



Full wwPDB EM Validation Report ⓘ

Mar 25, 2026 – 12:05 AM UTC

PDB ID : 5IVW / pdb_00005ivw
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)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

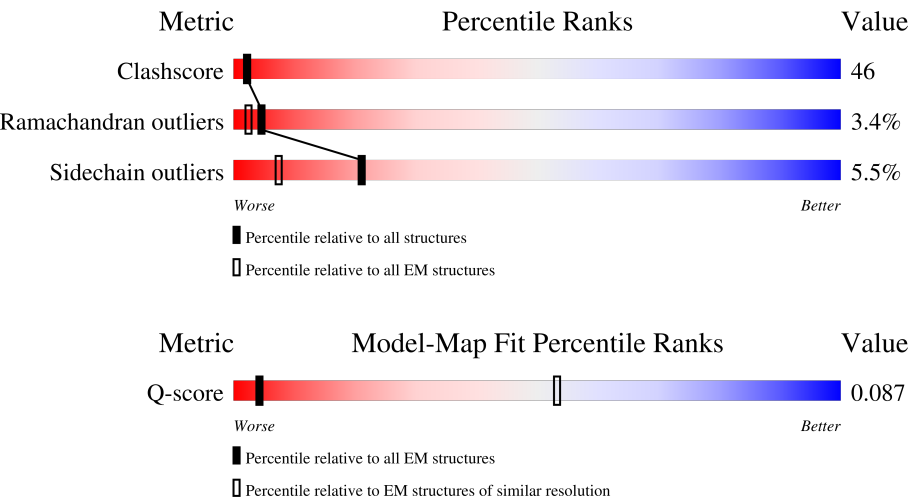
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	147 (9.50 - 10.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	V	782	14% 24%28%7%•39%
2	W	760	18% 38%42%7%•12%
3	0	395	6% 25%20%•52%
4	1	71	11% 14%52%20%•13%

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Mol	Chain	Length	Quality of chain
5	2	462	8% 19% 32% 7% 41%
6	3	308	10% 14% 41% 7% 37%
7	X	19	21% 47% 32%
8	Y	20	20% 40% 40%

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 TFIID 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 TFIID 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.

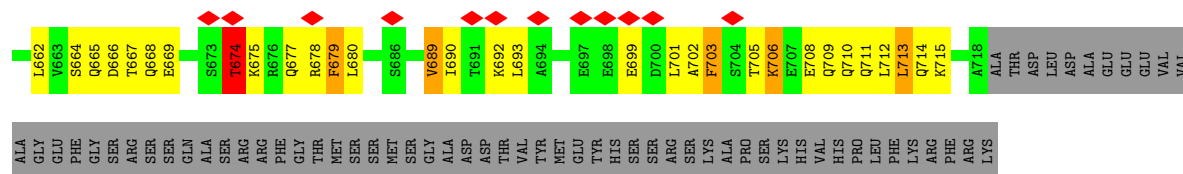
Mol	Chain	Residues	Atoms					AltConf	Trace
6	3	193	Total	C	N	O	S	0	0
			1526	978	252	284	12		

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

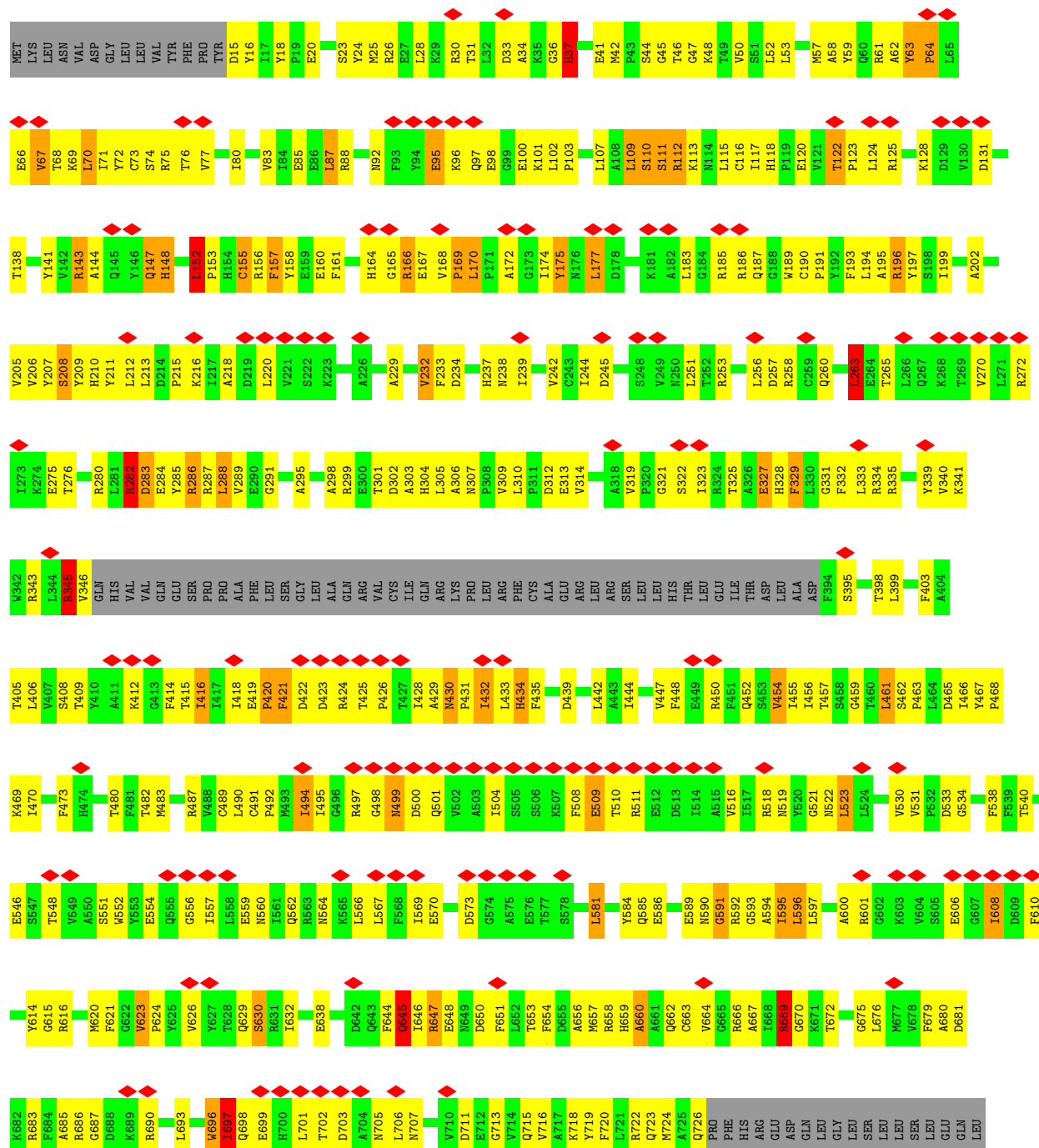
Mol	Chain	Residues	Atoms					AltConf	Trace
7	X	19	Total	C	N	O	P	0	0
			392	187	83	104	18		

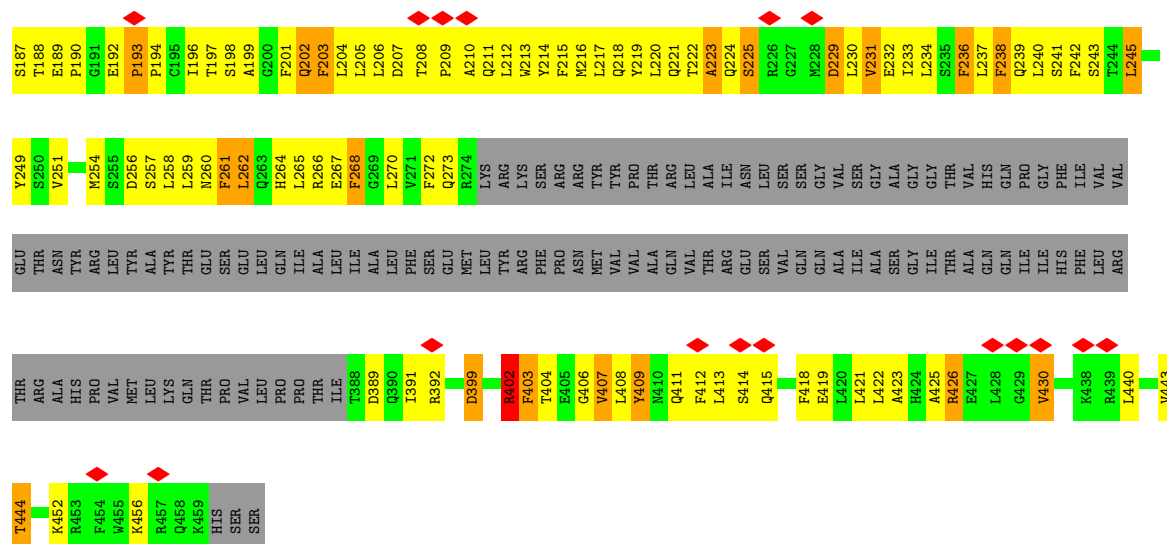
- Molecule 8 is a DNA chain called scp-Y.

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

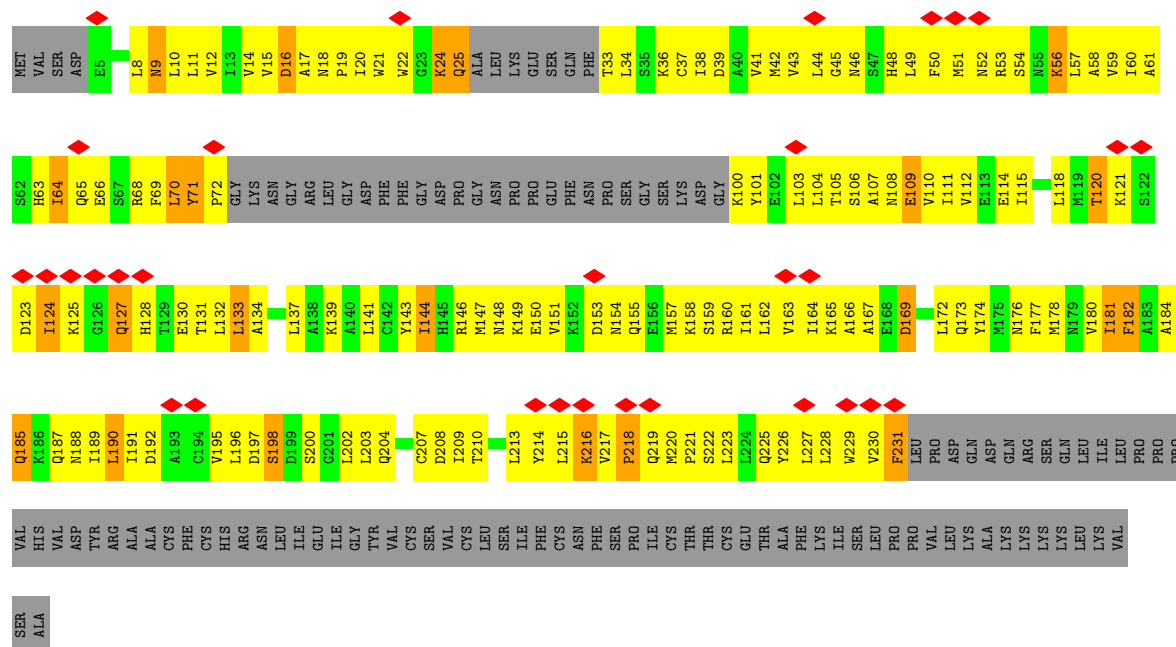


• Molecule 2: TFIIH basal transcription factor complex helicase XPD subunit

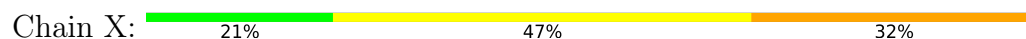




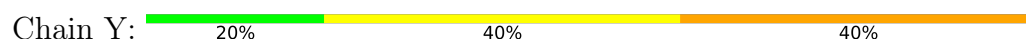
• Molecule 6: General transcription factor IIH subunit 3

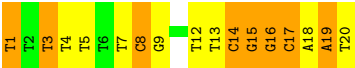


• Molecule 7: scp-X



• Molecule 8: scp-Y





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	219771	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	42	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	27500	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.181	Depositor
Minimum map value	-0.086	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	503.03998, 503.03998, 503.03998	wwPDB
Map dimensions	192, 192, 192	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.62, 2.62, 2.62	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 > 5$	RMSZ	# $ Z > 5$
1	V	1.88	79/3931 (2.0%)	2.33	250/5298 (4.7%)
2	W	2.00	125/5460 (2.3%)	2.36	328/7390 (4.4%)
3	0	2.00	29/1506 (1.9%)	2.24	65/2038 (3.2%)
4	1	1.29	1/496 (0.2%)	1.74	13/669 (1.9%)
5	2	1.23	0/2243	1.70	40/3024 (1.3%)
6	3	1.27	0/1548	1.55	15/2090 (0.7%)
7	X	1.46	2/443 (0.5%)	2.09	15/682 (2.2%)
8	Y	1.58	2/445 (0.4%)	2.26	22/685 (3.2%)
All	All	1.77	238/16072 (1.5%)	2.17	748/21876 (3.4%)

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 (238) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	0	142	GLU	N-CA	-10.05	1.37	1.45
3	0	158	HIS	CA-C	9.99	1.65	1.52
2	W	465	ASP	CA-C	9.07	1.64	1.52
1	V	590	MET	CA-C	8.93	1.64	1.52
1	V	255	MET	N-CA	8.58	1.54	1.47
1	V	376	ALA	CA-C	8.44	1.63	1.52
2	W	237	HIS	CE1-NE2	8.40	1.41	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	0	142	GLU	CA-C	8.37	1.60	1.52
1	V	374	TRP	CA-CB	8.21	1.66	1.53
3	0	122	GLY	N-CA	8.08	1.55	1.45
3	0	186	ILE	N-CA	7.75	1.55	1.46
2	W	670	GLY	CA-C	7.71	1.59	1.52
2	W	302	ASP	CA-C	7.71	1.62	1.53
2	W	606	GLU	CA-CB	7.67	1.65	1.53
1	V	289	TYR	N-CA	7.55	1.54	1.46
1	V	554	ARG	NE-CZ	7.39	1.41	1.33
1	V	391	ARG	CZ-NH2	-7.32	1.24	1.33
2	W	168	VAL	CA-CB	7.28	1.58	1.54
3	0	112	LYS	N-CA	7.28	1.56	1.46
2	W	566	LEU	CA-C	7.25	1.61	1.52
3	0	135	VAL	N-CA	7.21	1.55	1.46
2	W	521	GLY	N-CA	7.18	1.55	1.45
2	W	556	GLY	N-CA	7.13	1.52	1.45
3	0	203	ALA	CA-C	7.11	1.61	1.52
2	W	706	LEU	CA-C	7.10	1.62	1.52
2	W	272	ARG	CA-CB	7.09	1.64	1.53
2	W	531	VAL	C-N	7.04	1.39	1.33
3	0	169	ILE	CA-CB	7.03	1.63	1.54
2	W	546	GLU	C-N	7.02	1.43	1.33
2	W	327	GLU	CA-C	7.00	1.61	1.52
1	V	626	ILE	N-CA	6.92	1.54	1.46
2	W	272	ARG	N-CA	6.88	1.54	1.45
2	W	615	GLY	N-CA	6.88	1.52	1.44
1	V	382	SER	N-CA	6.81	1.54	1.46
2	W	429	ALA	CA-C	6.73	1.61	1.52
2	W	698	GLN	N-CA	6.65	1.54	1.46
3	0	188	THR	N-CA	6.63	1.54	1.46
1	V	353	ALA	C-N	6.61	1.42	1.33
1	V	425	ARG	C-O	-6.61	1.16	1.24
1	V	706	LYS	N-CA	-6.59	1.38	1.46
2	W	115	LEU	N-CA	6.58	1.54	1.46
2	W	683	ARG	CZ-NH2	-6.52	1.25	1.33
3	0	202	SER	CA-C	6.47	1.62	1.53
3	0	99	ASN	CA-CB	6.47	1.63	1.53
2	W	522	ASN	CA-C	6.47	1.61	1.52
1	V	453	ARG	CZ-NH2	-6.44	1.25	1.33
1	V	348	LEU	C-O	-6.44	1.16	1.24
2	W	321	GLY	N-CA	6.44	1.54	1.45
3	0	171	PHE	CA-C	6.43	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	W	291	GLY	CA-C	6.41	1.59	1.52
1	V	712	LEU	CA-C	6.31	1.60	1.52
1	V	479	ASP	N-CA	-6.28	1.38	1.46
2	W	685	ALA	N-CA	6.26	1.54	1.46
2	W	245	ASP	N-CA	6.25	1.53	1.46
1	V	414	GLY	CA-C	6.25	1.58	1.51
2	W	523	LEU	N-CA	6.25	1.53	1.46
2	W	47	GLY	N-CA	6.24	1.54	1.45
2	W	494	ILE	C-O	-6.24	1.17	1.24
2	W	490	LEU	CA-C	6.23	1.59	1.52
2	W	265	THR	N-CA	6.21	1.54	1.46
2	W	608	ILE	CA-CB	6.20	1.63	1.54
3	0	128	ILE	CA-C	6.16	1.60	1.52
2	W	67	VAL	N-CA	6.16	1.54	1.46
2	W	693	LEU	CA-CB	6.14	1.61	1.54
1	V	618	PRO	C-O	6.14	1.31	1.23
1	V	252	TYR	CA-CB	6.12	1.62	1.53
2	W	432	ILE	CA-CB	6.12	1.62	1.54
1	V	332	ARG	CA-C	6.12	1.60	1.52
2	W	675	GLY	N-CA	6.12	1.52	1.45
2	W	158	TYR	N-CA	6.11	1.54	1.46
2	W	491	CYS	N-CA	6.09	1.53	1.46
2	W	301	THR	N-CA	6.08	1.53	1.45
2	W	698	GLN	CA-C	6.07	1.60	1.52
2	W	511	ARG	NE-CZ	-6.06	1.26	1.33
3	0	199	ILE	C-N	6.05	1.41	1.33
2	W	69	LYS	CA-C	6.03	1.59	1.52
3	0	142	GLU	CA-CB	-6.03	1.46	1.54
2	W	559	GLU	C-O	-6.02	1.16	1.23
2	W	492	PRO	CA-C	6.02	1.59	1.52
2	W	18	TYR	CA-CB	6.00	1.62	1.53
3	0	171	PHE	N-CA	-6.00	1.39	1.46
2	W	83	VAL	CA-C	5.99	1.60	1.52
1	V	306	ILE	N-CA	-5.98	1.38	1.46
1	V	286	HIS	N-CA	5.97	1.53	1.46
1	V	609	LYS	N-CA	5.96	1.54	1.46
1	V	383	THR	CB-OG1	-5.95	1.34	1.43
2	W	701	LEU	N-CA	5.94	1.54	1.46
1	V	620	ALA	N-CA	5.92	1.54	1.46
1	V	633	ARG	CZ-NH1	-5.92	1.24	1.32
1	V	638	GLN	N-CA	5.91	1.53	1.46
2	W	244	ILE	CA-CB	5.89	1.61	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	V	286	HIS	CB-CG	5.87	1.58	1.50
1	V	551	HIS	CA-C	5.85	1.60	1.52
2	W	508	PHE	CA-CB	5.84	1.57	1.53
1	V	534	TYR	N-CA	5.83	1.53	1.46
1	V	468	ALA	N-CA	5.82	1.53	1.46
1	V	269	SER	N-CA	5.81	1.53	1.46
1	V	690	ILE	CA-CB	5.80	1.61	1.54
2	W	237	HIS	CA-C	5.80	1.60	1.52
1	V	332	ARG	CZ-NH2	-5.80	1.25	1.33
2	W	648	GLU	C-N	5.78	1.41	1.33
3	0	162	HIS	CA-C	5.76	1.60	1.52
1	V	437	LEU	C-N	5.75	1.41	1.33
2	W	242	VAL	N-CA	5.75	1.53	1.46
2	W	448	PHE	CA-C	5.75	1.60	1.52
2	W	632	ILE	N-CA	5.73	1.53	1.46
2	W	42	MET	CA-C	5.71	1.60	1.52
1	V	474	ASP	N-CA	5.70	1.53	1.46
2	W	666	ARG	NE-CZ	-5.70	1.26	1.33
2	W	705	ASN	C-O	-5.69	1.16	1.24
2	W	286	ARG	CZ-NH2	-5.67	1.26	1.33
3	0	207	VAL	CA-CB	5.67	1.61	1.54
1	V	461	HIS	CG-CD2	5.66	1.42	1.35
3	0	147	ASN	CA-C	5.66	1.60	1.52
2	W	256	LEU	C-N	-5.65	1.26	1.33
1	V	657	ALA	CA-C	5.64	1.59	1.52
8	Y	3	DT	C3'-C2'	-5.64	1.41	1.52
2	W	343	ARG	CA-C	5.64	1.60	1.52
2	W	152	LEU	N-CA	5.64	1.54	1.46
2	W	334	ARG	CZ-NH2	-5.64	1.26	1.33
2	W	160	GLU	CA-C	5.63	1.60	1.52
1	V	452	ARG	CZ-NH2	-5.62	1.26	1.33
3	0	190	LYS	N-CA	5.61	1.53	1.46
3	0	131	LEU	CA-C	5.60	1.60	1.52
1	V	640	LEU	CA-C	5.60	1.60	1.52
2	W	155	CYS	C-N	5.58	1.43	1.34
1	V	565	VAL	N-CA	5.57	1.53	1.46
2	W	600	ALA	N-CA	5.57	1.53	1.46
1	V	252	TYR	C-N	5.57	1.41	1.33
1	V	392	PHE	C-N	5.57	1.38	1.33
2	W	703	ASP	CA-C	5.56	1.60	1.53
2	W	291	GLY	C-N	5.55	1.41	1.34
1	V	639	ARG	N-CA	5.55	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	V	642	ARG	CD-NE	5.55	1.54	1.46
2	W	331	GLY	N-CA	-5.53	1.39	1.45
4	1	47	ALA	CA-C	-5.53	1.48	1.53
3	0	195	ARG	CA-CB	5.52	1.61	1.53
1	V	560	VAL	N-CA	-5.50	1.39	1.46
2	W	283	ASP	CA-CB	5.49	1.62	1.53
2	W	663	CYS	N-CA	-5.49	1.39	1.46
2	W	693	LEU	N-CA	5.46	1.51	1.45
2	W	518	ARG	CZ-NH2	-5.46	1.26	1.33
1	V	699	GLU	CA-C	5.45	1.59	1.52
1	V	310	LEU	CA-C	5.45	1.60	1.52
2	W	405	THR	N-CA	5.44	1.52	1.46
2	W	185	ARG	CA-CB	5.43	1.62	1.53
1	V	626	ILE	CB-CG1	5.43	1.64	1.53
1	V	296	ASP	CA-C	5.42	1.59	1.52
2	W	552	TRP	C-O	-5.42	1.17	1.24
2	W	77	VAL	CA-C	5.42	1.57	1.52
1	V	323	SER	CA-C	5.41	1.59	1.52
2	W	630	SER	CA-C	5.38	1.59	1.52
2	W	110	SER	CA-CB	5.38	1.62	1.53
3	0	217	GLY	N-CA	5.35	1.53	1.45
2	W	263	LEU	N-CA	5.32	1.52	1.46
2	W	510	THR	CA-C	-5.32	1.45	1.52
1	V	705	THR	CB-OG1	-5.32	1.35	1.43
2	W	426	PRO	CA-CB	-5.31	1.47	1.53
2	W	229	ALA	N-CA	5.31	1.52	1.46
2	W	298	ALA	CA-C	5.31	1.59	1.52
1	V	618	PRO	CA-CB	5.31	1.62	1.53
2	W	548	THR	N-CA	5.30	1.52	1.46
1	V	332	ARG	NE-CZ	-5.30	1.27	1.33
3	0	136	ASP	N-CA	5.29	1.52	1.46
1	V	692	LYS	CA-C	5.29	1.59	1.52
1	V	367	SER	N-CA	-5.28	1.39	1.46
2	W	66	GLU	N-CA	5.28	1.53	1.46
2	W	412	LYS	N-CA	5.27	1.53	1.46
8	Y	8	DC	P-O5'	-5.26	1.50	1.60
2	W	592	ARG	CD-NE	5.26	1.53	1.46
2	W	341	LYS	CA-CB	5.25	1.61	1.53
2	W	85	GLU	CA-C	5.25	1.59	1.52
2	W	95	GLU	CA-C	5.25	1.59	1.52
2	W	310	LEU	CA-CB	5.25	1.60	1.53
2	W	713	GLY	CA-C	5.25	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	X	10	DG	N7-C5	5.23	1.49	1.39
2	W	482	THR	N-CA	5.23	1.52	1.46
1	V	561	PHE	C-N	5.22	1.40	1.33
2	W	48	LYS	N-CA	5.22	1.52	1.46
1	V	420	SER	N-CA	5.22	1.52	1.46
2	W	398	THR	CB-OG1	-5.22	1.35	1.43
1	V	303	ASN	C-N	5.22	1.37	1.33
1	V	521	GLU	CA-CB	5.21	1.61	1.53
2	W	658	ARG	CZ-NH2	-5.20	1.26	1.33
1	V	636	GLU	N-CA	5.20	1.52	1.46
1	V	316	LEU	CA-CB	5.19	1.61	1.53
2	W	567	LEU	N-CA	-5.18	1.40	1.45
1	V	598	HIS	CB-CG	5.18	1.57	1.50
1	V	386	ASP	N-CA	5.17	1.51	1.46
2	W	257	ASP	CA-C	5.17	1.59	1.52
2	W	96	LYS	N-CA	5.17	1.52	1.46
2	W	168	VAL	N-CA	5.17	1.52	1.46
2	W	418	ILE	N-CA	5.16	1.52	1.46
1	V	398	ASP	N-CA	5.15	1.52	1.45
1	V	410	TYR	N-CA	5.15	1.52	1.46
1	V	607	ILE	C-O	-5.14	1.18	1.24
1	V	693	LEU	CA-C	5.14	1.59	1.53
2	W	30	ARG	N-CA	5.14	1.52	1.46
3	O	140	HIS	ND1-CE1	5.14	1.37	1.32
1	V	333	ALA	CA-C	-5.13	1.45	1.52
2	W	75	ARG	CZ-NH2	-5.13	1.26	1.33
3	O	197	SER	N-CA	-5.13	1.39	1.46
1	V	623	LEU	C-O	-5.13	1.18	1.24
2	W	491	CYS	CA-C	5.13	1.58	1.53
1	V	532	LEU	CA-CB	5.12	1.61	1.53
2	W	699	GLU	N-CA	5.12	1.52	1.46
2	W	501	GLN	CA-C	5.12	1.59	1.52
1	V	408	SER	CA-C	-5.12	1.46	1.52
2	W	20	GLU	C-N	-5.11	1.26	1.33
2	W	531	VAL	C-O	-5.10	1.18	1.24
3	O	105	GLY	C-N	5.09	1.40	1.33
3	O	195	ARG	CZ-NH1	-5.08	1.25	1.32
2	W	679	PHE	CA-CB	5.08	1.62	1.53
2	W	452	GLN	CA-CB	5.08	1.61	1.53
2	W	672	THR	N-CA	5.08	1.52	1.46
2	W	303	ALA	CA-C	5.08	1.59	1.52
2	W	61	ARG	CA-C	5.08	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	W	626	VAL	N-CA	5.07	1.52	1.46
2	W	122	THR	CA-C	5.07	1.58	1.52
1	V	702	ALA	N-CA	5.06	1.52	1.45
1	V	633	ARG	N-CA	5.06	1.52	1.46
2	W	629	GLN	N-CA	-5.06	1.39	1.46
1	V	419	ARG	CA-C	5.05	1.57	1.52
1	V	617	LEU	N-CA	5.05	1.51	1.45
2	W	651	PHE	N-CA	-5.05	1.40	1.46
7	X	8	DA	C1'-N9	5.05	1.56	1.46
2	W	286	ARG	CZ-NH1	-5.04	1.25	1.32
2	W	498	GLY	CA-C	-5.04	1.47	1.52
1	V	489	TYR	CA-C	5.04	1.58	1.52
1	V	338	ILE	CA-C	5.04	1.58	1.52
2	W	686	ARG	CD-NE	5.02	1.53	1.46
2	W	322	SER	N-CA	5.02	1.52	1.46
2	W	185	ARG	NE-CZ	-5.02	1.27	1.33
2	W	210	HIS	CE1-NE2	5.01	1.37	1.32
2	W	275	GLU	C-N	5.01	1.40	1.33
2	W	335	ARG	CA-C	-5.01	1.46	1.52
1	V	289	TYR	CA-C	5.00	1.58	1.52
2	W	466	ILE	C-O	-5.00	1.18	1.24

