



wwPDB EM Map/Model Validation Report ⓘ

Jun 14, 2016 – 12:09 PM EDT

PDB ID : 5IVW
EMDB ID: : EMD-8131
Title : Human core TFIIH bound to DNA within the PIC
Authors : He, Y.; Yan, C.; Fang, J.; Inouye, C.; Tjian, R.; Ivanov, I.; Nogales, E.
Deposited on : 2016-03-21
Resolution : 10.00 Å(reported)
Based on PDB ID : ?

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

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

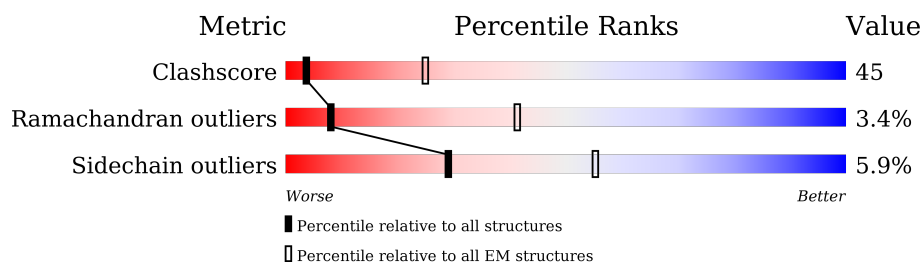
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 10.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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

Mol	Chain	Length	Quality of chain
1	V	782	38% 17% 5% • 39%
2	W	760	59% 24% • • 13%
3	0	395	31% 15% • 52%
4	1	71	18% 59% 10% 13%
5	2	462	22% 34% • 41%
6	3	308	16% 41% 6% 37%
7	X	19	53% 47%
8	Y	20	40% 60%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 15688 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 TFIIF basal transcription factor complex helicase XPB subunit.

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

- Molecule 2 is a protein called TFIIF basal transcription factor complex helicase XPD subunit.

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

- Molecule 3 is a protein called General transcription factor IIF subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	0	188	Total	C	N	O	S	0	0
			1479	935	258	276	10		

- Molecule 4 is a protein called General transcription factor IIF subunit 5.

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

- Molecule 5 is a protein called General transcription factor IIF subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	2	274	Total	C	N	O	S	0	0
			2196	1417	377	392	10		

- Molecule 6 is a protein called General transcription factor IIF subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	3	193	Total	C	N	O	S	0	0
			1526	978	252	284	12		

- Molecule 7 is a DNA chain called scp-X.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	X	19	Total	C	N	O	P	0	0
			392	187	83	104	18		

- Molecule 8 is a DNA chain called scp-Y.

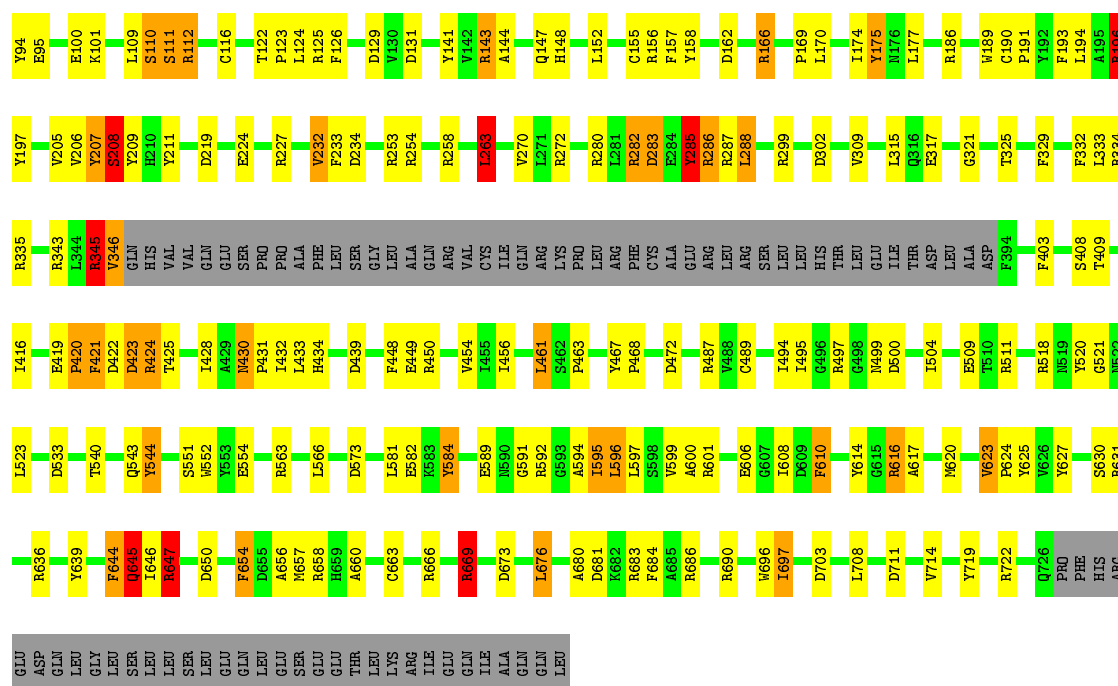
Mol	Chain	Residues	Atoms					AltConf	Trace
8	Y	20	Total	C	N	O	P	0	0
			401	196	59	127	19		

- Molecule 1: TFIIH basal transcription factor complex helicase XPB subunit

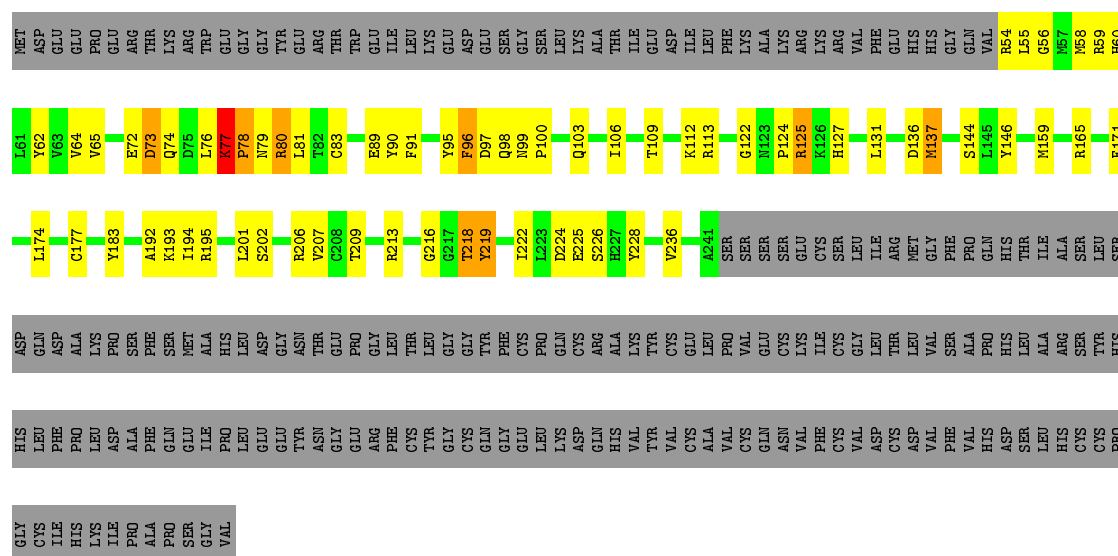
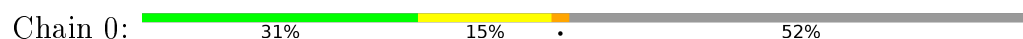
[illegible]

- Molecule 2: TFIIH basal transcription factor complex helicase XPD subunit

Met	Lys	Leu	Asp	Val	Gly	Leu	Leu	Val	Tyr	Phe	Pro	Tyr	D15	M25	R26	E27	L28	K29	R30	D33	G36	H37	E41	G45	T46	G47	V50	S51	L52	A58	Y59	G60	R61	A62	Y63	P64	V67	L70	T71	Y72	C73	T74	R75	T76	V77	L87	R88
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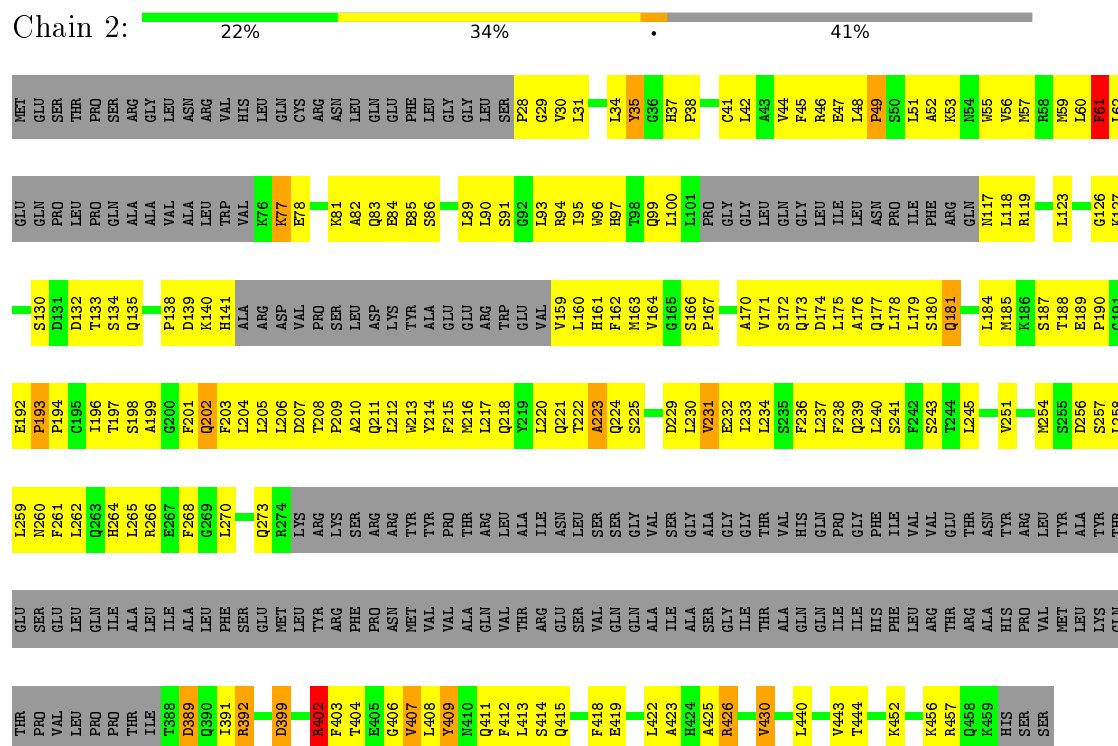
• Molecule 3: General transcription factor IIH subunit 2



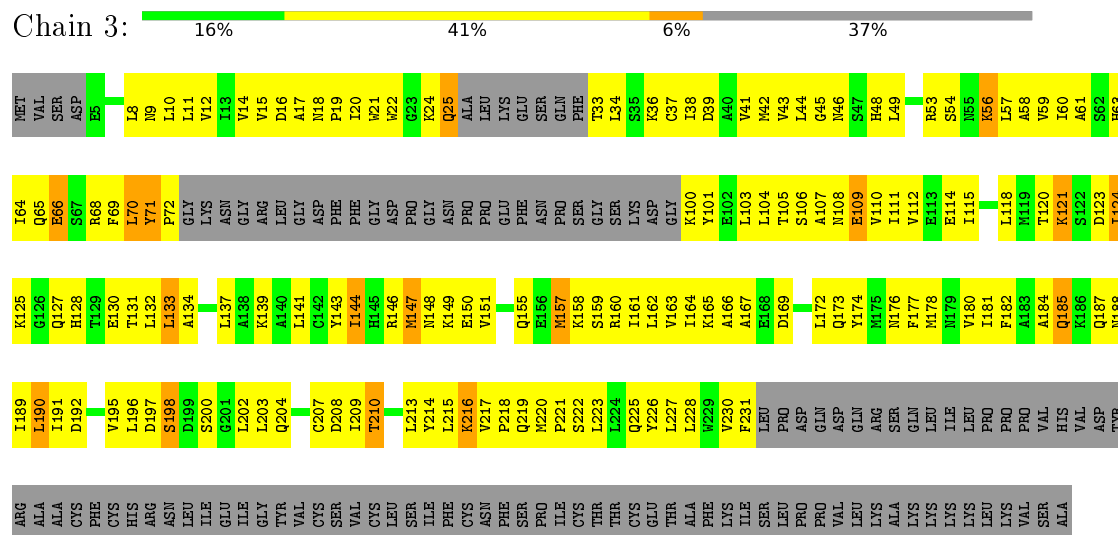
• Molecule 4: General transcription factor IIH subunit 5



- Molecule 5: General transcription factor IIH subunit 4



- Molecule 6: General transcription factor IIH subunit 3



- Molecule 7: scp-X



- Molecule 8: scp-Y



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	219771	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	27500	Depositor
Image detector	Not provided	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	V	1.44	15/3931 (0.4%)	1.95	110/5298 (2.1%)
2	W	1.50	21/5460 (0.4%)	2.00	150/7390 (2.0%)
3	0	1.45	5/1506 (0.3%)	1.92	42/2038 (2.1%)
4	1	0.83	0/496	1.12	0/669
5	2	0.88	0/2243	1.18	9/3024 (0.3%)
6	3	0.85	0/1548	1.13	2/2090 (0.1%)
7	X	3.20	45/443 (10.2%)	3.95	129/682 (18.9%)
8	Y	3.42	58/445 (13.0%)	4.25	126/685 (18.4%)
All	All	1.51	144/16072 (0.9%)	2.00	568/21876 (2.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	V	0	12
2	W	0	8
5	2	0	8
7	X	0	7
8	Y	0	12
All	All	0	47

All (144) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	X	10	DG	N7-C5	17.61	1.49	1.39
8	Y	6	DT	C5-C7	15.71	1.59	1.50
8	Y	2	DT	C5-C7	11.35	1.56	1.50
7	X	1	DA	N3-C4	10.46	1.41	1.34
8	Y	4	DT	C5-C6	9.83	1.41	1.34
8	Y	8	DC	P-O5'	-9.82	1.50	1.59
8	Y	20	DT	N1-C2	9.82	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	X	19	DA	N3-C4	9.77	1.40	1.34
8	Y	20	DT	C5-C6	9.37	1.41	1.34
8	Y	4	DT	N1-C6	9.09	1.44	1.38
8	Y	3	DT	C3'-C2'	-8.82	1.41	1.52
8	Y	16	DG	C5'-C4'	8.68	1.60	1.51
8	Y	16	DG	N3-C4	8.68	1.41	1.35
8	Y	5	DT	N1-C2	8.65	1.45	1.38
8	Y	6	DT	C4'-C3'	8.56	1.61	1.53
7	X	19	DA	N9-C4	8.25	1.42	1.37
7	X	12	DC	C4-N4	-8.09	1.26	1.33
8	Y	16	DG	C6-N1	-8.07	1.33	1.39
7	X	5	DC	C4'-C3'	8.05	1.61	1.53
7	X	8	DA	C6-N6	-8.02	1.27	1.33
8	Y	18	DA	N7-C5	-8.01	1.34	1.39
2	W	158	TYR	CE1-CZ	8.01	1.49	1.38
7	X	10	DG	P-O5'	7.98	1.67	1.59
1	V	672	TYR	CE1-CZ	7.94	1.48	1.38
7	X	9	DA	N7-C5	7.91	1.44	1.39
8	Y	14	DC	C5-C6	7.91	1.40	1.34
8	Y	14	DC	C5'-C4'	7.88	1.60	1.51
7	X	13	DG	C2-N2	-7.88	1.26	1.34
8	Y	3	DT	C4'-C3'	7.78	1.61	1.53
7	X	8	DA	O4'-C1'	-7.73	1.32	1.42
8	Y	18	DA	C5-C6	7.54	1.47	1.41
7	X	16	DA	N9-C4	-7.47	1.33	1.37
7	X	13	DG	N1-C2	-7.37	1.31	1.37
8	Y	1	DT	C4-C5	7.37	1.51	1.45
7	X	4	DG	N7-C5	7.31	1.43	1.39
8	Y	18	DA	C5'-C4'	7.27	1.59	1.51
7	X	19	DA	C5-C4	-7.19	1.33	1.38
7	X	6	DC	N3-C4	-7.18	1.28	1.33
7	X	7	DG	P-O5'	-7.10	1.52	1.59
7	X	16	DA	C6-N1	-7.04	1.30	1.35
1	V	391	ARG	CZ-NH2	-7.01	1.24	1.33
8	Y	5	DT	P-O5'	6.99	1.66	1.59
8	Y	20	DT	C5-C7	6.98	1.54	1.50
8	Y	7	DT	N1-C2	6.93	1.43	1.38
7	X	4	DG	C2-N3	6.83	1.38	1.32
7	X	4	DG	C2'-C1'	6.83	1.59	1.52
8	Y	17	DC	C4'-C3'	6.78	1.60	1.53
7	X	16	DA	N7-C5	6.73	1.43	1.39
7	X	3	DT	C2-N3	-6.71	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	Y	9	DG	C6-N1	-6.69	1.34	1.39
2	W	110	SER	CA-CB	6.68	1.62	1.52
7	X	8	DA	C2-N3	6.65	1.39	1.33
7	X	2	DT	C4'-O4'	-6.63	1.38	1.45
1	V	633	ARG	CZ-NH1	-6.61	1.24	1.33
7	X	18	DA	N1-C2	-6.60	1.28	1.34
8	Y	15	DG	C8-N7	-6.54	1.27	1.30
7	X	13	DG	N7-C5	6.54	1.43	1.39
2	W	521	GLY	N-CA	6.49	1.55	1.46
2	W	208	SER	CB-OG	-6.46	1.33	1.42
8	Y	19	DA	C2-N3	6.44	1.39	1.33
8	Y	12	DT	C5'-C4'	6.41	1.58	1.51
3	0	122	GLY	N-CA	6.39	1.55	1.46
1	V	606	PHE	CG-CD1	6.38	1.48	1.38
7	X	17	DA	C2'-C1'	6.38	1.58	1.52
7	X	15	DA	P-O5'	-6.37	1.53	1.59
8	Y	14	DC	C4-C5	6.37	1.48	1.43
8	Y	18	DA	C8-N7	-6.35	1.27	1.31
8	Y	12	DT	C4'-O4'	-6.31	1.38	1.45
8	Y	4	DT	C5-C7	6.30	1.53	1.50
7	X	16	DA	C5-C4	-6.26	1.34	1.38
1	V	554	ARG	NE-CZ	6.26	1.41	1.33
8	Y	3	DT	C5-C6	6.23	1.38	1.34
2	W	683	ARG	CZ-NH2	-6.21	1.25	1.33
7	X	7	DG	O4'-C1'	-6.21	1.34	1.42
7	X	13	DG	N9-C8	6.14	1.42	1.37
1	V	453	ARG	CZ-NH2	-6.14	1.25	1.33
8	Y	8	DC	C3'-C2'	6.12	1.59	1.52
8	Y	12	DT	C2-N3	6.11	1.42	1.37
8	Y	8	DC	C4'-O4'	-6.07	1.39	1.45
8	Y	6	DT	C4-C5	6.05	1.50	1.45
8	Y	9	DG	N3-C4	-6.05	1.31	1.35
8	Y	9	DG	C2'-C1'	6.00	1.58	1.52
8	Y	18	DA	P-O5'	5.98	1.65	1.59
7	X	8	DA	C5-C4	-5.97	1.34	1.38
8	Y	2	DT	O4'-C1'	-5.96	1.35	1.42
8	Y	7	DT	C5-C6	5.94	1.38	1.34
7	X	8	DA	C5'-C4'	5.90	1.57	1.51
8	Y	11	DC	N1-C6	5.90	1.40	1.37
1	V	319	TYR	CE1-CZ	5.87	1.46	1.38
1	V	435	TRP	CD2-CE2	5.87	1.48	1.41
7	X	8	DA	C4'-O4'	-5.86	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	X	18	DA	N9-C8	5.81	1.42	1.37
7	X	9	DA	N3-C4	5.78	1.38	1.34
7	X	19	DA	C8-N7	-5.77	1.27	1.31
2	W	321	GLY	N-CA	5.77	1.54	1.46
1	V	252	TYR	CE1-CZ	5.75	1.46	1.38
3	0	195	ARG	CZ-NH1	-5.71	1.25	1.33
7	X	1	DA	C5-C6	5.67	1.46	1.41
2	W	286	ARG	CZ-NH1	-5.66	1.25	1.33
8	Y	20	DT	P-O5'	5.64	1.65	1.59
8	Y	7	DT	C5-C7	5.63	1.53	1.50
1	V	374	TRP	CA-CB	5.63	1.66	1.53
7	X	8	DA	C1'-N9	5.61	1.56	1.49
7	X	19	DA	N7-C5	5.60	1.42	1.39
2	W	47	GLY	N-CA	5.58	1.54	1.46
8	Y	3	DT	P-O5'	-5.55	1.54	1.59
7	X	4	DG	N3-C4	-5.52	1.31	1.35
8	Y	11	DC	C4-N4	-5.50	1.28	1.33
1	V	332	ARG	CZ-NH2	-5.49	1.25	1.33
8	Y	12	DT	C2-O2	5.46	1.26	1.22
2	W	610	PHE	CG-CD1	5.45	1.47	1.38
2	W	606	GLU	CA-CB	5.43	1.65	1.53
7	X	18	DA	C2-N3	-5.41	1.28	1.33
7	X	16	DA	N9-C8	-5.41	1.33	1.37
8	Y	20	DT	N1-C6	5.38	1.42	1.38
8	Y	5	DT	C5-C6	5.37	1.38	1.34
2	W	286	ARG	CZ-NH2	-5.37	1.26	1.33
7	X	17	DA	N1-C2	-5.35	1.29	1.34
8	Y	13	DT	O3'-P	5.34	1.67	1.61
2	W	334	ARG	CZ-NH2	-5.33	1.26	1.33
8	Y	19	DA	C6-N6	-5.33	1.29	1.33
1	V	452	ARG	CZ-NH2	-5.32	1.26	1.33
2	W	448	PHE	CE1-CZ	5.30	1.47	1.37
2	W	253	ARG	CZ-NH1	-5.30	1.26	1.33
8	Y	3	DT	N3-C4	-5.25	1.34	1.38
8	Y	13	DT	N1-C6	5.22	1.42	1.38
1	V	659	PHE	CG-CD2	5.18	1.46	1.38
2	W	254	ARG	CZ-NH1	-5.17	1.26	1.33
2	W	518	ARG	CZ-NH2	-5.15	1.26	1.33
8	Y	8	DC	N1-C6	5.15	1.40	1.37
2	W	639	TYR	CZ-OH	-5.13	1.29	1.37
2	W	511	ARG	NE-CZ	-5.13	1.26	1.33
2	W	654	PHE	CG-CD1	5.12	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	0	95	TYR	CG-CD1	5.11	1.45	1.39
2	W	345	ARG	CZ-NH1	-5.10	1.26	1.33
3	0	112	LYS	N-CA	5.10	1.56	1.46
1	V	451	PHE	CG-CD2	5.09	1.46	1.38
8	Y	19	DA	N3-C4	5.08	1.37	1.34
2	W	520	TYR	CZ-OH	-5.07	1.29	1.37
8	Y	3	DT	C4'-O4'	-5.05	1.40	1.45
3	0	146	TYR	CD2-CE2	5.04	1.47	1.39
7	X	2	DT	C5'-C4'	5.04	1.56	1.51
8	Y	18	DA	C6-N6	-5.04	1.29	1.33
1	V	685	TYR	CG-CD1	5.00	1.45	1.39

