wwPDB EM Map/Model Validation Report (i)

Jun 14, 2016 – 01:45 PM EDT

PDB ID	:	5IY9
EMDB ID:	:	EMD-8134
Title	:	Human holo-PIC in the initial transcribing state (no IIS)
Authors	:	He, Y.; Yan, C.; Fang, J.; Inouye, C.; Tjian, R.; Ivanov, I.; Nogales, E.
Deposited on	:	2016-03-24
Resolution	:	6.30 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

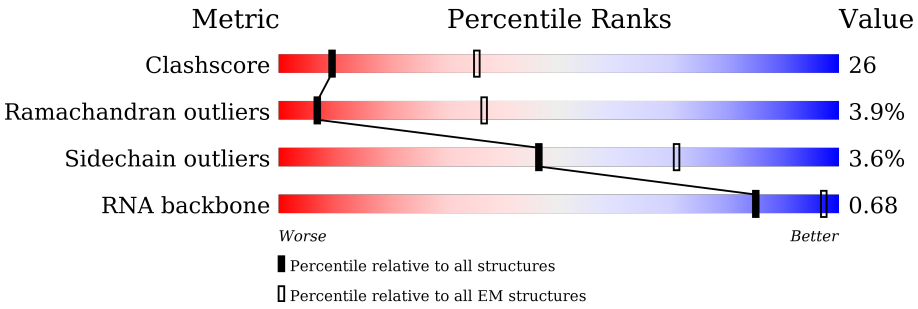
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027790

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 6.30 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
RNA backbone	3027	244

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	50% 21% • • 26%
2	B	1174	61% 34% • ••
3	C	275	66% 31% •
4	D	142	75% 15% • 9%
5	E	210	72% 26% ••
6	F	127	57% 11% 32%
7	G	172	69% 29% ••
8	H	150	56% 39% 5% •

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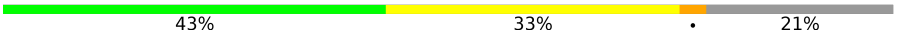
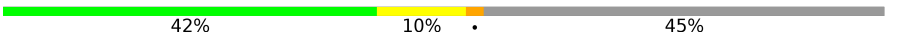
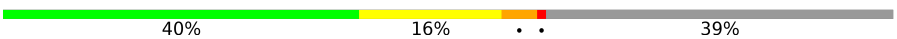
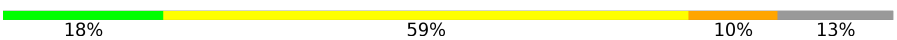
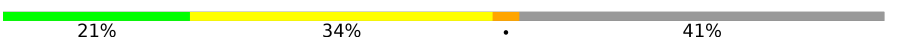
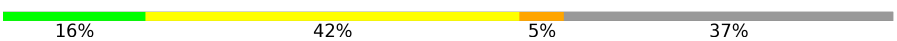
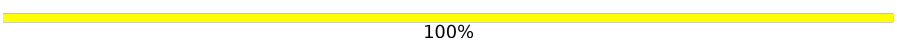
Mol	Chain	Length	Quality of chain
9	I	125	
10	J	67	
11	K	117	
12	L	58	
13	M	316	
14	N	376	
15	O	109	
16	P	339	
17	Q	439	
18	R	291	
19	S	517	
20	T	249	
21	V	782	
22	W	760	
23	0	395	
24	1	71	
25	2	462	
26	3	308	
27	X	83	
28	Y	83	
29	Z	6	

2 Entry composition

There are 31 unique types of molecules in this entry. The entry contains 61725 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 TFIIH basal transcription factor complex helicase XPB subunit.

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

- Molecule 22 is a protein called TFIIH basal transcription factor complex helicase XPD subunit.

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

- Molecule 23 is a protein called General transcription factor IIH subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	0	188	Total	C	N	O	S	0	0
			1479	935	258	276	10		

- Molecule 24 is a protein called General transcription factor IIH subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	1	62	Total	C	N	O	S	0	0
			491	317	77	93	4		

- Molecule 25 is a protein called General transcription factor IIH subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	2	274	Total	C	N	O	S	0	0
			2196	1417	377	392	10		

- Molecule 26 is a protein called General transcription factor IIH subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	3	193	Total	C	N	O	S	0	0
			1526	978	252	284	12		

- Molecule 27 is a DNA chain called SCP-X.

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

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

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

- Molecule 29 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Z	6	Total	C	N	O	P	0	0
			125	57	23	40	5		

- 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).

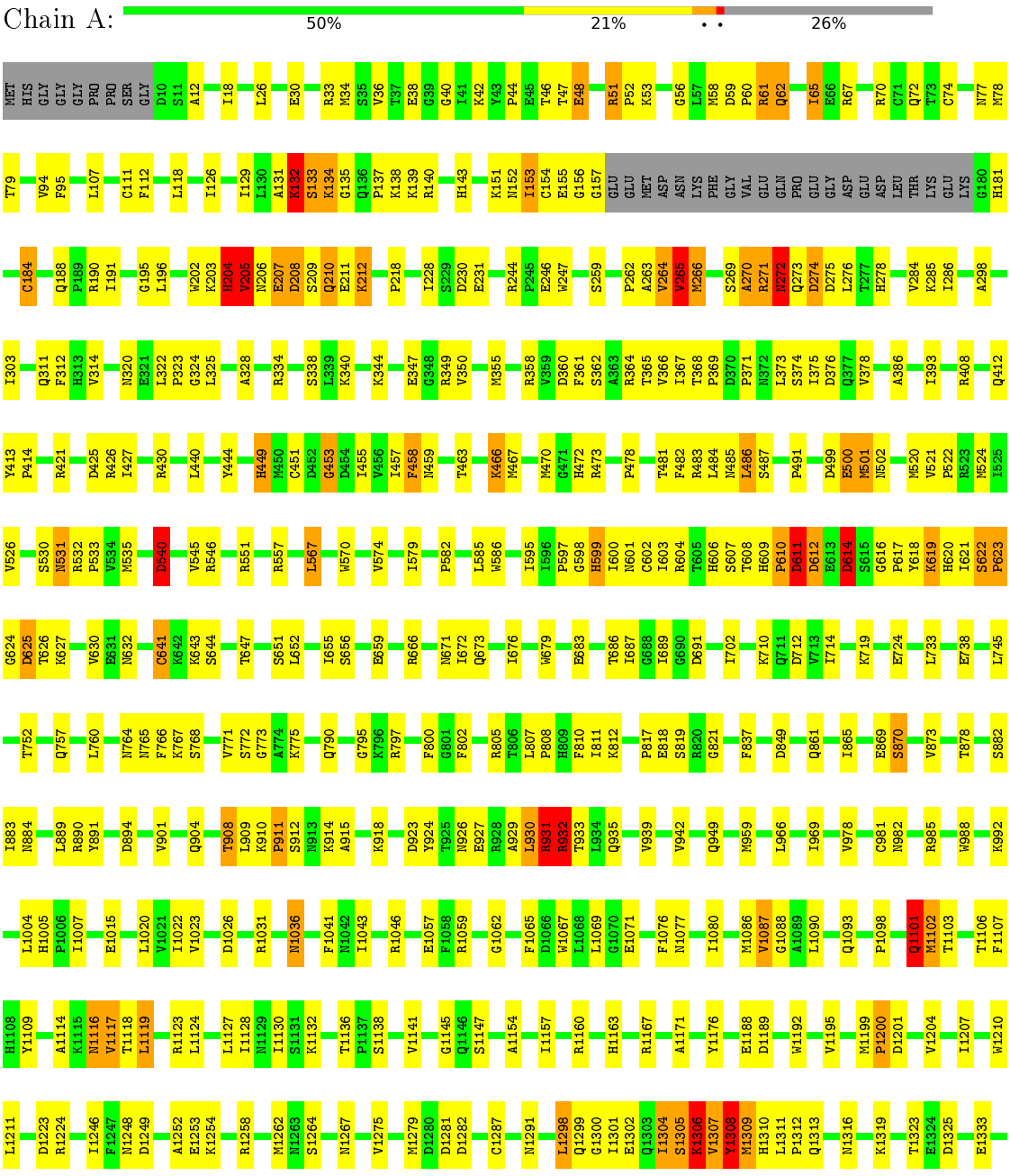
Mol	Chain	Residues	Atoms		AltConf
31	J	1	Total	Zn	0
			1	1	
31	Q	1	Total	Zn	0
			1	1	
31	B	1	Total	Zn	0
			1	1	
31	I	2	Total	Zn	0
			2	2	
31	C	1	Total	Zn	0
			1	1	
31	A	2	Total	Zn	0
			2	2	
31	L	1	Total	Zn	0
			1	1	
31	M	1	Total	Zn	0
			1	1	

3 Residue-property plots (i)

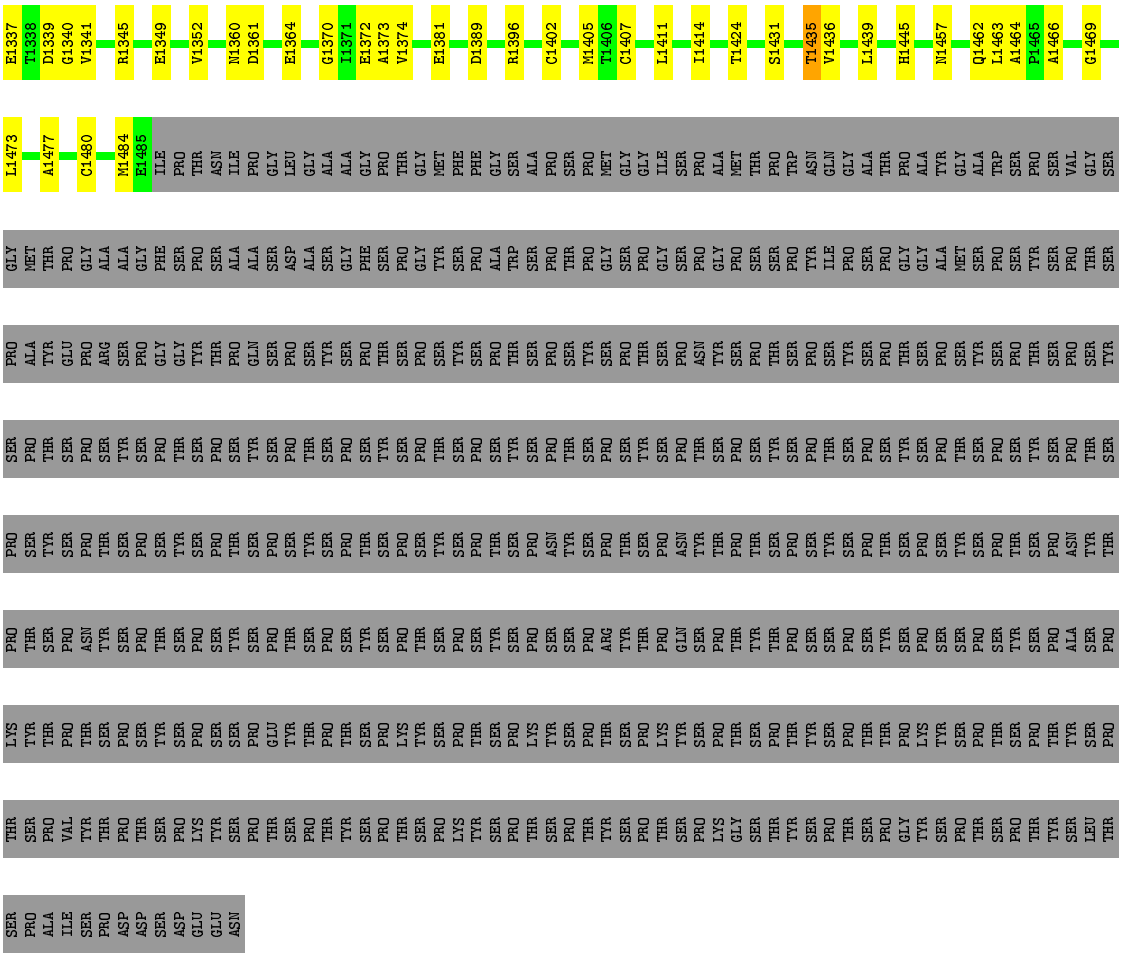
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric 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:

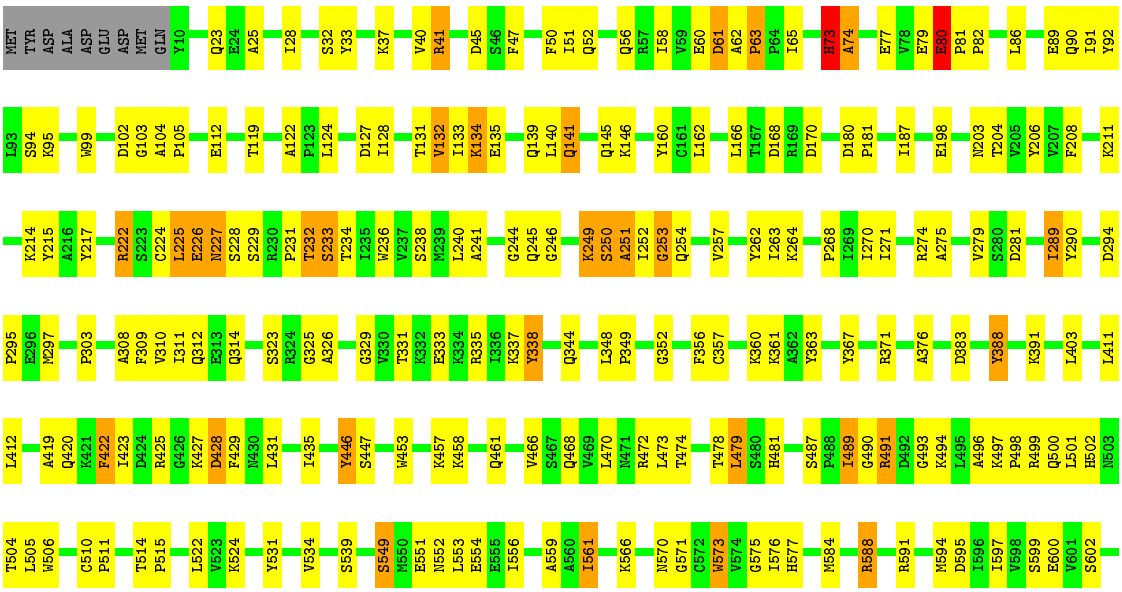


WORLDWIDE PDB PROTEIN DATA BANK
EMDataBank Unified Data Resource for 3DEM

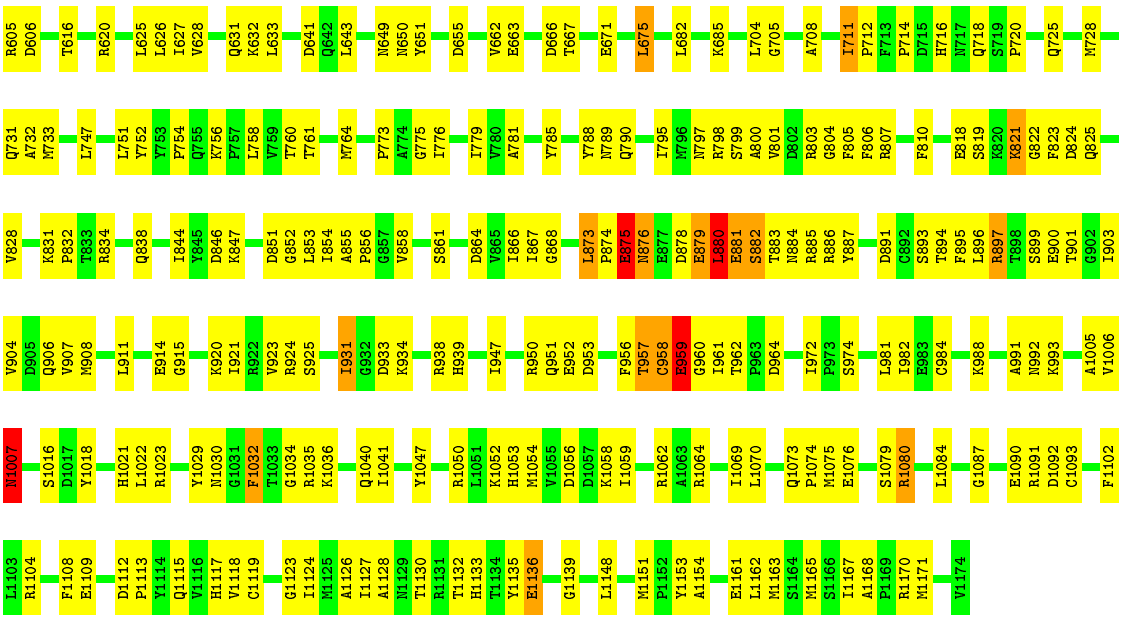


• Molecule 2: DNA-directed RNA polymerase II subunit RPB2

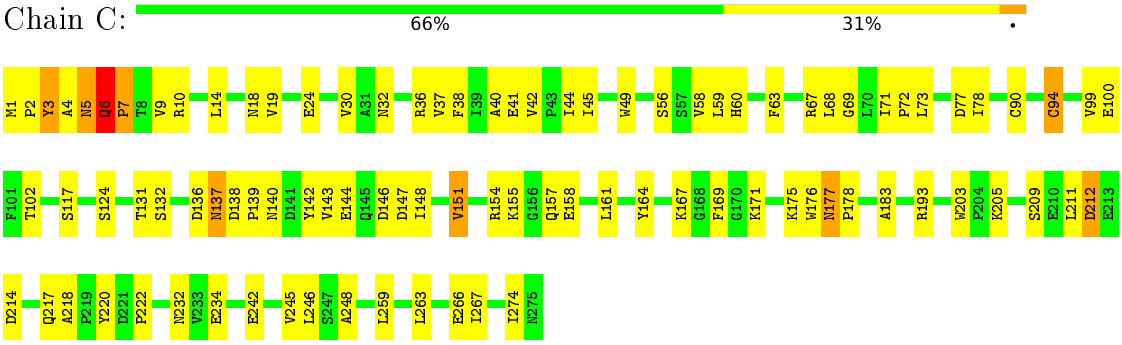
Chain B:



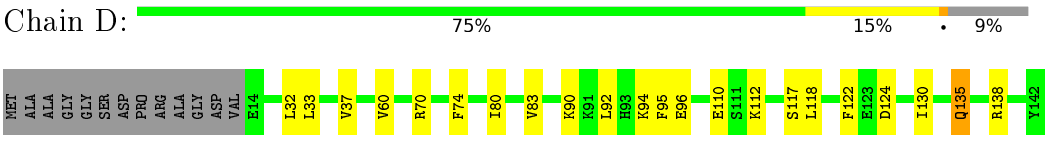
WORLDWIDE PDB PROTEIN DATA BANK
EMDataBank Unified Data Resource for 3DEM



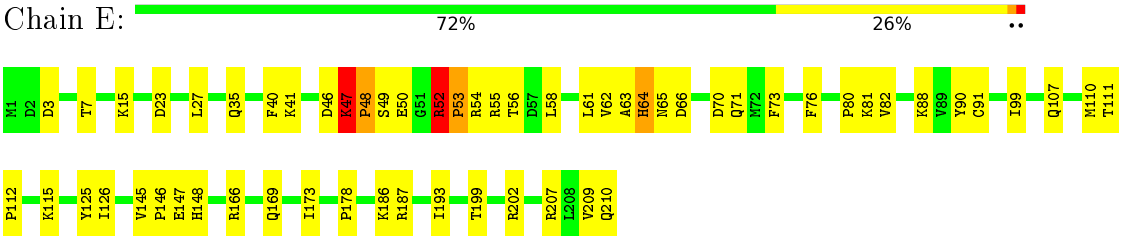
• Molecule 3: DNA-directed RNA polymerase II subunit RPB3



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

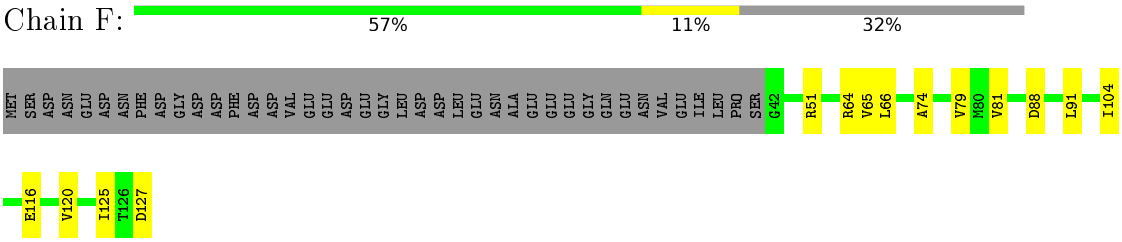


• Molecule 5: DNA-directed RNA polymerase II subunit RPB5



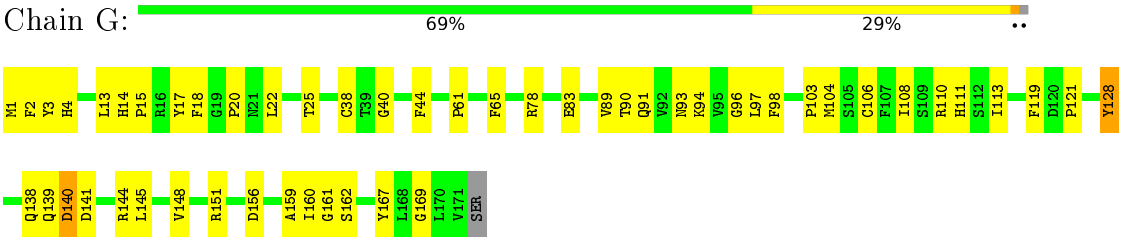
• Molecule 6: DNA-directed RNA polymerase II subunit RPB6

Chain F:



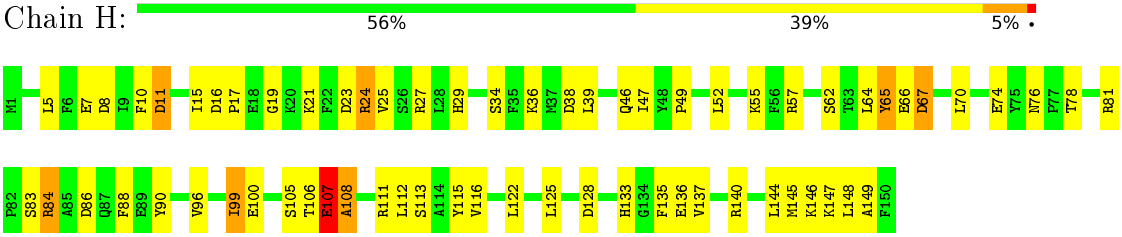
- Molecule 7: DNA-directed RNA polymerase II subunit RPB7

Chain G:



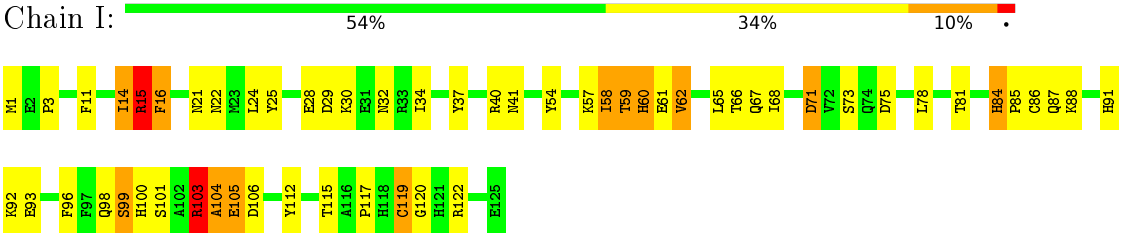
- Molecule 8: DNA-directed RNA polymerase II subunit RPB8

Chain H:



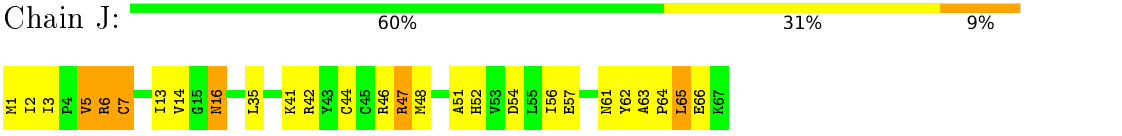
- Molecule 9: DNA-directed RNA polymerase II subunit RPB9

Chain I:



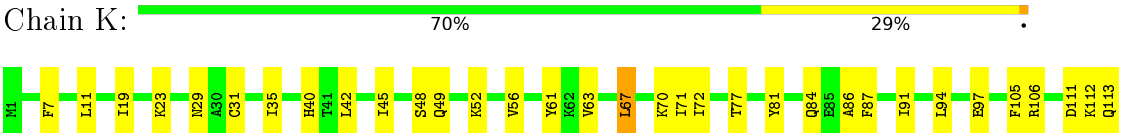
- Molecule 10: DNA-directed RNA polymerase II subunit RPB10

Chain J:



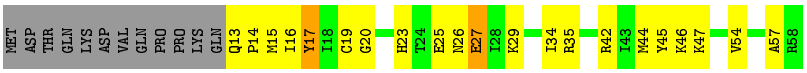
- Molecule 11: DNA-directed RNA polymerase II subunit RPB11-a

Chain K:



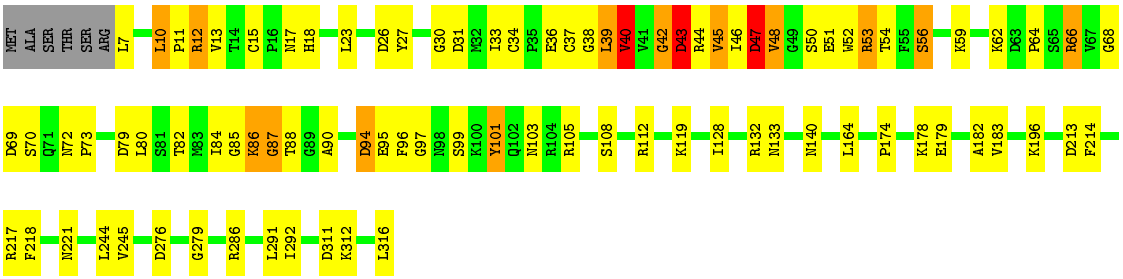
• Molecule 12: DNA-directed RNA polymerase II subunit RPB12

Chain L:



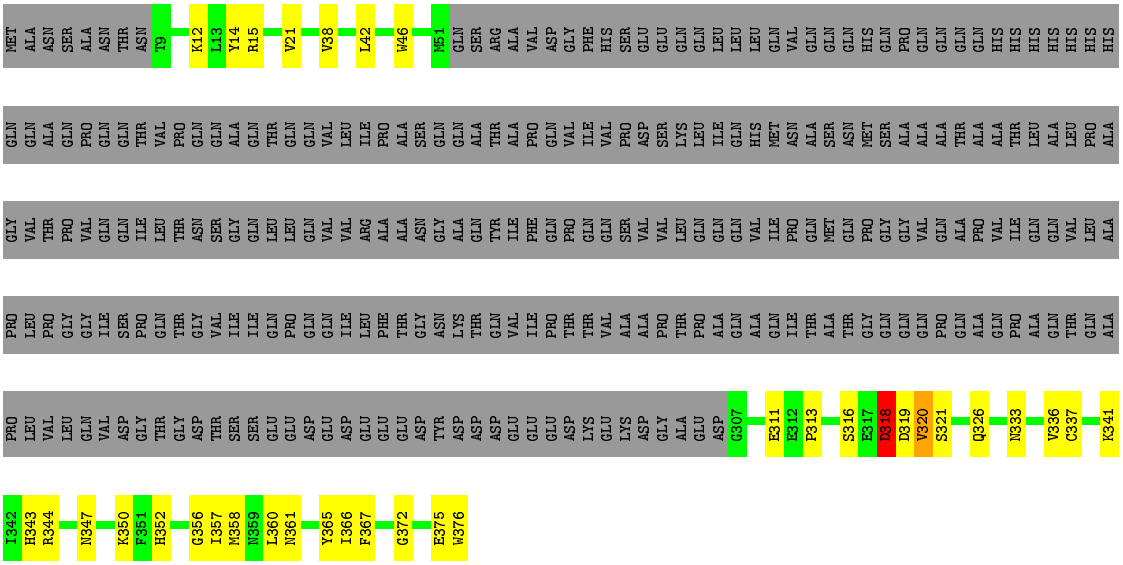
• Molecule 13: Transcription initiation factor IIB

Chain M:



• Molecule 14: Transcription initiation factor IIA subunit 1

Chain N:

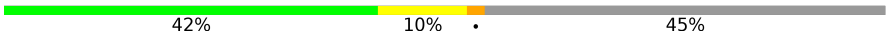


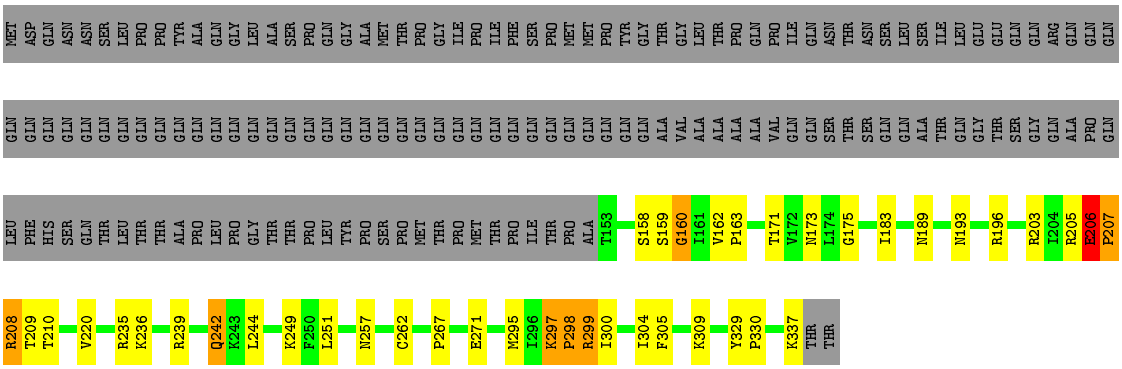
• Molecule 15: Transcription initiation factor IIA subunit 2

Chain O:

- Molecule 16: TATA-box-binding protein

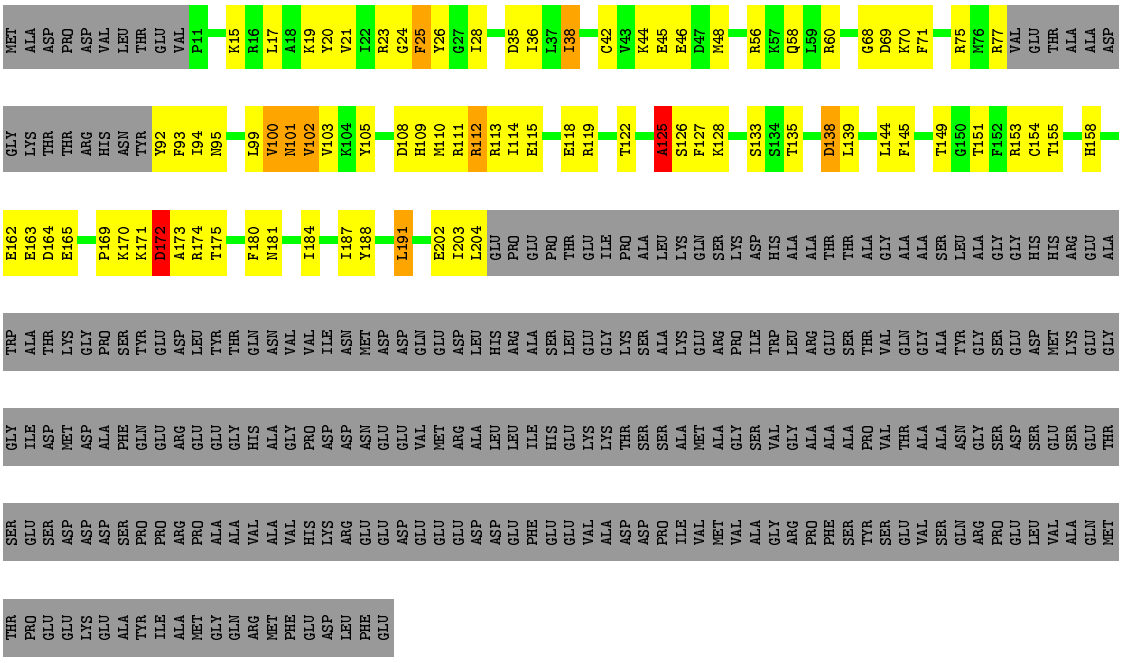
Chain P:





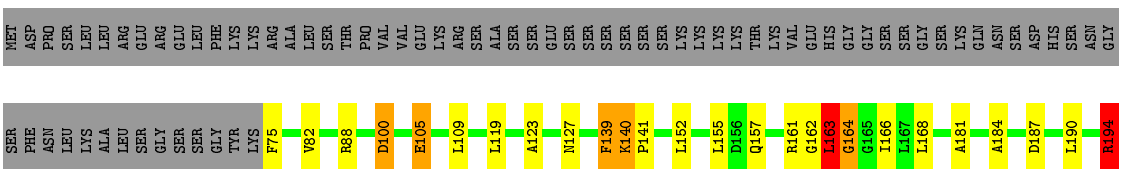
- Molecule 17: General transcription factor IIE subunit 1

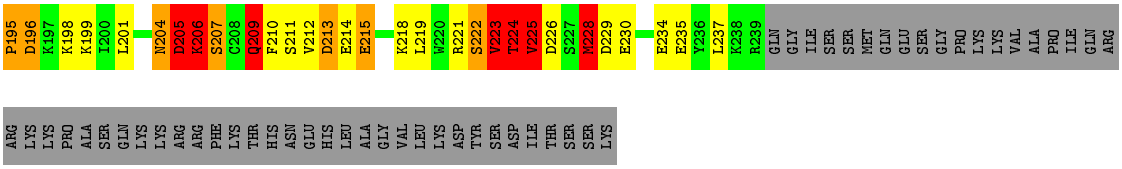
Chain Q:



- Molecule 18: Transcription initiation factor IIE subunit beta

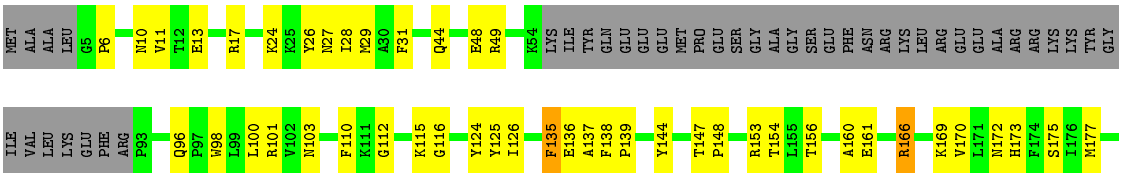
Chain R:

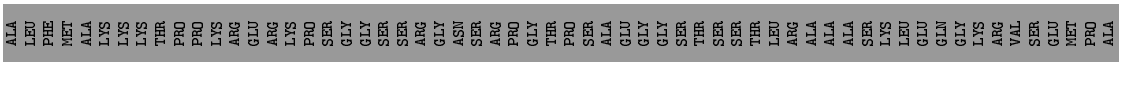




• Molecule 19: General transcription factor IIF subunit 1

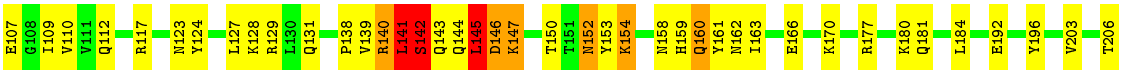
Chain S:





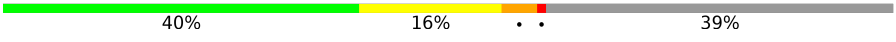
• Molecule 20: General transcription factor IIF subunit 2

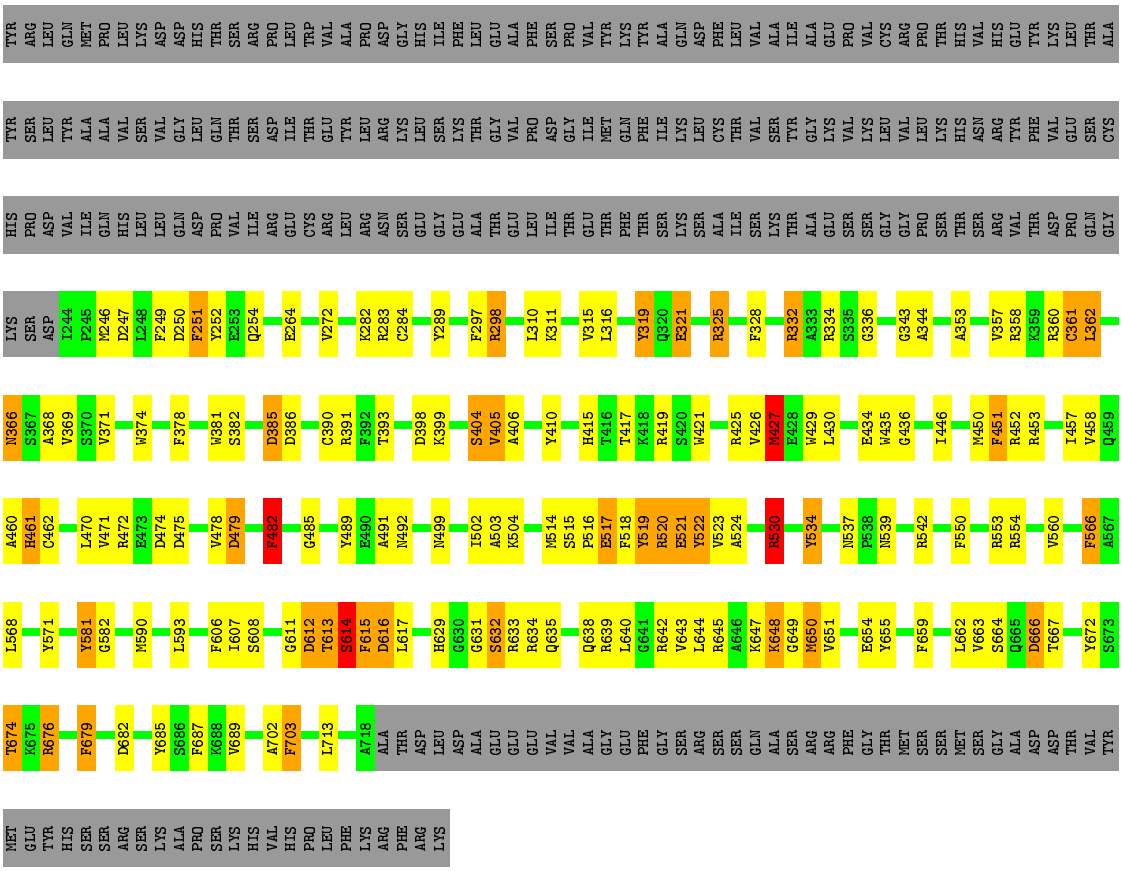
Chain T:



• Molecule 21: TFIIH basal transcription factor complex helicase XPB subunit

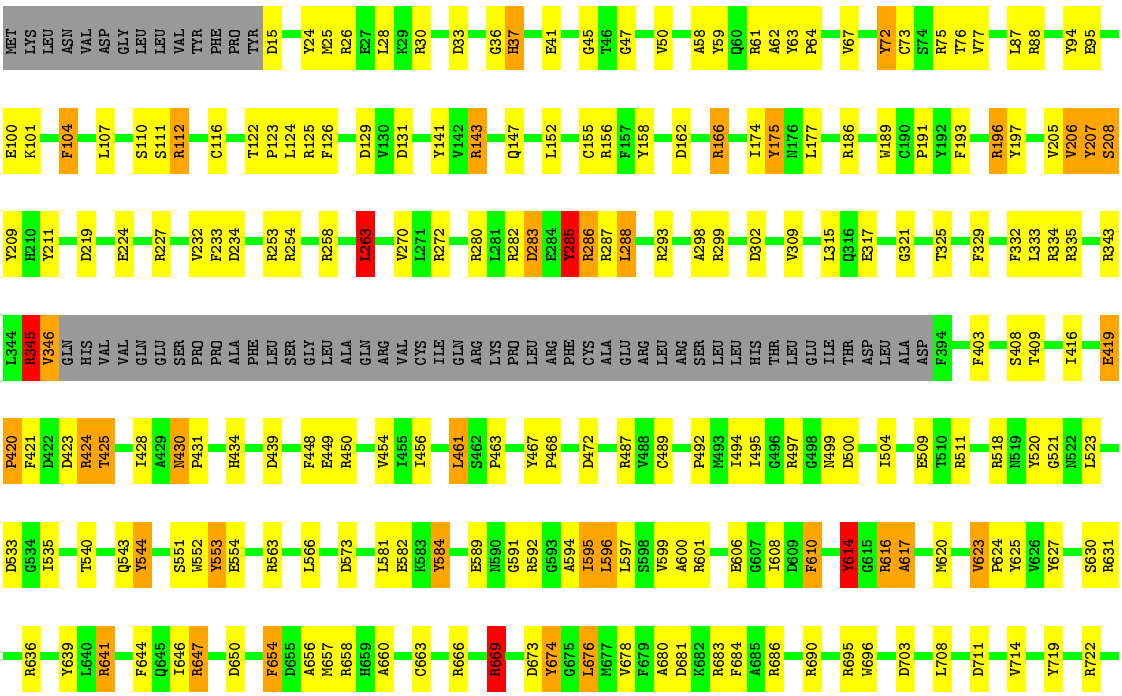
Chain V:





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

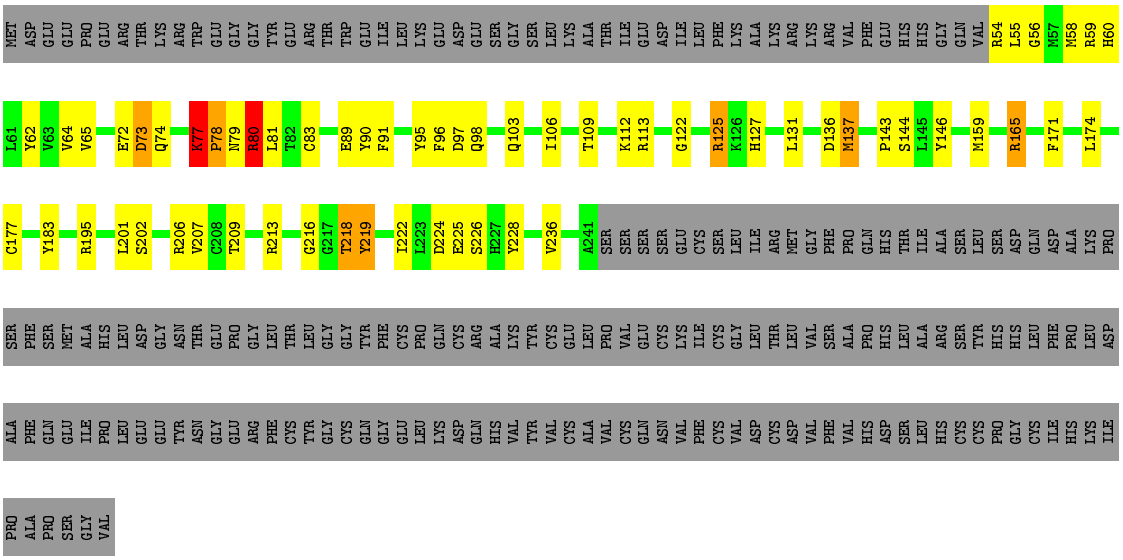
Chain W:



WORLDWIDE PDB PROTEIN DATA BANK
EMDataBank Unified Data Resource for 3DEM

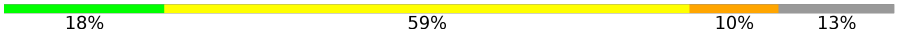
• Molecule 23: General transcription factor IIH subunit 2

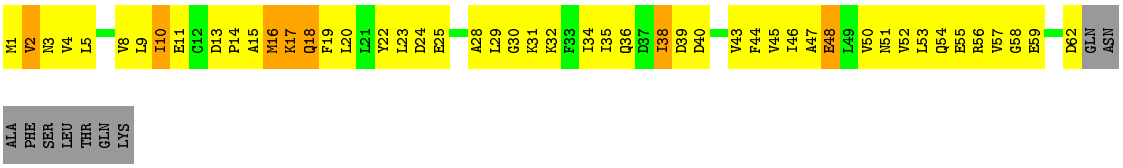
Chain 0:



• Molecule 24: General transcription factor IIH subunit 5

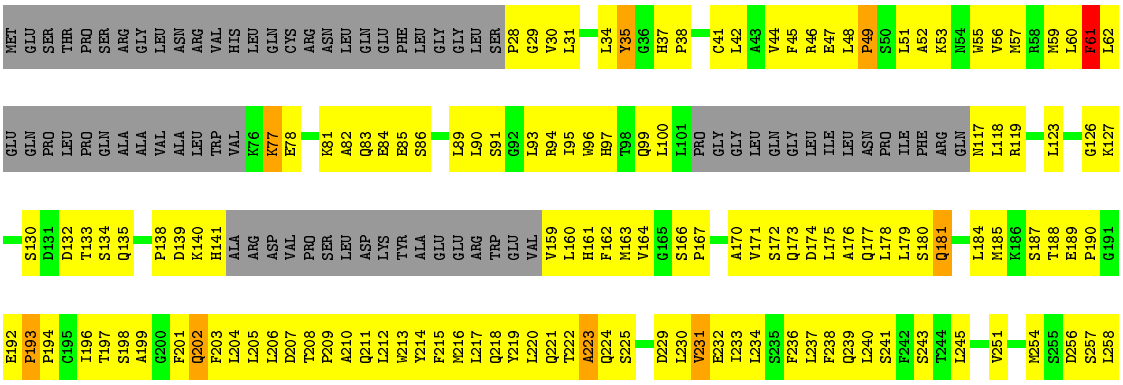
Chain 1:





• Molecule 25: General transcription factor IIH subunit 4

Chain 2:



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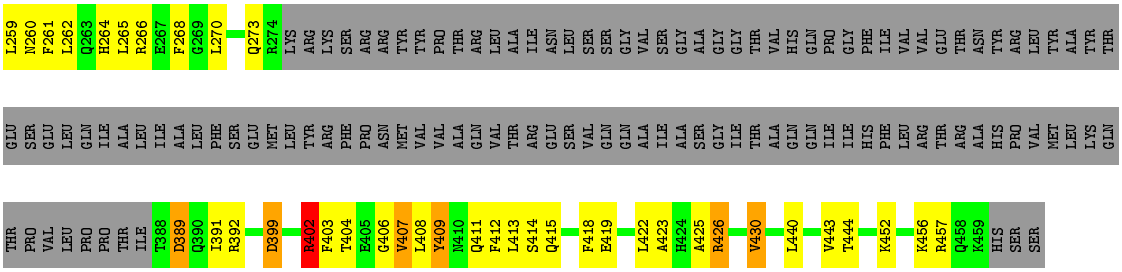
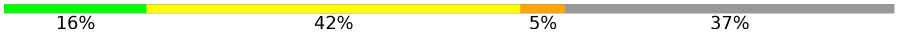
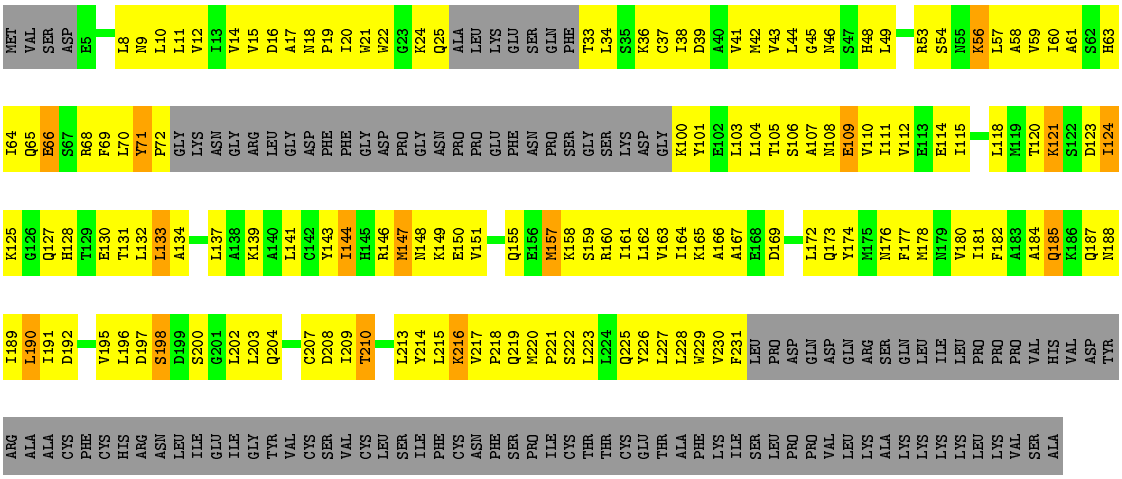
EMDataBank Unified Data Resource for 3DEM