All (748) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	0	77	LYS	C-N-CD	-14.05	67.39	125.00
6	3	71	TYR	C-N-CD	-12.17	75.09	125.00
2	W	175	TYR	N-CA-C	11.98	127.85	110.24
1	V	520	ARG	O-C-N	11.82	135.70	122.11
2	W	26	ARG	NE-CZ-NH2	11.67	129.70	119.20
1	V	520	ARG	CA-C-N	-11.62	100.72	120.58
1	V	520	ARG	C-N-CA	-11.62	100.72	120.58
5	2	236	PHE	CA-CB-CG	-11.13	102.67	113.80
1	V	550	PHE	CA-CB-CG	11.12	124.92	113.80
1	V	358	ARG	NE-CZ-NH2	10.95	129.06	119.20
2	W	335	ARG	NE-CZ-NH1	-10.94	110.56	121.50
1	V	270	PHE	CA-CB-CG	10.59	124.39	113.80
1	V	649	GLY	N-CA-C	-10.45	88.41	113.18
2	W	167	GLU	CA-C-N	10.42	128.67	120.33
2	W	167	GLU	C-N-CA	10.42	128.67	120.33
2	W	26	ARG	NH1-CZ-NH2	-9.82	106.53	119.30
2	W	287	ARG	NE-CZ-NH2	9.82	128.03	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	V	586	GLN	OE1-CD-NE2	-9.80	112.80	122.60
2	W	117	ILE	N-CA-C	9.68	119.63	110.53
4	1	44	PHE	CA-CB-CG	-9.65	104.15	113.80
1	V	638	GLN	OE1-CD-NE2	-9.64	112.96	122.60
1	V	634	ARG	NE-CZ-NH2	9.54	127.79	119.20
1	V	388	GLN	OE1-CD-NE2	-9.54	113.06	122.60
2	W	147	GLN	OE1-CD-NE2	-9.46	113.14	122.60
1	V	621	ASN	CA-CB-CG	9.42	122.02	112.60
1	V	377	GLN	OE1-CD-NE2	-9.36	113.24	122.60
6	3	231	PHE	CA-CB-CG	-9.12	104.68	113.80
2	W	335	ARG	NE-CZ-NH2	9.05	127.34	119.20
1	V	649	GLY	CA-C-O	-9.04	104.84	120.57
1	V	668	GLN	OE1-CD-NE2	-9.03	113.58	122.60
5	2	61	PHE	CB-CA-C	-8.97	97.04	110.95
1	V	421	TRP	CD2-CE3-CZ3	8.96	130.24	118.60
2	W	530	VAL	N-CA-CB	8.93	120.74	110.65
1	V	334	ARG	CD-NE-CZ	8.90	136.86	124.40
2	W	270	VAL	CA-C-O	8.85	131.85	120.78
2	W	112	ARG	CA-C-N	8.81	132.09	120.28
2	W	112	ARG	C-N-CA	8.81	132.09	120.28
1	V	665	GLN	OE1-CD-NE2	-8.78	113.83	122.60
2	W	76	THR	CA-CB-OG1	8.73	122.69	109.60
2	W	332	PHE	CA-CB-CG	8.70	122.50	113.80
4	1	34	ILE	CA-C-N	-8.68	111.83	123.12
4	1	34	ILE	C-N-CA	-8.68	111.83	123.12
5	2	268	PHE	CA-CB-CG	-8.68	105.12	113.80
4	1	47	ALA	CB-CA-C	-8.56	106.69	116.54
1	V	484	ILE	N-CA-C	8.46	119.08	111.81
2	W	469	LYS	CA-C-N	8.44	131.37	120.56
2	W	469	LYS	C-N-CA	8.44	131.37	120.56
2	W	193	PHE	CA-CB-CG	8.42	122.22	113.80
2	W	263	LEU	N-CA-CB	-8.39	97.78	110.12
2	W	343	ARG	NE-CZ-NH2	8.35	126.71	119.20
2	W	77	VAL	N-CA-CB	-8.23	105.31	110.50
1	V	392	PHE	CA-CB-CG	8.18	121.98	113.80
2	W	157	PHE	CA-CB-CG	8.18	121.98	113.80
1	V	433	GLN	N-CA-C	8.16	121.79	112.57
2	W	521	GLY	CA-C-N	8.15	131.04	120.44
2	W	521	GLY	C-N-CA	8.15	131.04	120.44
5	2	47	GLU	N-CA-C	8.13	120.05	111.03
2	W	667	ALA	N-CA-C	7.99	119.62	111.07
2	W	395	SER	CA-C-O	-7.96	110.61	118.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	V	333	ALA	N-CA-C	7.95	121.92	111.75
1	V	421	TRP	CE2-CD2-CE3	-7.94	110.86	118.80
2	W	16	TYR	N-CA-C	7.84	118.33	108.45
1	V	394	SER	N-CA-C	7.84	121.94	112.38
2	W	696	TRP	N-CA-C	7.83	120.87	110.53
2	W	345	ARG	N-CA-C	7.82	122.17	112.47
5	2	160	LEU	N-CA-C	-7.80	102.78	111.28
1	V	648	LYS	N-CA-C	7.79	121.53	110.23
2	W	107	LEU	N-CA-C	7.77	120.75	107.93
8	Y	14	DC	N3-C2-O2	-7.76	110.25	121.90
5	2	162	PHE	CA-CB-CG	-7.76	106.04	113.80
8	Y	15	DG	N9-C1'-C2'	7.75	125.12	113.50
2	W	499	ASN	OD1-CG-ND2	-7.73	114.87	122.60
2	W	724	MET	CA-C-N	7.73	130.63	120.28
2	W	724	MET	C-N-CA	7.73	130.63	120.28
2	W	304	HIS	CB-CG-CD2	-7.67	121.22	131.20
1	V	640	LEU	O-C-N	7.63	130.25	122.08
1	V	710	GLN	CA-C-N	7.63	130.35	120.44
1	V	710	GLN	C-N-CA	7.63	130.35	120.44
8	Y	20	DT	O4'-C1'-N1	7.62	119.83	108.40
2	W	497	ARG	CD-NE-CZ	7.62	135.06	124.40
6	3	182	PHE	CA-CB-CG	-7.57	106.23	113.80
3	0	237	SER	CA-C-N	7.57	128.17	120.38
3	0	237	SER	C-N-CA	7.57	128.17	120.38
1	V	422	GLU	CA-C-O	7.56	128.79	119.11
2	W	509	GLU	N-CA-C	7.54	122.15	112.34
2	W	295	ALA	N-CA-C	7.54	119.28	111.14
6	3	127	GLN	N-CA-C	-7.54	103.14	111.36
2	W	165	GLY	CA-C-N	7.53	130.99	120.29
2	W	165	GLY	C-N-CA	7.53	130.99	120.29
1	V	355	CYS	CA-C-N	7.51	130.66	120.44
1	V	355	CYS	C-N-CA	7.51	130.66	120.44
5	2	35	TYR	CA-CB-CG	-7.50	100.39	113.90
2	W	329	PHE	CA-CB-CG	7.47	121.27	113.80
3	0	206	ARG	NH1-CZ-NH2	-7.45	109.61	119.30
1	V	669	GLU	CA-C-N	7.44	131.61	120.31
1	V	669	GLU	C-N-CA	7.44	131.61	120.31
2	W	41	GLU	O-C-N	7.42	131.66	123.27
3	0	123	ASN	CA-C-N	7.41	127.42	119.28
3	0	123	ASN	C-N-CA	7.41	127.42	119.28
5	2	245	LEU	N-CA-C	-7.38	101.33	110.41
2	W	302	ASP	CA-C-O	7.36	126.80	119.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	W	487	ARG	N-CA-C	7.35	120.16	111.71
2	W	654	PHE	CA-C-N	7.34	130.11	120.28
2	W	654	PHE	C-N-CA	7.34	130.11	120.28
3	0	92	VAL	O-C-N	7.33	129.10	121.91
8	Y	12	DT	C6-C5-C7	-7.33	113.00	124.00
2	W	690	ARG	NE-CZ-NH2	7.28	125.75	119.20
6	3	16	ASP	CA-C-N	7.28	132.87	120.72
6	3	16	ASP	C-N-CA	7.28	132.87	120.72
2	W	683	ARG	NE-CZ-NH2	7.27	125.74	119.20
3	0	195	ARG	NE-CZ-NH1	7.26	128.76	121.50
1	V	486	PRO	CA-C-N	7.25	132.79	121.99
1	V	486	PRO	C-N-CA	7.25	132.79	121.99
1	V	580	ILE	CA-C-O	7.22	128.01	120.36
1	V	641	GLY	N-CA-C	7.20	120.85	112.50
2	W	288	LEU	O-C-N	-7.20	114.55	122.03
5	2	89	LEU	N-CA-C	-7.13	103.58	111.36
2	W	323	ILE	CA-C-N	7.13	129.84	120.28
2	W	323	ILE	C-N-CA	7.13	129.84	120.28
1	V	393	THR	O-C-N	-7.07	113.84	122.68
1	V	598	HIS	CB-CG-CD2	-7.06	122.02	131.20
8	Y	4	DT	C6-C5-C7	-7.06	113.40	124.00
2	W	232	VAL	CA-CB-CG1	7.06	122.41	110.40
5	2	193	PRO	N-CA-C	7.05	119.31	110.70
2	W	715	GLN	OE1-CD-NE2	-7.04	115.56	122.60
8	Y	17	DC	N3-C4-N4	-7.03	107.35	117.90
1	V	267	THR	CA-C-O	-7.01	112.04	120.32
1	V	421	TRP	NE1-CE2-CD2	-7.00	98.30	107.40
2	W	653	THR	CA-C-N	6.99	129.65	120.28
2	W	653	THR	C-N-CA	6.99	129.65	120.28
3	0	147	ASN	OD1-CG-ND2	-6.98	115.62	122.60
2	W	340	VAL	CA-C-N	6.97	129.63	120.28
2	W	340	VAL	C-N-CA	6.97	129.63	120.28
5	2	225	SER	N-CA-C	-6.97	103.61	111.14
1	V	274	GLN	O-C-N	-6.96	116.57	123.46
8	Y	19	DA	C4'-C3'-O3'	-6.96	99.57	110.00
1	V	558	ILE	N-CA-CB	-6.94	101.39	111.52
2	W	98	GLU	CA-C-N	6.94	130.27	122.15
2	W	98	GLU	C-N-CA	6.94	130.27	122.15
4	1	45	VAL	CA-C-N	-6.93	113.43	122.51
4	1	45	VAL	C-N-CA	-6.93	113.43	122.51
2	W	186	ARG	NE-CZ-NH1	6.92	128.43	121.50
1	V	715	LYS	N-CA-C	6.88	118.77	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	W	562	GLN	OE1-CD-NE2	-6.87	115.73	122.60
2	W	328	HIS	CB-CG-CD2	-6.86	122.29	131.20
3	0	145	LEU	N-CA-C	6.85	118.74	111.28
2	W	497	ARG	NE-CZ-NH1	6.81	128.31	121.50
5	2	193	PRO	CA-N-CD	-6.81	102.47	112.00
2	W	462	SER	CA-C-N	6.80	126.48	119.82
2	W	462	SER	C-N-CA	6.80	126.48	119.82
1	V	317	ARG	CA-C-O	-6.80	113.01	120.69
2	W	34	ALA	CA-C-N	6.80	132.47	122.82
2	W	34	ALA	C-N-CA	6.80	132.47	122.82
1	V	348	LEU	CA-C-O	-6.79	113.35	120.55
2	W	703	ASP	N-CA-C	6.79	120.91	111.74
2	W	66	GLU	CA-C-N	6.79	134.19	121.97
2	W	66	GLU	C-N-CA	6.79	134.19	121.97
2	W	343	ARG	NE-CZ-NH1	-6.79	114.71	121.50
2	W	97	GLN	OE1-CD-NE2	-6.77	115.83	122.60
2	W	595	ILE	CB-CA-C	6.76	122.38	111.29
2	W	659	HIS	CA-CB-CG	6.76	120.56	113.80
1	V	608	SER	O-C-N	-6.74	113.85	122.20
2	W	263	LEU	O-C-N	-6.73	114.99	122.12
2	W	467	TYR	CA-C-N	6.73	126.68	119.28
2	W	467	TYR	C-N-CA	6.73	126.68	119.28
3	0	64	VAL	O-C-N	-6.72	116.00	123.26
2	W	473	PHE	CA-CB-CG	-6.72	107.08	113.80
2	W	591	GLY	CA-C-O	-6.72	113.74	121.47
1	V	331	GLY	CA-C-N	6.72	129.28	120.28
1	V	331	GLY	C-N-CA	6.72	129.28	120.28
2	W	270	VAL	CA-C-N	6.72	130.51	120.17
2	W	270	VAL	C-N-CA	6.72	130.51	120.17
2	W	131	ASP	CA-C-N	6.71	127.43	119.98
2	W	131	ASP	C-N-CA	6.71	127.43	119.98
2	W	723	GLN	OE1-CD-NE2	-6.69	115.91	122.60
3	0	236	VAL	CA-CB-CG1	6.69	121.78	110.40
1	V	553	ARG	NE-CZ-NH2	6.69	125.22	119.20
3	0	59	ARG	NE-CZ-NH2	6.66	125.20	119.20
3	0	92	VAL	CA-C-O	-6.65	114.12	121.17
2	W	80	ILE	N-CA-CB	6.60	119.52	110.54
1	V	711	GLN	OE1-CD-NE2	-6.60	116.00	122.60
2	W	629	GLN	CA-C-O	-6.59	113.77	120.96
5	2	242	PHE	CA-CB-CG	-6.59	107.21	113.80
1	V	714	GLN	OE1-CD-NE2	-6.58	116.02	122.60
2	W	187	GLN	OE1-CD-NE2	-6.58	116.02	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	V	598	HIS	CB-CG-ND1	6.57	132.55	122.70
1	V	388	GLN	CG-CD-NE2	6.57	126.25	116.40
7	X	1	DA	N1-C6-N6	-6.57	109.15	119.00
1	V	358	ARG	NH1-CZ-NH2	-6.56	110.77	119.30
7	X	4	DG	O4'-C1'-N9	6.55	118.23	108.40
1	V	701	LEU	O-C-N	-6.55	115.57	123.10
5	2	272	PHE	CA-CB-CG	-6.55	107.25	113.80
1	V	366	ASN	CA-CB-CG	6.53	119.13	112.60
2	W	314	VAL	N-CA-CB	6.53	118.19	110.55
2	W	152	LEU	O-C-N	-6.51	113.83	121.32
2	W	120	GLU	CA-C-N	6.50	128.89	120.56
2	W	120	GLU	C-N-CA	6.50	128.89	120.56
1	V	374	TRP	O-C-N	-6.50	114.74	122.15
2	W	406	LEU	CA-C-O	-6.50	114.17	121.00
1	V	281	GLN	O-C-N	6.50	128.84	122.09
2	W	540	THR	O-C-N	-6.49	114.29	122.27
1	V	624	ILE	N-CA-CB	-6.49	103.21	111.64
1	V	467	THR	N-CA-C	6.48	118.71	108.79
1	V	409	THR	CA-C-N	6.48	131.06	120.63
1	V	409	THR	C-N-CA	6.48	131.06	120.63
1	V	328	PHE	CA-C-N	6.47	134.09	121.41
1	V	328	PHE	C-N-CA	6.47	134.09	121.41
2	W	491	CYS	CA-C-N	6.46	126.84	119.92
2	W	491	CYS	C-N-CA	6.46	126.84	119.92
2	W	138	THR	CA-C-O	-6.45	113.71	120.55
1	V	454	VAL	CA-C-N	6.45	129.45	120.29
1	V	454	VAL	C-N-CA	6.45	129.45	120.29
2	W	88	ARG	CA-C-N	6.45	129.45	120.29
2	W	88	ARG	C-N-CA	6.45	129.45	120.29
1	V	434	GLU	N-CA-C	6.45	118.39	111.36
2	W	161	PHE	CA-CB-CG	6.45	120.25	113.80
2	W	33	ASP	N-CA-C	6.45	119.12	111.71
2	W	511	ARG	NE-CZ-NH2	6.43	124.99	119.20
2	W	282	ARG	N-CA-C	-6.42	104.20	111.07
3	0	58	MET	O-C-N	6.42	131.10	123.27
2	W	210	HIS	ND1-CG-CD2	6.41	112.51	106.10
1	V	643	VAL	CA-CB-CG1	6.40	121.29	110.40
2	W	166	ARG	CD-NE-CZ	6.40	133.36	124.40
1	V	709	GLN	CA-C-N	6.39	128.85	120.28
1	V	709	GLN	C-N-CA	6.39	128.85	120.28
1	V	391	ARG	NE-CZ-NH1	-6.39	115.11	121.50
2	W	698	GLN	OE1-CD-NE2	-6.39	116.21	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	W	552	TRP	N-CA-C	-6.38	104.25	111.14
5	2	238	PHE	CA-CB-CG	-6.38	107.42	113.80
2	W	299	ARG	NE-CZ-NH1	6.38	127.88	121.50
2	W	416	ILE	CA-C-N	6.37	131.84	123.06
2	W	416	ILE	C-N-CA	6.37	131.84	123.06
2	W	257	ASP	CA-CB-CG	-6.36	106.24	112.60
6	3	218	PRO	N-CA-C	-6.36	99.16	111.69
3	0	224	ASP	N-CA-CB	-6.36	101.52	111.56
2	W	416	ILE	O-C-N	-6.35	115.71	122.95
3	0	105	GLY	CA-C-O	-6.35	116.05	121.57
2	W	83	VAL	CA-C-N	6.34	128.55	120.56
2	W	83	VAL	C-N-CA	6.34	128.55	120.56
1	V	396	ALA	CA-C-N	6.33	132.90	121.89
1	V	396	ALA	C-N-CA	6.33	132.90	121.89
2	W	70	LEU	CA-C-O	-6.32	113.59	120.36
2	W	258	ARG	CA-C-O	-6.31	113.73	120.42
3	0	111	SER	CA-C-N	6.28	132.91	123.05
3	0	111	SER	C-N-CA	6.28	132.91	123.05
1	V	373	GLN	OE1-CD-NE2	-6.27	116.33	122.60
1	V	449	LYS	N-CA-C	6.27	118.11	111.28
1	V	689	VAL	O-C-N	-6.26	116.60	123.18
2	W	299	ARG	N-CA-C	-6.26	104.85	113.18
2	W	242	VAL	CA-C-O	-6.26	114.21	120.85
2	W	461	LEU	CA-C-N	6.26	128.84	120.58
2	W	461	LEU	C-N-CA	6.26	128.84	120.58
1	V	545	GLN	N-CA-C	6.25	118.10	111.28
2	W	238	ASN	OD1-CG-ND2	-6.25	116.35	122.60
6	3	181	ILE	CB-CA-C	-6.24	103.98	111.97
1	V	341	PRO	CB-CA-C	-6.24	103.41	111.39
1	V	480	LEU	CA-C-N	6.24	128.64	120.28
1	V	480	LEU	C-N-CA	6.24	128.64	120.28
2	W	63	TYR	CA-C-N	6.23	126.13	119.28
2	W	63	TYR	C-N-CA	6.23	126.13	119.28
2	W	113	LYS	CA-C-O	-6.23	113.95	120.55
2	W	286	ARG	NE-CZ-NH2	6.23	124.80	119.20
2	W	662	GLN	OE1-CD-NE2	-6.22	116.38	122.60
1	V	341	PRO	N-CA-CB	6.22	108.54	103.32
8	Y	17	DC	C5-C4-N4	6.22	129.62	120.30
5	2	229	ASP	CA-CB-CG	-6.21	106.39	112.60
3	0	123	ASN	OD1-CG-ND2	-6.21	116.39	122.60
2	W	447	VAL	O-C-N	6.19	127.88	121.87
2	W	332	PHE	O-C-N	-6.19	115.56	122.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	W	585	GLN	O-C-N	6.18	130.26	122.23
3	0	206	ARG	NE-CZ-NH1	6.17	127.67	121.50
1	V	337	VAL	CA-C-N	6.17	131.57	122.99
1	V	337	VAL	C-N-CA	6.17	131.57	122.99
1	V	524	ALA	N-CA-C	6.17	118.01	111.28
2	W	50	VAL	CA-CB-CG1	6.17	120.89	110.40
2	W	125	ARG	CD-NE-CZ	6.17	133.04	124.40
2	W	272	ARG	NH1-CZ-NH2	-6.16	111.29	119.30
1	V	330	ASN	CA-C-O	-6.16	113.40	120.24
2	W	434	HIS	N-CA-C	6.16	118.13	108.96
8	Y	3	DT	O5'-C5'-C4'	6.15	120.03	110.80
2	W	592	ARG	NH1-CZ-NH2	-6.15	111.31	119.30
3	0	62	TYR	CA-C-O	6.15	126.94	120.54
2	W	662	GLN	CG-CD-NE2	6.14	125.61	116.40
1	V	286	HIS	CE1-NE2-CD2	-6.14	102.86	109.00
2	W	312	ASP	N-CA-C	6.14	117.77	111.14
1	V	367	SER	CA-C-N	6.13	129.00	120.29
1	V	367	SER	C-N-CA	6.13	129.00	120.29
1	V	474	ASP	CA-C-N	6.12	133.22	121.54
1	V	474	ASP	C-N-CA	6.12	133.22	121.54
2	W	301	THR	CA-C-N	6.11	130.44	120.23
2	W	301	THR	C-N-CA	6.11	130.44	120.23
2	W	345	ARG	CD-NE-CZ	6.11	132.95	124.40
2	W	463	PRO	N-CA-CB	6.10	109.32	103.52
3	0	140	HIS	CB-CG-CD2	-6.10	123.27	131.20
1	V	251	PHE	CA-C-N	6.10	130.22	121.50
1	V	251	PHE	C-N-CA	6.10	130.22	121.50
3	0	184	ASP	CA-CB-CG	6.08	118.68	112.60
2	W	183	LEU	CA-C-N	6.08	126.68	120.00
2	W	183	LEU	C-N-CA	6.08	126.68	120.00
2	W	314	VAL	N-CA-C	6.07	116.25	110.42
2	W	30	ARG	CD-NE-CZ	6.07	132.90	124.40
7	X	9	DA	P-O5'-C5'	6.07	129.10	120.00
1	V	529	LYS	O-C-N	-6.06	115.29	122.20
2	W	210	HIS	CB-CG-CD2	-6.06	123.32	131.20
1	V	337	VAL	CA-C-O	-6.04	115.65	121.63
1	V	709	GLN	OE1-CD-NE2	-6.03	116.57	122.60
1	V	713	LEU	CA-C-O	-6.03	114.45	120.90
5	2	171	VAL	CB-CA-C	-6.01	104.27	111.97
1	V	404	SER	CB-CA-C	6.00	122.37	110.42
1	V	278	GLU	CA-C-O	-6.00	112.69	120.25
1	V	651	VAL	CA-C-O	-6.00	113.28	120.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	W	621	PHE	CA-CB-CG	-6.00	107.80	113.80
2	W	164	HIS	CB-CG-CD2	-6.00	123.41	131.20
2	W	569	ILE	N-CA-CB	-6.00	105.23	112.07
5	2	79	PHE	CA-CB-CG	-5.99	107.81	113.80
1	V	379	LYS	N-CA-C	5.99	119.41	111.75
8	Y	3	DT	C6-C5-C7	-5.98	115.03	124.00
2	W	590	ASN	N-CA-C	5.97	119.82	110.32
1	V	410	TYR	CA-C-N	5.97	129.59	120.82
1	V	410	TYR	C-N-CA	5.97	129.59	120.82
2	W	470	ILE	CB-CG1-CD1	-5.97	101.27	113.80
1	V	561	PHE	O-C-N	-5.96	116.53	123.27
7	X	5	DC	O4'-C1'-N1	5.96	117.34	108.40
3	0	130	SER	N-CA-C	5.96	117.85	111.36
8	Y	14	DC	N1-C2-O2	5.96	128.13	119.20
2	W	161	PHE	O-C-N	-5.95	115.90	122.09
3	0	74	GLN	OE1-CD-NE2	-5.95	116.65	122.60
1	V	607	ILE	CA-CB-CG1	5.95	120.51	110.40
3	0	158	HIS	CB-CG-CD2	-5.94	123.47	131.20
5	2	203	PHE	CA-CB-CG	-5.94	107.86	113.80
1	V	403	CYS	N-CA-CB	-5.94	102.03	110.46
2	W	122	THR	CA-C-N	5.94	127.26	119.84
2	W	122	THR	C-N-CA	5.94	127.26	119.84
1	V	307	ASN	CA-CB-CG	5.94	118.54	112.60
1	V	603	ASN	CA-CB-CG	5.93	118.53	112.60
1	V	459	GLN	CA-C-N	5.92	132.85	121.54
1	V	459	GLN	C-N-CA	5.92	132.85	121.54
2	W	289	VAL	N-CA-C	5.92	116.66	110.62
7	X	19	DA	N1-C6-N6	-5.92	110.12	119.00
2	W	92	ASN	OD1-CG-ND2	-5.91	116.69	122.60
2	W	650	ASP	CA-C-O	-5.91	114.61	120.70
2	W	20	GLU	CA-C-O	-5.91	114.29	120.55
2	W	442	LEU	CA-C-N	5.91	128.68	120.29
2	W	442	LEU	C-N-CA	5.91	128.68	120.29
2	W	606	GLU	O-C-N	-5.91	115.31	122.22
1	V	642	ARG	NE-CZ-NH1	5.90	127.40	121.50
2	W	416	ILE	CA-C-O	5.90	127.38	120.71
2	W	480	THR	CA-CB-OG1	5.90	118.45	109.60
7	X	9	DA	O5'-C5'-C4'	5.90	119.65	110.80
2	W	592	ARG	NE-CZ-NH1	5.90	127.40	121.50
2	W	280	ARG	CA-C-O	-5.89	114.17	120.42
2	W	623	VAL	N-CA-C	-5.88	103.57	108.63
1	V	527	THR	CA-C-O	-5.86	115.31	121.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	W	37	HIS	N-CA-C	5.86	117.76	108.79
1	V	369	VAL	CA-CB-CG1	5.85	120.35	110.40
1	V	485	GLY	CA-C-N	5.85	126.18	119.92
1	V	485	GLY	C-N-CA	5.85	126.18	119.92
1	V	633	ARG	NE-CZ-NH2	-5.84	113.94	119.20
3	0	190	LYS	N-CA-C	-5.84	105.00	111.36
5	2	175	LEU	N-CA-CB	5.84	119.21	110.22
6	3	64	ILE	CB-CA-C	-5.83	104.51	111.97
2	W	239	ILE	N-CA-C	5.82	116.56	110.62
2	W	152	LEU	CA-C-N	5.82	125.77	119.78
2	W	152	LEU	C-N-CA	5.82	125.77	119.78
3	0	56	GLY	CA-C-N	5.82	131.76	122.10
3	0	56	GLY	C-N-CA	5.82	131.76	122.10
3	0	203	ALA	N-CA-C	5.82	118.95	108.48
2	W	683	ARG	CD-NE-CZ	5.81	132.54	124.40
6	3	153	ASP	N-CA-C	-5.81	104.94	111.28
2	W	548	THR	CA-C-O	-5.81	114.72	120.82
2	W	213	LEU	N-CA-C	5.81	118.39	111.71