All (568) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	0	77	LYS	C-N-CD	-24.19	67.39	120.60
6	3	71	TYR	C-N-CD	-20.68	75.09	120.60
2	W	335	ARG	NE-CZ-NH1	-19.48	110.56	120.30
2	W	26	ARG	NE-CZ-NH2	18.81	129.70	120.30
1	V	358	ARG	NE-CZ-NH2	17.52	129.06	120.30
3	0	195	ARG	NE-CZ-NH1	16.92	128.76	120.30
8	Y	20	DT	O4'-C1'-N1	16.90	119.83	108.00
8	Y	14	DC	N3-C2-O2	-16.64	110.25	121.90
8	Y	12	DT	C6-C5-C7	-16.49	113.00	122.90
2	W	186	ARG	NE-CZ-NH1	16.25	128.43	120.30
2	W	497	ARG	NE-CZ-NH1	16.02	128.31	120.30
8	Y	4	DT	C6-C5-C7	-15.83	113.40	122.90
7	X	1	DA	N1-C6-N6	-15.75	109.15	118.60
2	W	287	ARG	NE-CZ-NH2	15.47	128.03	120.30
8	Y	14	DC	N1-C2-O2	15.39	128.13	118.90
8	Y	14	DC	N3-C4-C5	15.31	128.02	121.90
8	Y	17	DC	N3-C4-N4	-15.21	107.35	118.00
2	W	299	ARG	NE-CZ-NH1	15.15	127.88	120.30
1	V	634	ARG	NE-CZ-NH2	14.98	127.79	120.30
8	Y	1	DT	N3-C2-O2	-14.80	113.42	122.30
3	0	206	ARG	NE-CZ-NH1	14.75	127.67	120.30
7	X	4	DG	O4'-C1'-N9	14.62	118.23	108.00
1	V	642	ARG	NE-CZ-NH1	14.20	127.40	120.30
2	W	592	ARG	NE-CZ-NH1	14.20	127.40	120.30
7	X	19	DA	N1-C6-N6	-14.13	110.12	118.60
2	W	335	ARG	NE-CZ-NH2	14.09	127.34	120.30
8	Y	11	DC	C2-N3-C4	-14.00	112.90	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	Y	11	DC	N3-C4-C5	13.98	127.49	121.90
2	W	112	ARG	NE-CZ-NH1	13.95	127.27	120.30
1	V	332	ARG	NE-CZ-NH1	13.87	127.23	120.30
2	W	669	ARG	NE-CZ-NH1	13.81	127.20	120.30
2	W	272	ARG	NE-CZ-NH1	13.68	127.14	120.30
8	Y	18	DA	C4-C5-C6	-13.53	110.23	117.00
8	Y	17	DC	C5-C4-N4	13.46	129.62	120.20
2	W	75	ARG	NE-CZ-NH1	13.38	126.99	120.30
7	X	5	DC	O4'-C1'-N1	13.35	117.34	108.00
8	Y	3	DT	C6-C5-C7	-13.12	115.03	122.90
2	W	343	ARG	NE-CZ-NH2	12.82	126.71	120.30
1	V	633	ARG	NE-CZ-NH2	-12.72	113.94	120.30
7	X	11	DA	C8-N9-C4	-12.45	100.82	105.80
8	Y	13	DT	N1-C2-N3	12.35	122.01	114.60
7	X	7	DG	N1-C6-O6	-12.22	112.57	119.90
2	W	467	TYR	CB-CG-CD1	-12.21	113.67	121.00
7	X	5	DC	N1-C2-O2	12.20	126.22	118.90
2	W	601	ARG	NE-CZ-NH2	-12.19	114.21	120.30
1	V	642	ARG	NE-CZ-NH2	-12.16	114.22	120.30
2	W	423	ASP	CB-CG-OD1	12.15	129.24	118.30
7	X	14	DA	C5-C6-N1	12.14	123.77	117.70
2	W	627	TYR	CB-CG-CD2	-12.08	113.75	121.00
7	X	16	DA	N9-C4-C5	12.05	110.62	105.80
2	W	631	ARG	NE-CZ-NH1	11.92	126.26	120.30
1	V	452	ARG	NE-CZ-NH1	11.70	126.15	120.30
2	W	26	ARG	NH1-CZ-NH2	-11.70	106.53	119.40
8	Y	13	DT	N3-C2-O2	-11.61	115.33	122.30
1	V	283	ARG	NE-CZ-NH2	-11.60	114.50	120.30
8	Y	12	DT	O4'-C1'-N1	11.59	116.11	108.00
2	W	487	ARG	NE-CZ-NH1	11.53	126.07	120.30
7	X	6	DC	N3-C2-O2	-11.52	113.83	121.90
2	W	636	ARG	NE-CZ-NH1	11.48	126.04	120.30
8	Y	4	DT	C5-C6-N1	-11.46	116.83	123.70
8	Y	1	DT	C5-C6-N1	-11.43	116.84	123.70
2	W	88	ARG	NE-CZ-NH1	11.39	126.00	120.30
7	X	1	DA	O4'-C1'-N9	11.24	115.87	108.00
2	W	343	ARG	NE-CZ-NH1	-11.18	114.71	120.30
2	W	647	ARG	NE-CZ-NH1	11.14	125.87	120.30
7	X	13	DG	N1-C6-O6	-11.10	113.24	119.90
8	Y	14	DC	C6-N1-C2	11.07	124.73	120.30
8	Y	16	DG	O4'-C4'-C3'	10.94	112.57	106.00
8	Y	1	DT	C6-C5-C7	-10.94	116.34	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	W	690	ARG	NE-CZ-NH2	10.90	125.75	120.30
2	W	683	ARG	NE-CZ-NH2	10.88	125.74	120.30
8	Y	14	DC	C5-C6-N1	-10.81	115.60	121.00
8	Y	4	DT	C4-C5-C7	10.68	125.41	119.00
7	X	15	DA	O4'-C4'-C3'	10.42	112.25	106.00
1	V	391	ARG	NE-CZ-NH1	-10.38	115.11	120.30
8	Y	16	DG	N3-C2-N2	-10.30	112.69	119.90
2	W	88	ARG	NE-CZ-NH2	-10.29	115.15	120.30
8	Y	6	DT	C6-C5-C7	-10.28	116.73	122.90
8	Y	18	DA	N1-C6-N6	-10.24	112.46	118.60
8	Y	20	DT	C6-N1-C2	-10.12	116.24	121.30
7	X	9	DA	C5-N7-C8	-10.11	98.84	103.90
8	Y	5	DT	C6-N1-C2	-10.10	116.25	121.30
7	X	9	DA	N1-C6-N6	-9.99	112.61	118.60
1	V	687	PHE	CB-CG-CD2	-9.97	113.82	120.80
1	V	452	ARG	NE-CZ-NH2	-9.90	115.35	120.30
8	Y	3	DT	N3-C2-O2	-9.90	116.36	122.30
2	W	497	ARG	NE-CZ-NH2	-9.89	115.35	120.30
1	V	649	GLY	N-CA-C	-9.88	88.41	113.10
8	Y	10	DT	O4'-C1'-C2'	9.85	113.78	105.90
1	V	553	ARG	NE-CZ-NH2	9.84	125.22	120.30
3	0	59	ARG	NE-CZ-NH2	9.80	125.20	120.30
8	Y	11	DC	N3-C2-O2	-9.79	115.05	121.90
1	V	283	ARG	NE-CZ-NH1	9.78	125.19	120.30
7	X	13	DG	N1-C2-N3	9.76	129.75	123.90
8	Y	19	DA	C5-C6-N1	9.75	122.57	117.70
1	V	520	ARG	CA-C-N	-9.72	95.82	117.20
7	X	16	DA	O4'-C1'-C2'	-9.64	98.19	105.90
8	Y	3	DT	C6-N1-C2	-9.55	116.53	121.30
7	X	5	DC	N3-C2-O2	-9.53	115.23	121.90
7	X	13	DG	N3-C2-N2	-9.52	113.23	119.90
8	Y	13	DT	C6-N1-C2	-9.49	116.56	121.30
7	X	6	DC	C6-N1-C2	-9.49	116.50	120.30
2	W	658	ARG	NE-CZ-NH2	-9.47	115.56	120.30
1	V	334	ARG	CD-NE-CZ	9.47	136.86	123.60
2	W	227	ARG	NE-CZ-NH1	9.46	125.03	120.30
8	Y	18	DA	C6-C5-N7	9.44	138.91	132.30
2	W	511	ARG	NE-CZ-NH2	9.38	124.99	120.30
7	X	11	DA	O4'-C4'-C3'	9.35	111.61	106.00
7	X	16	DA	C4-C5-N7	-9.33	106.03	110.70
7	X	14	DA	C2-N3-C4	9.30	115.25	110.60
7	X	7	DG	O4'-C1'-N9	-9.27	101.51	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	X	12	DC	N3-C2-O2	-9.23	115.44	121.90
7	X	2	DT	N3-C2-O2	-9.22	116.77	122.30
2	W	686	ARG	NE-CZ-NH1	9.20	124.90	120.30
8	Y	12	DT	C2-N3-C4	-9.19	121.69	127.20
8	Y	12	DT	N3-C4-O4	-9.19	114.39	119.90
1	V	645	ARG	NE-CZ-NH1	9.17	124.89	120.30
2	W	666	ARG	NE-CZ-NH1	9.15	124.88	120.30
1	V	264	GLU	OE1-CD-OE2	-9.14	112.34	123.30
3	0	219	TYR	CB-CG-CD1	-9.13	115.52	121.00
2	W	627	TYR	CG-CD2-CE2	-9.12	114.00	121.30
7	X	4	DG	N3-C2-N2	-9.12	113.52	119.90
8	Y	20	DT	N1-C2-N3	9.10	120.06	114.60
8	Y	1	DT	C4-C5-C6	9.08	123.45	118.00
7	X	11	DA	N7-C8-N9	9.03	118.32	113.80
1	V	421	TRP	NE1-CE2-CD2	-9.01	98.30	107.30
2	W	286	ARG	NE-CZ-NH2	9.01	124.80	120.30
7	X	8	DA	C5-C6-N1	8.97	122.19	117.70
8	Y	12	DT	C5-C4-O4	8.91	131.14	124.90
3	0	206	ARG	NH1-CZ-NH2	-8.90	109.61	119.40
2	W	703	ASP	CB-CG-OD2	8.89	126.30	118.30
7	X	14	DA	C4-C5-C6	-8.82	112.59	117.00
1	V	421	TRP	CD2-CE3-CZ3	8.80	130.24	118.80
1	V	550	PHE	CB-CG-CD1	-8.80	114.64	120.80
1	V	649	GLY	CA-C-O	-8.76	104.84	120.60
7	X	8	DA	C5-N7-C8	-8.74	99.53	103.90
7	X	13	DG	C4-C5-N7	8.74	114.30	110.80
8	Y	3	DT	N1-C2-N3	8.60	119.76	114.60
7	X	10	DG	C5-N7-C8	-8.60	100.00	104.30
8	Y	5	DT	N3-C2-O2	-8.59	117.14	122.30
8	Y	4	DT	N3-C2-O2	-8.58	117.15	122.30
8	Y	3	DT	C4-C5-C7	8.53	124.12	119.00
7	X	7	DG	C5-C6-N1	8.52	115.76	111.50
8	Y	16	DG	C4'-C3'-C2'	-8.51	95.44	103.10
7	X	11	DA	C5-N7-C8	-8.51	99.64	103.90
2	W	450	ARG	NE-CZ-NH1	8.49	124.55	120.30
8	Y	12	DT	C4-C5-C6	8.46	123.07	118.00
2	W	654	PHE	CB-CG-CD2	-8.42	114.90	120.80
8	Y	16	DG	C1'-O4'-C4'	-8.41	101.69	110.10
7	X	14	DA	O4'-C1'-N9	8.40	113.88	108.00
1	V	581	TYR	CG-CD1-CE1	-8.40	114.58	121.30
1	V	520	ARG	C-N-CA	-8.39	100.72	121.70
7	X	11	DA	C1'-O4'-C4'	-8.34	101.76	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	X	9	DA	N9-C4-C5	-8.34	102.47	105.80
7	X	13	DG	C6-N1-C2	-8.33	120.10	125.10
3	0	213	ARG	NE-CZ-NH1	8.32	124.46	120.30
8	Y	20	DT	C6-C5-C7	-8.31	117.91	122.90
1	V	685	TYR	CB-CG-CD2	8.29	125.98	121.00
1	V	419	ARG	NE-CZ-NH1	8.28	124.44	120.30
2	W	332	PHE	CB-CG-CD2	-8.27	115.01	120.80
7	X	9	DA	C4-C5-N7	8.23	114.81	110.70
8	Y	20	DT	C5-C4-O4	8.22	130.65	124.90
2	W	497	ARG	CD-NE-CZ	8.19	135.06	123.60
8	Y	8	DC	C5-C4-N4	-8.15	114.49	120.20
1	V	634	ARG	NE-CZ-NH1	-8.13	116.23	120.30
1	V	520	ARG	O-C-N	8.13	135.70	122.70
1	V	520	ARG	NE-CZ-NH2	8.11	124.36	120.30
8	Y	14	DC	C2-N3-C4	-8.06	115.87	119.90
7	X	15	DA	N1-C2-N3	-8.01	125.30	129.30
8	Y	19	DA	O4'-C1'-N9	-7.97	102.42	108.00
8	Y	17	DC	O4'-C1'-N1	-7.97	102.42	108.00
2	W	75	ARG	NE-CZ-NH2	-7.93	116.33	120.30
7	X	1	DA	C4-C5-C6	-7.92	113.04	117.00
2	W	601	ARG	NE-CZ-NH1	7.92	124.26	120.30
8	Y	12	DT	C4-C5-C7	7.90	123.74	119.00
7	X	10	DG	O4'-C4'-C3'	-7.87	101.28	106.00
2	W	126	PHE	CB-CG-CD2	7.87	126.31	120.80
7	X	15	DA	N1-C6-N6	-7.86	113.88	118.60
8	Y	20	DT	N3-C4-O4	-7.86	115.19	119.90
1	V	358	ARG	NH1-CZ-NH2	-7.85	110.77	119.40
7	X	11	DA	O4'-C1'-C2'	7.83	112.16	105.90
1	V	386	ASP	CB-CG-OD2	-7.82	111.27	118.30
1	V	410	TYR	CB-CG-CD1	-7.81	116.31	121.00
2	W	448	PHE	CB-CG-CD2	7.76	126.23	120.80
7	X	8	DA	O4'-C4'-C3'	7.76	110.66	106.00
2	W	644	PHE	CB-CG-CD1	7.75	126.22	120.80
2	W	143	ARG	NE-CZ-NH1	7.73	124.17	120.30
2	W	467	TYR	CB-CG-CD2	7.72	125.63	121.00
2	W	125	ARG	NE-CZ-NH1	7.71	124.15	120.30
8	Y	15	DG	N7-C8-N9	7.71	116.95	113.10
8	Y	9	DG	C8-N9-C4	-7.69	103.33	106.40
8	Y	16	DG	C4-C5-N7	-7.69	107.72	110.80
8	Y	15	DG	C5-N7-C8	-7.68	100.46	104.30
2	W	232	VAL	CA-CB-CG1	7.67	122.41	110.90
7	X	4	DG	N1-C6-O6	-7.66	115.31	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	Y	6	DT	N3-C2-O2	-7.64	117.72	122.30
8	Y	8	DC	C4-C5-C6	-7.63	113.59	117.40
1	V	542	ARG	NE-CZ-NH2	7.62	124.11	120.30
2	W	582	GLU	OE1-CD-OE2	-7.62	114.16	123.30
2	W	520	TYR	CG-CD1-CE1	-7.58	115.24	121.30
1	V	421	TRP	CE2-CD2-CG	7.57	113.36	107.30
3	O	90	TYR	CB-CG-CD2	-7.54	116.47	121.00
8	Y	10	DT	N3-C4-O4	-7.54	115.38	119.90
8	Y	8	DC	N1-C2-O2	7.53	123.42	118.90
7	X	8	DA	C4'-C3'-C2'	-7.51	96.34	103.10
1	V	474	ASP	CB-CG-OD2	7.50	125.05	118.30
7	X	8	DA	C4-C5-N7	7.50	114.45	110.70
7	X	1	DA	C5-C6-N1	7.49	121.45	117.70
5	2	402	ARG	NE-CZ-NH1	7.48	124.04	120.30
1	V	421	TRP	NE1-CE2-CZ2	7.46	138.61	130.40
8	Y	17	DC	C2-N3-C4	-7.46	116.17	119.90
8	Y	16	DG	C5-C6-N1	7.45	115.23	111.50
1	V	522	TYR	CB-CG-CD2	-7.45	116.53	121.00
7	X	6	DC	C2-N3-C4	-7.45	116.18	119.90
7	X	5	DC	C5-C4-N4	-7.44	114.99	120.20
8	Y	11	DC	N3-C4-N4	-7.43	112.80	118.00
2	W	193	PHE	CB-CG-CD1	-7.42	115.61	120.80
8	Y	6	DT	N1-C2-N3	7.41	119.05	114.60
3	O	95	TYR	CB-CG-CD1	-7.39	116.56	121.00
7	X	18	DA	N1-C2-N3	-7.38	125.61	129.30
2	W	272	ARG	NH1-CZ-NH2	-7.37	111.29	119.40
8	Y	17	DC	N3-C2-O2	-7.37	116.74	121.90
7	X	12	DC	C6-N1-C2	-7.37	117.35	120.30
2	W	592	ARG	NH1-CZ-NH2	-7.36	111.31	119.40
8	Y	2	DT	O4'-C1'-C2'	-7.35	100.02	105.90
1	V	685	TYR	CB-CG-CD1	-7.33	116.60	121.00
7	X	6	DC	N1-C2-N3	7.32	124.33	119.20
7	X	9	DA	N3-C4-C5	7.32	131.92	126.80
7	X	4	DG	N9-C4-C5	7.30	108.32	105.40
7	X	16	DA	N1-C6-N6	-7.30	114.22	118.60
3	O	73	ASP	CB-CG-OD2	-7.29	111.73	118.30
8	Y	14	DC	N3-C4-N4	-7.28	112.90	118.00
3	O	236	VAL	CA-CB-CG1	7.25	121.78	110.90
7	X	5	DC	O4'-C1'-C2'	-7.25	100.10	105.90
7	X	11	DA	C4-C5-C6	-7.22	113.39	117.00
2	W	186	ARG	NE-CZ-NH2	-7.21	116.69	120.30
1	V	421	TRP	CD1-NE1-CE2	7.20	115.48	109.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	V	249	PHE	CB-CG-CD2	7.18	125.82	120.80
7	X	2	DT	N1-C2-O2	7.14	128.81	123.10
7	X	1	DA	C4-C5-N7	7.14	114.27	110.70
7	X	1	DA	C5-C6-N6	7.13	129.40	123.70
2	W	280	ARG	NE-CZ-NH1	-7.11	116.75	120.30
8	Y	5	DT	C2-N3-C4	-7.09	122.94	127.20
1	V	554	ARG	NE-CZ-NH1	7.09	123.85	120.30
7	X	12	DC	N3-C4-N4	-7.06	113.06	118.00
2	W	317	GLU	OE1-CD-OE2	-7.05	114.84	123.30
3	0	89	GLU	OE1-CD-OE2	-7.04	114.85	123.30
7	X	1	DA	C5-N7-C8	-7.03	100.38	103.90
7	X	18	DA	C4-C5-C6	-7.03	113.48	117.00
1	V	639	ARG	NE-CZ-NH2	7.03	123.81	120.30
1	V	703	PHE	CB-CG-CD2	-7.00	115.90	120.80
2	W	627	TYR	CD1-CG-CD2	7.00	125.60	117.90
8	Y	16	DG	P-O3'-C3'	6.99	128.08	119.70
8	Y	16	DG	O4'-C1'-N9	6.98	112.89	108.00
2	W	166	ARG	CD-NE-CZ	6.97	133.36	123.60
7	X	7	DG	N9-C4-C5	-6.96	102.62	105.40
8	Y	12	DT	N1-C2-N3	6.95	118.77	114.60
7	X	19	DA	C5-C6-N1	6.95	121.17	117.70
8	Y	2	DT	N3-C2-O2	-6.93	118.14	122.30
1	V	643	VAL	CA-CB-CG1	6.92	121.29	110.90
1	V	385	ASP	CB-CG-OD1	-6.88	112.11	118.30
7	X	13	DG	C5-N7-C8	-6.87	100.87	104.30
3	0	136	ASP	CB-CG-OD1	6.86	124.47	118.30
7	X	13	DG	C5-C6-N1	6.85	114.92	111.50
8	Y	5	DT	O4'-C1'-N1	6.85	112.79	108.00
5	2	35	TYR	CA-CB-CG	-6.84	100.39	113.40
2	W	253	ARG	NE-CZ-NH1	6.84	123.72	120.30
8	Y	16	DG	C6-C5-N7	6.84	134.50	130.40
8	Y	2	DT	C4-C5-C7	-6.82	114.91	119.00
2	W	219	ASP	CB-CG-OD1	6.81	124.43	118.30
2	W	332	PHE	CB-CG-CD1	6.81	125.57	120.80
7	X	15	DA	C4'-C3'-C2'	-6.80	96.98	103.10
1	V	334	ARG	NE-CZ-NH1	6.77	123.69	120.30
1	V	581	TYR	CD1-CE1-CZ	6.77	125.89	119.80
2	W	644	PHE	CB-CG-CD2	-6.76	116.06	120.80
2	W	654	PHE	CB-CG-CD1	6.76	125.53	120.80
3	0	195	ARG	NE-CZ-NH2	-6.76	116.92	120.30
2	W	125	ARG	CD-NE-CZ	6.74	133.04	123.60
1	V	530	ARG	NE-CZ-NH2	-6.74	116.93	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	W	566	LEU	CB-CG-CD1	6.73	122.44	111.00
3	0	95	TYR	CD1-CE1-CZ	-6.73	113.74	119.80
2	W	196	ARG	NE-CZ-NH1	6.70	123.65	120.30
7	X	16	DA	C6-C5-N7	6.68	136.98	132.30
2	W	345	ARG	CD-NE-CZ	6.68	132.95	123.60
5	2	61	PHE	CB-CA-C	-6.68	97.04	110.40
7	X	9	DA	C2-N3-C4	-6.67	107.27	110.60
2	W	50	VAL	CA-CB-CG1	6.66	120.89	110.90
8	Y	1	DT	N1-C2-N3	6.66	118.59	114.60
1	V	298	ARG	NE-CZ-NH1	6.65	123.63	120.30
1	V	655	TYR	CB-CG-CD2	-6.65	117.01	121.00
2	W	26	ARG	NE-CZ-NH1	6.65	123.62	120.30
2	W	30	ARG	CD-NE-CZ	6.64	132.90	123.60
8	Y	13	DT	C2-N3-C4	-6.64	123.22	127.20
3	0	219	TYR	CG-CD1-CE1	-6.61	116.01	121.30
8	Y	15	DG	N9-C1'-C2'	6.59	125.12	112.60
2	W	302	ASP	CB-CG-OD1	6.57	124.21	118.30
7	X	14	DA	N1-C6-N6	-6.55	114.67	118.60
7	X	15	DA	C4-C5-C6	-6.54	113.73	117.00
1	V	421	TRP	CE2-CD2-CE3	-6.53	110.86	118.70
2	W	76	THR	CA-CB-OG1	6.52	122.69	109.00
2	W	125	ARG	NE-CZ-NH2	-6.52	117.04	120.30
8	Y	16	DG	N1-C6-O6	-6.52	115.99	119.90
8	Y	20	DT	C4-C5-C6	6.50	121.90	118.00
8	Y	2	DT	C4-C5-C6	6.50	121.90	118.00
2	W	315	LEU	CB-CG-CD1	6.49	122.03	111.00
7	X	11	DA	N1-C6-N6	-6.48	114.71	118.60
2	W	487	ARG	NH1-CZ-NH2	-6.48	112.27	119.40
2	W	299	ARG	NE-CZ-NH2	-6.46	117.07	120.30
8	Y	18	DA	N3-C4-C5	6.46	131.32	126.80
1	V	404	SER	CB-CA-C	6.46	122.37	110.10
2	W	616	ARG	NE-CZ-NH1	-6.45	117.07	120.30
5	2	193	PRO	CA-N-CD	-6.45	102.47	111.50
7	X	19	DA	C5-N7-C8	6.44	107.12	103.90
7	X	7	DG	C4-C5-N7	6.43	113.37	110.80
8	Y	5	DT	C6-C5-C7	-6.43	119.04	122.90
7	X	9	DA	C4-C5-C6	-6.41	113.80	117.00
7	X	18	DA	N7-C8-N9	-6.41	110.60	113.80
7	X	10	DG	O4'-C1'-C2'	-6.40	100.78	105.90
3	0	113	ARG	NE-CZ-NH1	6.39	123.50	120.30
8	Y	10	DT	O4'-C1'-N1	6.39	112.47	108.00
2	W	131	ASP	CB-CG-OD1	-6.39	112.55	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	X	12	DC	C4'-C3'-C2'	-6.39	97.35	103.10
2	W	669	ARG	NH1-CZ-NH2	-6.39	112.38	119.40
2	W	683	ARG	CD-NE-CZ	6.38	132.54	123.60
7	X	7	DG	N3-C2-N2	-6.38	115.43	119.90
7	X	12	DC	N1-C2-N3	6.38	123.67	119.20
2	W	639	TYR	CB-CG-CD2	-6.38	117.17	121.00
1	V	682	ASP	CB-CG-OD1	6.38	124.04	118.30
2	W	722	ARG	CD-NE-CZ	6.38	132.53	123.60
3	0	59	ARG	NH1-CZ-NH2	-6.37	112.39	119.40
7	X	17	DA	C2-N3-C4	-6.33	107.44	110.60
1	V	522	TYR	CB-CG-CD1	6.32	124.79	121.00
1	V	332	ARG	NH1-CZ-NH2	-6.32	112.45	119.40
2	W	263	LEU	N-CA-CB	-6.31	97.78	110.40
7	X	18	DA	C6-N1-C2	6.30	122.38	118.60
1	V	369	VAL	CA-CB-CG1	6.30	120.35	110.90
1	V	521	GLU	OE1-CD-OE2	-6.30	115.74	123.30
1	V	344	ALA	N-CA-CB	-6.29	101.29	110.10
8	Y	11	DC	C5-C6-N1	-6.27	117.86	121.00
8	Y	17	DC	C6-N1-C2	-6.27	117.79	120.30
8	Y	1	DT	O4'-C1'-N1	6.26	112.39	108.00
8	Y	17	DC	N1-C2-N3	6.26	123.59	119.20
7	X	16	DA	C5-C6-N1	6.26	120.83	117.70
7	X	1	DA	N9-C4-C5	-6.25	103.30	105.80
2	W	30	ARG	NE-CZ-NH1	6.25	123.42	120.30
7	X	7	DG	C6-N1-C2	-6.25	121.35	125.10
7	X	16	DA	N1-C2-N3	-6.25	126.17	129.30
8	Y	20	DT	C4'-C3'-C2'	-6.25	97.48	103.10
7	X	13	DG	O4'-C1'-N9	-6.24	103.63	108.00
2	W	175	TYR	N-CA-C	6.24	127.85	111.00
3	0	137	MET	CG-SD-CE	6.24	110.18	100.20
8	Y	3	DT	O4'-C1'-N1	6.23	112.36	108.00
8	Y	7	DT	O4'-C1'-N1	6.21	112.35	108.00
2	W	206	VAL	CA-CB-CG1	6.21	120.21	110.90
8	Y	8	DC	N3-C4-C5	6.18	124.37	121.90
7	X	13	DG	C4-C5-C6	-6.17	115.10	118.80
1	V	435	TRP	NE1-CE2-CD2	-6.15	101.15	107.30
8	Y	10	DT	C5-C4-O4	6.14	129.20	124.90
2	W	77	VAL	CG1-CB-CG2	-6.11	101.12	110.90
8	Y	19	DA	C6-N1-C2	-6.10	114.94	118.60
8	Y	9	DG	N1-C6-O6	-6.10	116.24	119.90
7	X	17	DA	N1-C6-N6	-6.08	114.95	118.60
8	Y	1	DT	N1-C2-O2	6.08	127.96	123.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	V	410	TYR	CZ-CE2-CD2	-6.07	114.34	119.80
7	X	6	DC	C5-C4-N4	-6.04	115.97	120.20
8	Y	20	DT	O4'-C1'-C2'	-6.04	101.07	105.90
3	0	183	TYR	CB-CG-CD1	-6.04	117.38	121.00
7	X	19	DA	O4'-C1'-C2'	-6.03	101.07	105.90
8	Y	7	DT	N3-C4-O4	-6.01	116.29	119.90
2	W	424	ARG	NE-CZ-NH1	6.01	123.30	120.30
8	Y	1	DT	C5-C4-O4	5.99	129.09	124.90
2	W	552	TRP	CD1-NE1-CE2	5.99	114.39	109.00
2	W	472	ASP	CB-CG-OD2	5.96	123.67	118.30
7	X	1	DA	N3-C4-N9	5.96	132.17	127.40
1	V	663	VAL	CG1-CB-CG2	-5.95	101.38	110.90
7	X	13	DG	C2-N3-C4	-5.95	108.92	111.90
2	W	673	ASP	CB-CG-OD1	5.95	123.65	118.30
8	Y	5	DT	N1-C2-N3	5.94	118.17	114.60
7	X	4	DG	N3-C4-N9	-5.94	122.44	126.00
8	Y	11	DC	N1-C2-N3	5.94	123.36	119.20
1	V	360	ARG	CD-NE-CZ	5.94	131.91	123.60
3	0	218	THR	CA-CB-CG2	-5.93	104.10	112.40
8	Y	16	DG	N3-C4-C5	-5.93	125.64	128.60
1	V	566	PHE	CB-CG-CD1	5.92	124.95	120.80
7	X	1	DA	P-O3'-C3'	5.92	126.80	119.70
1	V	472	ARG	NE-CZ-NH1	5.91	123.25	120.30
7	X	19	DA	C5-C6-N6	5.91	128.43	123.70
7	X	6	DC	O4'-C1'-C2'	5.90	110.62	105.90
7	X	10	DG	N7-C8-N9	5.90	116.05	113.10
2	W	156	ARG	CD-NE-CZ	5.89	131.85	123.60
8	Y	10	DT	C6-N1-C2	-5.89	118.35	121.30
8	Y	5	DT	C4-C5-C7	5.88	122.53	119.00
7	X	19	DA	C4-C5-N7	-5.88	107.76	110.70
2	W	131	ASP	CB-CG-OD2	5.87	123.58	118.30
7	X	10	DG	N3-C2-N2	-5.86	115.80	119.90
8	Y	8	DC	O4'-C1'-N1	5.85	112.09	108.00
8	Y	4	DT	N1-C2-O2	5.84	127.77	123.10
1	V	435	TRP	CD1-NE1-CE2	5.83	114.25	109.00
8	Y	6	DT	C4-C5-C7	5.82	122.49	119.00
8	Y	6	DT	C5-C6-N1	-5.81	120.21	123.70
8	Y	7	DT	C5-C4-O4	5.81	128.97	124.90
7	X	13	DG	N7-C8-N9	5.79	115.99	113.10
8	Y	20	DT	N3-C2-O2	-5.79	118.83	122.30
7	X	12	DC	C2-N3-C4	-5.78	117.01	119.90
1	V	410	TYR	CB-CG-CD2	5.78	124.47	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	W	112	ARG	NH1-CZ-NH2	-5.78	113.04	119.40
2	W	472	ASP	CB-CG-OD1	-5.77	113.11	118.30
3	0	171	PHE	CB-CG-CD1	-5.77	116.76	120.80
2	W	563	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	V	425	ARG	NE-CZ-NH1	5.75	123.18	120.30
1	V	542	ARG	NH1-CZ-NH2	-5.75	113.08	119.40
3	0	91	PHE	CG-CD2-CE2	-5.74	114.49	120.80
2	W	722	ARG	NE-CZ-NH1	-5.73	117.43	120.30
3	0	183	TYR	CD1-CE1-CZ	5.72	124.95	119.80
7	X	9	DA	N7-C8-N9	5.72	116.66	113.80
7	X	4	DG	C3'-C2'-C1'	-5.71	95.64	102.50
3	0	80	ARG	CD-NE-CZ	5.71	131.59	123.60
3	0	90	TYR	CG-CD2-CE2	-5.71	116.74	121.30
2	W	650	ASP	CB-CG-OD1	5.70	123.43	118.30
2	W	345	ARG	NE-CZ-NH2	-5.70	117.45	120.30
7	X	19	DA	C6-C5-N7	5.69	136.28	132.30
2	W	708	LEU	CB-CG-CD2	-5.69	101.33	111.00
3	0	177	CYS	CA-CB-SG	-5.69	103.76	114.00
1	V	251	PHE	CB-CG-CD1	-5.69	116.82	120.80
1	V	419	ARG	CD-NE-CZ	5.68	131.56	123.60
1	V	391	ARG	NE-CZ-NH2	5.68	123.14	120.30
8	Y	16	DG	N9-C4-C5	5.68	107.67	105.40
2	W	334	ARG	NE-CZ-NH2	-5.67	117.47	120.30
8	Y	14	DC	C4-C5-C6	-5.67	114.57	117.40
2	W	711	ASP	CB-CG-OD1	5.66	123.39	118.30
1	V	284	CYS	CA-CB-SG	-5.66	103.82	114.00
7	X	1	DA	C2-N3-C4	5.64	113.42	110.60
1	V	482	PHE	CB-CG-CD1	-5.63	116.86	120.80
7	X	12	DC	C6-N1-C1'	5.63	127.55	120.80
3	0	201	LEU	CB-CG-CD1	5.62	120.56	111.00
1	V	328	PHE	C-N-CA	5.62	134.09	122.30
1	V	430	LEU	CB-CG-CD1	5.62	120.55	111.00
8	Y	11	DC	C3'-C2'-C1'	-5.62	95.76	102.50
1	V	655	TYR	CB-CG-CD1	5.61	124.36	121.00
2	W	41	GLU	O-C-N	5.60	131.66	122.70
3	0	226	SER	N-CA-CB	-5.60	102.11	110.50
1	V	649	GLY	CA-C-N	5.59	129.51	117.20
2	W	270	VAL	CA-C-O	5.59	131.85	120.10
1	V	662	LEU	CB-CG-CD2	-5.59	101.50	111.00
1	V	640	LEU	CB-CG-CD2	5.59	120.50	111.00
2	W	544	TYR	CG-CD2-CE2	-5.58	116.84	121.30
1	V	679	PHE	CG-CD1-CE1	-5.58	114.67	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	V	289	TYR	CG-CD2-CE2	-5.57	116.84	121.30
7	X	8	DA	C5-C6-N6	-5.55	119.26	123.70
8	Y	17	DC	O4'-C4'-C3'	-5.55	102.28	104.50
2	W	684	PHE	CB-CG-CD1	-5.54	116.92	120.80
7	X	4	DG	C5-C6-O6	5.54	131.93	128.60
8	Y	13	DT	C4-C5-C7	-5.54	115.67	119.00
1	V	393	THR	O-C-N	-5.54	113.84	122.70
3	0	65	VAL	CA-CB-CG1	5.54	119.21	110.90
1	V	419	ARG	NH1-CZ-NH2	-5.54	113.31	119.40
1	V	608	SER	O-C-N	-5.53	113.85	122.70
2	W	129	ASP	CB-CG-OD1	5.53	123.28	118.30
1	V	634	ARG	CD-NE-CZ	5.51	131.31	123.60
8	Y	20	DT	C5-C6-N1	-5.51	120.39	123.70
3	0	183	TYR	CG-CD1-CE1	-5.50	116.90	121.30
1	V	272	VAL	CA-CB-CG2	-5.49	102.66	110.90
2	W	258	ARG	NE-CZ-NH1	5.49	123.04	120.30
7	X	7	DG	P-O3'-C3'	5.47	126.27	119.70
1	V	362	LEU	CB-CG-CD1	-5.47	101.71	111.00
2	W	224	GLU	OE1-CD-OE2	-5.46	116.74	123.30
1	V	571	TYR	CG-CD2-CE2	-5.46	116.93	121.30
2	W	177	LEU	CB-CG-CD1	5.46	120.29	111.00
1	V	571	TYR	CB-CG-CD1	-5.46	117.72	121.00
2	W	253	ARG	NH1-CZ-NH2	-5.46	113.39	119.40
7	X	12	DC	C4-C5-C6	-5.44	114.68	117.40
2	W	141	TYR	CG-CD2-CE2	5.44	125.65	121.30
1	V	382	SER	N-CA-CB	-5.44	102.35	110.50
2	W	280	ARG	NE-CZ-NH2	5.43	123.01	120.30
2	W	196	ARG	CD-NE-CZ	5.41	131.18	123.60
2	W	33	ASP	CB-CG-OD2	5.41	123.17	118.30
1	V	702	ALA	N-CA-CB	-5.41	102.53	110.10
2	W	631	ARG	NH1-CZ-NH2	-5.40	113.46	119.40
5	2	61	PHE	CB-CG-CD2	-5.40	117.02	120.80
2	W	595	ILE	CB-CA-C	5.39	122.38	111.60
2	W	625	TYR	CZ-CE2-CD2	-5.39	114.95	119.80
2	W	690	ARG	CD-NE-CZ	5.39	131.15	123.60
7	X	7	DG	C5-N7-C8	-5.38	101.61	104.30
2	W	285	TYR	CB-CG-CD1	-5.38	117.77	121.00
7	X	13	DG	C5-C6-O6	5.38	131.83	128.60
2	W	205	VAL	CA-CB-CG1	5.38	118.96	110.90
2	W	686	ARG	NE-CZ-NH2	-5.36	117.62	120.30
7	X	16	DA	C4'-C3'-C2'	-5.36	98.28	103.10
2	W	287	ARG	NH1-CZ-NH2	-5.35	113.51	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	W	616	ARG	NE-CZ-NH2	5.35	122.98	120.30
1	V	666	ASP	CB-CG-OD1	-5.33	113.50	118.30
1	V	319	TYR	CB-CG-CD1	-5.33	117.80	121.00
7	X	19	DA	C6-N1-C2	-5.33	115.40	118.60
2	W	663	CYS	CA-CB-SG	-5.33	104.41	114.00
1	V	479	ASP	CB-CG-OD2	5.32	123.09	118.30
1	V	560	VAL	CA-CB-CG2	5.32	118.88	110.90
3	0	207	VAL	CA-CB-CG1	5.31	118.87	110.90
3	0	125	ARG	NE-CZ-NH2	-5.31	117.64	120.30
5	2	35	TYR	CB-CA-C	5.31	121.02	110.40
8	Y	18	DA	C4'-C3'-C2'	-5.30	98.33	103.10
2	W	286	ARG	NH1-CZ-NH2	-5.29	113.58	119.40
3	0	90	TYR	CB-CG-CD1	5.28	124.17	121.00
8	Y	4	DT	C4-C5-C6	5.28	121.17	118.00
2	W	623	VAL	CG1-CB-CG2	-5.27	102.46	110.90
2	W	162	ASP	CB-CG-OD2	5.27	123.04	118.30
7	X	1	DA	O4'-C4'-C3'	5.27	109.16	106.00
8	Y	9	DG	C4-C5-C6	-5.26	115.64	118.80
2	W	540	THR	O-C-N	-5.26	114.29	122.70
3	0	213	ARG	NH1-CZ-NH2	-5.25	113.62	119.40
3	0	58	MET	O-C-N	5.25	131.10	122.70
3	0	64	VAL	CA-CB-CG1	5.24	118.76	110.90
8	Y	16	DG	C5-N7-C8	5.22	106.91	104.30
5	2	389	ASP	CB-CG-OD1	-5.22	113.60	118.30
2	W	617	ALA	N-CA-CB	5.21	117.40	110.10
1	V	478	VAL	CA-CB-CG2	-5.21	103.08	110.90
1	V	703	PHE	CG-CD1-CE1	-5.20	115.08	120.80
1	V	434	GLU	OE1-CD-OE2	5.19	129.53	123.30
1	V	289	TYR	CB-CG-CD2	-5.19	117.89	121.00
7	X	8	DA	O4'-C1'-N9	5.19	111.63	108.00
7	X	11	DA	C5-C6-N1	5.19	120.29	117.70
2	W	253	ARG	NE-CZ-NH2	5.17	122.89	120.30
3	0	62	TYR	CB-CG-CD1	5.17	124.10	121.00
3	0	131	LEU	CB-CG-CD1	5.17	119.79	111.00
2	W	143	ARG	NH1-CZ-NH2	-5.17	113.71	119.40
2	W	449	GLU	OE1-CD-OE2	-5.17	117.10	123.30
5	2	457	ARG	NE-CZ-NH1	5.17	122.88	120.30
8	Y	10	DT	C1'-O4'-C4'	-5.17	104.93	110.10
1	V	250	ASP	CB-CG-OD1	5.17	122.95	118.30
1	V	332	ARG	CA-CB-CG	5.17	124.76	113.40
2	W	61	ARG	NE-CZ-NH1	5.15	122.87	120.30
2	W	468	PRO	CA-N-CD	-5.14	104.30	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	V	644	LEU	CB-CG-CD2	-5.14	102.26	111.00
3	0	228	TYR	CB-CG-CD2	-5.14	117.92	121.00
5	2	392	ARG	NE-CZ-NH1	5.14	122.87	120.30
7	X	2	DT	C4-C5-C7	5.14	122.08	119.00
2	W	461	LEU	CA-CB-CG	5.14	127.11	115.30
1	V	679	PHE	CB-CG-CD1	-5.13	117.21	120.80
2	W	94	TYR	CB-CG-CD2	5.13	124.08	121.00
7	X	9	DA	P-O5'-C5'	5.12	129.10	120.90
2	W	439	ASP	CB-CG-OD2	5.12	122.91	118.30
3	0	90	TYR	CZ-CE2-CD2	5.12	124.41	119.80
8	Y	19	DA	C5-C6-N6	-5.12	119.61	123.70
1	V	362	LEU	CB-CG-CD2	5.11	119.69	111.00
7	X	7	DG	C5-C6-O6	5.11	131.66	128.60
1	V	360	ARG	NE-CZ-NH1	5.11	122.85	120.30
2	W	283	ASP	CB-CG-OD2	5.11	122.90	118.30
2	W	288	LEU	O-C-N	-5.10	114.55	122.70
2	W	676	LEU	CB-CG-CD2	5.07	119.61	111.00
2	W	714	VAL	CA-CB-CG2	5.07	118.50	110.90
1	V	289	TYR	CZ-CE2-CD2	5.07	124.36	119.80
1	V	678	ARG	NE-CZ-NH2	5.06	122.83	120.30
2	W	636	ARG	CD-NE-CZ	5.05	130.68	123.60
1	V	398	ASP	CB-CG-OD1	5.05	122.85	118.30
1	V	378	PHE	CB-CG-CD2	-5.05	117.27	120.80
2	W	600	ALA	N-CA-CB	-5.05	103.03	110.10
6	3	210	THR	CA-CB-CG2	-5.05	105.33	112.40
2	W	87	LEU	CB-CA-C	5.05	119.79	110.20
3	0	224	ASP	N-CA-CB	-5.05	101.52	110.60
2	W	599	VAL	CA-CB-CG1	5.02	118.43	110.90
7	X	8	DA	N7-C8-N9	5.02	116.31	113.80
2	W	463	PRO	N-CA-CB	5.01	109.32	103.30
7	X	12	DC	N3-C4-C5	5.01	123.91	121.90
8	Y	1	DT	N3-C4-C5	-5.01	112.19	115.20
7	X	16	DA	N3-C4-N9	-5.01	123.39	127.40
2	W	346	VAL	CA-CB-CG2	5.01	118.41	110.90
1	V	607	ILE	CA-CB-CG1	5.00	120.51	111.00
2	W	566	LEU	CB-CG-CD2	-5.00	102.50	111.00
7	X	4	DG	N1-C2-N2	5.00	120.70	116.20