• Molecule 26: General transcription factor IIH subunit 3

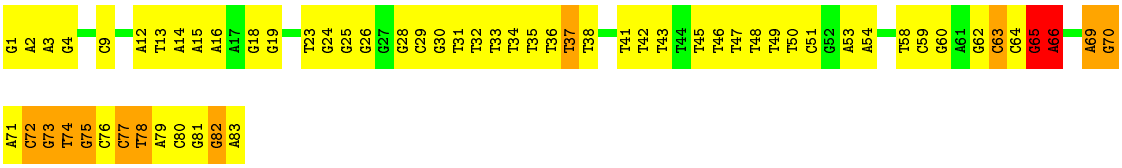
Chain 3:





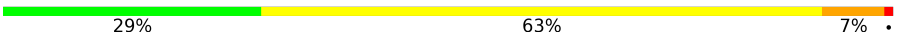
• Molecule 27: SCP-X

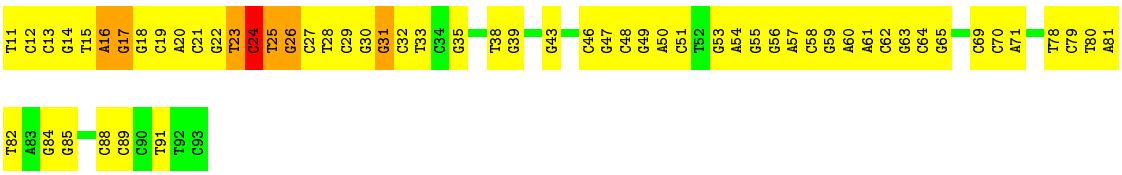
Chain X:



• Molecule 28: SCP-Y

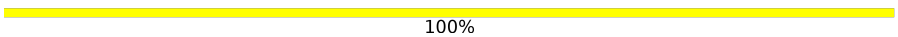
Chain Y:

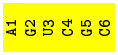




• Molecule 29: RNA

Chain Z:




A1
G2
U3
C4
G5
C6

4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	91642	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	0.56	1/11727 (0.0%)	0.81	15/15833 (0.1%)
10	J	0.66	1/542 (0.2%)	0.89	0/730
11	K	0.50	0/956	0.72	1/1294 (0.1%)
12	L	0.56	0/394	0.73	0/524
13	M	0.42	0/2429	0.73	3/3281 (0.1%)
14	N	0.24	0/945	0.52	0/1274
15	O	0.34	0/816	0.53	0/1105
16	P	0.29	0/1489	0.54	0/2005
17	Q	0.29	0/1507	0.63	1/2023 (0.0%)
18	R	0.67	4/1380 (0.3%)	1.13	6/1854 (0.3%)
19	S	0.27	0/1167	0.54	0/1576
2	B	0.67	3/9503 (0.0%)	0.87	8/12831 (0.1%)
20	T	0.28	0/1817	0.66	2/2445 (0.1%)
21	V	1.46	15/3931 (0.4%)	1.96	111/5298 (2.1%)
22	W	1.55	24/5460 (0.4%)	2.05	161/7390 (2.2%)
23	0	1.49	5/1506 (0.3%)	1.98	45/2038 (2.2%)
24	1	0.84	0/496	1.16	0/669
25	2	0.88	0/2243	1.18	8/3024 (0.3%)
26	3	0.85	0/1548	1.14	2/2090 (0.1%)
27	X	1.17	20/1917 (1.0%)	1.52	41/2962 (1.4%)
28	Y	1.16	13/1880 (0.7%)	1.48	43/2896 (1.5%)
29	Z	0.37	0/139	0.84	0/215
3	C	0.54	0/2259	0.76	1/3073 (0.0%)
4	D	0.27	0/1077	0.52	0/1446
5	E	0.43	0/1753	0.85	1/2368 (0.0%)
6	F	0.44	0/700	0.71	0/946
7	G	0.32	0/1382	0.58	0/1874
8	H	0.45	0/1227	0.71	1/1654 (0.1%)
9	I	0.38	0/1038	1.06	4/1407 (0.3%)
All	All	0.85	86/63228 (0.1%)	1.17	454/86125 (0.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
15	O	0	1
16	P	0	1
17	Q	0	2
18	R	0	20
20	T	0	1
21	V	0	16
22	W	0	18
23	0	0	2
24	1	0	1
25	2	0	8
27	X	0	3
28	Y	0	3
8	H	0	1
All	All	0	79

All (86) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	Y	25	DT	O3'-P	10.60	1.73	1.61
27	X	71	DA	P-O5'	-9.87	1.49	1.59
28	Y	31	DG	O3'-P	-9.02	1.50	1.61
27	X	79	DA	C5'-C4'	8.68	1.60	1.51
27	X	69	DA	C4'-C3'	8.62	1.61	1.53
28	Y	15	DT	C4'-C3'	8.01	1.61	1.53
22	W	158	TYR	CE1-CZ	8.01	1.49	1.38
28	Y	20	DA	P-O5'	7.96	1.67	1.59
28	Y	18	DG	O4'-C1'	-7.82	1.32	1.42
27	X	77	DC	C5'-C4'	7.82	1.59	1.51
21	V	672	TYR	CE1-CZ	7.79	1.48	1.38
27	X	81	DG	C5'-C4'	7.29	1.59	1.51
22	W	104	PHE	CG-CD1	7.18	1.49	1.38
28	Y	17	DG	P-O5'	-7.00	1.52	1.59
21	V	391	ARG	CZ-NH2	-6.99	1.24	1.33
28	Y	14	DG	C2'-C1'	6.86	1.59	1.52
22	W	110	SER	CA-CB	6.75	1.63	1.52
27	X	75	DG	C5'-C4'	6.67	1.58	1.51
27	X	80	DC	C4'-C3'	6.67	1.60	1.53
21	V	325	ARG	CZ-NH1	-6.60	1.24	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	V	633	ARG	CZ-NH1	-6.59	1.24	1.33
10	J	44	CYS	CB-SG	-6.55	1.71	1.82
28	Y	12	DC	C4'-O4'	-6.51	1.38	1.45
22	W	521	GLY	N-CA	6.48	1.55	1.46
23	0	122	GLY	N-CA	6.46	1.55	1.46
22	W	208	SER	CB-OG	-6.33	1.34	1.42
21	V	606	PHE	CG-CD1	6.31	1.48	1.38
22	W	683	ARG	CZ-NH2	-6.28	1.24	1.33
27	X	75	DG	C4'-O4'	-6.26	1.38	1.45
27	X	71	DA	C3'-C2'	6.22	1.59	1.52
21	V	554	ARG	NE-CZ	6.20	1.41	1.33
28	Y	25	DT	P-O5'	-6.19	1.53	1.59
28	Y	17	DG	O4'-C1'	-6.17	1.34	1.42
1	A	500	GLU	CG-CD	6.10	1.61	1.51
21	V	453	ARG	CZ-NH2	-6.04	1.25	1.33
27	X	71	DA	C4'-O4'	-6.01	1.39	1.45
28	Y	18	DG	C5'-C4'	5.93	1.57	1.51
21	V	319	TYR	CE1-CZ	5.90	1.46	1.38
27	X	72	DC	C2'-C1'	5.89	1.58	1.52
21	V	435	TRP	CD2-CE2	5.87	1.48	1.41
22	W	321	GLY	N-CA	5.84	1.54	1.46
28	Y	18	DG	C4'-O4'	-5.82	1.39	1.45
27	X	66	DA	C1'-N9	5.81	1.56	1.49
27	X	81	DG	P-O5'	5.77	1.65	1.59
18	R	205	ASP	N-CA	5.75	1.57	1.46
23	0	195	ARG	CZ-NH1	-5.73	1.25	1.33
2	B	984	CYS	CB-SG	-5.71	1.72	1.81
18	R	206	LYS	N-CA	5.68	1.57	1.46
22	W	286	ARG	CZ-NH1	-5.67	1.25	1.33
27	X	83	DA	P-O5'	5.63	1.65	1.59
21	V	252	TYR	CE1-CZ	5.62	1.45	1.38
21	V	374	TRP	CA-CB	5.62	1.66	1.53
2	B	959	GLU	CG-CD	5.60	1.60	1.51
27	X	75	DG	C1'-N9	-5.55	1.39	1.47
22	W	47	GLY	N-CA	5.54	1.54	1.46
27	X	76	DC	O3'-P	5.51	1.67	1.61
27	X	81	DG	C1'-N9	-5.42	1.39	1.47
22	W	610	PHE	CG-CD1	5.41	1.46	1.38
18	R	206	LYS	CA-C	5.37	1.67	1.52
21	V	452	ARG	CZ-NH2	-5.35	1.26	1.33
21	V	332	ARG	CZ-NH2	-5.35	1.26	1.33
22	W	606	GLU	CA-CB	5.34	1.65	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	W	286	ARG	CZ-NH2	-5.33	1.26	1.33
22	W	674	TYR	CE1-CZ	5.31	1.45	1.38
22	W	448	PHE	CE1-CZ	5.31	1.47	1.37
22	W	24	TYR	CE2-CZ	5.29	1.45	1.38
22	W	334	ARG	CZ-NH2	-5.28	1.26	1.33
22	W	253	ARG	CZ-NH1	-5.28	1.26	1.33
21	V	659	PHE	CG-CD2	5.22	1.46	1.38
18	R	205	ASP	CA-C	5.18	1.66	1.52
27	X	66	DA	C5'-C4'	5.16	1.57	1.51
2	B	112	GLU	CD-OE2	5.14	1.31	1.25
27	X	72	DC	C1'-N1	5.14	1.55	1.49
28	Y	12	DC	C5'-C4'	5.12	1.56	1.51
23	0	112	LYS	N-CA	5.10	1.56	1.46
22	W	511	ARG	NE-CZ	-5.10	1.26	1.33
22	W	639	TYR	CZ-OH	-5.09	1.29	1.37
23	0	95	TYR	CG-CD1	5.08	1.45	1.39
22	W	254	ARG	CZ-NH1	-5.06	1.26	1.33
27	X	65	DG	C2'-C1'	5.06	1.57	1.52
22	W	654	PHE	CG-CD1	5.05	1.46	1.38
22	W	518	ARG	CZ-NH2	-5.04	1.26	1.33
22	W	520	TYR	CZ-OH	-5.03	1.29	1.37
23	0	146	TYR	CD2-CE2	5.03	1.46	1.39
21	V	451	PHE	CG-CD2	5.02	1.46	1.38
22	W	345	ARG	CZ-NH1	-5.02	1.26	1.33

All (454) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	I	84	HIS	C-N-CD	-28.48	57.95	120.60
5	E	52	ARG	C-N-CD	-22.65	70.76	120.60
23	0	77	LYS	C-N-CD	-22.15	71.87	120.60
26	3	71	TYR	C-N-CD	-20.77	74.91	120.60
1	A	622	SER	C-N-CD	-20.67	75.13	120.60
22	W	335	ARG	NE-CZ-NH1	-19.62	110.49	120.30
28	Y	14	DG	O4'-C1'-N9	19.12	121.39	108.00
22	W	26	ARG	NE-CZ-NH2	18.75	129.67	120.30
18	R	194	ARG	C-N-CD	-17.75	81.55	120.60
21	V	358	ARG	NE-CZ-NH2	17.72	129.16	120.30
23	0	195	ARG	NE-CZ-NH1	16.68	128.64	120.30
22	W	186	ARG	NE-CZ-NH1	16.19	128.39	120.30
22	W	497	ARG	NE-CZ-NH1	15.94	128.27	120.30
22	W	287	ARG	NE-CZ-NH2	15.59	128.10	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	X	83	DA	O4'-C1'-N9	15.35	118.75	108.00
23	0	165	ARG	NE-CZ-NH2	-15.32	112.64	120.30
22	W	299	ARG	NE-CZ-NH1	15.13	127.86	120.30
21	V	634	ARG	NE-CZ-NH2	14.68	127.64	120.30
23	0	206	ARG	NE-CZ-NH1	14.67	127.64	120.30
22	W	592	ARG	NE-CZ-NH1	14.39	127.49	120.30
22	W	335	ARG	NE-CZ-NH2	14.20	127.40	120.30
28	Y	15	DT	O4'-C1'-N1	13.97	117.78	108.00
21	V	332	ARG	NE-CZ-NH1	13.94	127.27	120.30
22	W	112	ARG	NE-CZ-NH1	13.87	127.23	120.30
22	W	669	ARG	NE-CZ-NH1	13.77	127.18	120.30
22	W	272	ARG	NE-CZ-NH1	13.76	127.18	120.30
22	W	343	ARG	NE-CZ-NH2	13.23	126.91	120.30
22	W	75	ARG	NE-CZ-NH1	13.20	126.90	120.30
21	V	633	ARG	NE-CZ-NH2	-12.81	113.90	120.30
28	Y	24	DC	O4'-C1'-N1	12.72	116.90	108.00
22	W	467	TYR	CB-CG-CD1	-12.31	113.61	121.00
22	W	627	TYR	CB-CG-CD2	-12.20	113.68	121.00
22	W	601	ARG	NE-CZ-NH2	-12.10	114.25	120.30
22	W	631	ARG	NE-CZ-NH1	11.92	126.26	120.30
21	V	452	ARG	NE-CZ-NH1	11.73	126.16	120.30
22	W	26	ARG	NH1-CZ-NH2	-11.69	106.54	119.40
22	W	636	ARG	NE-CZ-NH1	11.61	126.10	120.30
22	W	487	ARG	NE-CZ-NH1	11.56	126.08	120.30
21	V	283	ARG	NE-CZ-NH2	-11.54	114.53	120.30
22	W	343	ARG	NE-CZ-NH1	-11.45	114.57	120.30
22	W	88	ARG	NE-CZ-NH1	11.34	125.97	120.30
22	W	647	ARG	NE-CZ-NH1	11.19	125.89	120.30
22	W	419	GLU	C-N-CD	-11.10	96.17	120.60
28	Y	11	DT	O4'-C1'-N1	11.06	115.74	108.00
27	X	79	DA	O4'-C4'-C3'	10.85	112.51	106.00
22	W	683	ARG	NE-CZ-NH2	10.74	125.67	120.30
27	X	79	DA	O4'-C1'-N9	10.72	115.51	108.00
22	W	690	ARG	NE-CZ-NH2	10.68	125.64	120.30
27	X	65	DG	O4'-C4'-C3'	10.68	112.41	106.00
27	X	62	DG	O3'-P-O5'	-10.67	83.72	104.00
27	X	66	DA	O4'-C1'-C2'	-10.60	97.42	105.90
28	Y	25	DT	O4'-C4'-C3'	10.36	112.22	106.00
21	V	391	ARG	NE-CZ-NH1	-10.34	115.13	120.30
28	Y	31	DG	O3'-P-O5'	10.33	123.63	104.00
22	W	88	ARG	NE-CZ-NH2	-10.30	115.15	120.30
27	X	75	DG	O4'-C1'-N9	10.06	115.04	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	V	687	PHE	CB-CG-CD2	-9.95	113.83	120.80
21	V	452	ARG	NE-CZ-NH2	-9.94	115.33	120.30
21	V	676	ARG	NE-CZ-NH2	-9.80	115.40	120.30
21	V	283	ARG	NE-CZ-NH1	9.78	125.19	120.30
22	W	497	ARG	NE-CZ-NH2	-9.73	115.44	120.30
27	X	73	DG	O4'-C1'-C2'	9.68	113.64	105.90
23	0	59	ARG	NE-CZ-NH2	9.67	125.14	120.30
21	V	520	ARG	CA-C-N	-9.66	95.95	117.20
21	V	553	ARG	NE-CZ-NH2	9.61	125.10	120.30
21	V	334	ARG	CD-NE-CZ	9.53	136.94	123.60
22	W	227	ARG	NE-CZ-NH1	9.42	125.01	120.30
22	W	658	ARG	NE-CZ-NH2	-9.38	115.61	120.30
21	V	645	ARG	NE-CZ-NH1	9.30	124.95	120.30
28	Y	21	DC	O4'-C4'-C3'	9.30	111.58	106.00
27	X	66	DA	O5'-P-OP1	9.28	121.84	110.70
22	W	511	ARG	NE-CZ-NH2	9.22	124.91	120.30
28	Y	17	DG	O4'-C1'-N9	-9.20	101.56	108.00
21	V	264	GLU	OE1-CD-OE2	-9.18	112.29	123.30
22	W	627	TYR	CG-CD2-CE2	-9.16	113.97	121.30
23	0	219	TYR	CB-CG-CD1	-9.16	115.50	121.00
22	W	686	ARG	NE-CZ-NH1	9.13	124.86	120.30
21	V	421	TRP	NE1-CE2-CD2	-9.05	98.25	107.30
22	W	666	ARG	NE-CZ-NH1	9.05	124.83	120.30
22	W	703	ASP	CB-CG-OD2	8.99	126.40	118.30
22	W	286	ARG	NE-CZ-NH2	8.96	124.78	120.30
28	Y	21	DC	C2-N1-C1'	-8.89	109.02	118.80
23	0	206	ARG	NH1-CZ-NH2	-8.85	109.67	119.40
21	V	421	TRP	CD2-CE3-CZ3	8.79	130.23	118.80
21	V	550	PHE	CB-CG-CD1	-8.72	114.70	120.80
27	X	70	DG	O4'-C1'-N9	8.64	114.05	108.00
27	X	79	DA	C4'-C3'-C2'	-8.55	95.40	103.10
22	W	654	PHE	CB-CG-CD2	-8.47	114.87	120.80
22	W	450	ARG	NE-CZ-NH1	8.41	124.50	120.30
27	X	79	DA	C1'-O4'-C4'	-8.40	101.70	110.10
9	I	103	ARG	N-CA-C	-8.38	88.38	111.00
2	B	112	GLU	OE1-CD-OE2	-8.38	113.25	123.30
21	V	581	TYR	CG-CD1-CE1	-8.36	114.61	121.30
20	T	141	LEU	N-CA-C	-8.33	88.52	111.00
21	V	520	ARG	C-N-CA	-8.32	100.90	121.70
21	V	419	ARG	NE-CZ-NH1	8.31	124.45	120.30
28	Y	21	DC	C1'-O4'-C4'	-8.28	101.82	110.10
22	W	332	PHE	CB-CG-CD2	-8.26	115.02	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	0	213	ARG	NE-CZ-NH1	8.22	124.41	120.30
28	Y	21	DC	C6-N1-C1'	8.22	130.66	120.80
22	W	497	ARG	CD-NE-CZ	8.18	135.06	123.60
21	V	685	TYR	CB-CG-CD2	8.17	125.90	121.00
21	V	520	ARG	NE-CZ-NH2	8.11	124.36	120.30
1	A	501	MET	CA-CB-CG	8.04	126.97	113.30
21	V	520	ARG	O-C-N	8.04	135.56	122.70
21	V	634	ARG	NE-CZ-NH1	-7.97	116.31	120.30
22	W	126	PHE	CB-CG-CD2	7.93	126.35	120.80
22	W	601	ARG	NE-CZ-NH1	7.93	124.26	120.30
21	V	386	ASP	CB-CG-OD2	-7.86	111.22	118.30
21	V	410	TYR	CB-CG-CD1	-7.86	116.28	121.00
28	Y	20	DA	O4'-C4'-C3'	-7.86	101.29	106.00
21	V	358	ARG	NH1-CZ-NH2	-7.85	110.76	119.40
22	W	75	ARG	NE-CZ-NH2	-7.83	116.38	120.30
22	W	614	TYR	CB-CG-CD2	-7.81	116.31	121.00
22	W	467	TYR	CB-CG-CD2	7.77	125.66	121.00
23	0	165	ARG	NE-CZ-NH1	7.76	124.18	120.30
22	W	644	PHE	CB-CG-CD1	7.73	126.21	120.80
28	Y	18	DG	O4'-C4'-C3'	7.73	110.64	106.00
28	Y	21	DC	O4'-C1'-C2'	7.72	112.08	105.90
22	W	232	VAL	CA-CB-CG1	7.69	122.44	110.90
22	W	125	ARG	NE-CZ-NH1	7.65	124.13	120.30
21	V	421	TRP	CE2-CD2-CG	7.64	113.41	107.30
22	W	520	TYR	CG-CD1-CE1	-7.64	115.19	121.30
22	W	448	PHE	CB-CG-CD2	7.64	126.15	120.80
2	B	588	ARG	CB-CG-CD	-7.63	91.75	111.60
13	M	94	ASP	N-CA-C	-7.62	90.41	111.00
22	W	582	GLU	OE1-CD-OE2	-7.58	114.20	123.30
21	V	542	ARG	NE-CZ-NH2	7.57	124.08	120.30
25	2	402	ARG	NE-CZ-NH1	7.54	124.07	120.30
21	V	474	ASP	CB-CG-OD2	7.53	125.08	118.30
21	V	421	TRP	NE1-CE2-CZ2	7.52	138.67	130.40
28	Y	18	DG	C4'-C3'-C2'	-7.52	96.33	103.10
23	0	90	TYR	CB-CG-CD2	-7.50	116.50	121.00
27	X	64	DC	N3-C2-O2	-7.48	116.67	121.90
22	W	553	TYR	CB-CG-CD2	7.47	125.48	121.00
22	W	592	ARG	NH1-CZ-NH2	-7.46	111.20	119.40
22	W	143	ARG	NE-CZ-NH1	7.46	124.03	120.30
28	Y	24	DC	C2-N1-C1'	-7.41	110.65	118.80
23	0	95	TYR	CB-CG-CD1	-7.41	116.56	121.00
2	B	882	SER	N-CA-C	-7.40	91.01	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	W	272	ARG	NH1-CZ-NH2	-7.39	111.27	119.40
21	V	522	TYR	CB-CG-CD2	-7.39	116.57	121.00
21	V	554	ARG	NE-CZ-NH1	7.37	123.98	120.30
22	W	193	PHE	CB-CG-CD1	-7.36	115.65	120.80
21	V	421	TRP	CD1-NE1-CE2	7.32	115.58	109.00
28	Y	15	DT	O4'-C1'-C2'	-7.31	100.05	105.90
21	V	249	PHE	CB-CG-CD2	7.29	125.91	120.80
23	0	73	ASP	CB-CG-OD2	-7.26	111.76	118.30
23	0	236	VAL	CA-CB-CG1	7.23	121.75	110.90
21	V	685	TYR	CB-CG-CD1	-7.20	116.68	121.00
21	V	639	ARG	NE-CZ-NH2	7.13	123.86	120.30
23	0	89	GLU	OE1-CD-OE2	-7.11	114.76	123.30
21	V	703	PHE	CB-CG-CD2	-7.10	115.83	120.80
27	X	66	DA	P-O5'-C5'	7.07	132.22	120.90
22	W	186	ARG	NE-CZ-NH2	-7.06	116.77	120.30
22	W	317	GLU	OE1-CD-OE2	-7.04	114.85	123.30
22	W	280	ARG	NE-CZ-NH1	-7.04	116.78	120.30
22	W	166	ARG	CD-NE-CZ	7.03	133.44	123.60
22	W	627	TYR	CD1-CG-CD2	6.99	125.59	117.90
2	B	479	LEU	CB-CG-CD2	-6.98	99.13	111.00
27	X	79	DA	P-O3'-C3'	6.93	128.02	119.70
9	I	15	ARG	N-CA-C	-6.92	92.30	111.00
21	V	643	VAL	CA-CB-CG1	6.91	121.27	110.90
22	W	614	TYR	CG-CD2-CE2	-6.91	115.77	121.30
21	V	385	ASP	CB-CG-OD1	-6.90	112.09	118.30
22	W	253	ARG	NE-CZ-NH1	6.89	123.74	120.30
28	Y	23	DT	O4'-C1'-N1	-6.88	103.18	108.00
22	W	654	PHE	CB-CG-CD1	6.88	125.61	120.80
22	W	332	PHE	CB-CG-CD1	6.87	125.61	120.80
23	0	95	TYR	CD1-CE1-CZ	-6.85	113.63	119.80
28	Y	29	DC	N3-C2-O2	-6.85	117.11	121.90
28	Y	25	DT	C4'-C3'-C2'	-6.84	96.94	103.10
22	W	219	ASP	CB-CG-OD1	6.82	124.44	118.30
25	2	35	TYR	CA-CB-CG	-6.81	100.46	113.40
22	W	196	ARG	NE-CZ-NH1	6.79	123.70	120.30
27	X	73	DG	O4'-C1'-N9	6.79	112.75	108.00
22	W	125	ARG	CD-NE-CZ	6.79	133.10	123.60
23	0	136	ASP	CB-CG-OD1	6.79	124.41	118.30
27	X	81	DG	C8-N9-C1'	6.78	135.82	127.00
27	X	37	DT	O4'-C1'-N1	6.77	112.74	108.00
23	0	195	ARG	NE-CZ-NH2	-6.77	116.91	120.30
22	W	566	LEU	CB-CG-CD1	6.75	122.48	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	W	644	PHE	CB-CG-CD2	-6.75	116.08	120.80
27	X	81	DG	C4-N9-C1'	-6.74	117.73	126.50
22	W	616	ARG	NE-CZ-NH1	-6.74	116.93	120.30
21	V	530	ARG	NE-CZ-NH2	-6.73	116.94	120.30
22	W	345	ARG	CD-NE-CZ	6.71	133.00	123.60
22	W	26	ARG	NE-CZ-NH1	6.70	123.65	120.30
22	W	50	VAL	CA-CB-CG1	6.69	120.94	110.90
22	W	299	ARG	NE-CZ-NH2	-6.64	116.98	120.30
21	V	581	TYR	CD1-CE1-CZ	6.64	125.78	119.80
25	2	61	PHE	CB-CA-C	-6.64	97.12	110.40
22	W	30	ARG	CD-NE-CZ	6.63	132.88	123.60
13	M	43	ASP	N-CA-C	-6.62	93.12	111.00
21	V	655	TYR	CB-CG-CD2	-6.62	117.03	121.00
21	V	334	ARG	NE-CZ-NH1	6.62	123.61	120.30
22	W	674	TYR	CB-CG-CD1	6.60	124.96	121.00
23	0	219	TYR	CG-CD1-CE1	-6.59	116.03	121.30
22	W	302	ASP	CB-CG-OD1	6.54	124.19	118.30
22	W	76	THR	CA-CB-OG1	6.53	122.72	109.00
21	V	421	TRP	CE2-CD2-CE3	-6.50	110.91	118.70
22	W	315	LEU	CB-CG-CD1	6.49	122.03	111.00
22	W	487	ARG	NH1-CZ-NH2	-6.49	112.26	119.40
2	B	880	LEU	N-CA-C	6.49	128.51	111.00
25	2	193	PRO	CA-N-CD	-6.48	102.43	111.50
21	V	298	ARG	NE-CZ-NH1	6.48	123.54	120.30
27	X	78	DT	N1-C1'-C2'	6.47	124.89	112.60
21	V	404	SER	CB-CA-C	6.46	122.38	110.10
28	Y	22	DG	C4'-C3'-C2'	-6.46	97.29	103.10
28	Y	20	DA	O4'-C1'-C2'	-6.46	100.73	105.90
18	R	88	ARG	NE-CZ-NH1	6.45	123.53	120.30
23	0	113	ARG	NE-CZ-NH1	6.45	123.52	120.30
8	H	148	LEU	CA-CB-CG	6.43	130.10	115.30
22	W	189	TRP	NE1-CE2-CD2	-6.43	100.87	107.30
22	W	131	ASP	CB-CG-OD1	-6.41	112.53	118.30
21	V	682	ASP	CB-CG-OD1	6.40	124.06	118.30
22	W	125	ARG	NE-CZ-NH2	-6.40	117.10	120.30
22	W	641	ARG	NE-CZ-NH1	6.40	123.50	120.30
22	W	669	ARG	NH1-CZ-NH2	-6.38	112.38	119.40
18	R	163	LEU	C-N-CA	-6.38	108.91	122.30
22	W	722	ARG	CD-NE-CZ	6.37	132.51	123.60
21	V	521	GLU	OE1-CD-OE2	-6.36	115.66	123.30
1	A	458	PHE	N-CA-CB	-6.36	99.15	110.60
22	W	30	ARG	NE-CZ-NH1	6.36	123.48	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	W	639	TYR	CB-CG-CD2	-6.36	117.19	121.00
22	W	683	ARG	CD-NE-CZ	6.35	132.50	123.60
21	V	369	VAL	CA-CB-CG1	6.33	120.40	110.90
22	W	263	LEU	N-CA-CB	-6.32	97.75	110.40
18	R	206	LYS	N-CA-C	6.32	128.07	111.00
21	V	332	ARG	NH1-CZ-NH2	-6.30	112.47	119.40
27	X	83	DA	C4'-C3'-C2'	-6.26	97.47	103.10
23	0	59	ARG	NH1-CZ-NH2	-6.23	112.55	119.40
21	V	344	ALA	N-CA-CB	-6.22	101.39	110.10
22	W	206	VAL	CA-CB-CG1	6.20	120.20	110.90
21	V	522	TYR	CB-CG-CD1	6.17	124.70	121.00
28	Y	27	DC	C2-N1-C1'	-6.15	112.03	118.80
23	0	137	MET	CG-SD-CE	6.14	110.02	100.20
21	V	410	TYR	CZ-CE2-CD2	-6.13	114.28	119.80
22	W	77	VAL	CG1-CB-CG2	-6.11	101.12	110.90
21	V	435	TRP	NE1-CE2-CD2	-6.08	101.22	107.30
27	X	63	DC	O4'-C4'-C3'	6.06	109.64	106.00
23	0	183	TYR	CB-CG-CD1	-6.06	117.36	121.00
21	V	676	ARG	NE-CZ-NH1	6.05	123.33	120.30
21	V	472	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	A	641	CYS	CA-CB-SG	-6.01	103.18	114.00
23	0	218	THR	CA-CB-CG2	-6.01	103.99	112.40
21	V	360	ARG	CD-NE-CZ	5.99	131.99	123.60
21	V	663	VAL	CG1-CB-CG2	-5.99	101.31	110.90
22	W	131	ASP	CB-CG-OD2	5.99	123.69	118.30
22	W	673	ASP	CB-CG-OD1	5.97	123.67	118.30
28	Y	21	DC	O4'-C1'-N1	-5.97	103.82	108.00
2	B	80	GLU	N-CA-C	5.95	127.06	111.00
27	X	83	DA	O4'-C1'-C2'	-5.95	101.14	105.90
27	X	63	DC	N3-C2-O2	-5.94	117.74	121.90
22	W	156	ARG	CD-NE-CZ	5.94	131.92	123.60
21	V	566	PHE	CB-CG-CD1	5.93	124.95	120.80
28	Y	11	DT	P-O3'-C3'	5.93	126.82	119.70
22	W	552	TRP	CD1-NE1-CE2	5.93	114.33	109.00
22	W	472	ASP	CB-CG-OD2	5.91	123.62	118.30
28	Y	16	DA	O4'-C1'-C2'	5.91	110.63	105.90
21	V	321	GLU	OE1-CD-OE2	-5.91	116.20	123.30
3	C	6	GLN	C-N-CD	-5.90	107.62	120.60
1	A	932	ARG	C-N-CA	-5.90	106.95	121.70
27	X	64	DC	N1-C2-O2	5.90	122.44	118.90
20	T	142	SER	N-CA-C	5.89	126.90	111.00
27	X	71	DA	O4'-C1'-N9	5.86	112.10	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	V	381	TRP	CZ3-CH2-CZ2	-5.86	114.57	121.60
23	0	171	PHE	CB-CG-CD1	-5.85	116.70	120.80
21	V	410	TYR	CB-CG-CD2	5.84	124.50	121.00
28	Y	25	DT	O4'-C1'-N1	-5.84	103.91	108.00
21	V	435	TRP	CD1-NE1-CE2	5.84	114.25	109.00
9	I	84	HIS	N-CA-C	5.82	126.72	111.00
22	W	563	ARG	NE-CZ-NH1	5.81	123.21	120.30
22	W	112	ARG	NH1-CZ-NH2	-5.79	113.03	119.40
22	W	650	ASP	CB-CG-OD1	5.79	123.51	118.30
22	W	472	ASP	CB-CG-OD1	-5.77	113.11	118.30
22	W	72	TYR	CB-CG-CD2	-5.74	117.55	121.00
21	V	542	ARG	NH1-CZ-NH2	-5.74	113.08	119.40
22	W	129	ASP	CB-CG-OD1	5.73	123.46	118.30
28	Y	14	DG	C3'-C2'-C1'	-5.72	95.63	102.50
28	Y	16	DA	O4'-C1'-N9	5.72	112.01	108.00
21	V	251	PHE	CB-CG-CD1	-5.70	116.81	120.80
22	W	641	ARG	CD-NE-CZ	5.70	131.58	123.60
18	R	205	ASP	N-CA-C	5.70	126.38	111.00
22	W	345	ARG	NE-CZ-NH2	-5.69	117.45	120.30
23	0	177	CYS	CA-CB-SG	-5.69	103.76	114.00
27	X	82	DG	O4'-C1'-N9	-5.69	104.02	108.00
22	W	544	TYR	CG-CD2-CE2	-5.68	116.75	121.30
21	V	419	ARG	CD-NE-CZ	5.68	131.56	123.60
27	X	64	DC	O4'-C1'-C2'	-5.68	101.35	105.90
23	0	80	ARG	CD-NE-CZ	5.68	131.55	123.60
1	A	1396	ARG	NE-CZ-NH2	-5.67	117.46	120.30
28	Y	27	DC	C6-N1-C1'	5.67	127.61	120.80
21	V	391	ARG	NE-CZ-NH2	5.67	123.14	120.30
23	0	91	PHE	CG-CD2-CE2	-5.67	114.56	120.80
22	W	41	GLU	O-C-N	5.66	131.76	122.70
23	0	96	PHE	CB-CG-CD1	-5.66	116.84	120.80
23	0	90	TYR	CG-CD2-CE2	-5.65	116.78	121.30
21	V	284	CYS	CA-CB-SG	-5.64	103.84	114.00
23	0	183	TYR	CD1-CE1-CZ	5.64	124.88	119.80
28	Y	24	DC	C6-N1-C1'	5.64	127.57	120.80
22	W	334	ARG	NE-CZ-NH2	-5.64	117.48	120.30
28	Y	14	DG	C4-N9-C1'	-5.63	119.17	126.50
21	V	482	PHE	CB-CG-CD1	-5.63	116.86	120.80
27	X	74	DT	C3'-C2'-C1'	-5.62	95.75	102.50
22	W	708	LEU	CB-CG-CD2	-5.62	101.45	111.00
23	0	201	LEU	CB-CG-CD1	5.62	120.55	111.00
22	W	711	ASP	CB-CG-OD1	5.61	123.35	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	540	ASP	CB-CG-OD2	-5.61	113.25	118.30
23	0	226	SER	N-CA-CB	-5.61	102.09	110.50
18	R	162	GLY	N-CA-C	5.60	127.11	113.10
28	Y	14	DG	C8-N9-C1'	5.59	134.27	127.00
21	V	430	LEU	CB-CG-CD1	5.58	120.49	111.00
22	W	722	ARG	NE-CZ-NH1	-5.58	117.51	120.30
21	V	328	PHE	C-N-CA	5.57	134.00	122.30
2	B	388	TYR	CB-CG-CD1	-5.57	117.66	121.00
21	V	640	LEU	CB-CG-CD2	5.57	120.47	111.00
22	W	270	VAL	CA-C-O	5.57	131.80	120.10
22	W	684	PHE	CB-CG-CD1	-5.57	116.90	120.80
28	Y	31	DG	O4'-C4'-C3'	5.56	109.34	106.00
22	W	207	TYR	CA-CB-CG	5.56	123.96	113.40
28	Y	23	DT	N1-C1'-C2'	5.56	123.16	112.60
22	W	616	ARG	NE-CZ-NH2	5.55	123.08	120.30
21	V	662	LEU	CB-CG-CD2	-5.55	101.57	111.00
21	V	571	TYR	CG-CD2-CE2	-5.55	116.86	121.30
13	M	42	GLY	N-CA-C	5.54	126.96	113.10
21	V	634	ARG	CD-NE-CZ	5.53	131.34	123.60
23	0	183	TYR	CG-CD1-CE1	-5.53	116.88	121.30
21	V	393	THR	O-C-N	-5.52	113.86	122.70
22	W	625	TYR	CZ-CE2-CD2	-5.52	114.83	119.80
28	Y	28	DT	C6-N1-C1'	5.52	128.68	120.40
21	V	362	LEU	CB-CG-CD1	-5.52	101.61	111.00
21	V	608	SER	O-C-N	-5.52	113.87	122.70
21	V	571	TYR	CB-CG-CD1	-5.52	117.69	121.00
22	W	177	LEU	CB-CG-CD1	5.52	120.38	111.00
27	X	65	DG	N1-C6-O6	-5.52	116.59	119.90
21	V	325	ARG	NE-CZ-NH1	5.51	123.06	120.30
21	V	419	ARG	NH1-CZ-NH2	-5.51	113.34	119.40
23	0	65	VAL	CA-CB-CG1	5.50	119.15	110.90
1	A	1090	LEU	CB-CG-CD2	-5.50	101.65	111.00
21	V	425	ARG	NE-CZ-NH1	5.49	123.05	120.30
28	Y	17	DG	P-O3'-C3'	5.49	126.29	119.70
21	V	679	PHE	CG-CD1-CE1	-5.47	114.78	120.80
22	W	253	ARG	NH1-CZ-NH2	-5.47	113.38	119.40
22	W	258	ARG	NE-CZ-NH1	5.46	123.03	120.30
27	X	65	DG	C4'-C3'-O3'	5.46	123.35	109.70
22	W	224	GLU	OE1-CD-OE2	-5.46	116.75	123.30
21	V	655	TYR	CB-CG-CD1	5.45	124.27	121.00
22	W	141	TYR	CG-CD2-CE2	5.44	125.65	121.30
21	V	272	VAL	CA-CB-CG2	-5.44	102.74	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	W	285	TYR	CB-CG-CD1	-5.44	117.74	121.00
22	W	280	ARG	NE-CZ-NH2	5.44	123.02	120.30
27	X	74	DT	O4'-C1'-N1	5.44	111.81	108.00
21	V	382	SER	N-CA-CB	-5.43	102.36	110.50
22	W	690	ARG	CD-NE-CZ	5.42	131.18	123.60
21	V	702	ALA	N-CA-CB	-5.41	102.52	110.10
22	W	595	ILE	CB-CA-C	5.41	122.42	111.60
1	A	1402	CYS	CA-CB-SG	-5.41	104.27	114.00
27	X	62	DG	OP1-P-O3'	5.41	117.09	105.20
22	W	205	VAL	CA-CB-CG1	5.40	119.00	110.90
22	W	207	TYR	CB-CG-CD2	-5.40	117.76	121.00
22	W	631	ARG	NH1-CZ-NH2	-5.39	113.47	119.40
22	W	196	ARG	CD-NE-CZ	5.38	131.13	123.60
21	V	289	TYR	CG-CD2-CE2	-5.38	117.00	121.30
27	X	62	DG	P-O3'-C3'	5.37	126.15	119.70
1	A	614	ASP	C-N-CA	-5.37	108.27	121.70
23	0	90	TYR	CB-CG-CD1	5.37	124.22	121.00
21	V	319	TYR	CB-CG-CD1	-5.37	117.78	121.00
21	V	479	ASP	CB-CG-OD2	5.37	123.13	118.30
28	Y	11	DT	O4'-C4'-C3'	5.36	109.22	106.00
22	W	540	THR	O-C-N	-5.36	114.13	122.70
27	X	80	DC	O4'-C4'-C3'	-5.36	102.36	104.50
22	W	663	CYS	CA-CB-SG	-5.35	104.38	114.00
23	0	125	ARG	NE-CZ-NH2	-5.34	117.63	120.30
28	Y	31	DG	N1-C6-O6	-5.34	116.69	119.90
22	W	287	ARG	NH1-CZ-NH2	-5.34	113.53	119.40
27	X	81	DG	C4'-C3'-C2'	-5.33	98.30	103.10
22	W	33	ASP	CB-CG-OD2	5.31	123.08	118.30
22	W	286	ARG	NH1-CZ-NH2	-5.31	113.56	119.40
21	V	560	VAL	CA-CB-CG2	5.30	118.86	110.90
25	2	35	TYR	CB-CA-C	5.30	121.00	110.40
22	W	696	TRP	CB-CG-CD2	5.29	133.47	126.60
25	2	61	PHE	CB-CG-CD2	-5.28	117.11	120.80
22	W	623	VAL	CG1-CB-CG2	-5.27	102.47	110.90
21	V	666	ASP	CB-CG-OD1	-5.27	113.56	118.30
21	V	703	PHE	CG-CD1-CE1	-5.27	115.00	120.80
22	W	162	ASP	CB-CG-OD2	5.27	123.04	118.30
23	0	64	VAL	CA-CB-CG1	5.25	118.77	110.90
23	0	207	VAL	CA-CB-CG1	5.25	118.77	110.90
25	2	457	ARG	NE-CZ-NH1	5.24	122.92	120.30
25	2	389	ASP	CB-CG-OD1	-5.23	113.59	118.30
23	0	213	ARG	NH1-CZ-NH2	-5.22	113.66	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	V	325	ARG	CD-NE-CZ	5.22	130.91	123.60
28	Y	19	DC	P-O5'-C5'	5.21	129.24	120.90
23	0	58	MET	O-C-N	5.21	131.04	122.70
22	W	617	ALA	N-CA-CB	5.21	117.39	110.10
22	W	449	GLU	OE1-CD-OE2	-5.20	117.06	123.30
22	W	686	ARG	NE-CZ-NH2	-5.20	117.70	120.30
23	0	131	LEU	CB-CG-CD1	5.20	119.83	111.00
21	V	478	VAL	CA-CB-CG2	-5.20	103.11	110.90
11	K	67	LEU	CA-CB-CG	-5.19	103.36	115.30
28	Y	30	DG	N1-C6-O6	-5.19	116.79	119.90
27	X	37	DT	C1'-O4'-C4'	-5.19	104.91	110.10
22	W	468	PRO	CA-N-CD	-5.18	104.24	111.50
1	A	807	LEU	CB-CG-CD2	-5.18	102.19	111.00
22	W	461	LEU	CA-CB-CG	5.18	127.21	115.30
22	W	695	ARG	NE-CZ-NH2	5.18	122.89	120.30
22	W	283	ASP	CB-CG-OD2	5.18	122.96	118.30
22	W	696	TRP	CB-CG-CD1	-5.17	120.28	127.00
27	X	64	DC	N3-C4-C5	5.17	123.97	121.90
22	W	94	TYR	CB-CG-CD2	5.17	124.10	121.00
28	Y	29	DC	P-O3'-C3'	5.16	125.89	119.70
21	V	415	HIS	CG-CD2-NE2	-5.15	99.41	109.20
22	W	253	ARG	NE-CZ-NH2	5.15	122.87	120.30
1	A	133	SER	N-CA-C	5.14	124.88	111.00
17	Q	172	ASP	N-CA-C	5.14	124.88	111.00
21	V	332	ARG	CA-CB-CG	5.12	124.67	113.40
22	W	61	ARG	NE-CZ-NH1	5.12	122.86	120.30
22	W	714	VAL	CA-CB-CG2	5.12	118.59	110.90
23	0	62	TYR	CB-CG-CD1	5.12	124.07	121.00
27	X	77	DC	O4'-C1'-N1	-5.12	104.41	108.00
2	B	751	LEU	CB-CG-CD1	-5.12	102.30	111.00
21	V	362	LEU	CB-CG-CD2	5.12	119.70	111.00
21	V	250	ASP	CB-CG-OD1	5.12	122.90	118.30
28	Y	28	DT	C2-N1-C1'	-5.11	110.02	118.20
27	X	73	DG	C1'-O4'-C4'	-5.11	104.99	110.10
21	V	644	LEU	CB-CG-CD2	-5.11	102.31	111.00
21	V	434	GLU	OE1-CD-OE2	5.10	129.43	123.30
22	W	288	LEU	O-C-N	-5.10	114.53	122.70
23	0	228	TYR	CB-CG-CD2	-5.09	117.94	121.00
22	W	24	TYR	CB-CG-CD2	-5.08	117.95	121.00
21	V	398	ASP	CB-CG-OD1	5.08	122.87	118.30
22	W	600	ALA	N-CA-CB	-5.07	103.00	110.10
22	W	636	ARG	CD-NE-CZ	5.07	130.70	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	486	LEU	CA-CB-CG	-5.06	103.67	115.30
22	W	439	ASP	CB-CG-OD2	5.06	122.85	118.30
22	W	676	LEU	CB-CG-CD2	5.05	119.58	111.00
21	V	679	PHE	CB-CG-CD1	-5.05	117.27	120.80
23	0	90	TYR	CZ-CE2-CD2	5.05	124.34	119.80
21	V	289	TYR	CZ-CE2-CD2	5.04	124.34	119.80
22	W	143	ARG	NH1-CZ-NH2	-5.04	113.86	119.40
21	V	344	ALA	CB-CA-C	5.03	117.65	110.10
27	X	65	DG	C4'-C3'-C2'	-5.03	98.57	103.10
22	W	599	VAL	CA-CB-CG1	5.03	118.44	110.90
21	V	374	TRP	O-C-N	-5.02	114.66	122.70
22	W	463	PRO	N-CA-CB	5.02	109.33	103.30
22	W	87	LEU	CB-CA-C	5.02	119.74	110.20
1	A	894	ASP	CB-CG-OD1	5.02	122.81	118.30
21	V	361	CYS	N-CA-CB	-5.01	101.58	110.60
21	V	607	ILE	CA-CB-CG1	5.01	120.52	111.00
26	3	210	THR	CA-CB-CG2	-5.01	105.39	112.40
1	A	655	ILE	CG1-CB-CG2	-5.01	100.38	111.40
22	W	346	VAL	CA-CB-CG2	5.01	118.41	110.90
23	0	224	ASP	N-CA-CB	-5.01	101.59	110.60

There are no chirality outliers.