1	V	335	SER	N-CA-C	5.80	117.89	109.07
2	W	92	ASN	CB-CG-ND2	5.80	125.11	116.40
2	W	722	ARG	CD-NE-CZ	5.80	132.53	124.40
2	W	685	ALA	N-CA-C	5.80	118.35	111.33
2	W	312	ASP	N-CA-CB	-5.80	101.66	110.07
1	V	674	THR	CA-C-N	5.79	127.97	120.44
1	V	674	THR	C-N-CA	5.79	127.97	120.44
1	V	412	MET	O-C-N	-5.79	115.03	122.21
1	V	461	HIS	CB-CG-CD2	-5.79	123.67	131.20
1	V	594	GLN	O-C-N	-5.79	115.84	122.09
2	W	716	VAL	N-CA-CB	5.79	119.26	110.58
1	V	435	TRP	CE2-CD2-CE3	-5.78	113.02	118.80
4	1	34	ILE	N-CA-C	5.78	115.96	110.42
2	W	112	ARG	NE-CZ-NH1	5.77	127.27	121.50
2	W	206	VAL	CA-CB-CG1	5.77	120.21	110.40
1	V	281	GLN	N-CA-C	5.77	118.03	111.11
1	V	276	MET	CA-C-O	-5.77	114.80	121.26
2	W	415	THR	CA-C-O	5.75	127.62	120.54
2	W	586	GLU	N-CA-C	5.75	117.22	111.07
4	1	48	GLU	N-CA-C	-5.75	98.55	110.80
1	V	665	GLN	CG-CD-NE2	5.74	125.02	116.40
2	W	672	THR	N-CA-C	5.74	119.91	113.02
1	V	338	ILE	CA-C-O	-5.74	114.27	120.36
2	W	593	GLY	CA-C-N	5.74	132.87	122.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	W	593	GLY	C-N-CA	5.74	132.87	122.02
3	0	160	PRO	CA-C-N	5.74	132.65	121.41
3	0	160	PRO	C-N-CA	5.74	132.65	121.41
1	V	332	ARG	NE-CZ-NH1	5.73	127.23	121.50
1	V	520	ARG	NE-CZ-NH2	5.73	124.36	119.20
1	V	479	ASP	N-CA-C	5.72	118.46	111.82
2	W	218	ALA	N-CA-C	5.72	117.52	111.28
1	V	526	LYS	CA-C-N	5.72	131.81	121.06
1	V	526	LYS	C-N-CA	5.72	131.81	121.06
8	Y	1	DT	N3-C2-O2	-5.72	113.42	122.00
1	V	354	ALA	N-CA-C	5.72	117.51	111.28
1	V	497	GLN	OE1-CD-NE2	-5.72	116.88	122.60
1	V	656	ASN	CA-CB-CG	5.72	118.32	112.60
3	0	92	VAL	CB-CA-C	-5.71	104.66	111.97
1	V	488	LEU	N-CA-C	5.71	117.59	111.36
1	V	567	ALA	CA-C-N	5.71	128.25	120.54
1	V	567	ALA	C-N-CA	5.71	128.25	120.54
6	3	120	THR	CA-C-N	5.71	127.93	120.28
6	3	120	THR	C-N-CA	5.71	127.93	120.28
1	V	679	PHE	CA-CB-CG	5.71	119.51	113.80
2	W	669	ARG	NE-CZ-NH1	5.71	127.20	121.50
3	0	178	ASP	O-C-N	-5.70	116.22	121.30
5	2	403	PHE	CA-C-N	5.70	132.69	122.09
5	2	403	PHE	C-N-CA	5.70	132.69	122.09
2	W	447	VAL	CA-C-O	-5.70	115.03	120.95
1	V	527	THR	N-CA-C	5.69	117.41	110.41
1	V	636	GLU	N-CA-C	-5.69	105.08	111.28
2	W	216	LYS	CA-C-O	-5.69	114.52	120.55
1	V	393	THR	N-CA-C	5.69	115.53	108.19
2	W	414	PHE	CA-CB-CG	5.69	119.49	113.80
8	Y	12	DT	C5-C4-O4	5.69	131.14	122.60
1	V	532	LEU	N-CA-C	5.68	118.41	111.82
1	V	702	ALA	N-CA-CB	-5.68	102.53	110.25
5	2	444	THR	CA-CB-OG1	5.68	118.11	109.60
1	V	421	TRP	NE1-CE2-CZ2	5.67	138.61	130.10
2	W	651	PHE	CA-CB-CG	5.67	119.47	113.80
2	W	215	PRO	CA-C-N	5.67	127.88	120.28
2	W	215	PRO	C-N-CA	5.67	127.88	120.28
2	W	702	THR	N-CA-C	5.67	119.81	113.01
1	V	307	ASN	N-CA-CB	-5.66	102.21	111.66
8	Y	1	DT	O3'-P-O5'	-5.65	95.53	104.00
2	W	109	LEU	CA-C-N	5.65	133.38	121.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	W	109	LEU	C-N-CA	5.65	133.38	121.91
2	W	16	TYR	CA-C-N	5.64	129.90	122.51
2	W	16	TYR	C-N-CA	5.64	129.90	122.51
1	V	295	TYR	N-CA-C	5.64	117.98	110.53
5	2	61	PHE	N-CA-CB	5.64	118.16	109.98
7	X	5	DC	O3'-P-O5'	5.64	112.46	104.00
2	W	272	ARG	NE-CZ-NH1	5.64	127.14	121.50
1	V	579	TYR	N-CA-C	5.64	118.41	109.50
2	W	305	LEU	CA-C-N	5.63	127.83	120.28
2	W	305	LEU	C-N-CA	5.63	127.83	120.28
1	V	477	ILE	CA-CB-CG1	5.63	119.97	110.40
2	W	177	LEU	N-CA-C	5.63	117.09	111.07
2	W	339	TYR	CA-C-N	5.63	128.41	120.42
2	W	339	TYR	C-N-CA	5.63	128.41	120.42
2	W	270	VAL	O-C-N	-5.63	115.54	122.57
1	V	506	GLN	OE1-CD-NE2	-5.62	116.98	122.60
2	W	697	ILE	N-CA-C	5.62	121.04	109.34
2	W	103	PRO	CB-CA-C	5.62	120.83	111.56
2	W	53	LEU	CA-C-O	-5.62	114.60	120.55
2	W	306	ALA	CA-C-O	-5.61	114.60	120.55
3	0	113	ARG	N-CA-C	5.61	117.94	109.41
2	W	193	PHE	N-CA-C	5.60	117.39	111.28
1	V	444	HIS	CA-C-N	5.60	128.55	120.38
1	V	444	HIS	C-N-CA	5.60	128.55	120.38
1	V	703	PHE	N-CA-CB	-5.60	103.50	111.84
1	V	405	VAL	CB-CA-C	5.59	120.46	111.29
5	2	262	LEU	CB-CA-C	-5.59	102.10	110.88
2	W	44	SER	CA-C-O	5.58	126.25	119.49
2	W	220	LEU	O-C-N	-5.58	115.78	122.15
1	V	551	HIS	CA-CB-CG	-5.58	108.22	113.80
1	V	439	ILE	CB-CG1-CD1	5.57	125.50	113.80
2	W	703	ASP	CA-C-N	5.57	132.19	121.54
2	W	703	ASP	C-N-CA	5.57	132.19	121.54
1	V	375	LYS	CA-C-N	5.55	127.72	120.28
1	V	375	LYS	C-N-CA	5.55	127.72	120.28
1	V	420	SER	O-C-N	-5.55	116.35	122.07
2	W	601	ARG	NE-CZ-NH2	-5.55	114.21	119.20
2	W	685	ALA	CA-C-O	5.55	126.62	120.63
1	V	355	CYS	O-C-N	-5.54	116.24	122.12
1	V	429	TRP	CA-C-N	5.54	133.17	122.53
1	V	429	TRP	C-N-CA	5.54	133.17	122.53
2	W	439	ASP	CA-C-O	5.54	127.25	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	V	268	VAL	CA-C-N	5.54	129.11	120.75
1	V	268	VAL	C-N-CA	5.54	129.11	120.75
3	0	194	ILE	CA-C-O	5.54	127.16	120.74
1	V	642	ARG	NE-CZ-NH2	-5.54	114.22	119.20
2	W	686	ARG	CA-C-N	5.53	127.05	120.14
2	W	686	ARG	C-N-CA	5.53	127.05	120.14
2	W	726	GLN	OE1-CD-NE2	-5.52	117.08	122.60
5	2	182	ALA	N-CA-C	-5.52	102.84	110.35
3	0	227	HIS	CA-CB-CG	5.52	119.32	113.80
2	W	68	THR	CA-C-O	-5.51	115.81	121.87
2	W	590	ASN	CA-C-N	5.51	128.99	121.83
2	W	590	ASN	C-N-CA	5.51	128.99	121.83
5	2	45	PHE	CA-CB-CG	-5.50	108.30	113.80
2	W	468	PRO	CA-N-CD	-5.50	104.30	112.00
1	V	567	ALA	O-C-N	5.49	128.41	122.15
1	V	677	GLN	N-CA-C	5.49	116.94	111.07
2	W	75	ARG	NE-CZ-NH1	5.49	126.99	121.50
2	W	606	GLU	CA-C-O	5.49	126.30	120.10
2	W	334	ARG	N-CA-CB	-5.49	102.06	110.01
3	0	236	VAL	CB-CA-C	-5.48	104.86	112.04
7	X	16	DA	O4'-C1'-C2'	-5.48	98.19	106.40
8	Y	12	DT	N3-C4-O4	-5.47	114.39	122.60
1	V	514	MET	CB-CA-C	5.47	118.90	110.14
1	V	637	ALA	N-CA-C	5.46	118.16	111.82
1	V	457	ILE	N-CA-CB	-5.46	102.22	111.23
3	0	186	ILE	N-CA-C	5.46	116.19	110.62
1	V	675	LYS	N-CA-C	5.46	116.91	111.07
1	V	542	ARG	NE-CZ-NH2	5.46	124.11	119.20
3	0	226	SER	N-CA-CB	-5.45	102.11	110.12
2	W	454	VAL	CA-C-N	5.45	131.05	122.33
2	W	454	VAL	C-N-CA	5.45	131.05	122.33
1	V	572	ALA	N-CA-C	5.45	117.22	111.28
3	0	123	ASN	O-C-N	-5.45	114.91	121.12
2	W	76	THR	N-CA-C	5.43	117.33	109.07
1	V	662	LEU	N-CA-CB	-5.43	101.58	110.43
3	0	142	GLU	O-C-N	5.43	125.78	121.55
5	2	98	THR	CA-C-N	5.43	128.09	120.28
5	2	98	THR	C-N-CA	5.43	128.09	120.28
1	V	564	ASN	CA-C-N	5.42	127.88	120.46
1	V	564	ASN	C-N-CA	5.42	127.88	120.46
2	W	463	PRO	CA-C-N	5.42	131.89	121.54
2	W	463	PRO	C-N-CA	5.42	131.89	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	1	51	ASN	CA-CB-CG	-5.42	107.18	112.60
2	W	489	CYS	CA-C-N	5.42	130.41	122.39
2	W	489	CYS	C-N-CA	5.42	130.41	122.39
5	2	267	GLU	CA-C-N	-5.41	115.80	122.84
5	2	267	GLU	C-N-CA	-5.41	115.80	122.84
2	W	57	MET	CA-C-N	5.41	129.26	120.60
2	W	57	MET	C-N-CA	5.41	129.26	120.60
2	W	487	ARG	NH1-CZ-NH2	-5.41	112.27	119.30
3	0	178	ASP	CA-C-N	5.41	124.92	119.19
3	0	178	ASP	C-N-CA	5.41	124.92	119.19
8	Y	16	DG	C2'-C3'-O3'	5.39	119.59	111.50
3	0	75	ASP	N-CA-C	5.39	117.16	111.28
1	V	576	ASN	CA-C-O	5.39	127.79	121.54
5	2	35	TYR	CB-CA-C	5.39	121.02	110.67
4	1	33	PHE	CA-CB-CG	-5.38	108.42	113.80
1	V	576	ASN	N-CA-CB	-5.38	103.82	111.84
2	W	153	PRO	CB-CA-C	5.38	118.11	111.23
1	V	253	GLU	CA-C-N	5.38	131.81	121.54
1	V	253	GLU	C-N-CA	5.38	131.81	121.54
7	X	6	DC	N3-C2-O2	-5.38	113.83	121.90
2	W	455	ILE	N-CA-C	5.37	115.63	108.27
8	Y	20	DT	C5-C4-O4	5.37	130.65	122.60
1	V	360	ARG	CD-NE-CZ	5.37	131.91	124.40
8	Y	18	DA	C2'-C3'-O3'	5.36	119.54	111.50
3	0	134	ALA	CA-C-O	5.36	126.10	120.42
1	V	433	GLN	OE1-CD-NE2	-5.36	117.24	122.60
1	V	265	THR	CA-C-O	-5.36	115.29	121.07
1	V	555	ASN	N-CA-C	5.35	118.82	111.54
2	W	141	TYR	N-CA-C	5.35	117.11	111.28
8	Y	16	DG	C1'-O4'-C4'	-5.34	101.69	109.70
2	W	313	GLU	N-CA-C	5.34	116.78	111.07
1	V	339	VAL	CA-C-O	5.34	126.00	120.39
2	W	118	HIS	CB-CG-CD2	-5.33	124.26	131.20
3	0	131	LEU	O-C-N	-5.33	115.71	122.27
1	V	332	ARG	CA-CB-CG	5.33	124.76	114.10
1	V	366	ASN	N-CA-C	5.33	119.50	112.89
7	X	11	DA	C8-N9-C1'	5.33	135.05	127.05
2	W	202	ALA	N-CA-C	5.33	118.23	109.76
3	0	99	ASN	OD1-CG-ND2	-5.33	117.27	122.60
2	W	669	ARG	NH1-CZ-NH2	-5.33	112.38	119.30
7	X	12	DC	C2'-C3'-O3'	5.33	119.49	111.50
2	W	156	ARG	CD-NE-CZ	5.32	131.85	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	V	575	LEU	CA-C-N	5.32	129.68	122.07
1	V	575	LEU	C-N-CA	5.32	129.68	122.07
3	O	73	ASP	CA-CB-CG	5.32	117.92	112.60
2	W	253	ARG	N-CA-C	5.32	117.07	111.28
3	O	59	ARG	NH1-CZ-NH2	-5.32	112.39	119.30
2	W	37	HIS	CA-C-N	5.31	127.83	120.92
2	W	37	HIS	C-N-CA	5.31	127.83	120.92
2	W	621	PHE	O-C-N	5.31	129.39	122.38
1	V	703	PHE	N-CA-C	5.31	118.76	111.54
2	W	148	HIS	N-CA-C	5.31	122.11	110.80
2	W	435	PHE	CA-C-N	5.31	128.38	120.95
2	W	435	PHE	C-N-CA	5.31	128.38	120.95
1	V	469	THR	CA-C-N	5.31	131.68	121.54
1	V	469	THR	C-N-CA	5.31	131.68	121.54
1	V	361	CYS	N-CA-CB	-5.30	101.60	110.83
2	W	562	GLN	CB-CG-CD	5.30	121.62	112.60
2	W	600	ALA	CA-C-N	5.30	127.92	120.28
2	W	600	ALA	C-N-CA	5.30	127.92	120.28
1	V	286	HIS	CG-CD2-NE2	5.30	112.50	107.20
1	V	574	ARG	O-C-N	-5.30	116.11	122.15
2	W	46	THR	CA-CB-OG1	5.29	117.54	109.60
2	W	450	ARG	N-CA-C	5.29	122.07	110.80
2	W	560	ASN	CA-CB-CG	-5.29	107.31	112.60
7	X	11	DA	C1'-O4'-C4'	-5.29	101.76	109.70
2	W	534	GLY	O-C-N	-5.29	118.86	122.62
3	O	90	TYR	CA-C-N	5.29	127.37	120.28
3	O	90	TYR	C-N-CA	5.29	127.37	120.28
1	V	677	GLN	OE1-CD-NE2	-5.29	117.31	122.60
2	W	169	PRO	N-CA-CB	5.29	109.10	103.39
3	O	170	ILE	CA-CB-CG1	5.29	119.39	110.40
2	W	494	ILE	O-C-N	-5.29	117.18	123.05
2	W	457	THR	N-CA-CB	-5.28	103.38	111.56
6	3	50	PHE	CA-CB-CG	-5.27	108.53	113.80
1	V	272	VAL	O-C-N	5.27	126.98	121.87
1	V	332	ARG	NH1-CZ-NH2	-5.27	112.45	119.30
1	V	634	ARG	NE-CZ-NH1	-5.26	116.23	121.50
2	W	516	VAL	N-CA-C	5.26	115.99	110.62
2	W	87	LEU	CB-CA-C	5.26	119.79	110.85
8	Y	16	DG	P-O3'-C3'	5.25	128.08	120.20
1	V	282	LYS	CG-CD-CE	5.25	123.39	111.30
3	O	237	SER	N-CA-C	5.25	116.03	109.57
2	W	284	GLU	N-CA-CB	5.24	117.61	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	V	317	ARG	O-C-N	5.24	127.30	121.43
1	V	341	PRO	CA-C-N	5.24	129.94	122.08
1	V	341	PRO	C-N-CA	5.24	129.94	122.08
1	V	552	GLU	N-CA-C	5.24	117.74	111.71
6	3	169	ASP	CA-CB-CG	-5.24	107.36	112.60
1	V	435	TRP	CA-C-O	-5.24	114.91	121.46
7	X	12	DC	C6-N1-C1'	5.23	127.55	119.70
2	W	199	ILE	O-C-N	-5.23	116.80	121.87
2	W	455	ILE	CA-C-O	-5.23	115.05	120.64
5	2	261	PHE	CB-CA-C	-5.23	102.67	110.88
2	W	319	VAL	CA-C-N	5.23	126.37	119.84
2	W	319	VAL	C-N-CA	5.23	126.37	119.84
1	V	699	GLU	N-CA-C	5.22	116.75	108.96
1	V	283	ARG	NE-CZ-NH2	-5.22	114.50	119.20
1	V	305	ASP	CA-C-N	5.22	131.36	121.97
1	V	305	ASP	C-N-CA	5.22	131.36	121.97
2	W	454	VAL	N-CA-CB	-5.21	105.87	112.60
1	V	252	TYR	O-C-N	-5.21	116.95	123.04
1	V	341	PRO	N-CA-C	5.20	119.38	111.11
2	W	71	ILE	N-CA-C	5.20	115.97	108.48
1	V	562	ALA	CA-C-N	5.20	131.47	121.54
1	V	562	ALA	C-N-CA	5.20	131.47	121.54
5	2	60	LEU	CB-CA-C	-5.20	102.71	110.88
1	V	251	PHE	N-CA-C	5.20	116.97	109.07
1	V	525	ILE	CA-C-O	-5.20	114.57	120.65
2	W	102	LEU	CA-C-N	5.20	126.34	119.84
2	W	102	LEU	C-N-CA	5.20	126.34	119.84
3	0	179	PRO	CA-C-O	-5.20	111.70	119.34
1	V	297	PHE	N-CA-C	5.19	116.96	109.07
5	2	402	ARG	N-CA-C	5.19	117.56	110.24
2	W	711	ASP	CA-CB-CG	-5.19	107.41	112.60
1	V	285	ILE	CA-CB-CG2	5.19	119.32	110.50
1	V	545	GLN	CA-C-N	5.19	127.23	120.28
1	V	545	GLN	C-N-CA	5.19	127.23	120.28
2	W	96	LYS	N-CA-C	5.19	121.85	110.80
1	V	678	ARG	CA-C-O	-5.18	115.05	120.55
1	V	611	GLY	O-C-N	5.18	127.17	122.19
3	0	65	VAL	CA-CB-CG1	5.18	119.21	110.40
1	V	344	ALA	N-CA-CB	-5.18	101.29	111.60
2	W	128	LYS	CA-C-N	5.18	128.06	120.71
2	W	128	LYS	C-N-CA	5.18	128.06	120.71
2	W	564	ASN	OD1-CG-ND2	-5.16	117.44	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	V	315	VAL	CA-C-O	-5.16	114.97	120.39
1	V	564	ASN	CB-CA-C	5.15	118.56	109.80
1	V	382	SER	O-C-N	-5.15	116.50	122.89
2	W	152	LEU	N-CA-C	5.15	121.20	109.81
2	W	98	GLU	O-C-N	-5.14	115.75	122.59
2	W	660	ALA	CA-C-N	5.14	127.69	120.28
2	W	660	ALA	C-N-CA	5.14	127.69	120.28
2	W	399	LEU	CA-C-O	-5.14	115.40	120.70
1	V	708	GLU	O-C-N	5.14	127.57	122.12
1	V	399	LYS	CA-C-N	5.14	124.75	119.56
1	V	399	LYS	C-N-CA	5.14	124.75	119.56
2	W	707	ASN	OD1-CG-ND2	-5.14	117.46	122.60
8	Y	12	DT	O4'-C1'-N1	5.14	116.11	108.40
1	V	357	VAL	N-CA-CB	5.14	117.53	110.54
3	O	80	ARG	CD-NE-CZ	5.13	131.59	124.40
1	V	363	VAL	CA-C-N	-5.13	115.92	123.00
1	V	363	VAL	C-N-CA	-5.13	115.92	123.00
1	V	421	TRP	CE2-CD2-CG	5.13	113.36	107.20
1	V	639	ARG	NE-CZ-NH2	5.13	123.81	119.20
2	W	50	VAL	O-C-N	5.13	127.11	121.83
2	W	69	LYS	CG-CD-CE	5.13	123.09	111.30
2	W	205	VAL	CA-C-N	5.12	130.26	122.98
2	W	205	VAL	C-N-CA	5.12	130.26	122.98
2	W	511	ARG	CA-C-N	5.12	131.34	122.32
2	W	511	ARG	C-N-CA	5.12	131.34	122.32
2	W	87	LEU	CA-C-N	5.12	127.14	120.28
2	W	87	LEU	C-N-CA	5.12	127.14	120.28
2	W	251	LEU	CB-CA-C	5.12	119.42	109.33
2	W	64	PRO	CA-N-CD	-5.12	104.83	112.00
7	X	11	DA	C4'-C3'-O3'	-5.12	102.33	110.00
7	X	13	DG	N9-C1'-C2'	5.12	121.17	113.50
2	W	143	ARG	CA-CB-CG	-5.11	103.87	114.10
1	V	419	ARG	CD-NE-CZ	5.11	131.56	124.40
2	W	170	LEU	O-C-N	-5.11	115.93	120.48
2	W	538	PHE	O-C-N	5.11	129.09	123.16
8	Y	1	DT	C6-C5-C7	-5.11	116.34	124.00
2	W	693	LEU	CB-CA-C	5.11	116.89	109.08
3	O	212	ALA	CA-C-N	5.11	127.38	120.44
3	O	212	ALA	C-N-CA	5.11	127.38	120.44
1	V	680	LEU	N-CA-C	5.10	116.84	111.28
2	W	31	THR	CA-CB-CG2	5.10	119.17	110.50
1	V	397	LYS	CA-CB-CG	5.10	124.30	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	V	543	ALA	N-CA-C	5.10	116.84	111.28
3	0	124	PRO	CA-C-N	5.10	127.11	120.28
3	0	124	PRO	C-N-CA	5.10	127.11	120.28
1	V	580	ILE	O-C-N	-5.09	117.70	123.20
2	W	519	ASN	CA-CB-CG	5.09	117.69	112.60
2	W	23	SER	CB-CA-C	-5.09	102.89	110.88
3	0	233	THR	CA-CB-OG1	5.09	117.23	109.60
1	V	452	ARG	CA-CB-CG	5.09	124.27	114.10
2	W	158	TYR	CA-C-N	5.08	127.60	120.28
2	W	158	TYR	C-N-CA	5.08	127.60	120.28
2	W	672	THR	CA-C-N	5.08	130.72	122.39
2	W	672	THR	C-N-CA	5.08	130.72	122.39
2	W	720	PHE	CA-CB-CG	5.08	118.88	113.80
5	2	249	TYR	CA-C-N	-5.08	114.53	122.05
5	2	249	TYR	C-N-CA	-5.08	114.53	122.05
1	V	466	LEU	N-CA-CB	-5.08	102.02	110.80
2	W	260	GLN	CA-C-N	5.08	125.62	119.98
2	W	260	GLN	C-N-CA	5.08	125.62	119.98
4	1	62	ASP	CA-CB-CG	-5.08	107.53	112.60
1	V	465	GLY	CA-C-O	-5.07	115.97	120.94
1	V	634	ARG	N-CA-C	5.07	117.70	111.82
2	W	299	ARG	O-C-N	-5.06	116.28	122.25
5	2	128	ALA	CA-C-N	-5.06	115.63	123.17
5	2	128	ALA	C-N-CA	-5.06	115.63	123.17
1	V	316	LEU	CB-CA-C	-5.06	101.48	111.60
2	W	483	MET	N-CA-CB	-5.06	102.73	110.42
2	W	24	TYR	N-CA-C	5.06	119.60	111.81
5	2	48	LEU	N-CA-C	5.06	120.98	109.81
2	W	172	ALA	CA-C-N	5.05	131.31	121.41
2	W	172	ALA	C-N-CA	5.05	131.31	121.41
2	W	699	GLU	CB-CA-C	5.05	118.39	109.80
6	3	9	ASN	CA-CB-CG	-5.05	107.55	112.60
1	V	395	ASP	CA-CB-CG	5.05	117.65	112.60
1	V	560	VAL	O-C-N	-5.04	117.20	123.10
4	1	3	ASN	CA-C-N	-5.04	115.12	122.58
4	1	3	ASN	C-N-CA	-5.04	115.12	122.58
3	0	207	VAL	CA-C-N	5.04	127.45	120.29
3	0	207	VAL	C-N-CA	5.04	127.45	120.29
2	W	468	PRO	N-CA-CB	5.04	108.83	103.39
2	W	205	VAL	CA-CB-CG1	5.04	118.96	110.40
1	V	366	ASN	OD1-CG-ND2	5.03	127.63	122.60
2	W	638	GLU	CA-C-O	-5.03	115.54	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	V	581	TYR	CA-C-O	-5.03	115.93	121.31
2	W	276	THR	CA-C-N	5.03	132.11	121.91
2	W	276	THR	C-N-CA	5.03	132.11	121.91
2	W	444	ILE	N-CA-C	5.03	117.37	111.09
2	W	459	GLY	O-C-N	5.02	129.23	122.70
1	V	487	LYS	CA-C-N	5.02	127.42	120.29
1	V	487	LYS	C-N-CA	5.02	127.42	120.29
2	W	687	GLY	CA-C-N	5.02	127.42	120.29
2	W	687	GLY	C-N-CA	5.02	127.42	120.29
2	W	570	GLU	CA-C-N	5.02	129.74	122.36
2	W	570	GLU	C-N-CA	5.02	129.74	122.36
2	W	718	LYS	CA-C-N	5.02	127.00	120.28
2	W	718	LYS	C-N-CA	5.02	127.00	120.28
2	W	195	ALA	O-C-N	5.02	127.24	122.07
2	W	557	ILE	CA-CB-CG1	5.01	118.92	110.40
2	W	629	GLN	OE1-CD-NE2	-5.01	117.59	122.60
1	V	311	LYS	CA-C-O	-5.01	113.30	120.16