There are no chirality outliers.

All (47) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	2	389	ASP	Sidechain,Mainchain
5	2	399	ASP	Sidechain
5	2	403	PHE	Mainchain,Peptide
5	2	406	GLY	Peptide
5	2	409	TYR	Sidechain
5	2	425	ALA	Mainchain
1	V	247	ASP	Mainchain
1	V	251	PHE	Sidechain
1	V	319	TYR	Sidechain
1	V	378	PHE	Sidechain
1	V	489	TYR	Sidechain
1	V	519	TYR	Sidechain
1	V	530	ARG	Sidechain
1	V	534	TYR	Sidechain
1	V	642	ARG	Sidechain
1	V	674	THR	Mainchain
1	V	679	PHE	Sidechain
1	V	703	PHE	Sidechain
2	W	208	SER	Mainchain
2	W	211	TYR	Sidechain
2	W	286	ARG	Sidechain
2	W	409	THR	Peptide
2	W	423	ASP	Peptide
2	W	616	ARG	Sidechain
2	W	669	ARG	Sidechain
2	W	719	TYR	Sidechain
7	X	10	DG	Sidechain
7	X	13	DG	Sidechain
7	X	14	DA	Sidechain
7	X	16	DA	Sidechain
7	X	19	DA	Sidechain
7	X	2	DT	Sidechain
7	X	4	DG	Sidechain
8	Y	1	DT	Sidechain
8	Y	13	DT	Sidechain
8	Y	14	DC	Sidechain
8	Y	15	DG	Sidechain
8	Y	16	DG	Sidechain
8	Y	17	DC	Sidechain
8	Y	19	DA	Sidechain
8	Y	3	DT	Sidechain
8	Y	5	DT	Sidechain
8	Y	7	DT	Sidechain

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Mol	Chain	Res	Type	Group
8	Y	8	DC	Sidechain
8	Y	9	DG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	V	3855	0	3872	163	0
2	W	5348	0	5371	175	0
3	0	1479	0	1524	69	0
4	1	491	0	507	227	0
5	2	2196	0	2206	587	0
6	3	1526	0	1561	454	0
7	X	392	0	207	1	0
8	Y	401	0	231	0	0
All	All	15688	0	15479	1391	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 45.