All (79) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
23	0	143	PRO	Mainchain
23	0	165	ARG	Sidechain
24	1	17	LYS	Mainchain
25	2	389	ASP	Sidechain,Mainchain
25	2	399	ASP	Sidechain
25	2	403	PHE	Mainchain,Peptide
25	2	406	GLY	Peptide
25	2	409	TYR	Sidechain
25	2	425	ALA	Mainchain
1	A	1291	ASN	Sidechain
1	A	210	GLN	Mainchain
8	H	99	ILE	Peptide
15	O	86	GLU	Sidechain
16	P	242	GLN	Sidechain
17	Q	112	ARG	Sidechain
17	Q	125	ALA	Peptide
18	R	100	ASP	Sidechain

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Mol	Chain	Res	Type	Group
18	R	105	GLU	Sidechain
18	R	109	LEU	Mainchain
18	R	139	PHE	Mainchain,Peptide
18	R	204	ASN	Mainchain
18	R	209	GLN	Sidechain
18	R	213	ASP	Sidechain,Peptide
18	R	215	GLU	Mainchain
18	R	222	SER	Peptide
18	R	223	VAL	Mainchain,Peptide
18	R	224	THR	Mainchain,Peptide
18	R	225	VAL	Mainchain
18	R	228	MET	Mainchain,Peptide
18	R	229	ASP	Sidechain
18	R	235	GLU	Sidechain
20	T	123	ASN	Peptide
21	V	247	ASP	Mainchain
21	V	251	PHE	Sidechain
21	V	319	TYR	Sidechain
21	V	378	PHE	Sidechain
21	V	417	THR	Peptide
21	V	427	MET	Mainchain,Peptide
21	V	489	TYR	Sidechain
21	V	503	ALA	Peptide
21	V	519	TYR	Sidechain
21	V	530	ARG	Sidechain
21	V	534	TYR	Sidechain
21	V	674	THR	Mainchain
21	V	676	ARG	Sidechain
21	V	679	PHE	Sidechain
21	V	703	PHE	Sidechain
22	W	104	PHE	Sidechain
22	W	175	TYR	Sidechain
22	W	197	TYR	Sidechain
22	W	206	VAL	Mainchain
22	W	208	SER	Mainchain
22	W	211	TYR	Sidechain
22	W	282	ARG	Sidechain
22	W	286	ARG	Sidechain
22	W	293	ARG	Sidechain
22	W	409	THR	Peptide
22	W	553	TYR	Sidechain
22	W	614	TYR	Sidechain

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Mol	Chain	Res	Type	Group
22	W	616	ARG	Sidechain
22	W	641	ARG	Sidechain
22	W	669	ARG	Sidechain
22	W	674	TYR	Sidechain
22	W	719	TYR	Sidechain
22	W	72	TYR	Sidechain
27	X	65	DG	Sidechain
27	X	66	DA	Sidechain
27	X	72	DC	Sidechain
28	Y	23	DT	Sidechain
28	Y	24	DC	Sidechain
28	Y	26	DG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11515	0	11608	512	0
2	B	9317	0	9307	414	0
3	C	2213	0	2153	98	0
4	D	1062	0	1042	15	0
5	E	1723	0	1745	65	0
6	F	689	0	715	11	0
7	G	1351	0	1358	42	0
8	H	1205	0	1167	48	0
9	I	1013	0	930	78	0
10	J	533	0	553	39	0
11	K	937	0	959	25	0
12	L	388	0	393	24	0
13	M	2391	0	2410	164	0
14	N	930	0	888	34	0
15	O	806	0	818	25	0
16	P	1462	0	1548	53	0
17	Q	1484	0	1498	212	0
18	R	1357	0	1381	224	0
19	S	1138	0	1103	42	0
20	T	1788	0	1819	92	0
21	V	3855	0	3871	131	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	W	5348	0	5373	122	0
23	0	1479	0	1524	43	0
24	1	491	0	507	228	0
25	2	2196	0	2206	571	0
26	3	1526	0	1561	461	0
27	X	1710	0	941	67	0
28	Y	1681	0	932	56	0
29	Z	125	0	67	10	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
All	All	61725	0	60377	3159	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 26.

All (3159) 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)
26:3:59:VAL:HG12	26:3:71:TYR:CD1	1.24	1.66
21:V:516:PRO:CG	24:1:15:ALA:HB3	1.21	1.65
1:A:1171:ALA:CB	9:I:59:THR:HG21	1.18	1.59
18:R:223:VAL:CG2	18:R:224:THR:HG21	1.29	1.59
21:V:315:VAL:HG13	22:W:500:ASP:CB	1.21	1.57
13:M:34:CYS:CB	13:M:39:LEU:HD23	1.28	1.56
26:3:59:VAL:CG1	26:3:71:TYR:HD1	1.15	1.56
23:0:54:ARG:HG3	26:3:182:PHE:CE1	1.42	1.55
18:R:223:VAL:CA	18:R:224:THR:HG23	1.09	1.53
25:2:31:LEU:HD11	26:3:33:THR:CB	1.39	1.52
21:V:516:PRO:HG3	24:1:15:ALA:CB	1.11	1.52
13:M:34:CYS:HB3	13:M:39:LEU:CD2	1.35	1.51
16:P:206:GLU:HB3	16:P:207:PRO:CD	1.34	1.50
1:A:202:TRP:CD1	1:A:212:LYS:HE2	1.47	1.47
1:A:1171:ALA:HB1	9:I:59:THR:CG2	1.42	1.47
21:V:315:VAL:CG1	22:W:500:ASP:HB2	1.01	1.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:223:VAL:CG2	18:R:224:THR:CG2	1.84	1.46
25:2:117:ASN:ND2	26:3:108:ASN:CB	1.76	1.46
3:C:157:GLN:NE2	10:J:65:LEU:HB3	1.29	1.45
25:2:117:ASN:HD21	26:3:108:ASN:CB	1.27	1.45
13:M:37:CYS:SG	13:M:39:LEU:HD22	1.53	1.45
25:2:31:LEU:HD11	26:3:33:THR:CG2	1.42	1.44
25:2:28:PRO:N	26:3:25:GLN:HA	1.29	1.43
17:Q:113:ARG:NE	18:R:222:SER:HB3	1.24	1.42
21:V:321:GLU:HB3	22:W:499:ASN:ND2	1.25	1.42
17:Q:113:ARG:HE	18:R:222:SER:CB	1.33	1.41
5:E:40:PHE:CE2	5:E:46:ASP:OD2	1.72	1.40
21:V:321:GLU:HB3	22:W:499:ASN:CG	1.38	1.40
25:2:117:ASN:CG	26:3:108:ASN:HB2	1.39	1.39
23:0:54:ARG:CG	26:3:182:PHE:HE1	1.35	1.38
1:A:1171:ALA:CB	9:I:59:THR:CG2	1.95	1.38
25:2:29:GLY:N	26:3:25:GLN:HG3	1.32	1.37
17:Q:180:PHE:CE2	18:R:213:ASP:OD1	1.76	1.37
18:R:223:VAL:CA	18:R:224:THR:CG2	1.75	1.36
27:X:15:DA:H61	28:Y:79:DC:N4	1.23	1.35
25:2:31:LEU:HD21	26:3:33:THR:N	1.34	1.34
25:2:117:ASN:OD1	26:3:108:ASN:ND2	1.57	1.34
17:Q:188:TYR:CE2	18:R:210:PHE:CD1	2.15	1.34
25:2:30:VAL:HG23	26:3:25:GLN:CB	1.57	1.33
1:A:202:TRP:CD1	1:A:212:LYS:CE	2.11	1.33
1:A:152:ASN:O	1:A:153:ILE:CG1	1.75	1.33
21:V:325:ARG:NH2	22:W:499:ASN:HB3	1.02	1.32
25:2:118:LEU:CD2	26:3:39:ASP:OD1	1.75	1.32
27:X:15:DA:N6	28:Y:79:DC:H42	1.25	1.32
21:V:615:PHE:O	21:V:617:LEU:N	1.60	1.32
25:2:118:LEU:HD22	26:3:39:ASP:OD1	1.16	1.31
24:1:1:MET:O	25:2:413:LEU:HG	1.28	1.30
21:V:321:GLU:HB3	22:W:499:ASN:OD1	1.30	1.30
18:R:194:ARG:HB3	18:R:195:PRO:CD	1.57	1.30
13:M:178:LYS:O	20:T:154:LYS:HB3	1.22	1.30
17:Q:113:ARG:HD3	18:R:221:ARG:C	1.50	1.30
18:R:194:ARG:CB	18:R:195:PRO:HD3	1.58	1.29
25:2:28:PRO:N	26:3:25:GLN:CA	1.94	1.29
1:A:1171:ALA:CA	9:I:59:THR:CG2	2.09	1.28
21:V:321:GLU:CB	22:W:499:ASN:HD21	1.45	1.28
1:A:202:TRP:CB	1:A:212:LYS:HB3	1.64	1.28
21:V:325:ARG:NH2	22:W:499:ASN:CB	1.97	1.27