There are no chirality outliers.

All (47) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	2	389	ASP	Mainchain,Sidechain
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

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

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	V	3855	0	3872	171	0
2	W	5348	0	5371	180	0
3	0	1479	0	1524	73	0
4	1	491	0	507	237	0
5	2	2196	0	2206	596	0
6	3	1526	0	1561	469	0
7	X	392	0	207	1	0
8	Y	401	0	231	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	15688	0	15479	1438	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 46.

All (1438) 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
5:2:117:ASN:CG	6:3:108:ASN:HB2	1.39	1.44
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
1:V:516:PRO:CG	1:V:706:LYS:HZ3	1.30	1.42
2:W:421:PHE:HB3	2:W:431:PRO:N	1.31	1.40
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
5:2:28:PRO:N	6:3:25:GLN:HA	1.03	1.34
5:2:117:ASN:OD1	6:3:108:ASN:ND2	1.57	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:2:31:LEU:CD1	6:3:33:THR:CG2	2.10	1.28
5:2:118:LEU:HD21	6:3:39:ASP:O	1.23	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
1:V:428:GLU:O	1:V:433:GLN:HA	1.38	1.20
6:3:59:VAL:HG13	6:3:70:LEU:CB	1.69	1.20
2:W:209:TYR:OH	2:W:233:PHE:HA	1.38	1.19
4:1:59:GLU:OE2	5:2:402:ARG:NH2	1.73	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
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
4:1:28:ALA:HB1	4:1:31:LYS:HD2	1.27	1.16
5:2:117:ASN:ND2	6:3:108:ASN:HB2	0.85	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
3:0:54:ARG:CG	6:3:182:PHE:CE1	2.17	1.12
4:1:5:LEU:CD2	5:2:408:LEU:HD13	1.79	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
1:V:315:VAL:CG1	2:W:500:ASP:CB	1.94	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:2:42:LEU:HD21	5:2:55:TRP:HB2	1.20	1.11
5:2:160:LEU:HD23	5:2:206:LEU:HD21	1.25	1.11
2:W:110:SER:C	2:W:207:TYR:OH	1.94	1.10
5:2:163:MET:HE2	5:2:206:LEU:HD12	1.30	1.10
4:1:2:VAL:HG11	5:2:456:LYS:CG	1.81	1.10
5:2:171:VAL:HG22	5:2:213:TRP:HA	1.27	1.10
3:0:77:LYS:CG	3:0:83:CYS:CB	2.22	1.10
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
2:W:169:PRO:C	2:W:175:TYR:OH	1.95	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
1:V:415:HIS:CD2	1:V:416:THR:HG23	1.87	1.08
5:2:29:GLY:N	6:3:25:GLN:CG	2.15	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
1:V:516:PRO:HG2	1:V:706:LYS:NZ	1.69	1.08
5:2:29:GLY:CA	6:3:25:GLN:HG3	1.83	1.08
5:2:31:LEU:HD11	6:3:33:THR:HG22	1.30	1.08
5:2:159:VAL:HG13	5:2:161:HIS:H	1.16	1.08
1:V:611:GLY:HA2	1:V:615:PHE:HD2	1.18	1.07
5:2:30:VAL:CG2	6:3:25:GLN:CB	2.32	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:516:PRO:HG2	1:V:706:LYS:HZ3	0.96	1.06
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
4:1:5:LEU:HD12	5:2:409:TYR:O	1.55	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
1:V:502:ILE:HG23	1:V:503:ALA:N	1.47	1.05
5:2:117:ASN:CG	6:3:108:ASN:CB	2.20	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:72:TYR:CD2	2:W:232:VAL:CG1	2.41	1.04
1:V:426:VAL:O	1:V:427:MET:O	1.76	1.04
1:V:516:PRO:CG	1:V:706:LYS:NZ	2.18	1.04
3:0:77:LYS:CG	3:0:83:CYS:SG	2.46	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
3:0:54:ARG:NE	6:3:182:PHE:CE1	2.26	1.02
4:1:4:VAL:HG12	5:2:411:GLN:O	1.56	1.02
3:0:54:ARG:CD	6:3:182:PHE:HE1	1.72	1.02
3:0:77:LYS:HB2	3:0:83:CYS:HB3	1.37	1.02
3:0:98:GLN:OE1	6:3:209:ILE:HA	1.58	1.02
4:1:34:ILE:HG12	4:1:50:VAL:HG11	1.39	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
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
5:2:199:ALA:HB3	5:2:202:GLN:HE22	1.22	1.01
4:1:1:MET:HE1	5:2:440:LEU:HD13	1.41	1.00
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
1:V:315:VAL:HG11	2:W:500:ASP:HB2	1.42	1.00
2:W:110:SER:HA	2:W:207:TYR:CZ	1.97	1.00
6:3:148:ASN:HB2	6:3:157:MET:HE2	1.42	0.99
2:W:209:TYR:OH	2:W:233:PHE:CA	2.09	0.99
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
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
5:2:196:ILE:HD11	5:2:210:ALA:HB2	1.45	0.98
2:W:584:TYR:CD1	2:W:594:ALA:HB2	1.99	0.97
6:3:173:GLN:HA	6:3:176:ASN:HD21	1.28	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
2:W:110:SER:CA	2:W:207:TYR:CZ	2.49	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:3:133:LEU:HD23	6:3:177:PHE:CD1	2.01	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
5:2:211: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
2:W:170:LEU:CD1	2:W:175:TYR:CZ	2.50	0.95
3:0:77:LYS:HG2	3:0:83:CYS:CB	1.89	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
2:W:170:LEU:HD12	2:W:175:TYR:OH	1.65	0.94
5:2:28:PRO:CD	6:3:25:GLN:HA	1.97	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
1:V:523:VAL:CG1	4:1:20:LEU:HD23	1.93	0.94
5:2:35:TYR:CE1	5:2:62:LEU:HG	2.02	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
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
2:W:696:TRP:CD1	2:W:697:ILE:HG12	2.04	0.92
4:1:1:MET:HB3	5:2:413:LEU:HB3	1.50	0.92
6:3:133:LEU:HD13	6:3:133:LEU:H	1.33	0.92
6:3:11:LEU:HD22	6:3:160:ARG:HG2	1.52	0.92
2:W:72:TYR:CD2	2:W:232:VAL:HG13	2.04	0.92
6:3:165:LYS:HE3	6:3:200:SER:CB	2.00	0.92
3:0:74:GLN:HA	3:0:78:PRO:C	1.93	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
5:2:118:LEU:HD22	6:3:39:ASP:CG	1.93	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:CD	1:V:706:LYS:HZ3	1.84	0.91
2:W:170:LEU:N	2:W:175:TYR:OH	2.01	0.91
5:2:81:LYS:CE	5:2:93:LEU:HD21	2.00	0.91
1:V:612:ASP:OD2	1:V:635:GLN:OE1	1.89	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:3:137:LEU:CB	6:3:180:VAL:HG11	2.01	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
2:W:430:ASN:HB3	2:W:431:PRO:HD2	1.54	0.90
5:2:81:LYS:HD2	5:2:89:LEU:HD21	1.52	0.90
2:W:169:PRO:HB2	2:W:175:TYR:HH	1.18	0.90
5:2:29:GLY:H	6:3:25:GLN:CG	1.81	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
4:1:13:ASP:CG	4:1:14:PRO:HD2	1.97	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
5:2:28:PRO:N	6:3:25:GLN:C	2.30	0.89
3:0:77:LYS:HA	3:0:77:LYS:CE	2.00	0.89
4:1:4:VAL:HG11	5:2:412:PHE:HD2	1.36	0.89
4:1:8:VAL:HG11	4:1:45:VAL:HG13	1.55	0.89
1:V:629:HIS:O	1:V:633:ARG:NH2	2.06	0.89
5:2:160:LEU:HB3	5:2:206:LEU:HD11	1.52	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
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
5:2:118:LEU:HD11	6:3:43:VAL:HG22	1.56	0.88
5:2:163:MET:SD	5:2:196:ILE:HG21	2.14	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
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
2:W:584:TYR:CE2	2:W:614:TYR:HB2	2.10	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:696:TRP:CD1	2:W:697:ILE:CG1	2.58	0.87
5:2:117:ASN:OD1	6:3:108:ASN:CB	2.23	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:3:165:LYS:HE3	6:3:200:SER:HB2	1.56	0.87
2:W:59:TYR:CG	2:W:62:ALA:HB2	2.10	0.86
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
5:2:48:LEU:HB3	5:2:49:PRO:HD3	1.57	0.86
5:2:138:PRO:HG3	5:2:189:GLU:HG3	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
6:3:178:MET:HE2	6:3:202:LEU:CD1	2.05	0.86
5:2:117:ASN:OD1	6:3:108:ASN:CG	2.18	0.86
5:2:224:GLN:HB2	5:2:268:PHE:CZ	2.10	0.86
2:W:421:PHE:HB3	2:W:430:ASN:C	2.00	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
2:W:59:TYR:CD2	2:W:62:ALA:HB2	2.12	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
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
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
2:W:70:LEU:CD2	2:W:72:TYR:CE1	2.55	0.84
2:W:169:PRO:C	2:W:175:TYR:CZ	2.50	0.84
5:2:78:GLU:O	5:2:81:LYS:HG2	1.77	0.84
1:V:502:ILE:HG23	1:V:503:ALA:H	0.68	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
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
6:3:49:LEU:HB3	6:3:101:TYR:CB	2.05	0.84
2:W:110:SER:C	2:W:207:TYR:HH	1.80	0.84
5:2:176:ALA:CB	5:2:178:LEU:HD13	2.07	0.84
6:3:178:MET:HE2	6:3:202:LEU:HD12	1.57	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:696:TRP:NE1	2:W:697:ILE:HG12	1.92	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
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
1:V:674:THR:CG2	5:2:392:ARG:CZ	2.55	0.83
5:2:160:LEU:HD23	5:2:206:LEU:CD2	2.07	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:315:VAL:HG12	2:W:500:ASP:HB2	1.54	0.82
2:W:109:LEU:O	2:W:207:TYR:CD1	2.32	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
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
1:V:392:PHE:O	1:V:418:LYS:HD2	1.78	0.82
3:0:97:ASP:O	6:3:208:ASP:HB3	1.79	0.82
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
1:V:427:MET:O	1:V:432:THR:O	1.98	0.81
4:1:1:MET:SD	5:2:415:GLN:O	2.38	0.81
5:2:174:ASP:OD1	5:2:179:LEU:HD12	1.80	0.81
5:2:174:ASP:O	5:2:220:LEU:HD23	1.79	0.81
5:2:175:LEU:HB3	5:2:216:MET:SD	2.20	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
2:W:144:ALA:HA	2:W:148:HIS:C	2.05	0.81
6:3:216:LYS:H	6:3:216:LYS:HD2	1.43	0.81
5:2:177:GLN:CD	5:2:220:LEU:HD22	2.06	0.81
2:W:59:TYR:CD1	2:W:62:ALA:HB2	2.16	0.81
5:2:37:HIS:HB3	5:2:38:PRO:HD3	1.61	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:1:9:LEU:CD1	4:1:48:GLU:HA	2.09	0.80
4:1:34:ILE:HG22	4:1:46:ILE:HD11	1.64	0.80
5:2:256:ASP:O	5:2:259:LEU:HG	1.81	0.80
6:3:144:ILE:CD1	6:3:147:MET:HE3	2.11	0.80
5:2:42:LEU:HD12	5:2:59:MET:CE	2.11	0.80
5:2:117:ASN:HB3	6:3:42:MET:HE3	1.62	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
5:2:35:TYR:CD1	5:2:62:LEU:HG	2.16	0.80
5:2:251:VAL:HG11	5:2:254:MET:HG3	1.62	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
1:V:516:PRO:CB	1:V:706:LYS:HZ3	1.95	0.80
6:3:22:TRP:O	6:3:25:GLN:NE2	2.15	0.80
2:W:52:LEU:HD23	2:W:72:TYR:OH	1.80	0.80
6:3:165:LYS:HE2	6:3:167:ALA:O	1.81	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
1:V:674:THR:CG2	5:2:392:ARG:NH2	2.39	0.79
3:0:96:PHE:CD2	3:0:124:PRO:HB3	2.17	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
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
5:2:117:ASN:CG	6:3:42:MET:CE	2.55	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:HB3	5:2:413:LEU:CD2	2.12	0.78
4:1:1:MET:HA	5:2:414:SER:H	1.47	0.78
6:3:59:VAL:HB	6:3:71:TYR:CE1	2.17	0.78
6:3:151:VAL:HG12	6:3:155:GLN:O	1.84	0.78
1:V:415:HIS:HD2	1:V:416:THR:HG23	1.45	0.78
5:2:234:LEU:O	5:2:234:LEU:HD23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:2:181:GLN:OE1	5:2:229:ASP:HB2	1.84	0.78
5:2:203:PHE:CD2	5:2:205:LEU:HD23	2.18	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
3:0:54:ARG:NE	6:3:182:PHE:HE1	1.73	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
2:W:169:PRO:CA	2:W:175:TYR:OH	2.32	0.78
5:2:53:LYS:O	5:2:56:VAL:HG22	1.84	0.78
5:2:118:LEU:CD1	6:3:39:ASP:OD1	2.31	0.78
6:3:71:TYR:CD2	6:3:72:PRO:HD2	2.19	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
1:V:393:THR:HA	1:V:418:LYS:CE	2.14	0.77
6:3:185:GLN:HA	6:3:185:GLN:HE21	1.48	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
6:3:185:GLN:NE2	6:3:210:THR:HA	2.00	0.77
1:V:516:PRO:CB	1:V:706:LYS:NZ	2.48	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
4:1:25:GLU:CD	4:1:35:ILE:HG12	2.09	0.77
5:2:117:ASN:CG	6:3:42:MET:HE2	2.10	0.77
5:2:211:GLN:HA	5:2:261:PHE:HZ	1.49	0.77
1:V:611:GLY:CA	1:V:615:PHE:HD2	1.98	0.76
5:2:42:LEU:HD21	5:2:55:TRP:CB	2.10	0.76
5:2:179:LEU:HB3	5:2:184:LEU:HD11	1.65	0.76
5:2:44:VAL:HG13	5:2:45:PHE:CD1	2.20	0.76
5:2:117:ASN:HD21	6:3:108:ASN:HB3	1.47	0.76
6:3:147:MET:HE1	6:3:157:MET:SD	2.25	0.76
6:3:190:LEU:HD23	6:3:190:LEU:H	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
4:1:1:MET:C	5:2:413:LEU:HG	2.09	0.76
6:3:59:VAL:CB	6:3:71:TYR:CE1	2.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:355:CYS:HG	1:V:381:TRP:CD1	2.05	0.75
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
4:1:1:MET:HG2	5:2:413:LEU:C	2.11	0.75
4:1:38:ILE:HD13	4:1:38:ILE:H	1.51	0.75
5:2:118:LEU:HD22	6:3:39:ASP:HA	1.65	0.75
5:2:163:MET:HE2	5:2:206:LEU:CD1	2.15	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
1:V:689:VAL:HB	5:2:391:ILE:HD11	1.67	0.75
4:1:24:ASP:OD2	4:1:57:VAL:HG11	1.85	0.75
1:V:444:HIS:O	1:V:447:PRO:HD2	1.86	0.75
6:3:8:LEU:HD23	6:3:54:SER:HB3	1.68	0.75
6:3:38:ILE:O	6:3:41:VAL:HG12	1.87	0.75
6:3:148:ASN:CB	6:3:157:MET:HE2	2.17	0.75
1:V:611:GLY:O	1:V:615:PHE:HB3	1.86	0.74
5:2:180:SER:O	5:2:184:LEU:HG	1.87	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
6:3:133:LEU:HD23	6:3:177:PHE:HD1	1.49	0.74
2:W:608:ILE:HG23	2:W:614:TYR:CE2	2.22	0.74
5:2:100:LEU:CD1	5:2:119:ARG:HG3	2.16	0.74
5:2:196:ILE:HD11	5:2:210:ALA:CB	2.17	0.74
2:W:430:ASN:HB3	2:W:431:PRO:CD	2.17	0.74
4:1:2:VAL:CG1	5:2:456:LYS:CG	2.53	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
1:V:516:PRO:HG2	1:V:706:LYS:CE	2.17	0.74
1:V:522:TYR:HE2	4:1:62:ASP:CG	1.96	0.74
5:2:51:LEU:HD23	5:2:51:LEU:O	1.87	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
2:W:52:LEU:HD23	2:W:72:TYR:CE2	2.22	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:110:SER:C	2:W:207:TYR:CZ	2.66	0.73
5:2:53:LYS:HE3	5:2:95:ILE:HD11	1.67	0.73
4:1:1:MET:HE3	5:2:415:GLN:C	2.13	0.73
4:1:34:ILE:HD13	4:1:54:GLN:OE1	1.88	0.73
1:V:674:THR:OG1	5:2:392:ARG:NE	2.21	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
6:3:214:TYR:HE2	6:3:216:LYS:HE2	1.53	0.73
1:V:612:ASP:CG	1:V:635:GLN:CD	2.57	0.73
4:1:34:ILE:HG12	4:1:50:VAL:CG1	2.18	0.73
5:2:118:LEU:HD21	6:3:39:ASP:C	2.12	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
6:3:144:ILE:HG12	6:3:147:MET:HE3	1.70	0.73
6:3:226:TYR:HA	6:3:230:VAL:HG23	1.71	0.73
2:W:73:CYS:HB2	2:W:209:TYR:CZ	2.23	0.73
5:2:41:CYS:O	5:2:44:VAL:HG12	1.88	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
2:W:59:TYR:CD2	2:W:62:ALA:CB	2.71	0.72
5:2:60:LEU:HD11	5:2:95:ILE:HB	1.71	0.72
5:2:218:GLN:HE22	5:2:265:LEU:HA	1.55	0.72
6:3:12:VAL:HG23	6:3:161:ILE:HG23	1.70	0.72
4:1:2:VAL:HG12	5:2:422:LEU:HD13	1.71	0.72
5:2:175:LEU:HD22	5:2:216:MET:SD	2.29	0.72
6:3:111:ILE:HG13	6:3:112:VAL:N	2.02	0.72
1:V:415:HIS:HD2	1:V:416:THR:CG2	1.99	0.72
4:1:2:VAL:HG12	5:2:456:LYS:HE2	1.72	0.72
5:2:117:ASN:ND2	6:3:42:MET:HE1	2.04	0.72
5:2:117:ASN:HB3	6:3:42:MET:CE	2.18	0.72
5:2:199:ALA:HB3	5:2:202:GLN:NE2	2.02	0.72
1:V:394:SER:HB3	1:V:416:THR:O	1.88	0.72
2:W:421:PHE:HB3	2:W:431:PRO:CA	2.17	0.72
5:2:31:LEU:CG	6:3:33:THR:HB	2.19	0.72
5:2:118:LEU:HD22	6:3:39:ASP:CA	2.19	0.72
6:3:222:SER:HB2	6:3:226:TYR:HE2	1.55	0.72
5:2:117:ASN:HB2	6:3:104:LEU:HD11	1.71	0.72
5:2:134:SER:O	5:2:138:PRO:HD2	1.89	0.72
6:3:217:VAL:HG13	6:3:226:TYR:CZ	2.24	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:315:VAL:HG12	2:W:500:ASP:CB	2.17	0.72
5:2:28:PRO:HD2	6:3:25:GLN:NE2	2.05	0.72
6:3:66:GLU:CA	6:3:132:LEU:HD12	2.13	0.72
5:2:192:GLU:HG3	5:2:193:PRO:CD	2.18	0.71
2:W:584:TYR:HD1	2:W:594:ALA:HB2	1.51	0.71
6:3:165:LYS:HG3	6:3:203:LEU:CD1	2.20	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
5:2:42:LEU:HD12	5:2:59:MET:HE1	1.71	0.71
5:2:171:VAL:HG12	5:2:216:MET:SD	2.31	0.71
2:W:73:CYS:C	2:W:209:TYR:CE2	2.68	0.71
3:0:98:GLN:OE1	6:3:209:ILE:CA	2.37	0.71
4:1:1:MET:HE2	5:2:413:LEU:O	1.91	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
6:3:18:ASN:CG	6:3:20:ILE:HD13	2.15	0.71
1:V:504:LYS:HB3	1:V:654:GLU:O	1.91	0.71
2:W:209:TYR:OH	2:W:234:ASP:N	2.23	0.71
1:V:366:ASN:ND2	1:V:613:THR:CG2	2.54	0.71
1:V:523:VAL:CB	4:1:20:LEU:HD23	2.21	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
3:0:77:LYS:HB2	3:0:83:CYS:HB2	0.80	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
4:1:29:LEU:HD23	4:1:30:GLY:N	2.06	0.70
5:2:126:GLY:C	5:2:178:LEU:HD23	2.16	0.70
2:W:589:GLU:O	2:W:594:ALA:HB1	1.91	0.70
5:2:31:LEU:N	6:3:25:GLN:O	2.24	0.70
6:3:177:PHE:CZ	6:3:203:LEU:HD23	2.27	0.70
1:V:515:SER:HB3	1:V:539:ASN:ND2	2.05	0.70
6:3:51:MET:HE3	6:3:52:ASN:ND2	2.07	0.70
2:W:109:LEU:C	2:W:207:TYR:CD1	2.70	0.70
2:W:209:TYR:HE1	2:W:233:PHE:CD1	2.09	0.70
5:2:218:GLN:CD	5:2:265:LEU:HA	2.16	0.70
1:V:393:THR:HA	1:V:418:LYS:HE3	1.74	0.70
5:2:218:GLN:OE1	5:2:265:LEU:HA	1.92	0.70
6:3:70:LEU:O	6:3:114:GLU:HG3	1.91	0.70
4:1:1:MET:HG3	5:2:418:PHE:HB2	1.73	0.70
2:W:70:LEU:HD21	2:W:72:TYR:CZ	2.27	0.70
4:1:8:VAL:HG11	4:1:45:VAL:HG12	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:3:133:LEU:HD22	6:3:134:ALA:H	1.56	0.70