All (1391) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:0:77:LYS:HB2	3:0:83:CYS:CB	1.26	1.61
2:W:110:SER:HA	2:W:207:TYR:CE1	1.10	1.58
5:2:31:LEU:HD11	6:3:33:THR:CB	1.33	1.55
3:0:54:ARG:HG3	6:3:182:PHE:CE1	1.42	1.55
1:V:315:VAL:HG13	2:W:500:ASP:CB	1.21	1.54
1:V:523:VAL:HG11	4:1:20:LEU:CD2	1.38	1.54
5:2:31:LEU:HD11	6:3:33:THR:CG2	1.33	1.51
2:W:110:SER:CA	2:W:207:TYR:CE1	1.92	1.50
1:V:315:VAL:CG1	2:W:500:ASP:HB2	1.01	1.48
3:0:77:LYS:CB	3:0:83:CYS:CB	1.79	1.47
5:2:117:ASN:ND2	6:3:108:ASN:CB	1.76	1.46
5:2:117:ASN:HD21	6:3:108:ASN:CB	1.27	1.46
6:3:59:VAL:HG12	6:3:71:TYR:CD1	1.49	1.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:2:29:GLY:N	6:3:25:GLN:HG3	1.21	1.43
5:2:30:VAL:HG23	6:3:25:GLN:CB	1.48	1.43
2:W:421:PHE:HB3	2:W:431:PRO:N	1.31	1.40
5:2:117:ASN:CG	6:3:108:ASN:HB2	1.39	1.39
2:W:170:LEU:HD12	2:W:175:TYR:CZ	1.57	1.39
5:2:28:PRO:N	6:3:25:GLN:CA	1.85	1.38
3:0:54:ARG:CG	6:3:182:PHE:HE1	1.36	1.38
5:2:31:LEU:HD21	6:3:33:THR:N	1.28	1.37
3:0:77:LYS:HG2	3:0:83:CYS:SG	1.63	1.37
5:2:117:ASN:OD1	6:3:108:ASN:ND2	1.57	1.34
5:2:28:PRO:N	6:3:25:GLN:HA	1.03	1.34
5:2:118:LEU:CD2	6:3:39:ASP:OD1	1.75	1.33
3:0:77:LYS:CB	3:0:83:CYS:HB2	0.85	1.32
4:1:1:MET:O	5:2:413:LEU:HG	1.25	1.31
5:2:118:LEU:HD22	6:3:39:ASP:OD1	1.16	1.31
3:0:74:GLN:CA	3:0:78:PRO:O	1.76	1.30
3:0:77:LYS:HD3	3:0:225:GLU:OE2	1.15	1.30
3:0:77:LYS:CG	3:0:83:CYS:HB2	1.62	1.30
2:W:169:PRO:HB2	2:W:175:TYR:OH	1.32	1.29
5:2:118:LEU:HD21	6:3:39:ASP:O	1.23	1.28
5:2:31:LEU:CD1	6:3:33:THR:CG2	2.10	1.28
2:W:432:ILE:HG12	2:W:434:HIS:CE1	1.68	1.27
6:3:59:VAL:CG1	6:3:71:TYR:CD1	2.19	1.25
5:2:31:LEU:CD1	6:3:33:THR:HB	1.64	1.25
3:0:165:ARG:NH1	3:0:192:ALA:O	1.70	1.25
2:W:421:PHE:HB3	2:W:431:PRO:CD	1.52	1.25
1:V:674:THR:HG23	5:2:392:ARG:NH2	1.50	1.24
1:V:321:GLU:OE2	2:W:500:ASP:HB3	1.11	1.23
1:V:502:ILE:CG2	1:V:503:ALA:H	1.45	1.23
2:W:59:TYR:CZ	2:W:62:ALA:CB	2.22	1.22
2:W:72:TYR:CE2	2:W:232:VAL:HG11	1.75	1.21
6:3:59:VAL:HG13	6:3:70:LEU:CB	1.69	1.20
1:V:428:GLU:O	1:V:433:GLN:HA	1.38	1.20
1:V:502:ILE:HG23	1:V:503:ALA:N	1.47	1.20
4:1:59:GLU:OE2	5:2:402:ARG:NH2	1.73	1.19
2:W:209:TYR:OH	2:W:233:PHE:HA	1.38	1.19
3:0:79:ASN:O	3:0:81:LEU:N	1.74	1.19
2:W:432:ILE:CG1	2:W:434:HIS:HE1	1.56	1.18
6:3:66:GLU:HA	6:3:132:LEU:HD12	1.22	1.18
2:W:59:TYR:CZ	2:W:62:ALA:HB1	1.77	1.17
5:2:31:LEU:CD1	6:3:33:THR:CB	2.20	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:110:SER:CA	2:W:207:TYR:HE1	1.40	1.17
4:1:1:MET:CG	5:2:413:LEU:HB3	1.73	1.17
5:2:117:ASN:ND2	6:3:108:ASN:HB2	0.85	1.16
4:1:28:ALA:HB1	4:1:31:LYS:HD2	1.27	1.16
5:2:30:VAL:H	6:3:25:GLN:HB3	1.08	1.15
4:1:2:VAL:CG1	5:2:456:LYS:HG2	1.75	1.15
4:1:2:VAL:HG13	5:2:422:LEU:HD11	1.19	1.14
6:3:59:VAL:CG1	6:3:70:LEU:HB2	1.78	1.14
5:2:211:GLN:HG3	5:2:257:SER:HB3	1.29	1.13
4:1:5:LEU:CD2	5:2:408:LEU:HD13	1.79	1.12
3:0:54:ARG:CG	6:3:182:PHE:CE1	2.17	1.12
1:V:523:VAL:HG11	4:1:20:LEU:HD23	1.29	1.12
2:W:421:PHE:CB	2:W:431:PRO:HD3	1.74	1.12
2:W:59:TYR:CE2	2:W:62:ALA:CB	2.32	1.12
3:0:77:LYS:HB3	3:0:83:CYS:HB2	1.13	1.12
4:1:9:LEU:HD13	4:1:48:GLU:HA	1.32	1.11
5:2:30:VAL:CG2	6:3:25:GLN:HB3	1.81	1.11
5:2:30:VAL:HG23	6:3:25:GLN:HB2	1.24	1.11
5:2:30:VAL:HG23	6:3:25:GLN:HB3	1.23	1.11
1:V:315:VAL:CG1	2:W:500:ASP:CB	1.94	1.11
5:2:160:LEU:HD23	5:2:206:LEU:HD21	1.25	1.11
5:2:42:LEU:HD21	5:2:55:TRP:HB2	1.20	1.11
5:2:171:VAL:HG22	5:2:213:TRP:HA	1.27	1.10
4:1:2:VAL:HG11	5:2:456:LYS:CG	1.81	1.10
3:0:77:LYS:CG	3:0:83:CYS:CB	2.22	1.10
1:V:516:PRO:CG	1:V:706:LYS:HZ3	1.64	1.09
5:2:30:VAL:H	6:3:25:GLN:CB	1.65	1.09
5:2:31:LEU:HD11	6:3:33:THR:HB	1.14	1.09
1:V:516:PRO:HG2	1:V:706:LYS:HZ3	1.12	1.09
5:2:192:GLU:HG3	5:2:193:PRO:HD2	1.33	1.09
4:1:5:LEU:HD21	5:2:408:LEU:CD1	1.81	1.09
6:3:49:LEU:HB3	6:3:101:TYR:HB3	1.14	1.09
5:2:29:GLY:N	6:3:25:GLN:CG	2.15	1.08
1:V:415:HIS:CD2	1:V:416:THR:HG23	1.87	1.08
4:1:5:LEU:HD11	5:2:408:LEU:HB3	1.15	1.08
6:3:137:LEU:HB3	6:3:180:VAL:HG11	1.34	1.08
4:1:1:MET:CB	5:2:413:LEU:HB3	1.83	1.08
6:3:59:VAL:HG12	6:3:71:TYR:CE1	1.89	1.08
5:2:31:LEU:HD11	6:3:33:THR:HG22	1.30	1.08
5:2:29:GLY:CA	6:3:25:GLN:HG3	1.83	1.08
5:2:159:VAL:HG13	5:2:161:HIS:H	1.16	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:516:PRO:HG2	1:V:706:LYS:NZ	1.69	1.08
5:2:30:VAL:CG2	6:3:25:GLN:CB	2.32	1.07
1:V:611:GLY:HA2	1:V:615:PHE:HD2	1.18	1.07
4:1:2:VAL:HG11	5:2:456:LYS:HG2	1.08	1.07
1:V:611:GLY:HA2	1:V:615:PHE:CD2	1.90	1.07
1:V:674:THR:HG23	5:2:392:ARG:CZ	1.83	1.07
1:V:523:VAL:CG1	4:1:20:LEU:CD2	2.31	1.06
2:W:169:PRO:CB	2:W:175:TYR:OH	2.02	1.06
2:W:432:ILE:HG12	2:W:434:HIS:HE1	1.03	1.06
3:0:54:ARG:HB2	6:3:209:ILE:HG23	1.36	1.06
1:V:516:PRO:CG	1:V:706:LYS:NZ	2.18	1.06
4:1:5:LEU:HD12	5:2:409:TYR:O	1.55	1.06
2:W:110:SER:C	2:W:207:TYR:OH	1.94	1.06
2:W:421:PHE:CB	2:W:431:PRO:CD	2.19	1.05
4:1:18:GLN:HB2	4:1:44:PHE:CE2	1.90	1.05
1:V:628:SER:O	1:V:629:HIS:O	1.71	1.05
2:W:70:LEU:HD21	2:W:72:TYR:CE1	1.92	1.05
1:V:321:GLU:OE2	2:W:500:ASP:CB	2.03	1.05
2:W:169:PRO:C	2:W:175:TYR:OH	1.95	1.04
2:W:72:TYR:CD2	2:W:232:VAL:CG1	2.41	1.04
3:0:77:LYS:CG	3:0:83:CYS:SG	2.46	1.04
1:V:426:VAL:O	1:V:427:MET:O	1.76	1.04
5:2:234:LEU:HD21	5:2:237:LEU:HD12	1.36	1.03
5:2:81:LYS:HE3	5:2:93:LEU:HD21	1.40	1.03
4:1:4:VAL:HG12	5:2:411:GLN:O	1.56	1.02
3:0:54:ARG:NE	6:3:182:PHE:CE1	2.26	1.02
3:0:77:LYS:HB2	3:0:83:CYS:HB3	1.37	1.02
4:1:34:ILE:HG12	4:1:50:VAL:HG11	1.39	1.02
3:0:54:ARG:CD	6:3:182:PHE:HE1	1.72	1.02
3:0:98:GLN:OE1	6:3:209:ILE:HA	1.58	1.02
3:0:74:GLN:HA	3:0:78:PRO:O	0.85	1.01
6:3:33:THR:HG23	6:3:36:LYS:H	1.22	1.01
6:3:196:LEU:HD21	6:3:223:LEU:HD23	1.42	1.01
5:2:199:ALA:HB3	5:2:202:GLN:HE22	1.22	1.01
1:V:515:SER:HB3	1:V:539:ASN:HD21	1.26	1.01
2:W:59:TYR:CE2	2:W:62:ALA:HB3	1.95	1.01
1:V:519:TYR:HB3	4:1:16:MET:O	1.62	1.00
2:W:70:LEU:CD2	2:W:72:TYR:HE1	1.73	1.00
2:W:110:SER:HA	2:W:207:TYR:CZ	1.97	1.00
1:V:315:VAL:HG11	2:W:500:ASP:HB2	1.42	1.00
2:W:209:TYR:OH	2:W:233:PHE:CA	2.09	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:2:31:LEU:CD2	6:3:33:THR:N	2.24	0.99
3:0:77:LYS:CD	3:0:225:GLU:OE2	2.09	0.99
1:V:366:ASN:HD21	1:V:613:THR:HG22	1.24	0.99
1:V:523:VAL:HG11	4:1:20:LEU:HD21	0.99	0.99
1:V:523:VAL:CG1	4:1:20:LEU:HD21	1.92	0.98
6:3:59:VAL:CG1	6:3:71:TYR:CE1	2.46	0.98
5:2:117:ASN:CG	6:3:108:ASN:CB	2.20	0.98
6:3:148:ASN:HB2	6:3:157:MET:HE2	1.44	0.98
5:2:196:ILE:HD11	5:2:210:ALA:HB2	1.45	0.98
4:1:1:MET:HB3	5:2:413:LEU:CG	1.94	0.98
5:2:118:LEU:CD2	6:3:39:ASP:O	2.12	0.98
6:3:173:GLN:HA	6:3:176:ASN:HD21	1.28	0.97
2:W:584:TYR:CD1	2:W:594:ALA:HB2	1.99	0.97
6:3:165:LYS:HD2	6:3:195:VAL:HG22	1.44	0.97
5:2:176:ALA:HB1	5:2:178:LEU:HD13	1.47	0.97
2:W:421:PHE:CB	2:W:431:PRO:N	2.28	0.97
5:2:100:LEU:HD11	5:2:119:ARG:HG3	1.46	0.96
6:3:133:LEU:HD23	6:3:177:PHE:CD1	2.01	0.96
2:W:110:SER:CA	2:W:207:TYR:CZ	2.49	0.96
4:1:18:GLN:CB	4:1:44:PHE:HE2	1.78	0.96
5:2:30:VAL:CB	6:3:25:GLN:HB3	1.95	0.95
4:1:2:VAL:CG1	5:2:422:LEU:HD11	1.96	0.95
5:2:117:ASN:ND2	6:3:42:MET:HE1	1.81	0.95
5:2:211:GLN:HA	5:2:261:PHE:CZ	2.02	0.95
2:W:59:TYR:CE1	2:W:62:ALA:HB1	2.02	0.95
3:0:77:LYS:HG2	3:0:83:CYS:CB	1.89	0.95
2:W:170:LEU:CD1	2:W:175:TYR:CZ	2.50	0.95
5:2:30:VAL:N	6:3:25:GLN:HB3	1.79	0.95
5:2:118:LEU:HD11	6:3:43:VAL:CG2	1.94	0.95
5:2:117:ASN:N	6:3:104:LEU:HD21	1.83	0.94
5:2:28:PRO:CD	6:3:25:GLN:HA	1.97	0.94
2:W:170:LEU:HD12	2:W:175:TYR:OH	1.65	0.94
2:W:209:TYR:HH	2:W:233:PHE:HA	1.32	0.94
2:W:72:TYR:CE2	2:W:232:VAL:CG1	2.49	0.94
2:W:110:SER:N	2:W:207:TYR:CE1	2.33	0.94
5:2:35:TYR:CE1	5:2:62:LEU:HG	2.02	0.94
1:V:523:VAL:CG1	4:1:20:LEU:HD23	1.93	0.94
1:V:515:SER:CB	1:V:539:ASN:HD21	1.80	0.94
2:W:70:LEU:HD21	2:W:72:TYR:HE1	1.30	0.94
4:1:9:LEU:HD22	4:1:51:ASN:HD22	1.34	0.93
6:3:187:GLN:HG3	6:3:189:ILE:HG12	1.51	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:2:177:GLN:HA	5:2:220:LEU:CD2	1.99	0.93
5:2:118:LEU:HD23	6:3:42:MET:HB2	1.50	0.93
6:3:190:LEU:HA	6:3:210:THR:HG22	1.50	0.93
4:1:1:MET:HB3	5:2:413:LEU:HB3	1.50	0.92
6:3:133:LEU:H	6:3:133:LEU:HD13	1.33	0.92
2:W:696:TRP:CD1	2:W:697:ILE:HG12	2.04	0.92
6:3:11:LEU:HD22	6:3:160:ARG:HG2	1.52	0.92
1:V:516:PRO:HB2	1:V:706:LYS:HZ1	1.33	0.92
6:3:165:LYS:HE3	6:3:200:SER:CB	2.00	0.92
2:W:72:TYR:CD2	2:W:232:VAL:HG13	2.04	0.92
5:2:29:GLY:H	6:3:25:GLN:HG3	1.15	0.91
6:3:59:VAL:HB	6:3:71:TYR:HE1	1.31	0.91
4:1:8:VAL:HG11	4:1:45:VAL:CG1	1.99	0.91
5:2:31:LEU:CD1	6:3:33:THR:HG22	1.87	0.91
1:V:516:PRO:CB	1:V:706:LYS:HZ1	1.83	0.91
5:2:81:LYS:CE	5:2:93:LEU:HD21	2.00	0.91
2:W:170:LEU:N	2:W:175:TYR:OH	2.01	0.91
6:3:137:LEU:CB	6:3:180:VAL:HG11	2.01	0.91
1:V:612:ASP:OD2	1:V:635:GLN:OE1	1.89	0.91
2:W:109:LEU:HG	2:W:207:TYR:CE2	2.06	0.90
3:0:54:ARG:HG3	6:3:182:PHE:CZ	2.05	0.90
4:1:2:VAL:HG13	5:2:422:LEU:CD1	2.01	0.90
5:2:159:VAL:HG22	5:2:160:LEU:HD12	1.51	0.90
2:W:59:TYR:CE1	2:W:62:ALA:CB	2.53	0.90
5:2:81:LYS:HD2	5:2:89:LEU:HD21	1.52	0.90
2:W:430:ASN:HB3	2:W:431:PRO:HD2	1.54	0.90
5:2:29:GLY:H	6:3:25:GLN:CG	1.81	0.90
2:W:169:PRO:HB2	2:W:175:TYR:HH	1.18	0.90
4:1:1:MET:HB3	5:2:413:LEU:CB	2.01	0.89
1:V:315:VAL:HG13	2:W:500:ASP:CA	2.03	0.89
6:3:165:LYS:HG3	6:3:203:LEU:HD12	1.52	0.89
4:1:47:ALA:CB	4:1:50:VAL:HB	2.03	0.89
3:0:77:LYS:HA	3:0:77:LYS:CE	2.00	0.89
4:1:8:VAL:HG11	4:1:45:VAL:HG13	1.55	0.89
4:1:4:VAL:HG11	5:2:412:PHE:HD2	1.36	0.89
5:2:160:LEU:HB3	5:2:206:LEU:HD11	1.52	0.89
1:V:629:HIS:O	1:V:633:ARG:NH2	2.06	0.89
5:2:30:VAL:H	6:3:25:GLN:CG	1.85	0.88
6:3:177:PHE:CE2	6:3:181:ILE:HD11	2.08	0.88
1:V:504:LYS:HD2	1:V:654:GLU:O	1.74	0.88
4:1:1:MET:O	5:2:413:LEU:CG	2.19	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:2:160:LEU:CA	5:2:206:LEU:HD11	2.04	0.88
5:2:243:SER:CB	5:2:258:LEU:HD22	2.04	0.88
6:3:59:VAL:CG1	6:3:70:LEU:CB	2.46	0.88
5:2:117:ASN:CB	6:3:42:MET:CE	2.51	0.88
5:2:163:MET:SD	5:2:196:ILE:HG21	2.14	0.88
5:2:118:LEU:HD11	6:3:43:VAL:HG22	1.56	0.88
6:3:177:PHE:CD2	6:3:181:ILE:HD11	2.08	0.87
2:W:37:HIS:CE1	2:W:454:VAL:HG13	2.08	0.87
5:2:45:PHE:HB2	5:2:51:LEU:HD13	1.56	0.87
3:0:74:GLN:HA	3:0:78:PRO:C	1.93	0.87
4:1:28:ALA:CB	4:1:31:LYS:HD2	2.04	0.87
5:2:218:GLN:HB3	5:2:264:HIS:CD2	2.08	0.87
5:2:160:LEU:CB	5:2:206:LEU:HD11	2.04	0.87
5:2:160:LEU:CD2	5:2:206:LEU:HD21	2.04	0.87
2:W:584:TYR:CE2	2:W:614:TYR:HB2	2.10	0.87
5:2:117:ASN:OD1	6:3:108:ASN:CB	2.23	0.87
6:3:165:LYS:HE3	6:3:200:SER:HB2	1.56	0.87
2:W:696:TRP:CD1	2:W:697:ILE:CG1	2.58	0.87
5:2:118:LEU:HD22	6:3:39:ASP:CG	1.93	0.87
6:3:14:VAL:HG21	6:3:163:VAL:HG22	1.57	0.86
6:3:64:ILE:HG13	6:3:123:ASP:HB3	1.57	0.86
2:W:59:TYR:CG	2:W:62:ALA:HB2	2.10	0.86
5:2:138:PRO:HG3	5:2:189:GLU:HG3	1.57	0.86
5:2:48:LEU:HB3	5:2:49:PRO:HD3	1.57	0.86
6:3:59:VAL:CG1	6:3:71:TYR:HD1	1.71	0.86
5:2:218:GLN:HB3	5:2:264:HIS:HD2	1.38	0.86
3:0:77:LYS:HG2	3:0:83:CYS:HG	1.40	0.86
5:2:224:GLN:HB2	5:2:268:PHE:CZ	2.10	0.86
5:2:171:VAL:HG22	5:2:213:TRP:CA	2.06	0.86
5:2:81:LYS:CD	5:2:89:LEU:HD21	2.06	0.85
6:3:100:LYS:HB3	6:3:103:LEU:HD13	1.58	0.85
5:2:211:GLN:HG3	5:2:257:SER:CB	2.05	0.85
6:3:160:ARG:HB3	6:3:190:LEU:HD21	1.57	0.85
5:2:118:LEU:CD2	6:3:42:MET:HB2	2.06	0.85
4:1:2:VAL:CG1	5:2:422:LEU:CD1	2.54	0.85
5:2:30:VAL:CG2	6:3:25:GLN:HB2	2.01	0.85
2:W:59:TYR:CD2	2:W:62:ALA:HB2	2.12	0.85
5:2:81:LYS:CD	5:2:93:LEU:HD21	2.07	0.85
1:V:523:VAL:HG21	4:1:20:LEU:HG	1.58	0.85
5:2:221:GLN:HG2	5:2:268:PHE:CZ	2.11	0.85
6:3:124:ILE:HD13	6:3:125:LYS:N	1.91	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:3:190:LEU:HA	6:3:210:THR:CG2	2.05	0.85
5:2:159:VAL:HG22	5:2:160:LEU:H	1.41	0.84
5:2:78:GLU:O	5:2:81:LYS:HG2	1.77	0.84
2:W:70:LEU:CD2	2:W:72:TYR:CE1	2.55	0.84
5:2:177:GLN:HA	5:2:220:LEU:HD21	1.56	0.84
6:3:57:LEU:HD23	6:3:58:ALA:N	1.92	0.84
1:V:502:ILE:HG23	1:V:503:ALA:H	0.68	0.84
6:3:49:LEU:CB	6:3:101:TYR:HB3	2.05	0.84
6:3:59:VAL:HG11	6:3:71:TYR:HD1	1.42	0.84
5:2:28:PRO:N	6:3:25:GLN:C	2.30	0.84
6:3:49:LEU:HB3	6:3:101:TYR:CB	2.05	0.84
4:1:13:ASP:CG	4:1:14:PRO:HD2	1.97	0.84
5:2:176:ALA:CB	5:2:178:LEU:HD13	2.07	0.84
4:1:18:GLN:CB	4:1:44:PHE:CE2	2.57	0.84
5:2:221:GLN:NE2	5:2:230:LEU:HB2	1.93	0.84
5:2:159:VAL:HG22	5:2:160:LEU:CD1	2.08	0.84
6:3:184:ALA:HA	6:3:187:GLN:HG2	1.57	0.84
2:W:696:TRP:NE1	2:W:697:ILE:HG12	1.92	0.84
5:2:118:LEU:CD2	6:3:39:ASP:HA	2.08	0.83
5:2:229:ASP:O	5:2:233:ILE:HG12	1.78	0.83
5:2:160:LEU:HD23	5:2:206:LEU:CD2	2.07	0.83
1:V:674:THR:CG2	5:2:392:ARG:CZ	2.55	0.83
5:2:118:LEU:HD12	5:2:119:ARG:N	1.92	0.83
5:2:57:MET:HA	5:2:60:LEU:CD1	2.09	0.83
6:3:59:VAL:HG13	6:3:70:LEU:HB2	0.85	0.83
5:2:167:PRO:O	5:2:171:VAL:HG23	1.76	0.83
3:0:97:ASP:O	3:0:100:PRO:HD3	1.78	0.83
6:3:196:LEU:HD21	6:3:223:LEU:CD2	2.09	0.83
4:1:52:VAL:HG23	4:1:53:LEU:HD12	1.60	0.83
5:2:160:LEU:O	5:2:164:VAL:HG23	1.79	0.83
4:1:1:MET:CB	5:2:413:LEU:CB	2.56	0.82
4:1:47:ALA:HB2	4:1:50:VAL:HB	1.61	0.82
5:2:259:LEU:HD12	5:2:260:ASN:N	1.94	0.82
1:V:516:PRO:CD	1:V:706:LYS:HZ3	1.92	0.82
4:1:59:GLU:OE1	5:2:402:ARG:NH1	2.11	0.82
5:2:221:GLN:OE1	5:2:224:GLN:HA	1.80	0.82
2:W:109:LEU:O	2:W:207:TYR:CD1	2.32	0.82
1:V:315:VAL:HG12	2:W:500:ASP:HB2	1.54	0.82
4:1:9:LEU:HB2	4:1:51:ASN:HD21	1.43	0.82
5:2:100:LEU:HG	5:2:119:ARG:HE	1.45	0.82
6:3:12:VAL:HG21	6:3:161:ILE:HG12	1.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1:52:VAL:CG2	4:1:53:LEU:HD12	2.09	0.82
5:2:86:SER:HB3	5:2:140:LYS:HE2	1.60	0.82
3:0:97:ASP:O	6:3:208:ASP:HB3	1.79	0.82
1:V:392:PHE:O	1:V:418:LYS:HD2	1.78	0.82
5:2:174:ASP:OD1	5:2:179:LEU:HD12	1.80	0.81
4:1:1:MET:SD	5:2:415:GLN:O	2.38	0.81
1:V:427:MET:O	1:V:432:THR:O	1.98	0.81
5:2:174:ASP:O	5:2:220:LEU:HD23	1.79	0.81
5:2:117:ASN:OD1	6:3:108:ASN:CG	2.18	0.81
5:2:175:LEU:HB3	5:2:216:MET:SD	2.20	0.81
2:W:421:PHE:HB3	2:W:430:ASN:C	2.00	0.81
6:3:12:VAL:CG2	6:3:161:ILE:HG12	2.11	0.81
1:V:415:HIS:CD2	1:V:416:THR:CG2	2.64	0.81
6:3:216:LYS:H	6:3:216:LYS:HD2	1.43	0.81
5:2:37:HIS:HB3	5:2:38:PRO:HD3	1.61	0.81
2:W:110:SER:C	2:W:207:TYR:HH	1.80	0.81
2:W:59:TYR:CD1	2:W:62:ALA:HB2	2.16	0.81
4:1:1:MET:HB3	5:2:413:LEU:HD23	1.63	0.81
4:1:50:VAL:HG12	4:1:54:GLN:HG2	1.62	0.81
4:1:34:ILE:HG22	4:1:46:ILE:HD11	1.64	0.80
4:1:9:LEU:CD1	4:1:48:GLU:HA	2.09	0.80
5:2:256:ASP:O	5:2:259:LEU:HG	1.81	0.80
2:W:169:PRO:C	2:W:175:TYR:CZ	2.50	0.80
5:2:42:LEU:HD12	5:2:59:MET:CE	2.11	0.80
6:3:121:LYS:O	6:3:124:ILE:HB	1.81	0.80
6:3:214:TYR:O	6:3:215:LEU:HD23	1.81	0.80
6:3:11:LEU:CD2	6:3:160:ARG:HG2	2.12	0.80
4:1:1:MET:HE2	5:2:440:LEU:HD13	1.63	0.80
5:2:251:VAL:HG11	5:2:254:MET:HG3	1.62	0.80
5:2:35:TYR:CD1	5:2:62:LEU:HG	2.16	0.80
4:1:1:MET:CE	5:2:440:LEU:HD13	2.12	0.80
5:2:93:LEU:HA	5:2:96:TRP:CD1	2.17	0.80
6:3:22:TRP:O	6:3:25:GLN:NE2	2.15	0.80
6:3:165:LYS:HE2	6:3:167:ALA:O	1.81	0.80
2:W:52:LEU:HD23	2:W:72:TYR:OH	1.80	0.80
2:W:432:ILE:CG1	2:W:434:HIS:CE1	2.43	0.79
5:2:224:GLN:HB2	5:2:268:PHE:CE2	2.17	0.79
3:0:96:PHE:CD2	3:0:124:PRO:HB3	2.17	0.79
1:V:674:THR:CG2	5:2:392:ARG:NH2	2.39	0.79
5:2:31:LEU:CD1	6:3:33:THR:HG21	2.10	0.79
6:3:64:ILE:HG23	6:3:128:HIS:CD2	2.17	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:2:205:LEU:O	5:2:209:PRO:HD2	1.81	0.79
6:3:14:VAL:CG2	6:3:163:VAL:HG22	2.13	0.79
5:2:42:LEU:HD12	5:2:59:MET:HE3	1.63	0.79
5:2:52:ALA:O	5:2:56:VAL:HG13	1.81	0.79
6:3:222:SER:O	6:3:225:GLN:HG2	1.83	0.79
2:W:170:LEU:HD12	2:W:175:TYR:CE2	2.16	0.79
1:V:520:ARG:HB2	4:1:19:PHE:HB3	1.64	0.78
4:1:1:MET:HA	5:2:414:SER:H	1.47	0.78
4:1:1:MET:HB3	5:2:413:LEU:CD2	2.12	0.78
6:3:151:VAL:HG12	6:3:155:GLN:O	1.84	0.78
6:3:59:VAL:HB	6:3:71:TYR:CE1	2.17	0.78
1:V:415:HIS:HD2	1:V:416:THR:HG23	1.45	0.78
3:0:55:LEU:HD12	6:3:178:MET:HE3	1.62	0.78
5:2:234:LEU:HD23	5:2:234:LEU:O	1.82	0.78
4:1:18:GLN:HB3	4:1:44:PHE:HE2	1.49	0.78
4:1:38:ILE:HA	4:1:44:PHE:HD1	1.48	0.78
5:2:118:LEU:CG	6:3:39:ASP:OD1	2.32	0.78
5:2:203:PHE:CD2	5:2:205:LEU:HD23	2.18	0.78
5:2:163:MET:HE2	5:2:206:LEU:HD12	1.66	0.78
5:2:181:GLN:OE1	5:2:229:ASP:HB2	1.84	0.78
4:1:34:ILE:CG2	4:1:46:ILE:HD11	2.13	0.78
5:2:34:LEU:O	5:2:38:PRO:HD2	1.84	0.78
5:2:77:LYS:HD3	5:2:78:GLU:N	1.97	0.78
5:2:159:VAL:HG13	5:2:161:HIS:N	1.96	0.78
5:2:190:PRO:O	5:2:194:PRO:HD2	1.82	0.78
5:2:207:ASP:O	5:2:211:GLN:HG2	1.84	0.78
5:2:211:GLN:CG	5:2:257:SER:HB3	2.13	0.78
3:0:54:ARG:NE	6:3:182:PHE:HE1	1.73	0.78
5:2:118:LEU:CD1	6:3:39:ASP:OD1	2.31	0.78
5:2:53:LYS:O	5:2:56:VAL:HG22	1.84	0.78
6:3:71:TYR:CD2	6:3:72:PRO:HD2	2.19	0.78
2:W:169:PRO:CA	2:W:175:TYR:OH	2.32	0.78
5:2:189:GLU:HB2	5:2:190:PRO:HD3	1.66	0.78
5:2:196:ILE:CD1	5:2:210:ALA:HB2	2.13	0.78
6:3:147:MET:O	6:3:151:VAL:HG23	1.84	0.78
6:3:185:GLN:HE21	6:3:185:GLN:HA	1.48	0.77
1:V:393:THR:HA	1:V:418:LYS:CE	2.14	0.77
5:2:221:GLN:HE22	5:2:230:LEU:HB2	1.47	0.77
5:2:163:MET:CE	5:2:206:LEU:HD12	2.14	0.77
4:1:1:MET:HG3	5:2:415:GLN:O	1.84	0.77
6:3:144:ILE:CD1	6:3:147:MET:HE3	2.14	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:3:185:GLN:NE2	6:3:210:THR:HA	2.00	0.77
4:1:38:ILE:HG22	4:1:44:PHE:CD1	2.19	0.77
5:2:208:THR:HG23	5:2:209:PRO:HD3	1.66	0.77
5:2:211:GLN:HA	5:2:261:PHE:HZ	1.49	0.77
5:2:179:LEU:HB3	5:2:184:LEU:HD11	1.65	0.76
5:2:42:LEU:HD21	5:2:55:TRP:CB	2.10	0.76
1:V:611:GLY:CA	1:V:615:PHE:HD2	1.98	0.76
5:2:117:ASN:HD21	6:3:108:ASN:HB3	1.47	0.76
5:2:44:VAL:HG13	5:2:45:PHE:CD1	2.20	0.76
6:3:190:LEU:H	6:3:190:LEU:HD23	1.51	0.76
5:2:208:THR:HG23	5:2:209:PRO:CD	2.16	0.76
6:3:172:LEU:HD13	6:3:172:LEU:O	1.85	0.76
3:0:54:ARG:HB2	6:3:209:ILE:CG2	2.14	0.76
5:2:177:GLN:CD	5:2:220:LEU:HD22	2.06	0.76
6:3:59:VAL:CB	6:3:71:TYR:CE1	2.67	0.76
2:W:144:ALA:HA	2:W:148:HIS:C	2.05	0.76
4:1:10:ILE:CG2	5:2:407:VAL:HG21	2.16	0.76
5:2:218:GLN:NE2	5:2:265:LEU:HA	2.00	0.76
6:3:14:VAL:CG2	6:3:163:VAL:HA	2.16	0.76
4:1:1:MET:SD	5:2:413:LEU:HB3	2.25	0.76
5:2:86:SER:HB3	5:2:140:LYS:CE	2.16	0.76
1:V:366:ASN:ND2	1:V:613:THR:HG22	2.00	0.75
3:0:77:LYS:HA	3:0:77:LYS:HE3	1.65	0.75
5:2:127:LYS:N	5:2:178:LEU:HD23	2.01	0.75
5:2:234:LEU:CD2	5:2:237:LEU:HD12	2.14	0.75
4:1:38:ILE:H	4:1:38:ILE:HD13	1.51	0.75
5:2:243:SER:HB3	5:2:258:LEU:HD22	1.69	0.75
6:3:11:LEU:HD22	6:3:160:ARG:CG	2.16	0.75
5:2:118:LEU:HD22	6:3:39:ASP:HA	1.65	0.75
4:1:24:ASP:OD2	4:1:57:VAL:HG11	1.85	0.75
1:V:689:VAL:HB	5:2:391:ILE:HD11	1.67	0.75
1:V:516:PRO:CB	1:V:706:LYS:NZ	2.48	0.75
6:3:8:LEU:HD23	6:3:54:SER:HB3	1.68	0.75
1:V:444:HIS:O	1:V:447:PRO:HD2	1.86	0.75
6:3:38:ILE:O	6:3:41:VAL:HG12	1.87	0.75
5:2:180:SER:O	5:2:184:LEU:HG	1.87	0.74
1:V:611:GLY:O	1:V:615:PHE:HB3	1.86	0.74
5:2:117:ASN:CG	6:3:42:MET:CE	2.55	0.74
1:V:412:MET:CA	1:V:417:THR:HG21	2.17	0.74
2:W:644:PHE:O	2:W:645:GLN:HB2	1.86	0.74
4:1:1:MET:HG2	5:2:413:LEU:HB3	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:3:133:LEU:HD23	6:3:177:PHE:HD1	1.49	0.74
5:2:100:LEU:CD1	5:2:119:ARG:HG3	2.16	0.74
2:W:608:ILE:HG23	2:W:614:TYR:CE2	2.22	0.74
5:2:196:ILE:HD11	5:2:210:ALA:CB	2.17	0.74
4:1:2:VAL:CG1	5:2:456:LYS:CG	2.53	0.74
2:W:430:ASN:HB3	2:W:431:PRO:CD	2.17	0.74
5:2:35:TYR:CD2	5:2:62:LEU:HB3	2.22	0.74
6:3:59:VAL:HG11	6:3:71:TYR:CD1	2.17	0.74
5:2:51:LEU:O	5:2:51:LEU:HD23	1.87	0.74
1:V:516:PRO:HG2	1:V:706:LYS:CE	2.17	0.74
5:2:132:ASP:O	5:2:135:GLN:HG2	1.88	0.74
5:2:160:LEU:HA	5:2:206:LEU:HD11	1.70	0.74
5:2:53:LYS:HE3	5:2:95:ILE:HD11	1.67	0.73
2:W:52:LEU:HD23	2:W:72:TYR:CE2	2.22	0.73
4:1:34:ILE:HD13	4:1:54:GLN:OE1	1.88	0.73
5:2:251:VAL:HG11	5:2:254:MET:CG	2.18	0.73
6:3:141:LEU:O	6:3:144:ILE:HG22	1.88	0.73
1:V:674:THR:OG1	5:2:392:ARG:NE	2.21	0.73
6:3:214:TYR:HE2	6:3:216:LYS:HE2	1.53	0.73
4:1:34:ILE:HG12	4:1:50:VAL:CG1	2.18	0.73
1:V:667:THR:HA	4:1:62:ASP:OD1	1.89	0.73
5:2:172:SER:HA	5:2:175:LEU:CD2	2.19	0.73
1:V:366:ASN:HD21	1:V:613:THR:CG2	1.98	0.73
5:2:243:SER:HB2	5:2:258:LEU:HD22	1.71	0.73
6:3:226:TYR:HA	6:3:230:VAL:HG23	1.71	0.73
5:2:41:CYS:O	5:2:44:VAL:HG12	1.88	0.73
2:W:73:CYS:HB2	2:W:209:TYR:CZ	2.23	0.73
4:1:9:LEU:HD22	4:1:51:ASN:ND2	2.04	0.72
5:2:237:LEU:O	5:2:240:LEU:HD13	1.88	0.72
5:2:218:GLN:HE22	5:2:265:LEU:HA	1.55	0.72
5:2:60:LEU:HD11	5:2:95:ILE:HB	1.71	0.72
6:3:12:VAL:HG23	6:3:161:ILE:HG23	1.70	0.72
2:W:59:TYR:CD2	2:W:62:ALA:CB	2.71	0.72
5:2:175:LEU:HD22	5:2:216:MET:SD	2.29	0.72
4:1:2:VAL:HG12	5:2:422:LEU:HD13	1.71	0.72
6:3:111:ILE:HG13	6:3:112:VAL:N	2.02	0.72
4:1:2:VAL:HG12	5:2:456:LYS:HE2	1.72	0.72
5:2:199:ALA:HB3	5:2:202:GLN:NE2	2.02	0.72
5:2:117:ASN:HB3	6:3:42:MET:CE	2.18	0.72
1:V:415:HIS:HD2	1:V:416:THR:CG2	1.99	0.72