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:103:ARG:O	9:I:105:GLU:N	1.66	1.27
17:Q:188:TYR:CE2	18:R:210:PHE:HD1	1.51	1.26
17:Q:21:VAL:O	18:R:210:PHE:CE2	1.87	1.26
25:2:118:LEU:HD21	26:3:39:ASP:O	1.23	1.25
25:2:30:VAL:CG2	26:3:25:GLN:HB3	1.66	1.25
23:0:97:ASP:O	26:3:208:ASP:HB3	1.12	1.25
18:R:223:VAL:C	18:R:224:THR:HG23	1.52	1.24
21:V:523:VAL:HG11	24:1:20:LEU:CD2	1.64	1.24
26:3:59:VAL:CG1	26:3:71:TYR:CD1	1.98	1.24
21:V:321:GLU:OE2	22:W:500:ASP:CB	1.85	1.24
1:A:202:TRP:CG	1:A:212:LYS:HD2	1.71	1.24
18:R:223:VAL:HB	18:R:224:THR:CB	1.68	1.24
2:B:51:ILE:O	20:T:141:LEU:HD23	1.34	1.23
13:M:34:CYS:CB	13:M:39:LEU:CD2	2.03	1.23
17:Q:113:ARG:CD	18:R:221:ARG:C	2.06	1.23
17:Q:113:ARG:HD3	18:R:221:ARG:O	1.36	1.23
5:E:7:THR:OG1	5:E:47:LYS:HD3	1.35	1.23
22:W:59:TYR:CZ	22:W:62:ALA:CB	2.21	1.22
21:V:321:GLU:CB	22:W:499:ASN:OD1	1.88	1.22
26:3:58:ALA:N	26:3:71:TYR:OH	1.74	1.21
25:2:31:LEU:CD1	26:3:33:THR:HB	1.69	1.21
21:V:674:THR:HG23	25:2:392:ARG:NH2	1.53	1.21
17:Q:188:TYR:CZ	18:R:210:PHE:CD1	2.29	1.21
2:B:56:GLN:CG	20:T:140:ARG:HG3	1.68	1.20
17:Q:180:PHE:HE2	18:R:213:ASP:OD1	1.05	1.20
17:Q:113:ARG:HD2	18:R:221:ARG:CB	1.70	1.20
22:W:209:TYR:OH	22:W:233:PHE:HA	1.37	1.20
16:P:297:LYS:HB3	16:P:298:PRO:CD	1.71	1.19
24:1:59:GLU:OE2	25:2:402:ARG:NH2	1.75	1.19
22:W:59:TYR:CZ	22:W:62:ALA:HB1	1.76	1.19
1:A:202:TRP:HB2	1:A:212:LYS:CB	1.71	1.19
1:A:1098:PRO:O	1:A:1101:GLN:NE2	1.74	1.18
21:V:516:PRO:CG	24:1:15:ALA:CB	1.91	1.18
17:Q:188:TYR:CZ	18:R:210:PHE:HD1	1.61	1.18
26:3:66:GLU:HA	26:3:132:LEU:HD12	1.22	1.18
2:B:880:LEU:O	2:B:881:GLU:HB2	1.37	1.17
25:2:31:LEU:CD1	26:3:33:THR:CG2	2.21	1.17
2:B:225:LEU:HB3	2:B:228:SER:CB	1.73	1.17
25:2:117:ASN:ND2	26:3:108:ASN:HB2	0.85	1.16
2:B:225:LEU:CB	2:B:228:SER:HB3	1.76	1.16
10:J:63:ALA:HB3	10:J:64:PRO:HD3	1.17	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:V:325:ARG:HH22	22:W:499:ASN:CB	1.55	1.16
25:2:30:VAL:HB	26:3:25:GLN:O	1.46	1.16
26:3:57:LEU:O	26:3:71:TYR:HE2	1.28	1.16
16:P:206:GLU:HB3	16:P:207:PRO:HD2	1.17	1.16
1:A:1171:ALA:CA	9:I:59:THR:HG22	1.73	1.16
17:Q:113:ARG:CZ	18:R:222:SER:HB3	1.76	1.16
1:A:608:THR:C	1:A:610:PRO:HD2	1.66	1.16
24:1:2:VAL:CG1	25:2:456:LYS:HG2	1.74	1.16
13:M:37:CYS:SG	13:M:39:LEU:CD2	2.34	1.16
21:V:613:THR:O	21:V:614:SER:HB2	1.44	1.15
25:2:211:GLN:HG3	25:2:257:SER:HB3	1.28	1.15
23:0:77:LYS:HB2	23:0:83:CYS:HB2	1.18	1.15
24:1:28:ALA:HB1	24:1:31:LYS:HD2	1.27	1.14
1:A:206:ASN:O	1:A:207:GLU:CB	1.92	1.14
5:E:47:LYS:HB3	5:E:48:PRO:HD3	1.23	1.14
17:Q:23:ARG:NH2	18:R:207:SER:O	1.78	1.14
8:H:107:GLU:O	8:H:108:ALA:O	1.66	1.14
24:1:1:MET:CG	25:2:413:LEU:HB3	1.76	1.14
16:P:206:GLU:CB	16:P:207:PRO:CD	2.25	1.14
2:B:56:GLN:HG2	20:T:140:ARG:CG	1.77	1.13
21:V:321:GLU:CB	22:W:499:ASN:ND2	2.05	1.13
22:W:419:GLU:HB3	22:W:420:PRO:CD	1.77	1.13
21:V:516:PRO:HB3	24:1:15:ALA:HB1	1.25	1.13
26:3:59:VAL:N	26:3:71:TYR:CE1	2.15	1.13
24:1:2:VAL:HG13	25:2:422:LEU:HD11	1.20	1.13
23:0:54:ARG:CG	26:3:182:PHE:CE1	2.17	1.13
22:W:59:TYR:CE2	22:W:62:ALA:CB	2.32	1.12
16:P:206:GLU:HB3	16:P:207:PRO:HD3	1.18	1.12
1:A:156:GLY:HA2	1:A:181:HIS:ND1	1.62	1.12
24:1:9:LEU:HD13	24:1:48:GLU:HA	1.32	1.12
26:3:33:THR:HG23	26:3:36:LYS:H	1.13	1.12
1:A:426:ARG:O	13:M:40:VAL:HG22	1.49	1.12
2:B:225:LEU:HD13	2:B:228:SER:OG	1.49	1.12
2:B:133:ILE:HG23	2:B:139:GLN:HG2	1.29	1.11
17:Q:113:ARG:NE	18:R:222:SER:CB	1.97	1.11
24:1:5:LEU:CD2	25:2:408:LEU:HD13	1.80	1.11
17:Q:187:ILE:HG21	18:R:211:SER:HA	1.20	1.10
17:Q:187:ILE:HG22	18:R:210:PHE:O	1.49	1.10
18:R:194:ARG:O	18:R:196:ASP:N	1.84	1.10
18:R:223:VAL:CG1	18:R:224:THR:CG2	2.30	1.10
25:2:192:GLU:HG3	25:2:193:PRO:HD2	1.33	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:2:42:LEU:HD21	25:2:55:TRP:HB2	1.20	1.10
25:2:31:LEU:CD1	26:3:33:THR:CB	2.27	1.10
17:Q:188:TYR:OH	18:R:210:PHE:CE1	2.02	1.10
24:1:5:LEU:HD11	25:2:408:LEU:HB3	1.17	1.09
24:1:2:VAL:HG11	25:2:456:LYS:CG	1.81	1.09
21:V:315:VAL:CG1	22:W:500:ASP:CB	1.94	1.09
1:A:118:LEU:HD21	1:A:151:LYS:O	1.48	1.09
1:A:426:ARG:HB3	13:M:40:VAL:HG21	1.31	1.09
25:2:160:LEU:HD23	25:2:206:LEU:HD21	1.25	1.09
1:A:206:ASN:O	1:A:207:GLU:HB2	1.34	1.09
2:B:879:GLU:O	2:B:880:LEU:HB2	1.32	1.09
24:1:18:GLN:HB2	24:1:44:PHE:CE2	1.86	1.09
26:3:137:LEU:HB3	26:3:180:VAL:HG11	1.34	1.09
17:Q:113:ARG:NH1	18:R:218:LYS:O	1.86	1.09
18:R:194:ARG:CB	18:R:195:PRO:CD	2.20	1.09
25:2:31:LEU:HD11	26:3:33:THR:HB	1.15	1.09
21:V:321:GLU:OE2	22:W:500:ASP:HB3	0.91	1.09
21:V:516:PRO:CB	24:1:15:ALA:HB1	1.81	1.08
26:3:59:VAL:HB	26:3:71:TYR:CE1	1.89	1.08
25:2:171:VAL:HG22	25:2:213:TRP:HA	1.27	1.08
2:B:225:LEU:CB	2:B:228:SER:CB	2.31	1.08
25:2:159:VAL:HG13	25:2:161:HIS:H	1.16	1.08
8:H:64:LEU:HB3	8:H:84:ARG:HD3	1.14	1.08
24:1:5:LEU:HD21	25:2:408:LEU:CD1	1.82	1.08
25:2:28:PRO:N	26:3:25:GLN:C	2.07	1.08
1:A:152:ASN:O	1:A:153:ILE:HG12	0.91	1.08
8:H:64:LEU:HB3	8:H:84:ARG:CD	1.84	1.08
17:Q:188:TYR:OH	18:R:210:PHE:CD1	2.07	1.08
1:A:202:TRP:CD1	1:A:212:LYS:HD2	1.89	1.07
24:1:13:ASP:CG	24:1:14:PRO:HD2	1.74	1.07
26:3:59:VAL:HG13	26:3:70:LEU:HB2	1.27	1.07
26:3:49:LEU:HB3	26:3:101:TYR:HB3	1.14	1.07
24:1:2:VAL:HG11	25:2:456:LYS:HG2	1.09	1.07
26:3:57:LEU:C	26:3:71:TYR:OH	1.93	1.07
23:0:97:ASP:O	26:3:208:ASP:CB	2.02	1.06
1:A:1171:ALA:HA	9:I:59:THR:HG22	1.08	1.06
2:B:225:LEU:HB3	2:B:228:SER:HB2	1.32	1.06
22:W:424:ARG:O	22:W:425:THR:HG23	1.52	1.06
23:0:54:ARG:HB2	26:3:209:ILE:HG23	1.36	1.06
1:A:202:TRP:CD1	1:A:212:LYS:CD	2.37	1.06
1:A:1117:VAL:O	1:A:1119:LEU:N	1.87	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:LYS:O	1:A:204:HIS:HB2	1.39	1.06
17:Q:184:ILE:HD11	18:R:213:ASP:CG	1.76	1.06
25:2:234:LEU:HD21	25:2:237:LEU:HD12	1.36	1.06
1:A:131:ALA:O	1:A:133:SER:N	1.87	1.06
24:1:1:MET:CB	25:2:413:LEU:HB3	1.86	1.05
22:W:419:GLU:CB	22:W:420:PRO:HD2	1.78	1.05
21:V:674:THR:HG23	25:2:392:ARG:CZ	1.85	1.05
3:C:157:GLN:CD	10:J:65:LEU:HB3	1.76	1.05
17:Q:184:ILE:HD13	18:R:211:SER:HB2	1.36	1.04
24:1:4:VAL:HG12	25:2:411:GLN:O	1.55	1.04
26:3:57:LEU:O	26:3:71:TYR:CE2	2.10	1.04
17:Q:110:MET:HG2	18:R:222:SER:HB2	1.08	1.04
25:2:28:PRO:CD	26:3:25:GLN:HA	1.88	1.03
1:A:609:HIS:N	1:A:610:PRO:HD2	1.72	1.03
16:P:297:LYS:CB	16:P:298:PRO:CD	2.34	1.03
13:M:179:GLU:HA	20:T:154:LYS:HG2	1.38	1.03
1:A:1116:ASN:HD21	1:A:1138:SER:HB3	1.20	1.03
1:A:265:VAL:C	1:A:272:ASN:CG	2.17	1.03
17:Q:187:ILE:HG21	18:R:211:SER:CA	1.88	1.03
24:1:5:LEU:HD12	25:2:409:TYR:O	1.56	1.03
25:2:81:LYS:HE3	25:2:93:LEU:HD21	1.40	1.03
21:V:523:VAL:HG11	24:1:20:LEU:HD21	1.06	1.03
17:Q:113:ARG:HD2	18:R:221:ARG:HB2	1.32	1.03
13:M:94:ASP:OD2	13:M:97:GLY:O	1.76	1.02
23:0:54:ARG:CD	26:3:182:PHE:HE1	1.72	1.02
1:A:273:GLN:O	1:A:274:ASP:O	1.76	1.02
23:0:54:ARG:NE	26:3:182:PHE:CE1	2.26	1.02
25:2:31:LEU:HD11	26:3:33:THR:HG22	1.37	1.02
3:C:157:GLN:NE2	10:J:65:LEU:CB	2.23	1.02
16:P:297:LYS:HB3	16:P:298:PRO:HD3	1.06	1.02
17:Q:188:TYR:CE1	18:R:211:SER:HB3	1.93	1.02
21:V:516:PRO:CB	24:1:15:ALA:CB	2.37	1.02
25:2:199:ALA:HB3	25:2:202:GLN:HE22	1.22	1.01
21:V:315:VAL:HG11	22:W:500:ASP:HB2	1.42	1.01
13:M:178:LYS:O	20:T:154:LYS:CB	2.07	1.01
26:3:196:LEU:HD21	26:3:223:LEU:HD23	1.42	1.01
22:W:59:TYR:CE2	22:W:62:ALA:HB3	1.94	1.01
26:3:59:VAL:CB	26:3:71:TYR:CE1	2.44	1.01
13:M:46:ILE:O	13:M:47:ASP:HB2	1.54	1.01
21:V:515:SER:HB3	21:V:539:ASN:HD21	1.26	1.01
24:1:34:ILE:HG12	24:1:50:VAL:HG11	1.39	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:875:GLU:O	2:B:876:ASN:HB2	1.57	1.00
13:M:94:ASP:HB2	13:M:99:SER:H	1.26	1.00
22:W:419:GLU:HB3	22:W:420:PRO:HD2	1.03	1.00
1:A:1171:ALA:HB2	9:I:59:THR:HG21	1.41	1.00
26:3:58:ALA:CA	26:3:71:TYR:CZ	2.44	1.00
1:A:67:ARG:NH2	13:M:45:VAL:O	1.94	1.00
16:P:298:PRO:O	16:P:300:ILE:HG12	1.61	1.00
17:Q:20:TYR:O	18:R:210:PHE:CD2	2.14	1.00
9:I:59:THR:O	9:I:60:HIS:CG	2.14	1.00
1:A:265:VAL:N	1:A:272:ASN:HB3	1.76	1.00
17:Q:105:TYR:OH	18:R:234:GLU:OE1	1.80	1.00
26:3:59:VAL:HB	26:3:71:TYR:HE1	1.24	1.00
1:A:265:VAL:N	1:A:272:ASN:CB	2.25	1.00
2:B:225:LEU:HB2	2:B:228:SER:HB3	1.39	1.00
17:Q:113:ARG:CD	18:R:222:SER:N	2.25	1.00
1:A:211:GLU:O	1:A:212:LYS:HB2	1.62	0.99
16:P:206:GLU:CB	16:P:207:PRO:HD3	1.88	0.99
1:A:263:ALA:O	1:A:265:VAL:N	1.96	0.99
22:W:209:TYR:OH	22:W:233:PHE:CA	2.09	0.99
2:B:225:LEU:O	2:B:227:ASN:N	1.94	0.99
25:2:117:ASN:CG	26:3:108:ASN:CB	2.20	0.99
18:R:223:VAL:CG1	18:R:224:THR:HG21	1.93	0.99
13:M:94:ASP:CB	13:M:99:SER:H	1.76	0.99
1:A:1171:ALA:HA	9:I:59:THR:CG2	1.80	0.98
10:J:63:ALA:CB	10:J:64:PRO:HD3	1.89	0.98
1:A:79:THR:HG21	13:M:43:ASP:HB2	1.46	0.98
25:2:196:ILE:HD11	25:2:210:ALA:HB2	1.45	0.98
1:A:133:SER:O	1:A:135:GLY:N	1.94	0.98
17:Q:188:TYR:HE2	18:R:210:PHE:CD1	1.76	0.98
25:2:100:LEU:HD11	25:2:119:ARG:HG3	1.46	0.98
25:2:118:LEU:CD2	26:3:39:ASP:O	2.12	0.98
22:W:584:TYR:CD1	22:W:594:ALA:HB2	1.99	0.98
13:M:34:CYS:HB3	13:M:39:LEU:CG	1.94	0.98
25:2:29:GLY:N	26:3:25:GLN:CG	2.27	0.97
26:3:165:LYS:HD2	26:3:195:VAL:HG22	1.44	0.97
5:E:47:LYS:CB	5:E:48:PRO:HD3	1.94	0.97
13:M:34:CYS:SG	13:M:39:LEU:HD23	2.02	0.97
18:R:223:VAL:HG21	18:R:224:THR:HG21	1.47	0.97
1:A:1116:ASN:O	1:A:1117:VAL:HG23	1.64	0.97
1:A:265:VAL:O	1:A:272:ASN:OD1	1.81	0.97
23:0:77:LYS:CB	23:0:83:CYS:HB2	1.95	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:2:176:ALA:HB1	25:2:178:LEU:HD13	1.47	0.97
17:Q:113:ARG:CZ	18:R:218:LYS:O	2.13	0.97
26:3:173:GLN:HA	26:3:176:ASN:HD21	1.28	0.96
13:M:34:CYS:CB	13:M:39:LEU:CG	2.42	0.96
26:3:59:VAL:CB	26:3:71:TYR:CD1	2.48	0.96
17:Q:184:ILE:HD12	18:R:218:LYS:NZ	1.81	0.96
23:0:77:LYS:HA	23:0:77:LYS:HE3	1.43	0.96
26:3:133:LEU:HD23	26:3:177:PHE:CD1	2.01	0.96
22:W:59:TYR:CE1	22:W:62:ALA:HB1	2.01	0.96
1:A:156:GLY:HA2	1:A:181:HIS:CG	2.01	0.96
21:V:321:GLU:CA	22:W:499:ASN:HD21	1.78	0.96
21:V:612:ASP:OD2	21:V:635:GLN:OE1	1.83	0.95
22:W:209:TYR:HH	22:W:233:PHE:HA	1.30	0.95
25:2:118:LEU:HD11	26:3:43:VAL:CG2	1.95	0.95
25:2:211:GLN:HA	25:2:261:PHE:CZ	2.01	0.95
24:1:13:ASP:OD2	24:1:17:LYS:HB3	1.65	0.95
25:2:29:GLY:CA	26:3:25:GLN:HG3	1.95	0.95
21:V:631:GLY:O	21:V:632:SER:CB	2.14	0.95
1:A:79:THR:CG2	13:M:43:ASP:HB2	1.96	0.94
24:1:1:MET:HB3	25:2:413:LEU:CG	1.98	0.94
25:2:35:TYR:CE1	25:2:62:LEU:HG	2.02	0.94
25:2:117:ASN:ND2	26:3:42:MET:HE1	1.82	0.94
24:1:2:VAL:CG1	25:2:422:LEU:HD11	1.96	0.94
25:2:117:ASN:N	26:3:104:LEU:HD21	1.83	0.94
13:M:34:CYS:HB2	13:M:39:LEU:HG	1.49	0.94
17:Q:113:ARG:NE	18:R:222:SER:CA	2.31	0.94
2:B:51:ILE:O	20:T:141:LEU:CD2	2.15	0.94
1:A:47:THR:O	1:A:48:GLU:HG2	1.68	0.94
25:2:31:LEU:CD2	26:3:33:THR:N	2.30	0.94
17:Q:24:GLY:N	18:R:210:PHE:CD2	2.35	0.94
21:V:325:ARG:HH21	22:W:499:ASN:HB3	1.19	0.94
26:3:133:LEU:H	26:3:133:LEU:HD13	1.33	0.93
17:Q:187:ILE:CG2	18:R:210:PHE:O	2.15	0.93
21:V:515:SER:CB	21:V:539:ASN:HD21	1.80	0.93
17:Q:24:GLY:CA	18:R:210:PHE:CE2	2.51	0.93
1:A:1116:ASN:ND2	1:A:1138:SER:CB	2.30	0.93
2:B:879:GLU:O	2:B:880:LEU:CB	2.16	0.93
9:I:59:THR:O	9:I:60:HIS:CB	2.17	0.93
24:1:8:VAL:HG11	24:1:45:VAL:CG1	1.99	0.93
25:2:177:GLN:HA	25:2:220:LEU:CD2	1.99	0.93
17:Q:113:ARG:HE	18:R:222:SER:CA	1.82	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:110:MET:HG2	18:R:222:SER:CB	1.98	0.93
17:Q:24:GLY:HA3	18:R:210:PHE:CD2	2.04	0.93
2:B:133:ILE:O	2:B:134:LYS:O	1.86	0.92
25:2:29:GLY:H	26:3:25:GLN:CG	1.83	0.92
1:A:202:TRP:HD1	1:A:212:LYS:HE2	0.83	0.92
24:1:9:LEU:HD22	24:1:51:ASN:HD22	1.34	0.92
26:3:11:LEU:HD22	26:3:160:ARG:HG2	1.51	0.92
26:3:187:GLN:HG3	26:3:189:ILE:HG12	1.51	0.92
26:3:148:ASN:HB2	26:3:157:MET:HE2	1.48	0.92
18:R:223:VAL:HG23	18:R:224:THR:CG2	1.98	0.92
26:3:190:LEU:HA	26:3:210:THR:HG22	1.50	0.92
17:Q:180:PHE:CE2	18:R:213:ASP:CG	2.27	0.92
21:V:516:PRO:HA	24:1:15:ALA:O	1.67	0.92
5:E:47:LYS:HB3	5:E:48:PRO:CD	1.97	0.92
24:1:18:GLN:HB2	24:1:44:PHE:HE2	1.26	0.92
26:3:165:LYS:HE3	26:3:200:SER:CB	2.00	0.92
1:A:426:ARG:O	13:M:40:VAL:CG2	2.17	0.92
25:2:118:LEU:HD23	26:3:42:MET:HB2	1.50	0.91
14:N:319:ASP:O	14:N:321:SER:N	2.03	0.91
1:A:265:VAL:H	1:A:272:ASN:HB3	1.30	0.91
25:2:159:VAL:HG22	25:2:160:LEU:HD12	1.51	0.91
20:T:142:SER:OG	20:T:143:GLN:OE1	1.87	0.91
17:Q:24:GLY:N	18:R:210:PHE:CE2	2.38	0.91
17:Q:188:TYR:CE2	18:R:210:PHE:CE1	2.58	0.91
1:A:265:VAL:HA	1:A:272:ASN:HB2	1.52	0.91
25:2:163:MET:HE2	25:2:206:LEU:HD12	1.52	0.91
25:2:81:LYS:HD2	25:2:89:LEU:HD21	1.52	0.91
1:A:202:TRP:CG	1:A:212:LYS:CD	2.52	0.91
18:R:163:LEU:O	18:R:164:GLY:C	2.05	0.91
22:W:59:TYR:CE1	22:W:62:ALA:CB	2.52	0.91
17:Q:109:HIS:CE1	18:R:225:VAL:HG21	2.05	0.91
17:Q:184:ILE:HD11	18:R:213:ASP:OD2	1.68	0.91
1:A:265:VAL:CA	1:A:272:ASN:CB	2.49	0.90
16:P:206:GLU:O	16:P:208:ARG:N	2.01	0.90
17:Q:113:ARG:HH22	18:R:218:LYS:HG2	1.34	0.90
25:2:81:LYS:CE	25:2:93:LEU:HD21	2.00	0.90
23:0:98:GLN:OE1	26:3:209:ILE:HA	1.70	0.90
2:B:880:LEU:O	2:B:881:GLU:CB	2.15	0.90
5:E:46:ASP:O	5:E:47:LYS:HB2	1.71	0.90
18:R:223:VAL:CB	18:R:224:THR:CG2	0.90	0.90
17:Q:58:GLN:OE1	18:R:194:ARG:HD2	1.71	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:0:54:ARG:HG3	26:3:182:PHE:CZ	2.05	0.90
23:0:97:ASP:OD1	26:3:208:ASP:OD1	1.88	0.90
17:Q:110:MET:CG	18:R:222:SER:HB2	1.99	0.90
26:3:137:LEU:CB	26:3:180:VAL:HG11	2.01	0.90
2:B:132:VAL:HG23	2:B:141:GLN:HG3	1.54	0.90
25:2:160:LEU:HB3	25:2:206:LEU:HD11	1.53	0.90
1:A:202:TRP:HE3	1:A:212:LYS:O	1.54	0.90
1:A:426:ARG:CB	13:M:40:VAL:HG21	2.02	0.90
17:Q:188:TYR:CE1	18:R:211:SER:CB	2.55	0.90
22:W:430:ASN:HB3	22:W:431:PRO:HD2	1.54	0.89
21:V:315:VAL:HG13	22:W:500:ASP:CA	2.03	0.89
24:1:8:VAL:HG11	24:1:45:VAL:HG13	1.55	0.89
26:3:165:LYS:HG3	26:3:203:LEU:HD12	1.52	0.89
24:1:47:ALA:CB	24:1:50:VAL:HB	2.03	0.89
26:3:177:PHE:CD2	26:3:181:ILE:HD11	2.08	0.89
3:C:132:SER:HB3	3:C:147:ASP:HB2	1.54	0.89
18:R:194:ARG:C	18:R:196:ASP:H	1.71	0.89
1:A:1171:ALA:HB1	9:I:59:THR:HG23	1.51	0.89
3:C:5:ASN:HB3	3:C:7:PRO:HD3	1.55	0.89
1:A:926:ASN:OD1	1:A:931:ARG:HG2	1.71	0.89
26:3:58:ALA:HA	26:3:71:TYR:CE2	2.08	0.88
1:A:1307:VAL:HG11	1:A:1339:ASP:HB3	1.52	0.88
24:1:4:VAL:HG11	25:2:412:PHE:HD2	1.36	0.88
26:3:70:LEU:HD13	26:3:115:ILE:HD11	1.55	0.88
3:C:157:GLN:HE21	10:J:65:LEU:HB3	1.07	0.88
26:3:177:PHE:CE2	26:3:181:ILE:HD11	2.08	0.88
26:3:71:TYR:CD2	26:3:72:PRO:HD2	2.08	0.88
25:2:117:ASN:CB	26:3:42:MET:CE	2.51	0.88
25:2:163:MET:SD	25:2:196:ILE:HG21	2.14	0.88
5:E:40:PHE:HE2	5:E:46:ASP:OD2	1.52	0.88
13:M:94:ASP:HB2	13:M:97:GLY:O	1.74	0.88
24:1:1:MET:HB3	25:2:413:LEU:CB	2.04	0.88
16:P:159:SER:HB3	16:P:329:TYR:CE2	2.08	0.88
24:1:1:MET:O	25:2:413:LEU:CG	2.21	0.88
25:2:243:SER:CB	25:2:258:LEU:HD22	2.04	0.88
1:A:929:ALA:O	1:A:931:ARG:N	2.06	0.88
1:A:265:VAL:CA	1:A:272:ASN:CG	2.35	0.88
24:1:28:ALA:CB	24:1:31:LYS:HD2	2.04	0.87
25:2:160:LEU:CB	25:2:206:LEU:HD11	2.04	0.87
25:2:118:LEU:HD11	26:3:43:VAL:HG22	1.56	0.87
1:A:265:VAL:HA	1:A:272:ASN:CB	2.04	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:49:SER:O	5:E:52:ARG:NH1	2.07	0.87
17:Q:187:ILE:HD13	18:R:211:SER:HA	1.57	0.87
21:V:523:VAL:CG1	24:1:20:LEU:CD2	2.53	0.87
25:2:160:LEU:CA	25:2:206:LEU:HD11	2.04	0.87
1:A:609:HIS:N	1:A:610:PRO:CD	2.37	0.87
2:B:549:SER:HG	2:B:577:HIS:HE2	1.19	0.87
26:3:59:VAL:CG1	26:3:70:LEU:HB2	2.03	0.87
24:1:2:VAL:HG13	25:2:422:LEU:CD1	2.03	0.87
25:2:218:GLN:HB3	25:2:264:HIS:CD2	2.08	0.87
25:2:118:LEU:HD22	26:3:39:ASP:CG	1.94	0.87
25:2:224:GLN:HB2	25:2:268:PHE:CZ	2.10	0.87
2:B:716:HIS:HD2	2:B:982:ILE:HG13	1.38	0.87
8:H:66:GLU:O	8:H:67:ASP:HB2	1.72	0.87
25:2:160:LEU:CD2	25:2:206:LEU:HD21	2.04	0.87
25:2:28:PRO:HD2	26:3:25:GLN:NE2	1.89	0.87
5:E:15:LYS:NZ	5:E:35:GLN:O	2.07	0.87
22:W:37:HIS:CE1	22:W:454:VAL:HG13	2.09	0.87
22:W:59:TYR:CG	22:W:62:ALA:HB2	2.10	0.87
24:1:1:MET:HB3	25:2:413:LEU:HB3	1.52	0.87
25:2:117:ASN:OD1	26:3:108:ASN:CB	2.23	0.87
25:2:45:PHE:HB2	25:2:51:LEU:HD13	1.56	0.87
17:Q:21:VAL:O	18:R:210:PHE:HE2	1.36	0.87
13:M:46:ILE:O	13:M:47:ASP:CB	2.21	0.87
17:Q:24:GLY:HA3	18:R:210:PHE:CE2	2.09	0.86
25:2:138:PRO:HG3	25:2:189:GLU:HG3	1.57	0.86
25:2:29:GLY:H	26:3:25:GLN:HG3	1.12	0.86
26:3:64:ILE:HG13	26:3:123:ASP:HB3	1.57	0.86
5:E:41:LYS:HA	5:E:46:ASP:HB2	1.56	0.86
25:2:221:GLN:HG2	25:2:268:PHE:CZ	2.11	0.86
1:A:1116:ASN:ND2	1:A:1138:SER:HB3	1.89	0.86
26:3:58:ALA:C	26:3:71:TYR:CZ	2.49	0.86
21:V:516:PRO:CG	24:1:15:ALA:HB1	1.96	0.86
14:N:313:PRO:HG2	16:P:235:ARG:HH22	1.41	0.86
20:T:154:LYS:H	20:T:154:LYS:HD2	1.41	0.86
26:3:69:PHE:CZ	26:3:139:LYS:HB3	2.10	0.86
17:Q:188:TYR:HE1	18:R:211:SER:CB	1.89	0.86
17:Q:113:ARG:HD2	18:R:221:ARG:C	1.90	0.86
25:2:48:LEU:HB3	25:2:49:PRO:HD3	1.57	0.86
26:3:190:LEU:HA	26:3:210:THR:CG2	2.05	0.86
26:3:165:LYS:HE3	26:3:200:SER:HB2	1.56	0.86
25:2:81:LYS:CD	25:2:89:LEU:HD21	2.05	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:3:160:ARG:HB3	26:3:190:LEU:HD21	1.57	0.85
21:V:316:LEU:HB2	21:V:321:GLU:HG3	1.58	0.85
25:2:218:GLN:HB3	25:2:264:HIS:HD2	1.38	0.85
21:V:631:GLY:O	21:V:632:SER:HB2	1.76	0.85
1:A:133:SER:C	1:A:135:GLY:H	1.79	0.85
25:2:118:LEU:CD2	26:3:42:MET:HB2	2.06	0.85
25:2:171:VAL:HG22	25:2:213:TRP:CA	2.06	0.85
22:W:59:TYR:CD2	22:W:62:ALA:HB2	2.11	0.85
23:0:77:LYS:HB2	23:0:83:CYS:CB	2.04	0.85
25:2:177:GLN:HA	25:2:220:LEU:HD21	1.56	0.85
24:1:1:MET:SD	25:2:415:GLN:O	2.34	0.85
1:A:890:ARG:HH21	1:A:1023:VAL:HG13	1.42	0.85
26:3:14:VAL:HG21	26:3:163:VAL:HG22	1.57	0.85
26:3:59:VAL:HG12	26:3:71:TYR:CG	2.07	0.85
2:B:880:LEU:HD12	2:B:881:GLU:OE1	1.77	0.85
5:E:7:THR:HG1	5:E:47:LYS:HD3	1.38	0.85
17:Q:113:ARG:HE	18:R:222:SER:HB3	0.68	0.85
17:Q:24:GLY:CA	18:R:210:PHE:CD2	2.59	0.85
25:2:81:LYS:CD	25:2:93:LEU:HD21	2.07	0.85
2:B:874:PRO:O	2:B:876:ASN:N	2.09	0.85
26:3:124:ILE:HD13	26:3:125:LYS:N	1.91	0.85
26:3:59:VAL:HG11	26:3:71:TYR:HD1	1.39	0.85
1:A:1098:PRO:C	1:A:1101:GLN:HE21	1.80	0.85
1:A:79:THR:HG21	13:M:43:ASP:CB	2.06	0.85
25:2:167:PRO:O	25:2:171:VAL:HG23	1.76	0.84
25:2:31:LEU:CD1	26:3:33:THR:HG22	1.96	0.84
1:A:202:TRP:CE3	1:A:212:LYS:O	2.30	0.84
1:A:265:VAL:O	1:A:272:ASN:CG	2.14	0.84
5:E:3:ASP:O	5:E:47:LYS:HE3	1.77	0.84
3:C:157:GLN:CG	10:J:65:LEU:CB	2.55	0.84
1:A:1116:ASN:HD21	1:A:1138:SER:CB	1.89	0.84
9:I:103:ARG:C	9:I:105:GLU:H	1.80	0.84
24:1:2:VAL:CG1	25:2:422:LEU:CD1	2.55	0.84
26:3:100:LYS:HB3	26:3:103:LEU:HD13	1.58	0.84
26:3:184:ALA:HA	26:3:187:GLN:HG2	1.57	0.84
1:A:1307:VAL:HG11	1:A:1339:ASP:CB	2.07	0.84
17:Q:113:ARG:NH2	18:R:222:SER:HB3	1.92	0.84
25:2:160:LEU:HD23	25:2:206:LEU:CD2	2.07	0.84
2:B:250:SER:O	2:B:251:ALA:CB	2.25	0.84
17:Q:20:TYR:O	18:R:210:PHE:HD2	1.57	0.84
23:0:55:LEU:HD12	26:3:178:MET:HE3	1.58	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:2:176:ALA:CB	25:2:178:LEU:HD13	2.07	0.84
25:2:211:GLN:HG3	25:2:257:SER:CB	2.05	0.84
23:0:79:ASN:O	23:0:81:LEU:N	2.10	0.84
25:2:159:VAL:HG22	25:2:160:LEU:H	1.41	0.84
25:2:229:ASP:O	25:2:233:ILE:HG12	1.78	0.84
24:1:52:VAL:HG23	24:1:53:LEU:HD12	1.59	0.83
25:2:118:LEU:HD12	25:2:119:ARG:N	1.92	0.83
26:3:49:LEU:CB	26:3:101:TYR:HB3	2.05	0.83
21:V:615:PHE:O	21:V:616:ASP:C	2.16	0.83
25:2:159:VAL:HG22	25:2:160:LEU:CD1	2.08	0.83
1:A:265:VAL:C	1:A:272:ASN:ND2	2.30	0.83
25:2:78:GLU:O	25:2:81:LYS:HG2	1.77	0.83
1:A:1246:ILE:HD11	1:A:1258:ARG:HD2	1.60	0.83
25:2:118:LEU:CD2	26:3:39:ASP:HA	2.08	0.83
26:3:57:LEU:HD23	26:3:58:ALA:N	1.91	0.83
2:B:56:GLN:HG2	20:T:140:ARG:HG3	0.85	0.83
5:E:52:ARG:HH21	5:E:54:ARG:CG	1.90	0.83
19:S:31:PHE:HB2	20:T:92:THR:HB	1.60	0.83
21:V:366:ASN:HD21	21:V:613:THR:HG22	1.43	0.83
25:2:86:SER:HB3	25:2:140:LYS:HE2	1.60	0.83
25:2:57:MET:HA	25:2:60:LEU:CD1	2.09	0.83
21:V:321:GLU:HB2	22:W:499:ASN:OD1	1.77	0.83
24:1:9:LEU:HB2	24:1:51:ASN:HD21	1.44	0.82
24:1:9:LEU:CD1	24:1:48:GLU:HA	2.09	0.82
2:B:61:ASP:HB3	2:B:63:PRO:HD3	1.61	0.82
2:B:803:ARG:NH2	3:C:177:ASN:OD1	2.10	0.82
18:R:223:VAL:HB	18:R:224:THR:CG2	0.49	0.82
25:2:221:GLN:NE2	25:2:230:LEU:HB2	1.93	0.82
25:2:259:LEU:HD12	25:2:260:ASN:N	1.94	0.82
2:B:289:ILE:HG12	2:B:297:MET:HG2	1.61	0.82
17:Q:101:ASN:C	17:Q:103:VAL:H	1.81	0.82
24:1:47:ALA:HB2	24:1:50:VAL:HB	1.61	0.82
26:3:12:VAL:HG21	26:3:161:ILE:HG12	1.61	0.82
25:2:174:ASP:O	25:2:220:LEU:HD23	1.79	0.82
17:Q:21:VAL:C	18:R:210:PHE:CE2	2.52	0.82
17:Q:21:VAL:O	18:R:210:PHE:CZ	2.32	0.82
5:E:52:ARG:HH21	5:E:54:ARG:HG2	1.45	0.82
17:Q:113:ARG:HD3	18:R:222:SER:N	1.90	0.82
25:2:160:LEU:O	25:2:164:VAL:HG23	1.79	0.82
26:3:49:LEU:HB3	26:3:101:TYR:CB	2.05	0.82
26:3:196:LEU:HD21	26:3:223:LEU:CD2	2.09	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:113:ARG:HD2	18:R:221:ARG:CA	2.10	0.82
17:Q:105:TYR:CZ	18:R:234:GLU:OE1	2.33	0.82
24:1:52:VAL:CG2	24:1:53:LEU:HD12	2.09	0.82
1:A:623:PRO:O	1:A:625:ASP:N	2.12	0.82
21:V:523:VAL:HG11	24:1:20:LEU:HD23	1.62	0.82
1:A:266:MET:HG2	1:A:272:ASN:OD1	1.79	0.81
1:A:269:SER:O	1:A:270:ALA:HB3	1.79	0.81
2:B:225:LEU:C	2:B:227:ASN:H	1.81	0.81
2:B:92:TYR:CB	20:T:145:LEU:HD12	2.10	0.81
24:1:59:GLU:OE1	25:2:402:ARG:NH1	2.13	0.81
25:2:221:GLN:OE1	25:2:224:GLN:HA	1.80	0.81
26:3:12:VAL:CG2	26:3:161:ILE:HG12	2.10	0.81
2:B:957:THR:O	2:B:960:GLY:N	2.10	0.81
9:I:14:ILE:HG13	9:I:16:PHE:CZ	2.14	0.81
1:A:156:GLY:CA	1:A:181:HIS:ND1	2.43	0.81
5:E:126:ILE:HD13	5:E:186:LYS:HE3	1.60	0.81
21:V:315:VAL:HG12	22:W:500:ASP:HB2	1.54	0.81
25:2:100:LEU:HG	25:2:119:ARG:HE	1.45	0.81
1:A:659:GLU:OE1	1:A:985:ARG:NH1	2.13	0.81
2:B:92:TYR:HB2	20:T:145:LEU:HD12	1.61	0.81
12:L:26:ASN:HB2	12:L:44:MET:CE	2.09	0.81
18:R:195:PRO:O	18:R:196:ASP:HB2	1.81	0.81
25:2:117:ASN:OD1	26:3:108:ASN:CG	2.18	0.81
21:V:674:THR:CG2	25:2:392:ARG:CZ	2.59	0.81
1:A:455:ILE:HD13	1:A:520:MET:HE1	1.63	0.81
2:B:133:ILE:HG23	2:B:139:GLN:CG	2.09	0.81
26:3:216:LYS:H	26:3:216:LYS:HD2	1.43	0.81
17:Q:112:ARG:NH2	18:R:237:LEU:HB2	1.95	0.81
22:W:59:TYR:CD1	22:W:62:ALA:HB2	2.16	0.81
25:2:174:ASP:OD1	25:2:179:LEU:HD12	1.80	0.81
25:2:37:HIS:HB3	25:2:38:PRO:HD3	1.61	0.81
25:2:175:LEU:HB3	25:2:216:MET:SD	2.20	0.81
25:2:251:VAL:HG11	25:2:254:MET:HG3	1.62	0.81
3:C:6:GLN:N	3:C:7:PRO:HD3	1.95	0.81
3:C:157:GLN:CG	10:J:65:LEU:HB3	2.10	0.81
17:Q:24:GLY:H	18:R:210:PHE:HD2	1.28	0.81
24:1:34:ILE:HG22	24:1:46:ILE:HD11	1.63	0.81
26:3:165:LYS:HE2	26:3:167:ALA:O	1.81	0.80
9:I:14:ILE:HG13	9:I:16:PHE:CE2	2.15	0.80
25:2:256:ASP:O	25:2:259:LEU:HG	1.81	0.80
26:3:121:LYS:O	26:3:124:ILE:HB	1.81	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:73:HIS:O	2:B:74:ALA:HB3	1.82	0.80
5:E:40:PHE:CD2	5:E:46:ASP:OD2	2.35	0.80
26:3:214:TYR:O	26:3:215:LEU:HD23	1.82	0.80
1:A:910:LYS:HD2	1:A:911:PRO:HD2	1.63	0.80
1:A:1171:ALA:HB1	9:I:59:THR:HG21	0.82	0.80
24:1:50:VAL:HG12	24:1:54:GLN:HG2	1.62	0.80
25:2:224:GLN:HB2	25:2:268:PHE:CE2	2.17	0.80
25:2:52:ALA:O	25:2:56:VAL:HG13	1.81	0.80
13:M:34:CYS:SG	13:M:39:LEU:CD2	2.64	0.80
26:3:11:LEU:CD2	26:3:160:ARG:HG2	2.12	0.80
26:3:64:ILE:HG23	26:3:128:HIS:CD2	2.17	0.80
17:Q:109:HIS:ND1	18:R:225:VAL:HG21	1.96	0.80
20:T:145:LEU:O	20:T:147:LYS:N	2.14	0.80
25:2:42:LEU:HD12	25:2:59:MET:CE	2.11	0.80
1:A:269:SER:O	1:A:270:ALA:CB	2.30	0.80
25:2:93:LEU:HA	25:2:96:TRP:CD1	2.17	0.80
2:B:225:LEU:HD13	2:B:228:SER:CB	2.12	0.80
24:1:1:MET:CB	25:2:413:LEU:CB	2.60	0.79
25:2:35:TYR:CD1	25:2:62:LEU:HG	2.16	0.79
1:A:204:HIS:O	1:A:205:VAL:O	1.99	0.79
17:Q:113:ARG:NH2	18:R:222:SER:CB	2.45	0.79
1:A:1117:VAL:C	1:A:1119:LEU:H	1.86	0.79
17:Q:113:ARG:CD	18:R:221:ARG:O	2.22	0.79
22:W:419:GLU:CB	22:W:420:PRO:CD	2.46	0.79
26:3:144:ILE:CD1	26:3:147:MET:HE3	2.12	0.79
25:2:221:GLN:HE22	25:2:230:LEU:HB2	1.47	0.79
1:A:608:THR:OG1	1:A:610:PRO:CG	2.30	0.79
2:B:132:VAL:CG2	2:B:141:GLN:HG3	2.13	0.79
16:P:207:PRO:O	16:P:209:THR:HG23	1.83	0.79
18:R:194:ARG:HB3	18:R:195:PRO:HD3	0.82	0.79
24:1:1:MET:HA	25:2:414:SER:H	1.46	0.79
1:A:926:ASN:HD22	1:A:932:ARG:HG3	1.47	0.79
5:E:52:ARG:NH2	5:E:54:ARG:CG	2.44	0.79
18:R:223:VAL:CB	18:R:224:THR:HG21	0.92	0.79
23:0:77:LYS:O	23:0:79:ASN:N	2.15	0.79
25:2:205:LEU:O	25:2:209:PRO:HD2	1.81	0.79
26:3:58:ALA:N	26:3:71:TYR:CZ	2.51	0.79
25:2:190:PRO:O	25:2:194:PRO:HD2	1.83	0.79
26:3:58:ALA:C	26:3:71:TYR:CE1	2.57	0.79
5:E:52:ARG:HG3	5:E:53:PRO:N	1.98	0.79
25:2:159:VAL:HG13	25:2:161:HIS:N	1.96	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:3:222:SER:O	26:3:225:GLN:HG2	1.83	0.79
1:A:926:ASN:ND2	1:A:932:ARG:CG	2.46	0.79
8:H:107:GLU:O	8:H:108:ALA:C	2.18	0.79
26:3:14:VAL:CG2	26:3:163:VAL:HG22	2.13	0.78
18:R:223:VAL:CB	18:R:224:THR:CB	2.41	0.78
25:2:118:LEU:CD1	26:3:39:ASP:OD1	2.31	0.78
8:H:64:LEU:CB	8:H:84:ARG:HD3	2.07	0.78
13:M:10:LEU:HB3	13:M:13:VAL:O	1.84	0.78
24:1:13:ASP:OD1	24:1:14:PRO:HD2	1.82	0.78
24:1:1:MET:HB3	25:2:413:LEU:HD23	1.65	0.78
9:I:59:THR:O	9:I:60:HIS:HB2	1.83	0.78
17:Q:184:ILE:CD1	18:R:218:LYS:NZ	2.45	0.78
25:2:203:PHE:CD2	25:2:205:LEU:HD23	2.18	0.78
25:2:181:GLN:OE1	25:2:229:ASP:HB2	1.83	0.78
26:3:151:VAL:HG12	26:3:155:GLN:O	1.84	0.78
1:A:206:ASN:O	1:A:207:GLU:CG	2.31	0.78
13:M:34:CYS:HB2	13:M:39:LEU:CG	2.07	0.78
22:W:298:ALA:HA	22:W:421:PHE:CD2	2.19	0.78
25:2:207:ASP:O	25:2:211:GLN:HG2	1.84	0.78
18:R:195:PRO:O	18:R:196:ASP:CB	2.31	0.78
25:2:42:LEU:HD12	25:2:59:MET:HE3	1.64	0.78
25:2:118:LEU:CG	26:3:39:ASP:OD1	2.32	0.78
1:A:926:ASN:OD1	1:A:931:ARG:CG	2.30	0.78
2:B:80:GLU:O	2:B:82:PRO:HD3	1.83	0.78
13:M:94:ASP:CB	13:M:97:GLY:O	2.32	0.78
18:R:223:VAL:CG2	18:R:224:THR:HG23	1.77	0.78
24:1:13:ASP:OD2	24:1:17:LYS:CB	2.31	0.78
25:2:196:ILE:CD1	25:2:210:ALA:HB2	2.13	0.78
25:2:53:LYS:O	25:2:56:VAL:HG22	1.84	0.78
21:V:516:PRO:CD	24:1:15:ALA:HB3	2.11	0.78
25:2:234:LEU:HD23	25:2:234:LEU:O	1.83	0.78
25:2:77:LYS:HD3	25:2:78:GLU:N	1.97	0.78
24:1:1:MET:HG3	25:2:415:GLN:O	1.84	0.78
25:2:34:LEU:O	25:2:38:PRO:HD2	1.84	0.78
26:3:147:MET:O	26:3:151:VAL:HG23	1.84	0.78
1:A:478:PRO:O	1:A:483:ARG:NH2	2.16	0.78
1:A:926:ASN:HD21	1:A:932:ARG:HG2	1.47	0.78
17:Q:113:ARG:HH21	18:R:222:SER:CB	1.96	0.78
24:1:34:ILE:CG2	24:1:46:ILE:HD11	2.13	0.77
24:1:38:ILE:HA	24:1:44:PHE:HD1	1.47	0.77
25:2:30:VAL:H	26:3:25:GLN:HB3	1.49	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:551:ARG:HD3	1:A:625:ASP:OD2	1.83	0.77
26:3:58:ALA:HA	26:3:71:TYR:CZ	2.18	0.77
23:0:54:ARG:NE	26:3:182:PHE:HE1	1.73	0.77
1:A:129:ILE:O	1:A:132:LYS:HB2	1.84	0.77
23:0:54:ARG:HB2	26:3:209:ILE:CG2	2.14	0.77
25:2:30:VAL:HG23	26:3:25:GLN:HB3	0.80	0.77
2:B:1080:ARG:HH21	13:M:50:SER:HB3	1.49	0.77
3:C:6:GLN:N	3:C:7:PRO:CD	2.48	0.77
7:G:151:ARG:HG3	17:Q:139:LEU:HD22	1.66	0.77
13:M:15:CYS:SG	13:M:39:LEU:HD21	2.25	0.77
25:2:179:LEU:HB3	25:2:184:LEU:HD11	1.65	0.77
26:3:185:GLN:HE21	26:3:185:GLN:HA	1.48	0.77
25:2:163:MET:CE	25:2:206:LEU:HD12	2.14	0.77
24:1:10:ILE:CG2	25:2:407:VAL:HG21	2.15	0.77
13:M:279:GLY:HA2	20:T:153:TYR:HE1	1.49	0.77
21:V:519:TYR:CE2	24:1:20:LEU:HG	2.20	0.77
25:2:211:GLN:CG	25:2:257:SER:HB3	2.13	0.77
28:Y:24:DC:H2"	28:Y:25:DT:H72	1.67	0.77
25:2:189:GLU:HB2	25:2:190:PRO:HD3	1.66	0.76
25:2:211:GLN:HA	25:2:261:PHE:HZ	1.49	0.76
26:3:185:GLN:NE2	26:3:210:THR:HA	2.00	0.76
17:Q:187:ILE:CD1	18:R:212:VAL:H	1.99	0.76
24:1:38:ILE:HG22	24:1:44:PHE:CD1	2.19	0.76
24:1:1:MET:CE	25:2:440:LEU:HD13	2.16	0.76
1:A:211:GLU:O	1:A:212:LYS:CB	2.33	0.76
2:B:490:GLY:O	2:B:491:ARG:HB2	1.84	0.76
25:2:44:VAL:HG13	25:2:45:PHE:CD1	2.20	0.76
1:A:1116:ASN:O	1:A:1117:VAL:CG2	2.33	0.76
17:Q:113:ARG:NE	18:R:222:SER:N	2.32	0.76
26:3:14:VAL:CG2	26:3:163:VAL:HA	2.16	0.76
25:2:177:GLN:CD	25:2:220:LEU:HD22	2.06	0.76
13:M:10:LEU:N	13:M:10:LEU:HD22	2.01	0.76
21:V:516:PRO:HA	24:1:15:ALA:C	2.05	0.76
25:2:234:LEU:CD2	25:2:237:LEU:HD12	2.14	0.76
2:B:958:CYS:SG	2:B:959:GLU:N	2.56	0.76
3:C:157:GLN:CG	10:J:65:LEU:HB2	2.16	0.76
9:I:57:LYS:O	9:I:58:ILE:HG12	1.85	0.76
14:N:343:HIS:NE2	27:X:9:DC:OP1	2.19	0.76
17:Q:184:ILE:HD13	18:R:211:SER:CB	2.15	0.76
24:1:38:ILE:H	24:1:38:ILE:HD13	1.51	0.76
26:3:133:LEU:HD23	26:3:177:PHE:HD1	1.49	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:222:ARG:HB3	2:B:222:ARG:HH11	1.49	0.76
9:I:57:LYS:C	9:I:58:ILE:HG12	2.05	0.76
16:P:297:LYS:CB	16:P:298:PRO:HD2	2.15	0.76
25:2:208:THR:HG23	25:2:209:PRO:CD	2.16	0.76
21:V:674:THR:CG2	25:2:392:ARG:NH2	2.43	0.76
24:1:1:MET:SD	25:2:413:LEU:HB3	2.25	0.76
26:3:172:LEU:HD13	26:3:172:LEU:O	1.86	0.76
1:A:360:ASP:OD1	1:A:361:PHE:N	2.17	0.76
18:R:223:VAL:CA	18:R:224:THR:HG22	1.78	0.76
21:V:612:ASP:C	21:V:614:SER:H	1.87	0.76
25:2:118:LEU:HD22	26:3:39:ASP:HA	1.65	0.76
24:1:1:MET:HB3	25:2:413:LEU:CD2	2.15	0.75
24:1:24:ASP:OD2	24:1:57:VAL:HG11	1.85	0.75
26:3:190:LEU:H	26:3:190:LEU:HD23	1.51	0.75
2:B:225:LEU:CB	2:B:228:SER:HB2	2.05	0.75
5:E:64:HIS:C	5:E:66:ASP:H	1.89	0.75
25:2:208:THR:HG23	25:2:209:PRO:HD3	1.66	0.75
25:2:42:LEU:HD21	25:2:55:TRP:CB	2.10	0.75
13:M:53:ARG:HH22	28:Y:54:DA:H61	1.34	0.75
17:Q:113:ARG:CD	18:R:221:ARG:CB	2.60	0.75
25:2:243:SER:HB3	25:2:258:LEU:HD22	1.69	0.75
26:3:8:LEU:HD23	26:3:54:SER:HB3	1.68	0.75
2:B:496:ALA:HB1	2:B:498:PRO:HD2	1.66	0.75
2:B:875:GLU:O	2:B:876:ASN:CB	2.35	0.75
10:J:5:VAL:HG12	10:J:6:ARG:HG3	1.65	0.75
21:V:523:VAL:HG21	24:1:20:LEU:HG	1.68	0.75
1:A:1117:VAL:C	1:A:1119:LEU:N	2.35	0.75
1:A:202:TRP:CD2	1:A:212:LYS:HD2	2.21	0.75
25:2:218:GLN:NE2	25:2:265:LEU:HA	2.00	0.75
25:2:53:LYS:HE3	25:2:95:ILE:HD11	1.67	0.75
25:2:86:SER:HB3	25:2:140:LYS:CE	2.16	0.75
5:E:47:LYS:CB	5:E:48:PRO:CD	2.59	0.75
2:B:132:VAL:HG21	2:B:141:GLN:OE1	1.86	0.75
25:2:100:LEU:CD1	25:2:119:ARG:HG3	2.16	0.75
25:2:196:ILE:HD11	25:2:210:ALA:CB	2.17	0.75
25:2:35:TYR:CD2	25:2:62:LEU:HB3	2.22	0.75
25:2:117:ASN:CG	26:3:42:MET:CE	2.55	0.75
3:C:157:GLN:CD	10:J:65:LEU:CB	2.54	0.75
10:J:65:LEU:N	10:J:65:LEU:HD13	2.01	0.75
17:Q:188:TYR:HE2	18:R:210:PHE:CE1	2.00	0.75
26:3:11:LEU:HD22	26:3:160:ARG:CG	2.16	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1040:GLN:N	2:B:1040:GLN:OE1	2.20	0.75
2:B:428:ASP:OD1	20:T:158:ASN:ND2	2.18	0.75
25:2:180:SER:O	25:2:184:LEU:HG	1.87	0.74
26:3:38:ILE:O	26:3:41:VAL:HG12	1.87	0.74
1:A:679:TRP:CH2	1:A:683:GLU:HG3	2.22	0.74
18:R:163:LEU:O	18:R:164:GLY:O	2.05	0.74
9:I:92:LYS:NZ	9:I:93:GLU:OE2	2.20	0.74
17:Q:113:ARG:NH2	18:R:222:SER:OG	2.21	0.74
22:W:73:CYS:HB2	22:W:209:TYR:CZ	2.22	0.74
27:X:41:DT:H3'	27:X:42:DT:H4'	1.67	0.74
26:3:24:LYS:O	26:3:25:GLN:O	2.06	0.74
26:3:57:LEU:C	26:3:71:TYR:CZ	2.61	0.74
2:B:250:SER:O	2:B:251:ALA:HB2	1.87	0.74
2:B:310:VAL:HG13	19:S:161:GLU:HB3	1.70	0.74
2:B:907:VAL:HG13	2:B:921:ILE:HG22	1.69	0.74
24:1:1:MET:HB2	25:2:418:PHE:CB	2.18	0.74
17:Q:113:ARG:CZ	18:R:222:SER:CB	2.51	0.74
21:V:321:GLU:OE1	22:W:499:ASN:OD1	2.06	0.74
22:W:430:ASN:HB3	22:W:431:PRO:CD	2.17	0.74
25:2:117:ASN:HD21	26:3:108:ASN:HB3	1.47	0.74
25:2:51:LEU:O	25:2:51:LEU:HD23	1.87	0.74
2:B:91:ILE:HD11	2:B:124:LEU:HD21	1.69	0.74
22:W:298:ALA:HA	22:W:421:PHE:HD2	1.50	0.74
22:W:424:ARG:O	22:W:425:THR:CG2	2.32	0.74
22:W:59:TYR:CD2	22:W:62:ALA:CB	2.70	0.74
25:2:127:LYS:N	25:2:178:LEU:HD23	2.01	0.73
26:3:141:LEU:O	26:3:144:ILE:HG22	1.88	0.73
1:A:1439:LEU:HD13	2:B:1162:LEU:HD21	1.70	0.73
18:R:223:VAL:HG23	18:R:224:THR:OG1	1.88	0.73
24:1:1:MET:HE2	25:2:440:LEU:HD13	1.70	0.73
2:B:591:ARG:NH1	2:B:663:GLU:OE2	2.21	0.73
26:3:12:VAL:HG23	26:3:161:ILE:HG23	1.70	0.73
26:3:214:TYR:HE2	26:3:216:LYS:HE2	1.53	0.73
26:3:59:VAL:CA	26:3:71:TYR:CE1	2.69	0.73
22:W:584:TYR:HD1	22:W:594:ALA:HB2	1.52	0.73
24:1:18:GLN:CB	24:1:44:PHE:HE2	2.01	0.73
24:1:34:ILE:HD13	24:1:54:GLN:OE1	1.88	0.73
1:A:623:PRO:C	1:A:625:ASP:H	1.88	0.73
12:L:19:CYS:SG	12:L:20:GLY:N	2.62	0.73
17:Q:184:ILE:HD12	18:R:218:LYS:HZ3	1.54	0.73
25:2:251:VAL:HG11	25:2:254:MET:CG	2.18	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:3:33:THR:HG23	26:3:36:LYS:N	1.98	0.73
1:A:1307:VAL:CG1	1:A:1339:ASP:HB3	2.18	0.73
1:A:18:ILE:HD12	2:B:1171:MET:HB2	1.69	0.73
17:Q:122:THR:HA	17:Q:169:PRO:HD2	1.70	0.73
1:A:47:THR:O	1:A:48:GLU:CG	2.37	0.73
14:N:343:HIS:HB3	14:N:350:LYS:HB2	1.70	0.73
14:N:42:LEU:HB2	15:O:22:LEU:HD11	1.69	0.73
16:P:206:GLU:C	16:P:208:ARG:H	1.91	0.73
24:1:34:ILE:HG12	24:1:50:VAL:CG1	2.18	0.73
25:2:41:CYS:O	25:2:44:VAL:HG12	1.88	0.73
3:C:157:GLN:HE21	10:J:65:LEU:CB	1.94	0.73
5:E:47:LYS:O	5:E:49:SER:N	2.22	0.73
24:1:25:GLU:CD	24:1:35:ILE:HG12	2.09	0.73
24:1:2:VAL:CG1	25:2:456:LYS:CG	2.53	0.73
25:2:160:LEU:HA	25:2:206:LEU:HD11	1.70	0.73
25:2:60:LEU:HD11	25:2:95:ILE:HB	1.71	0.73
1:A:1223:ASP:OD2	1:A:1224:ARG:NH1	2.22	0.73
19:S:49:ARG:NH1	19:S:96:GLN:O	2.21	0.73
25:2:30:VAL:CB	26:3:25:GLN:O	2.34	0.73
8:H:99:ILE:HG22	8:H:136:GLU:HG3	1.70	0.73
14:N:333:ASN:HB3	14:N:360:LEU:HA	1.71	0.73
25:2:172:SER:HA	25:2:175:LEU:CD2	2.19	0.73
1:A:61:ARG:HB3	1:A:72:GLN:HG2	1.69	0.73
22:W:59:TYR:CE2	22:W:62:ALA:HB2	2.22	0.73
25:2:132:ASP:O	25:2:135:GLN:HG2	1.88	0.72
26:3:222:SER:HB2	26:3:226:TYR:HE2	1.54	0.72
24:1:1:MET:HG3	25:2:418:PHE:HB2	1.69	0.72
24:1:9:LEU:HD22	24:1:51:ASN:ND2	2.04	0.72
21:V:667:THR:HA	24:1:62:ASP:OD1	1.89	0.72
26:3:111:ILE:HG13	26:3:112:VAL:N	2.02	0.72
1:A:691:ASP:HB3	1:A:766:PHE:HB2	1.71	0.72
2:B:89:GLU:HB3	2:B:127:ASP:HB3	1.70	0.72
2:B:73:HIS:O	2:B:74:ALA:CB	2.37	0.72
2:B:906:GLN:HG2	12:L:45:TYR:HE1	1.52	0.72
26:3:66:GLU:CA	26:3:132:LEU:HD12	2.13	0.72
26:3:226:TYR:HA	26:3:230:VAL:HG23	1.71	0.72
26:3:57:LEU:C	26:3:71:TYR:CE2	2.62	0.72
1:A:926:ASN:ND2	1:A:932:ARG:HG2	2.05	0.72
2:B:487:SER:OG	2:B:524:LYS:NZ	2.22	0.72
10:J:3:ILE:HD12	10:J:3:ILE:H	1.54	0.72
17:Q:188:TYR:CE1	18:R:211:SER:OG	2.42	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:2:35:TYR:CG	25:2:62:LEU:HD12	2.25	0.72
25:2:134:SER:O	25:2:138:PRO:HD2	1.89	0.72
25:2:218:GLN:HE22	25:2:265:LEU:HA	1.54	0.72
25:2:243:SER:HB2	25:2:258:LEU:HD22	1.71	0.72
21:V:689:VAL:HB	25:2:391:ILE:HD11	1.70	0.72
24:1:5:LEU:HD21	25:2:408:LEU:HD13	0.87	0.72
26:3:69:PHE:CE1	26:3:139:LYS:HD2	2.25	0.72
1:A:926:ASN:ND2	1:A:932:ARG:HG3	2.04	0.72
1:A:426:ARG:HD2	13:M:40:VAL:HG11	1.72	0.72
25:2:175:LEU:HD22	25:2:216:MET:SD	2.29	0.72
1:A:1101:GLN:OE1	1:A:1389:ASP:OD2	2.07	0.72
22:W:209:TYR:HE1	22:W:233:PHE:CD1	2.07	0.72
2:B:51:ILE:CG2	20:T:141:LEU:HD21	2.18	0.72
25:2:117:ASN:HB3	26:3:42:MET:CE	2.18	0.72
1:A:426:ARG:CA	13:M:40:VAL:HG21	2.20	0.72
17:Q:184:ILE:HD11	18:R:213:ASP:OD1	1.90	0.72
25:2:117:ASN:HB2	26:3:104:LEU:HD11	1.71	0.72
26:3:165:LYS:HG3	26:3:203:LEU:CD1	2.20	0.72
3:C:59:LEU:HD22	3:C:151:VAL:HG23	1.72	0.72
21:V:504:LYS:HB3	21:V:654:GLU:O	1.90	0.72
24:1:2:VAL:HG12	25:2:422:LEU:HD13	1.72	0.71
26:3:217:VAL:HG13	26:3:226:TYR:CZ	2.25	0.71
3:C:193:ARG:HH12	3:C:218:ALA:HB1	1.54	0.71
17:Q:188:TYR:CZ	18:R:210:PHE:CE1	2.65	0.71
28:Y:53:DG:H2"	28:Y:55:DG:H5'	1.73	0.71
25:2:171:VAL:HG12	25:2:216:MET:SD	2.31	0.71
25:2:237:LEU:O	25:2:240:LEU:HD13	1.88	0.71
25:2:118:LEU:CD2	26:3:39:ASP:CA	2.68	0.71
25:2:118:LEU:HD22	26:3:39:ASP:CA	2.19	0.71
25:2:86:SER:CB	25:2:140:LYS:HE2	2.20	0.71
1:A:1171:ALA:CA	9:I:59:THR:HG21	1.91	0.71
21:V:611:GLY:HA2	21:V:615:PHE:HB3	1.71	0.71
25:2:199:ALA:HB3	25:2:202:GLN:NE2	2.02	0.71
24:1:1:MET:HG2	25:2:413:LEU:HB3	1.71	0.71
27:X:42:DT:H3'	27:X:43:DT:H5"	1.72	0.71
27:X:47:DT:H3'	27:X:48:DT:H5"	1.71	0.71
13:M:10:LEU:C	13:M:12:ARG:H	1.90	0.71
22:W:209:TYR:OH	22:W:234:ASP:N	2.23	0.71
16:P:159:SER:HB3	16:P:329:TYR:CD2	2.25	0.71
14:N:316:SER:OG	16:P:235:ARG:NH1	2.23	0.71
22:W:589:GLU:O	22:W:594:ALA:HB1	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:356:PHE:HB3	19:S:116:GLY:HA2	1.71	0.71
21:V:648:LYS:O	21:V:650:MET:N	2.24	0.71
24:1:29:LEU:HD23	24:1:30:GLY:N	2.06	0.70
25:2:163:MET:O	25:2:167:PRO:HD2	1.91	0.70
7:G:97:LEU:HB2	7:G:108:ILE:HB	1.71	0.70
8:H:147:LYS:HE2	8:H:149:ALA:HA	1.73	0.70
22:W:59:TYR:CE1	22:W:62:ALA:HB2	2.26	0.70
23:0:74:GLN:HA	23:0:78:PRO:O	1.92	0.70
1:A:1192:TRP:HE1	1:A:1249:ASP:H	1.35	0.70
1:A:1305:SER:C	1:A:1306:LYS:HG3	2.10	0.70
13:M:279:GLY:HA2	20:T:153:TYR:CE1	2.27	0.70
21:V:315:VAL:HG12	22:W:500:ASP:CB	2.16	0.70
25:2:192:GLU:HG3	25:2:193:PRO:CD	2.18	0.70
2:B:854:ILE:HD11	2:B:921:ILE:HD12	1.73	0.70
9:I:101:SER:O	9:I:104:ALA:HB2	1.91	0.70
24:1:28:ALA:HB3	24:1:31:LYS:HB2	1.71	0.70
25:2:199:ALA:CB	25:2:202:GLN:HE22	2.02	0.70
23:0:54:ARG:NE	26:3:182:PHE:CD1	2.60	0.70
24:1:2:VAL:HG12	25:2:456:LYS:HE2	1.74	0.70
26:3:177:PHE:CZ	26:3:203:LEU:HD23	2.27	0.70
25:2:117:ASN:CB	26:3:42:MET:HE3	2.21	0.70
26:3:162:LEU:HA	26:3:192:ASP:OD1	1.92	0.70
1:A:190:ARG:NH2	27:X:58:DT:OP2	2.24	0.70
2:B:102:ASP:OD1	2:B:103:GLY:N	2.24	0.70
2:B:514:THR:HG22	2:B:524:LYS:HA	1.72	0.70
1:A:79:THR:HG21	13:M:43:ASP:CA	2.22	0.70
17:Q:114:ILE:HD11	18:R:218:LYS:HE3	1.74	0.70
28:Y:49:DG:H2'	28:Y:50:DA:H8	1.56	0.70
1:A:203:LYS:O	1:A:204:HIS:CB	2.25	0.70
2:B:225:LEU:C	2:B:227:ASN:N	2.39	0.70
2:B:51:ILE:HG22	20:T:141:LEU:HD21	1.71	0.70
25:2:185:MET:SD	25:2:232:GLU:HB2	2.32	0.70
26:3:69:PHE:CZ	26:3:139:LYS:HD2	2.27	0.70
28:Y:24:DC:H2"	28:Y:25:DT:C7	2.22	0.70
24:1:53:LEU:HD12	24:1:53:LEU:H	1.57	0.70
25:2:218:GLN:OE1	25:2:265:LEU:HA	1.92	0.70
2:B:851:ASP:HB2	12:L:14:PRO:HG3	1.72	0.69
14:N:311:GLU:HG2	16:P:251:LEU:HD21	1.72	0.69
1:A:1171:ALA:C	9:I:59:THR:CG2	2.59	0.69
21:V:515:SER:HB3	21:V:539:ASN:ND2	2.05	0.69
21:V:674:THR:OG1	25:2:392:ARG:NE	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1076:GLU:HG3	13:M:54:THR:OG1	1.93	0.69
7:G:93:ASN:ND2	17:Q:151:THR:HA	2.08	0.69
13:M:7:LEU:CD1	13:M:10:LEU:HD11	2.22	0.69
24:1:1:MET:CG	25:2:415:GLN:O	2.41	0.69
1:A:263:ALA:C	1:A:265:VAL:H	1.94	0.69
13:M:11:PRO:O	13:M:12:ARG:HB3	1.91	0.69
24:1:34:ILE:CG1	24:1:50:VAL:HG11	2.21	0.69
25:2:189:GLU:HA	25:2:192:GLU:HG2	1.71	0.69
13:M:7:LEU:HD11	13:M:10:LEU:HD11	1.74	0.69
25:2:81:LYS:HD2	25:2:89:LEU:CD2	2.20	0.69
26:3:215:LEU:HD12	26:3:230:VAL:CG1	2.23	0.69
14:N:319:ASP:O	14:N:320:VAL:C	2.28	0.69
17:Q:187:ILE:HD13	18:R:212:VAL:H	1.56	0.69
25:2:81:LYS:HE3	25:2:93:LEU:CD2	2.20	0.69
1:A:612:ASP:HB3	1:A:617:PRO:HD3	1.75	0.69
5:E:52:ARG:NE	5:E:54:ARG:HG3	2.06	0.69
24:1:8:VAL:HG11	24:1:45:VAL:HG12	1.74	0.69
25:2:140:LYS:HD3	25:2:162:PHE:HE1	1.58	0.69
25:2:130:SER:O	25:2:133:THR:HG22	1.92	0.69
13:M:94:ASP:CG	13:M:97:GLY:O	2.30	0.69
24:1:55:GLU:OE2	25:2:402:ARG:HG3	1.93	0.69
24:1:1:MET:C	25:2:413:LEU:HG	2.12	0.69
26:3:133:LEU:HD22	26:3:134:ALA:H	1.56	0.69
2:B:834:ARG:O	2:B:885:ARG:NH1	2.24	0.69
25:2:118:LEU:HD11	26:3:43:VAL:HG23	1.75	0.69
13:M:7:LEU:CG	13:M:10:LEU:HD11	2.23	0.69
13:M:94:ASP:HB3	13:M:99:SER:H	1.57	0.69
17:Q:109:HIS:ND1	18:R:225:VAL:CG2	2.55	0.69
26:3:34:LEU:HD13	26:3:34:LEU:O	1.92	0.68
26:3:33:THR:HG22	26:3:36:LYS:HB2	1.73	0.68
2:B:80:GLU:O	2:B:82:PRO:CD	2.41	0.68
3:C:157:GLN:HG2	10:J:65:LEU:CB	2.22	0.68
13:M:108:SER:HB3	13:M:112:ARG:HH11	1.58	0.68
25:2:163:MET:CE	25:2:206:LEU:HB3	2.23	0.68
24:1:1:MET:HG2	25:2:413:LEU:C	2.14	0.68
25:2:251:VAL:HG12	25:2:254:MET:H	1.58	0.68
5:E:52:ARG:CG	5:E:53:PRO:N	2.50	0.68
9:I:119:CYS:SG	9:I:120:GLY:N	2.64	0.68
21:V:522:TYR:HE2	24:1:62:ASP:CG	1.96	0.68
2:B:329:GLY:H	2:B:335:ARG:HH21	1.39	0.68
26:3:114:GLU:O	26:3:118:LEU:HD23	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:71:GLN:HE21	5:E:99:ILE:HA	1.59	0.68
25:2:48:LEU:CB	25:2:49:PRO:HD3	2.19	0.68
26:3:130:GLU:HB2	26:3:173:GLN:NE2	2.09	0.68
25:2:118:LEU:HD13	26:3:39:ASP:OD1	1.93	0.68
1:A:686:THR:OG1	1:A:687:ILE:N	2.26	0.68
22:W:73:CYS:C	22:W:209:TYR:CE2	2.67	0.68
26:3:59:VAL:N	26:3:71:TYR:CD1	2.62	0.68
12:L:26:ASN:O	12:L:27:GLU:HB3	1.94	0.68
17:Q:101:ASN:C	17:Q:103:VAL:N	2.45	0.68
25:2:211:GLN:HA	25:2:261:PHE:CE1	2.28	0.68
26:3:187:GLN:HG3	26:3:189:ILE:CG1	2.24	0.68
25:2:118:LEU:HD21	26:3:39:ASP:C	2.12	0.68
5:E:52:ARG:HE	5:E:54:ARG:HG3	1.59	0.68
17:Q:184:ILE:CD1	18:R:218:LYS:HZ3	2.05	0.68
24:1:39:ASP:OD1	24:1:43:VAL:HB	1.94	0.67
1:A:1086:MET:O	1:A:1088:GLY:N	2.27	0.67
20:T:154:LYS:N	20:T:154:LYS:HD2	2.08	0.67
25:2:170:ALA:HB1	25:2:213:TRP:CZ3	2.29	0.67
24:1:4:VAL:CG1	25:2:411:GLN:O	2.39	0.67
25:2:30:VAL:H	26:3:25:GLN:CB	2.07	0.67
1:A:112:PHE:H	1:A:188:GLN:HE22	1.40	0.67
1:A:153:ILE:O	1:A:155:GLU:HG2	1.94	0.67
2:B:1029:TYR:HE1	2:B:1036:LYS:HE2	1.59	0.67
21:V:321:GLU:CB	22:W:499:ASN:CG	2.32	0.67
25:2:211:GLN:HB3	25:2:261:PHE:HE1	1.59	0.67
1:A:207:GLU:O	1:A:209:SER:N	2.27	0.67
2:B:775:GLY:N	2:B:1047:TYR:OH	2.28	0.67
2:B:875:GLU:HA	2:B:875:GLU:OE2	1.92	0.67
17:Q:187:ILE:CG2	18:R:210:PHE:C	2.62	0.67
18:R:223:VAL:CB	18:R:224:THR:HG22	1.24	0.67
18:R:223:VAL:HB	18:R:224:THR:HG22	0.75	0.67
21:V:516:PRO:HB3	24:1:15:ALA:CB	2.05	0.67
26:3:159:SER:OG	26:3:189:ILE:HD12	1.94	0.67
1:A:358:ARG:NH2	2:B:1076:GLU:OE1	2.23	0.67
18:R:223:VAL:CG1	18:R:224:THR:HG22	2.07	0.67
25:2:176:ALA:HB1	25:2:178:LEU:CD1	2.23	0.67
26:3:111:ILE:O	26:3:115:ILE:HD13	1.94	0.67
2:B:895:PHE:O	2:B:897:ARG:NE	2.27	0.67
13:M:10:LEU:HD23	13:M:10:LEU:O	1.95	0.67
25:2:117:ASN:HD21	26:3:108:ASN:CA	2.04	0.67
25:2:172:SER:O	25:2:175:LEU:HD23	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:1:10:ILE:HG21	25:2:407:VAL:HG21	1.76	0.67
1:A:923:ASP:O	1:A:932:ARG:NH1	2.28	0.67
2:B:882:SER:HB2	2:B:887:TYR:CZ	2.30	0.67
1:A:271:ARG:HG2	13:M:73:PRO:HG3	1.76	0.67
20:T:228:ILE:HG22	27:X:29:DC:H1'	1.75	0.67
26:3:187:GLN:CG	26:3:189:ILE:HG12	2.24	0.67
13:M:62:LYS:HB2	29:Z:1:A:H5"	1.76	0.67
21:V:516:PRO:HG3	24:1:15:ALA:HB2	1.58	0.67
24:1:59:GLU:OE2	25:2:402:ARG:CZ	2.41	0.67
26:3:24:LYS:HE2	26:3:220:MET:SD	2.33	0.67
25:2:56:VAL:HG11	25:2:91:SER:HB2	1.77	0.67
14:N:319:ASP:C	14:N:321:SER:N	2.46	0.67
11:K:111:ASP:O	11:K:113:GLN:N	2.29	0.67
16:P:206:GLU:CG	16:P:207:PRO:HD3	2.23	0.67
1:A:67:ARG:H	1:A:78:MET:HE1	1.59	0.66
25:2:56:VAL:O	25:2:60:LEU:HG	1.94	0.66
26:3:18:ASN:CG	26:3:20:ILE:HD13	2.15	0.66
1:A:775:LYS:HB3	2:B:974:SER:OG	1.96	0.66
14:N:358:MET:HB2	14:N:365:TYR:HB2	1.78	0.66
17:Q:188:TYR:HH	18:R:210:PHE:HE1	1.29	0.66
21:V:631:GLY:O	21:V:632:SER:HB3	1.95	0.66
25:2:160:LEU:H	25:2:160:LEU:HD12	1.60	0.66
26:3:146:ARG:O	26:3:149:LYS:HG2	1.95	0.66
25:2:117:ASN:HB3	26:3:42:MET:HE3	1.75	0.66
1:A:228:ILE:O	1:A:244:ARG:NH2	2.26	0.66
26:3:144:ILE:HG12	26:3:147:MET:HE2	1.76	0.66
3:C:267:ILE:HG21	11:K:84:GLN:HE22	1.60	0.66
13:M:10:LEU:C	13:M:12:ARG:N	2.48	0.66
17:Q:23:ARG:NH2	18:R:206:LYS:O	2.27	0.66
18:R:223:VAL:CB	18:R:224:THR:HG23	1.10	0.66
27:X:69:DA:C2	28:Y:26:DG:C2	2.84	0.66
26:3:207:CYS:SG	26:3:214:TYR:HB2	2.34	0.66
1:A:79:THR:HG21	13:M:43:ASP:HA	1.78	0.66
13:M:52:TRP:O	13:M:52:TRP:CD1	2.48	0.66
14:N:318:ASP:OD1	16:P:239:ARG:NE	2.28	0.66
24:1:35:ILE:HG22	24:1:46:ILE:HD12	1.78	0.66
25:2:218:GLN:CG	25:2:268:PHE:HB3	2.26	0.66
26:3:217:VAL:HG13	26:3:226:TYR:CE2	2.30	0.66
25:2:117:ASN:HD22	26:3:42:MET:HE1	1.60	0.66
3:C:212:ASP:C	3:C:214:ASP:N	2.49	0.66
24:1:8:VAL:HG12	24:1:9:LEU:N	2.10	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:2:163:MET:HE2	25:2:206:LEU:CD1	2.26	0.66
1:A:611:ASP:O	1:A:612:ASP:HB2	1.95	0.66
2:B:224:CYS:O	2:B:226:GLU:OE1	2.12	0.66
17:Q:109:HIS:CE1	18:R:225:VAL:CG2	2.79	0.66
17:Q:113:ARG:HH12	18:R:218:LYS:CG	2.09	0.66
2:B:225:LEU:HD13	2:B:228:SER:HG	1.59	0.66
24:1:19:PHE:O	24:1:22:TYR:HB3	1.96	0.66
26:3:144:ILE:O	26:3:147:MET:HG3	1.96	0.66
26:3:184:ALA:CA	26:3:187:GLN:HG2	2.25	0.66
26:3:33:THR:CG2	26:3:36:LYS:HB2	2.26	0.66
26:3:45:GLY:O	26:3:49:LEU:HD23	1.96	0.66
11:K:81:TYR:HE2	11:K:86:ALA:HB2	1.61	0.66
13:M:7:LEU:HG	13:M:10:LEU:HD11	1.77	0.66
16:P:205:ARG:O	16:P:206:GLU:O	2.13	0.66
21:V:612:ASP:C	21:V:614:SER:N	2.49	0.66
25:2:218:GLN:CD	25:2:265:LEU:HA	2.17	0.65
24:1:1:MET:SD	25:2:419:GLU:HB2	2.37	0.65
1:A:133:SER:C	1:A:135:GLY:N	2.45	0.65
1:A:421:ARG:NH2	1:A:425:ASP:OD2	2.29	0.65
2:B:801:VAL:HA	2:B:805:PHE:HB3	1.77	0.65
2:B:873:LEU:H	2:B:874:PRO:HD2	1.61	0.65
16:P:239:ARG:NH1	16:P:242:GLN:OE1	2.29	0.65
17:Q:113:ARG:HH12	18:R:218:LYS:HG3	1.61	0.65
25:2:270:LEU:HD23	25:2:273:GLN:HE21	1.62	0.65
2:B:490:GLY:O	2:B:491:ARG:CB	2.43	0.65
16:P:206:GLU:CB	16:P:207:PRO:HD2	2.10	0.65
25:2:42:LEU:CD2	25:2:55:TRP:HB2	2.13	0.65
26:3:137:LEU:HB3	26:3:180:VAL:CG1	2.20	0.65
2:B:309:PHE:CE2	9:I:40:ARG:HD2	2.31	0.65
13:M:178:LYS:C	20:T:154:LYS:HB3	2.14	0.65
24:1:13:ASP:CG	24:1:14:PRO:CD	2.61	0.65
25:2:171:VAL:HG13	25:2:216:MET:CB	2.26	0.65
17:Q:68:GLY:O	18:R:226:ASP:OD2	2.14	0.65
25:2:126:GLY:C	25:2:178:LEU:HD23	2.16	0.65
24:1:10:ILE:HG22	25:2:407:VAL:HG21	1.79	0.65
25:2:44:VAL:HG13	25:2:45:PHE:HD1	1.59	0.65
26:3:106:SER:O	26:3:110:VAL:HG23	1.97	0.65
21:V:612:ASP:CG	21:V:635:GLN:CD	2.55	0.65
24:1:22:TYR:HD1	24:1:23:LEU:HD23	1.61	0.65
25:2:117:ASN:ND2	26:3:108:ASN:CA	2.57	0.65
1:A:610:PRO:HB2	1:A:626:THR:CG2	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:W:584:TYR:CE1	22:W:614:TYR:O	2.46	0.65
27:X:32:DT:H4'	27:X:33:DT:H5'	1.78	0.65
1:A:929:ALA:C	1:A:931:ARG:H	2.00	0.65
2:B:249:LYS:O	2:B:249:LYS:HG2	1.96	0.65
8:H:106:THR:C	8:H:108:ALA:H	1.99	0.65
10:J:63:ALA:HB3	10:J:64:PRO:CD	2.11	0.65
25:2:189:GLU:HA	25:2:192:GLU:CG	2.26	0.65
25:2:270:LEU:HD23	25:2:270:LEU:O	1.96	0.65
1:A:266:MET:CG	1:A:272:ASN:OD1	2.45	0.65
17:Q:101:ASN:O	17:Q:103:VAL:N	2.29	0.65
25:2:57:MET:HA	25:2:60:LEU:HD11	1.77	0.65
8:H:105:SER:HB2	8:H:108:ALA:HB2	1.79	0.65
1:A:152:ASN:O	1:A:153:ILE:CB	2.44	0.65
17:Q:24:GLY:HA2	18:R:209:GLN:CD	2.17	0.65
25:2:236:PHE:CZ	25:2:262:LEU:HD22	2.32	0.64
1:A:890:ARG:NH2	1:A:1023:VAL:HG13	2.12	0.64
3:C:212:ASP:C	3:C:214:ASP:H	1.99	0.64
26:3:17:ALA:CB	26:3:63:HIS:HD2	2.10	0.64
1:A:202:TRP:HB2	1:A:212:LYS:HB3	0.75	0.64
1:A:610:PRO:HB2	1:A:626:THR:HG21	1.79	0.64
1:A:738:GLU:OE2	1:A:797:ARG:HD3	1.97	0.64
2:B:241:ALA:HA	2:B:253:GLY:HA2	1.78	0.64
2:B:326:ALA:HB2	2:B:338:TYR:HE2	1.61	0.64
24:1:13:ASP:OD1	24:1:14:PRO:CD	2.46	0.64
25:2:266:ARG:O	25:2:270:LEU:HB2	1.97	0.64
26:3:131:THR:O	26:3:133:LEU:HD13	1.97	0.64
26:3:192:ASP:HB2	26:3:231:PHE:CE1	2.32	0.64
2:B:489:ILE:HG21	2:B:522:LEU:HD13	1.79	0.64
3:C:67:ARG:NH2	10:J:3:ILE:O	2.28	0.64
25:2:211:GLN:CB	25:2:261:PHE:HE1	2.11	0.64
26:3:149:LYS:HG3	26:3:150:GLU:N	2.12	0.64
1:A:157:GLY:H	1:A:181:HIS:CE1	2.15	0.64
1:A:375:ILE:HB	1:A:666:ARG:HD2	1.80	0.64
3:C:3:TYR:O	11:K:52:LYS:HE3	1.96	0.64
2:B:312:GLN:HB3	19:S:153:ARG:HH22	1.62	0.64
21:V:523:VAL:CG1	24:1:20:LEU:HD23	2.21	0.64
23:0:54:ARG:CD	26:3:182:PHE:CE1	2.60	0.64
24:1:35:ILE:HG22	24:1:46:ILE:CD1	2.27	0.64
25:2:31:LEU:CD1	26:3:33:THR:HG21	2.22	0.64
25:2:45:PHE:HB2	25:2:51:LEU:CD1	2.26	0.64
26:3:14:VAL:HG22	26:3:163:VAL:HA	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:3:58:ALA:CA	26:3:71:TYR:OH	2.39	0.64
1:A:426:ARG:HB3	13:M:40:VAL:CG2	2.19	0.64
2:B:934:LYS:NZ	29:Z:6:C:OP1	2.31	0.64
17:Q:188:TYR:HE1	18:R:211:SER:OG	1.80	0.64
25:2:258:LEU:HG	25:2:262:LEU:CD2	2.28	0.64
25:2:28:PRO:CA	26:3:25:GLN:C	2.66	0.64
26:3:130:GLU:HB2	26:3:173:GLN:HE22	1.61	0.64
26:3:64:ILE:HB	26:3:123:ASP:OD2	1.98	0.64
21:V:517:GLU:HB2	21:V:713:LEU:HD22	1.80	0.64
25:2:140:LYS:HG2	25:2:162:PHE:CE1	2.33	0.64
2:B:1124:ILE:HG22	2:B:1126:ALA:H	1.63	0.64
2:B:602:SER:OG	2:B:620:ARG:NH1	2.31	0.64
13:M:17:ASN:OD1	13:M:18:HIS:N	2.30	0.64
17:Q:113:ARG:HD2	18:R:221:ARG:HB3	1.75	0.64