2:W:189:TRP:HE1	2:W:194:LEU:HB2	1.55	0.70
3:0:54:ARG:NE	6:3:182:PHE:CD1	2.60	0.70
2:W:59:TYR:CE1	2:W:62:ALA:HB2	2.27	0.69
5:2:163:MET:O	5:2:167:PRO:HD2	1.91	0.69
5:2:29:GLY:CA	6:3:25:GLN:CG	2.66	0.69
5:2:189:GLU:HA	5:2:192:GLU:HG2	1.72	0.69
1:V:516:PRO:HB2	1:V:706:LYS:NZ	2.07	0.69
6:3:162:LEU:HA	6:3:192:ASP:OD1	1.92	0.69
5:2:118:LEU:HD11	6:3:43:VAL:HG23	1.75	0.69
6:3:144:ILE:CG1	6:3:147:MET:HE3	2.23	0.69
5:2:185:MET:SD	5:2:232:GLU:HB2	2.32	0.69
5:2:30:VAL:N	6:3:25:GLN:CG	2.55	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
5:2:163:MET:CE	5:2:206:LEU:HB3	2.23	0.69
5:2:199:ALA:CB	5:2:202:GLN:HE22	2.02	0.69
3:0:54:ARG:CD	6:3:182:PHE:CE1	2.60	0.69
6:3:69:PHE:CE1	6:3:139:LYS:HD2	2.27	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
2:W:111:SER:N	2:W:207:TYR:OH	2.24	0.68
5:2:48:LEU:CB	5:2:49:PRO:HD3	2.19	0.68
5:2:181:GLN:HG3	5:2:229:ASP:CG	2.18	0.68
5:2:211:GLN:HA	5:2:261:PHE:CE1	2.28	0.68
6:3:215:LEU:HD12	6:3:230:VAL:CG1	2.23	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
6:3:18:ASN:CG	6:3:64:ILE:HD11	2.19	0.68
1:V:502:ILE:CG2	1:V:503:ALA:N	2.17	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
4:1:1:MET:SD	5:2:419:GLU:HB2	2.34	0.67
4:1:4:VAL:CG1	5:2:411:GLN:O	2.40	0.67
5:2:170:ALA:HB1	5:2:213:TRP:CZ3	2.29	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
1:V:516:PRO:CD	1:V:706:LYS:NZ	2.53	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:2:117:ASN:CB	6:3:42:MET:HE3	2.22	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
1:V:667:THR:HA	4:1:62:ASP:CG	2.19	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
5:2:181:GLN:CD	5:2:229:ASP:HB2	2.20	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
2:W:52:LEU:HD23	2:W:72:TYR:CZ	2.29	0.67
5:2:117:ASN:HD21	6:3:108:ASN:CA	2.04	0.67
1:V:520:ARG:HB2	4:1:19:PHE:CB	2.25	0.66
5:2:56:VAL:HG11	5:2:91:SER:HB2	1.77	0.66
1:V:612:ASP:CG	1:V:635:GLN:OE1	2.38	0.66
1:V:514:MET:HE3	4:1:16:MET:CE	2.25	0.66
4:1:10:ILE:HG21	5:2:407:VAL:HG21	1.77	0.66
5:2:160:LEU:HD12	5:2:160:LEU:H	1.60	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
6:3:207:CYS:SG	6:3:214:TYR:HB2	2.34	0.66
2:W:432:ILE:CD1	2:W:434:HIS:HE1	2.07	0.66
6:3:45:GLY:O	6:3:49:LEU:HD23	1.96	0.66
6:3:146:ARG:O	6:3:149:LYS:HG2	1.95	0.66
1:V:412:MET:HA	1:V:417:THR:HG21	1.77	0.66
4:1:8:VAL:HG12	4:1:9:LEU:N	2.10	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
4:1:35:ILE:HG22	4:1:46:ILE:HD12	1.78	0.66
5:2:117:ASN:CG	6:3:108:ASN:ND2	2.50	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
5:2:270:LEU:HD23	5:2:270:LEU:O	1.96	0.65
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
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
1:V:523:VAL:HG21	4:1:20:LEU:CG	2.25	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:316:LEU:HB2	1:V:321:GLU:HG3	1.78	0.65
5:2:189:GLU:HA	5:2:192:GLU:CG	2.26	0.65
5:2:28:PRO:C	6:3:25:GLN:HG3	2.17	0.65
6:3:184:ALA:CA	6:3:187:GLN:HG2	2.25	0.65
1:V:503:ALA:HB2	1:V:646:ALA:N	2.11	0.65
5:2:57:MET:HA	5:2:60:LEU:HD11	1.76	0.65
5:2:45:PHE:HB2	5:2:51:LEU:CD1	2.26	0.65
5:2:117:ASN:ND2	6:3:42:MET:CE	2.60	0.65
5:2:173:GLN:CD	5:2:179:LEU:HD21	2.22	0.65
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
5:2:29:GLY:H	6:3:25:GLN:CD	2.04	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
1:V:517:GLU:HB2	1:V:713:LEU:HD22	1.79	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:426:VAL:HG13	1:V:427:MET:H	1.62	0.64
5:2:42:LEU:CD2	5:2:55:TRP:HB2	2.13	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
3:0:98:GLN:CD	6:3:209:ILE:HA	2.21	0.64
4:1:59:GLU:CD	5:2:402:ARG:NH1	2.56	0.64
5:2:202:GLN:H	5:2:202:GLN:HE21	1.44	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
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
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:O	5:2:220:LEU:HD13	1.98	0.64
2:W:696:TRP:HD1	2:W:697:ILE:HG13	1.63	0.64
4:1:1:MET:HA	5:2:413:LEU:HA	1.80	0.64
6:3:69:PHE:CZ	6:3:139:LYS:HB3	2.33	0.64
6:3:149:LYS:HG3	6:3:150:GLU:N	2.12	0.63
2:W:584:TYR:CZ	2:W:614:TYR:HB2	2.32	0.63
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
6:3:144:ILE:HD13	6:3:147:MET:HE3	1.80	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
5:2:28:PRO:HA	6:3:33:THR:HB	1.80	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
6:3:214:TYR:CE2	6:3:216:LYS:HE2	2.32	0.63
2:W:432:ILE:CD1	2:W:434:HIS:CE1	2.80	0.63
5:2:28:PRO:CA	6:3:25:GLN:C	2.71	0.63
5:2:123:LEU:O	5:2:123:LEU:HD23	1.98	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
4:1:1:MET:HE3	5:2:415:GLN:CA	2.28	0.62
5:2:30:VAL:CA	6:3:25:GLN:HB3	2.28	0.62
5:2:93:LEU:HA	5:2:96:TRP:HD1	1.64	0.62
5:2:173:GLN:HG2	5:2:179:LEU:HG	1.81	0.62
4:1:38:ILE:HB	4:1:44:PHE:CE1	2.34	0.62
5:2:197:THR:HG21	5:2:239:GLN:CD	2.24	0.62
2:W:584:TYR:CG	2:W:594:ALA:HB2	2.34	0.62
4:1:5:LEU:HD21	5:2:408:LEU:HD13	0.85	0.62
5:2:218:GLN:HG2	5:2:268:PHE:HB3	1.82	0.62
2:W:209:TYR:OH	2:W:233:PHE:C	2.42	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:O	6:3:165:LYS:HD3	1.98	0.62
6:3:184:ALA:HA	6:3:187:GLN:CG	2.28	0.62
2:W:37:HIS:CE1	2:W:454:VAL:CG1	2.82	0.62
6:3:9:ASN:O	6:3:56:LYS:HD3	1.99	0.62
3:0:98:GLN:OE1	6:3:209:ILE:HG23	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1:47:ALA:HB1	4:1:50:VAL:HB	1.81	0.61
5:2:117:ASN:CG	6:3:108:ASN:CG	2.65	0.61
6:3:46:ASN:CG	6:3:104:LEU:HD22	2.25	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
6:3:18:ASN:O	6:3:21:TRP:HD1	1.83	0.61
6:3:133:LEU:HD22	6:3:134:ALA:N	2.14	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
1:V:520:ARG:HG3	4:1:23:LEU:HD11	1.82	0.61
4:1:1:MET:HG2	5:2:414:SER:N	2.16	0.61
5:2:203:PHE:HD2	5:2:205:LEU:HD23	1.64	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
2:W:584:TYR:HB2	2:W:594:ALA:HB2	1.82	0.61
5:2:31:LEU:HD13	6:3:33:THR:HG22	1.76	0.61
5:2:236:PHE:CE2	5:2:262:LEU:HD13	2.36	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
1:V:368:ALA:O	1:V:371:VAL:HG22	2.00	0.61
2:W:59:TYR:OH	2:W:63:TYR:CE2	2.53	0.60
4:1:1:MET:HA	5:2:414:SER:N	2.14	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
2:W:109:LEU:C	2:W:207:TYR:CE1	2.79	0.60
3:0:55:LEU:HD12	6:3:178:MET:CE	2.31	0.60
4:1:10:ILE:HD13	4:1:10:ILE:C	2.26	0.60
6:3:33:THR:CG2	6:3:36:LYS:HB2	2.30	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
5:2:42:LEU:HD12	5:2:59:MET:HE3	1.83	0.60
6:3:42:MET:HE2	6:3:108:ASN:CG	2.27	0.60
3:0:54:ARG:C	6:3:209:ILE:HD11	2.25	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
5:2:164:VAL:HG13	5:2:209:PRO:HG2	1.83	0.59
5:2:259:LEU:HD12	5:2:259:LEU:C	2.27	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
6:3:59:VAL:CG1	6:3:70:LEU:HB3	2.32	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
5:2:56:VAL:HG11	5:2:91:SER:CB	2.32	0.59
5:2:206:LEU:N	5:2:206:LEU:HD22	2.17	0.59
6:3:110:VAL:O	6:3:114:GLU:HG2	2.02	0.59
1:V:519:TYR:CE2	4:1:20:LEU:HG	2.37	0.59
5:2:171:VAL:HG13	5:2:216:MET:HB2	1.83	0.59
2:W:584:TYR:HB2	2:W:594:ALA:CB	2.32	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:37:HIS:ND1	2:W:454:VAL:HG13	2.15	0.59
5:2:31:LEU:HG	6:3:25:GLN:O	2.01	0.59
5:2:202:GLN:NE2	5:2:202:GLN:H	2.00	0.59
6:3:160:ARG:HB3	6:3:190:LEU:CD2	2.32	0.59
2:W:73:CYS:CB	2:W:209:TYR:CZ	2.85	0.59
4:1:29:LEU:HD23	4:1:29:LEU:C	2.27	0.59
5:2:30:VAL:HB	6:3:25:GLN:HB3	1.84	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
1:V:519:TYR:HB2	4:1:16:MET:CG	2.32	0.59
4:1:2:VAL:CG1	5:2:456:LYS:CD	2.81	0.59
5:2:44:VAL:HG13	5:2:45:PHE:N	2.17	0.59
5:2:160:LEU:HD12	5:2:160:LEU:N	2.18	0.59
6:3:174:TYR:CE1	6:3:178:MET:HE3	2.37	0.59
6:3:215:LEU:CD1	6:3:230:VAL:HG13	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
2:W:70:LEU:CG	2:W:72:TYR:CE1	2.86	0.58
4:1:38:ILE:H	4:1:38:ILE:CD1	2.16	0.58
5:2:217:LEU:HD23	5:2:233:ILE:CD1	2.33	0.58
5:2:177:GLN:HE22	5:2:220:LEU:HA	1.68	0.58
6:3:24:LYS:HE2	6:3:220:MET:SD	2.42	0.58
6:3:169:ASP:CG	6:3:202:LEU:HD23	2.29	0.58
6:3:190:LEU:HD23	6:3:190:LEU:N	2.18	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
5:2:220:LEU:HD13	5:2:220:LEU:C	2.29	0.58
6:3:21:TRP:CD2	6:3:34:LEU:HD23	2.39	0.58
6:3:131:THR:CG2	6:3:133:LEU:HD12	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:3:169:ASP:CB	6:3:202:LEU:HD23	2.33	0.58
2:W:209:TYR:CE1	2:W:233:PHE:CD1	2.90	0.58
4:1:4:VAL:HG11	5:2:412:PHE:CD2	2.28	0.58
4:1:13:ASP:OD2	4:1:17:LYS:HB3	2.03	0.58
4:1:34:ILE:HG22	4:1:46:ILE:CD1	2.32	0.58
5:2:35:TYR:CB	5:2:62:LEU:HD12	2.33	0.58
5:2:62:LEU:HD13	5:2:62:LEU:C	2.28	0.58
4:1:1:MET:HB2	5:2:418:PHE:HB3	1.84	0.58
5:2:28:PRO:HD2	6:3:25:GLN:CD	2.29	0.58
2:W:645:GLN:O	2:W:647:ARG:HD2	2.03	0.58
5:2:118:LEU:CD2	6:3:39:ASP:C	2.72	0.58
5:2:236:PHE:CZ	5:2:258:LEU:HD11	2.39	0.58
5:2:118:LEU:HD12	5:2:118:LEU:C	2.29	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
6:3:216:LYS:H	6:3:216:LYS:CD	2.13	0.57
1:V:612:ASP:OD2	1:V:635:GLN:CD	2.48	0.57
6:3:172:LEU:HD13	6:3:172:LEU:C	2.29	0.57
6:3:14:VAL:HG23	6:3:163:VAL:HG13	1.86	0.57
6:3:44:LEU:C	6:3:44:LEU:HD13	2.30	0.57
1:V:520:ARG:HD3	4:1:19:PHE:CD1	2.40	0.57
3:0:109:THR:HB	3:0:144:SER:H	1.67	0.57
6:3:187:GLN:NE2	6:3:189:ILE:HG13	2.20	0.57
2:W:584:TYR:CB	2:W:594:ALA:HB2	2.33	0.57
6:3:16:ASP:O	6:3:21:TRP:NE1	2.28	0.57
5:2:185:MET:HB2	5:2:229:ASP:OD1	2.04	0.57
1:V:514:MET:SD	1:V:537:ASN:ND2	2.78	0.57
6:3:223:LEU:HD11	6:3:227:LEU:HD11	1.87	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
6:3:57:LEU:HD23	6:3:58:ALA:C	2.30	0.56
6:3:144:ILE:HG12	6:3:147:MET:CE	2.34	0.56
1:V:519:TYR:HB3	4:1:16:MET:HG3	1.86	0.56
2:W:110:SER:N	2:W:207:TYR:CZ	2.71	0.56
5:2:60:LEU:HD11	5:2:95:ILE:CG2	2.35	0.56
5:2:117:ASN:HD22	6:3:42:MET:HE1	1.70	0.56
6:3:178:MET:SD	6:3:181:ILE:HD12	2.46	0.56
6:3:210:THR:HG22	6:3:210:THR:O	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1:18:GLN:HB2	4:1:44:PHE:CZ	2.39	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
2:W:209:TYR:HH	2:W:233:PHE:CA	2.10	0.56
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
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:HA	1:V:428:GLU:OE1	2.06	0.56
6:3:57:LEU:C	6:3:71:TYR:OH	2.48	0.56
4:1:3:ASN:CB	5:2:412:PHE:O	2.52	0.56
4:1:31:LYS:O	4:1:32:LYS:HB2	2.06	0.56
4:1:36:GLN:HB3	4:1:45:VAL:HG12	1.88	0.56
5:2:206:LEU:HD22	5:2:206:LEU:H	1.71	0.56
6:3:165:LYS:HD3	6:3:165:LYS:C	2.31	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
1:V:689:VAL:CB	5:2:391:ILE:HD11	2.36	0.55
4:1:38:ILE:HA	4:1:44:PHE:CD1	2.37	0.55
5:2:28:PRO:HA	6:3:33:THR:CB	2.36	0.55
6:3:44:LEU:HD13	6:3:44:LEU:O	2.06	0.55
3:0:97:ASP:C	6:3:208:ASP:HB3	2.32	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
5:2:53:LYS:CE	5:2:95:ILE:HD11	2.36	0.55
5:2:123:LEU:HD21	5:2:178:LEU:CD1	2.37	0.55
6:3:223:LEU:HD13	6:3:227:LEU:HG	1.88	0.55
1:V:631:GLY:O	1:V:632:SER:HB2	2.06	0.54
2:W:608:ILE:O	2:W:614:TYR:OH	2.21	0.54
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:520:ARG:NE	1:V:521:GLU:OE2	2.29	0.54
3:0:77:LYS:HA	3:0:77:LYS:NZ	2.22	0.54
1:V:519:TYR:CB	4:1:16:MET:CG	2.84	0.54
2:W:70:LEU:HD21	2:W:72:TYR:OH	2.07	0.54
6:3:64:ILE:HG23	6:3:128:HIS:CG	2.42	0.54
6:3:100:LYS:O	6:3:103:LEU:HB2	2.08	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
5:2:37:HIS:HB3	5:2:38:PRO:CD	2.35	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
2:W:416:ILE:HA	2:W:434:HIS:O	2.08	0.54
4:1:59:GLU:CD	5:2:402:ARG:HH12	2.12	0.54
5:2:211:GLN:HB3	5:2:261:PHE:CE1	2.40	0.54
6:3:223:LEU:HD13	6:3:223:LEU:C	2.32	0.54
4:1:18:GLN:HA	4:1:21:LEU:HG	1.90	0.54
4:1:34:ILE:HG21	4:1:54:GLN:CD	2.32	0.54
6:3:59:VAL:CB	6:3:71:TYR:HE1	2.01	0.54
2:W:189:TRP:NE1	2:W:194:LEU:HB2	2.22	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:428:ILE:HA	2:W:430:ASN:ND2	2.23	0.54
5:2:86:SER:O	5:2:90:LEU:HD13	2.08	0.54
1:V:667:THR:HA	4:1:62:ASP:OD2	2.07	0.53
6:3:106:SER:O	6:3:109:GLU:HG3	2.08	0.53
3:0:54:ARG:CB	6:3:209:ILE:HG23	2.25	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
3:0:76:LEU:HD11	3:0:225:GLU:N	2.22	0.53
4:1:1:MET:HB2	5:2:418:PHE:HB2	1.90	0.53
1:V:514:MET:CE	4:1:16:MET:HE1	2.38	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
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
6:3:191:ILE:N	6:3:210:THR:HG21	2.24	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
1:V:498:ASN:ND2	1:V:504:LYS:HG3	2.24	0.53
6:3:160:ARG:NH2	6:3:192:ASP:HB3	2.23	0.53
5:2:30:VAL:O	5:2:34:LEU:HD23	2.09	0.53
5:2:241:SER:O	5:2:245:LEU:HD23	2.09	0.53
6:3:15:VAL:O	6:3:15:VAL:HG23	2.08	0.53
2:W:52:LEU:HD23	2:W:72:TYR:HE2	1.71	0.53
3:0:74:GLN:N	3:0:78:PRO:O	2.40	0.53
5:2:234:LEU:HD23	5:2:234:LEU:C	2.34	0.53
6:3:34:LEU:HD13	6:3:34:LEU:C	2.33	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:3:204:GLN:HG2	6:3:214:TYR:CZ	2.44	0.53
6:3:105:THR:HG23	6:3:106:SER:N	2.23	0.53
4:1:1:MET:HE1	5:2:440:LEU:CD1	2.27	0.53
6:3:10:LEU:HD21	6:3:143:TYR:CE2	2.44	0.53
6:3:133:LEU:HD13	6:3:133:LEU:N	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
4:1:4:VAL:HG12	5:2:411:GLN:C	2.30	0.52
5:2:221:GLN:CD	5:2:230:LEU:HB2	2.34	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
1:V:519:TYR:HB2	4:1:16:MET:HG2	1.91	0.52
1:V:612:ASP:O	1:V:613:THR:O	2.28	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
2:W:433:LEU:C	2:W:434:HIS:ND1	2.68	0.52
6:3:42:MET:CG	6:3:111:ILE:HD11	2.40	0.52
1:V:514:MET:HE3	4:1:16:MET:HE1	1.91	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
5:2:31:LEU:HD13	6:3:33:THR:CG2	2.28	0.52
6:3:226:TYR:O	6:3:230:VAL:HB	2.10	0.52
5:2:257:SER:O	5:2:261:PHE:HD1	1.93	0.51
6:3:64:ILE:HG21	6:3:128:HIS:CB	2.40	0.51
6:3:71:TYR:HA	6:3:110:VAL:HG11	1.92	0.51
6:3:141:LEU:HG	6:3:187:GLN:HE22	1.75	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
6:3:14:VAL:HG23	6:3:14:VAL:O	2.09	0.51
1:V:412:MET:N	1:V:417:THR:HG21	2.25	0.51
1:V:689:VAL:CG2	5:2:391:ILE:CD1	2.88	0.51
2:W:209:TYR:HH	2:W:234:ASP:H	1.57	0.51
5:2:160:LEU:HB3	5:2:206:LEU:HD21	1.93	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
2:W:110:SER:C	2:W:207:TYR:CE1	2.79	0.51
4:1:3:ASN:HB2	5:2:412:PHE:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:2:179:LEU:CB	5:2:184:LEU:HD11	2.40	0.51
1:V:428:GLU:OE1	1:V:460:ALA:HA	2.10	0.51
2:W:581:LEU:HD13	2:W:581:LEU:C	2.36	0.51
5:2:207:ASP:OD2	5:2:254:MET:HE2	2.10	0.51
6:3:71:TYR:CG	6:3:72:PRO:HD2	2.21	0.51
6:3:121:LYS:HD3	6:3:121:LYS:N	2.25	0.51
5:2:46:ARG:HD3	5:2:85:GLU:HB2	1.93	0.51
5:2:51:LEU:CD2	5:2:55:TRP:CD1	2.94	0.51
5:2:215:PHE:CE2	5:2:264:HIS:HB2	2.46	0.51
5:2:236:PHE:CZ	5:2:262:LEU:CD2	2.94	0.51
5:2:236:PHE:CE1	5:2:261:PHE:CB	2.94	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
3:0:55:LEU:HD12	6:3:178:MET:HE3	1.93	0.50
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:HG12	5:2:456:LYS:HG2	1.81	0.50
5:2:199:ALA:HB1	5:2:201:PHE:CE2	2.47	0.50
2:W:73:CYS:O	2:W:209:TYR:CE2	2.64	0.50
5:2:30:VAL:CG1	5:2:34:LEU:HD23	2.40	0.50
5:2:35:TYR:CD1	5:2:35:TYR:N	2.79	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
6:3:60:ILE:HG22	6:3:61:ALA:N	2.26	0.50
1:V:321:GLU:HB3	2:W:499:ASN:HB2	1.93	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
4:1:1:MET:CE	5:2:415:GLN:C	2.84	0.50
5:2:93:LEU:CD2	5:2:96:TRP:HE1	2.25	0.50
5:2:214:TYR:CB	5:2:261:PHE:CE2	2.95	0.50
6:3:64:ILE:CG2	6:3:128:HIS:HB3	2.42	0.50
1:V:393:THR:CA	1:V:418:LYS:HE3	2.41	0.50
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
6:3:108:ASN:O	6:3:111:ILE:HG12	2.12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:2:181:GLN:HE22	5:2:220:LEU:HD12	1.76	0.50
6:3:178:MET:HE2	6:3:202:LEU:HD13	1.93	0.50
6:3:216:LYS:O	6:3:216:LYS:HG2	2.11	0.50
2:W:325:THR:HG22	2:W:329:PHE:CE2	2.47	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:N	6:3:202:LEU:HD22	2.27	0.50
1:V:502:ILE:O	1:V:646:ALA:HB2	2.12	0.49
1:V:667:THR:CA	4:1:62:ASP:OD1	2.59	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
5:2:188:THR:HG23	5:2:189:GLU:N	2.27	0.49
6:3:12:VAL:HG23	6:3:12:VAL:O	2.10	0.49
6:3:216:LYS:HD2	6:3:216:LYS:N	2.22	0.49
5:2:51:LEU:HD23	5:2:51:LEU:C	2.37	0.49
5:2:57:MET:HA	5:2:60:LEU:HG	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
6:3:53:ARG:HA	6:3:101:TYR:HE1	1.77	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
1:V:418:LYS:CE	1:V:418:LYS:HA	2.41	0.49
5:2:81:LYS:CE	5:2:89:LEU:HD21	2.42	0.49
