	524	MET
1	A	534	VAL
1	A	538	VAL
1	A	545	VAL
1	A	607	SER
1	A	613	GLU
1	A	619	LYS
1	A	625	ASP
1	A	644	SER
1	A	687	ILE
1	A	691	ASP
1	A	766	PHE
1	A	792	ASN
1	A	818	GLU
1	A	849	ASP
1	A	853	LYS
1	A	864	LEU
1	A	873	VAL
1	A	908	THR
1	A	931	ARG
1	A	932	ARG
1	A	940	LYS
1	A	1036	ASN
1	A	1077	ASN
1	A	1128	ILE
1	A	1160	ARG
1	A	1165	THR
1	A	1168	LYS
1	A	1203	ASP
1	A	1281	ASP
1	A	1282	ASP
1	A	1298	LEU
1	A	1306	LYS
1	A	1308	TYR
1	A	1318	LYS
1	A	1341	VAL
1	A	1485	GLU
2	B	41	ARG
2	B	57	ARG

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Mol	Chain	Res	Type
2	B	61	ASP
2	B	67	LEU
2	B	80	GLU
2	B	132	VAL
2	B	224	CYS
2	B	225	LEU
2	B	250	SER
2	B	269	ILE
2	B	282	ARG
2	B	330	VAL
2	B	371	ARG
2	B	388	TYR
2	B	416	ARG
2	B	422	PHE
2	B	448	LEU
2	B	485	LEU
2	B	621	ILE
2	B	655	ASP
2	B	667	THR
2	B	711	ILE
2	B	733	MET
2	B	735	VAL
2	B	737	ILE
2	B	747	LEU
2	B	784	SER
2	B	785	TYR
2	B	853	LEU
2	B	875	GLU
2	B	880	LEU
2	B	881	GLU
2	B	921	ILE
2	B	958	CYS
2	B	1018	TYR
2	B	1035	ARG
2	B	1071	ASN
2	B	1091	ARG
2	B	1092	ASP
2	B	1156	LYS
3	C	6	GLN
3	C	35	ARG
3	C	58	VAL
3	C	63	PHE

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Mol	Chain	Res	Type
3	C	70	LEU
3	C	136	ASP
3	C	148	ILE
3	C	242	GLU
5	E	38	GLU
5	E	47	LYS
5	E	64	HIS
5	E	113	SER
5	E	205	THR
6	F	54	THR
6	F	64	ARG
7	G	158	PHE
8	H	65	TYR
8	H	66	GLU
8	H	74	GLU
8	H	84	ARG
8	H	107	GLU
8	H	144	LEU
9	I	60	HIS
9	I	61	GLU
9	I	84	HIS
9	I	103	ARG
9	I	105	GLU
9	I	111	TYR
10	J	7	CYS
10	J	14	VAL
10	J	46	ARG
10	J	47	ARG
10	J	54	ASP
10	J	59	LEU
10	J	65	LEU
11	K	39	ASP
11	K	48	SER
11	K	63	VAL
12	L	16	ILE
12	L	27	GLU
13	M	10	LEU
13	M	40	VAL
13	M	43	ASP
13	M	47	ASP
13	M	48	VAL
13	M	111	ASP

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Mol	Chain	Res	Type
13	M	132	ARG
13	M	133	ASN
13	M	282	ASP
14	N	20	ASP
14	N	318	ASP
14	N	319	ASP
14	N	351	PHE
15	O	63	ASN
15	O	88	ILE
16	P	180	LEU
16	P	206	GLU
16	P	297	LYS
17	Q	17	LEU
17	Q	76	MET
17	Q	101	ASN
17	Q	138	ASP
17	Q	171	LYS
17	Q	177	LEU
17	Q	191	LEU
18	R	163	LEU
18	R	169	GLU
18	R	205	ASP
18	R	206	LYS
18	R	209	GLN
18	R	228	MET
19	S	135	PHE
19	S	163	GLU
19	S	166	ARG
19	S	177	MET
20	T	141	LEU
20	T	148	VAL
20	T	154	LYS
21	U	194	ARG
21	U	226	GLU
21	U	248	HIS
21	U	252	LYS
21	U	253	THR
21	U	257	GLN
21	U	276	VAL
22	V	246	MET
22	V	332	ARG
22	V	362	LEU