7:G:94:LYS:NZ	17:Q:162:GLU:OE2	2.30	0.64
17:Q:113:ARG:NH2	18:R:218:LYS:HG2	2.10	0.64
25:2:181:GLN:HG3	25:2:229:ASP:CG	2.17	0.63
25:2:220:LEU:HD13	25:2:220:LEU:O	1.98	0.63
26:3:17:ALA:HB1	26:3:63:HIS:HD2	1.63	0.63
1:A:1116:ASN:C	1:A:1117:VAL:HG23	2.18	0.63
1:A:467:MET:SD	1:A:524:MET:HB3	2.37	0.63
24:1:35:ILE:HA	24:1:46:ILE:HG13	1.80	0.63
25:2:159:VAL:HG11	25:2:161:HIS:HD2	1.62	0.63
1:A:367:ILE:HG21	1:A:501:MET:CG	2.28	0.63
18:R:127:ASN:ND2	20:T:238:GLU:OE1	2.31	0.63
22:W:581:LEU:HD21	22:W:608:ILE:HG21	1.78	0.63
25:2:202:GLN:H	25:2:202:GLN:HE21	1.44	0.63
25:2:177:GLN:OE1	25:2:220:LEU:HD22	1.98	0.63
1:A:1192:TRP:CD1	1:A:1248:ASN:HA	2.34	0.63
1:A:271:ARG:HG2	13:M:73:PRO:CG	2.28	0.63
1:A:271:ARG:CG	13:M:73:PRO:HG3	2.29	0.63
24:1:38:ILE:HB	24:1:44:PHE:HE1	1.63	0.63
26:3:70:LEU:HD13	26:3:115:ILE:CD1	2.28	0.63
2:B:52:GLN:OE1	2:B:160:TYR:OH	2.15	0.63
8:H:57:ARG:HD3	8:H:146:LYS:HD3	1.78	0.63
11:K:56:VAL:HA	11:K:77:THR:HG22	1.81	0.63
26:3:214:TYR:CE2	26:3:216:LYS:HE2	2.32	0.63
23:0:77:LYS:HG2	23:0:225:GLU:OE2	1.99	0.63
25:2:100:LEU:HG	25:2:119:ARG:NE	2.13	0.63
25:2:35:TYR:CZ	25:2:62:LEU:HG	2.34	0.63
26:3:134:ALA:HB2	26:3:176:ASN:OD1	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:691:ASP:OD2	1:A:765:ASN:HB2	1.98	0.63
13:M:10:LEU:CB	13:M:13:VAL:O	2.47	0.63
13:M:44:ARG:HH11	13:M:46:ILE:HG22	1.62	0.63
26:3:64:ILE:CG1	26:3:123:ASP:HB3	2.29	0.63
24:1:18:GLN:NE2	24:1:44:PHE:HZ	1.97	0.63
25:2:123:LEU:HD23	25:2:123:LEU:O	1.99	0.63
26:3:184:ALA:HA	26:3:187:GLN:CG	2.29	0.63
26:3:18:ASN:CG	26:3:64:ILE:HD11	2.19	0.63
26:3:59:VAL:CB	26:3:71:TYR:HE1	1.94	0.63
2:B:453:TRP:CE3	2:B:466:VAL:HG21	2.33	0.63
8:H:23:ASP:O	8:H:25:VAL:N	2.31	0.63
27:X:42:DT:H2'	27:X:43:DT:H71	1.81	0.63
1:A:1116:ASN:OD1	1:A:1136:THR:O	2.17	0.63
2:B:933:ASP:OD2	2:B:1050:ARG:NH2	2.32	0.63
2:B:95:LYS:HD3	2:B:162:LEU:HD21	1.80	0.63
6:F:125:ILE:HG22	6:F:127:ASP:H	1.63	0.63
8:H:7:GLU:OE2	8:H:57:ARG:NH2	2.32	0.63
20:T:12:ALA:HB2	20:T:106:LEU:HD23	1.81	0.63
25:2:60:LEU:HD11	25:2:95:ILE:CB	2.29	0.62
1:A:157:GLY:N	1:A:181:HIS:CE1	2.68	0.62
2:B:882:SER:O	2:B:887:TYR:CG	2.52	0.62
13:M:34:CYS:HB3	13:M:39:LEU:CB	2.29	0.62
13:M:34:CYS:HB3	13:M:39:LEU:HD23	0.64	0.62
17:Q:112:ARG:HH21	18:R:237:LEU:HD22	1.63	0.62
25:2:117:ASN:ND2	26:3:42:MET:CE	2.60	0.62
2:B:626:LEU:HD23	2:B:662:VAL:HG12	1.79	0.62
9:I:99:SER:OG	9:I:100:HIS:N	2.32	0.62
24:1:2:VAL:HG12	25:2:422:LEU:CD1	2.27	0.62
25:2:160:LEU:HB3	25:2:206:LEU:CD1	2.27	0.62
26:3:165:LYS:HD3	26:3:165:LYS:O	1.98	0.62
25:2:30:VAL:CG2	26:3:25:GLN:CB	2.48	0.62
1:A:208:ASP:OD1	1:A:209:SER:N	2.32	0.62
3:C:42:VAL:HB	3:C:178:PRO:HG2	1.81	0.62
12:L:26:ASN:HB2	12:L:44:MET:HE2	1.78	0.62
19:S:166:ARG:HH11	19:S:166:ARG:HG3	1.64	0.62
22:W:59:TYR:OH	22:W:63:TYR:CE2	2.52	0.62
25:2:181:GLN:CD	25:2:229:ASP:HB2	2.20	0.62
24:1:1:MET:HB2	25:2:418:PHE:HB3	1.81	0.62
26:3:18:ASN:O	26:3:21:TRP:HD1	1.82	0.62
8:H:106:THR:O	8:H:108:ALA:N	2.32	0.62
17:Q:180:PHE:HE2	18:R:213:ASP:CG	1.68	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:99:LEU:O	17:Q:101:ASN:N	2.25	0.62
17:Q:184:ILE:CD1	18:R:211:SER:HB2	2.20	0.62
25:2:173:GLN:HG2	25:2:179:LEU:HG	1.81	0.62
1:A:355:MET:HE1	1:A:1431:SER:HB2	1.82	0.62
2:B:956:PHE:HB3	2:B:962:THR:HG22	1.81	0.62
21:V:612:ASP:CG	21:V:635:GLN:OE1	2.37	0.62
22:W:584:TYR:CG	22:W:594:ALA:HB2	2.34	0.62
21:V:516:PRO:CA	24:1:15:ALA:O	2.45	0.62
25:2:93:LEU:HA	25:2:96:TRP:HD1	1.64	0.62
26:3:160:ARG:NH2	26:3:190:LEU:HD12	2.13	0.62
26:3:58:ALA:CA	26:3:71:TYR:CE2	2.78	0.62
21:V:667:THR:HA	24:1:62:ASP:CG	2.19	0.62
25:2:203:PHE:HD2	25:2:205:LEU:HD23	1.64	0.62
25:2:218:GLN:HG2	25:2:268:PHE:HB3	1.82	0.62
26:3:133:LEU:HD22	26:3:134:ALA:N	2.14	0.62
26:3:216:LYS:H	26:3:216:LYS:CD	2.13	0.62
25:2:31:LEU:CG	26:3:33:THR:HB	2.28	0.62
14:N:319:ASP:C	14:N:321:SER:H	2.03	0.62
1:A:47:THR:O	1:A:48:GLU:CB	2.47	0.62
2:B:810:PHE:N	2:B:925:SER:O	2.29	0.62
12:L:35:ARG:NH1	12:L:42:ARG:HH21	1.98	0.62
17:Q:35:ASP:OD2	18:R:161:ARG:NH2	2.26	0.62
17:Q:114:ILE:CD1	18:R:218:LYS:HE3	2.29	0.62
24:1:50:VAL:HA	24:1:53:LEU:HD13	1.82	0.62
24:1:38:ILE:HB	24:1:44:PHE:CE1	2.34	0.62
25:2:189:GLU:O	25:2:193:PRO:HD2	2.00	0.62
25:2:46:ARG:CD	25:2:85:GLU:HB2	2.30	0.62
25:2:89:LEU:HD23	25:2:89:LEU:O	1.99	0.62
1:A:531:ASN:HD22	1:A:901:VAL:HG23	1.65	0.62
1:A:1372:GLU:HG3	5:E:193:ILE:HD13	1.81	0.62
2:B:899:SER:O	2:B:901:THR:N	2.33	0.61
6:F:65:VAL:HG22	6:F:104:ILE:HD11	1.81	0.61
21:V:613:THR:O	21:V:614:SER:CB	2.30	0.61
22:W:37:HIS:CE1	22:W:454:VAL:CG1	2.82	0.61
24:1:1:MET:HG2	25:2:414:SER:N	2.15	0.61
1:A:1480:CYS:O	1:A:1484:MET:HG3	2.00	0.61
21:V:612:ASP:O	21:V:614:SER:N	2.33	0.61
24:1:8:VAL:O	25:2:407:VAL:HG12	1.99	0.61
25:2:60:LEU:CD1	25:2:95:ILE:HB	2.31	0.61
1:A:935:GLN:HG2	1:A:1059:ARG:HH12	1.65	0.61
2:B:1115:GLN:HB2	2:B:1148:LEU:HD21	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:2:236:PHE:CE2	25:2:262:LEU:HD13	2.36	0.61
2:B:225:LEU:CD1	2:B:228:SER:CB	2.78	0.61
13:M:7:LEU:HD11	13:M:10:LEU:CD1	2.31	0.61
15:O:41:ASP:OD1	15:O:45:ASN:ND2	2.33	0.61
17:Q:165:GLU:HB3	17:Q:170:LYS:HE2	1.82	0.61
26:3:9:ASN:O	26:3:56:LYS:HD3	1.99	0.61
2:B:329:GLY:O	2:B:335:ARG:NE	2.34	0.61
21:V:368:ALA:O	21:V:371:VAL:HG22	2.00	0.61
22:W:584:TYR:HB2	22:W:594:ALA:HB2	1.81	0.61
26:3:70:LEU:CD1	26:3:115:ILE:HD11	2.27	0.61
26:3:8:LEU:HA	26:3:54:SER:HB3	1.83	0.61
1:A:376:ASP:HB3	1:A:522:PRO:HD3	1.82	0.61
2:B:489:ILE:HG13	2:B:490:GLY:H	1.65	0.61
8:H:65:TYR:HE1	8:H:84:ARG:HE	1.47	0.61
18:R:163:LEU:HD12	18:R:163:LEU:O	2.01	0.61
28:Y:24:DC:C2'	28:Y:25:DT:H72	2.30	0.61
24:1:1:MET:HA	25:2:414:SER:N	2.15	0.61
25:2:30:VAL:HG23	26:3:25:GLN:HB2	1.74	0.61
26:3:190:LEU:H	26:3:190:LEU:CD2	2.12	0.61
1:A:1116:ASN:ND2	1:A:1138:SER:HB2	2.14	0.61
1:A:202:TRP:CB	1:A:212:LYS:CB	2.53	0.61
5:E:166:ARG:HB2	5:E:169:GLN:HG3	1.80	0.61
8:H:65:TYR:CE2	8:H:70:LEU:HB3	2.36	0.61
12:L:15:MET:HB3	12:L:29:LYS:HB3	1.83	0.61
21:V:316:LEU:HB2	21:V:321:GLU:CG	2.29	0.61
21:V:366:ASN:HD21	21:V:613:THR:CG2	2.11	0.61
28:Y:49:DG:N2	29:Z:4:C:O2	2.34	0.61
24:1:47:ALA:HB1	24:1:50:VAL:HB	1.81	0.61
26:3:173:GLN:CA	26:3:176:ASN:HD21	2.10	0.61
1:A:1305:SER:OG	1:A:1306:LYS:N	2.33	0.61
1:A:608:THR:CB	1:A:610:PRO:HD2	2.30	0.61
1:A:60:PRO:HD2	1:A:62:GLN:HG2	1.83	0.61
4:D:70:ARG:NH2	7:G:140:ASP:O	2.33	0.61
13:M:178:LYS:C	20:T:154:LYS:CB	2.69	0.61
16:P:206:GLU:HG3	16:P:207:PRO:HD3	1.82	0.61
21:V:520:ARG:HD3	24:1:19:PHE:HB3	1.82	0.61
21:V:523:VAL:CB	24:1:20:LEU:HD23	2.31	0.61
25:2:83:GLN:OE1	25:2:83:GLN:HA	2.01	0.61
1:A:206:ASN:O	1:A:207:GLU:HG3	1.99	0.61
1:A:426:ARG:CD	13:M:40:VAL:HG11	2.31	0.61
13:M:27:TYR:HE2	13:M:46:ILE:CD1	2.14	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:42:CYS:C	17:Q:95:ASN:HD21	2.04	0.61
25:2:251:VAL:CG1	25:2:254:MET:HG3	2.30	0.61
26:3:143:TYR:O	26:3:146:ARG:HG2	2.01	0.61
26:3:178:MET:HE2	26:3:202:LEU:CD1	2.30	0.61
2:B:1130:THR:HB	2:B:1133:HIS:HB2	1.83	0.61
10:J:3:ILE:HG13	10:J:52:HIS:CE1	2.36	0.61
13:M:52:TRP:O	13:M:54:THR:N	2.31	0.61
22:W:209:TYR:CE1	22:W:233:PHE:CD1	2.89	0.61
22:W:73:CYS:CB	22:W:209:TYR:CZ	2.84	0.61
21:V:520:ARG:HG3	24:1:23:LEU:HD11	1.82	0.60
25:2:173:GLN:CD	25:2:179:LEU:HD21	2.22	0.60
25:2:164:VAL:HG13	25:2:209:PRO:HG2	1.83	0.60
26:3:100:LYS:HG3	26:3:101:TYR:N	2.16	0.60
26:3:148:ASN:CB	26:3:157:MET:HE2	2.27	0.60
2:B:461:GLN:NE2	27:X:43:DT:O2	2.34	0.60
16:P:297:LYS:HB2	16:P:298:PRO:HD2	1.82	0.60
26:3:222:SER:HB2	26:3:226:TYR:CE2	2.36	0.60
1:A:486:LEU:HD22	2:B:790:GLN:CD	2.22	0.60
1:A:608:THR:OG1	1:A:610:PRO:HG3	2.01	0.60
1:A:865:ILE:O	1:A:869:GLU:HB3	2.01	0.60
9:I:14:ILE:HG13	9:I:16:PHE:CE1	2.36	0.60
17:Q:108:ASP:OD2	18:R:237:LEU:HD22	2.01	0.60
22:W:423:ASP:C	22:W:425:THR:H	2.04	0.60
22:W:423:ASP:O	22:W:425:THR:N	2.34	0.60
25:2:159:VAL:HG13	25:2:160:LEU:N	2.17	0.60
2:B:553:LEU:HD13	2:B:573:TRP:CZ3	2.36	0.60
9:I:29:ASP:OD2	9:I:32:ASN:ND2	2.28	0.60
24:1:1:MET:HA	25:2:413:LEU:HA	1.83	0.60
9:I:58:ILE:O	9:I:58:ILE:HG22	2.00	0.60
20:T:94:THR:HG23	20:T:109:ILE:HG22	1.83	0.60
22:W:584:TYR:CE2	22:W:614:TYR:HB2	2.36	0.60
2:B:80:GLU:OE1	2:B:134:LYS:HE2	2.00	0.60
10:J:63:ALA:CB	10:J:64:PRO:CD	2.73	0.60
18:R:223:VAL:CG2	18:R:224:THR:CB	2.77	0.60
25:2:30:VAL:HG12	25:2:34:LEU:HD23	1.82	0.60
2:B:712:PRO:O	2:B:939:HIS:HE1	1.84	0.60
20:T:146:ASP:O	20:T:147:LYS:HB3	2.01	0.60
24:1:9:LEU:CB	24:1:51:ASN:HD21	2.14	0.60
24:1:1:MET:HB3	25:2:413:LEU:HG	1.83	0.60
1:A:931:ARG:O	1:A:933:THR:N	2.35	0.60
17:Q:171:LYS:O	17:Q:173:ALA:N	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:28:ILE:HD13	20:T:95:VAL:HG22	1.82	0.60
21:V:366:ASN:ND2	21:V:613:THR:CG2	2.65	0.60
2:B:861:SER:N	2:B:864:ASP:OD2	2.34	0.60
18:R:166:ILE:HG22	18:R:168:LEU:H	1.66	0.60
23:0:55:LEU:HD12	26:3:178:MET:CE	2.31	0.60
25:2:206:LEU:HD22	25:2:206:LEU:N	2.17	0.60
2:B:959:GLU:OE2	2:B:961:ILE:HB	2.01	0.60
17:Q:113:ARG:CD	18:R:222:SER:CA	2.77	0.60
21:V:366:ASN:ND2	21:V:613:THR:HG22	2.15	0.60
26:3:21:TRP:O	26:3:24:LYS:HB2	2.02	0.60
2:B:552:ASN:OD1	2:B:553:LEU:N	2.35	0.60
13:M:10:LEU:H	13:M:10:LEU:HD22	1.65	0.60
13:M:94:ASP:O	13:M:96:PHE:N	2.35	0.60
20:T:82:PRO:HG2	20:T:117:ARG:HB2	1.83	0.60
24:1:53:LEU:HD12	24:1:53:LEU:N	2.17	0.59
25:2:171:VAL:HG13	25:2:216:MET:HB2	1.83	0.59
26:3:14:VAL:HG23	26:3:163:VAL:HA	1.84	0.59
2:B:866:ILE:HD12	2:B:921:ILE:HD11	1.82	0.59
1:A:1188:GLU:HG3	9:I:1:MET:HG2	1.83	0.59
13:M:36:GLU:OE1	13:M:36:GLU:N	2.34	0.59
2:B:51:ILE:HG22	20:T:141:LEU:CD2	2.32	0.59
24:1:18:GLN:HB2	24:1:44:PHE:CZ	2.37	0.59
25:2:202:GLN:H	25:2:202:GLN:NE2	2.00	0.59
26:3:213:LEU:HD23	26:3:230:VAL:HG12	1.84	0.59
1:A:890:ARG:HE	1:A:1023:VAL:HG22	1.67	0.59
1:A:263:ALA:HA	1:A:272:ASN:O	2.02	0.59
1:A:545:VAL:HG22	1:A:676:ILE:HG13	1.84	0.59
9:I:15:ARG:HD2	9:I:37:TYR:CD2	2.37	0.59
28:Y:49:DG:H2'	28:Y:50:DA:C8	2.37	0.59
26:3:110:VAL:O	26:3:114:GLU:HG2	2.02	0.59
1:A:1026:ASP:O	1:A:1031:ARG:NH1	2.36	0.59
1:A:930:LEU:O	1:A:931:ARG:O	2.19	0.59
2:B:225:LEU:HB3	2:B:228:SER:HB3	1.49	0.59
2:B:881:GLU:C	2:B:883:THR:H	2.05	0.59
8:H:96:VAL:HG22	8:H:116:VAL:HG13	1.84	0.59
13:M:86:LYS:HE3	13:M:86:LYS:HA	1.83	0.59
18:R:223:VAL:HA	18:R:224:THR:HG22	1.79	0.59
22:W:584:TYR:HB2	22:W:594:ALA:CB	2.32	0.59
28:Y:48:DC:H2'	28:Y:49:DG:C8	2.37	0.59
25:2:56:VAL:HG11	25:2:91:SER:CB	2.31	0.59
1:A:579:ILE:HB	1:A:585:LEU:HB2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:347:ASN:ND2	14:N:375:GLU:OE2	2.35	0.59
20:T:158:ASN:HB3	20:T:161:TYR:HB2	1.84	0.59
22:W:37:HIS:ND1	22:W:454:VAL:HG13	2.15	0.59
5:E:52:ARG:NH2	5:E:54:ARG:HD3	2.18	0.59
13:M:59:LYS:HB2	29:Z:1:A:H5'	1.83	0.59
24:1:59:GLU:CD	25:2:402:ARG:NH1	2.56	0.59
1:A:1022:ILE:HG23	1:A:1023:VAL:HG23	1.84	0.59
2:B:226:GLU:O	2:B:227:ASN:HB2	2.00	0.59
2:B:631:GLN:HB3	2:B:685:LYS:NZ	2.18	0.59
17:Q:24:GLY:HA2	18:R:209:GLN:HG2	1.83	0.59
25:2:215:PHE:CD2	25:2:264:HIS:HB2	2.38	0.59
1:A:33:ARG:HB3	2:B:1139:GLY:HA2	1.85	0.59
1:A:926:ASN:OD1	1:A:931:ARG:CB	2.51	0.59
3:C:154:ARG:NH2	10:J:61:ASN:OD1	2.35	0.59
26:3:215:LEU:CD1	26:3:230:VAL:HG13	2.32	0.59
25:2:30:VAL:CB	26:3:25:GLN:HB3	2.32	0.59
1:A:386:ALA:HA	1:A:449:HIS:CD2	2.38	0.59
3:C:147:ASP:O	10:J:16:ASN:HB3	2.03	0.59
5:E:64:HIS:C	5:E:66:ASP:N	2.56	0.59
18:R:194:ARG:C	18:R:196:ASP:N	2.40	0.59
24:1:38:ILE:CD1	24:1:38:ILE:H	2.16	0.59
2:B:226:GLU:O	2:B:226:GLU:HG2	2.01	0.59
19:S:44:GLN:HB2	19:S:103:ASN:HA	1.84	0.59
24:1:34:ILE:HG22	24:1:46:ILE:CD1	2.32	0.59
26:3:131:THR:HG23	26:3:133:LEU:CD1	2.33	0.59
1:A:1116:ASN:O	1:A:1117:VAL:CB	2.51	0.59
1:A:154:CYS:O	1:A:184:CYS:O	2.21	0.59
1:A:486:LEU:HD22	2:B:790:GLN:OE1	2.03	0.59
1:A:51:ARG:H	1:A:52:PRO:HD2	1.66	0.59
2:B:419:ALA:O	2:B:423:ILE:HG12	2.03	0.59
25:2:160:LEU:HD12	25:2:160:LEU:N	2.18	0.58
25:2:196:ILE:HA	25:2:202:GLN:OE1	2.02	0.58
25:2:217:LEU:HD23	25:2:233:ILE:CD1	2.32	0.58
2:B:1005:ALA:C	2:B:1007:ASN:H	2.04	0.58
19:S:10:ASN:OD1	19:S:11:VAL:N	2.36	0.58
24:1:2:VAL:HB	25:2:456:LYS:HD3	1.86	0.58
26:3:21:TRP:CD2	26:3:34:LEU:HD23	2.38	0.58
2:B:798:ARG:O	2:B:801:VAL:HG22	2.03	0.58
9:I:14:ILE:HG13	9:I:16:PHE:CD2	2.37	0.58
24:1:19:PHE:O	24:1:23:LEU:HG	2.02	0.58
24:1:34:ILE:O	24:1:46:ILE:HG13	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:2:203:PHE:CE2	25:2:205:LEU:HD23	2.38	0.58
25:2:177:GLN:HE22	25:2:220:LEU:HA	1.68	0.58
24:1:2:VAL:CG1	25:2:456:LYS:CD	2.82	0.58
2:B:1079:SER:O	2:B:1080:ARG:HD2	2.03	0.58
2:B:1117:HIS:HB2	2:B:1127:ILE:HG12	1.84	0.58
2:B:133:ILE:CG2	2:B:139:GLN:HG2	2.18	0.58
2:B:225:LEU:HD22	2:B:228:SER:HB2	1.85	0.58
2:B:470:LEU:HD21	2:B:478:THR:HG23	1.83	0.58
13:M:311:ASP:OD2	13:M:312:LYS:NZ	2.36	0.58
25:2:28:PRO:HA	26:3:33:THR:HB	1.85	0.58
26:3:215:LEU:HD12	26:3:230:VAL:HG13	1.85	0.58
13:M:27:TYR:HE2	13:M:46:ILE:HD13	1.68	0.58
26:3:59:VAL:HB	26:3:71:TYR:CD1	2.25	0.58
2:B:510:CYS:HB2	2:B:705:GLY:HA3	1.84	0.58
3:C:4:ALA:HA	11:K:52:LYS:NZ	2.18	0.58
13:M:179:GLU:HA	20:T:154:LYS:CG	2.24	0.58
26:3:131:THR:CG2	26:3:133:LEU:HD12	2.33	0.58
1:A:1464:ALA:O	1:A:1469:GLY:HA3	2.03	0.58
1:A:320:ASN:HB2	1:A:338:SER:OG	2.03	0.58
2:B:357:CYS:HB2	2:B:360:LYS:HD2	1.85	0.58
17:Q:113:ARG:HH22	18:R:218:LYS:CG	2.11	0.58
22:W:419:GLU:O	22:W:420:PRO:O	2.20	0.58
23:0:109:THR:HB	23:0:144:SER:H	1.67	0.58
25:2:236:PHE:CZ	25:2:258:LEU:HD11	2.39	0.58
1:A:131:ALA:C	1:A:133:SER:H	2.00	0.58
2:B:906:GLN:CG	12:L:45:TYR:HE1	2.17	0.58
3:C:274:ILE:HD11	11:K:31:CYS:SG	2.43	0.58
13:M:27:TYR:CE2	13:M:46:ILE:HD13	2.39	0.58
1:A:30:GLU:OE1	1:A:33:ARG:NH2	2.24	0.58
2:B:880:LEU:O	2:B:881:GLU:OE1	2.22	0.58
11:K:63:VAL:HG22	11:K:71:ILE:HG22	1.86	0.58
25:2:44:VAL:HG13	25:2:45:PHE:N	2.17	0.58
26:3:169:ASP:CB	26:3:202:LEU:HD23	2.33	0.58
1:A:1372:GLU:OE2	5:E:207:ARG:NH1	2.36	0.58
21:V:612:ASP:OD2	21:V:635:GLN:CD	2.42	0.58
26:3:160:ARG:HB3	26:3:190:LEU:CD2	2.32	0.58
26:3:16:ASP:O	26:3:21:TRP:NE1	2.27	0.58
1:A:1307:VAL:HG11	1:A:1339:ASP:HB2	1.86	0.58
2:B:881:GLU:C	2:B:883:THR:N	2.55	0.58
1:A:79:THR:HG23	13:M:43:ASP:HB2	1.81	0.58
13:M:59:LYS:HG3	13:M:64:PRO:HG2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:3:190:LEU:HD23	26:3:190:LEU:N	2.18	0.57
25:2:30:VAL:N	26:3:25:GLN:HB3	2.19	0.57
2:B:290:TYR:OH	2:B:566:LYS:NZ	2.36	0.57
7:G:144:ARG:N	7:G:169:GLY:O	2.34	0.57
13:M:94:ASP:HB2	13:M:99:SER:N	2.09	0.57
17:Q:113:ARG:HD3	18:R:222:SER:CA	2.34	0.57
22:W:584:TYR:CB	22:W:594:ALA:HB2	2.33	0.57
25:2:35:TYR:CB	25:2:62:LEU:HD12	2.33	0.57
26:3:196:LEU:CD2	26:3:223:LEU:HD23	2.25	0.57
2:B:80:GLU:O	2:B:82:PRO:N	2.37	0.57
26:3:210:THR:O	26:3:210:THR:HG22	2.04	0.57
26:3:46:ASN:CG	26:3:104:LEU:HD22	2.25	0.57
2:B:92:TYR:HE2	2:B:146:LYS:HE2	1.69	0.57
2:B:446:TYR:HB2	28:Y:59:DG:OP1	2.05	0.57
2:B:895:PHE:O	2:B:897:ARG:HG3	2.04	0.57
1:A:426:ARG:H	13:M:40:VAL:HG21	1.69	0.57
16:P:171:THR:HG22	16:P:220:VAL:HG22	1.87	0.57
24:1:8:VAL:HG12	24:1:9:LEU:H	1.69	0.57
25:2:29:GLY:CA	26:3:25:GLN:CG	2.78	0.57
2:B:92:TYR:HB3	20:T:145:LEU:HD12	1.87	0.57
2:B:94:SER:O	2:B:122:ALA:HB1	2.04	0.57
25:2:197:THR:HG21	25:2:239:GLN:CD	2.24	0.57
25:2:82:ALA:HA	25:2:89:LEU:HD11	1.85	0.57
26:3:14:VAL:HG23	26:3:163:VAL:HG13	1.86	0.57
1:A:935:GLN:HA	1:A:1059:ARG:HH22	1.67	0.57
1:A:1123:ARG:NH2	1:A:1381:GLU:OE1	2.31	0.57
2:B:81:PRO:HD2	2:B:135:GLU:HG3	1.87	0.57
27:X:49:DT:H2'	27:X:50:DT:H4'	1.86	0.57
25:2:163:MET:HE1	25:2:206:LEU:HB3	1.84	0.57
26:3:144:ILE:HG12	26:3:147:MET:CE	2.34	0.57
26:3:187:GLN:NE2	26:3:189:ILE:HG13	2.20	0.57
1:A:608:THR:OG1	1:A:610:PRO:CD	2.52	0.57
10:J:64:PRO:C	10:J:66:GLU:H	2.08	0.57
1:A:334:ARG:NH2	13:M:66:ARG:O	2.37	0.57
17:Q:24:GLY:HA2	18:R:209:GLN:CG	2.34	0.57
26:3:178:MET:HE2	26:3:202:LEU:HD12	1.87	0.57
1:A:927:GLU:HB3	1:A:931:ARG:HD3	1.87	0.57
2:B:761:THR:OG1	2:B:764:MET:HG3	2.05	0.57
3:C:90:CYS:SG	3:C:94:CYS:HB3	2.43	0.57
6:F:88:ASP:OD1	6:F:91:LEU:N	2.33	0.57
21:V:321:GLU:HA	22:W:499:ASN:HD21	1.65	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:805:ARG:NH2	2:B:671:GLU:O	2.37	0.57
25:2:117:ASN:CG	26:3:42:MET:HE2	2.24	0.57
25:2:118:LEU:CD2	26:3:39:ASP:C	2.72	0.57
25:2:185:MET:HB2	25:2:229:ASP:OD1	2.04	0.57
25:2:47:GLU:HG3	25:2:48:LEU:N	2.20	0.57
25:2:60:LEU:HD11	25:2:95:ILE:CG2	2.35	0.57
1:A:426:ARG:N	13:M:40:VAL:HG21	2.20	0.57
5:E:52:ARG:CZ	5:E:54:ARG:HG3	2.35	0.57
3:C:5:ASN:N	11:K:97:GLU:OE2	2.38	0.57
2:B:1053:HIS:CE1	2:B:1058:LYS:HG3	2.40	0.57
21:V:514:MET:SD	21:V:537:ASN:ND2	2.78	0.57
25:2:160:LEU:H	25:2:160:LEU:CD1	2.18	0.56
26:3:195:VAL:HG21	26:3:214:TYR:OH	2.05	0.56
1:A:1123:ARG:NH2	1:A:1360:ASN:HB2	2.19	0.56
1:A:355:MET:CE	1:A:1431:SER:HB2	2.35	0.56
2:B:422:PHE:CD1	2:B:422:PHE:C	2.77	0.56
9:I:15:ARG:O	9:I:24:LEU:HD12	2.04	0.56
9:I:84:HIS:HB3	9:I:92:LYS:HB3	1.86	0.56
18:R:155:LEU:HD13	18:R:204:ASN:HD22	1.70	0.56
1:A:322:LEU:HD12	1:A:323:PRO:HD2	1.87	0.56
1:A:567:LEU:HG	1:A:671:ASN:OD1	2.04	0.56
2:B:1029:TYR:CE1	2:B:1036:LYS:HE2	2.38	0.56
2:B:232:THR:HG23	2:B:233:SER:H	1.69	0.56
2:B:716:HIS:CD2	2:B:982:ILE:HG13	2.30	0.56
17:Q:125:ALA:HB1	17:Q:138:ASP:HB3	1.87	0.56
25:2:117:ASN:HB2	26:3:104:LEU:CD1	2.35	0.56
25:2:423:ALA:HA	25:2:426:ARG:HE	1.70	0.56
2:B:718:GLN:HG2	2:B:720:PRO:HD2	1.87	0.56
17:Q:77:ARG:HB2	17:Q:93:PHE:HB3	1.86	0.56
22:W:209:TYR:OH	22:W:233:PHE:C	2.42	0.56
25:2:28:PRO:HD2	26:3:25:GLN:CD	2.25	0.56
1:A:904:GLN:NE2	1:A:982:ASN:HA	2.20	0.56
3:C:60:HIS:CE1	3:C:63:PHE:HB2	2.39	0.56
14:N:313:PRO:HG2	16:P:235:ARG:NH2	2.17	0.56
17:Q:115:GLU:HA	17:Q:118:GLU:HB3	1.88	0.56
26:3:144:ILE:HD13	26:3:147:MET:HE3	1.85	0.56
1:A:1466:ALA:O	1:A:1469:GLY:N	2.39	0.56
2:B:133:ILE:O	2:B:133:ILE:HG22	2.06	0.56
3:C:5:ASN:C	3:C:7:PRO:HD3	2.25	0.56
13:M:72:ASN:HB2	28:Y:58:DC:H42	1.70	0.56
17:Q:21:VAL:HA	18:R:210:PHE:CE2	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:3:223:LEU:HD11	26:3:227:LEU:HD11	1.87	0.56
26:3:42:MET:SD	26:3:111:ILE:HD13	2.46	0.56
1:A:1004:LEU:HD13	1:A:1062:GLY:HA2	1.88	0.56
1:A:1211:LEU:HD11	1:A:1258:ARG:HG3	1.86	0.56
1:A:455:ILE:HG12	1:A:473:ARG:HG2	1.87	0.56
16:P:158:SER:C	16:P:160:GLY:H	2.07	0.56
16:P:257:ASN:ND2	27:X:14:DA:N3	2.54	0.56
26:3:19:PRO:HG2	26:3:123:ASP:O	2.05	0.56
1:A:1154:ALA:HB1	1:A:1310:HIS:CE1	2.41	0.56
1:A:375:ILE:HB	1:A:666:ARG:CD	2.35	0.56
1:A:65:ILE:HA	1:A:78:MET:HE2	1.87	0.56
2:B:166:LEU:HB3	2:B:170:ASP:HB2	1.87	0.56
2:B:758:LEU:HD13	2:B:991:ALA:HB2	1.88	0.56
13:M:103:ASN:HB3	13:M:105:ARG:HH22	1.69	0.56
21:V:426:VAL:HG13	21:V:427:MET:H	1.69	0.56
24:1:17:LYS:O	24:1:20:LEU:HB3	2.05	0.56
25:2:130:SER:HB2	25:2:173:GLN:OE1	2.06	0.56
25:2:206:LEU:H	25:2:206:LEU:HD22	1.71	0.56
24:1:1:MET:CB	25:2:418:PHE:HB2	2.35	0.56
26:3:223:LEU:O	26:3:223:LEU:HD13	2.06	0.56
1:A:1188:GLU:O	1:A:1192:TRP:HZ3	1.87	0.56
1:A:790:GLN:HE22	1:A:821:GLY:HA3	1.71	0.56
2:B:501:LEU:HD12	2:B:505:LEU:HD12	1.86	0.56
5:E:62:VAL:O	5:E:63:ALA:HB2	2.05	0.56
17:Q:113:ARG:NH1	18:R:218:LYS:C	2.59	0.56
23:0:73:ASP:O	23:0:79:ASN:HA	2.06	0.56
26:3:24:LYS:O	26:3:25:GLN:C	2.44	0.56
1:A:139:LYS:HE2	1:A:143:HIS:NE2	2.20	0.56
7:G:94:LYS:O	7:G:110:ARG:NH1	2.34	0.56
8:H:8:ASP:HB3	8:H:10:PHE:CE1	2.39	0.56
13:M:17:ASN:OD1	13:M:18:HIS:ND1	2.39	0.56
15:O:28:ILE:HB	15:O:32:LEU:HD23	1.86	0.56
26:3:178:MET:SD	26:3:181:ILE:HD12	2.46	0.56
2:B:206:TYR:HD1	2:B:208:PHE:HE1	1.54	0.56
2:B:625:LEU:HD13	2:B:675:LEU:HD11	1.87	0.56
3:C:157:GLN:HG2	10:J:65:LEU:HB2	1.83	0.56
2:B:605:ARG:NH2	9:I:71:ASP:OD2	2.39	0.56
9:I:96:PHE:HB3	9:I:112:TYR:HD1	1.72	0.56
18:R:181:ALA:HA	18:R:184:ALA:HB3	1.88	0.56
18:R:184:ALA:HA	18:R:187:ASP:HB3	1.87	0.56
24:1:10:ILE:C	24:1:10:ILE:HD13	2.26	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:1:52:VAL:HG22	24:1:53:LEU:HD12	1.87	0.55
24:1:1:MET:CG	25:2:418:PHE:HB2	2.35	0.55
2:B:270:ILE:HG21	2:B:308:ALA:HB2	1.87	0.55
1:A:264:VAL:HG21	13:M:68:GLY:HA3	1.88	0.55
16:P:158:SER:C	16:P:160:GLY:N	2.60	0.55
17:Q:149:THR:HG23	17:Q:151:THR:H	1.72	0.55
24:1:34:ILE:HG23	24:1:50:VAL:HG11	1.89	0.55
25:2:159:VAL:HG22	25:2:160:LEU:N	2.16	0.55
25:2:37:HIS:HB3	25:2:38:PRO:CD	2.35	0.55
26:3:133:LEU:CD1	26:3:133:LEU:H	2.10	0.55
2:B:474:THR:HG23	2:B:732:ALA:O	2.05	0.55
5:E:64:HIS:O	5:E:66:ASP:N	2.37	0.55
8:H:16:ASP:HB3	8:H:19:GLY:HA2	1.89	0.55
3:C:154:ARG:NH1	10:J:61:ASN:HA	2.21	0.55
13:M:94:ASP:HB3	13:M:99:SER:N	2.21	0.55
17:Q:108:ASP:O	17:Q:111:ARG:HG2	2.06	0.55
17:Q:25:PHE:N	18:R:210:PHE:CE2	2.74	0.55
19:S:27:ASN:O	20:T:95:VAL:HG13	2.06	0.55
1:A:644:SER:O	1:A:651:SER:HB3	2.06	0.55
5:E:52:ARG:NH2	5:E:54:ARG:CD	2.70	0.55
7:G:138:GLN:HG2	7:G:139:GLN:HG2	1.89	0.55
1:A:298:ALA:H	17:Q:60:ARG:HE	1.53	0.55
25:2:181:GLN:HA	25:2:181:GLN:HE21	1.70	0.55
2:B:225:LEU:CG	2:B:228:SER:CB	2.84	0.55
1:A:1287:CYS:HA	2:B:250:SER:HB2	1.88	0.55
24:1:1:MET:HE1	25:2:440:LEU:HD13	1.88	0.55
1:A:138:LYS:N	1:A:1445:HIS:HE1	2.04	0.55
1:A:1036:ASN:ND2	5:E:202:ARG:O	2.29	0.55
13:M:27:TYR:CD2	13:M:46:ILE:CG2	2.89	0.55
18:R:204:ASN:OD1	18:R:205:ASP:N	2.39	0.55
17:Q:112:ARG:HH22	18:R:237:LEU:HB2	1.72	0.55
20:T:93:LEU:HB2	20:T:110:VAL:HB	1.89	0.55
27:X:70:DG:N2	28:Y:25:DT:O2	2.39	0.55
24:1:1:MET:HB2	25:2:418:PHE:HB2	1.88	0.55
24:1:31:LYS:O	24:1:32:LYS:HB2	2.06	0.55
24:1:36:GLN:HB3	24:1:45:VAL:HG12	1.88	0.55
24:1:3:ASN:CB	25:2:412:PHE:O	2.54	0.55
19:S:6:PRO:HG3	19:S:10:ASN:HD22	1.71	0.55
25:2:117:ASN:CG	26:3:108:ASN:ND2	2.50	0.55
1:A:263:ALA:O	1:A:265:VAL:HG22	2.07	0.55
1:A:47:THR:C	1:A:48:GLU:CG	2.75	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:546:ARG:NH1	1:A:768:SER:OG	2.39	0.55
1:A:1373:ALA:HB2	5:E:145:VAL:HG22	1.88	0.55
2:B:906:GLN:HG2	12:L:45:TYR:CE1	2.39	0.55
20:T:177:ARG:NH2	27:X:19:DG:OP1	2.39	0.55
26:3:44:LEU:HD13	26:3:44:LEU:O	2.06	0.55
1:A:328:ALA:HA	13:M:84:ILE:HG22	1.89	0.55
2:B:45:ASP:HB3	2:B:534:VAL:HG11	1.88	0.55
2:B:649:ASN:OD1	2:B:650:ASN:N	2.40	0.55
17:Q:188:TYR:OH	18:R:210:PHE:HE1	1.79	0.55
20:T:203:VAL:HG11	20:T:210:VAL:HG22	1.88	0.55
23:0:72:GLU:O	23:0:79:ASN:CB	2.55	0.55
24:1:38:ILE:HA	24:1:44:PHE:CD1	2.37	0.55
25:2:177:GLN:NE2	25:2:220:LEU:HA	2.22	0.55
25:2:211:GLN:HB3	25:2:261:PHE:CE1	2.40	0.55
1:A:265:VAL:HG21	13:M:48:VAL:HB	1.88	0.55
1:A:601:ASN:HD21	1:A:632:ASN:H	1.55	0.55
2:B:894:THR:HG23	2:B:897:ARG:NH1	2.22	0.55
12:L:26:ASN:HB2	12:L:44:MET:HE1	1.86	0.55
17:Q:170:LYS:HG2	17:Q:171:LYS:H	1.72	0.55
2:B:1087:GLY:HA3	28:Y:48:DC:OP1	2.07	0.55
13:M:119:LYS:HD3	28:Y:60:DA:H62	1.72	0.55
25:2:123:LEU:HD21	25:2:178:LEU:CD1	2.38	0.54
1:A:611:ASP:OD1	1:A:626:THR:HG23	2.07	0.54
8:H:106:THR:C	8:H:108:ALA:N	2.60	0.54
17:Q:187:ILE:HG21	18:R:210:PHE:C	2.27	0.54
21:V:504:LYS:HD2	21:V:654:GLU:O	2.07	0.54
21:V:325:ARG:HH22	22:W:499:ASN:HB3	0.72	0.54
24:1:52:VAL:HG23	24:1:53:LEU:N	2.21	0.54
25:2:208:THR:O	25:2:212:LEU:HG	2.07	0.54
25:2:214:TYR:CD2	25:2:261:PHE:CD2	2.95	0.54
26:3:64:ILE:HG23	26:3:128:HIS:CG	2.42	0.54
1:A:1199:MET:SD	1:A:1200:PRO:HD2	2.47	0.54
1:A:196:LEU:HB2	1:A:325:LEU:HD21	1.90	0.54
27:X:42:DT:H3'	27:X:43:DT:C5'	2.37	0.54
28:Y:64:DC:H2"	28:Y:65:DG:H5'	1.89	0.54
25:2:123:LEU:CD2	25:2:178:LEU:HD11	2.37	0.54
1:A:129:ILE:HG22	1:A:140:ARG:HG3	1.90	0.54
1:A:608:THR:CA	1:A:610:PRO:HD2	2.37	0.54
2:B:855:ALA:O	2:B:858:VAL:HG12	2.07	0.54
17:Q:23:ARG:CZ	18:R:207:SER:O	2.51	0.54
25:2:62:LEU:HD13	25:2:62:LEU:C	2.28	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:88:PHE:HD2	8:H:144:LEU:HB3	1.72	0.54
16:P:163:PRO:HA	16:P:262:CYS:HB3	1.88	0.54
18:R:223:VAL:HG23	18:R:224:THR:HG1	1.71	0.54
26:3:100:LYS:O	26:3:103:LEU:HB2	2.08	0.54
26:3:106:SER:O	26:3:109:GLU:HG3	2.08	0.54
26:3:144:ILE:HD11	26:3:147:MET:HE3	1.89	0.54
26:3:223:LEU:HD13	26:3:227:LEU:HG	1.89	0.54
1:A:131:ALA:C	1:A:133:SER:N	2.57	0.54
1:A:870:SER:HB2	1:A:882:SER:HB3	1.90	0.54
3:C:209:SER:O	3:C:211:LEU:N	2.41	0.54
9:I:15:ARG:HD2	9:I:37:TYR:HD2	1.72	0.54
3:C:157:GLN:HG2	10:J:65:LEU:HB3	1.85	0.54
13:M:174:PRO:HD2	13:M:213:ASP:HB3	1.89	0.54
1:A:285:LYS:HD2	13:M:80:LEU:HD23	1.89	0.54
27:X:69:DA:C2	28:Y:26:DG:N2	2.76	0.54
1:A:760:LEU:HD13	1:A:767:LYS:HB2	1.89	0.54
2:B:254:GLN:HG3	2:B:303:PRO:HG2	1.90	0.54
7:G:108:ILE:HG23	7:G:162:SER:HA	1.90	0.54
24:1:29:LEU:HD23	24:1:29:LEU:C	2.27	0.54
25:2:199:ALA:HB1	25:2:201:PHE:CD2	2.43	0.54
25:2:259:LEU:C	25:2:259:LEU:HD12	2.27	0.54
25:2:53:LYS:CE	25:2:95:ILE:HD11	2.36	0.54
26:3:169:ASP:CG	26:3:202:LEU:HD23	2.28	0.54
13:M:27:TYR:CD2	13:M:46:ILE:HG21	2.43	0.54
17:Q:187:ILE:HG21	18:R:211:SER:N	2.21	0.54
17:Q:21:VAL:CA	18:R:210:PHE:CE2	2.91	0.54
20:T:177:ARG:HH22	27:X:19:DG:P	2.31	0.54
21:V:667:THR:HA	24:1:62:ASP:OD2	2.07	0.54
1:A:373:LEU:O	1:A:485:ASN:ND2	2.41	0.54
12:L:26:ASN:O	12:L:27:GLU:CB	2.55	0.54
27:X:24:DG:H2"	27:X:25:DG:H5'	1.89	0.54
26:3:22:TRP:O	26:3:25:GLN:NE2	2.39	0.54
13:M:182:ALA:HB2	20:T:154:LYS:HA	1.89	0.54
1:A:271:ARG:CG	13:M:73:PRO:CG	2.86	0.54
28:Y:31:DG:C5	28:Y:32:DC:C4	2.96	0.54
24:1:25:GLU:HG2	24:1:32:LYS:HA	1.89	0.54
1:A:522:PRO:HB3	1:A:666:ARG:HB2	1.89	0.54
2:B:132:VAL:HG23	2:B:141:GLN:CG	2.31	0.54
2:B:252:ILE:O	2:B:254:GLN:N	2.35	0.54
5:E:52:ARG:NH2	5:E:54:ARG:HG3	2.21	0.54
20:T:140:ARG:O	20:T:142:SER:N	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:V:638:GLN:O	21:V:642:ARG:HG2	2.08	0.54
22:W:209:TYR:CZ	22:W:233:PHE:HA	2.38	0.54
26:3:133:LEU:N	26:3:133:LEU:HD13	2.14	0.53
1:A:1171:ALA:C	9:I:59:THR:HG23	2.27	0.53
1:A:155:GLU:C	1:A:181:HIS:HD1	2.12	0.53
2:B:1053:HIS:HE1	2:B:1058:LYS:HG3	1.73	0.53
2:B:911:LEU:HD13	2:B:915:GLY:HA2	1.90	0.53
7:G:106:CYS:HA	7:G:159:ALA:O	2.08	0.53
13:M:45:VAL:CG1	13:M:48:VAL:HG13	2.38	0.53
13:M:94:ASP:CB	13:M:99:SER:N	2.58	0.53
19:S:48:GLU:OE1	19:S:101:ARG:NH2	2.41	0.53
19:S:13:GLU:OE1	20:T:44:ARG:NH1	2.41	0.53
23:0:79:ASN:O	23:0:80:ARG:C	2.46	0.53
24:1:18:GLN:CD	24:1:44:PHE:HZ	2.12	0.53
24:1:8:VAL:CG1	24:1:45:VAL:HG13	2.35	0.53
25:2:141:HIS:HA	25:2:162:PHE:CE2	2.43	0.53
25:2:86:SER:O	25:2:90:LEU:HD13	2.09	0.53
26:3:105:THR:HG23	26:3:106:SER:N	2.23	0.53
1:A:1253:GLU:HG2	9:I:3:PRO:HB2	1.89	0.53
1:A:152:ASN:C	1:A:153:ILE:CG1	2.63	0.53
1:A:623:PRO:C	1:A:625:ASP:N	2.54	0.53
2:B:752:TYR:CG	3:C:63:PHE:HE1	2.26	0.53
25:2:160:LEU:CG	25:2:206:LEU:HD21	2.39	0.53
25:2:81:LYS:HG3	25:2:82:ALA:N	2.21	0.53
1:A:375:ILE:HG13	1:A:666:ARG:HH11	1.74	0.53
2:B:352:GLY:HA3	2:B:357:CYS:SG	2.48	0.53
2:B:708:ALA:O	2:B:711:ILE:HG23	2.08	0.53
2:B:309:PHE:HE2	9:I:40:ARG:HD2	1.72	0.53
17:Q:144:LEU:HD22	17:Q:154:CYS:HA	1.91	0.53
19:S:172:ASN:HD21	19:S:175:SER:HB2	1.72	0.53
25:2:220:LEU:HD13	25:2:220:LEU:C	2.29	0.53
25:2:222:THR:HG23	25:2:222:THR:O	2.07	0.53
1:A:153:ILE:HG22	1:A:155:GLU:OE2	2.08	0.53
2:B:92:TYR:CE2	2:B:146:LYS:HE2	2.42	0.53
11:K:116:ILE:HG13	11:K:117:GLU:HG3	1.90	0.53
26:3:191:ILE:N	26:3:210:THR:HG21	2.24	0.53
1:A:1204:VAL:HA	1:A:1207:ILE:HG12	1.89	0.53
3:C:183:ALA:HB3	3:C:232:ASN:HB3	1.91	0.53
25:2:241:SER:O	25:2:245:LEU:HD23	2.09	0.53
24:1:2:VAL:HG12	25:2:456:LYS:HG2	1.79	0.53
26:3:18:ASN:O	26:3:21:TRP:CD1	2.62	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:THR:C	1:A:48:GLU:HG2	2.28	0.53
22:W:428:ILE:HA	22:W:430:ASN:ND2	2.24	0.53
27:X:45:DT:O2	27:X:46:DT:N3	2.41	0.53
29:Z:1:A:H2'	29:Z:2:G:O4'	2.08	0.53
25:2:118:LEU:HD12	25:2:118:LEU:C	2.28	0.53
25:2:211:GLN:HE21	25:2:257:SER:CB	2.21	0.53
1:A:156:GLY:CA	1:A:181:HIS:CE1	2.92	0.53
2:B:627:ILE:HD11	2:B:663:GLU:HB2	1.89	0.53
7:G:93:ASN:HD22	17:Q:151:THR:HA	1.73	0.53
16:P:207:PRO:O	16:P:208:ARG:C	2.47	0.53
17:Q:25:PHE:HA	18:R:219:LEU:HD13	1.91	0.53
17:Q:113:ARG:HD3	18:R:222:SER:HA	1.91	0.53
24:1:35:ILE:HG13	24:1:35:ILE:O	2.08	0.53
26:3:15:VAL:O	26:3:15:VAL:HG23	2.08	0.53
26:3:160:ARG:NH2	26:3:192:ASP:HB3	2.23	0.53
1:A:270:ALA:O	1:A:272:ASN:N	2.42	0.53
1:A:426:ARG:H	13:M:40:VAL:CG2	2.21	0.53
4:D:135:GLN:HA	4:D:138:ARG:HG2	1.91	0.53
4:D:33:LEU:HD12	4:D:80:ILE:HG23	1.91	0.53
1:A:1370:GLY:HA2	5:E:178:PRO:HD2	1.91	0.53
17:Q:180:PHE:CE1	18:R:214:GLU:N	2.70	0.53
1:A:367:ILE:HG21	1:A:501:MET:HG2	1.91	0.53
1:A:557:ARG:HA	1:A:586:TRP:CZ3	2.44	0.53
2:B:800:ALA:O	2:B:805:PHE:HB2	2.09	0.53
17:Q:203:ILE:HG23	17:Q:204:LEU:HG	1.91	0.53
23:0:54:ARG:CG	26:3:182:PHE:CZ	2.80	0.52
25:2:138:PRO:O	25:2:139:ASP:HB2	2.08	0.52
25:2:159:VAL:CG1	25:2:161:HIS:H	2.06	0.52
26:3:100:LYS:HG3	26:3:101:TYR:H	1.74	0.52
1:A:440:LEU:HB2	1:A:444:TYR:HD2	1.73	0.52
23:0:54:ARG:C	26:3:209:ILE:HD11	2.25	0.52
2:B:712:PRO:HD2	2:B:939:HIS:CE1	2.44	0.52
1:A:1477:ALA:HB2	7:G:22:LEU:HD23	1.90	0.52
2:B:295:PRO:HB3	9:I:11:PHE:HD2	1.75	0.52
19:S:125:TYR:CD1	19:S:139:PRO:HA	2.44	0.52
21:V:689:VAL:CB	25:2:391:ILE:HD11	2.39	0.52
23:0:54:ARG:CB	26:3:209:ILE:CG2	2.87	0.52
1:A:205:VAL:HG21	1:A:212:LYS:NZ	2.24	0.52
1:A:618:TYR:C	1:A:620:HIS:H	2.12	0.52
2:B:51:ILE:HG23	20:T:141:LEU:HD21	1.90	0.52
13:M:34:CYS:SG	13:M:39:LEU:HD21	2.46	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:102:VAL:O	17:Q:102:VAL:HG23	2.09	0.52
27:X:26:DG:N2	28:Y:69:DC:N3	2.57	0.52
2:B:489:ILE:HA	27:X:47:DT:O2	2.09	0.52
25:2:29:GLY:H	26:3:25:GLN:CD	2.12	0.52
26:3:204:GLN:HG2	26:3:214:TYR:CZ	2.44	0.52
26:3:44:LEU:HD13	26:3:44:LEU:C	2.30	0.52
1:A:837:PHE:HB2	2:B:506:TRP:HZ3	1.74	0.52
2:B:473:LEU:HD21	2:B:1052:LYS:HB2	1.90	0.52
2:B:838:GLN:O	2:B:891:ASP:N	2.43	0.52
2:B:844:ILE:HG22	2:B:846:ASP:H	1.74	0.52
26:3:14:VAL:HG23	26:3:14:VAL:O	2.09	0.52
1:A:1022:ILE:HD13	1:A:1080:ILE:HD12	1.92	0.52
2:B:133:ILE:C	2:B:134:LYS:O	2.46	0.52
20:T:229:HIS:NE2	27:X:28:DG:H1'	2.25	0.52
25:2:30:VAL:O	25:2:34:LEU:HD23	2.09	0.52
24:1:1:MET:HE3	25:2:415:GLN:N	2.25	0.52
26:3:10:LEU:HD21	26:3:143:TYR:CD2	2.45	0.52
26:3:222:SER:HB3	26:3:225:GLN:HG2	1.92	0.52
2:B:1073:GLN:NE2	2:B:1154:ALA:HB2	2.25	0.52
3:C:157:GLN:HG3	10:J:65:LEU:HB2	1.90	0.52
12:L:35:ARG:HH11	12:L:42:ARG:HH21	1.57	0.52
13:M:196:LYS:NZ	27:X:13:DT:OP1	2.32	0.52
28:Y:48:DC:O2	29:Z:5:G:N2	2.26	0.52
26:3:10:LEU:HD21	26:3:143:TYR:CE2	2.44	0.52
1:A:924:TYR:CZ	1:A:949:GLN:HG3	2.45	0.52
22:W:584:TYR:HB2	22:W:591:GLY:HA3	1.92	0.52
25:2:257:SER:O	25:2:261:PHE:HD1	1.93	0.52
1:A:95:PHE:CE1	1:A:218:PRO:HG3	2.44	0.52
2:B:1053:HIS:CE1	2:B:1058:LYS:HE3	2.45	0.52
2:B:553:LEU:O	2:B:556:ILE:HG12	2.10	0.52
2:B:914:GLU:HG3	13:M:132:ARG:HB3	1.91	0.52
8:H:17:PRO:C	8:H:19:GLY:H	2.13	0.52
19:S:100:LEU:HD23	19:S:110:PHE:HD2	1.75	0.52
24:1:59:GLU:CD	25:2:402:ARG:HH12	2.13	0.52
1:A:926:ASN:OD1	1:A:931:ARG:HB3	2.10	0.52
8:H:76:ASN:OD1	8:H:78:THR:OG1	2.26	0.52
17:Q:172:ASP:HA	17:Q:175:THR:HB	1.91	0.52
21:V:504:LYS:CB	21:V:654:GLU:O	2.58	0.52
25:2:193:PRO:HB2	25:2:194:PRO:HD3	1.92	0.52
2:B:225:LEU:CG	2:B:228:SER:HB2	2.40	0.52
2:B:854:ILE:HG13	2:B:866:ILE:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:988:LYS:O	2:B:992:ASN:HB2	2.10	0.52
16:P:309:LYS:HD3	28:Y:82:DT:H5"	1.91	0.52
17:Q:24:GLY:HA2	18:R:209:GLN:OE1	2.09	0.52
21:V:520:ARG:NE	21:V:521:GLU:OE2	2.30	0.52
22:W:423:ASP:C	22:W:425:THR:N	2.63	0.52
28:Y:80:DT:H2"	28:Y:81:DA:C8	2.45	0.52
26:3:10:LEU:HD22	26:3:147:MET:HG2	1.92	0.51
26:3:165:LYS:HD3	26:3:165:LYS:C	2.31	0.51
1:A:1305:SER:O	1:A:1306:LYS:HG3	2.10	0.51
1:A:1128:ILE:HG23	1:A:1414:ILE:HG13	1.92	0.51
1:A:451:CYS:O	1:A:453:GLY:N	2.38	0.51
1:A:47:THR:HG23	1:A:53:LYS:HA	1.92	0.51
1:A:606:HIS:HB3	1:A:627:LYS:HA	1.92	0.51
1:A:679:TRP:CZ3	1:A:683:GLU:HG3	2.44	0.51
1:A:601:ASN:HB3	1:A:988:TRP:CZ3	2.45	0.51
2:B:1053:HIS:ND1	2:B:1058:LYS:HE3	2.25	0.51
2:B:331:THR:O	2:B:333:GLU:N	2.42	0.51
9:I:91:HIS:ND1	9:I:92:LYS:O	2.43	0.51
28:Y:53:DG:H4'	28:Y:54:DA:OP1	2.09	0.51
26:3:42:MET:CG	26:3:111:ILE:HD11	2.40	0.51
26:3:64:ILE:HG21	26:3:128:HIS:CB	2.40	0.51
26:3:131:THR:HG23	26:3:133:LEU:HD12	1.92	0.51
26:3:57:LEU:HD23	26:3:58:ALA:C	2.31	0.51
1:A:40:GLY:O	1:A:42:LYS:HG2	2.10	0.51
2:B:584:MET:HE3	2:B:588:ARG:HH12	1.75	0.51
13:M:128:ILE:HG23	13:M:183:VAL:HG11	1.92	0.51
17:Q:112:ARG:NH2	18:R:237:LEU:HD22	2.25	0.51
21:V:611:GLY:HA2	21:V:615:PHE:CB	2.38	0.51
26:3:121:LYS:HD3	26:3:121:LYS:N	2.25	0.51
26:3:226:TYR:O	26:3:230:VAL:HB	2.10	0.51
1:A:347:GLU:OE1	1:A:347:GLU:N	2.42	0.51
2:B:1016:SER:HB3	2:B:1022:LEU:CB	2.40	0.51
25:2:181:GLN:HE21	25:2:181:GLN:CA	2.23	0.51
25:2:171:VAL:CG2	25:2:213:TRP:HA	2.20	0.51
26:3:70:LEU:HD22	26:3:114:GLU:HB3	1.91	0.51
26:3:172:LEU:HD13	26:3:172:LEU:C	2.29	0.51
1:A:1313:GLN:OE1	1:A:1316:ASN:ND2	2.43	0.51
1:A:44:PRO:HG3	1:A:284:VAL:HG13	1.91	0.51
2:B:631:GLN:HB3	2:B:685:LYS:HZ3	1.74	0.51
3:C:99:VAL:HG13	3:C:124:SER:OG	2.10	0.51
3:C:136:ASP:OD1	3:C:136:ASP:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:193:ASN:HD21	16:P:196:ARG:HD3	1.74	0.51
16:P:203:ARG:NH2	16:P:210:THR:OG1	2.43	0.51
2:B:214:LYS:O	2:B:240:LEU:HD12	2.11	0.51
2:B:56:GLN:NE2	2:B:60:GLU:OE2	2.44	0.51
21:V:523:VAL:HG21	24:1:20:LEU:CG	2.38	0.51
27:X:50:DT:H3'	27:X:51:DC:H5"	1.92	0.51
25:2:231:VAL:O	25:2:234:LEU:HB3	2.11	0.51
25:2:215:PHE:CE2	25:2:264:HIS:HB2	2.46	0.51
1:A:1304:ILE:HA	1:A:1340:GLY:HA3	1.93	0.51
1:A:26:LEU:HB2	2:B:1168:ALA:HB2	1.92	0.51
1:A:530:SER:O	1:A:532:ARG:N	2.43	0.51
2:B:250:SER:O	2:B:251:ALA:HB3	2.09	0.51
7:G:13:LEU:HD21	7:G:22:LEU:HD11	1.93	0.51
15:O:48:LEU:HD23	15:O:52:VAL:HG21	1.93	0.51
7:G:111:HIS:CE1	17:Q:125:ALA:H	2.28	0.51
26:3:141:LEU:HG	26:3:187:GLN:HE22	1.75	0.51
25:2:31:LEU:HD13	26:3:33:THR:HG22	1.86	0.51
1:A:1323:THR:HG23	1:A:1325:ASP:H	1.75	0.51
6:F:64:ARG:HH12	7:G:61:PRO:HB3	1.75	0.51
10:J:54:ASP:OD2	10:J:57:GLU:HG2	2.11	0.51
19:S:26:TYR:CD2	19:S:138:PHE:HB3	2.46	0.51
27:X:24:DG:H2'	27:X:25:DG:C8	2.45	0.51
25:2:138:PRO:HG3	25:2:189:GLU:CG	2.35	0.51
25:2:160:LEU:HB3	25:2:206:LEU:HD21	1.93	0.51
25:2:51:LEU:CD2	25:2:55:TRP:CD1	2.94	0.51
26:3:165:LYS:HE3	26:3:200:SER:OG	2.09	0.51
2:B:234:THR:O	2:B:236:TRP:HD1	1.93	0.51
2:B:881:GLU:HA	2:B:883:THR:HG23	1.92	0.51
17:Q:46:GLU:OE2	17:Q:56:ARG:NH1	2.34	0.51
25:2:236:PHE:CE2	25:2:262:LEU:CD1	2.94	0.51
26:3:216:LYS:O	26:3:216:LYS:HG2	2.11	0.51
1:A:883:ILE:HG21	1:A:1424:THR:HA	1.92	0.51
1:A:367:ILE:HG12	1:A:499:ASP:O	2.10	0.51
2:B:822:GLY:HA3	2:B:825:GLN:HG2	1.92	0.51
9:I:86:CYS:O	9:I:88:LYS:N	2.43	0.51
13:M:45:VAL:HG11	13:M:48:VAL:HG13	1.93	0.51
17:Q:42:CYS:O	17:Q:95:ASN:ND2	2.40	0.51
17:Q:184:ILE:CD1	18:R:213:ASP:OD1	2.59	0.51
27:X:23:DT:H2"	27:X:24:DG:H8	1.75	0.51
1:A:1264:SER:OG	1:A:1267:ASN:ND2	2.38	0.51
1:A:616:GLY:O	1:A:619:LYS:HB2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:56:SER:OG	3:C:158:GLU:N	2.28	0.51
7:G:104:MET:HE2	7:G:159:ALA:HB2	1.91	0.51
13:M:34:CYS:HB3	13:M:39:LEU:HB2	1.93	0.51
25:2:140:LYS:CG	25:2:162:PHE:CE1	2.94	0.50
25:2:236:PHE:CE1	25:2:261:PHE:CB	2.94	0.50
25:2:46:ARG:HD3	25:2:85:GLU:HB2	1.93	0.50
26:3:64:ILE:CG2	26:3:128:HIS:HB3	2.42	0.50
1:A:152:ASN:OD1	1:A:188:GLN:HB2	2.11	0.50
1:A:202:TRP:N	1:A:212:LYS:O	2.33	0.50
1:A:710:LYS:HE3	1:A:818:GLU:OE2	2.11	0.50
1:A:930:LEU:O	1:A:931:ARG:C	2.49	0.50
5:E:40:PHE:CZ	5:E:46:ASP:OD2	2.54	0.50
6:F:51:ARG:HA	6:F:116:GLU:OE1	2.10	0.50
13:M:87:GLY:O	13:M:88:THR:CB	2.59	0.50
9:I:93:GLU:O	9:I:115:THR:HG22	2.10	0.50
17:Q:44:LYS:HG3	17:Q:46:GLU:H	1.76	0.50
17:Q:180:PHE:CE1	18:R:212:VAL:O	2.65	0.50
18:R:223:VAL:HG23	18:R:224:THR:CB	2.40	0.50
20:T:138:PRO:O	20:T:140:ARG:N	2.44	0.50
25:2:181:GLN:HE22	25:2:220:LEU:HD12	1.76	0.50
25:2:77:LYS:CD	25:2:78:GLU:HG3	2.41	0.50
26:3:12:VAL:HG12	26:3:58:ALA:HB3	1.92	0.50
1:A:603:ILE:HG12	1:A:604:ARG:H	1.76	0.50
13:M:10:LEU:N	13:M:10:LEU:CD2	2.73	0.50
17:Q:113:ARG:HH12	18:R:218:LYS:CA	2.25	0.50
17:Q:184:ILE:CD1	18:R:211:SER:CB	2.86	0.50
17:Q:23:ARG:HH12	18:R:206:LYS:HB3	1.75	0.50
28:Y:48:DC:H2'	28:Y:49:DG:H8	1.76	0.50
25:2:192:GLU:CG	25:2:193:PRO:HD2	2.23	0.50
25:2:208:THR:HG23	25:2:209:PRO:HD2	1.91	0.50
25:2:223:ALA:O	25:2:224:GLN:HB3	2.12	0.50
25:2:57:MET:HA	25:2:60:LEU:HG	1.93	0.50
26:3:24:LYS:HE2	26:3:196:LEU:HB3	1.93	0.50
1:A:1114:ALA:HB2	1:A:1309:MET:HE1	1.92	0.50
1:A:710:LYS:O	1:A:714:ILE:HG12	2.11	0.50
2:B:1029:TYR:CE1	2:B:1036:LYS:HG3	2.46	0.50
5:E:53:PRO:HB2	5:E:56:THR:HB	1.92	0.50
2:B:312:GLN:HB3	19:S:153:ARG:NH2	2.24	0.50
22:W:116:CYS:SG	22:W:191:PRO:HD2	2.51	0.50
22:W:73:CYS:O	22:W:209:TYR:CE2	2.63	0.50
27:X:3:DA:H1'	27:X:4:DG:H5'	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:2:57:MET:HA	25:2:60:LEU:CG	2.41	0.50
25:2:42:LEU:HD12	25:2:59:MET:HE1	1.90	0.50
26:3:107:ALA:O	26:3:111:ILE:HG23	2.11	0.50
1:A:1319:LYS:HB2	1:A:1333:GLU:OE2	2.11	0.50
13:M:34:CYS:CB	13:M:39:LEU:CB	2.89	0.50
17:Q:28:ILE:HD12	18:R:190:LEU:HD21	1.92	0.50
25:2:199:ALA:CB	25:2:201:PHE:CE2	2.95	0.50
25:2:245:LEU:HD22	25:2:245:LEU:N	2.27	0.50
25:2:30:VAL:CG1	25:2:34:LEU:HD23	2.40	0.50
26:3:137:LEU:CD1	26:3:177:PHE:CE1	2.95	0.50
26:3:202:LEU:HD22	26:3:202:LEU:N	2.27	0.50
1:A:1361:ASP:OD2	1:A:1364:GLU:HB2	2.12	0.50
1:A:1473:LEU:HD13	6:F:104:ILE:HD12	1.94	0.50
1:A:196:LEU:HD22	1:A:325:LEU:HD21	1.94	0.50
2:B:367:TYR:OH	2:B:371:ARG:NH1	2.45	0.50
2:B:747:LEU:HD21	2:B:810:PHE:HE1	1.75	0.50
9:I:15:ARG:O	9:I:16:PHE:O	2.30	0.50
9:I:81:THR:HB	9:I:96:PHE:CE2	2.46	0.50
27:X:36:DT:H71	27:X:37:DT:H3	1.77	0.50
25:2:100:LEU:HD11	25:2:119:ARG:CG	2.31	0.50
24:1:1:MET:CE	25:2:415:GLN:C	2.80	0.50
1:A:366:VAL:O	1:A:481:THR:HB	2.12	0.50
3:C:136:ASP:HB2	3:C:138:ASP:HB2	1.94	0.50
3:C:259:LEU:HD22	11:K:42:LEU:HD21	1.94	0.50
1:A:298:ALA:N	17:Q:60:ARG:HE	2.09	0.50
22:W:494:ILE:HD11	22:W:680:ALA:HB2	1.93	0.50
24:1:22:TYR:O	24:1:25:GLU:HB3	2.11	0.50
21:V:520:ARG:CG	24:1:23:LEU:HD11	2.42	0.50
25:2:199:ALA:HB1	25:2:201:PHE:CE2	2.47	0.50
25:2:236:PHE:CZ	25:2:262:LEU:CD2	2.94	0.50
26:3:12:VAL:O	26:3:12:VAL:HG23	2.10	0.50
26:3:10:LEU:CD2	26:3:143:TYR:HE2	2.25	0.50
26:3:187:GLN:O	26:3:188:ASN:HB2	2.12	0.50
1:A:137:PRO:HB2	1:A:1445:HIS:CE1	2.47	0.50
1:A:426:ARG:CG	13:M:40:VAL:HG11	2.42	0.50
2:B:1075:MET:CE	13:M:51:GLU:HG2	2.40	0.50
17:Q:36:ILE:HG21	17:Q:48:MET:HG2	1.93	0.50
25:2:189:GLU:CA	25:2:192:GLU:HG2	2.41	0.50
26:3:215:LEU:HD12	26:3:230:VAL:CG2	2.42	0.50
1:A:1207:ILE:HG22	1:A:1262:MET:HG3	1.92	0.50
1:A:772:SER:OG	1:A:773:GLY:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:28:GLU:HG2	9:I:30:LYS:HG3	1.94	0.50
18:R:195:PRO:HB2	18:R:199:LYS:CD	2.41	0.50
19:S:26:TYR:HB2	19:S:139:PRO:O	2.12	0.50
20:T:181:GLN:HA	20:T:184:LEU:HD12	1.93	0.50
20:T:34:ALA:O	20:T:37:ARG:HG3	2.12	0.50
20:T:95:VAL:O	20:T:107:GLU:N	2.45	0.50
27:X:33:DT:H2"	27:X:34:DT:C5	2.47	0.50
24:1:2:VAL:O	24:1:2:VAL:HG23	2.11	0.49
24:1:34:ILE:HG21	24:1:54:GLN:CD	2.32	0.49
25:2:176:ALA:O	25:2:177:GLN:HB2	2.12	0.49
25:2:214:TYR:CB	25:2:261:PHE:CE2	2.95	0.49
25:2:35:TYR:CD1	25:2:62:LEU:CD1	2.95	0.49
26:3:10:LEU:CD2	26:3:143:TYR:CE2	2.95	0.49
1:A:802:PHE:CE2	1:A:808:PRO:HD3	2.47	0.49
1:A:930:LEU:C	1:A:931:ARG:O	2.50	0.49
2:B:1162:LEU:HD23	2:B:1165:MET:HE3	1.94	0.49
5:E:46:ASP:O	5:E:47:LYS:CB	2.51	0.49
6:F:79:VAL:HG12	6:F:81:VAL:H	1.77	0.49
22:W:430:ASN:CB	22:W:431:PRO:CD	2.85	0.49
25:2:89:LEU:HD23	25:2:93:LEU:HG	1.94	0.49
26:3:166:ALA:O	26:3:198:SER:HB2	2.13	0.49
26:3:60:ILE:HG22	26:3:61:ALA:N	2.26	0.49
1:A:1098:PRO:CA	1:A:1101:GLN:NE2	2.74	0.49
1:A:60:PRO:O	1:A:61:ARG:HG3	2.12	0.49
2:B:883:THR:O	2:B:885:ARG:N	2.45	0.49
5:E:52:ARG:NH2	5:E:54:ARG:HG2	2.19	0.49
8:H:88:PHE:CE1	8:H:146:LYS:HD2	2.46	0.49
14:N:326:GLN:OE1	15:O:92:LYS:NZ	2.30	0.49
16:P:206:GLU:C	16:P:208:ARG:N	2.55	0.49
24:1:18:GLN:HG3	24:1:19:PHE:H	1.78	0.49
26:3:53:ARG:HA	26:3:101:TYR:HE1	1.78	0.49
1:A:138:LYS:H	1:A:1445:HIS:HE1	1.60	0.49
1:A:111:CYS:SG	1:A:154:CYS:CB	3.01	0.49
14:N:344:ARG:HH21	28:Y:78:DT:H3'	1.77	0.49
18:R:82:VAL:HG22	18:R:140:LYS:HE2	1.94	0.49
18:R:75:PHE:HD2	20:T:192:GLU:OE2	1.96	0.49
22:W:209:TYR:HH	22:W:234:ASP:H	1.59	0.49
28:Y:46:DC:H2'	28:Y:47:DG:C8	2.48	0.49
25:2:35:TYR:CD2	25:2:62:LEU:CB	2.95	0.49
25:2:426:ARG:HD2	25:2:444:THR:CG2	2.43	0.49
25:2:81:LYS:CE	25:2:89:LEU:HD21	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:2:93:LEU:CD2	25:2:96:TRP:HE1	2.25	0.49
26:3:220:MET:N	26:3:221:PRO:HD2	2.28	0.49
26:3:59:VAL:HG13	26:3:59:VAL:O	2.12	0.49
1:A:107:LEU:HD23	1:A:191:ILE:HD13	1.94	0.49
2:B:323:SER:HB3	2:B:335:ARG:NH1	2.27	0.49
2:B:468:GLN:OE1	2:B:481:HIS:NE2	2.44	0.49
2:B:882:SER:HB2	2:B:887:TYR:CE1	2.46	0.49
8:H:10:PHE:CE2	8:H:39:LEU:HD22	2.47	0.49
14:N:347:ASN:O	14:N:375:GLU:HA	2.11	0.49
14:N:21:VAL:HG21	15:O:40:PHE:HD1	1.77	0.49
25:2:203:PHE:CE2	25:2:205:LEU:CD2	2.96	0.49
25:2:35:TYR:N	25:2:35:TYR:CD1	2.79	0.49
26:3:108:ASN:O	26:3:111:ILE:HG12	2.12	0.49
1:A:1457:ASN:OD1	1:A:1462:GLN:NE2	2.39	0.49
2:B:356:PHE:HB3	19:S:116:GLY:CA	2.39	0.49
22:W:325:THR:HG22	22:W:329:PHE:CE2	2.47	0.49
24:1:3:ASN:HB2	25:2:412:PHE:O	2.13	0.49
24:1:1:MET:HA	25:2:413:LEU:CA	2.42	0.49
26:3:147:MET:HE3	26:3:157:MET:SD	2.52	0.49
26:3:21:TRP:HA	26:3:24:LYS:CG	2.42	0.49
26:3:223:LEU:C	26:3:223:LEU:HD13	2.33	0.49
1:A:1130:ILE:HD13	1:A:1411:LEU:HB3	1.95	0.49
1:A:641:CYS:SG	1:A:643:LYS:N	2.86	0.49
2:B:363:TYR:CD2	2:B:553:LEU:HD11	2.48	0.49
2:B:422:PHE:CE2	2:B:429:PHE:HB2	2.48	0.49
3:C:137:ASN:ND2	3:C:137:ASN:H	2.10	0.49
3:C:36:ARG:NH2	11:K:40:HIS:HB2	2.28	0.49
17:Q:25:PHE:CE2	18:R:219:LEU:HD11	2.35	0.49
24:1:45:VAL:HG21	25:2:409:TYR:CE2	2.48	0.49
25:2:188:THR:HG23	25:2:189:GLU:N	2.27	0.49
25:2:198:SER:OG	25:2:238:PHE:HE2	1.96	0.49
25:2:42:LEU:HD22	25:2:52:ALA:HA	1.95	0.49
26:3:190:LEU:HA	26:3:210:THR:HG21	1.91	0.49
26:3:174:TYR:HD1	26:3:202:LEU:HD11	1.78	0.49
2:B:819:SER:HB3	2:B:821:LYS:HB2	1.94	0.49
3:C:100:GLU:HG3	3:C:164:TYR:CE1	2.48	0.49
3:C:142:TYR:O	3:C:144:GLU:N	2.45	0.49
8:H:99:ILE:HD11	8:H:112:LEU:HD21	1.94	0.49
13:M:178:LYS:HB3	20:T:154:LYS:HB2	1.93	0.49
21:V:667:THR:CA	24:1:62:ASP:OD1	2.59	0.49
22:W:624:PRO:O	22:W:656:ALA:HB1	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:3:100:LYS:HB3	26:3:103:LEU:CD1	2.37	0.49
26:3:12:VAL:HG22	26:3:161:ILE:HA	1.94	0.49
1:A:1147:SER:HB3	1:A:1157:ILE:HD11	1.95	0.49
1:A:156:GLY:HA2	1:A:181:HIS:CE1	2.38	0.49
1:A:702:ILE:HG12	1:A:752:THR:HG23	1.94	0.49
2:B:422:PHE:O	2:B:425:ARG:N	2.46	0.49
3:C:146:ASP:O	3:C:148:ILE:N	2.45	0.49
3:C:6:GLN:O	3:C:7:PRO:C	2.51	0.49
13:M:85:GLY:O	13:M:86:LYS:HB2	2.13	0.49
22:W:596:LEU:HG	22:W:597:LEU:N	2.27	0.49
25:2:35:TYR:CE2	25:2:62:LEU:CB	2.96	0.49
26:3:217:VAL:CG1	26:3:226:TYR:CE2	2.95	0.49
26:3:58:ALA:C	26:3:71:TYR:OH	2.50	0.49
1:A:36:VAL:HG11	1:A:72:GLN:NE2	2.26	0.49
2:B:203:ASN:O	2:B:204:THR:OG1	2.27	0.49
9:I:86:CYS:O	9:I:87:GLN:C	2.50	0.49
13:M:245:VAL:HG12	13:M:291:LEU:HD23	1.95	0.49
17:Q:70:LYS:NZ	18:R:230:GLU:OE2	2.45	0.49
28:Y:46:DC:H2'	28:Y:47:DG:H8	1.77	0.49
24:1:43:VAL:HG12	24:1:44:PHE:N	2.27	0.49
24:1:4:VAL:HG12	25:2:411:GLN:C	2.30	0.49
25:2:236:PHE:CZ	25:2:258:LEU:CD1	2.95	0.49
25:2:77:LYS:HD3	25:2:78:GLU:HG3	1.94	0.49
26:3:195:VAL:HG23	26:3:214:TYR:CE1	2.48	0.49
2:B:852:GLY:O	2:B:868:GLY:N	2.31	0.49
2:B:952:GLU:OE2	3:C:40:ALA:HB2	2.13	0.49
2:B:1080:ARG:NH1	13:M:53:ARG:HD2	2.28	0.49
17:Q:105:TYR:OH	18:R:234:GLU:CD	2.50	0.49
20:T:217:LEU:HB3	20:T:233:TRP:CE3	2.48	0.49
20:T:47:LYS:HG2	20:T:52:THR:HG23	1.95	0.49
24:1:45:VAL:CG2	25:2:409:TYR:CE2	2.95	0.48
1:A:1076:PHE:CE2	1:A:1080:ILE:HD11	2.47	0.48
1:A:1463:LEU:HA	2:B:1104:ARG:HD3	1.95	0.48
1:A:611:ASP:CG	1:A:626:THR:OG1	2.51	0.48
2:B:58:ILE:O	2:B:61:ASP:HB2	2.13	0.48
2:B:752:TYR:O	10:J:1:MET:HG3	2.13	0.48
19:S:110:PHE:HD1	19:S:148:PRO:HA	1.78	0.48
13:M:56:SER:O	28:Y:51:DC:N4	2.45	0.48
23:0:55:LEU:N	26:3:209:ILE:HD11	2.28	0.48
25:2:170:ALA:CB	25:2:213:TRP:CZ3	2.95	0.48
25:2:179:LEU:CB	25:2:184:LEU:HD11	2.40	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:2:211:GLN:HE21	25:2:257:SER:HB3	1.78	0.48
26:3:12:VAL:CG2	26:3:161:ILE:HA	2.42	0.48
1:A:1020:LEU:HD22	1:A:1076:PHE:CD2	2.48	0.48
1:A:371:PRO:HD2	2:B:788:TYR:CE1	2.48	0.48
1:A:606:HIS:O	1:A:608:THR:N	2.44	0.48
1:A:608:THR:CB	1:A:610:PRO:CD	2.91	0.48
1:A:358:ARG:HE	2:B:1076:GLU:CD	2.16	0.48
17:Q:191:LEU:HD21	18:R:210:PHE:HB2	1.95	0.48
22:W:37:HIS:NE2	22:W:454:VAL:CG1	2.76	0.48
27:X:82:DG:N2	28:Y:13:DC:C2	2.81	0.48
25:2:117:ASN:CG	26:3:108:ASN:CG	2.65	0.48
25:2:133:THR:HG23	25:2:134:SER:N	2.28	0.48
25:2:211:GLN:CA	25:2:261:PHE:CE1	2.95	0.48
1:A:1020:LEU:HD13	1:A:1041:PHE:HE2	1.76	0.48
2:B:1104:ARG:O	2:B:1108:PHE:HB3	2.14	0.48
2:B:838:GLN:HG3	2:B:886:ARG:NH2	2.28	0.48
2:B:799:SER:HB2	2:B:951:GLN:HB2	1.96	0.48
3:C:69:GLY:HA3	12:L:57:ALA:HB1	1.95	0.48
7:G:145:LEU:HD13	7:G:161:GLY:HA3	1.94	0.48
20:T:146:ASP:OD2	20:T:147:LYS:HG2	2.13	0.48
21:V:315:VAL:CG1	22:W:500:ASP:HB3	2.26	0.48
21:V:325:ARG:HH21	22:W:499:ASN:CB	1.95	0.48
25:2:178:LEU:HD12	25:2:178:LEU:N	2.28	0.48
25:2:211:GLN:CB	25:2:261:PHE:CE1	2.95	0.48
25:2:35:TYR:CD1	25:2:62:LEU:CG	2.92	0.48
26:3:160:ARG:HE	26:3:190:LEU:HG	1.78	0.48
1:A:485:ASN:C	1:A:485:ASN:OD1	2.52	0.48
2:B:102:ASP:OD1	2:B:104:ALA:N	2.38	0.48
2:B:89:GLU:HG3	2:B:90:GLN:H	1.78	0.48
3:C:154:ARG:HG2	3:C:155:LYS:H	1.77	0.48
19:S:110:PHE:CD1	19:S:148:PRO:HA	2.48	0.48
21:V:321:GLU:CA	22:W:499:ASN:ND2	2.57	0.48
25:2:90:LEU:CD2	25:2:140:LYS:HD3	2.42	0.48
26:3:177:PHE:CZ	26:3:203:LEU:CD2	2.95	0.48
26:3:21:TRP:CG	26:3:34:LEU:HD23	2.48	0.48
1:A:137:PRO:HB2	1:A:1445:HIS:NE2	2.29	0.48
1:A:206:ASN:C	1:A:207:GLU:HG3	2.33	0.48
1:A:77:ASN:N	1:A:77:ASN:OD1	2.47	0.48
2:B:62:ALA:N	2:B:63:PRO:HD3	2.28	0.48
12:L:25:GLU:OE1	12:L:25:GLU:N	2.36	0.48
15:O:79:VAL:HG21	15:O:93:VAL:HG12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:113:ARG:HH11	18:R:221:ARG:HB2	1.79	0.48
17:Q:21:VAL:HA	18:R:210:PHE:CD2	2.49	0.48
17:Q:75:ARG:HB3	17:Q:95:ASN:HB3	1.95	0.48
27:X:13:DT:H3	28:Y:81:DA:H61	1.60	0.48
25:2:100:LEU:CG	25:2:119:ARG:HE	2.22	0.48
25:2:159:VAL:N	25:2:162:PHE:HB3	2.28	0.48
25:2:89:LEU:CD2	25:2:93:LEU:HG	2.44	0.48
2:B:198:GLU:OE2	2:B:391:LYS:NZ	2.35	0.48
4:D:60:VAL:HG13	7:G:103:PRO:HG3	1.95	0.48
8:H:64:LEU:CB	8:H:84:ARG:CD	2.76	0.48
13:M:86:LYS:HA	13:M:86:LYS:CE	2.42	0.48
18:R:140:LYS:H	18:R:141:PRO:HD2	1.79	0.48
20:T:180:LYS:HE3	20:T:184:LEU:HD11	1.95	0.48
22:W:73:CYS:CB	22:W:209:TYR:CE1	2.97	0.48
23:0:209:THR:HA	23:0:219:TYR:CD1	2.48	0.48
24:1:34:ILE:HG22	24:1:46:ILE:CG1	2.44	0.48
26:3:34:LEU:HD13	26:3:38:ILE:HG12	1.96	0.48
1:A:1319:LYS:HD3	1:A:1333:GLU:OE1	2.13	0.48
1:A:118:LEU:CD2	1:A:151:LYS:O	2.40	0.48
2:B:1162:LEU:HD23	2:B:1165:MET:CE	2.43	0.48
2:B:274:ARG:NH2	2:B:279:VAL:O	2.47	0.48
2:B:728:MET:HA	2:B:731:GLN:HB2	1.95	0.48
7:G:97:LEU:HG	7:G:113:ILE:HD11	1.95	0.48
9:I:96:PHE:HB3	9:I:112:TYR:CD1	2.47	0.48
9:I:21:ASN:O	9:I:22:ASN:ND2	2.47	0.48
12:L:13:GLN:C	12:L:15:MET:H	2.17	0.48
17:Q:58:GLN:NE2	18:R:194:ARG:NH1	2.61	0.48
20:T:166:GLU:O	20:T:170:LYS:HG3	2.13	0.48
22:W:73:CYS:HB2	22:W:209:TYR:CE1	2.48	0.48
22:W:285:TYR:CE1	22:W:403:PHE:CZ	3.01	0.48
25:2:166:SER:HB3	25:2:167:PRO:CD	2.43	0.48
1:A:360:ASP:CG	2:B:1064:ARG:H	2.17	0.48
1:A:371:PRO:HD2	2:B:788:TYR:CZ	2.49	0.48
2:B:880:LEU:CD1	2:B:881:GLU:OE1	2.56	0.48
3:C:37:VAL:HG12	3:C:248:ALA:HB1	1.96	0.48