5:2:245:LEU:N	5:2:245:LEU:HD22	2.27	0.49
6:3:59:VAL:HG13	6:3:59:VAL:O	2.12	0.49
6:3:217:VAL:CG1	6:3:226:TYR:CE2	2.95	0.49
2:W:37:HIS:NE2	2:W:454:VAL:CG1	2.75	0.49
3:0:54:ARG:CB	6:3:209:ILE:CG2	2.87	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
6:3:215:LEU:HD12	6:3:230:VAL:CG2	2.42	0.49
1:V:515:SER:C	4:1:16:MET:HB2	2.36	0.49
4:1:2:VAL:HG23	4:1:2:VAL:O	2.11	0.49
5:2:89:LEU:HD23	5:2:93:LEU:HG	1.94	0.49
6:3:10:LEU:CD2	6:3:143:TYR:HE2	2.25	0.49
5:2:35:TYR:CD1	5:2:62:LEU:CD1	2.95	0.49
5:2:236:PHE:CZ	5:2:258:LEU:CD1	2.95	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:CE2	2.95	0.49
6:3:12:VAL:CG2	6:3:161:ILE:HA	2.42	0.49
1:V:428:GLU:HB3	1:V:432:THR:O	2.13	0.49
3:0:55:LEU:N	6:3:209:ILE:HD11	2.28	0.49
6:3:174:TYR:HD1	6:3:202:LEU:HD11	1.78	0.49
1:V:393:THR:HA	1:V:418:LYS:CG	2.42	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
2:W:624:PRO:O	2:W:656:ALA:HB1	2.12	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
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
5:2:166: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
2:W:596:LEU:HG	2:W:597:LEU:N	2.27	0.48
5:2:77:LYS:HD3	5:2:78:GLU:HG3	1.94	0.48
5:2:170:ALA:CB	5:2:213:TRP:CZ3	2.95	0.48
6:3:21:TRP:CG	6:3:34:LEU:HD23	2.47	0.48
6:3:42:MET:HE2	6:3:108:ASN:CB	2.42	0.48
6:3:177:PHE:CZ	6:3:203:LEU:CD2	2.95	0.48
1:V:516:PRO:HB2	1:V:706:LYS:HZ1	1.77	0.48
5:2:133:THR:HG23	5:2:134:SER:N	2.29	0.48
3:0:54:ARG:CG	6:3:182:PHE:CZ	2.80	0.48
3:0:209:THR:HA	3:0:219:TYR:CD1	2.48	0.48
5:2:28:PRO:C	6:3:25:GLN:O	2.56	0.48
5:2:35:TYR:CE2	5:2:62:LEU:CB	2.96	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
1:V:516:PRO:HG2	1:V:706:LYS:HE2	1.91	0.48
4:1:21:LEU:N	4:1:21:LEU:HD23	2.29	0.48
5:2:60:LEU:CD1	5:2:95:ILE:CG2	2.91	0.48
1:V:514:MET:SD	1:V:537:ASN:CG	2.97	0.48
3:0:55:LEU:HD12	6:3:178:MET:HE1	1.95	0.48
6:3:69:PHE:HE1	6:3:139:LYS:HD2	1.77	0.48
4:1:22:TYR:CD1	4:1:22:TYR:C	2.92	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:2:251:VAL:HG11	5:2:254:MET:SD	2.53	0.48
2:W:608:ILE:HG23	2:W:614:TYR:CZ	2.48	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
6:3:165:LYS:HZ1	6:3:200:SER:H	1.62	0.48
2:W:421:PHE:CB	2:W:430:ASN:C	2.80	0.48
5:2:100:LEU:HD11	5:2:119:ARG:CG	2.31	0.48
1:V:522:TYR:CE2	4:1:62:ASP:CG	2.69	0.48
2:W:285:TYR:CE1	2:W:403:PHE:CZ	3.01	0.48
2:W:419:GLU:O	2:W:420:PRO:C	2.55	0.48
6:3:124:ILE:O	6:3:127:GLN:HB2	2.14	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:H	4:1:53:LEU:CD1	2.26	0.48
6:3:165:LYS:NZ	6:3:200:SER:H	2.12	0.48
2:W:28:LEU:C	2:W:28:LEU:HD13	2.38	0.47
2:W:263:LEU:C	2:W:263:LEU:HD23	2.39	0.47
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
5:2:30:VAL:N	6:3:25:GLN:HG3	2.23	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
5:2:35:TYR:CD1	5:2:62:LEU:CG	2.92	0.47
5:2:163:MET:HE1	5:2:206:LEU:HB3	1.94	0.47
5:2:203:PHE:CD2	5:2:204:LEU:N	2.82	0.47
5:2:218:GLN:HG2	5:2:268:PHE:CB	2.44	0.47
5:2:236:PHE:CD1	5:2:261:PHE:HB3	2.49	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
2:W:70:LEU:HG	2:W:72:TYR:CE1	2.49	0.47
5:2:117:ASN:CB	6:3:42:MET:HE1	2.42	0.47
6:3:10:LEU:CD1	6:3:56:LYS:HG2	2.44	0.47
6:3:34:LEU:HD22	6:3:37:CYS:SG	2.55	0.47
6:3:124:ILE:HD13	6:3:124:ILE:C	2.38	0.47
6:3:226:TYR:CA	6:3:230:VAL:HG23	2.42	0.47
1:V:361:CYS:HB3	1:V:405:VAL:HG21	1.96	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
4:1:57:VAL:CG2	4:1:61:MET:HE3	2.44	0.47
5:2:205:LEU:N	5:2:205:LEU:HD22	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
5:2:28:PRO:CD	6:3:25:GLN:NE2	2.75	0.47
5:2:93:LEU:CA	5:2:96:TRP:CD1	2.94	0.47
5:2:138:PRO:HD3	5:2:189:GLU:CD	2.40	0.47
6:3:10:LEU:HA	6:3:56:LYS:HG2	1.96	0.47
1:V:315:VAL:CG1	2:W:500:ASP:CG	2.81	0.47
2:W:52:LEU:CD2	2:W:72:TYR:OH	2.55	0.47
2:W:432:ILE:HD11	2:W:434:HIS:CE1	2.48	0.47
4:1:9:LEU:N	4:1:9:LEU:HD12	2.29	0.47
4:1:45:VAL:CG2	5:2:409:TYR:CE2	2.98	0.47
4:1:50:VAL:CG1	4:1:54:GLN:HG2	2.41	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
5:2:211:GLN:CB	5:2:261:PHE:CE1	2.95	0.47
6:3:24:LYS:HE2	6:3:196:LEU:HB3	1.96	0.47
2:W:73:CYS:CB	2:W:209:TYR:CE1	2.98	0.47
4:1:22:TYR:O	4:1:25:GLU:HB3	2.15	0.47
6:3:64:ILE:HG21	6:3:128:HIS:HB3	1.97	0.47
2:W:37:HIS:CG	2:W:454:VAL:HG13	2.50	0.47
2:W:73:CYS:HB3	2:W:209:TYR:CD1	2.50	0.47
2:W:143:ARG:HH11	2:W:143:ARG:HG2	1.80	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
6:3:56:LYS:HD3	6:3:56:LYS:N	2.30	0.47
6:3:137:LEU:HD11	6:3:177:PHE:CE1	2.50	0.47
2:W:657:MET:O	2:W:660:ALA:HB3	2.15	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
5:2:240:LEU:HD12	5:2:240:LEU:N	2.30	0.47
1:V:514:MET:HE3	4:1:16:MET:HE2	1.95	0.46
2:W:170:LEU:CD1	2:W:175:TYR:OH	2.51	0.46
4:1:38:ILE:HG12	4:1:38:ILE:O	2.15	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:109:LEU:HG	2:W:207:TYR:CZ	2.50	0.46
6:3:12:VAL:CG2	6:3:161:ILE:HG23	2.43	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
4:1:5:LEU:HD11	5:2:408:LEU:CB	2.11	0.46
4:1:38:ILE:CG2	4:1:44:PHE:CD1	2.94	0.46
5:2:223:ALA:C	5:2:225:SER:H	2.24	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
1:V:504:LYS:HB3	1:V:655:TYR:HA	1.97	0.46
1:V:689:VAL:CG2	5:2:391:ILE:HD13	2.46	0.46
4:1:10:ILE:HG12	4:1:43:VAL:CG1	2.45	0.46
6:3:196:LEU:HB3	6:3:220:MET:SD	2.56	0.46
1:V:514:MET:CE	4:1:16:MET:CE	2.93	0.46
5:2:96:TRP:CZ2	5:2:97:HIS:NE2	2.83	0.46
5:2:123:LEU:HD23	5:2:123:LEU:C	2.41	0.46
5:2:217:LEU:CD2	5:2:233:ILE:HD11	2.45	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
4:1:22: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
2:W:37:HIS:NE2	2:W:454:VAL:HG11	2.31	0.46
4:1:57:VAL:HG13	4:1:58:GLY:N	2.31	0.46
5:2:118:LEU:HD21	6:3:39:ASP:OD1	1.95	0.46
5:2:170:ALA:C	5:2:213:TRP:CZ3	2.94	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
6:3:9:ASN:C	6:3:56:LYS:HE3	2.41	0.46
6:3:15:VAL:HG12	6:3:164:ILE:HD12	1.97	0.46
6:3:125:LYS:C	6:3:127:GLN:H	2.24	0.46
1:V:628:SER:C	1:V:629:HIS:O	2.49	0.45
4:1:59:GLU:CD	5:2:402:ARG:CZ	2.88	0.45
5:2:211:GLN:CD	5:2:261:PHE:CE1	2.94	0.45
6:3:64:ILE:CG2	6:3:128:HIS:CB	2.94	0.45
6:3:141:LEU:C	6:3:144:ILE:HG22	2.41	0.45
2:W:37:HIS:CD2	2:W:454:VAL:CG1	2.99	0.45
4:1:13:ASP:CG	4:1:14:PRO:CD	2.80	0.45
5:2:35:TYR:CD2	5:2:62:LEU:CB	2.95	0.45
5:2:203:PHE:CG	5:2:204:LEU:N	2.84	0.45
6:3:8:LEU:HD23	6:3:54:SER:CB	2.42	0.45
6:3:64:ILE:CG2	6:3:128:HIS:CG	2.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:517:GLU:CB	1:V:713:LEU:HD22	2.46	0.45
1:V:519:TYR:CE2	4:1:20:LEU:CB	3.00	0.45
5:2:236:PHE:CD1	5:2:239:GLN:CD	2.95	0.45
5:2:117:ASN:HB2	6:3:104:LEU:CG	2.47	0.45
5:2:221:GLN:HG2	5:2:268:PHE:HZ	1.75	0.45
1:V:370:SER:OG	1:V:614:SER:OG	2.34	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
6:3:228:LEU:HD23	6:3:228:LEU:C	2.41	0.45
4:1:54:GLN:O	4:1:57:VAL:HG12	2.16	0.45
5:2:30:VAL:CG1	5:2:34:LEU:CD2	2.94	0.45
5:2:84:GLU:HA	5:2:84:GLU:OE1	2.15	0.45
5:2:89:LEU:HD23	5:2:89:LEU:C	2.42	0.45
5:2:90:LEU:HD21	5:2:140:LYS:HD3	1.98	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
6:3:21:TRP:HA	6:3:24:LYS:CG	2.46	0.45
6:3:219:GLN:OE1	6:3:219:GLN:HA	2.17	0.45
1:V:444:HIS:O	1:V:447:PRO:CD	2.62	0.45
1:V:514:MET:HE2	1:V:664:SER:HB3	1.99	0.45
3:0:79:ASN:C	3:0:81:LEU:N	2.63	0.45
5:2:203:PHE:CD2	5:2:205:LEU:CD2	2.95	0.45
6:3:121:LYS:HD3	6:3:121:LYS:H	1.81	0.45
6:3:148:ASN:CG	6:3:157:MET:HE2	2.42	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
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
2:W:433:LEU:C	2:W:434:HIS:HD1	2.25	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
2:W:432:ILE:HG12	2:W:434:HIS:ND1	2.23	0.44
2:W:421:PHE:HB2	2:W:431:PRO:HD3	1.84	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
5:2:219:TYR:CD1	5:2:219:TYR:C	2.95	0.44
2:W:207:TYR:CD1	2:W:208:SER:N	2.86	0.44
3:0:54:ARG:HA	6:3:209:ILE:HD13	1.06	0.44
3:0:106:ILE:HD11	3:0:127:HIS:HB3	2.00	0.44
6:3:160:ARG:HE	6:3:160:ARG:HB2	1.58	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:3:228:LEU:HD23	6:3:228:LEU:O	2.17	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
6:3:60:ILE:HG23	6:3:68:ARG:O	2.17	0.44
6:3:144:ILE:O	6:3:144:ILE:HD13	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
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
4:1:7:GLY:C	4:1:8:VAL:HG23	2.43	0.44
5:2:159:VAL:HG12	5:2:161:HIS:HB2	1.99	0.44
6:3:65:GLN:O	6:3:132:LEU:HD11	2.18	0.44
6:3:160:ARG:CB	6:3:190:LEU:CD2	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
3:0:98:GLN:C	3:0:100:PRO:HD3	2.42	0.44
5:2:60:LEU:CD1	5:2:95:ILE:CB	2.95	0.44
5:2:206:LEU:CD2	5:2:206:LEU:H	2.30	0.44
2:W:421:PHE:HB2	2:W:430:ASN:HA	2.00	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
6:3:124:ILE:O	6:3:124:ILE:HG23	2.18	0.44
1:V:519:TYR:HA	1:V:522:TYR:HB3	2.00	0.43
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
6:3:64:ILE:HB	6:3:123:ASP:CG	2.43	0.43
7:X:6:DC:H2'	7:X:7:DG:C8	2.53	0.43
1:V:282:LYS:HE3	1:V:482:PHE:CD1	2.54	0.43
1:V:409:THR:H	1:V:418:LYS:CB	2.31	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
5:2:56:VAL:HG23	5:2:57:MET:N	2.31	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
6:3:184:ALA:C	6:3:187:GLN:HG2	2.43	0.43
6:3:187:GLN:CD	6:3:189:ILE:HG13	2.43	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
5:2:35:TYR:CD1	5:2:62:LEU:HD12	2.52	0.43
5:2:117:ASN:ND2	6:3:108:ASN:N	2.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
6:3:178:MET:O	6:3:182:PHE:HD2	2.01	0.43
6:3:178:MET:HA	6:3:181:ILE:HD12	1.99	0.43
6:3:222:SER:HB3	6:3:225:GLN:CD	2.43	0.43
2:W:645:GLN:C	2:W:647:ARG:H	2.24	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:411:SER:O	1:V:417:THR:HB	2.19	0.43
1:V:519:TYR:CE2	4:1:20:LEU:HB2	2.54	0.43
1:V:519:TYR:H	4:1:16:MET:HG3	1.83	0.43
5:2:87:THR:C	5:2:89:LEU:H	2.26	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
5:2:214:TYR:OH	5:2:265:LEU:HD13	2.18	0.43
5:2:270:LEU:HD23	5:2:270:LEU:C	2.43	0.43
5:2:270:LEU:HA	5:2:273:GLN:HG3	2.00	0.43
1:V:504:LYS:CB	1:V:655:TYR:HA	2.48	0.43
1:V:514:MET:SD	4:1:16:MET:HE1	2.59	0.43
1:V:514:MET:HB3	4:1:16:MET:SD	2.58	0.43
3:0:77:LYS:CB	3:0:83:CYS:SG	2.89	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
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
6:3:174:TYR:HE1	6:3:178:MET:HE3	1.77	0.43
2:W:73:CYS:CB	2:W:209:TYR:CE2	3.02	0.43
4:1:1:MET:CA	5:2:413:LEU:HA	2.48	0.43
5:2:29:GLY:C	6:3:25:GLN:HG3	2.40	0.43
5:2:30:VAL:HB	6:3:24:LYS:O	2.19	0.43
5:2:34:LEU:N	5:2:34:LEU:HD22	2.33	0.43
5:2:201:PHE:CD1	5:2:201:PHE:C	2.96	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
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
3:0:96:PHE:CG	3:0:124:PRO:HB3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
6:3:229:TRP:CD1	6:3:229:TRP:C	2.96	0.43
1:V:689:VAL:CG2	5:2:391:ILE:HD11	2.48	0.43
2:W:584:TYR:CB	2:W:591:GLY:HA3	2.49	0.43
4:1:8:VAL:CG1	4:1:9:LEU:N	2.80	0.43
5:2:31:LEU:HG	6:3:33:THR:HB	1.95	0.43
6:3:57:LEU:HD23	6:3:57:LEU:C	2.43	0.43
5:2:236:PHE:CE1	5:2:239:GLN:NE2	2.87	0.42
6:3:154:ASN:CG	6:3:155:GLN:H	2.26	0.42
6:3:184:ALA:O	6:3:187:GLN:HG2	2.19	0.42
5:2:230:LEU:C	5:2:230:LEU:HD13	2.44	0.42
6:3:137:LEU:HD12	6:3:177:PHE:CE1	2.54	0.42
6:3:141:LEU:HA	6:3:144:ILE:HG22	2.01	0.42
3:0:73:ASP:O	3:0:78:PRO:O	2.37	0.42
5:2:35:TYR:CG	5:2:62:LEU:CD1	2.99	0.42
5:2:159:VAL:HG11	5:2:161:HIS:CD2	2.49	0.42
6:3:8:LEU:CD2	6:3:54:SER:HB3	2.45	0.42
1:V:666:ASP:CB	4:1:17:LYS:HZ3	2.32	0.42
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
6:3:159:SER:HG	6:3:189:ILE:HD12	1.85	0.42
5:2:57:MET:CA	5:2:60:LEU:HG	2.49	0.42
5:2:188:THR:CG2	5:2:189:GLU:N	2.83	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
6:3:42:MET:SD	6:3:111:ILE:CD1	3.07	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
2:W:282:ARG:HA	2:W:285:TYR:CD2	2.54	0.42
3:0:96:PHE:CE2	3:0:124:PRO:HA	2.54	0.42
4:1:1:MET:SD	5:2:419:GLU:N	2.92	0.42
5:2:89:LEU:CD2	5:2:89:LEU:C	2.93	0.42
5:2:171:VAL:CG1	5:2:216:MET:SD	3.06	0.42
6:3:9:ASN:OD1	6:3:158:LYS:HB3	2.19	0.42
6:3:100:LYS:CB	6:3:103:LEU:HD13	2.41	0.42
6:3:165:LYS:HZ1	6:3:200:SER:N	2.17	0.42
5:2:77:LYS:HD3	5:2:78:GLU:CG	2.50	0.42
5:2:123:LEU:CD2	5:2:123:LEU:C	2.93	0.42
5:2:140:LYS:CD	5:2:162:PHE:HE1	2.29	0.42
5:2:172:SER:C	5:2:175:LEU:HD23	2.43	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:2:236:PHE:CE1	5:2:261:PHE:HB3	2.54	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
1:V:315:VAL:HG13	2:W:500:ASP:HB2	0.42	0.42
1:V:503:ALA:HB2	1:V:646:ALA:H	1.82	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
6:3:18:ASN:ND2	6:3:64:ILE:HD11	2.35	0.42
6:3:197:ASP:O	6:3:198:SER:HB3	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
5:2:171:VAL:HG13	5:2:216:MET:HB3	1.98	0.42
6:3:64:ILE:CB	6:3:123:ASP:HB3	2.49	0.42
6:3:105:THR:CG2	6:3:106:SER:N	2.82	0.42
6:3:217:VAL:HG12	6:3:218:PRO:O	2.20	0.42
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
3:0:165:ARG:HD3	3:0:194:ILE:HG12	2.02	0.41
6:3:100:LYS:HB2	6:3:100:LYS:HE2	1.89	0.41
6:3:228:LEU:C	6:3:228:LEU:CD2	2.93	0.41
3:0:73:ASP:C	3:0:78:PRO:O	2.63	0.41
4:1:10:ILE:C	4:1:10:ILE:CD1	2.93	0.41
6:3:70:LEU:HD13	6:3:115:ILE:HD11	2.02	0.41
6:3:221:PRO:C	6:3:223:LEU:H	2.27	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
5:2:202:GLN:HE21	5:2:202:GLN:N	2.15	0.41
5:2:204:LEU:HD23	5:2:254:MET:HE3	2.02	0.41
5:2:270:LEU:C	5:2:270:LEU:CD2	2.94	0.41
1:V:514:MET:HE2	1:V:667:THR:HG21	2.01	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
4:1:31:LYS:C	4:1:33:PHE:H	2.28	0.41
4:1:43:VAL:CG1	4:1:44:PHE:N	2.82	0.41
5:2:62:LEU:C	5:2:62:LEU:CD1	2.94	0.41
5:2:170:ALA:C	5:2:213:TRP:HZ3	2.27	0.41
5:2:175:LEU:CD2	5:2:216:MET:SD	3.07	0.41
5:2:176:ALA:HB3	5:2:178:LEU:HD13	1.98	0.41
6:3:14:VAL:HG22	6:3:162:LEU:O	2.21	0.41
1:V:426:VAL:C	1:V:427:MET:O	2.51	0.41
4:1:13:ASP:OD1	4:1:14:PRO:HD2	2.17	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:2:93:LEU:HD23	5:2:96:TRP:HE1	1.85	0.41
5:2:221:GLN:O	5:2:268:PHE:CE1	2.74	0.41
6:3:109:GLU:HG3	6:3:110:VAL:N	2.35	0.41
1:V:408:SER:HB3	1:V:418:LYS:HB3	2.03	0.41
4:1:52:VAL:CG2	4:1:53:LEU:N	2.83	0.41
6:3:41:VAL:HG13	6:3:42:MET:N	2.35	0.41
1:V:390:CYS:SG	1:V:399:LYS:HE3	2.61	0.41
1:V:612:ASP:O	1:V:613:THR:C	2.63	0.41
2:W:212:LEU:C	2:W:212:LEU:HD13	2.46	0.41
5:2:206:LEU:CD2	5:2:206:LEU:N	2.84	0.41
6:3:34:LEU:C	6:3:34:LEU:CD1	2.94	0.41
1:V:631:GLY:O	1:V:632:SER:CB	2.69	0.41
4:1:1:MET:N	5:2:418:PHE:CB	2.84	0.41
5:2:181:GLN:HA	5:2:181:GLN:NE2	2.34	0.41
5:2:236:PHE:HZ	5:2:258:LEU:CD1	2.34	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:353:ALA:O	1:V:357:VAL:HG23	2.21	0.41
3:0:76:LEU:HD11	3:0:224:ASP:C	2.46	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:CD2	5:2:236:PHE:C	2.94	0.41
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
2:W:74:SER:OG	2:W:207:TYR:O	2.37	0.40
5:2:93:LEU:CA	5:2:96:TRP:HD1	2.31	0.40
6:3:44:LEU:C	6:3:44:LEU:CD1	2.94	0.40
6:3:187:GLN:CG	6:3:189:ILE:CG1	2.94	0.40
5:2:34:LEU:CD2	5:2:34:LEU:N	2.84	0.40
5:2:224:GLN:CB	5:2:268:PHE:CZ	2.94	0.40
5:2:236:PHE:HZ	5:2:262:LEU:CD2	2.35	0.40
6:3:60:ILE:CG2	6:3:61:ALA:N	2.83	0.40
4:1:7:GLY:C	4:1:8:VAL:CG2	2.94	0.40
4:1:38:ILE:CB	4:1:44:PHE:CD1	3.04	0.40
5:2:51:LEU:CD2	5:2:51:LEU:C	2.94	0.40
5:2:93:LEU:O	5:2:96:TRP:CD1	2.74	0.40
5:2:251:VAL:CG1	5:2:254:MET:CG	2.95	0.40
6:3:42:MET:HG2	6:3:111:ILE:CD1	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:3:222:SER:HB3	6:3:225:GLN:OE1	2.21	0.40
1:V:413:LEU:H	1:V:417:THR:CG2	2.35	0.40
5:2:94:ARG:HD2	5:2:95:ILE:HD13	2.02	0.40
5:2:411:GLN:C	5:2:413:LEU:HD12	2.47	0.40
2:W:233:PHE:HB2	2:W:456:ILE:HG22	2.02	0.40
5:2:93:LEU:HA	5:2:93:LEU:HD23	1.77	0.40
5:2:399:ASP:OD1	5:2:402:ARG:NH1	2.55	0.40
6:3:18:ASN:OD1	6:3:19:PRO:HD2	2.21	0.40
6:3:172:LEU:C	6:3:172:LEU:CD1	2.94	0.40
6:3:187:GLN:HE21	6:3:189:ILE:HB	1.86	0.40
6:3:222:SER:O	6:3:226:TYR:CD2	2.75	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	V	473/782 (60%)	401 (85%)	47 (10%)	25 (5%)	1	15
2	W	661/760 (87%)	569 (86%)	68 (10%)	24 (4%)	2	20
3	0	186/395 (47%)	166 (89%)	15 (8%)	5 (3%)	4	25
4	1	60/71 (84%)	49 (82%)	9 (15%)	2 (3%)	3	21
5	2	264/462 (57%)	246 (93%)	14 (5%)	4 (2%)	8	40
6	3	187/308 (61%)	175 (94%)	10 (5%)	2 (1%)	11	46
All	All	1831/2778 (66%)	1606 (88%)	163 (9%)	62 (3%)	4	21