1:V:394:SER:HB3	1:V:416:THR:O	1.88	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:421:PHE:HB3	2:W:431:PRO:CA	2.17	0.72
5:2:118:LEU:HD22	6:3:39:ASP:CA	2.19	0.72
5:2:31:LEU:CG	6:3:33:THR:HB	2.19	0.72
4:1:25:GLU:CD	4:1:35:ILE:HG12	2.09	0.72
6:3:148:ASN:CB	6:3:157:MET:HE2	2.20	0.72
6:3:222:SER:HB2	6:3:226:TYR:HE2	1.55	0.72
5:2:134:SER:O	5:2:138:PRO:HD2	1.89	0.72
5:2:117:ASN:HB2	6:3:104:LEU:HD11	1.71	0.72
6:3:217:VAL:HG13	6:3:226:TYR:CZ	2.24	0.72
6:3:66:GLU:CA	6:3:132:LEU:HD12	2.13	0.72
5:2:28:PRO:HD2	6:3:25:GLN:NE2	2.05	0.72
1:V:315:VAL:HG12	2:W:500:ASP:CB	2.17	0.72
5:2:192:GLU:HG3	5:2:193:PRO:CD	2.18	0.71
6:3:165:LYS:HG3	6:3:203:LEU:CD1	2.20	0.71
2:W:584:TYR:HD1	2:W:594:ALA:HB2	1.51	0.71
5:2:35:TYR:CG	5:2:62:LEU:HD12	2.25	0.71
4:1:28:ALA:HB3	4:1:31:LYS:HB2	1.71	0.71
5:2:171:VAL:HG12	5:2:216:MET:SD	2.31	0.71
3:0:98:GLN:OE1	6:3:209:ILE:CA	2.37	0.71
4:1:1:MET:C	5:2:413:LEU:HG	2.09	0.71
4:1:1:MET:HB2	5:2:418:PHE:CB	2.21	0.71
5:2:118:LEU:CD2	6:3:39:ASP:CA	2.68	0.71
1:V:502:ILE:CG2	1:V:503:ALA:N	2.17	0.71
1:V:504:LYS:HB3	1:V:654:GLU:O	1.91	0.71
1:V:516:PRO:CD	1:V:706:LYS:NZ	2.53	0.71
2:W:209:TYR:OH	2:W:234:ASP:N	2.23	0.71
3:0:77:LYS:HB2	3:0:83:CYS:HB2	0.80	0.71
1:V:523:VAL:CB	4:1:20:LEU:HD23	2.21	0.71
4:1:55:GLU:OE2	5:2:402:ARG:HG3	1.90	0.71
5:2:86:SER:CB	5:2:140:LYS:HE2	2.20	0.71
1:V:366:ASN:ND2	1:V:613:THR:CG2	2.54	0.71
2:W:170:LEU:HD12	2:W:175:TYR:HH	1.53	0.71
2:W:696:TRP:CD1	2:W:697:ILE:HG13	2.26	0.71
4:1:1:MET:HG2	5:2:413:LEU:C	2.11	0.70
4:1:29:LEU:HD23	4:1:30:GLY:N	2.06	0.70
2:W:589:GLU:O	2:W:594:ALA:HB1	1.91	0.70
6:3:177:PHE:CZ	6:3:203:LEU:HD23	2.27	0.70
5:2:31:LEU:N	6:3:25:GLN:O	2.24	0.70
1:V:515:SER:HB3	1:V:539:ASN:ND2	2.05	0.70
2:W:209:TYR:HE1	2:W:233:PHE:CD1	2.09	0.70
5:2:218:GLN:OE1	5:2:265:LEU:HA	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:3:70:LEU:O	6:3:114:GLU:HG3	1.91	0.70
1:V:393:THR:HA	1:V:418:LYS:HE3	1.74	0.70
6:3:144:ILE:HG12	6:3:147:MET:HE2	1.74	0.70
4:1:1:MET:HG3	5:2:418:PHE:HB2	1.73	0.70
4:1:8:VAL:HG11	4:1:45:VAL:HG12	1.74	0.70
6:3:133:LEU:HD22	6:3:134:ALA:H	1.56	0.70
2:W:70:LEU:HD21	2:W:72:TYR:CZ	2.27	0.70
3:0:54:ARG:NE	6:3:182:PHE:CD1	2.60	0.70
2:W:189:TRP:HE1	2:W:194:LEU:HB2	1.55	0.70
5:2:163:MET:O	5:2:167:PRO:HD2	1.91	0.69
2:W:59:TYR:CE1	2:W:62:ALA:HB2	2.27	0.69
5:2:189:GLU:HA	5:2:192:GLU:HG2	1.72	0.69
5:2:29:GLY:CA	6:3:25:GLN:CG	2.66	0.69
6:3:162:LEU:HA	6:3:192:ASP:OD1	1.92	0.69
1:V:516:PRO:HB2	1:V:706:LYS:NZ	2.07	0.69
5:2:117:ASN:CB	6:3:42:MET:HE3	2.22	0.69
5:2:118:LEU:HD11	6:3:43:VAL:HG23	1.75	0.69
5:2:185:MET:SD	5:2:232:GLU:HB2	2.32	0.69
1:V:522:TYR:HE2	4:1:62:ASP:CG	1.96	0.69
5:2:130:SER:O	5:2:133:THR:HG22	1.92	0.69
5:2:140:LYS:HD3	5:2:162:PHE:HE1	1.58	0.69
5:2:199:ALA:CB	5:2:202:GLN:HE22	2.02	0.69
5:2:163:MET:CE	5:2:206:LEU:HB3	2.23	0.69
5:2:30:VAL:N	6:3:25:GLN:CG	2.55	0.69
6:3:69:PHE:CE1	6:3:139:LYS:HD2	2.27	0.69
3:0:54:ARG:CD	6:3:182:PHE:CE1	2.60	0.69
4:1:53:LEU:HD12	4:1:53:LEU:H	1.57	0.69
5:2:81:LYS:HD2	5:2:89:LEU:CD2	2.20	0.69
5:2:81:LYS:HE3	5:2:93:LEU:CD2	2.20	0.69
5:2:211:GLN:HA	5:2:261:PHE:CE1	2.28	0.68
5:2:48:LEU:CB	5:2:49:PRO:HD3	2.19	0.68
6:3:215:LEU:HD12	6:3:230:VAL:CG1	2.23	0.68
2:W:111:SER:N	2:W:207:TYR:OH	2.24	0.68
2:W:110:SER:C	2:W:207:TYR:CZ	2.66	0.68
6:3:34:LEU:HD13	6:3:34:LEU:O	1.92	0.68
5:2:251:VAL:HG12	5:2:254:MET:H	1.58	0.68
6:3:114:GLU:O	6:3:118:LEU:HD23	1.92	0.68
5:2:176:ALA:HB1	5:2:178:LEU:CD1	2.23	0.68
4:1:1:MET:CG	5:2:415:GLN:O	2.42	0.68
6:3:70:LEU:HD11	6:3:115:ILE:HD11	1.74	0.68
5:2:170:ALA:HB1	5:2:213:TRP:CZ3	2.29	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1:4:VAL:CG1	5:2:411:GLN:O	2.40	0.67
4:1:1:MET:SD	5:2:419:GLU:HB2	2.34	0.67
4:1:39:ASP:OD1	4:1:43:VAL:HB	1.94	0.67
6:3:187:GLN:HG3	6:3:189:ILE:CG1	2.24	0.67
5:2:172:SER:O	5:2:175:LEU:HD23	1.95	0.67
5:2:211:GLN:HB3	5:2:261:PHE:HE1	1.60	0.67
6:3:159:SER:OG	6:3:189:ILE:HD12	1.93	0.67
5:2:118:LEU:HD13	6:3:39:ASP:OD1	1.92	0.67
6:3:130:GLU:HB2	6:3:173:GLN:NE2	2.09	0.67
6:3:178:MET:HE2	6:3:202:LEU:CD1	2.24	0.67
6:3:187:GLN:CG	6:3:189:ILE:HG12	2.24	0.67
1:V:519:TYR:CB	4:1:16:MET:HG3	2.25	0.67
5:2:56:VAL:O	5:2:60:LEU:HG	1.94	0.67
6:3:111:ILE:O	6:3:115:ILE:HD13	1.94	0.67
6:3:217:VAL:HG13	6:3:226:TYR:CE2	2.30	0.67
5:2:117:ASN:HD21	6:3:108:ASN:CA	2.04	0.67
2:W:52:LEU:HD23	2:W:72:TYR:CZ	2.29	0.67
5:2:56:VAL:HG11	5:2:91:SER:HB2	1.77	0.66
1:V:520:ARG:HB2	4:1:19:PHE:CB	2.25	0.66
2:W:73:CYS:C	2:W:209:TYR:CE2	2.68	0.66
5:2:160:LEU:H	5:2:160:LEU:HD12	1.60	0.66
4:1:10:ILE:HG21	5:2:407:VAL:HG21	1.77	0.66
4:1:59:GLU:OE2	5:2:402:ARG:CZ	2.42	0.66
5:2:218:GLN:CG	5:2:268:PHE:HB3	2.26	0.66
6:3:18:ASN:CG	6:3:20:ILE:HD13	2.15	0.66
6:3:207:CYS:SG	6:3:214:TYR:HB2	2.34	0.66
6:3:146:ARG:O	6:3:149:LYS:HG2	1.95	0.66
6:3:45:GLY:O	6:3:49:LEU:HD23	1.96	0.66
2:W:432:ILE:CD1	2:W:434:HIS:HE1	2.07	0.66
4:1:8:VAL:HG12	4:1:9:LEU:N	2.10	0.66
1:V:412:MET:HA	1:V:417:THR:HG21	1.77	0.66
5:2:126:GLY:C	5:2:178:LEU:HD23	2.16	0.66
6:3:144:ILE:O	6:3:147:MET:HG3	1.96	0.66
3:0:73:ASP:O	3:0:79:ASN:HA	1.95	0.66
5:2:117:ASN:HB3	6:3:42:MET:HE3	1.76	0.66
4:1:35:ILE:HG22	4:1:46:ILE:HD12	1.78	0.66
6:3:70:LEU:CD1	6:3:115:ILE:HD11	2.26	0.66
5:2:171:VAL:HG13	5:2:216:MET:CB	2.26	0.66
1:V:516:PRO:HD2	1:V:706:LYS:HZ3	1.60	0.66
5:2:218:GLN:CD	5:2:265:LEU:HA	2.16	0.65
5:2:270:LEU:HD23	5:2:270:LEU:O	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:2:270:LEU:HD23	5:2:273:GLN:HE21	1.62	0.65
6:3:33:THR:HG22	6:3:36:LYS:HB2	1.76	0.65
2:W:109:LEU:C	2:W:207:TYR:CD1	2.70	0.65
6:3:137:LEU:HB3	6:3:180:VAL:CG1	2.20	0.65
5:2:236:PHE:CZ	5:2:262:LEU:HD22	2.32	0.65
4:1:34:ILE:CG1	4:1:50:VAL:HG11	2.21	0.65
6:3:106:SER:O	6:3:110:VAL:HG23	1.97	0.65
1:V:523:VAL:HG21	4:1:20:LEU:CG	2.25	0.65
5:2:189:GLU:HA	5:2:192:GLU:CG	2.26	0.65
1:V:316:LEU:HB2	1:V:321:GLU:HG3	1.78	0.65
6:3:184:ALA:CA	6:3:187:GLN:HG2	2.25	0.65
5:2:57:MET:HA	5:2:60:LEU:HD11	1.76	0.65
1:V:503:ALA:HB2	1:V:646:ALA:N	2.11	0.65
5:2:45:PHE:HB2	5:2:51:LEU:CD1	2.26	0.65
5:2:118:LEU:HD21	6:3:39:ASP:C	2.12	0.64
6:3:178:MET:HE2	6:3:202:LEU:HD12	1.79	0.64
6:3:17:ALA:CB	6:3:63:HIS:HD2	2.10	0.64
1:V:519:TYR:CD2	4:1:20:LEU:HB2	2.32	0.64
5:2:198:SER:HG	5:2:238:PHE:HE2	1.45	0.64
6:3:130:GLU:HB2	6:3:173:GLN:HE22	1.61	0.64
5:2:266:ARG:O	5:2:270:LEU:HB2	1.97	0.64
6:3:149:LYS:HG3	6:3:150:GLU:N	2.12	0.64
4:1:35:ILE:HG22	4:1:46:ILE:CD1	2.27	0.64
5:2:211:GLN:CB	5:2:261:PHE:HE1	2.11	0.64
6:3:192:ASP:HB2	6:3:231:PHE:CE1	2.32	0.64
1:V:517:GLU:HB2	1:V:713:LEU:HD22	1.79	0.64
5:2:42:LEU:CD2	5:2:55:TRP:HB2	2.13	0.64
1:V:426:VAL:HG13	1:V:427:MET:H	1.62	0.64
5:2:202:GLN:H	5:2:202:GLN:HE21	1.44	0.64
2:W:170:LEU:CD1	2:W:175:TYR:CE2	2.79	0.64
2:W:581:LEU:HD21	2:W:608:ILE:HG21	1.78	0.64
5:2:159:VAL:HG11	5:2:161:HIS:HD2	1.62	0.64
5:2:160:LEU:HB3	5:2:206:LEU:CD1	2.27	0.64
5:2:181:GLN:HG3	5:2:229:ASP:CG	2.18	0.64
6:3:14:VAL:HG22	6:3:163:VAL:HA	1.78	0.64
6:3:64:ILE:HB	6:3:123:ASP:OD2	1.98	0.64
1:V:612:ASP:CG	1:V:635:GLN:CD	2.57	0.64
2:W:59:TYR:CZ	2:W:62:ALA:HB2	2.29	0.64
4:1:10:ILE:HG22	5:2:407:VAL:HG21	1.80	0.64
5:2:220:LEU:HD13	5:2:220:LEU:O	1.98	0.64
4:1:1:MET:HA	5:2:413:LEU:HA	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:3:69:PHE:CZ	6:3:139:LYS:HB3	2.33	0.64
2:W:696:TRP:HD1	2:W:697:ILE:HG13	1.63	0.64
4:1:38:ILE:HB	4:1:44:PHE:HE1	1.63	0.63
5:2:117:ASN:ND2	6:3:108:ASN:CA	2.57	0.63
2:W:584:TYR:CZ	2:W:614:TYR:HB2	2.32	0.63
5:2:177:GLN:OE1	5:2:220:LEU:HD22	1.98	0.63
6:3:17:ALA:HB1	6:3:63:HIS:HD2	1.63	0.63
6:3:33:THR:HG23	6:3:36:LYS:N	2.06	0.63
6:3:18:ASN:CG	6:3:64:ILE:HD11	2.19	0.63
1:V:393:THR:HA	1:V:418:LYS:CD	2.28	0.63
3:0:72:GLU:HA	3:0:79:ASN:HB2	1.81	0.63
5:2:35:TYR:CZ	5:2:62:LEU:HG	2.34	0.63
5:2:44:VAL:HG13	5:2:45:PHE:HD1	1.59	0.63
6:3:64:ILE:CG1	6:3:123:ASP:HB3	2.29	0.63
6:3:160:ARG:NH2	6:3:190:LEU:HD12	2.13	0.63
4:1:35:ILE:HA	4:1:46:ILE:HG13	1.80	0.63
5:2:60:LEU:HD11	5:2:95:ILE:CB	2.29	0.63
6:3:131:THR:O	6:3:133:LEU:HD13	1.97	0.63
5:2:100:LEU:HG	5:2:119:ARG:NE	2.13	0.63
5:2:140:LYS:HG2	5:2:162:PHE:CE1	2.33	0.63
5:2:28:PRO:HA	6:3:33:THR:HB	1.80	0.63
6:3:214:TYR:CE2	6:3:216:LYS:HE2	2.32	0.63
5:2:123:LEU:HD23	5:2:123:LEU:O	1.98	0.63
2:W:432:ILE:CD1	2:W:434:HIS:CE1	2.80	0.63
5:2:163:MET:HE1	5:2:206:LEU:HB3	1.81	0.63
5:2:258:LEU:HG	5:2:262:LEU:CD2	2.28	0.63
6:3:134:ALA:HB2	6:3:176:ASN:OD1	1.99	0.63
4:1:2:VAL:HG12	5:2:422:LEU:CD1	2.27	0.62
5:2:89:LEU:HD23	5:2:89:LEU:O	1.99	0.62
5:2:173:GLN:HG2	5:2:179:LEU:HG	1.81	0.62
5:2:93:LEU:HA	5:2:96:TRP:HD1	1.64	0.62
5:2:30:VAL:CA	6:3:25:GLN:HB3	2.28	0.62
4:1:38:ILE:HB	4:1:44:PHE:CE1	2.34	0.62
1:V:667:THR:HA	4:1:62:ASP:CG	2.19	0.62
5:2:181:GLN:CD	5:2:229:ASP:HB2	2.20	0.62
5:2:218:GLN:HG2	5:2:268:PHE:HB3	1.82	0.62
4:1:5:LEU:HD21	5:2:408:LEU:HD13	0.85	0.62
2:W:584:TYR:CG	2:W:594:ALA:HB2	2.34	0.62
5:2:189:GLU:O	5:2:193:PRO:HD2	2.00	0.62
4:1:50:VAL:HA	4:1:53:LEU:HD13	1.82	0.62
6:3:165:LYS:HD3	6:3:165:LYS:O	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:3:184:ALA:HA	6:3:187:GLN:CG	2.28	0.62
6:3:9:ASN:O	6:3:56:LYS:HD3	1.99	0.62
2:W:37:HIS:CE1	2:W:454:VAL:CG1	2.82	0.62
3:0:98:GLN:OE1	6:3:209:ILE:HG23	1.98	0.62
4:1:47:ALA:HB1	4:1:50:VAL:HB	1.81	0.61
1:V:612:ASP:CG	1:V:635:GLN:OE1	2.38	0.61
4:1:8:VAL:O	5:2:407:VAL:HG12	2.00	0.61
5:2:60:LEU:CD1	5:2:95:ILE:HB	2.31	0.61
6:3:133:LEU:HD22	6:3:134:ALA:N	2.14	0.61
6:3:18:ASN:O	6:3:21:TRP:HD1	1.83	0.61
6:3:190:LEU:H	6:3:190:LEU:CD2	2.11	0.61
5:2:46:ARG:CD	5:2:85:GLU:HB2	2.30	0.61
4:1:1:MET:HG2	5:2:414:SER:N	2.16	0.61
5:2:117:ASN:HD22	6:3:42:MET:HE1	1.60	0.61
5:2:203:PHE:HD2	5:2:205:LEU:HD23	1.64	0.61
1:V:520:ARG:HG3	4:1:23:LEU:HD11	1.82	0.61
4:1:1:MET:HB3	5:2:413:LEU:HG	1.81	0.61
5:2:251:VAL:CG1	5:2:254:MET:HG3	2.30	0.61
6:3:100:LYS:HG3	6:3:101:TYR:N	2.16	0.61
5:2:236:PHE:CE2	5:2:262:LEU:HD13	2.36	0.61
5:2:31:LEU:HD13	6:3:33:THR:HG22	1.76	0.61
2:W:584:TYR:HB2	2:W:594:ALA:HB2	1.82	0.61
3:0:77:LYS:HB2	3:0:83:CYS:SG	2.40	0.61
6:3:8:LEU:HA	6:3:54:SER:HB3	1.83	0.61
4:1:9:LEU:CB	4:1:51:ASN:HD21	2.14	0.61
5:2:117:ASN:ND2	6:3:42:MET:CE	2.60	0.61
1:V:368:ALA:O	1:V:371:VAL:HG22	2.00	0.61
4:1:1:MET:HA	5:2:414:SER:N	2.14	0.60
2:W:59:TYR:OH	2:W:63:TYR:CE2	2.53	0.60
5:2:30:VAL:HG12	5:2:34:LEU:HD23	1.82	0.60
6:3:143:TYR:O	6:3:146:ARG:HG2	2.01	0.60
6:3:33:THR:CG2	6:3:36:LYS:HB2	2.30	0.60
5:2:173:GLN:CD	5:2:179:LEU:HD21	2.22	0.60
1:V:520:ARG:CB	4:1:19:PHE:HB3	2.31	0.60
5:2:83:GLN:OE1	5:2:83:GLN:HA	2.01	0.60
6:3:222:SER:HB2	6:3:226:TYR:CE2	2.37	0.60
6:3:69:PHE:CZ	6:3:139:LYS:HD2	2.37	0.60
5:2:159:VAL:HG13	5:2:160:LEU:N	2.17	0.60
5:2:29:GLY:H	6:3:25:GLN:CD	2.04	0.60
5:2:164:VAL:HG13	5:2:209:PRO:HG2	1.83	0.59
6:3:14:VAL:HG23	6:3:163:VAL:HA	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:2:196:ILE:HA	5:2:202:GLN:OE1	2.02	0.59
6:3:173:GLN:CA	6:3:176:ASN:HD21	2.10	0.59
6:3:213:LEU:HD23	6:3:230:VAL:HG12	1.84	0.59
6:3:59:VAL:CG1	6:3:70:LEU:HB3	2.32	0.59
5:2:206:LEU:HD22	5:2:206:LEU:N	2.17	0.59
5:2:56:VAL:HG11	5:2:91:SER:CB	2.32	0.59
6:3:110:VAL:O	6:3:114:GLU:HG2	2.02	0.59
5:2:171:VAL:HG13	5:2:216:MET:HB2	1.83	0.59
3:0:55:LEU:HD12	6:3:178:MET:CE	2.31	0.59
3:0:98:GLN:CD	6:3:209:ILE:HA	2.21	0.59
1:V:519:TYR:CE2	4:1:20:LEU:HG	2.37	0.59
4:1:53:LEU:HD12	4:1:53:LEU:N	2.18	0.59
6:3:196:LEU:CD2	6:3:223:LEU:HD23	2.25	0.59
2:W:584:TYR:HB2	2:W:594:ALA:CB	2.32	0.59
5:2:31:LEU:HG	6:3:25:GLN:O	2.01	0.59
2:W:37:HIS:ND1	2:W:454:VAL:HG13	2.15	0.59
5:2:202:GLN:H	5:2:202:GLN:NE2	2.00	0.59
6:3:160:ARG:HB3	6:3:190:LEU:CD2	2.32	0.59
5:2:30:VAL:HB	6:3:25:GLN:HB3	1.84	0.59
2:W:73:CYS:CB	2:W:209:TYR:CZ	2.85	0.59
4:1:34:ILE:O	4:1:46:ILE:HG13	2.03	0.59
5:2:203:PHE:CE2	5:2:205:LEU:HD23	2.38	0.59
4:1:2:VAL:CG1	5:2:456:LYS:CD	2.81	0.59
5:2:160:LEU:HD12	5:2:160:LEU:N	2.18	0.59
5:2:44:VAL:HG13	5:2:45:PHE:N	2.17	0.59
6:3:215:LEU:CD1	6:3:230:VAL:HG13	2.32	0.59
1:V:519:TYR:HB2	4:1:16:MET:CG	2.32	0.59
5:2:215:PHE:CD2	5:2:264:HIS:HB2	2.38	0.58
6:3:131:THR:HG23	6:3:133:LEU:CD1	2.33	0.58
4:1:38:ILE:CD1	4:1:38:ILE:H	2.16	0.58
5:2:217:LEU:HD23	5:2:233:ILE:CD1	2.33	0.58
2:W:70:LEU:CG	2:W:72:TYR:CE1	2.86	0.58
5:2:177:GLN:HE22	5:2:220:LEU:HA	1.68	0.58
6:3:190:LEU:HD23	6:3:190:LEU:N	2.18	0.58
6:3:24:LYS:HE2	6:3:220:MET:SD	2.42	0.58
3:0:72:GLU:O	3:0:72:GLU:HG2	2.02	0.58
4:1:2:VAL:HB	5:2:456:LYS:HD3	1.86	0.58
6:3:131:THR:CG2	6:3:133:LEU:HD12	2.33	0.58
6:3:169:ASP:CB	6:3:202:LEU:HD23	2.33	0.58
6:3:21:TRP:CD2	6:3:34:LEU:HD23	2.39	0.58
4:1:13:ASP:OD2	4:1:17:LYS:HB3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1:34:ILE:HG22	4:1:46:ILE:CD1	2.32	0.58
4:1:4:VAL:HG11	5:2:412:PHE:CD2	2.28	0.58
5:2:35:TYR:CB	5:2:62:LEU:HD12	2.33	0.58
2:W:209:TYR:CE1	2:W:233:PHE:CD1	2.90	0.58
4:1:1:MET:HB2	5:2:418:PHE:HB3	1.84	0.58
5:2:28:PRO:CA	6:3:25:GLN:C	2.71	0.58
5:2:117:ASN:CG	6:3:108:ASN:ND2	2.50	0.58
5:2:236:PHE:CZ	5:2:258:LEU:HD11	2.39	0.58
2:W:645:GLN:O	2:W:647:ARG:HD2	2.03	0.58
4:1:8:VAL:HG12	4:1:9:LEU:H	1.69	0.57
5:2:82:ALA:HA	5:2:89:LEU:HD11	1.85	0.57
6:3:215:LEU:HD12	6:3:230:VAL:HG13	1.85	0.57
4:1:59:GLU:CD	5:2:402:ARG:NH1	2.56	0.57
6:3:144:ILE:HG12	6:3:147:MET:CE	2.34	0.57
6:3:216:LYS:H	6:3:216:LYS:CD	2.13	0.57
5:2:117:ASN:CG	6:3:42:MET:HE1	2.21	0.57
2:W:209:TYR:OH	2:W:233:PHE:C	2.42	0.57
6:3:14:VAL:HG23	6:3:163:VAL:HG13	1.86	0.57
3:0:109:THR:HB	3:0:144:SER:H	1.67	0.57
1:V:520:ARG:HD3	4:1:19:PHE:CD1	2.40	0.57
6:3:187:GLN:NE2	6:3:189:ILE:HG13	2.20	0.57
5:2:197:THR:HG21	5:2:239:GLN:CD	2.24	0.57
6:3:16:ASP:O	6:3:21:TRP:NE1	2.28	0.57
6:3:46:ASN:CG	6:3:104:LEU:HD22	2.25	0.57
2:W:584:TYR:CB	2:W:594:ALA:HB2	2.33	0.57
5:2:185:MET:HB2	5:2:229:ASP:OD1	2.04	0.57
6:3:223:LEU:HD11	6:3:227:LEU:HD11	1.87	0.57
1:V:514:MET:SD	1:V:537:ASN:ND2	2.78	0.57
4:1:52:VAL:HG22	4:1:53:LEU:HD12	1.87	0.56
6:3:19:PRO:HG2	6:3:123:ASP:O	2.04	0.56
6:3:195:VAL:HG21	6:3:214:TYR:OH	2.05	0.56
5:2:117:ASN:HB2	6:3:104:LEU:CD1	2.35	0.56
6:3:210:THR:O	6:3:210:THR:HG22	2.04	0.56
1:V:519:TYR:HB3	4:1:16:MET:HG3	1.86	0.56
5:2:60:LEU:HD11	5:2:95:ILE:CG2	2.35	0.56
6:3:178:MET:SD	6:3:181:ILE:HD12	2.46	0.56
2:W:110:SER:N	2:W:207:TYR:CZ	2.71	0.56
4:1:18:GLN:HB2	4:1:44:PHE:CZ	2.39	0.56
5:2:117:ASN:CG	6:3:42:MET:HE2	2.25	0.56
5:2:130:SER:HB2	5:2:173:GLN:OE1	2.06	0.56
6:3:42:MET:SD	6:3:111:ILE:HD13	2.46	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:2:47:GLU:HG3	5:2:48:LEU:N	2.20	0.56
6:3:223:LEU:HD13	6:3:223:LEU:O	2.06	0.56
2:W:209:TYR:HH	2:W:233:PHE:CA	2.10	0.56
5:2:160:LEU:H	5:2:160:LEU:CD1	2.17	0.56
5:2:423:ALA:HA	5:2:426:ARG:HE	1.69	0.56
1:V:428:GLU:OE1	1:V:428:GLU:HA	2.06	0.56
4:1:31:LYS:O	4:1:32:LYS:HB2	2.06	0.56
4:1:3:ASN:CB	5:2:412:PHE:O	2.52	0.56
4:1:36:GLN:HB3	4:1:45:VAL:HG12	1.88	0.56
5:2:163:MET:HE2	5:2:206:LEU:CD1	2.35	0.56
5:2:163:MET:HE3	5:2:206:LEU:HD12	1.88	0.56
5:2:206:LEU:H	5:2:206:LEU:HD22	1.71	0.56
2:W:109:LEU:C	2:W:207:TYR:CE1	2.79	0.56
4:1:19:PHE:O	4:1:23:LEU:HG	2.06	0.55
5:2:181:GLN:HE21	5:2:181:GLN:HA	1.70	0.55
4:1:38:ILE:HA	4:1:44:PHE:CD1	2.37	0.55
3:0:54:ARG:C	6:3:209:ILE:HD11	2.25	0.55
5:2:28:PRO:HA	6:3:33:THR:CB	2.36	0.55
1:V:689:VAL:CB	5:2:391:ILE:HD11	2.36	0.55
6:3:44:LEU:HD13	6:3:44:LEU:O	2.06	0.55
4:1:10:ILE:C	4:1:10:ILE:HD13	2.26	0.55
5:2:259:LEU:C	5:2:259:LEU:HD12	2.27	0.55
1:V:516:PRO:HD2	1:V:706:LYS:NZ	2.22	0.55
4:1:34:ILE:HG23	4:1:50:VAL:HG11	1.89	0.55
4:1:52:VAL:HG23	4:1:53:LEU:N	2.21	0.55
5:2:123:LEU:HD21	5:2:178:LEU:CD1	2.37	0.55
5:2:53:LYS:CE	5:2:95:ILE:HD11	2.36	0.55
6:3:223:LEU:HD13	6:3:227:LEU:HG	1.88	0.55
5:2:123:LEU:CD2	5:2:178:LEU:HD11	2.37	0.54
5:2:177:GLN:NE2	5:2:220:LEU:HA	2.22	0.54
5:2:208:THR:O	5:2:212:LEU:HG	2.07	0.54
6:3:133:LEU:H	6:3:133:LEU:CD1	2.10	0.54
1:V:631:GLY:O	1:V:632:SER:HB2	2.06	0.54
3:0:77:LYS:HA	3:0:77:LYS:NZ	2.22	0.54
1:V:520:ARG:NE	1:V:521:GLU:OE2	2.29	0.54
1:V:519:TYR:CB	4:1:16:MET:CG	2.84	0.54
4:1:29:LEU:HD23	4:1:29:LEU:C	2.27	0.54
6:3:100:LYS:O	6:3:103:LEU:HB2	2.08	0.54
6:3:64:ILE:HG23	6:3:128:HIS:CG	2.42	0.54
2:W:70:LEU:HD21	2:W:72:TYR:OH	2.07	0.54
1:V:518:PHE:HB2	4:1:16:MET:SD	2.48	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1:13:ASP:OD2	4:1:17:LYS:CB	2.55	0.54
5:2:159:VAL:HG22	5:2:160:LEU:N	2.16	0.54
5:2:199:ALA:HB1	5:2:201:PHE:CD2	2.43	0.54
5:2:37:HIS:HB3	5:2:38:PRO:CD	2.35	0.54
6:3:147:MET:HE3	6:3:157:MET:SD	2.48	0.54
1:V:667:THR:HA	4:1:62:ASP:OD2	2.07	0.54
5:2:211:GLN:HB3	5:2:261:PHE:CE1	2.40	0.54
5:2:117:ASN:CG	6:3:108:ASN:CG	2.65	0.54
6:3:144:ILE:HD13	6:3:147:MET:HE3	1.88	0.54
2:W:416:ILE:HA	2:W:434:HIS:O	2.08	0.54
4:1:18:GLN:HA	4:1:21:LEU:HG	1.90	0.54
6:3:59:VAL:CB	6:3:71:TYR:HE1	2.01	0.54
4:1:25:GLU:HG2	4:1:32:LYS:HA	1.89	0.54
5:2:214:TYR:CD2	5:2:261:PHE:CD2	2.95	0.54
2:W:189:TRP:NE1	2:W:194:LEU:HB2	2.22	0.54
5:2:220:LEU:HD13	5:2:220:LEU:C	2.29	0.54
5:2:86:SER:O	5:2:90:LEU:HD13	2.08	0.54
6:3:169:ASP:CG	6:3:202:LEU:HD23	2.29	0.54
2:W:428:ILE:HA	2:W:430:ASN:ND2	2.23	0.54
6:3:106:SER:O	6:3:109:GLU:HG3	2.08	0.53
4:1:1:MET:HA	5:2:413:LEU:CA	2.38	0.53
5:2:159:VAL:CG1	5:2:161:HIS:H	2.06	0.53
5:2:222:THR:HG23	5:2:222:THR:O	2.07	0.53
5:2:62:LEU:HD13	5:2:62:LEU:C	2.28	0.53
3:0:54:ARG:CB	6:3:209:ILE:HG23	2.25	0.53
3:0:76:LEU:HD11	3:0:225:GLU:N	2.22	0.53
5:2:28:PRO:HD2	6:3:25:GLN:CD	2.29	0.53
4:1:1:MET:HB2	5:2:418:PHE:HB2	1.90	0.53
5:2:141:HIS:HA	5:2:162:PHE:CE2	2.43	0.53
5:2:160:LEU:CG	5:2:206:LEU:HD21	2.39	0.53
4:1:1:MET:CB	5:2:418:PHE:HB2	2.39	0.53
5:2:81:LYS:HG3	5:2:82:ALA:N	2.21	0.53
6:3:191:ILE:N	6:3:210:THR:HG21	2.24	0.53
5:2:118:LEU:CD2	6:3:39:ASP:C	2.72	0.53
5:2:138:PRO:O	5:2:139:ASP:HB2	2.08	0.53
5:2:211:GLN:HE21	5:2:257:SER:CB	2.21	0.53
5:2:118:LEU:HD12	5:2:118:LEU:C	2.29	0.53
6:3:160:ARG:NH2	6:3:192:ASP:HB3	2.23	0.53
1:V:498:ASN:ND2	1:V:504:LYS:HG3	2.24	0.53
5:2:241:SER:O	5:2:245:LEU:HD23	2.09	0.53
5:2:30:VAL:O	5:2:34:LEU:HD23	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:3:15:VAL:HG23	6:3:15:VAL:O	2.08	0.53
3:0:74:GLN:N	3:0:78:PRO:O	2.40	0.53
4:1:1:MET:HE1	5:2:440:LEU:HD13	1.89	0.53
6:3:204:GLN:HG2	6:3:214:TYR:CZ	2.44	0.53
2:W:52:LEU:HD23	2:W:72:TYR:HE2	1.71	0.53
6:3:105:THR:HG23	6:3:106:SER:N	2.23	0.53
6:3:10:LEU:HD21	6:3:143:TYR:CE2	2.44	0.53
1:V:612:ASP:OD2	1:V:635:GLN:CD	2.48	0.53
6:3:144:ILE:HD11	6:3:147:MET:HE3	1.89	0.52
1:V:514:MET:HE1	4:1:16:MET:HE1	1.91	0.52
6:3:44:LEU:C	6:3:44:LEU:HD13	2.30	0.52
6:3:133:LEU:N	6:3:133:LEU:HD13	2.14	0.52
6:3:222:SER:HB3	6:3:225:GLN:HG2	1.92	0.52
5:2:138:PRO:HG3	5:2:189:GLU:CG	2.35	0.52
6:3:18:ASN:O	6:3:21:TRP:CD1	2.63	0.52
4:1:35:ILE:HG13	4:1:35:ILE:O	2.08	0.52
5:2:192:GLU:CG	5:2:193:PRO:HD2	2.23	0.52
6:3:172:LEU:HD13	6:3:172:LEU:C	2.29	0.52
6:3:57:LEU:C	6:3:71:TYR:OH	2.48	0.52
1:V:519:TYR:HB2	4:1:16:MET:HG2	1.91	0.52
4:1:8:VAL:CG1	4:1:45:VAL:HG13	2.35	0.52
5:2:193:PRO:HB2	5:2:194:PRO:HD3	1.92	0.52
6:3:10:LEU:HD21	6:3:143:TYR:CD2	2.45	0.52
6:3:10:LEU:HD22	6:3:147:MET:HG2	1.92	0.52
6:3:57:LEU:HD23	6:3:58:ALA:C	2.30	0.52
1:V:612:ASP:O	1:V:613:THR:O	2.28	0.52
6:3:42:MET:CG	6:3:111:ILE:HD11	2.40	0.52
4:1:1:MET:CG	5:2:413:LEU:CB	2.68	0.52
4:1:1:MET:CG	5:2:418:PHE:HB2	2.38	0.52
6:3:226:TYR:O	6:3:230:VAL:HB	2.10	0.52
5:2:31:LEU:HD13	6:3:33:THR:CG2	2.28	0.52
5:2:257:SER:O	5:2:261:PHE:HD1	1.93	0.51
6:3:71:TYR:HA	6:3:110:VAL:HG11	1.92	0.51
6:3:64:ILE:HG21	6:3:128:HIS:CB	2.40	0.51
6:3:141:LEU:HG	6:3:187:GLN:HE22	1.75	0.51
6:3:14:VAL:HG23	6:3:14:VAL:O	2.09	0.51
2:W:209:TYR:CZ	2:W:233:PHE:HA	2.39	0.51
2:W:584:TYR:HB2	2:W:591:GLY:HA3	1.92	0.51
5:2:160:LEU:HB3	5:2:206:LEU:HD21	1.93	0.51
1:V:689:VAL:CG2	5:2:391:ILE:CD1	2.88	0.51
1:V:412:MET:N	1:V:417:THR:HG21	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:209:TYR:HH	2:W:234:ASP:H	1.57	0.51
6:3:21:TRP:O	6:3:24:LYS:HB2	2.11	0.51
6:3:131:THR:HG23	6:3:133:LEU:HD12	1.92	0.51
6:3:165:LYS:HE3	6:3:200:SER:OG	2.09	0.51
4:1:3:ASN:HB2	5:2:412:PHE:O	2.10	0.51
5:2:179:LEU:CB	5:2:184:LEU:HD11	2.40	0.51
6:3:165:LYS:HD3	6:3:165:LYS:C	2.31	0.51
6:3:121:LYS:HD3	6:3:121:LYS:N	2.25	0.51
6:3:71:TYR:CG	6:3:72:PRO:HD2	2.21	0.51
1:V:428:GLU:OE1	1:V:460:ALA:HA	2.10	0.51
5:2:236:PHE:CE1	5:2:261:PHE:CB	2.94	0.51
5:2:236:PHE:CZ	5:2:262:LEU:CD2	2.94	0.51
5:2:215:PHE:CE2	5:2:264:HIS:HB2	2.46	0.51
5:2:51:LEU:CD2	5:2:55:TRP:CD1	2.94	0.51
5:2:46:ARG:HD3	5:2:85:GLU:HB2	1.93	0.51
5:2:236:PHE:CE2	5:2:262:LEU:CD1	2.94	0.51
6:3:12:VAL:HG12	6:3:58:ALA:HB3	1.92	0.51