8:H:65:TYR:HE1	8:H:84:ARG:NE	2.11	0.48
22:W:73:CYS:HB3	22:W:209:TYR:CG	2.48	0.48
24:1:38:ILE:HG22	24:1:44:PHE:CE1	2.48	0.48
24:1:38:ILE:CG2	24:1:44:PHE:CE1	2.96	0.48
25:2:251:VAL:HG11	25:2:254:MET:SD	2.53	0.48
26:3:34:LEU:HD13	26:3:34:LEU:C	2.33	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1162:LEU:HA	2:B:1165:MET:HE3	1.96	0.48
2:B:206:TYR:HD1	2:B:208:PHE:CE1	2.32	0.48
2:B:628:VAL:HG12	2:B:633:LEU:HA	1.94	0.48
14:N:360:LEU:HD11	15:O:81:PHE:HD2	1.79	0.48
24:1:53:LEU:CD1	24:1:53:LEU:H	2.26	0.48
26:3:124:ILE:O	26:3:127:GLN:HB2	2.14	0.48
2:B:1016:SER:HB3	2:B:1022:LEU:HB3	1.96	0.48
2:B:531:TYR:HE2	2:B:599:SER:HB3	1.79	0.48
8:H:90:TYR:HB3	8:H:145:MET:HB3	1.96	0.48
1:A:430:ARG:NH2	13:M:26:ASP:OD2	2.47	0.48
19:S:135:PHE:HE2	20:T:43:LEU:HD23	1.79	0.48
21:V:321:GLU:OE2	22:W:500:ASP:CA	2.59	0.48
1:A:344:LYS:NZ	28:Y:43:DG:H5"	2.28	0.48
25:2:221:GLN:CD	25:2:230:LEU:HB2	2.34	0.47
25:2:30:VAL:H	26:3:25:GLN:CG	2.27	0.47
25:2:60:LEU:CD1	25:2:95:ILE:CG2	2.91	0.47
25:2:93:LEU:CA	25:2:96:TRP:CD1	2.94	0.47
26:3:165:LYS:NZ	26:3:200:SER:H	2.12	0.47
26:3:160:ARG:HB2	26:3:190:LEU:HG	1.96	0.47
1:A:34:MET:SD	2:B:1124:ILE:HG21	2.54	0.47
2:B:344:GLN:O	2:B:361:LYS:NZ	2.38	0.47
2:B:573:TRP:O	2:B:573:TRP:HE3	1.97	0.47
4:D:112:LYS:HD2	4:D:124:ASP:OD1	2.14	0.47
8:H:65:TYR:CE2	8:H:70:LEU:CB	2.96	0.47
14:N:333:ASN:O	15:O:93:VAL:HG23	2.14	0.47
19:S:126:ILE:O	19:S:137:ALA:HA	2.13	0.47
25:2:205:LEU:N	25:2:205:LEU:HD22	2.30	0.47
25:2:236:PHE:HE2	25:2:262:LEU:CD1	2.27	0.47
26:3:10:LEU:HA	26:3:56:LYS:HG2	1.96	0.47
26:3:216:LYS:O	26:3:218:PRO:HD3	2.14	0.47
1:A:614:ASP:O	1:A:618:TYR:CE2	2.67	0.47
1:A:719:LYS:HG2	1:A:724:GLU:OE1	2.13	0.47
2:B:1029:TYR:HE1	2:B:1036:LYS:CE	2.25	0.47
2:B:1163:MET:HA	2:B:1167:ILE:O	2.14	0.47
2:B:312:GLN:O	19:S:153:ARG:NH2	2.47	0.47
2:B:497:LYS:O	2:B:500:GLN:HG2	2.14	0.47
3:C:100:GLU:HG3	3:C:164:TYR:HE1	1.79	0.47
3:C:131:THR:HB	3:C:147:ASP:OD1	2.15	0.47
11:K:67:LEU:HD23	11:K:67:LEU:HA	1.63	0.47
16:P:183:ILE:HG12	16:P:244:LEU:HD13	1.96	0.47
22:W:209:TYR:HH	22:W:233:PHE:CA	2.08	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:3:131:THR:HG23	26:3:133:LEU:HD13	1.95	0.47
1:A:522:PRO:HG3	1:A:666:ARG:HG2	1.95	0.47
2:B:295:PRO:HB3	9:I:11:PHE:CD2	2.49	0.47
5:E:112:PRO:HA	5:E:115:LYS:HE2	1.95	0.47
17:Q:25:PHE:H	18:R:210:PHE:HE2	1.61	0.47
19:S:172:ASN:OD1	19:S:173:HIS:N	2.45	0.47
22:W:73:CYS:HB3	22:W:209:TYR:CD1	2.49	0.47
24:1:9:LEU:HD12	24:1:9:LEU:N	2.29	0.47
25:2:221:GLN:HG2	25:2:268:PHE:HZ	1.75	0.47
2:B:1123:GLY:HA3	2:B:1170:ARG:HB3	1.97	0.47
11:K:87:PHE:CE1	11:K:91:ILE:HD11	2.49	0.47
1:A:312:PHE:HB2	13:M:101:TYR:OH	2.14	0.47
13:M:276:ASP:O	20:T:153:TYR:HD1	1.98	0.47
16:P:206:GLU:HB2	16:P:236:LYS:NZ	2.29	0.47
16:P:298:PRO:O	16:P:299:ARG:C	2.52	0.47
17:Q:118:GLU:HB2	17:Q:181:ASN:ND2	2.29	0.47
18:R:119:LEU:HA	18:R:123:ALA:HB3	1.97	0.47
25:2:203:PHE:CD2	25:2:204:LEU:N	2.82	0.47
25:2:234:LEU:HD23	25:2:234:LEU:C	2.34	0.47
25:2:236:PHE:CD1	25:2:261:PHE:HB3	2.49	0.47
25:2:85:GLU:O	25:2:89:LEU:HB2	2.14	0.47
26:3:137:LEU:HD11	26:3:177:PHE:CE1	2.50	0.47
1:A:1067:TRP:CZ2	1:A:1071:GLU:HG3	2.50	0.47
2:B:257:VAL:HA	2:B:268:PRO:HA	1.97	0.47
4:D:95:PHE:HZ	7:G:83:GLU:HG3	1.80	0.47
10:J:7:CYS:SG	10:J:48:MET:HE3	2.55	0.47
13:M:214:PHE:HB3	13:M:218:PHE:CE2	2.48	0.47
17:Q:187:ILE:HD13	18:R:212:VAL:N	2.25	0.47
19:S:136:GLU:HG2	19:S:138:PHE:CE1	2.49	0.47
25:2:201:PHE:CD1	25:2:202:GLN:N	2.83	0.47
25:2:46:ARG:CD	25:2:85:GLU:CB	2.93	0.47
26:3:226:TYR:CA	26:3:230:VAL:HG23	2.42	0.47
26:3:34:LEU:HD22	26:3:37:CYS:SG	2.54	0.47
26:3:71:TYR:CG	26:3:72:PRO:HD2	2.18	0.47
2:B:561:ILE:HD11	2:B:576:ILE:HG21	1.97	0.47
7:G:40:GLY:O	7:G:78:ARG:NH1	2.48	0.47
8:H:24:ARG:NH1	8:H:46:GLN:OE1	2.48	0.47
18:R:194:ARG:O	18:R:196:ASP:O	2.33	0.47
2:B:56:GLN:CD	20:T:140:ARG:HG3	2.31	0.47
28:Y:57:DA:H5"	28:Y:58:DC:H2'	1.95	0.47
24:1:38:ILE:O	24:1:38:ILE:HG12	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:3:177:PHE:O	26:3:181:ILE:HG13	2.15	0.47
2:B:217:TYR:CE2	2:B:376:ALA:HA	2.50	0.47
2:B:873:LEU:HB3	2:B:874:PRO:HD3	1.97	0.47
2:B:908:MET:HE3	2:B:920:LYS:HB2	1.97	0.47
3:C:14:LEU:HD13	3:C:19:VAL:HG23	1.95	0.47
18:R:157:GLN:O	18:R:161:ARG:N	2.47	0.47
21:V:361:CYS:HB3	21:V:405:VAL:HG21	1.96	0.47
24:1:38:ILE:CB	24:1:44:PHE:CE1	2.98	0.47
25:2:96:TRP:CZ2	25:2:97:HIS:NE2	2.83	0.47
1:A:1374:VAL:HG11	1:A:1411:LEU:HD21	1.96	0.47
1:A:362:SER:OG	2:B:1084:LEU:HD13	2.15	0.47
1:A:466:LYS:HA	2:B:1093:CYS:SG	2.55	0.47
1:A:926:ASN:CG	1:A:931:ARG:HB3	2.35	0.47
5:E:173:ILE:CG2	5:E:209:VAL:HG22	2.44	0.47
2:B:595:ASP:OD1	20:T:129:ARG:NH1	2.48	0.47
28:Y:16:DA:H2'	28:Y:17:DG:C8	2.50	0.47
24:1:53:LEU:O	24:1:57:VAL:HG12	2.15	0.47
21:V:689:VAL:CG2	25:2:391:ILE:CD1	2.93	0.47
25:2:84:GLU:HA	25:2:84:GLU:OE1	2.15	0.47
26:3:69:PHE:HE1	26:3:139:LYS:HD2	1.77	0.47
25:2:28:PRO:CD	26:3:25:GLN:NE2	2.72	0.47
26:3:70:LEU:HD22	26:3:114:GLU:CB	2.44	0.47
1:A:540:ASP:HB3	2:B:790:GLN:HG2	1.96	0.47
1:A:810:PHE:CZ	1:A:819:SER:HA	2.50	0.47
1:A:365:THR:HG22	2:B:1059:ILE:HG22	1.97	0.47
2:B:348:LEU:N	2:B:349:PRO:HD3	2.30	0.47
2:B:804:GLY:HA2	2:B:807:ARG:HE	1.80	0.47
3:C:212:ASP:HB2	3:C:214:ASP:HB2	1.97	0.47
7:G:139:GLN:O	7:G:141:ASP:N	2.47	0.47
9:I:15:ARG:O	9:I:24:LEU:CD1	2.62	0.47
13:M:52:TRP:C	13:M:52:TRP:CD1	2.88	0.47
17:Q:169:PRO:HA	17:Q:174:ARG:HG2	1.96	0.47
2:B:494:LYS:HG3	27:X:49:DT:C2	2.50	0.47
25:2:51:LEU:HD21	25:2:55:TRP:CD1	2.50	0.47
25:2:96:TRP:CH2	25:2:97:HIS:CE1	3.03	0.47
26:3:174:TYR:CE1	26:3:178:MET:HE2	2.50	0.47
1:A:1306:LYS:HD3	1:A:1306:LYS:O	2.15	0.47
1:A:322:LEU:HD23	1:A:325:LEU:HD22	1.97	0.47
3:C:5:ASN:CB	3:C:7:PRO:HD3	2.35	0.47
5:E:173:ILE:HG23	5:E:209:VAL:HG22	1.97	0.47
22:W:657:MET:O	22:W:660:ALA:HB3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:3:64:ILE:HG21	26:3:128:HIS:HB3	1.97	0.47
1:A:274:ASP:OD2	1:A:276:LEU:N	2.46	0.47
1:A:745:LEU:HD21	1:A:817:PRO:HB3	1.95	0.47
3:C:100:GLU:CG	3:C:164:TYR:HE1	2.28	0.47
4:D:96:GLU:OE2	4:D:117:SER:OG	2.22	0.47
9:I:66:THR:O	9:I:68:ILE:N	2.44	0.47
22:W:143:ARG:HG2	22:W:143:ARG:HH11	1.80	0.47
28:Y:63:DG:H5'	28:Y:65:DG:OP1	2.15	0.47
25:2:217:LEU:CD2	25:2:233:ILE:HD11	2.45	0.46
25:2:240:LEU:HD12	25:2:240:LEU:N	2.31	0.46
26:3:56:LYS:HD3	26:3:56:LYS:N	2.30	0.46
1:A:152:ASN:O	1:A:153:ILE:CD1	2.55	0.46
1:A:582:PRO:HD2	8:H:47:ILE:HD12	1.98	0.46
1:A:608:THR:C	1:A:610:PRO:CD	2.60	0.46
1:A:601:ASN:ND2	1:A:992:LYS:HD2	2.30	0.46
2:B:1022:LEU:HD12	2:B:1023:ARG:HG3	1.97	0.46
2:B:551:GLU:HB2	2:B:576:ILE:HD11	1.97	0.46
2:B:733:MET:HG2	2:B:1050:ARG:O	2.14	0.46
14:N:333:ASN:CG	14:N:361:ASN:H	2.19	0.46
17:Q:188:TYR:CD2	17:Q:191:LEU:HD22	2.50	0.46
17:Q:188:TYR:OH	18:R:211:SER:OG	2.19	0.46
5:E:81:LYS:HD3	27:X:63:DC:OP1	2.15	0.46
24:1:10:ILE:HG12	24:1:43:VAL:CG1	2.45	0.46
26:3:25:GLN:NE2	26:3:25:GLN:HA	2.30	0.46
26:3:10:LEU:CD1	26:3:56:LYS:HG2	2.44	0.46
1:A:597:PRO:O	1:A:599:HIS:N	2.48	0.46
2:B:80:GLU:OE1	2:B:134:LYS:HB3	2.16	0.46
2:B:878:ASP:O	2:B:882:SER:OG	2.33	0.46
11:K:61:TYR:HA	11:K:72:ILE:O	2.15	0.46
14:N:376:TRP:HD1	15:O:62:LEU:O	1.98	0.46
17:Q:135:THR:HG23	17:Q:164:ASP:OD1	2.15	0.46
2:B:594:MET:O	20:T:129:ARG:NH1	2.49	0.46
27:X:73:DG:C2	27:X:74:DT:C2	3.04	0.46
23:0:77:LYS:HA	23:0:77:LYS:CE	2.18	0.46
25:2:218:GLN:HG2	25:2:268:PHE:CB	2.44	0.46
1:A:891:TYR:CE1	1:A:1087:VAL:HG13	2.49	0.46
1:A:133:SER:O	1:A:134:LYS:HB2	2.14	0.46
2:B:1108:PHE:CD2	2:B:1109:GLU:HG3	2.51	0.46
2:B:924:ARG:HG3	2:B:924:ARG:O	2.15	0.46
3:C:56:SER:HG	3:C:158:GLU:H	1.55	0.46
3:C:169:PHE:CE1	3:C:171:LYS:HB3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:80:PRO:HA	5:E:107:GLN:HB3	1.97	0.46
5:E:27:LEU:HB2	5:E:64:HIS:HB3	1.97	0.46
9:I:98:GLN:O	9:I:100:HIS:N	2.47	0.46
9:I:32:ASN:HB2	9:I:34:ILE:HG12	1.98	0.46
13:M:53:ARG:NH1	28:Y:55:DG:O6	2.48	0.46
14:N:337:CYS:O	15:O:97:ALA:HA	2.14	0.46
17:Q:113:ARG:CD	18:R:221:ARG:HB3	2.40	0.46
19:S:98:TRP:HB2	19:S:112:GLY:HA3	1.97	0.46
21:V:514:MET:HE2	21:V:664:SER:HB3	1.97	0.46
24:1:2:VAL:HG12	25:2:456:LYS:CE	2.44	0.46
2:B:952:GLU:N	2:B:952:GLU:OE1	2.46	0.46
3:C:117:SER:OG	3:C:147:ASP:HB3	2.14	0.46
3:C:68:LEU:HD12	3:C:71:ILE:HD12	1.97	0.46
7:G:94:LYS:HA	7:G:119:PHE:CD2	2.50	0.46
15:O:41:ASP:O	15:O:45:ASN:ND2	2.37	0.46
15:O:84:VAL:HG13	15:O:85:THR:HG23	1.97	0.46
16:P:249:LYS:HB3	16:P:251:LEU:HG	1.97	0.46
25:2:117:ASN:CB	26:3:42:MET:HE2	2.43	0.46
26:3:10:LEU:N	26:3:56:LYS:HE3	2.31	0.46
1:A:350:VAL:HG21	1:A:1435:THR:HG23	1.98	0.46
1:A:610:PRO:HB2	1:A:626:THR:HG22	1.98	0.46
1:A:262:PRO:CG	2:B:1070:LEU:HG	2.46	0.46
2:B:312:GLN:OE1	19:S:153:ARG:NH1	2.49	0.46
3:C:138:ASP:O	3:C:139:PRO:C	2.52	0.46
11:K:49:GLN:HG3	11:K:94:LEU:HB2	1.97	0.46
1:A:427:ILE:HG23	13:M:38:GLY:HA3	1.98	0.46
24:1:50:VAL:CG1	24:1:54:GLN:HG2	2.41	0.46
26:3:165:LYS:HZ1	26:3:200:SER:H	1.63	0.46
1:A:687:ILE:HA	1:A:691:ASP:OD2	2.15	0.46
2:B:584:MET:HG3	2:B:605:ARG:HD2	1.97	0.46
3:C:138:ASP:O	3:C:140:ASN:N	2.49	0.46
3:C:246:LEU:HD11	11:K:106:ARG:NH2	2.31	0.46
1:A:1252:ALA:HB1	9:I:3:PRO:HB3	1.96	0.46
12:L:35:ARG:NH1	12:L:42:ARG:NH2	2.62	0.46
17:Q:184:ILE:HD12	18:R:218:LYS:HZ1	1.74	0.46
22:W:420:PRO:O	22:W:421:PHE:CG	2.68	0.46
26:3:196:LEU:HB3	26:3:220:MET:SD	2.56	0.46
26:3:71:TYR:HD2	26:3:72:PRO:HD2	1.69	0.46
1:A:760:LEU:HD22	1:A:764:ASN:HD22	1.81	0.46
2:B:1135:TYR:O	2:B:1136:GLU:HG2	2.16	0.46
2:B:489:ILE:HG13	2:B:490:GLY:N	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:561:ILE:HD11	2:B:576:ILE:HG12	1.97	0.46
3:C:72:PRO:HG3	10:J:13:ILE:HD13	1.97	0.46
21:V:321:GLU:CG	22:W:499:ASN:ND2	2.76	0.46
22:W:581:LEU:HD13	22:W:581:LEU:C	2.36	0.46
27:X:77:DC:H2"	27:X:78:DT:H72	1.98	0.46
24:1:40:ASP:HB2	24:1:43:VAL:H	1.81	0.46
24:1:57:VAL:HG13	24:1:58:GLY:N	2.31	0.46
26:3:59:VAL:N	26:3:71:TYR:CZ	2.69	0.46
1:A:472:HIS:NE2	1:A:521:VAL:HG21	2.30	0.46
1:A:687:ILE:HG13	1:A:691:ASP:OD2	2.16	0.46
2:B:309:PHE:HA	2:B:312:GLN:NE2	2.31	0.46
8:H:96:VAL:HG13	8:H:115:TYR:O	2.16	0.46
18:R:198:LYS:HE3	18:R:199:LYS:HE3	1.98	0.46
27:X:31:DT:H2'	27:X:32:DT:C2	2.50	0.46
26:3:10:LEU:HB2	26:3:56:LYS:HE3	1.97	0.46
1:A:939:VAL:O	1:A:942:VAL:HG22	2.16	0.46
2:B:1054:MET:HB2	2:B:1054:MET:HE3	1.78	0.46
2:B:99:TRP:NE1	2:B:105:PRO:HB3	2.31	0.46
3:C:138:ASP:C	3:C:140:ASN:N	2.69	0.46
2:B:950:ARG:HH12	3:C:171:LYS:HG3	1.79	0.46
3:C:175:LYS:NZ	12:L:57:ALA:HB3	2.30	0.46
7:G:98:PHE:CZ	17:Q:145:PHE:HB2	2.51	0.46
9:I:60:HIS:C	9:I:62:VAL:H	2.15	0.46
13:M:217:ARG:O	13:M:221:ASN:ND2	2.46	0.46
13:M:94:ASP:HB3	13:M:99:SER:C	2.36	0.46
20:T:196:TYR:HB2	20:T:232:THR:HB	1.98	0.46
27:X:48:DT:OP1	27:X:48:DT:H4'	2.15	0.46
27:X:60:DG:N3	28:Y:35:DG:N2	2.64	0.46
24:1:38:ILE:CG2	24:1:44:PHE:CD1	2.94	0.46
25:2:164:VAL:HG13	25:2:209:PRO:CG	2.45	0.46
25:2:189:GLU:HB2	25:2:190:PRO:CD	2.43	0.46
1:A:567:LEU:HD11	1:A:595:ILE:HG12	1.96	0.46
2:B:959:GLU:OE2	10:J:42:ARG:HB3	2.15	0.46
11:K:35:ILE:HB	11:K:71:ILE:HG12	1.98	0.46
15:O:50:GLN:O	15:O:53:ARG:NH1	2.49	0.46
22:W:37:HIS:CG	22:W:454:VAL:HG13	2.50	0.46
25:2:203:PHE:CD2	25:2:205:LEU:CD2	2.95	0.45
26:3:64:ILE:CG2	26:3:128:HIS:CB	2.94	0.45
2:B:127:ASP:HA	2:B:145:GLN:O	2.16	0.45
1:A:334:ARG:HE	13:M:66:ARG:HD3	1.80	0.45
27:X:30:DG:N2	28:Y:64:DC:O2	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:2:203:PHE:CG	25:2:204:LEU:N	2.84	0.45
1:A:1128:ILE:HG23	1:A:1414:ILE:CG1	2.46	0.45
1:A:421:ARG:HA	1:A:444:TYR:CD1	2.52	0.45
2:B:225:LEU:CD2	2:B:228:SER:HB2	2.45	0.45
13:M:59:LYS:HA	29:Z:1:A:N7	2.32	0.45
14:N:46:TRP:CZ2	15:O:11:LEU:HD11	2.51	0.45
17:Q:184:ILE:CD1	18:R:213:ASP:OD2	2.53	0.45
20:T:128:LYS:HA	20:T:131:GLN:HB3	1.98	0.45
27:X:37:DT:H1'	27:X:38:DT:O5'	2.16	0.45
25:2:118:LEU:HD23	26:3:42:MET:CB	2.34	0.45
25:2:51:LEU:C	25:2:51:LEU:HD23	2.37	0.45
25:2:81:LYS:CG	25:2:82:ALA:N	2.79	0.45
26:3:165:LYS:CG	26:3:203:LEU:HD12	2.36	0.45
26:3:219:GLN:HA	26:3:219:GLN:OE1	2.17	0.45
1:A:1114:ALA:C	1:A:1116:ASN:H	2.18	0.45
2:B:972:ILE:HG12	2:B:981:LEU:HD21	1.97	0.45
4:D:74:PHE:CZ	4:D:83:VAL:HG21	2.51	0.45
9:I:58:ILE:HB	9:I:61:GLU:OE1	2.16	0.45
2:B:756:LYS:HG2	10:J:51:ALA:O	2.16	0.45
18:R:139:PHE:HA	18:R:140:LYS:HB2	1.98	0.45
18:R:194:ARG:CB	18:R:195:PRO:HD2	2.30	0.45
25:2:187:SER:OG	25:2:190:PRO:HD2	2.16	0.45
1:A:196:LEU:HD21	1:A:311:GLN:HG3	1.99	0.45
2:B:65:ILE:HD11	2:B:86:LEU:HD12	1.98	0.45
5:E:73:PHE:HD2	5:E:90:TYR:HH	1.62	0.45
13:M:286:ARG:HG3	13:M:316:LEU:HD23	1.98	0.45
20:T:211:VAL:O	20:T:215:GLU:HG2	2.15	0.45
25:2:30:VAL:CG1	25:2:34:LEU:CD2	2.94	0.45
26:3:160:ARG:HB2	26:3:160:ARG:HE	1.58	0.45
26:3:12:VAL:CG2	26:3:161:ILE:HG23	2.43	0.45
26:3:64:ILE:CG2	26:3:128:HIS:CG	2.99	0.45
1:A:1160:ARG:NH1	1:A:1349:GLU:OE2	2.50	0.45
1:A:470:MET:HG2	1:A:524:MET:HG3	1.98	0.45
1:A:485:ASN:O	1:A:487:SER:N	2.49	0.45
1:A:600:ILE:HD12	1:A:656:SER:HA	1.99	0.45
1:A:795:GLY:HA3	1:A:1107:PHE:HD2	1.80	0.45
1:A:959:MET:HE1	1:A:1046:ARG:O	2.17	0.45
2:B:1029:TYR:HD1	2:B:1036:LYS:HA	1.82	0.45
13:M:73:PRO:HB3	13:M:79:ASP:OD1	2.17	0.45
20:T:154:LYS:N	20:T:154:LYS:CD	2.74	0.45
20:T:94:THR:HA	20:T:109:ILE:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:LYS:HZ1	28:Y:43:DG:H5"	1.82	0.45
24:1:4:VAL:HG11	25:2:412:PHE:CD2	2.29	0.45
26:3:42:MET:CG	26:3:111:ILE:CD1	2.95	0.45
26:3:8:LEU:HD23	26:3:54:SER:CB	2.42	0.45
1:A:601:ASN:ND2	1:A:988:TRP:HZ3	2.14	0.45
2:B:489:ILE:HD12	27:X:47:DT:O2	2.17	0.45
2:B:957:THR:HG23	2:B:961:ILE:HG23	1.98	0.45
3:C:1:MET:O	3:C:3:TYR:N	2.37	0.45
3:C:37:VAL:HG13	3:C:41:GLU:HB2	1.98	0.45
5:E:55:ARG:NE	5:E:107:GLN:OE1	2.46	0.45
7:G:14:HIS:CG	7:G:15:PRO:HD2	2.51	0.45
13:M:244:LEU:HD21	13:M:292:ILE:HA	1.98	0.45
13:M:34:CYS:H	13:M:39:LEU:CB	2.29	0.45
17:Q:92:TYR:CE2	17:Q:94:ILE:HB	2.52	0.45
20:T:99:SER:HB2	20:T:103:LYS:H	1.81	0.45
21:V:647:LYS:O	21:V:648:LYS:O	2.35	0.45
16:P:171:THR:HG21	27:X:16:DA:H4'	1.99	0.45
27:X:53:DA:C6	27:X:54:DA:C6	3.05	0.45
12:L:17:TYR:HB2	12:L:26:ASN:HB3	1.99	0.45
17:Q:69:ASP:HB3	17:Q:71:PHE:CD2	2.52	0.45
13:M:179:GLU:CA	20:T:154:LYS:HG2	2.27	0.45
20:T:31:TRP:HD1	20:T:62:LEU:HD21	1.82	0.45
21:V:461:HIS:CE1	21:V:462:CYS:HG	2.35	0.45
22:W:37:HIS:NE2	22:W:454:VAL:HG11	2.32	0.45
22:W:623:VAL:HG23	22:W:681:ASP:HB2	1.98	0.45
27:X:65:DG:N1	27:X:66:DA:C2	2.85	0.45
21:V:522:TYR:CE2	24:1:62:ASP:CG	2.69	0.45
25:2:214:TYR:CE1	25:2:233:ILE:HG23	2.51	0.45
1:A:112:PHE:H	1:A:188:GLN:NE2	2.09	0.45
1:A:322:LEU:HA	1:A:323:PRO:HD3	1.84	0.45
1:A:46:THR:HG23	1:A:58:MET:HG2	1.98	0.45
12:L:19:CYS:HB3	12:L:23:HIS:H	1.81	0.45
16:P:295:MET:HG2	16:P:297:LYS:H	1.81	0.45
17:Q:114:ILE:HD11	18:R:218:LYS:CE	2.43	0.45
17:Q:184:ILE:HG13	18:R:218:LYS:HZ2	1.82	0.45
20:T:140:ARG:HA	20:T:140:ARG:HD3	1.40	0.45
27:X:24:DG:H4'	27:X:25:DG:OP1	2.16	0.45
25:2:117:ASN:HB2	26:3:104:LEU:CG	2.46	0.45
26:3:144:ILE:HD13	26:3:144:ILE:O	2.17	0.45
26:3:148:ASN:ND2	26:3:157:MET:HG3	2.32	0.45
1:A:1005:HIS:ND1	1:A:1007:ILE:HG22	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1411:LEU:HD23	1:A:1411:LEU:HA	1.80	0.45
1:A:531:ASN:ND2	1:A:901:VAL:HG23	2.31	0.45
2:B:225:LEU:O	2:B:228:SER:N	2.49	0.45
2:B:234:THR:O	2:B:236:TRP:CD1	2.69	0.45
2:B:56:GLN:CD	20:T:140:ARG:HD2	2.38	0.45
5:E:146:PRO:O	5:E:148:HIS:ND1	2.48	0.45
15:O:71:VAL:HG22	15:O:98:CYS:HB3	1.99	0.45
17:Q:112:ARG:NH2	18:R:237:LEU:CB	2.73	0.45
25:2:90:LEU:HD21	25:2:140:LYS:HD3	1.98	0.45
26:3:15:VAL:HG12	26:3:164:ILE:HD12	1.97	0.45
1:A:1308:TYR:CD1	1:A:1308:TYR:O	2.71	0.45
1:A:374:SER:C	1:A:485:ASN:HD22	2.20	0.45
1:A:810:PHE:CE2	1:A:819:SER:HA	2.52	0.45
2:B:275:ALA:O	2:B:314:GLN:NE2	2.48	0.45
2:B:838:GLN:HG3	2:B:886:ARG:HH22	1.82	0.45
3:C:18:ASN:HB2	3:C:234:GLU:HG2	1.99	0.45
1:A:1484:MET:SD	7:G:20:PRO:HA	2.57	0.45
7:G:14:HIS:CD2	7:G:65:PHE:HE1	2.35	0.45
7:G:89:VAL:HA	7:G:98:PHE:O	2.17	0.45
9:I:14:ILE:CG1	9:I:16:PHE:CG	3.00	0.45
9:I:58:ILE:C	9:I:60:HIS:H	2.21	0.45
18:R:195:PRO:HG2	18:R:201:LEU:HD21	1.97	0.45
19:S:17:ARG:HG2	20:T:38:GLY:O	2.17	0.45
2:B:556:ILE:O	20:T:91:GLN:NE2	2.49	0.45
24:1:22:TYR:CD1	24:1:23:LEU:HD23	2.48	0.44
24:1:54:GLN:O	24:1:57:VAL:HG12	2.16	0.44
24:1:4:VAL:HG22	24:1:5:LEU:N	2.32	0.44
25:2:56:VAL:HG23	25:2:57:MET:N	2.31	0.44
26:3:228:LEU:O	26:3:228:LEU:HD23	2.17	0.44
26:3:33:THR:CG2	26:3:36:LYS:CB	2.95	0.44
26:3:71:TYR:O	26:3:71:TYR:CG	2.70	0.44
2:B:132:VAL:CG2	2:B:141:GLN:OE1	2.62	0.44
2:B:119:THR:HG23	2:B:187:ILE:HD13	1.99	0.44
2:B:867:ILE:O	2:B:893:SER:HB2	2.17	0.44
5:E:88:LYS:O	5:E:91:CYS:HB2	2.17	0.44
13:M:11:PRO:O	13:M:12:ARG:CB	2.63	0.44
15:O:3:TYR:HE2	15:O:99:ASP:HA	1.82	0.44
16:P:267:PRO:HG2	16:P:337:LYS:HB2	1.99	0.44
20:T:177:ARG:NH1	27:X:19:DG:H3'	2.31	0.44
27:X:29:DC:H2"	27:X:30:DG:H5'	1.99	0.44
28:Y:56:DG:N2	28:Y:58:DC:OP1	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:Y:61:DA:H3'	28:Y:62:DC:H5"	1.98	0.44
26:3:60:ILE:HG23	26:3:68:ARG:O	2.17	0.44
1:A:1308:TYR:CG	1:A:1308:TYR:O	2.70	0.44
1:A:1130:ILE:HD11	1:A:1405:MET:CE	2.47	0.44
1:A:574:VAL:O	8:H:74:GLU:HA	2.16	0.44
2:B:1079:SER:C	2:B:1080:ARG:HD2	2.38	0.44
2:B:133:ILE:HA	2:B:139:GLN:HA	1.98	0.44
2:B:632:LYS:HA	2:B:682:LEU:HD21	1.99	0.44
2:B:861:SER:O	2:B:896:LEU:HD23	2.17	0.44
1:A:393:ILE:CG2	6:F:74:ALA:HB1	2.47	0.44
8:H:38:ASP:OD1	8:H:39:LEU:N	2.51	0.44
8:H:65:TYR:HE1	8:H:84:ARG:HH21	1.66	0.44
9:I:65:LEU:HD23	9:I:122:ARG:NH2	2.32	0.44
13:M:52:TRP:O	13:M:54:THR:HG22	2.18	0.44
18:R:163:LEU:C	18:R:164:GLY:O	2.55	0.44
18:R:198:LYS:HG3	18:R:199:LYS:HG3	1.98	0.44
27:X:37:DT:H4'	27:X:38:DT:OP1	2.15	0.44
24:1:11:GLU:HG2	25:2:404:THR:OG1	2.17	0.44
25:2:243:SER:HB3	25:2:258:LEU:CD2	2.45	0.44
26:3:121:LYS:H	26:3:121:LYS:HD3	1.81	0.44
26:3:33:THR:HG22	26:3:36:LYS:CB	2.44	0.44
1:A:1210:TRP:CD1	1:A:1281:ASP:HB3	2.52	0.44
1:A:231:GLU:H	1:A:231:GLU:CD	2.19	0.44
1:A:275:ASP:OD1	1:A:276:LEU:N	2.50	0.44
1:A:457:ILE:HG21	1:A:457:ILE:HD13	1.75	0.44
1:A:546:ARG:O	1:A:546:ARG:HG2	2.18	0.44
2:B:880:LEU:C	2:B:881:GLU:OE1	2.56	0.44
2:B:1040:GLN:HG2	3:C:203:TRP:CZ2	2.52	0.44
8:H:15:ILE:HD11	8:H:52:LEU:N	2.32	0.44
11:K:7:PHE:CD1	11:K:11:LEU:HD12	2.53	0.44
14:N:38:VAL:HG13	15:O:22:LEU:HD22	1.99	0.44
17:Q:144:LEU:O	17:Q:153:ARG:N	2.44	0.44
17:Q:17:LEU:HD11	17:Q:191:LEU:HB3	1.99	0.44
24:1:3:ASN:HB3	25:2:412:PHE:O	2.17	0.44
25:2:223:ALA:H	25:2:268:PHE:HE1	1.64	0.44
25:2:217:LEU:CD2	25:2:233:ILE:CD1	2.95	0.44
24:1:1:MET:SD	25:2:419:GLU:N	2.90	0.44
26:3:42:MET:HE1	26:3:108:ASN:HB2	1.99	0.44
1:A:1298:LEU:O	1:A:1300:GLY:N	2.50	0.44
2:B:403:LEU:HD21	2:B:447:SER:HB2	2.00	0.44
2:B:760:THR:OG1	2:B:761:THR:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:853:LEU:HD13	2:B:907:VAL:HG11	1.97	0.44
4:D:118:LEU:HB2	4:D:122:PHE:CD2	2.52	0.44
7:G:96:GLY:O	7:G:128:TYR:HE2	2.00	0.44
8:H:11:ASP:OD2	8:H:55:LYS:HG2	2.17	0.44
18:R:206:LYS:HG3	18:R:207:SER:H	1.82	0.44
19:S:124:TYR:HE1	20:T:22:LYS:HG3	1.83	0.44
28:Y:70:DC:H2"	28:Y:71:DA:H8	1.83	0.44
23:0:60:HIS:CE1	23:0:159:MET:SD	3.11	0.44
23:0:77:LYS:HD2	23:0:77:LYS:N	2.32	0.44
24:1:4:VAL:CG1	25:2:412:PHE:HD2	2.20	0.44
26:3:178:MET:CE	26:3:202:LEU:CD1	2.95	0.44
1:A:1057:GLU:O	1:A:1059:ARG:HG3	2.17	0.44
1:A:1176:TYR:HB2	1:A:1211:LEU:HD23	1.98	0.44
1:A:1298:LEU:C	1:A:1300:GLY:H	2.21	0.44
1:A:811:ILE:HD12	1:A:811:ILE:HA	1.87	0.44
1:A:926:ASN:OD1	1:A:927:GLU:N	2.50	0.44
1:A:924:TYR:CE1	1:A:949:GLN:HG3	2.53	0.44
2:B:244:GLY:O	2:B:246:GLY:N	2.50	0.44
2:B:903:ILE:O	2:B:923:VAL:HG13	2.18	0.44
3:C:136:ASP:C	3:C:138:ASP:H	2.20	0.44
2:B:1021:HIS:HB2	3:C:203:TRP:CZ3	2.53	0.44
10:J:2:ILE:HD13	10:J:2:ILE:HG21	1.74	0.44
10:J:62:TYR:O	10:J:65:LEU:CD1	2.65	0.44
17:Q:114:ILE:CG1	18:R:218:LYS:HE3	2.47	0.44
18:R:206:LYS:O	18:R:207:SER:O	2.35	0.44
25:2:61:PHE:CE1	25:2:99:GLN:NE2	2.85	0.44
1:A:1127:LEU:HD11	1:A:1381:GLU:HB3	2.00	0.44
1:A:1114:ALA:HB2	1:A:1309:MET:CE	2.48	0.44
1:A:408:ARG:HD3	1:A:412:GLN:OE1	2.17	0.44
1:A:426:ARG:O	13:M:40:VAL:HG21	2.12	0.44
1:A:459:ASN:C	1:A:459:ASN:OD1	2.56	0.44
2:B:1062:ARG:CZ	2:B:1074:PRO:HB3	2.48	0.44
2:B:882:SER:CB	2:B:887:TYR:CE1	3.00	0.44
22:W:73:CYS:CB	22:W:209:TYR:CE2	3.00	0.44
24:1:13:ASP:OD2	24:1:17:LYS:HB2	2.16	0.44
25:2:123:LEU:CD2	25:2:178:LEU:CD1	2.95	0.44
25:2:159:VAL:HG12	25:2:161:HIS:HB2	1.99	0.44
25:2:218:GLN:HE22	25:2:265:LEU:CA	2.28	0.44
1:A:601:ASN:ND2	1:A:632:ASN:H	2.15	0.44
1:A:800:PHE:HA	1:A:805:ARG:O	2.18	0.44
2:B:420:GLN:HA	2:B:423:ILE:HG12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:818:GLU:OE2	2:B:828:VAL:HA	2.17	0.44
3:C:9:VAL:HG21	11:K:105:PHE:HA	2.00	0.44
9:I:11:PHE:HE1	9:I:54:TYR:HA	1.82	0.44
17:Q:70:LYS:HZ2	18:R:226:ASP:HA	1.83	0.44
19:S:125:TYR:HD1	19:S:139:PRO:HA	1.82	0.44
20:T:146:ASP:O	20:T:147:LYS:CB	2.65	0.44
20:T:225:VAL:HA	20:T:231:ASN:HA	1.99	0.44
22:W:37:HIS:CD2	22:W:454:VAL:CG1	3.00	0.44
23:0:72:GLU:O	23:0:79:ASN:HB3	2.17	0.44
2:B:132:VAL:O	2:B:139:GLN:HA	2.17	0.44
2:B:25:ALA:HA	2:B:28:ILE:HD12	2.00	0.44
2:B:854:ILE:HD13	2:B:904:VAL:HG21	1.99	0.44
2:B:931:ILE:HD11	2:B:947:ILE:HA	1.99	0.44
7:G:1:MET:HB3	7:G:3:TYR:CZ	2.53	0.44
17:Q:113:ARG:HH12	18:R:218:LYS:HA	1.83	0.44
17:Q:115:GLU:O	17:Q:119:ARG:N	2.40	0.44
27:X:30:DG:H5"	27:X:31:DT:O4'	2.18	0.44
28:Y:60:DA:H2"	28:Y:61:DA:C8	2.53	0.44
23:0:106:ILE:HD11	23:0:127:HIS:HB3	2.00	0.44
25:2:130:SER:HB2	25:2:179:LEU:HD23	1.99	0.44
25:2:35:TYR:CG	25:2:62:LEU:CD1	2.99	0.44
25:2:35:TYR:HB2	25:2:62:LEU:HD12	1.98	0.44
26:3:178:MET:HA	26:3:181:ILE:HD12	1.99	0.44
1:A:1477:ALA:O	1:A:1480:CYS:HB2	2.18	0.44
1:A:230:ASP:OD1	1:A:244:ARG:NH1	2.51	0.44
2:B:1080:ARG:HH21	13:M:50:SER:CB	2.27	0.44
2:B:128:ILE:HG21	2:B:431:LEU:HD21	2.00	0.44
2:B:882:SER:O	2:B:887:TYR:CD1	2.70	0.44
10:J:35:LEU:HD13	10:J:46:ARG:HG2	1.99	0.44
12:L:16:ILE:HG21	12:L:47:LYS:CD	2.48	0.44
13:M:27:TYR:HD2	13:M:46:ILE:HB	1.82	0.44
1:A:278:HIS:HB3	13:M:82:THR:HG23	2.00	0.44
17:Q:69:ASP:HB3	17:Q:71:PHE:HD2	1.83	0.44
18:R:223:VAL:O	18:R:224:THR:HG23	2.05	0.44
20:T:159:HIS:CG	20:T:160:GLN:N	2.85	0.44
20:T:180:LYS:HZ2	20:T:216:ILE:HD12	1.83	0.44
21:V:282:LYS:HE3	21:V:482:PHE:CD1	2.53	0.44
27:X:77:DC:C2'	27:X:78:DT:H72	2.48	0.44
28:Y:88:DC:H2"	28:Y:89:DC:O4'	2.18	0.44
25:2:203:PHE:HD2	25:2:205:LEU:H	1.65	0.43
25:2:214:TYR:HB3	25:2:261:PHE:CE2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1116:ASN:O	1:A:1117:VAL:HB	2.18	0.43
1:A:126:ILE:HD13	1:A:129:ILE:HD12	2.00	0.43
2:B:203:ASN:O	2:B:571:GLY:HA3	2.18	0.43
2:B:32:SER:OG	2:B:643:LEU:HD22	2.17	0.43
2:B:754:PRO:HB2	2:B:773:PRO:HB2	1.99	0.43
13:M:86:LYS:HD2	13:M:86:LYS:N	2.32	0.43
14:N:336:VAL:HG23	14:N:357:ILE:HB	2.00	0.43
25:2:127:LYS:CA	25:2:178:LEU:HD23	2.48	0.43
25:2:215:PHE:CE2	25:2:264:HIS:ND1	2.86	0.43
25:2:117:ASN:ND2	26:3:108:ASN:N	2.65	0.43
8:H:65:TYR:CD1	8:H:65:TYR:N	2.85	0.43
13:M:108:SER:HB3	13:M:112:ARG:NH1	2.30	0.43
14:N:372:GLY:HA3	15:O:58:PHE:CZ	2.53	0.43
25:2:140:LYS:HD3	25:2:162:PHE:CE1	2.47	0.43
26:3:160:ARG:CB	26:3:190:LEU:CD2	2.95	0.43
1:A:134:LYS:HA	1:A:140:ARG:NH2	2.33	0.43
1:A:285:LYS:HB3	1:A:285:LYS:HE3	1.83	0.43
1:A:53:LYS:HE3	1:A:59:ASP:HB3	2.00	0.43
1:A:882:SER:C	1:A:884:ASN:H	2.22	0.43
2:B:333:GLU:HG2	2:B:337:LYS:HE3	2.00	0.43
3:C:212:ASP:O	3:C:214:ASP:N	2.52	0.43
3:C:44:ILE:O	3:C:167:LYS:HA	2.18	0.43
3:C:45:ILE:HG22	3:C:73:LEU:HD12	2.00	0.43
8:H:5:LEU:HD11	8:H:62:SER:HB3	2.00	0.43
14:N:356:GLY:HA3	14:N:367:PHE:CZ	2.54	0.43
17:Q:24:GLY:N	18:R:210:PHE:HD2	1.98	0.43
18:R:155:LEU:HA	18:R:161:ARG:HB2	2.00	0.43
21:V:405:VAL:HG12	21:V:406:ALA:H	1.82	0.43
21:V:517:GLU:CB	21:V:713:LEU:HD22	2.46	0.43
25:2:206:LEU:CD2	25:2:206:LEU:H	2.30	0.43
25:2:117:ASN:ND2	26:3:104:LEU:O	2.52	0.43
1:A:1192:TRP:O	1:A:1195:VAL:HB	2.19	0.43
2:B:993:LYS:HA	2:B:1018:TYR:OH	2.19	0.43
2:B:625:LEU:CD1	2:B:675:LEU:HD11	2.49	0.43
2:B:896:LEU:C	2:B:897:ARG:HG3	2.35	0.43
3:C:274:ILE:O	11:K:23:LYS:NZ	2.33	0.43
3:C:4:ALA:HA	11:K:52:LYS:HZ2	1.83	0.43
9:I:75:ASP:OD2	9:I:78:LEU:HG	2.18	0.43
1:A:271:ARG:HG2	13:M:73:PRO:CD	2.47	0.43
22:W:28:LEU:C	22:W:28:LEU:HD13	2.38	0.43
22:W:73:CYS:HB3	22:W:209:TYR:CD2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:2:166:SER:HB3	25:2:167:PRO:HD3	2.01	0.43
25:2:409:TYR:CD2	25:2:443:VAL:HG22	2.54	0.43
25:2:117:ASN:CA	26:3:104:LEU:HD21	2.47	0.43
25:2:118:LEU:CD1	26:3:43:VAL:HG22	2.39	0.43
1:A:1086:MET:SD	1:A:1466:ALA:HB1	2.58	0.43
1:A:275:ASP:HA	1:A:278:HIS:HD2	1.84	0.43
1:A:324:GLY:HA2	13:M:90:ALA:HB3	1.99	0.43
1:A:861:GLN:HE22	1:A:1093:GLN:HA	1.83	0.43
1:A:909:LEU:HD23	1:A:909:LEU:HA	1.68	0.43
2:B:281:ASP:H	9:I:22:ASN:HD22	1.66	0.43
2:B:573:TRP:CZ3	2:B:575:GLY:HA2	2.54	0.43
2:B:651:TYR:HA	2:B:655:ASP:OD2	2.19	0.43
2:B:725:GLN:HG2	2:B:938:ARG:O	2.18	0.43
3:C:263:LEU:HD13	11:K:19:ILE:HD13	2.00	0.43
11:K:63:VAL:HG13	11:K:70:LYS:O	2.18	0.43
14:N:319:ASP:O	14:N:321:SER:O	2.36	0.43
21:V:524:ALA:HB2	24:1:23:LEU:HD13	2.01	0.43
27:X:41:DT:H2'	27:X:42:DT:O3'	2.19	0.43
25:2:117:ASN:HB3	26:3:42:MET:HE2	2.00	0.43
25:2:94:ARG:HD2	25:2:95:ILE:CD1	2.47	0.43
26:3:124:ILE:HD13	26:3:124:ILE:C	2.38	0.43
25:2:118:LEU:HD21	26:3:39:ASP:OD1	1.95	0.43
1:A:413:TYR:CD1	1:A:414:PRO:HD3	2.54	0.43
2:B:779:ILE:HG23	2:B:779:ILE:HD12	1.76	0.43
5:E:111:THR:HG21	27:X:63:DC:O3'	2.19	0.43
15:O:64:THR:HA	16:P:189:ASN:OD1	2.18	0.43
17:Q:187:ILE:CD1	18:R:211:SER:HA	2.36	0.43
21:V:446:ILE:HD12	21:V:451:PHE:HB3	2.00	0.43
21:V:666:ASP:CB	24:1:17:LYS:HZ3	2.32	0.43
25:2:214:TYR:OH	25:2:265:LEU:HD13	2.18	0.43
25:2:34:LEU:N	25:2:34:LEU:HD22	2.33	0.43
26:3:65:GLN:O	26:3:132:LEU:HD11	2.18	0.43
26:3:69:PHE:HZ	26:3:139:LYS:HD2	1.80	0.43
1:A:246:GLU:HG3	1:A:247:TRP:CD1	2.53	0.43
1:A:367:ILE:HG21	1:A:501:MET:HG3	1.99	0.43
1:A:802:PHE:CE1	2:B:504:THR:HG22	2.53	0.43
3:C:45:ILE:O	3:C:73:LEU:HB2	2.18	0.43
13:M:52:TRP:C	13:M:54:THR:H	2.18	0.43
16:P:206:GLU:HB2	16:P:236:LYS:HZ1	1.83	0.43
17:Q:113:ARG:NH1	18:R:218:LYS:CA	2.82	0.43
20:T:30:GLN:NE2	20:T:62:LEU:O	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:W:584:TYR:CB	22:W:591:GLY:HA3	2.49	0.43
28:Y:55:DG:H21	28:Y:56:DG:H1	1.67	0.43
24:1:50:VAL:HG12	24:1:50:VAL:O	2.18	0.43
26:3:124:ILE:HG23	26:3:124:ILE:O	2.18	0.43
1:A:364:ARG:HD3	1:A:500:GLU:OE1	2.19	0.43
1:A:914:LYS:O	1:A:918:LYS:HG2	2.19	0.43
2:B:549:SER:OG	2:B:577:HIS:NE2	2.25	0.43
9:I:14:ILE:CG1	9:I:16:PHE:CD1	3.02	0.43
9:I:58:ILE:O	9:I:60:HIS:N	2.51	0.43
12:L:19:CYS:HB3	12:L:23:HIS:N	2.33	0.43
17:Q:92:TYR:HE2	17:Q:94:ILE:HB	1.84	0.43
20:T:141:LEU:HB3	20:T:142:SER:H	1.57	0.43
20:T:159:HIS:O	20:T:162:ASN:HB3	2.19	0.43
21:V:519:TYR:HA	21:V:522:TYR:HB3	2.00	0.43
16:P:305:PHE:CZ	28:Y:82:DT:H1'	2.54	0.43
23:0:77:LYS:HB3	23:0:78:PRO:HD2	1.79	0.43
24:1:18:GLN:CD	24:1:44:PHE:CZ	2.92	0.43
25:2:171:VAL:HG13	25:2:216:MET:HB3	1.98	0.43
25:2:270:LEU:HA	25:2:273:GLN:HG3	2.00	0.43
26:3:11:LEU:CD1	26:3:48:HIS:NE2	2.82	0.43
26:3:133:LEU:CD2	26:3:134:ALA:N	2.82	0.43
1:A:526:VAL:HA	1:A:533:PRO:HA	2.00	0.43
2:B:271:ILE:HG12	2:B:311:ILE:HD11	2.00	0.43
2:B:797:ASN:HB2	2:B:964:ASP:HA	2.00	0.43
5:E:49:SER:HB2	5:E:52:ARG:HH12	1.83	0.43
16:P:304:ILE:N	16:P:304:ILE:HD12	2.33	0.43
18:R:195:PRO:HB2	18:R:199:LYS:CB	2.48	0.43
20:T:127:LEU:O	20:T:131:GLN:N	2.44	0.43
21:V:514:MET:SD	21:V:537:ASN:CG	2.97	0.43
22:W:416:ILE:HA	22:W:434:HIS:O	2.19	0.43
24:1:8:VAL:CG1	24:1:9:LEU:N	2.80	0.43
25:2:171:VAL:CG1	25:2:216:MET:SD	3.06	0.43
25:2:236:PHE:CE1	25:2:239:GLN:NE2	2.87	0.43
25:2:236:PHE:HZ	25:2:258:LEU:HD11	1.83	0.43
25:2:44:VAL:CG1	25:2:45:PHE:N	2.82	0.43
2:B:1151:MET:HE2	2:B:1151:MET:HB3	1.78	0.43
5:E:52:ARG:HH21	5:E:54:ARG:HG3	1.79	0.43
8:H:81:ARG:C	8:H:83:SER:H	2.23	0.43
2:B:758:LEU:HD11	10:J:47:ARG:HB3	2.01	0.43
17:Q:15:LYS:HE3	17:Q:38:ILE:HG23	2.01	0.43
25:2:258:LEU:HG	25:2:262:LEU:HD21	1.99	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:2:35:TYR:CD1	25:2:62:LEU:HD12	2.52	0.42
26:3:121:LYS:CD	26:3:121:LYS:H	2.32	0.42
26:3:137:LEU:HD12	26:3:177:PHE:CE1	2.54	0.42
1:A:274:ASP:OD2	1:A:276:LEU:HB3	2.18	0.42
1:A:760:LEU:HD22	1:A:764:ASN:ND2	2.34	0.42
3:C:212:ASP:N	3:C:212:ASP:OD1	2.41	0.42
7:G:38:CYS:SG	7:G:156:ASP:HA	2.59	0.42
1:A:1254:LYS:HE3	9:I:3:PRO:HA	2.00	0.42
17:Q:105:TYR:CE1	18:R:234:GLU:CD	2.93	0.42
17:Q:127:PHE:HA	17:Q:163:GLU:C	2.38	0.42
17:Q:58:GLN:HE22	18:R:194:ARG:HH11	1.65	0.42
20:T:86:GLN:O	20:T:112:GLN:NE2	2.52	0.42
20:T:128:LYS:NZ	20:T:131:GLN:OE1	2.52	0.42
27:X:2:DA:N6	28:Y:91:DT:O4	2.52	0.42
24:1:25:GLU:OE2	24:1:35:ILE:HG12	2.18	0.42
25:2:117:ASN:HD21	26:3:108:ASN:N	2.16	0.42
25:2:159:VAL:HG11	25:2:161:HIS:CD2	2.49	0.42
25:2:93:LEU:HD23	25:2:93:LEU:HA	1.76	0.42
1:A:1301:ILE:O	1:A:1345:ARG:HD3	2.19	0.42
2:B:1069:ILE:HD12	2:B:1070:LEU:HD12	2.00	0.42
2:B:40:VAL:HG21	2:B:181:PRO:HB2	2.01	0.42
2:B:411:LEU:HD11	2:B:435:ILE:HG23	2.01	0.42
5:E:61:LEU:HD21	5:E:71:GLN:HB2	2.02	0.42
4:D:37:VAL:HG21	7:G:2:PHE:CD2	2.54	0.42
14:N:366:ILE:O	15:O:54:ASN:ND2	2.50	0.42
16:P:297:LYS:HA	16:P:297:LYS:HD3	1.39	0.42
17:Q:19:LYS:O	17:Q:23:ARG:HG3	2.19	0.42
17:Q:113:ARG:NH1	18:R:218:LYS:HA	2.33	0.42
19:S:135:PHE:HA	19:S:135:PHE:HD1	1.71	0.42
22:W:263:LEU:C	22:W:263:LEU:HD23	2.39	0.42
21:V:514:MET:HB3	24:1:16:MET:SD	2.59	0.42
24:1:34:ILE:CG2	24:1:50:VAL:HG11	2.48	0.42
26:3:178:MET:O	26:3:182:PHE:HD2	2.01	0.42
1:A:1103:THR:HG21	1:A:1106:THR:OG1	2.18	0.42
1:A:1128:ILE:HG23	1:A:1414:ILE:HD11	2.01	0.42
1:A:491:PRO:HG3	1:A:535:MET:HE2	2.01	0.42
2:B:570:ASN:OD1	2:B:616:THR:HG22	2.19	0.42
2:B:899:SER:C	2:B:901:THR:H	2.21	0.42
2:B:921:ILE:HG13	2:B:921:ILE:O	2.19	0.42
1:A:1171:ALA:C	9:I:59:THR:HG22	2.30	0.42
15:O:64:THR:HG22	15:O:75:VAL:HB	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:114:ILE:HG12	18:R:218:LYS:HE3	2.00	0.42
17:Q:108:ASP:CG	18:R:237:LEU:HD22	2.39	0.42
24:1:10:ILE:HG22	25:2:407:VAL:CG2	2.49	0.42
25:2:133:THR:CG2	25:2:134:SER:N	2.82	0.42
25:2:28:PRO:HA	26:3:33:THR:CB	2.49	0.42
26:3:128:HIS:NE2	26:3:130:GLU:CG	2.82	0.42
26:3:147:MET:CE	26:3:157:MET:SD	3.07	0.42
26:3:64:ILE:CB	26:3:123:ASP:HB3	2.50	0.42
26:3:18:ASN:ND2	26:3:64:ILE:HD11	2.35	0.42
1:A:1132:LYS:HE3	27:X:53:DA:H5'	2.01	0.42
1:A:567:LEU:HD22	1:A:570:TRP:HB2	2.00	0.42
2:B:33:TYR:CE1	2:B:37:LYS:HG3	2.54	0.42
2:B:499:ARG:CZ	2:B:522:LEU:HD11	2.49	0.42
2:B:894:THR:HG23	2:B:897:ARG:HH11	1.83	0.42
2:B:924:ARG:HH11	3:C:60:HIS:HB2	1.84	0.42
13:M:164:LEU:HD12	13:M:164:LEU:HA	1.80	0.42
22:W:107:LEU:HB2	22:W:175:TYR:CZ	2.54	0.42
27:X:77:DC:H2"	27:X:78:DT:C7	2.50	0.42
23:0:74:GLN:CA	23:0:78:PRO:O	2.66	0.42
24:1:18:GLN:HG3	24:1:19:PHE:N	2.34	0.42
25:2:188:THR:CG2	25:2:189:GLU:N	2.83	0.42
25:2:224:GLN:N	25:2:268:PHE:HZ	2.16	0.42
25:2:236:PHE:CE1	25:2:261:PHE:HB3	2.54	0.42
26:3:42:MET:SD	26:3:111:ILE:CD1	3.07	0.42
26:3:144:ILE:HG13	26:3:159:SER:OG	2.20	0.42
1:A:1171:ALA:O	9:I:59:THR:CG2	2.67	0.42
1:A:94:VAL:HG21	1:A:314:VAL:HG21	2.01	0.42
2:B:711:ILE:O	2:B:714:PRO:HD3	2.19	0.42
4:D:110:GLU:HA	7:G:167:TYR:CE2	2.55	0.42
13:M:10:LEU:O	13:M:12:ARG:N	2.52	0.42
14:N:12:LYS:O	14:N:15:ARG:HB2	2.19	0.42
22:W:419:GLU:HB3	22:W:420:PRO:HD3	1.84	0.42
25:2:176:ALA:HB3	25:2:178:LEU:HD13	1.98	0.42
25:2:138:PRO:HD3	25:2:189:GLU:CD	2.40	0.42
26:3:184:ALA:O	26:3:187:GLN:HG2	2.19	0.42
2:B:776:ILE:HD12	2:B:806:PHE:CD1	2.55	0.42
2:B:931:ILE:CD1	2:B:947:ILE:HA	2.48	0.42
5:E:52:ARG:HB2	5:E:53:PRO:HD2	1.13	0.42
8:H:122:LEU:HA	8:H:122:LEU:HD23	1.82	0.42
8:H:135:PHE:O	8:H:137:VAL:HG22	2.19	0.42
8:H:34:SER:O	8:H:36:LYS:HG2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:214:PHE:HB3	13:M:218:PHE:HE2	1.84	0.42
17:Q:128:LYS:HB3	17:Q:164:ASP:HA	2.02	0.42
17:Q:70:LYS:NZ	18:R:226:ASP:HA	2.34	0.42
21:V:523:VAL:HG21	24:1:20:LEU:CD2	2.50	0.42
23:0:72:GLU:O	23:0:79:ASN:HB2	2.20	0.42
24:1:1:MET:SD	25:2:413:LEU:CB	3.04	0.42
25:2:47:GLU:HG3	25:2:48:LEU:H	1.83	0.42
1:A:375:ILE:HD13	1:A:485:ASN:ND2	2.35	0.42
1:A:878:THR:HA	1:A:889:LEU:O	2.20	0.42
2:B:908:MET:CE	2:B:920:LYS:HB2	2.50	0.42
1:A:689:ILE:HD11	2:B:981:LEU:CB	2.50	0.42
3:C:220:TYR:CE2	3:C:222:PRO:HB3	2.55	0.42
3:C:263:LEU:O	3:C:266:GLU:HB2	2.19	0.42
5:E:99:ILE:O	5:E:125:TYR:HE1	2.03	0.42
7:G:138:GLN:HG2	7:G:139:GLN:N	2.35	0.42
9:I:14:ILE:HG12	9:I:16:PHE:CG	2.54	0.42
18:R:223:VAL:HG23	18:R:224:THR:HG23	1.79	0.42
21:V:519:TYR:HB3	24:1:16:MET:HG3	2.00	0.42
25:2:118:LEU:HD22	26:3:39:ASP:CB	2.50	0.42
25:2:57:MET:CA	25:2:60:LEU:HG	2.49	0.42
26:3:105:THR:CG2	26:3:106:SER:N	2.83	0.42
26:3:160:ARG:CZ	26:3:190:LEU:CD1	2.97	0.42
1:A:942:VAL:HG21	1:A:1005:HIS:NE2	2.35	0.42
1:A:1141:VAL:HG13	1:A:1352:VAL:HG13	2.02	0.42
1:A:156:GLY:HA2	1:A:181:HIS:HD1	1.71	0.42
1:A:901:VAL:HB	1:A:978:VAL:HG13	2.02	0.42
2:B:47:PHE:O	2:B:50:PHE:HB3	2.20	0.42
3:C:44:ILE:HG23	3:C:176:TRP:HD1	1.84	0.42
6:F:66:LEU:HA	6:F:66:LEU:HD23	1.92	0.42
13:M:62:LYS:HD3	29:Z:1:A:H4'	2.02	0.42
18:R:194:ARG:HA	18:R:194:ARG:HD3	1.49	0.42
22:W:584:TYR:CD1	22:W:594:ALA:CB	2.88	0.42
27:X:1:DG:H2"	27:X:2:DA:C8	2.55	0.42
21:V:689:VAL:CG2	25:2:391:ILE:HD13	2.50	0.42
26:3:202:LEU:CD2	26:3:202:LEU:N	2.82	0.42
26:3:9:ASN:OD1	26:3:158:LYS:HB3	2.19	0.42
1:A:375:ILE:HG13	1:A:666:ARG:NH1	2.34	0.42
1:A:47:THR:O	1:A:48:GLU:HB2	2.20	0.42
1:A:672:ILE:HG23	1:A:673:GLN:N	2.35	0.42
1:A:800:PHE:HD1	1:A:805:ARG:C	2.23	0.42
2:B:180:ASP:OD1	2:B:181:PRO:HD2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:10:ARG:HH21	3:C:24:GLU:CD	2.23	0.42
13:M:79:ASP:N	13:M:79:ASP:OD1	2.53	0.42
15:O:9:THR:O	15:O:13:ASN:N	2.48	0.42
2:B:246:GLY:HA3	19:S:169:LYS:HD2	2.02	0.42
21:V:450:MET:HG3	27:X:75:DG:H3'	2.02	0.42
21:V:615:PHE:O	21:V:615:PHE:CG	2.71	0.42
24:1:14:PRO:HG2	24:1:17:LYS:HB2	2.01	0.42
26:3:141:LEU:HA	26:3:144:ILE:HG22	2.01	0.42
1:A:365:THR:CG2	2:B:1059:ILE:HG22	2.50	0.42
2:B:224:CYS:O	2:B:226:GLU:N	2.51	0.42
2:B:779:ILE:HA	2:B:779:ILE:HD13	1.86	0.42
5:E:187:ARG:HG3	5:E:210:GLN:HA	2.02	0.42
9:I:14:ILE:CG1	9:I:16:PHE:CD2	3.02	0.42
13:M:34:CYS:H	13:M:39:LEU:HB3	1.85	0.42
17:Q:202:GLU:C	17:Q:204:LEU:H	2.23	0.42
22:W:25:MET:SD	22:W:58:ALA:HB2	2.59	0.42
26:3:197:ASP:O	26:3:198:SER:HB3	2.20	0.41
1:A:368:THR:HB	1:A:369:PRO:HD2	2.01	0.41
1:A:532:ARG:HD2	1:A:647:THR:O	2.20	0.41
1:A:805:ARG:HG2	1:A:812:LYS:HA	2.01	0.41
1:A:904:GLN:HE22	1:A:982:ASN:HA	1.85	0.41
2:B:479:LEU:HD12	2:B:479:LEU:HA	1.80	0.41
2:B:506:TRP:CD1	2:B:506:TRP:O	2.73	0.41
2:B:597:ILE:HB	2:B:600:GLU:HB2	2.02	0.41
2:B:874:PRO:C	2:B:876:ASN:N	2.70	0.41
2:B:953:ASP:OD1	3:C:36:ARG:NH1	2.51	0.41
17:Q:154:CYS:SG	17:Q:155:THR:N	2.93	0.41
21:V:315:VAL:HG13	22:W:500:ASP:HB2	0.42	0.41
25:2:181:GLN:HA	25:2:181:GLN:NE2	2.34	0.41
1:A:265:VAL:C	1:A:272:ASN:OD1	2.40	0.41
1:A:273:GLN:H	1:A:273:GLN:HG2	1.69	0.41
1:A:603:ILE:HG12	1:A:604:ARG:N	2.34	0.41
1:A:689:ILE:HD12	1:A:689:ILE:HG23	1.75	0.41
5:E:82:VAL:HB	5:E:110:MET:SD	2.60	0.41
5:E:48:PRO:O	5:E:49:SER:OG	2.29	0.41
7:G:90:THR:O	7:G:91:GLN:HG3	2.20	0.41
9:I:11:PHE:CE1	9:I:54:TYR:HA	2.55	0.41
13:M:69:ASP:OD1	13:M:70:SER:N	2.53	0.41
16:P:271:GLU:OE1	16:P:271:GLU:N	2.50	0.41
17:Q:23:ARG:HH22	18:R:206:LYS:C	2.21	0.41
20:T:143:GLN:O	20:T:144:GLN:C	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:Y:38:DT:H2"	28:Y:39:DG:O4'	2.20	0.41
26:3:109:GLU:HG3	26:3:110:VAL:N	2.35	0.41
26:3:14:VAL:HG22	26:3:162:LEU:O	2.21	0.41
26:3:217:VAL:HG12	26:3:218:PRO:O	2.20	0.41
1:A:1302:GLU:HG3	1:A:1304:ILE:HG12	2.02	0.41
1:A:340:LYS:HG3	1:A:1436:VAL:HG21	2.02	0.41
4:D:90:LYS:HE3	4:D:130:ILE:HD11	2.01	0.41
4:D:92:LEU:HD23	4:D:122:PHE:CE2	2.56	0.41
4:D:94:LYS:HD3	4:D:94:LYS:HA	1.78	0.41
5:E:58:LEU:HD23	5:E:76:PHE:CE2	2.55	0.41
9:I:15:ARG:HG3	9:I:15:ARG:O	2.19	0.41
10:J:62:TYR:O	10:J:65:LEU:HD11	2.20	0.41
13:M:30:GLY:CA	13:M:44:ARG:HG2	2.50	0.41
2:B:1075:MET:HE3	13:M:51:GLU:HG2	2.02	0.41
17:Q:24:GLY:O	18:R:215:GLU:OE2	2.38	0.41
19:S:147:THR:HA	19:S:148:PRO:HD3	1.89	0.41
23:0:54:ARG:HA	26:3:209:ILE:HD13	1.06	0.41
24:1:43:VAL:CG1	24:1:44:PHE:N	2.83	0.41
25:2:211:GLN:CD	25:2:261:PHE:CE1	2.94	0.41
26:3:33:THR:CG2	26:3:36:LYS:H	2.04	0.41
26:3:41:VAL:HG13	26:3:42:MET:N	2.34	0.41
1:A:273:GLN:C	1:A:274:ASP:O	2.55	0.41
2:B:1032:PHE:O	3:C:32:ASN:ND2	2.53	0.41
2:B:1132:THR:HG23	2:B:1133:HIS:ND1	2.36	0.41
9:I:25:TYR:HD2	9:I:40:ARG:HG3	1.85	0.41
3:C:49:TRP:CE3	12:L:54:VAL:HG21	2.56	0.41
15:O:63:ASN:HB3	15:O:75:VAL:O	2.20	0.41
19:S:166:ARG:CG	19:S:166:ARG:HH11	2.32	0.41
22:W:420:PRO:O	22:W:431:PRO:HB3	2.20	0.41
25:2:77:LYS:HD3	25:2:78:GLU:CG	2.50	0.41
26:3:165:LYS:HZ1	26:3:200:SER:N	2.18	0.41
1:A:602:CYS:H	1:A:630:VAL:CG1	2.33	0.41
1:A:889:LEU:HA	1:A:889:LEU:HD23	1.88	0.41
1:A:901:VAL:HB	1:A:978:VAL:CG1	2.51	0.41
2:B:831:LYS:HA	2:B:832:PRO:HD3	1.90	0.41
9:I:15:ARG:HD3	9:I:24:LEU:HD12	2.02	0.41
13:M:44:ARG:HD2	13:M:45:VAL:H	1.85	0.41
2:B:1075:MET:HE1	13:M:51:GLU:HG2	2.02	0.41
17:Q:184:ILE:CG1	18:R:213:ASP:OD1	2.68	0.41
20:T:213:LEU:HD23	20:T:213:LEU:HA	1.78	0.41
27:X:18:DG:OP2	27:X:18:DG:H2'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:2:123:LEU:HD23	25:2:123:LEU:C	2.41	0.41
25:2:224:GLN:CB	25:2:268:PHE:CZ	2.94	0.41
26:3:146:ARG:HG3	26:3:147:MET:N	2.35	0.41
26:3:228:LEU:C	26:3:228:LEU:HD23	2.41	0.41
1:A:205:VAL:HB	1:A:206:ASN:H	1.63	0.41
1:A:457:ILE:HD11	2:B:1102:PHE:CE2	2.55	0.41
2:B:1040:GLN:O	2:B:1041:ILE:HD13	2.21	0.41
2:B:262:TYR:O	2:B:263:ILE:HD13	2.20	0.41
2:B:823:PHE:HA	13:M:140:ASN:HD21	1.86	0.41
2:B:856:PRO:HG2	12:L:46:LYS:O	2.20	0.41
3:C:67:ARG:HB3	3:C:67:ARG:NH1	2.36	0.41
5:E:41:LYS:HA	5:E:46:ASP:CB	2.40	0.41
6:F:104:ILE:O	6:F:120:VAL:HG23	2.21	0.41
7:G:148:VAL:HG23	7:G:160:ILE:CD1	2.50	0.41
7:G:18:PHE:HA	7:G:22:LEU:HD13	2.02	0.41
1:A:265:VAL:HG21	13:M:48:VAL:CG2	2.51	0.41
21:V:353:ALA:O	21:V:357:VAL:HG23	2.21	0.41
21:V:519:TYR:CE2	21:V:523:VAL:HG21	2.55	0.41
27:X:25:DG:N2	28:Y:70:DC:O2	2.53	0.41
24:1:52:VAL:CG2	24:1:53:LEU:N	2.83	0.41
25:2:211:GLN:HE21	25:2:257:SER:HB2	1.84	0.41
25:2:221:GLN:O	25:2:268:PHE:CE1	2.74	0.41
24:1:1:MET:N	25:2:418:PHE:CB	2.83	0.41
26:3:14:VAL:CG2	26:3:163:VAL:HG13	2.48	0.41
1:A:1201:ASP:O	1:A:1204:VAL:HG22	2.20	0.41
1:A:378:VAL:HG23	1:A:484:LEU:HD23	2.02	0.41
1:A:679:TRP:CZ2	1:A:683:GLU:HG3	2.55	0.41
2:B:215:TYR:CD1	2:B:238:SER:HB3	2.55	0.41
2:B:510:CYS:HB2	2:B:705:GLY:CA	2.49	0.41
2:B:704:LEU:HD23	2:B:704:LEU:HA	1.85	0.41
3:C:30:VAL:HG22	11:K:45:ILE:HD11	2.02	0.41
5:E:15:LYS:HA	5:E:15:LYS:HD3	1.80	0.41
10:J:2:ILE:HG12	10:J:3:ILE:N	2.36	0.41
17:Q:187:ILE:O	17:Q:191:LEU:HD13	2.21	0.41
2:B:554:GLU:OE1	19:S:115:LYS:HG3	2.20	0.41
20:T:150:THR:C	20:T:152:ASN:H	2.22	0.41
2:B:211:LYS:HE3	27:X:48:DT:H2'	2.02	0.41
27:X:59:DC:H2"	27:X:60:DG:O5'	2.21	0.41
29:Z:3:U:H2'	29:Z:4:C:O4'	2.20	0.41
24:1:2:VAL:HG11	25:2:456:LYS:CB	2.44	0.41
26:3:24:LYS:CE	26:3:220:MET:SD	3.07	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:3:9:ASN:C	26:3:56:LYS:HE3	2.41	0.41
1:A:908:THR:C	1:A:910:LYS:H	2.24	0.41
1:A:912:SER:HB3	1:A:915:ALA:HB3	2.02	0.41
2:B:132:VAL:CG2	2:B:141:GLN:CG	2.93	0.41
2:B:264:LYS:H	2:B:325:GLY:HA2	1.86	0.41
2:B:510:CYS:SG	2:B:511:PRO:HD2	2.61	0.41
2:B:847:LYS:O	2:B:854:ILE:HG22	2.21	0.41
7:G:17:TYR:HB3	7:G:25:THR:HG21	2.03	0.41
6:F:64:ARG:NH1	7:G:61:PRO:HB3	2.35	0.41
13:M:178:LYS:HD3	13:M:279:GLY:HA3	2.01	0.41
1:A:271:ARG:HG3	13:M:73:PRO:HG3	2.03	0.41
22:W:15:ASP:HA	22:W:100:GLU:OE2	2.21	0.41
27:X:12:DA:C2	27:X:13:DT:C4	3.09	0.41
27:X:45:DT:H4'	27:X:46:DT:O4'	2.21	0.41
13:M:119:LYS:HD3	28:Y:60:DA:N6	2.34	0.41
24:1:1:MET:HG2	25:2:413:LEU:CB	2.47	0.41
26:3:125:LYS:C	26:3:127:GLN:H	2.24	0.41
26:3:141:LEU:C	26:3:144:ILE:HG22	2.41	0.41
1:A:1102:MET:HE2	1:A:1102:MET:HB2	1.95	0.41
1:A:1124:LEU:HD12	1:A:1124:LEU:HA	1.84	0.41
1:A:458:PHE:HE1	1:A:501:MET:HE3	1.85	0.41
1:A:966:LEU:HA	1:A:969:ILE:HD12	2.03	0.41
8:H:113:SER:HA	8:H:125:LEU:O	2.20	0.41
8:H:137:VAL:HG21	8:H:140:ARG:HD2	2.01	0.41
9:I:41:ASN:CG	19:S:153:ARG:HD2	2.40	0.41
9:I:58:ILE:C	9:I:60:HIS:N	2.74	0.41
16:P:159:SER:CB	16:P:329:TYR:CE2	2.93	0.41
17:Q:187:ILE:HD13	18:R:211:SER:CA	2.39	0.41
17:Q:26:TYR:OH	17:Q:69:ASP:OD2	2.25	0.41
21:V:390:CYS:SG	21:V:399:LYS:HE3	2.61	0.41
21:V:518:PHE:CD1	21:V:713:LEU:HD13	2.55	0.41
22:W:233:PHE:HB2	22:W:456:ILE:HG22	2.02	0.41
28:Y:56:DG:C4	28:Y:57:DA:H1'	2.56	0.41
24:1:38:ILE:CB	24:1:44:PHE:CD1	3.04	0.41
25:2:42:LEU:HA	25:2:42:LEU:HD23	1.78	0.41
25:2:93:LEU:O	25:2:96:TRP:CD1	2.74	0.41
25:2:93:LEU:HD23	25:2:96:TRP:HE1	1.85	0.41
26:3:100:LYS:HB2	26:3:100:LYS:HE2	1.89	0.41
26:3:185:GLN:NE2	26:3:185:GLN:HA	2.26	0.41
1:A:266:MET:HB3	13:M:52:TRP:CE3	2.56	0.41
2:B:1005:ALA:C	2:B:1007:ASN:N	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:56:ILE:HD12	10:J:56:ILE:HG23	1.76	0.41
17:Q:188:TYR:CZ	18:R:210:PHE:HE1	2.34	0.41
28:Y:32:DC:H2"	28:Y:33:DT:C6	2.55	0.41
1:A:499:ASP:OD1	29:Z:6:C:H4'	2.20	0.41
24:1:22:TYR:CD1	24:1:22:TYR:C	2.94	0.41
25:2:140:LYS:CD	25:2:162:PHE:HE1	2.29	0.41
25:2:236:PHE:HZ	25:2:258:LEU:CD1	2.34	0.41
25:2:89:LEU:HD23	25:2:89:LEU:C	2.42	0.41
26:3:100:LYS:CB	26:3:103:LEU:HD13	2.41	0.41
26:3:114:GLU:OE1	26:3:114:GLU:HA	2.21	0.41
1:A:966:LEU:HD13	1:A:1043:ILE:HD11	2.03	0.41
1:A:367:ILE:HG22	1:A:482:PHE:HB2	2.02	0.41
1:A:520:MET:HG3	1:A:522:PRO:HD2	2.03	0.41
1:A:618:TYR:C	1:A:620:HIS:N	2.73	0.41
2:B:497:LYS:HE2	2:B:497:LYS:HB3	1.77	0.41
2:B:502:HIS:CE1	2:B:504:THR:HG1	2.39	0.41
3:C:205:LYS:HZ1	3:C:217:GLN:HA	1.85	0.41
3:C:38:PHE:HE1	3:C:245:VAL:HA	1.86	0.41
5:E:46:ASP:O	5:E:48:PRO:HD2	2.20	0.41
7:G:119:PHE:CE2	7:G:121:PRO:HB3	2.56	0.41
21:V:518:PHE:HB2	24:1:16:MET:SD	2.61	0.40
25:2:34:LEU:N	25:2:34:LEU:CD2	2.84	0.40
24:1:59:GLU:CD	25:2:402:ARG:CZ	2.89	0.40
24:1:1:MET:HE3	25:2:415:GLN:CA	2.51	0.40
25:2:89:LEU:O	25:2:93:LEU:HG	2.21	0.40
26:3:111:ILE:HG13	26:3:112:VAL:H	1.84	0.40
26:3:222:SER:HB3	26:3:225:GLN:CG	2.51	0.40
1:A:1189:ASP:HA	1:A:1192:TRP:CZ3	2.56	0.40
1:A:1307:VAL:HG13	1:A:1308:TYR:H	1.86	0.40
1:A:466:LYS:HE3	1:A:466:LYS:HB2	1.88	0.40
2:B:1030:ASN:N	2:B:1035:ARG:O	2.42	0.40
2:B:1112:ASP:OD2	2:B:1153:TYR:N	2.55	0.40
2:B:51:ILE:HG22	20:T:141:LEU:CG	2.52	0.40
13:M:23:LEU:HD12	13:M:33:ILE:O	2.21	0.40
17:Q:71:PHE:CD1	17:Q:102:VAL:CG2	3.05	0.40
21:V:297:PHE:CG	21:V:298:ARG:N	2.89	0.40
22:W:535:ILE:HG12	22:W:617:ALA:HB3	2.04	0.40
24:1:18:GLN:OE1	24:1:19:PHE:CD1	2.74	0.40
25:2:202:GLN:HE21	25:2:202:GLN:N	2.15	0.40
25:2:60:LEU:CD1	25:2:95:ILE:CB	2.95	0.40
25:2:93:LEU:CA	25:2:96:TRP:HD1	2.31	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:3:165:LYS:HE3	26:3:200:SER:N	2.36	0.40
26:3:174:TYR:CZ	26:3:178:MET:HG3	2.56	0.40
26:3:60:ILE:CG2	26:3:61:ALA:N	2.84	0.40
26:3:59:VAL:CA	26:3:71:TYR:CD1	3.02	0.40
1:A:202:TRP:CB	1:A:212:LYS:CG	2.97	0.40
1:A:818:GLU:N	1:A:818:GLU:OE1	2.50	0.40
1:A:912:SER:HB3	1:A:915:ALA:CB	2.51	0.40
2:B:23:GLN:OE1	2:B:23:GLN:N	2.40	0.40
2:B:573:TRP:CH2	2:B:576:ILE:HG23	2.56	0.40
2:B:861:SER:O	2:B:896:LEU:CD2	2.69	0.40
14:N:14:TYR:CE1	15:O:11:LEU:HD22	2.56	0.40
19:S:169:LYS:HE3	19:S:169:LYS:HB3	1.83	0.40
19:S:24:LYS:HB2	20:T:99:SER:HA	2.04	0.40
19:S:29:MET:HB2	20:T:96:PHE:CD1	2.57	0.40
22:W:492:PRO:HG2	22:W:678:VAL:HG22	2.03	0.40
27:X:35:DT:H4'	27:X:36:DT:OP1	2.20	0.40
27:X:70:DG:N2	28:Y:25:DT:C2	2.90	0.40
25:2:159:VAL:HG22	25:2:160:LEU:HD13	1.95	0.40
25:2:206:LEU:CD2	25:2:206:LEU:N	2.84	0.40
25:2:41:CYS:SG	25:2:42:LEU:N	2.95	0.40
26:3:222:SER:HB3	26:3:225:GLN:OE1	2.21	0.40
26:3:222:SER:O	26:3:226:TYR:CD2	2.75	0.40
1:A:672:ILE:HG21	1:A:672:ILE:HD13	1.79	0.40
2:B:1118:VAL:HG12	2:B:1119:CYS:O	2.21	0.40
2:B:1127:ILE:HB	2:B:1128:ALA:H	1.75	0.40
2:B:781:ALA:HB1	2:B:1041:ILE:HG21	2.03	0.40
2:B:789:ASN:HB3	2:B:795:ILE:HG13	2.03	0.40
8:H:5:LEU:HD22	8:H:133:HIS:HB3	2.02	0.40
14:N:341:LYS:H	14:N:352:HIS:HB2	1.86	0.40
16:P:329:TYR:N	16:P:330:PRO:HD2	2.36	0.40
17:Q:100:VAL:HG23	17:Q:101:ASN:N	2.37	0.40
18:R:195:PRO:HB2	18:R:199:LYS:HD2	2.04	0.40
20:T:51:ARG:NE	20:T:53:GLU:OE2	2.39	0.40
24:1:52:VAL:O	24:1:56:ARG:HG2	2.21	0.40
25:2:170:ALA:C	25:2:213:TRP:CZ3	2.94	0.40
25:2:174:ASP:OD2	25:2:213:TRP:CZ3	2.74	0.40
25:2:223:ALA:C	25:2:225:SER:H	2.24	0.40
25:2:236:PHE:HZ	25:2:262:LEU:CD2	2.35	0.40
25:2:399:ASP:OD1	25:2:402:ARG:NH1	2.55	0.40
25:2:94:ARG:HD2	25:2:95:ILE:HD13	2.02	0.40
26:3:42:MET:HG2	26:3:111:ILE:CD1	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:733:LEU:HA	1:A:733:LEU:HD12	1.90	0.40
1:A:360:ASP:HA	2:B:1062:ARG:HD3	2.04	0.40
1:A:349:ARG:HG3	2:B:1161:GLU:OE1	2.22	0.40
2:B:758:LEU:HA	2:B:758:LEU:HD23	1.91	0.40
2:B:824:ASP:OD2	2:B:875:GLU:CG	2.70	0.40
3:C:161:LEU:C	3:C:161:LEU:HD12	2.42	0.40
4:D:32:LEU:HD11	7:G:4:HIS:HB2	2.02	0.40
7:G:44:PHE:CD2	7:G:103:PRO:HG2	2.57	0.40
1:A:623:PRO:HB2	8:H:27:ARG:NH2	2.37	0.40
9:I:14:ILE:HG13	9:I:16:PHE:CD1	2.56	0.40
16:P:207:PRO:O	16:P:208:ARG:O	2.39	0.40
21:V:593:LEU:HD11	21:V:615:PHE:CZ	2.55	0.40
25:2:219:TYR:C	25:2:219:TYR:CD1	2.95	0.40
25:2:236:PHE:CD1	25:2:239:GLN:CD	2.95	0.40
26:3:187:GLN:HE21	26:3:189:ILE:HB	1.87	0.40
26:3:229:TRP:HD1	26:3:229:TRP:O	2.04	0.40
1:A:1065:PHE:CZ	1:A:1069:LEU:HD21	2.57	0.40
1:A:1163:HIS:HA	1:A:1300:GLY:HA2	2.04	0.40
1:A:265:VAL:HG21	13:M:48:VAL:CB	2.51	0.40
1:A:458:PHE:CZ	1:A:501:MET:HG3	2.57	0.40
2:B:294:ASP:HA	2:B:295:PRO:HD3	1.79	0.40
16:P:173:ASN:OD1	16:P:175:GLY:N	2.40	0.40
20:T:160:GLN:HA	20:T:163:ILE:HD12	2.03	0.40
19:S:144:TYR:CD2	20:T:96:PHE:HZ	2.39	0.40
21:V:336:GLY:HA3	21:V:485:GLY:HA3	2.04	0.40
28:Y:56:DG:H1'	28:Y:57:DA:H4'	2.03	0.40
28:Y:84:DG:C2	28:Y:85:DG:C4	3.09	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%)	1268 (87%)	120 (8%)	62 (4%)	3 34
2	B	1163/1174 (99%)	996 (86%)	116 (10%)	51 (4%)	3 33
3	C	273/275 (99%)	239 (88%)	25 (9%)	9 (3%)	5 40
4	D	127/142 (89%)	119 (94%)	8 (6%)	0	100 100
5	E	208/210 (99%)	191 (92%)	11 (5%)	6 (3%)	6 43
6	F	84/127 (66%)	82 (98%)	2 (2%)	0	100 100
7	G	169/172 (98%)	158 (94%)	10 (6%)	1 (1%)	30 74
8	H	148/150 (99%)	118 (80%)	20 (14%)	10 (7%)	1 23
9	I	123/125 (98%)	92 (75%)	16 (13%)	15 (12%)	0 8
10	J	65/67 (97%)	51 (78%)	9 (14%)	5 (8%)	1 20
11	K	115/117 (98%)	109 (95%)	4 (4%)	2 (2%)	11 55
12	L	44/58 (76%)	33 (75%)	9 (20%)	2 (4%)	3 33
13	M	308/316 (98%)	263 (85%)	32 (10%)	13 (4%)	3 34
14	N	109/376 (29%)	101 (93%)	6 (6%)	2 (2%)	11 53
15	O	97/109 (89%)	95 (98%)	2 (2%)	0	100 100
16	P	183/339 (54%)	170 (93%)	6 (3%)	7 (4%)	4 37
17	Q	176/439 (40%)	158 (90%)	10 (6%)	8 (4%)	3 33
18	R	163/291 (56%)	140 (86%)	14 (9%)	9 (6%)	2 28
19	S	134/517 (26%)	120 (90%)	10 (8%)	4 (3%)	5 42
20	T	218/249 (88%)	190 (87%)	20 (9%)	8 (4%)	4 37
21	V	473/782 (60%)	398 (84%)	47 (10%)	28 (6%)	2 26
22	W	661/760 (87%)	570 (86%)	69 (10%)	22 (3%)	5 40
23	0	186/395 (47%)	168 (90%)	13 (7%)	5 (3%)	6 44
24	1	60/71 (84%)	53 (88%)	5 (8%)	2 (3%)	5 40
25	2	264/462 (57%)	246 (93%)	14 (5%)	4 (2%)	13 57
26	3	187/308 (61%)	176 (94%)	9 (5%)	2 (1%)	17 63
All	All	7188/10001 (72%)	6304 (88%)	607 (8%)	277 (4%)	7 36