All (62) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	V	385	ASP

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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%)	402 (95%)	20 (5%)	23	45
2	W	577/664 (87%)	540 (94%)	37 (6%)	16	37
3	0	171/352 (49%)	163 (95%)	8 (5%)	23	45
4	1	56/64 (88%)	51 (91%)	5 (9%)	9	28
5	2	238/399 (60%)	229 (96%)	9 (4%)	29	50
6	3	171/272 (63%)	160 (94%)	11 (6%)	16	37
All	All	1635/2439 (67%)	1545 (94%)	90 (6%)	21	41

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	V	246	MET
1	V	271	GLU
1	V	332	ARG
1	V	362	LEU
1	V	371	VAL
1	V	418	LYS
1	V	427	MET
1	V	428	GLU
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	568	LEU
1	V	581	TYR
1	V	590	MET
1	V	614	SER
1	V	648	LYS
2	W	37	HIS
2	W	64	PRO
2	W	87	LEU
2	W	95	GLU
2	W	101	LYS
2	W	112	ARG
2	W	122	THR
2	W	123	PRO
2	W	152	LEU
2	W	166	ARG
2	W	177	LEU
2	W	196	ARG
2	W	263	LEU
2	W	282	ARG
2	W	283	ASP
2	W	288	LEU
2	W	307	ASN
2	W	309	VAL
2	W	327	GLU
2	W	333	LEU
2	W	345	ARG
2	W	346	VAL
2	W	421	PHE

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Mol	Chain	Res	Type
2	W	425	THR
2	W	461	LEU
2	W	523	LEU
2	W	533	ASP
2	W	554	GLU
2	W	581	LEU
2	W	596	LEU
2	W	610	PHE
2	W	620	MET
2	W	645	GLN
2	W	647	ARG
2	W	664	VAL
2	W	669	ARG
2	W	676	LEU
3	0	77	LYS
3	0	103	GLN
3	0	125	ARG
3	0	174	LEU
3	0	202	SER
3	0	218	THR
3	0	222	ILE
3	0	223	LEU
4	1	10	ILE
4	1	16	MET
4	1	18	GLN
4	1	21	LEU
4	1	38	ILE
5	2	77	LYS
5	2	181	GLN
5	2	202	GLN
5	2	402	ARG
5	2	407	VAL
5	2	421	LEU
5	2	426	ARG
5	2	430	VAL
5	2	452	LYS
6	3	24	LYS
6	3	25	GLN
6	3	56	LYS
6	3	70	LEU
6	3	109	GLU
6	3	124	ILE

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Mol	Chain	Res	Type
6	3	133	LEU
6	3	144	ILE
6	3	185	GLN
6	3	190	LEU
6	3	216	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	V	281	GLN
1	V	366	ASN
1	V	377	GLN
1	V	415	HIS
1	V	459	GLN
1	V	537	ASN
1	V	539	ASN
1	V	621	ASN
1	V	665	GLN
1	V	677	GLN
2	W	187	GLN
2	W	203	ASN
2	W	250	ASN
2	W	316	GLN
2	W	328	HIS
2	W	430	ASN
2	W	700	HIS
3	0	60	HIS
4	1	27	ASN
4	1	51	ASN
5	2	97	HIS
5	2	161	HIS
5	2	181	GLN
5	2	202	GLN
5	2	221	GLN
5	2	239	GLN
5	2	263	GLN
5	2	273	GLN
5	2	411	GLN
5	2	458	GLN
6	3	52	ASN
6	3	63	HIS
6	3	148	ASN

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Mol	Chain	Res	Type
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 oligosaccharides 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.

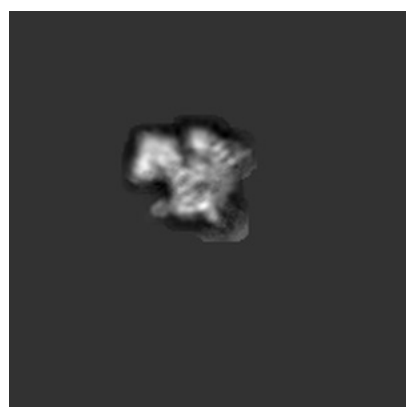
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8131. These allow visual inspection of the internal detail of the map and identification of artifacts.

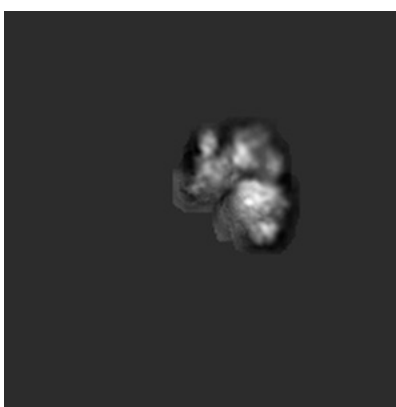
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

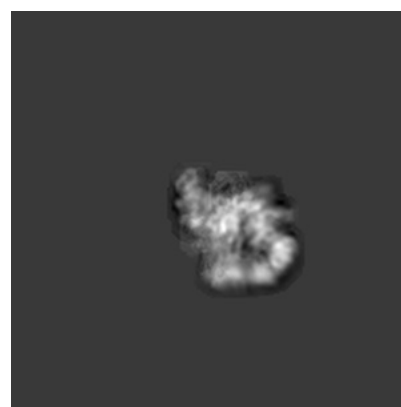
6.1.1 Primary map



X



Y

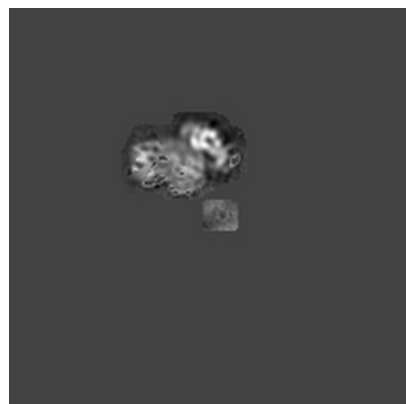


Z

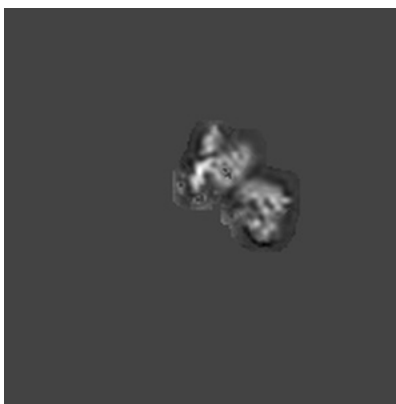
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

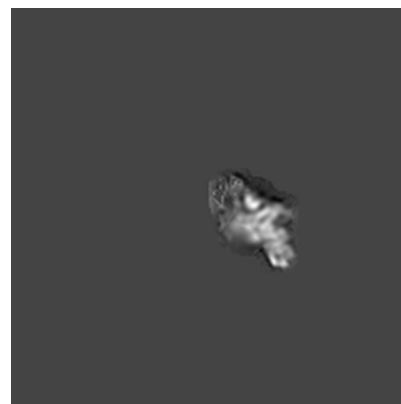
6.2.1 Primary map



X Index: 96



Y Index: 96

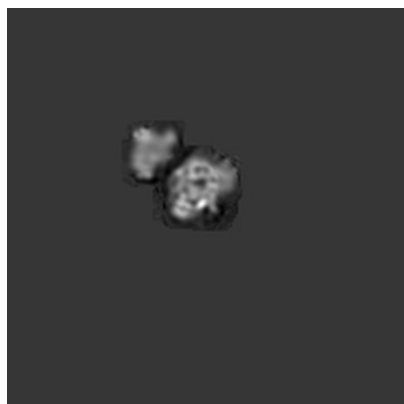


Z Index: 96

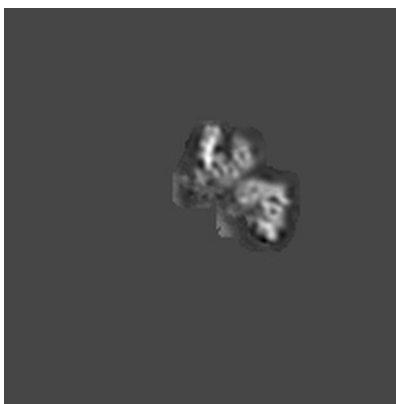
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