5:2:231:VAL:O	5:2:234:LEU:HB3	2.11	0.50
6:3:100:LYS:HG3	6:3:101:TYR:H	1.74	0.50
3:0:77:LYS:HB3	3:0:83:CYS:CB	1.95	0.50
5:2:57:MET:HA	5:2:60:LEU:CG	2.41	0.50
6:3:100:LYS:HB3	6:3:103:LEU:CD1	2.38	0.50
6:3:187:GLN:O	6:3:188:ASN:HB2	2.12	0.50
4:1:2:VAL:O	4:1:2:VAL:HG23	2.11	0.50
5:2:199:ALA:HB1	5:2:201:PHE:CE2	2.47	0.50
4:1:2:VAL:HG12	5:2:456:LYS:HG2	1.81	0.50
5:2:30:VAL:CG1	5:2:34:LEU:HD23	2.40	0.50
3:0:97:ASP:C	6:3:208:ASP:HB3	2.32	0.50
2:W:73:CYS:O	2:W:209:TYR:CE2	2.64	0.50
5:2:140:LYS:CG	5:2:162:PHE:CE1	2.94	0.50
5:2:223:ALA:O	5:2:224:GLN:HB3	2.12	0.50
5:2:35:TYR:N	5:2:35:TYR:CD1	2.79	0.50
6:3:60:ILE:HG22	6:3:61:ALA:N	2.26	0.50
5:2:214:TYR:CB	5:2:261:PHE:CE2	2.95	0.50
5:2:93:LEU:CD2	5:2:96:TRP:HE1	2.25	0.50
6:3:64:ILE:CG2	6:3:128:HIS:HB3	2.42	0.50
1:V:394:SER:CB	1:V:416:THR:O	2.59	0.50
1:V:520:ARG:CG	4:1:23:LEU:HD11	2.42	0.50
1:V:321:GLU:HB3	2:W:499:ASN:HB2	1.93	0.50
6:3:108:ASN:O	6:3:111:ILE:HG12	2.12	0.50
1:V:393:THR:CA	1:V:418:LYS:HE3	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:116:CYS:SG	2:W:191:PRO:HD2	2.51	0.50
2:W:430:ASN:CB	2:W:431:PRO:CD	2.85	0.50
5:2:181:GLN:HE22	5:2:220:LEU:HD12	1.76	0.50
4:1:4:VAL:CG1	5:2:412:PHE:HD2	2.19	0.50
5:2:77:LYS:CD	5:2:78:GLU:HG3	2.41	0.50
6:3:216:LYS:O	6:3:216:LYS:HG2	2.11	0.50
4:1:21:LEU:O	4:1:24:ASP:HB3	2.11	0.50
6:3:137:LEU:CD1	6:3:177:PHE:CE1	2.95	0.50
6:3:202:LEU:HD22	6:3:202:LEU:N	2.27	0.50
2:W:325:THR:HG22	2:W:329:PHE:CE2	2.47	0.50
1:V:667:THR:CA	4:1:62:ASP:OD1	2.59	0.49
5:2:188:THR:HG23	5:2:189:GLU:N	2.27	0.49
6:3:12:VAL:O	6:3:12:VAL:HG23	2.10	0.49
6:3:216:LYS:N	6:3:216:LYS:HD2	2.22	0.49
1:V:502:ILE:O	1:V:646:ALA:HB2	2.12	0.49
2:W:169:PRO:O	2:W:175:TYR:CZ	2.65	0.49
2:W:494:ILE:HD11	2:W:680:ALA:HB2	1.93	0.49
5:2:100:LEU:CG	5:2:119:ARG:HE	2.22	0.49
5:2:181:GLN:HE21	5:2:181:GLN:CA	2.23	0.49
5:2:57:MET:HA	5:2:60:LEU:HG	1.93	0.49
6:3:107:ALA:O	6:3:111:ILE:HG23	2.11	0.49
6:3:220:MET:N	6:3:221:PRO:HD2	2.27	0.49
6:3:53:ARG:HA	6:3:101:TYR:HE1	1.77	0.49
5:2:245:LEU:HD22	5:2:245:LEU:N	2.27	0.49
5:2:81:LYS:CE	5:2:89:LEU:HD21	2.42	0.49
6:3:217:VAL:CG1	6:3:226:TYR:CE2	2.95	0.49
6:3:59:VAL:HG13	6:3:59:VAL:O	2.12	0.49
1:V:418:LYS:HA	1:V:418:LYS:CE	2.41	0.49
4:1:17:LYS:O	4:1:20:LEU:N	2.43	0.49
5:2:199:ALA:CB	5:2:201:PHE:CE2	2.95	0.49
5:2:208:THR:HG23	5:2:209:PRO:HD2	1.91	0.49
5:2:426:ARG:HD2	5:2:444:THR:CG2	2.43	0.49
6:3:12:VAL:HG22	6:3:161:ILE:HA	1.94	0.49
6:3:166:ALA:O	6:3:198:SER:HB2	2.13	0.49
3:0:54:ARG:CB	6:3:209:ILE:CG2	2.87	0.49
6:3:215:LEU:HD12	6:3:230:VAL:CG2	2.42	0.49
6:3:223:LEU:HD13	6:3:223:LEU:C	2.32	0.49
2:W:37:HIS:NE2	2:W:454:VAL:CG1	2.75	0.49
4:1:34:ILE:HG21	4:1:54:GLN:CD	2.32	0.49
4:1:59:GLU:CD	5:2:402:ARG:HH12	2.12	0.49
5:2:89:LEU:HD23	5:2:93:LEU:HG	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:3:10:LEU:CD2	6:3:143:TYR:HE2	2.25	0.49
6:3:165:LYS:HZ1	6:3:200:SER:H	1.60	0.49
5:2:236:PHE:CZ	5:2:258:LEU:CD1	2.95	0.49
5:2:35:TYR:CD1	5:2:62:LEU:CD1	2.95	0.49
6:3:10:LEU:CD2	6:3:143:TYR:CE2	2.95	0.49
6:3:12:VAL:CG2	6:3:161:ILE:HA	2.42	0.49
6:3:174:TYR:HD1	6:3:202:LEU:HD11	1.78	0.49
3:0:55:LEU:N	6:3:209:ILE:HD11	2.28	0.49
1:V:428:GLU:HB3	1:V:432:THR:O	2.13	0.49
5:2:176:ALA:O	5:2:177:GLN:HB2	2.12	0.49
5:2:203:PHE:CE2	5:2:205:LEU:CD2	2.96	0.49
6:3:195:VAL:HG23	6:3:214:TYR:CE1	2.48	0.49
1:V:393:THR:HA	1:V:418:LYS:CG	2.42	0.49
3:0:54:ARG:HB2	3:0:98:GLN:OE1	2.13	0.49
5:2:42:LEU:HD22	5:2:52:ALA:HA	1.95	0.49
2:W:624:PRO:O	2:W:656:ALA:HB1	2.12	0.49
5:2:166:SER:HB3	5:2:167:PRO:CD	2.43	0.49
5:2:198:SER:OG	5:2:238:PHE:HE2	1.96	0.49
6:3:160:ARG:HE	6:3:190:LEU:HG	1.78	0.49
1:V:315:VAL:CG1	2:W:500:ASP:HB3	2.26	0.49
2:W:169:PRO:O	2:W:175:TYR:CE2	2.64	0.49
5:2:170:ALA:CB	5:2:213:TRP:CZ3	2.95	0.48
5:2:77:LYS:HD3	5:2:78:GLU:HG3	1.94	0.48
6:3:177:PHE:CZ	6:3:203:LEU:CD2	2.95	0.48
6:3:21:TRP:CG	6:3:34:LEU:HD23	2.47	0.48
2:W:596:LEU:HG	2:W:597:LEU:N	2.27	0.48
5:2:133:THR:HG23	5:2:134:SER:N	2.29	0.48
3:0:209:THR:HA	3:0:219:TYR:CD1	2.48	0.48
3:0:54:ARG:CG	6:3:182:PHE:CZ	2.80	0.48
5:2:90:LEU:CD2	5:2:140:LYS:HD3	2.42	0.48
5:2:159:VAL:N	5:2:162:PHE:HB3	2.28	0.48
5:2:189:GLU:CA	5:2:192:GLU:HG2	2.41	0.48
5:2:35:TYR:CE2	5:2:62:LEU:CB	2.96	0.48
4:1:21:LEU:HD23	4:1:21:LEU:N	2.29	0.48
5:2:60:LEU:CD1	5:2:95:ILE:CG2	2.91	0.48
1:V:516:PRO:HG2	1:V:706:LYS:HE2	1.91	0.48
6:3:69:PHE:HE1	6:3:139:LYS:HD2	1.77	0.48
4:1:38:ILE:CG2	4:1:44:PHE:CE1	2.96	0.48
5:2:211:GLN:HE21	5:2:257:SER:HB3	1.78	0.48
5:2:234:LEU:C	5:2:234:LEU:HD23	2.34	0.48
5:2:251:VAL:HG11	5:2:254:MET:SD	2.53	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:3:34:LEU:HD13	6:3:34:LEU:C	2.33	0.48
4:1:34:ILE:HG22	4:1:46:ILE:CG1	2.44	0.48
5:2:178:LEU:HD12	5:2:178:LEU:N	2.28	0.48
5:2:211:GLN:CA	5:2:261:PHE:CE1	2.95	0.48
2:W:608:ILE:HG23	2:W:614:TYR:CZ	2.48	0.48
5:2:100:LEU:HD11	5:2:119:ARG:CG	2.31	0.48
5:2:42:LEU:HD12	5:2:59:MET:HE1	1.91	0.48
6:3:124:ILE:O	6:3:127:GLN:HB2	2.14	0.48
2:W:285:TYR:CE1	2:W:403:PHE:CZ	3.01	0.48
4:1:2:VAL:HG12	5:2:456:LYS:CE	2.43	0.48
4:1:43:VAL:HG12	4:1:44:PHE:N	2.27	0.48
4:1:53:LEU:CD1	4:1:53:LEU:H	2.26	0.48
6:3:165:LYS:NZ	6:3:200:SER:H	2.12	0.48
3:0:97:ASP:O	6:3:208:ASP:CB	2.58	0.47
4:1:38:ILE:HG22	4:1:44:PHE:CE1	2.48	0.47
5:2:89:LEU:CD2	5:2:93:LEU:HG	2.44	0.47
6:3:160:ARG:HB2	6:3:190:LEU:HG	1.96	0.47
5:2:30:VAL:N	6:3:25:GLN:HG3	2.23	0.47
5:2:117:ASN:CB	6:3:42:MET:HE2	2.43	0.47
5:2:203:PHE:CD2	5:2:204:LEU:N	2.82	0.47
5:2:236:PHE:CD1	5:2:261:PHE:HB3	2.49	0.47
5:2:218:GLN:HG2	5:2:268:PHE:CB	2.44	0.47
5:2:35:TYR:CD1	5:2:62:LEU:CG	2.92	0.47
6:3:34:LEU:HD13	6:3:38:ILE:HG12	1.95	0.47
1:V:519:TYR:N	4:1:16:MET:HG3	2.29	0.47
6:3:10:LEU:CD1	6:3:56:LYS:HG2	2.44	0.47
6:3:226:TYR:CA	6:3:230:VAL:HG23	2.42	0.47
6:3:34:LEU:HD22	6:3:37:CYS:SG	2.55	0.47
1:V:461:HIS:CE1	1:V:462:CYS:HG	2.31	0.47
2:W:70:LEU:HG	2:W:72:TYR:CE1	2.49	0.47
3:0:165:ARG:HB2	3:0:193:LYS:O	2.14	0.47
4:1:11:GLU:HG2	5:2:404:THR:OG1	2.14	0.47
4:1:4:VAL:HG12	5:2:411:GLN:C	2.30	0.47
5:2:205:LEU:N	5:2:205:LEU:HD22	2.30	0.47
5:2:236:PHE:HE2	5:2:262:LEU:CD1	2.28	0.47
6:3:216:LYS:O	6:3:218:PRO:HD3	2.14	0.47
1:V:361:CYS:HB3	1:V:405:VAL:HG21	1.96	0.47
5:2:171:VAL:CG2	5:2:213:TRP:HA	2.20	0.47
6:3:59:VAL:HG21	6:3:70:LEU:HD12	1.97	0.47
2:W:73:CYS:HB2	2:W:209:TYR:CE1	2.49	0.47
2:W:73:CYS:HB3	2:W:209:TYR:CG	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:2:93:LEU:CA	5:2:96:TRP:CD1	2.94	0.47
5:2:28:PRO:CD	6:3:25:GLN:NE2	2.75	0.47
6:3:10:LEU:HA	6:3:56:LYS:HG2	1.96	0.47
4:1:50:VAL:CG1	4:1:54:GLN:HG2	2.41	0.47
5:2:211:GLN:CB	5:2:261:PHE:CE1	2.95	0.47
2:W:433:LEU:C	2:W:434:HIS:ND1	2.68	0.47
2:W:52:LEU:CD2	2:W:72:TYR:OH	2.55	0.47
4:1:45:VAL:CG2	5:2:409:TYR:CE2	2.98	0.47
4:1:9:LEU:HD12	4:1:9:LEU:N	2.29	0.47
5:2:46:ARG:CD	5:2:85:GLU:CB	2.93	0.47
5:2:85:GLU:O	5:2:89:LEU:HB2	2.14	0.47
6:3:24:LYS:HE2	6:3:196:LEU:HB3	1.96	0.47
2:W:432:ILE:HD11	2:W:434:HIS:CE1	2.48	0.47
4:1:22:TYR:O	4:1:25:GLU:HB3	2.15	0.47
5:2:84:GLU:HA	5:2:84:GLU:OE1	2.15	0.47
6:3:64:ILE:HG21	6:3:128:HIS:HB3	1.97	0.47
2:W:73:CYS:CB	2:W:209:TYR:CE1	2.98	0.47
4:1:38:ILE:CB	4:1:44:PHE:CE1	2.98	0.47
4:1:45:VAL:HG21	5:2:409:TYR:CE2	2.50	0.47
4:1:53:LEU:O	4:1:57:VAL:HG12	2.15	0.47
5:2:201:PHE:CD1	5:2:202:GLN:N	2.83	0.47
6:3:137:LEU:HD11	6:3:177:PHE:CE1	2.50	0.47
6:3:56:LYS:HD3	6:3:56:LYS:N	2.30	0.47
2:W:143:ARG:HH11	2:W:143:ARG:HG2	1.80	0.47
2:W:73:CYS:HB3	2:W:209:TYR:CD1	2.50	0.47
2:W:37:HIS:CG	2:W:454:VAL:HG13	2.50	0.47
5:2:240:LEU:HD12	5:2:240:LEU:N	2.30	0.47
5:2:51:LEU:HD21	5:2:55:TRP:CD1	2.50	0.47
5:2:96:TRP:CH2	5:2:97:HIS:CE1	3.03	0.47
2:W:657:MET:O	2:W:660:ALA:HB3	2.15	0.47
4:1:38:ILE:O	4:1:38:ILE:HG12	2.15	0.46
5:2:221:GLN:CD	5:2:230:LEU:HB2	2.34	0.46
6:3:131:THR:HG23	6:3:133:LEU:HD13	1.95	0.46
6:3:177:PHE:O	6:3:181:ILE:HG13	2.15	0.46
2:W:170:LEU:CD1	2:W:175:TYR:OH	2.51	0.46
5:2:78:GLU:HB3	5:2:81:LYS:HZ2	1.79	0.46
6:3:12:VAL:CG2	6:3:161:ILE:HG23	2.43	0.46
2:W:109:LEU:HG	2:W:207:TYR:CZ	2.50	0.46
6:3:42:MET:HE1	6:3:108:ASN:HB2	1.96	0.46
4:1:40:ASP:HB2	4:1:43:VAL:H	1.81	0.46
6:3:10:LEU:N	6:3:56:LYS:HE3	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:110:SER:C	2:W:207:TYR:CE1	2.79	0.46
1:V:514:MET:CE	4:1:16:MET:CE	2.93	0.46
4:1:5:LEU:HD11	5:2:408:LEU:CB	2.11	0.46
2:W:581:LEU:HD13	2:W:581:LEU:C	2.36	0.46
4:1:38:ILE:CG2	4:1:44:PHE:CD1	2.94	0.46
6:3:10:LEU:HB2	6:3:56:LYS:HE3	1.97	0.46
6:3:165:LYS:CG	6:3:203:LEU:HD12	2.36	0.46
4:1:10:ILE:HG12	4:1:43:VAL:CG1	2.45	0.46
1:V:689:VAL:CG2	5:2:391:ILE:HD13	2.46	0.46
6:3:196:LEU:HB3	6:3:220:MET:SD	2.56	0.46
1:V:504:LYS:HB3	1:V:655:TYR:HA	1.97	0.46
5:2:217:LEU:CD2	5:2:233:ILE:HD11	2.45	0.46
5:2:96:TRP:CZ2	5:2:97:HIS:NE2	2.83	0.46
4:1:22:TYR:HD1	4:1:23:LEU:HD23	1.80	0.46
5:2:81:LYS:CG	5:2:82:ALA:N	2.79	0.46
1:V:517:GLU:HA	4:1:19:PHE:CD2	2.51	0.46
2:W:623:VAL:HG23	2:W:681:ASP:HB2	1.97	0.46
4:1:1:MET:HE3	5:2:415:GLN:N	2.31	0.46
4:1:57:VAL:HG13	4:1:58:GLY:N	2.31	0.46
5:2:187:SER:OG	5:2:190:PRO:HD2	2.16	0.46
5:2:214:TYR:CE1	5:2:233:ILE:HG23	2.51	0.46
6:3:15:VAL:HG12	6:3:164:ILE:HD12	1.97	0.46
5:2:118:LEU:HD21	6:3:39:ASP:OD1	1.95	0.46
2:W:37:HIS:NE2	2:W:454:VAL:HG11	2.31	0.46
6:3:64:ILE:CG2	6:3:128:HIS:CB	2.94	0.45
4:1:1:MET:CE	5:2:415:GLN:C	2.84	0.45
5:2:117:ASN:HB3	6:3:42:MET:HE2	1.98	0.45
5:2:203:PHE:CG	5:2:204:LEU:N	2.84	0.45
5:2:35:TYR:CD2	5:2:62:LEU:CB	2.95	0.45
6:3:64:ILE:CG2	6:3:128:HIS:CG	2.99	0.45
6:3:8:LEU:HD23	6:3:54:SER:CB	2.42	0.45
2:W:37:HIS:CD2	2:W:454:VAL:CG1	2.99	0.45
1:V:519:TYR:CE2	4:1:20:LEU:CB	3.00	0.45
1:V:517:GLU:CB	1:V:713:LEU:HD22	2.46	0.45
5:2:221:GLN:HG2	5:2:268:PHE:HZ	1.75	0.45
5:2:117:ASN:HB2	6:3:104:LEU:CG	2.47	0.45
6:3:42:MET:CG	6:3:111:ILE:CD1	2.94	0.45
6:3:190:LEU:HA	6:3:210:THR:HG21	1.91	0.45
5:2:28:PRO:C	6:3:25:GLN:HG3	2.17	0.45
1:V:370:SER:OG	1:V:614:SER:OG	2.34	0.45
4:1:54:GLN:O	4:1:57:VAL:HG12	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:2:90:LEU:HD21	5:2:140:LYS:HD3	1.98	0.45
5:2:30:VAL:CG1	5:2:34:LEU:CD2	2.94	0.45
6:3:59:VAL:HG11	6:3:70:LEU:HB3	1.98	0.45
4:1:1:MET:SD	5:2:413:LEU:CB	3.03	0.45
5:2:30:VAL:HG23	6:3:25:GLN:CG	2.37	0.45
6:3:219:GLN:HA	6:3:219:GLN:OE1	2.17	0.45
6:3:21:TRP:HA	6:3:24:LYS:CG	2.46	0.45
5:2:203:PHE:CD2	5:2:205:LEU:CD2	2.95	0.45
5:2:51:LEU:C	5:2:51:LEU:HD23	2.37	0.45
6:3:121:LYS:H	6:3:121:LYS:HD3	1.81	0.45
1:V:444:HIS:O	1:V:447:PRO:CD	2.62	0.45
5:2:164:VAL:HG13	5:2:209:PRO:CG	2.45	0.45
6:3:148:ASN:ND2	6:3:157:MET:HG3	2.32	0.45
1:V:393:THR:HA	1:V:418:LYS:HG2	1.99	0.45
1:V:615:PHE:CD1	1:V:616:ASP:N	2.85	0.45
1:V:514:MET:CE	4:1:16:MET:HE1	2.46	0.45
4:1:1:MET:HG2	5:2:413:LEU:CB	2.44	0.45
5:2:35:TYR:HB2	5:2:62:LEU:HD12	1.98	0.45
1:V:515:SER:C	4:1:16:MET:HB2	2.36	0.44
2:W:432:ILE:HG12	2:W:434:HIS:ND1	2.23	0.44
5:2:130:SER:HB2	5:2:179:LEU:HD23	1.99	0.44
5:2:217:LEU:CD2	5:2:233:ILE:CD1	2.95	0.44
2:W:421:PHE:HB2	2:W:431:PRO:HD3	1.84	0.44
3:0:106:ILE:HD11	3:0:127:HIS:HB3	2.00	0.44
3:0:54:ARG:HA	6:3:209:ILE:HD13	1.06	0.44
6:3:160:ARG:HB2	6:3:160:ARG:HE	1.58	0.44
6:3:228:LEU:HD23	6:3:228:LEU:O	2.17	0.44
2:W:207:TYR:CD1	2:W:208:SER:N	2.86	0.44
5:2:123:LEU:CD2	5:2:178:LEU:CD1	2.95	0.44
5:2:189:GLU:HB2	5:2:190:PRO:CD	2.43	0.44
5:2:218:GLN:HE22	5:2:265:LEU:CA	2.28	0.44
6:3:144:ILE:HD13	6:3:144:ILE:O	2.17	0.44
6:3:60:ILE:HG23	6:3:68:ARG:O	2.17	0.44
4:1:4:VAL:HG22	4:1:5:LEU:N	2.32	0.44
5:2:140:LYS:HD3	5:2:162:PHE:CE1	2.47	0.44
5:2:204:LEU:HD23	5:2:254:MET:HE2	1.99	0.44
5:2:159:VAL:HG12	5:2:161:HIS:HB2	1.99	0.44
6:3:160:ARG:CB	6:3:190:LEU:CD2	2.95	0.44
6:3:65:GLN:O	6:3:132:LEU:HD11	2.18	0.44
1:V:514:MET:SD	4:1:16:MET:CE	3.05	0.44
2:W:170:LEU:CD1	2:W:175:TYR:HH	2.26	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:2:206:LEU:CD2	5:2:206:LEU:H	2.30	0.44
5:2:60:LEU:CD1	5:2:95:ILE:CB	2.95	0.44
1:V:612:ASP:OD2	1:V:639:ARG:NH1	2.50	0.44
2:W:189:TRP:CE3	2:W:190:CYS:N	2.86	0.44
5:2:166:SER:HB3	5:2:167:PRO:HD3	2.00	0.44
5:2:258:LEU:HG	5:2:262:LEU:HD21	1.99	0.44
5:2:28:PRO:C	6:3:25:GLN:O	2.56	0.44
6:3:124:ILE:HG23	6:3:124:ILE:O	2.18	0.44
2:W:421:PHE:HB2	2:W:430:ASN:HA	2.00	0.44
2:W:421:PHE:CB	2:W:430:ASN:C	2.80	0.44
4:1:3:ASN:HB3	5:2:412:PHE:O	2.18	0.43
5:2:61:PHE:CE1	5:2:99:GLN:NE2	2.85	0.43
1:V:519:TYR:HA	1:V:522:TYR:HB3	2.00	0.43
7:X:6:DC:H2'	7:X:7:DG:C8	2.53	0.43
3:0:60:HIS:CE1	3:0:159:MET:SD	3.11	0.43
4:1:34:ILE:CG2	4:1:50:VAL:HG11	2.48	0.43
5:2:117:ASN:ND2	6:3:104:LEU:O	2.52	0.43
5:2:214:TYR:HB3	5:2:261:PHE:CE2	2.54	0.43
5:2:56:VAL:HG23	5:2:57:MET:N	2.31	0.43
1:V:409:THR:H	1:V:418:LYS:CB	2.31	0.43
1:V:282:LYS:HE3	1:V:482:PHE:CD1	2.54	0.43
4:1:22:TYR:C	4:1:22:TYR:CD1	2.92	0.43
5:2:117:ASN:ND2	6:3:108:ASN:N	2.65	0.43
5:2:159:VAL:HG22	5:2:160:LEU:HD13	1.94	0.43
5:2:243:SER:HB3	5:2:258:LEU:CD2	2.45	0.43
5:2:35:TYR:CD1	5:2:62:LEU:HD12	2.52	0.43
6:3:178:MET:HA	6:3:181:ILE:HD12	1.99	0.43
6:3:178:MET:O	6:3:182:PHE:HD2	2.01	0.43
1:V:405:VAL:HG12	1:V:406:ALA:H	1.82	0.43
1:V:446:ILE:HD12	1:V:451:PHE:HB3	1.99	0.43
1:V:514:MET:SD	1:V:537:ASN:CG	2.97	0.43
3:0:77:LYS:HE3	3:0:78:PRO:HD3	2.00	0.43
5:2:236:PHE:HZ	5:2:258:LEU:HD11	1.82	0.43
1:V:519:TYR:H	4:1:16:MET:HG3	1.83	0.43
1:V:519:TYR:CE2	4:1:20:LEU:HB2	2.54	0.43
5:2:214:TYR:OH	5:2:265:LEU:HD13	2.18	0.43
5:2:270:LEU:HA	5:2:273:GLN:HG3	2.00	0.43
5:2:94:ARG:HD2	5:2:95:ILE:CD1	2.47	0.43
5:2:117:ASN:CA	6:3:104:LEU:HD21	2.47	0.43
1:V:411:SER:O	1:V:417:THR:HB	2.19	0.43
3:0:77:LYS:CB	3:0:83:CYS:SG	2.89	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:514:MET:HB3	4:1:16:MET:SD	2.58	0.43
4:1:50:VAL:HG12	4:1:50:VAL:O	2.18	0.43
5:2:223:ALA:H	5:2:268:PHE:HE1	1.64	0.43
5:2:224:GLN:N	5:2:268:PHE:HZ	2.16	0.43
5:2:409:TYR:CD2	5:2:443:VAL:HG22	2.54	0.43
6:3:121:LYS:H	6:3:121:LYS:CD	2.32	0.43
1:V:504:LYS:CB	1:V:655:TYR:HA	2.48	0.43
2:W:419:GLU:O	2:W:420:PRO:C	2.55	0.43
4:1:25:GLU:OE2	4:1:35:ILE:HG12	2.18	0.43
5:2:127:LYS:CA	5:2:178:LEU:HD23	2.48	0.43
6:3:59:VAL:O	6:3:70:LEU:HB2	2.19	0.43
5:2:203:PHE:HD2	5:2:205:LEU:H	1.65	0.43
5:2:215:PHE:CE2	5:2:264:HIS:ND1	2.86	0.43
5:2:30:VAL:HB	6:3:24:LYS:O	2.19	0.43
5:2:34:LEU:HD22	5:2:34:LEU:N	2.33	0.43
4:1:1:MET:CA	5:2:413:LEU:HA	2.48	0.43
2:W:73:CYS:CB	2:W:209:TYR:CE2	3.02	0.43
2:W:263:LEU:C	2:W:263:LEU:HD23	2.39	0.43
2:W:28:LEU:HD13	2:W:28:LEU:C	2.38	0.43
3:0:96:PHE:CG	3:0:124:PRO:HB3	2.53	0.43
5:2:117:ASN:HD21	6:3:108:ASN:N	2.16	0.43
5:2:118:LEU:HD23	6:3:42:MET:CB	2.35	0.43
1:V:524:ALA:HB2	4:1:23:LEU:HD13	2.01	0.43
2:W:73:CYS:HB3	2:W:209:TYR:CD2	2.53	0.43
4:1:8:VAL:CG1	4:1:9:LEU:N	2.80	0.43
1:V:689:VAL:CG2	5:2:391:ILE:HD11	2.48	0.43
6:3:165:LYS:HZ1	6:3:200:SER:N	2.16	0.43
5:2:31:LEU:HG	6:3:33:THR:HB	1.95	0.43
2:W:584:TYR:CB	2:W:591:GLY:HA3	2.49	0.43
5:2:118:LEU:HD22	6:3:39:ASP:CB	2.49	0.42
5:2:236:PHE:CE1	5:2:239:GLN:NE2	2.87	0.42
6:3:124:ILE:HD13	6:3:124:ILE:C	2.38	0.42
6:3:184:ALA:O	6:3:187:GLN:HG2	2.19	0.42
6:3:141:LEU:HA	6:3:144:ILE:HG22	2.01	0.42
6:3:137:LEU:HD12	6:3:177:PHE:CE1	2.54	0.42
3:0:73:ASP:O	3:0:78:PRO:O	2.37	0.42
5:2:138:PRO:HD3	5:2:189:GLU:CD	2.40	0.42
5:2:159:VAL:HG11	5:2:161:HIS:CD2	2.49	0.42
5:2:35:TYR:CG	5:2:62:LEU:CD1	2.99	0.42
6:3:178:MET:CE	6:3:202:LEU:CD1	2.95	0.42
6:3:8:LEU:CD2	6:3:54:SER:HB3	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:2:133:THR:CG2	5:2:134:SER:N	2.83	0.42
6:3:144:ILE:HG13	6:3:159:SER:OG	2.20	0.42
1:V:666:ASP:CB	4:1:17:LYS:HZ3	2.32	0.42
5:2:188:THR:CG2	5:2:189:GLU:N	2.83	0.42
5:2:57:MET:CA	5:2:60:LEU:HG	2.49	0.42
6:3:133:LEU:CD2	6:3:134:ALA:N	2.82	0.42
6:3:160:ARG:CZ	6:3:190:LEU:CD1	2.97	0.42
1:V:315:VAL:CG1	2:W:500:ASP:CG	2.81	0.42
6:3:111:ILE:HG13	6:3:112:VAL:H	1.83	0.42
6:3:128:HIS:NE2	6:3:130:GLU:CG	2.82	0.42
6:3:42:MET:SD	6:3:111:ILE:CD1	3.07	0.42
3:0:96:PHE:CE2	3:0:124:PRO:HA	2.54	0.42
5:2:171:VAL:CG1	5:2:216:MET:SD	3.06	0.42
4:1:1:MET:SD	5:2:419:GLU:N	2.92	0.42
6:3:100:LYS:CB	6:3:103:LEU:HD13	2.41	0.42
6:3:9:ASN:OD1	6:3:158:LYS:HB3	2.19	0.42
2:W:282:ARG:HA	2:W:285:TYR:CD2	2.54	0.42
5:2:140:LYS:CD	5:2:162:PHE:HE1	2.29	0.42
5:2:236:PHE:CE1	5:2:261:PHE:HB3	2.54	0.42
5:2:77:LYS:HD3	5:2:78:GLU:CG	2.50	0.42
6:3:14:VAL:CG2	6:3:163:VAL:HG13	2.48	0.42
6:3:202:LEU:N	6:3:202:LEU:CD2	2.82	0.42
5:2:47:GLU:HG3	5:2:48:LEU:H	1.83	0.42
6:3:11:LEU:CD1	6:3:48:HIS:NE2	2.82	0.42
6:3:197:ASP:O	6:3:198:SER:HB3	2.20	0.42
6:3:18:ASN:ND2	6:3:64:ILE:HD11	2.35	0.42
1:V:503:ALA:HB2	1:V:646:ALA:H	1.82	0.42
1:V:315:VAL:HG13	2:W:500:ASP:HB2	0.42	0.42
5:2:171:VAL:HG13	5:2:216:MET:HB3	1.98	0.42
6:3:105:THR:CG2	6:3:106:SER:N	2.82	0.42
6:3:64:ILE:CB	6:3:123:ASP:HB3	2.49	0.42
6:3:217:VAL:HG12	6:3:218:PRO:O	2.20	0.42
1:V:518:PHE:CD1	1:V:713:LEU:HD13	2.55	0.42
2:W:25:MET:SD	2:W:58:ALA:HB2	2.59	0.42
3:0:165:ARG:HD3	3:0:194:ILE:HG12	2.02	0.41
5:2:117:ASN:CB	6:3:42:MET:HE1	2.48	0.41
6:3:100:LYS:HE2	6:3:100:LYS:HB2	1.89	0.41
2:W:15:ASP:HA	2:W:100:GLU:OE2	2.20	0.41
2:W:421:PHE:HB2	2:W:422:ASP:H	1.59	0.41
5:2:159:VAL:CG2	5:2:160:LEU:N	2.81	0.41
6:3:70:LEU:HD13	6:3:115:ILE:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:3:147:MET:CE	6:3:157:MET:SD	3.07	0.41
5:2:202:GLN:HE21	5:2:202:GLN:N	2.15	0.41
5:2:223:ALA:C	5:2:225:SER:H	2.24	0.41
2:W:157:PHE:HA	2:W:189:TRP:CZ3	2.55	0.41
2:W:170:LEU:HG	2:W:175:TYR:CD2	2.55	0.41
4:1:43:VAL:CG1	4:1:44:PHE:N	2.82	0.41
5:2:176:ALA:HB3	5:2:178:LEU:HD13	1.98	0.41
5:2:175:LEU:CD2	5:2:216:MET:SD	3.07	0.41
6:3:14:VAL:HG22	6:3:162:LEU:O	2.21	0.41
1:V:519:TYR:CE2	1:V:523:VAL:HG21	2.54	0.41
2:W:196:ARG:CZ	2:W:197:TYR:HA	2.51	0.41
4:1:13:ASP:OD1	4:1:14:PRO:HD2	2.17	0.41
5:2:221:GLN:O	5:2:268:PHE:CE1	2.74	0.41
5:2:93:LEU:HD23	5:2:96:TRP:HE1	1.85	0.41
6:3:109:GLU:HG3	6:3:110:VAL:N	2.35	0.41
4:1:52:VAL:CG2	4:1:53:LEU:N	2.83	0.41
5:2:123:LEU:HD23	5:2:123:LEU:C	2.41	0.41
6:3:41:VAL:HG13	6:3:42:MET:N	2.35	0.41
1:V:408:SER:HB3	1:V:418:LYS:HB3	2.03	0.41
5:2:206:LEU:CD2	5:2:206:LEU:N	2.84	0.41
6:3:125:LYS:C	6:3:127:GLN:H	2.24	0.41
6:3:9:ASN:C	6:3:56:LYS:HE3	2.41	0.41
1:V:390:CYS:SG	1:V:399:LYS:HE3	2.61	0.41
5:2:181:GLN:NE2	5:2:181:GLN:HA	2.34	0.41
5:2:211:GLN:CD	5:2:261:PHE:CE1	2.94	0.41
5:2:236:PHE:HZ	5:2:258:LEU:CD1	2.34	0.41
4:1:59:GLU:CD	5:2:402:ARG:CZ	2.88	0.41
4:1:1:MET:N	5:2:418:PHE:CB	2.84	0.41
6:3:141:LEU:C	6:3:144:ILE:HG22	2.41	0.41
5:2:170:ALA:C	5:2:213:TRP:CZ3	2.94	0.41
6:3:114:GLU:OE1	6:3:114:GLU:HA	2.21	0.41
6:3:146:ARG:HG3	6:3:147:MET:N	2.35	0.41
6:3:191:ILE:H	6:3:210:THR:HG21	1.85	0.41
6:3:222:SER:HB3	6:3:225:GLN:CG	2.51	0.41
1:V:631:GLY:O	1:V:632:SER:CB	2.69	0.41
4:1:52:VAL:O	4:1:56:ARG:HG2	2.21	0.41
5:2:86:SER:HB2	5:2:140:LYS:HE2	2.03	0.41
5:2:174:ASP:OD2	5:2:213:TRP:CZ3	2.74	0.41
5:2:236:PHE:CD1	5:2:239:GLN:CD	2.95	0.41
1:V:353:ALA:O	1:V:357:VAL:HG23	2.21	0.41
4:1:13:ASP:CG	4:1:14:PRO:CD	2.80	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:2:196:ILE:HG13	5:2:197:THR:N	2.36	0.40
5:2:93:LEU:CA	5:2:96:TRP:HD1	2.31	0.40
6:3:187:GLN:CG	6:3:189:ILE:CG1	2.94	0.40
1:V:297:PHE:CG	1:V:298:ARG:N	2.89	0.40
1:V:409:THR:H	1:V:418:LYS:HG3	1.84	0.40
5:2:236:PHE:HZ	5:2:262:LEU:CD2	2.35	0.40
5:2:224:GLN:CB	5:2:268:PHE:CZ	2.94	0.40
5:2:34:LEU:N	5:2:34:LEU:CD2	2.84	0.40
6:3:60:ILE:CG2	6:3:61:ALA:N	2.83	0.40
4:1:10:ILE:HG23	4:1:10:ILE:O	2.21	0.40
4:1:38:ILE:CB	4:1:44:PHE:CD1	3.04	0.40
5:2:251:VAL:CG1	5:2:254:MET:CG	2.95	0.40
5:2:89:LEU:HD23	5:2:89:LEU:C	2.42	0.40
5:2:93:LEU:O	5:2:96:TRP:CD1	2.74	0.40
6:3:42:MET:HG2	6:3:111:ILE:CD1	2.52	0.40
6:3:222:SER:HB3	6:3:225:GLN:OE1	2.21	0.40
6:3:228:LEU:HD23	6:3:228:LEU:C	2.41	0.40
5:2:94:ARG:HD2	5:2:95:ILE:HD13	2.02	0.40
1:V:413:LEU:H	1:V:417:THR:CG2	2.35	0.40
5:2:399:ASP:OD1	5:2:402:ARG:NH1	2.55	0.40
5:2:93:LEU:HA	5:2:93:LEU:HD23	1.77	0.40
6:3:187:GLN:HE21	6:3:189:ILE:HB	1.86	0.40
6:3:18:ASN:OD1	6:3:19:PRO:HD2	2.21	0.40
6:3:222:SER:O	6:3:226:TYR:CD2	2.75	0.40
2:W:233:PHE:HB2	2:W:456:ILE:HG22	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	V	473/782 (60%)	401 (85%)	47 (10%)	25 (5%)	2	29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	W	661/760 (87%)	569 (86%)	68 (10%)	24 (4%)	4	38
3	0	186/395 (47%)	166 (89%)	15 (8%)	5 (3%)	6	45
4	1	60/71 (84%)	49 (82%)	9 (15%)	2 (3%)	5	40
5	2	264/462 (57%)	246 (93%)	14 (5%)	4 (2%)	13	57
6	3	187/308 (61%)	175 (94%)	10 (5%)	2 (1%)	17	63
All	All	1831/2778 (66%)	1606 (88%)	163 (9%)	62 (3%)	8	40