All (277) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	132	LYS
1	A	153	ILE
1	A	204	HIS

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Mol	Chain	Res	Type
1	A	205	VAL
1	A	207	GLU
1	A	208	ASP
1	A	210	GLN
1	A	212	LYS
1	A	264	VAL
1	A	265	VAL
1	A	272	ASN
1	A	274	ASP
1	A	531	ASN
1	A	598	GLY
1	A	607	SER
1	A	610	PRO
1	A	623	PRO
1	A	911	PRO
1	A	930	LEU
1	A	931	ARG
1	A	1087	VAL
1	A	1101	GLN
1	A	1117	VAL
1	A	1118	THR
1	A	1200	PRO
1	A	1275	VAL
1	A	1299	GLN
1	A	1306	LYS
2	B	63	PRO
2	B	74	ALA
2	B	79	GLU
2	B	80	GLU
2	B	134	LYS
2	B	226	GLU
2	B	227	ASN
2	B	231	PRO
2	B	249	LYS
2	B	251	ALA
2	B	383	ASP
2	B	428	ASP
2	B	876	ASN
2	B	880	LEU
2	B	881	GLU
2	B	958	CYS
2	B	1007	ASN

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Mol	Chain	Res	Type
2	B	1136	GLU
3	C	7	PRO
5	E	47	LYS
5	E	52	ARG
5	E	53	PRO
8	H	67	ASP
8	H	86	ASP
8	H	108	ALA
9	I	15	ARG
9	I	16	PHE
9	I	60	HIS
9	I	62	VAL
9	I	85	PRO
9	I	103	ARG
9	I	104	ALA
9	I	106	ASP
9	I	119	CYS
11	K	112	LYS
13	M	12	ARG
13	M	42	GLY
13	M	43	ASP
13	M	47	ASP
13	M	95	GLU
13	M	101	TYR
14	N	320	VAL
16	P	160	GLY
16	P	162	VAL
16	P	206	GLU
16	P	208	ARG
17	Q	100	VAL
17	Q	102	VAL
17	Q	172	ASP
18	R	140	LYS
18	R	195	PRO
18	R	196	ASP
18	R	207	SER
20	T	124	TYR
20	T	145	LEU
20	T	146	ASP
21	V	385	ASP
21	V	461	HIS
21	V	491	ALA