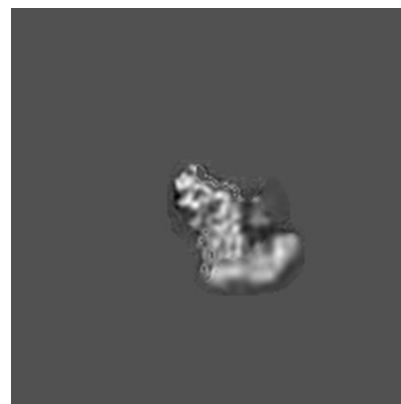
6.3.1 Primary map



X Index: 119



Y Index: 93

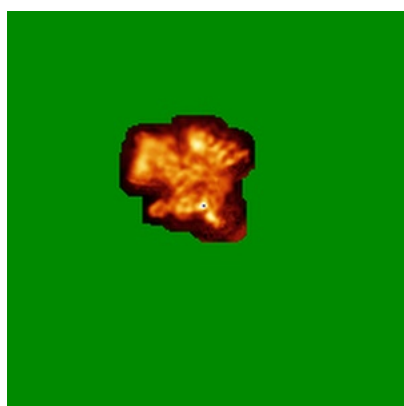


Z Index: 120

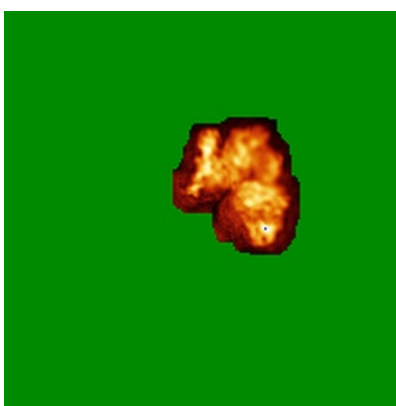
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

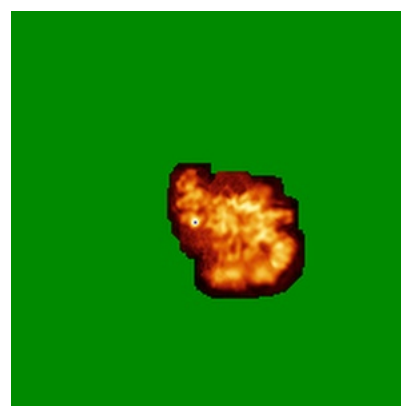
6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

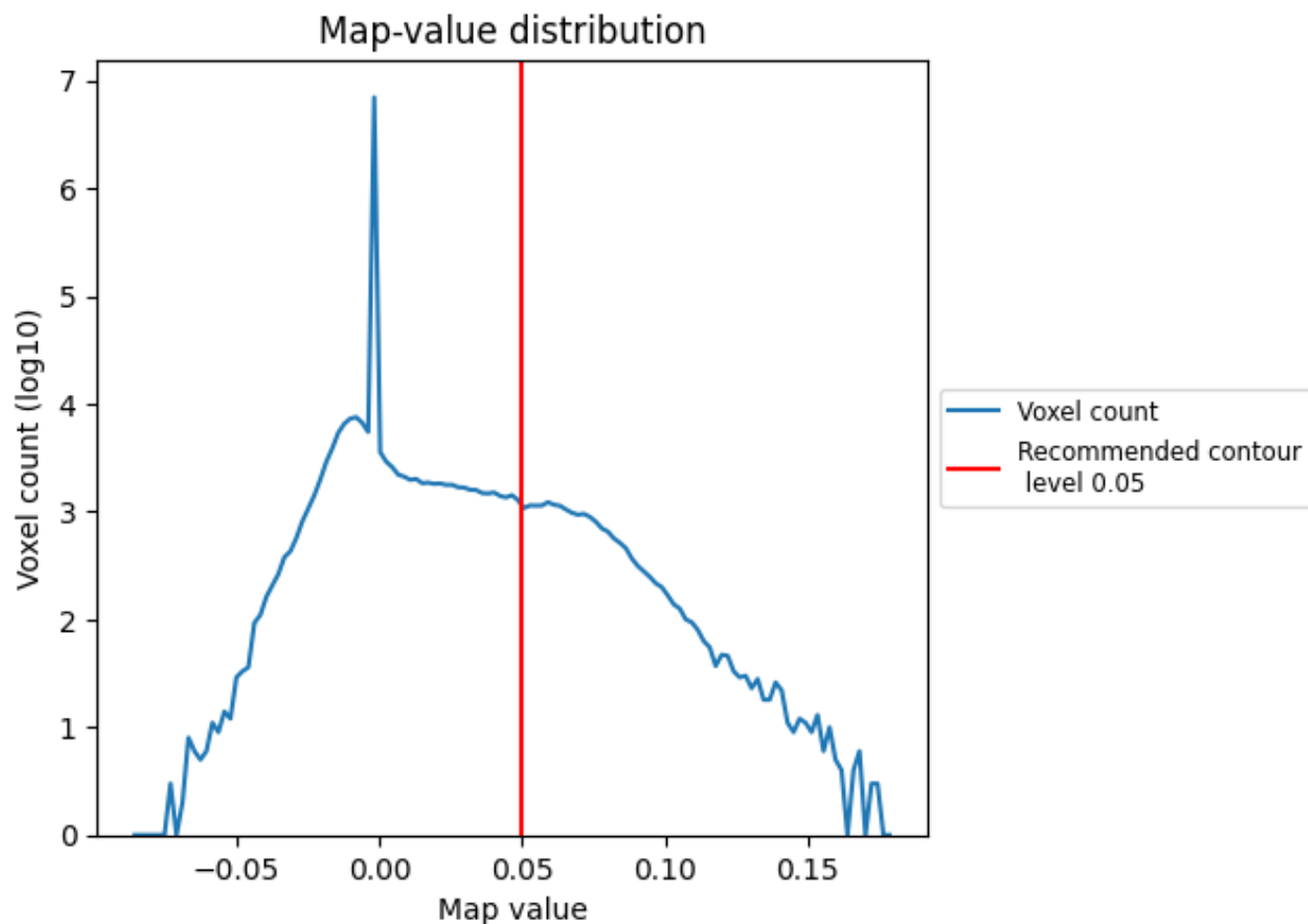
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

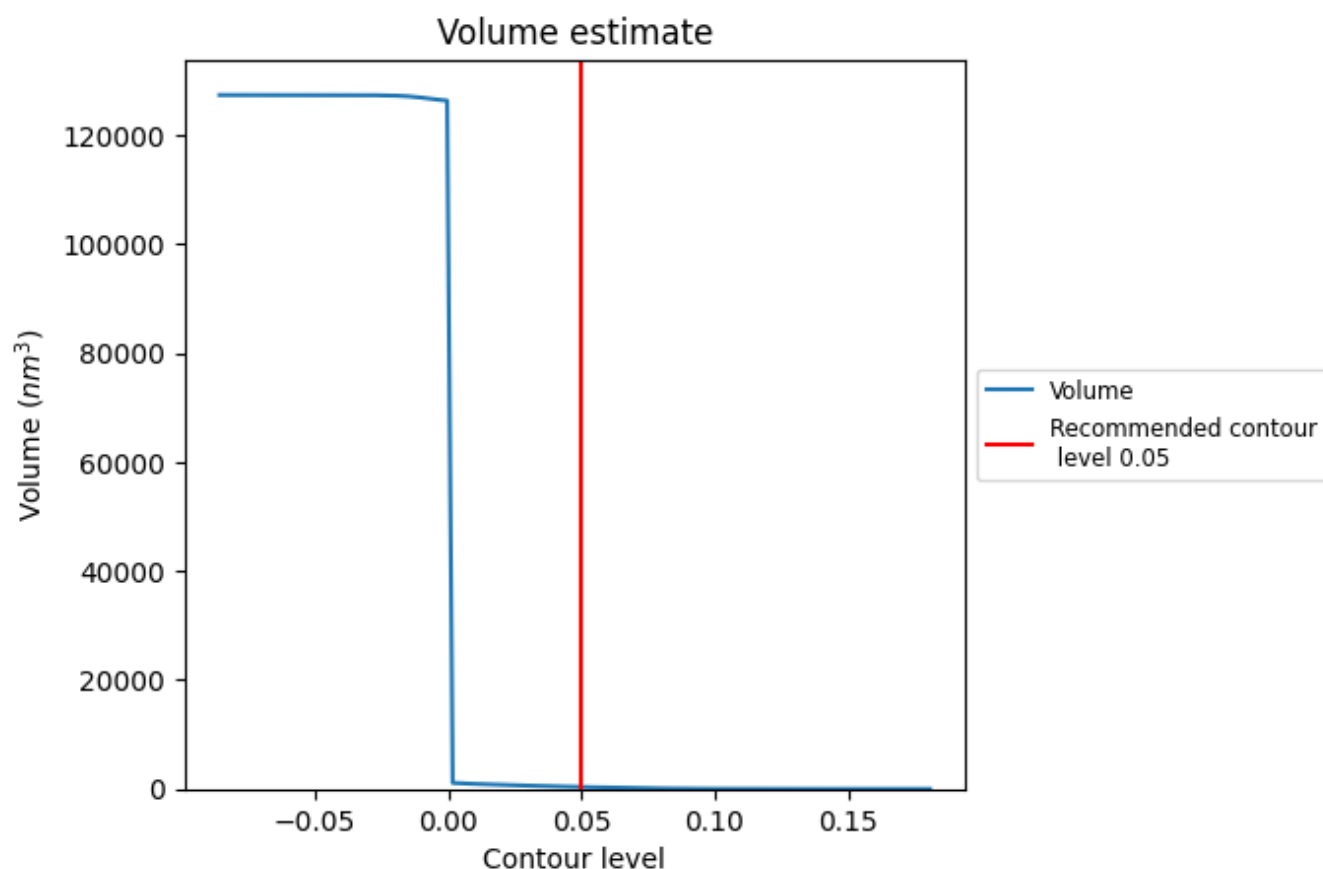
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

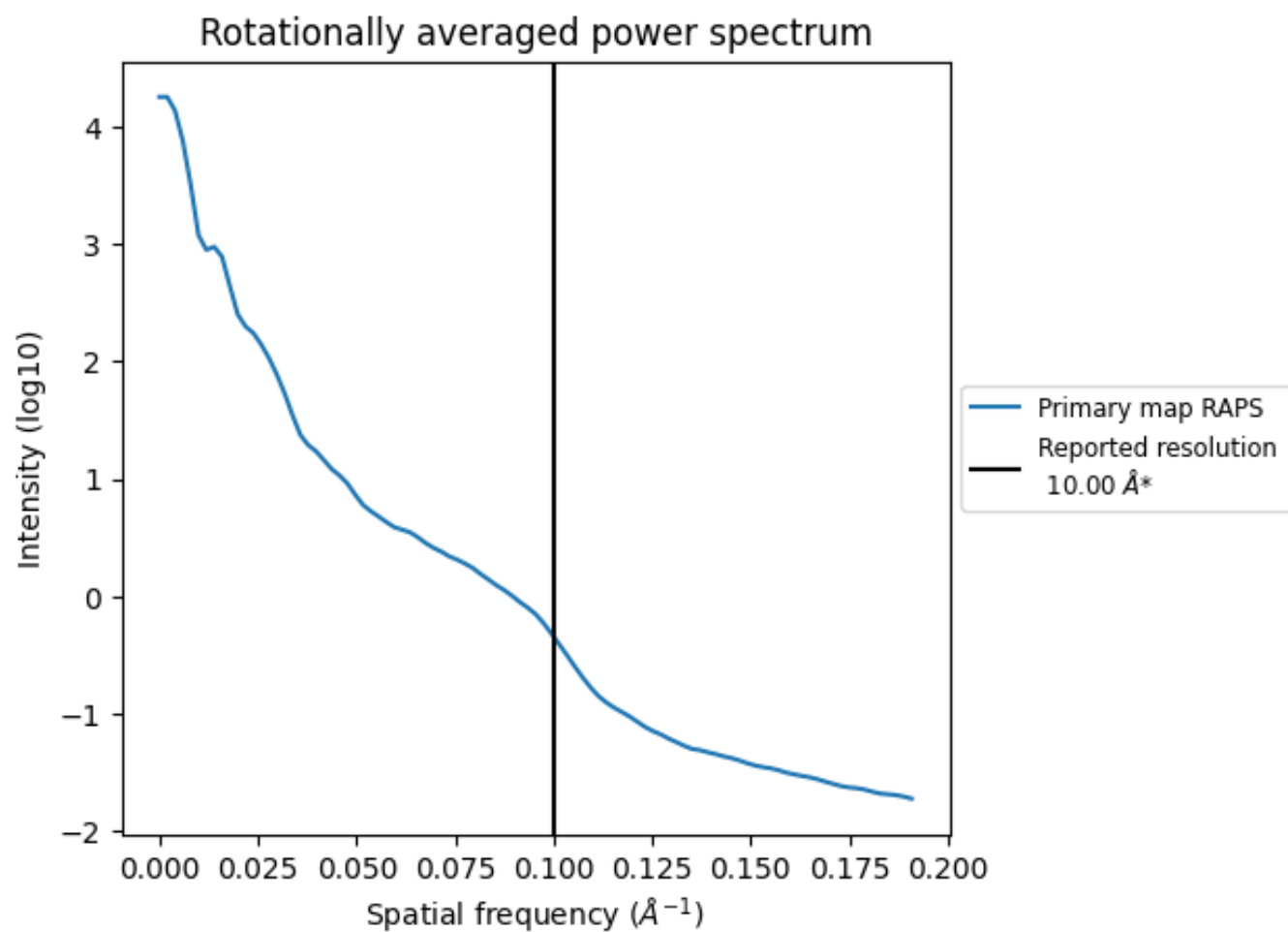
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 356 nm³; this corresponds to an approximate mass of 321 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.100 Å⁻¹

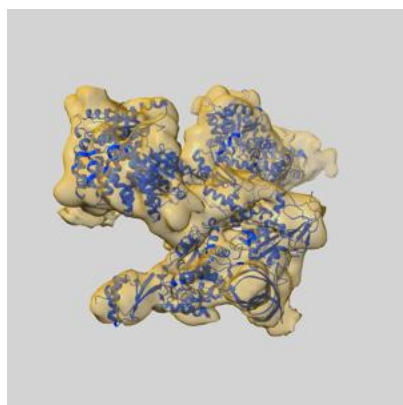
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

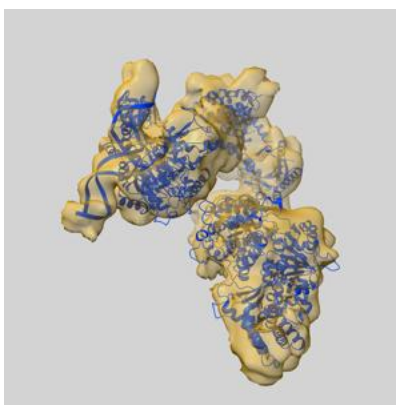
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-8131 and PDB model 5IVW. Per-residue inclusion information can be found in section 3 on page 6.

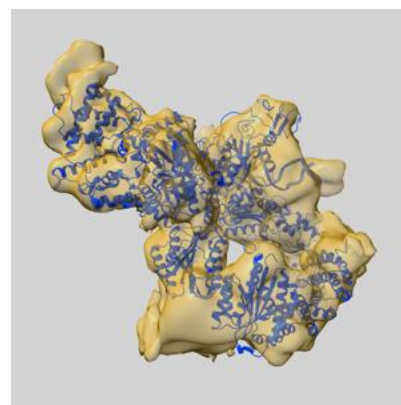
9.1 Map-model overlay [i](#)



X



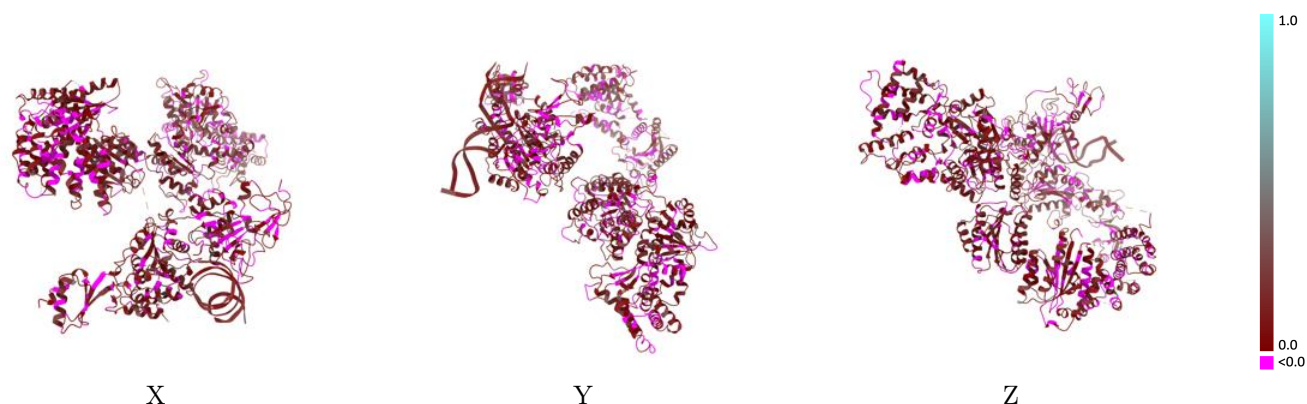
Y



Z

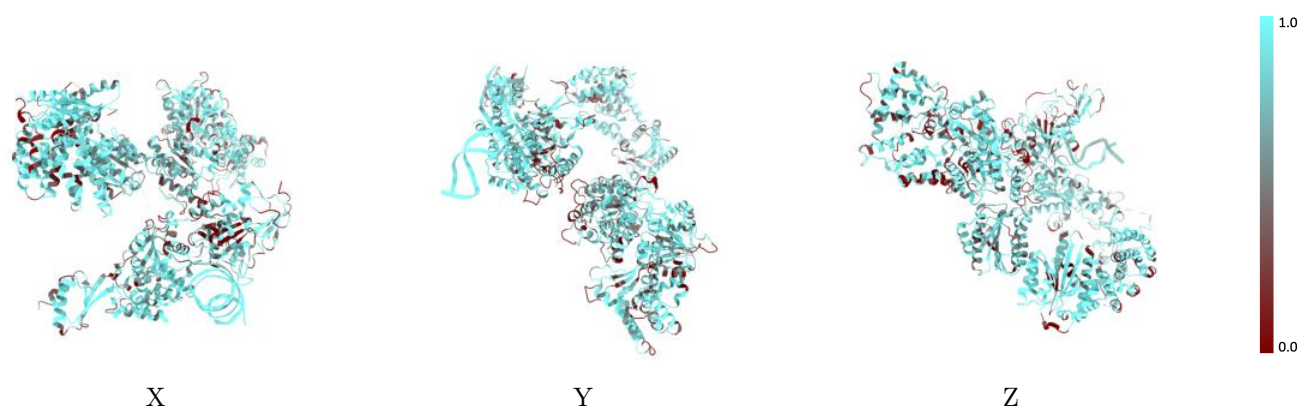
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



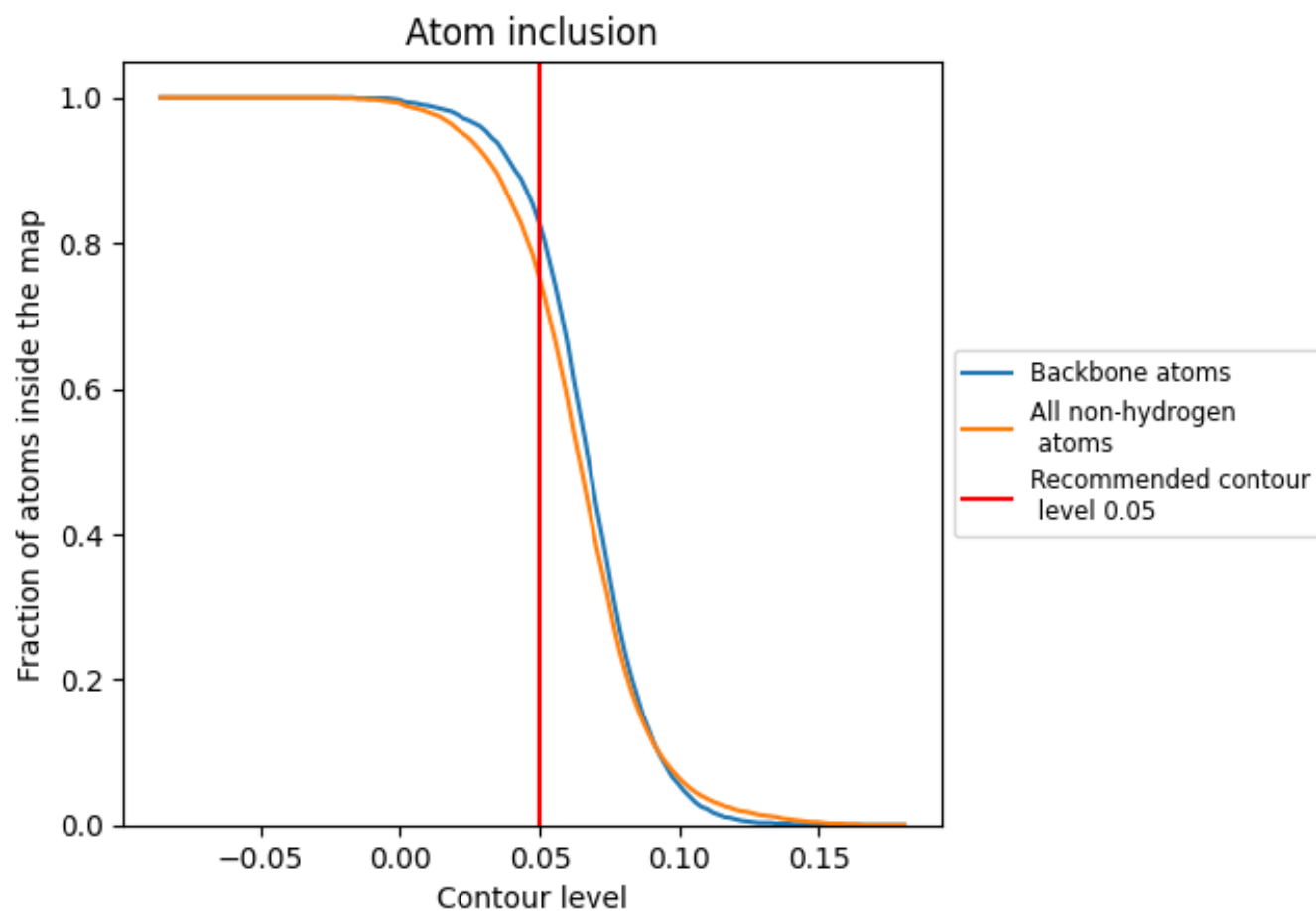
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.05).

9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 75% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7510	0.0870
0	0.7660	0.1070
1	0.7660	0.1130
2	0.8010	0.0780
3	0.7830	0.0650
V	0.7200	0.0770
W	0.7120	0.0840
X	0.8780	0.1600
Y	0.9730	0.1650

1.0

0.0

<0.0