All (62) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	V	385	ASP
1	V	427	MET
1	V	461	HIS
1	V	491	ALA
1	V	499	ASN
1	V	502	ILE
1	V	613	THR
1	V	629	HIS
1	V	650	MET
2	W	67	VAL
2	W	424	ARG
2	W	430	ASN
2	W	504	ILE
2	W	573	ASP
2	W	595	ILE
2	W	630	SER
2	W	646	ILE
3	0	78	PRO
3	0	80	ARG
4	1	48	GLU
5	2	49	PRO
6	3	120	THR
1	V	254	GLN
1	V	404	SER
1	V	460	ALA
1	V	632	SER
2	W	124	LEU
2	W	408	SER
2	W	645	GLN
5	2	223	ALA

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Mol	Chain	Res	Type
5	2	231	VAL
1	V	343	GLY
1	V	418	LYS
2	W	147	GLN
2	W	155	CYS
2	W	509	GLU
6	3	198	SER
1	V	310	LEU
1	V	436	GLY
1	V	470	LEU
1	V	475	ASP
2	W	420	PRO
2	W	152	LEU
2	W	551	SER
5	2	430	VAL
1	V	582	GLY
2	W	36	GLY
2	W	111	SER
2	W	345	ARG
2	W	697	ILE
1	V	311	LYS
1	V	651	VAL
1	V	426	VAL
1	V	457	ILE
2	W	495	ILE
3	0	216	GLY
1	V	405	VAL
2	W	174	ILE
4	1	2	VAL
3	0	56	GLY
2	W	45	GLY
3	0	99	ASN