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Mol	Chain	Res	Type
22	V	366	ASN
22	V	427	MET
22	V	429	TRP
22	V	458	VAL
22	V	471	VAL
22	V	479	ASP
22	V	482	PHE
22	V	492	ASN
22	V	517	GLU
22	V	530	ARG
22	V	534	TYR
22	V	566	PHE
22	V	568	LEU
22	V	581	TYR
22	V	590	MET
22	V	614	SER
23	W	37	HIS
23	W	64	PRO
23	W	95	GLU
23	W	101	LYS
23	W	112	ARG
23	W	122	THR
23	W	123	PRO
23	W	166	ARG
23	W	196	ARG
23	W	207	TYR
23	W	263	LEU
23	W	283	ASP
23	W	285	TYR
23	W	288	LEU
23	W	309	VAL
23	W	333	LEU
23	W	345	ARG
23	W	346	VAL
23	W	425	THR
23	W	461	LEU
23	W	489	CYS
23	W	523	LEU
23	W	533	ASP
23	W	543	GLN
23	W	544	TYR
23	W	554	GLU

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Mol	Chain	Res	Type
23	W	584	TYR
23	W	596	LEU
23	W	610	PHE
23	W	620	MET
23	W	647	ARG
23	W	654	PHE
23	W	669	ARG
23	W	676	LEU
24	0	77	LYS
24	0	103	GLN
24	0	125	ARG
24	0	137	MET
24	0	174	LEU
24	0	202	SER
24	0	218	THR
24	0	222	ILE
25	1	10	ILE
25	1	16	MET
25	1	18	GLN
25	1	21	LEU
25	1	38	ILE
26	2	61	PHE
26	2	77	LYS
26	2	181	GLN
26	2	202	GLN
26	2	402	ARG
26	2	407	VAL
26	2	426	ARG
26	2	430	VAL
26	2	452	LYS
27	3	56	LYS
27	3	66	GLU
27	3	109	GLU
27	3	121	LYS
27	3	124	ILE
27	3	133	LEU
27	3	144	ILE
27	3	147	MET
27	3	157	MET
27	3	185	GLN
27	3	190	LEU
27	3	216	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	122	ASN
1	A	181	HIS
1	A	222	HIS
1	A	507	GLN
1	A	529	GLN
1	A	673	GLN
1	A	757	GLN
1	A	989	ASN
1	A	1194	ASN
1	A	1445	HIS
2	B	72	GLN
2	B	90	GLN
2	B	175	ASN
2	B	452	ASN
2	B	790	GLN
2	B	941	GLN
2	B	1101	GLN
3	C	5	ASN
3	C	275	ASN
4	D	48	ASN
6	F	46	GLN
9	I	22	ASN
9	I	41	ASN
9	I	84	HIS
10	J	52	HIS
11	K	89	ASN
13	M	102	GLN
17	Q	109	HIS
18	R	204	ASN
22	V	281	GLN
22	V	366	ASN
22	V	539	ASN
22	V	677	GLN
23	W	187	GLN
23	W	430	ASN
23	W	499	ASN
23	W	590	ASN
24	0	60	HIS
24	0	103	GLN
25	1	51	ASN

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Mol	Chain	Res	Type
26	2	117	ASN
26	2	161	HIS
26	2	181	GLN
26	2	202	GLN
26	2	221	GLN
26	2	239	GLN
26	2	263	GLN
26	2	273	GLN
27	3	25	GLN
27	3	52	ASN
27	3	63	HIS
27	3	148	ASN
27	3	155	GLN
27	3	185	GLN
27	3	187	GLN
27	3	225	GLN

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 (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.