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Mol	Chain	Res	Type
21	V	499	ASN
21	V	614	SER
21	V	615	PHE
21	V	616	ASP
21	V	632	SER
21	V	648	LYS
21	V	649	GLY
22	W	67	VAL
22	W	420	PRO
22	W	424	ARG
22	W	430	ASN
22	W	504	ILE
22	W	573	ASP
22	W	595	ILE
22	W	630	SER
23	0	78	PRO
23	0	80	ARG
24	1	48	GLU
25	2	49	PRO
26	3	120	THR
1	A	12	ALA
1	A	184	CYS
1	A	270	ALA
1	A	271	ARG
1	A	466	LYS
1	A	624	GLY
1	A	932	ARG
1	A	1119	LEU
1	A	1145	GLY
1	A	1435	THR
2	B	41	ARG
2	B	73	HIS
2	B	77	GLU
2	B	141	GLN
2	B	229	SER
2	B	253	GLY
2	B	491	ARG
2	B	785	TYR
2	B	875	GLU
2	B	879	GLU
2	B	884	ASN
2	B	900	GLU

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Mol	Chain	Res	Type
3	C	5	ASN
3	C	143	VAL
5	E	70	ASP
8	H	21	LYS
8	H	107	GLU
9	I	58	ILE
9	I	59	THR
9	I	67	GLN
9	I	99	SER
10	J	5	VAL
10	J	6	ARG
13	M	40	VAL
13	M	48	VAL
13	M	53	ARG
14	N	318	ASP
16	P	299	ARG
17	Q	126	SER
17	Q	158	HIS
18	R	164	GLY
18	R	194	ARG
18	R	223	VAL
18	R	224	THR
21	V	254	GLN
21	V	404	SER
21	V	460	ALA
21	V	613	THR
22	W	124	LEU
22	W	408	SER
22	W	646	ILE
25	2	223	ALA
25	2	231	VAL
1	A	48	GLU
1	A	61	ARG
1	A	70	ARG
1	A	134	LYS
1	A	599	HIS
1	A	612	ASP
1	A	1109	TYR
1	A	1116	ASN
1	A	1305	SER
2	B	61	ASP
2	B	233	SER

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Mol	Chain	Res	Type
2	B	245	GLN
2	B	458	LYS
2	B	549	SER
2	B	873	LEU
3	C	3	TYR
5	E	48	PRO
5	E	65	ASN
7	G	140	ASP
8	H	111	ARG
12	L	17	TYR
13	M	87	GLY
16	P	207	PRO
16	P	298	PRO
17	Q	125	ALA
17	Q	133	SER
19	S	160	ALA
20	T	147	LYS
21	V	343	GLY
22	W	147	GLN
22	W	155	CYS
22	W	509	GLU
26	3	198	SER
1	A	38	GLU
1	A	62	GLN
1	A	266	MET
1	A	611	ASP
1	A	1308	TYR
2	B	225	LEU
2	B	427	LYS
2	B	559	ALA
2	B	821	LYS
2	B	1032	PHE
8	H	100	GLU
8	H	128	ASP
9	I	73	SER
9	I	117	PRO
10	J	16	ASN
10	J	41	LYS
11	K	29	ASN
13	M	45	VAL
13	M	56	SER
18	R	228	MET

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Mol	Chain	Res	Type
19	S	156	THR
19	S	170	VAL
20	T	139	VAL
20	T	141	LEU
20	T	142	SER
21	V	310	LEU
21	V	436	GLY
21	V	470	LEU
21	V	475	ASP
21	V	502	ILE
21	V	629	HIS
1	A	51	ARG
1	A	981	CYS
1	A	1307	VAL
2	B	457	LYS
2	B	515	PRO
8	H	24	ARG
12	L	34	ILE
13	M	66	ARG
17	Q	25	PHE
20	T	152	ASN
21	V	427	MET
21	V	650	MET
22	W	152	LEU
22	W	551	SER
25	2	430	VAL
1	A	195	GLY
1	A	453	GLY
1	A	621	ILE
1	A	622	SER
3	C	2	PRO
3	C	6	GLN
19	S	154	THR
21	V	582	GLY
22	W	36	GLY
22	W	111	SER
22	W	345	ARG
23	0	77	LYS
1	A	1304	ILE
2	B	493	GLY
2	B	1006	VAL
2	B	1113	PRO

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Mol	Chain	Res	Type
21	V	311	LYS
21	V	651	VAL
22	W	174	ILE
23	0	216	GLY
3	C	58	VAL
3	C	78	ILE
21	V	457	ILE
22	W	495	ILE
2	B	561	ILE
2	B	931	ILE
3	C	151	VAL
8	H	49	PRO
21	V	405	VAL
24	1	2	VAL
1	A	56	GLY
2	B	289	ILE
2	B	1034	GLY
10	J	14	VAL
1	A	1312	PRO
2	B	489	ILE
22	W	45	GLY
23	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%)	1235 (97%)	44 (3%)	44 75
2	B	1020/1028 (99%)	985 (97%)	35 (3%)	44 75
3	C	252/252 (100%)	244 (97%)	8 (3%)	46 76
4	D	119/126 (94%)	118 (99%)	1 (1%)	86 94
5	E	192/192 (100%)	186 (97%)	6 (3%)	47 77
6	F	74/111 (67%)	74 (100%)	0	100 100
7	G	152/153 (99%)	151 (99%)	1 (1%)	88 94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	H	131/131 (100%)	126 (96%)	5 (4%)	40	73
9	I	112/112 (100%)	108 (96%)	4 (4%)	42	74
10	J	56/56 (100%)	53 (95%)	3 (5%)	27	64
11	K	106/106 (100%)	105 (99%)	1 (1%)	84	93
12	L	43/55 (78%)	42 (98%)	1 (2%)	58	82
13	M	263/268 (98%)	256 (97%)	7 (3%)	52	79
14	N	105/324 (32%)	104 (99%)	1 (1%)	82	92
15	O	90/98 (92%)	89 (99%)	1 (1%)	80	91
16	P	159/293 (54%)	157 (99%)	2 (1%)	76	89
17	Q	164/373 (44%)	158 (96%)	6 (4%)	41	73
18	R	150/261 (58%)	139 (93%)	11 (7%)	17	54
19	S	121/448 (27%)	118 (98%)	3 (2%)	55	81
20	T	196/218 (90%)	190 (97%)	6 (3%)	47	77
21	V	422/688 (61%)	403 (96%)	19 (4%)	34	69
22	W	577/664 (87%)	543 (94%)	34 (6%)	24	61
23	0	171/352 (49%)	163 (95%)	8 (5%)	32	68
24	1	56/64 (88%)	52 (93%)	4 (7%)	18	55
25	2	238/399 (60%)	229 (96%)	9 (4%)	40	73
26	3	171/272 (63%)	159 (93%)	12 (7%)	19	56
All	All	6419/8792 (73%)	6187 (96%)	232 (4%)	46	74

All (232) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	ILE
1	A	74	CYS
1	A	132	LYS
1	A	204	HIS
1	A	205	VAL
1	A	259	SER
1	A	265	VAL
1	A	272	ASN
1	A	286	ILE
1	A	303	ILE
1	A	449	HIS

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Mol	Chain	Res	Type
1	A	463	THR
1	A	502	ASN
1	A	540	ASP
1	A	567	LEU
1	A	611	ASP
1	A	614	ASP
1	A	619	LYS
1	A	625	ASP
1	A	652	LEU
1	A	712	ASP
1	A	757	GLN
1	A	771	VAL
1	A	849	ASP
1	A	870	SER
1	A	873	VAL
1	A	908	THR
1	A	931	ARG
1	A	1015	GLU
1	A	1036	ASN
1	A	1077	ASN
1	A	1101	GLN
1	A	1102	MET
1	A	1167	ARG
1	A	1279	MET
1	A	1282	ASP
1	A	1298	LEU
1	A	1306	LYS
1	A	1308	TYR
1	A	1309	MET
1	A	1311	LEU
1	A	1337	GLU
1	A	1341	VAL
1	A	1407	CYS
2	B	41	ARG
2	B	73	HIS
2	B	80	GLU
2	B	131	THR
2	B	132	VAL
2	B	140	LEU
2	B	168	ASP
2	B	222	ARG
2	B	232	THR

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Mol	Chain	Res	Type
2	B	250	SER
2	B	338	TYR
2	B	388	TYR
2	B	412	LEU
2	B	422	PHE
2	B	446	TYR
2	B	472	ARG
2	B	539	SER
2	B	573	TRP
2	B	606	ASP
2	B	641	ASP
2	B	666	ASP
2	B	667	THR
2	B	675	LEU
2	B	711	ILE
2	B	875	GLU
2	B	880	LEU
2	B	897	ARG
2	B	957	THR
2	B	959	GLU
2	B	1007	ASN
2	B	1056	ASP
2	B	1080	ARG
2	B	1090	GLU
2	B	1091	ARG
2	B	1092	ASP
3	C	6	GLN
3	C	77	ASP
3	C	94	CYS
3	C	102	THR
3	C	137	ASN
3	C	177	ASN
3	C	212	ASP
3	C	242	GLU
4	D	135	GLN
5	E	23	ASP
5	E	47	LYS
5	E	50	GLU
5	E	64	HIS
5	E	147	GLU
5	E	199	THR
7	G	128	TYR

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Mol	Chain	Res	Type
8	H	11	ASP
8	H	29	HIS
8	H	65	TYR
8	H	84	ARG
8	H	107	GLU
9	I	14	ILE
9	I	15	ARG
9	I	71	ASP
9	I	105	GLU
10	J	7	CYS
10	J	47	ARG
10	J	65	LEU
11	K	48	SER
12	L	27	GLU
13	M	10	LEU
13	M	31	ASP
13	M	39	LEU
13	M	40	VAL
13	M	47	ASP
13	M	86	LYS
13	M	133	ASN
14	N	318	ASP
15	O	21	GLU
16	P	206	GLU
16	P	297	LYS
17	Q	38	ILE
17	Q	45	GLU
17	Q	101	ASN
17	Q	138	ASP
17	Q	172	ASP
17	Q	191	LEU
18	R	100	ASP
18	R	105	GLU
18	R	152	LEU
18	R	163	LEU
18	R	194	ARG
18	R	205	ASP
18	R	206	LYS
18	R	209	GLN
18	R	224	THR
18	R	225	VAL
18	R	228	MET

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Mol	Chain	Res	Type
19	S	135	PHE
19	S	166	ARG
19	S	177	MET
20	T	140	ARG
20	T	141	LEU
20	T	145	LEU
20	T	154	LYS
20	T	160	GLN
20	T	206	THR
21	V	246	MET
21	V	332	ARG
21	V	362	LEU
21	V	366	ASN
21	V	429	TRP
21	V	458	VAL
21	V	471	VAL
21	V	479	ASP
21	V	482	PHE
21	V	492	ASN
21	V	517	GLU
21	V	530	ARG
21	V	534	TYR
21	V	566	PHE
21	V	568	LEU
21	V	581	TYR
21	V	590	MET
21	V	612	ASP
21	V	614	SER
22	W	37	HIS
22	W	64	PRO
22	W	95	GLU
22	W	101	LYS
22	W	112	ARG
22	W	122	THR
22	W	123	PRO
22	W	166	ARG
22	W	196	ARG
22	W	207	TYR
22	W	263	LEU
22	W	283	ASP
22	W	285	TYR
22	W	288	LEU

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Mol	Chain	Res	Type
22	W	309	VAL
22	W	333	LEU
22	W	345	ARG
22	W	346	VAL
22	W	425	THR
22	W	461	LEU
22	W	489	CYS
22	W	523	LEU
22	W	533	ASP
22	W	543	GLN
22	W	544	TYR
22	W	554	GLU
22	W	584	TYR
22	W	596	LEU
22	W	610	PHE
22	W	620	MET
22	W	647	ARG
22	W	654	PHE
22	W	669	ARG
22	W	676	LEU
23	0	77	LYS
23	0	103	GLN
23	0	125	ARG
23	0	137	MET
23	0	174	LEU
23	0	202	SER
23	0	218	THR
23	0	222	ILE
24	1	10	ILE
24	1	16	MET
24	1	18	GLN
24	1	38	ILE
25	2	61	PHE
25	2	77	LYS
25	2	181	GLN
25	2	202	GLN
25	2	402	ARG
25	2	407	VAL
25	2	426	ARG
25	2	430	VAL
25	2	452	LYS
26	3	56	LYS

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Mol	Chain	Res	Type
26	3	66	GLU
26	3	109	GLU
26	3	121	LYS
26	3	124	ILE
26	3	133	LEU
26	3	144	ILE
26	3	147	MET
26	3	157	MET
26	3	185	GLN
26	3	190	LEU
26	3	216	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	188	GLN
1	A	449	HIS
1	A	601	ASN
1	A	1077	ASN
1	A	1101	GLN
1	A	1105	ASN
1	A	1116	ASN
1	A	1310	HIS
1	A	1313	GLN
1	A	1316	ASN
1	A	1445	HIS
2	B	716	HIS
2	B	1053	HIS
2	B	1097	HIS
3	C	6	GLN
3	C	137	ASN
8	H	126	GLN
9	I	84	HIS
11	K	84	GLN
17	Q	95	ASN
21	V	281	GLN
21	V	366	ASN
21	V	539	ASN
21	V	677	GLN
22	W	187	GLN
22	W	430	ASN
22	W	590	ASN

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Mol	Chain	Res	Type
23	0	60	HIS
23	0	103	GLN
24	1	51	ASN
25	2	117	ASN
25	2	161	HIS
25	2	181	GLN
25	2	202	GLN
25	2	221	GLN
25	2	239	GLN
25	2	263	GLN
25	2	273	GLN
26	3	25	GLN
26	3	52	ASN
26	3	63	HIS
26	3	148	ASN
26	3	155	GLN
26	3	185	GLN
26	3	187	GLN
26	3	225	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
29	Z	5/6 (83%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.