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	V	422/688 (61%)	400 (95%)	22 (5%)	29	65
2	W	577/664 (87%)	540 (94%)	37 (6%)	22	58
3	0	171/352 (49%)	162 (95%)	9 (5%)	28	64
4	1	56/64 (88%)	51 (91%)	5 (9%)	12	44
5	2	238/399 (60%)	229 (96%)	9 (4%)	40	73
6	3	171/272 (63%)	157 (92%)	14 (8%)	14	49
All	All	1635/2439 (67%)	1539 (94%)	96 (6%)	29	61

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	V	246	MET
1	V	332	ARG
1	V	362	LEU
1	V	366	ASN
1	V	418	LYS
1	V	427	MET
1	V	429	TRP
1	V	458	VAL
1	V	471	VAL
1	V	479	ASP
1	V	482	PHE
1	V	492	ASN
1	V	517	GLU
1	V	530	ARG
1	V	534	TYR
1	V	566	PHE
1	V	568	LEU
1	V	581	TYR
1	V	590	MET
1	V	612	ASP
1	V	614	SER
1	V	648	LYS
2	W	37	HIS
2	W	64	PRO
2	W	95	GLU
2	W	101	LYS
2	W	112	ARG
2	W	122	THR
2	W	123	PRO
2	W	166	ARG

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Mol	Chain	Res	Type
2	W	196	ARG
2	W	207	TYR
2	W	263	LEU
2	W	282	ARG
2	W	283	ASP
2	W	285	TYR
2	W	288	LEU
2	W	309	VAL
2	W	333	LEU
2	W	345	ARG
2	W	346	VAL
2	W	421	PHE
2	W	425	THR
2	W	461	LEU
2	W	489	CYS
2	W	523	LEU
2	W	533	ASP
2	W	543	GLN
2	W	544	TYR
2	W	554	GLU
2	W	584	TYR
2	W	596	LEU
2	W	610	PHE
2	W	620	MET
2	W	645	GLN
2	W	647	ARG
2	W	654	PHE
2	W	669	ARG
2	W	676	LEU
3	0	77	LYS
3	0	96	PHE
3	0	103	GLN
3	0	125	ARG
3	0	137	MET
3	0	174	LEU
3	0	202	SER
3	0	218	THR
3	0	222	ILE
4	1	10	ILE
4	1	13	ASP
4	1	18	GLN
4	1	21	LEU

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Mol	Chain	Res	Type
4	1	38	ILE
5	2	61	PHE
5	2	77	LYS
5	2	181	GLN
5	2	202	GLN
5	2	402	ARG
5	2	407	VAL
5	2	426	ARG
5	2	430	VAL
5	2	452	LYS
6	3	25	GLN
6	3	56	LYS
6	3	66	GLU
6	3	70	LEU
6	3	109	GLU
6	3	121	LYS
6	3	124	ILE
6	3	133	LEU
6	3	144	ILE
6	3	147	MET
6	3	157	MET
6	3	185	GLN
6	3	190	LEU
6	3	216	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	V	281	GLN
1	V	366	ASN
1	V	415	HIS
1	V	539	ASN
1	V	635	GLN
1	V	677	GLN
2	W	187	GLN
2	W	430	ASN
2	W	590	ASN
3	0	60	HIS
3	0	103	GLN
4	1	51	ASN
5	2	117	ASN
5	2	161	HIS

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Mol	Chain	Res	Type
5	2	181	GLN
5	2	202	GLN
5	2	221	GLN
5	2	239	GLN
5	2	263	GLN
5	2	273	GLN
6	3	25	GLN
6	3	52	ASN
6	3	63	HIS
6	3	148	ASN
6	3	155	GLN
6	3	185	GLN
6	3	187	GLN
6	3	225	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.