



Full wwPDB EM Validation Report ⓘ

Mar 29, 2026 – 05:33 AM UTC

PDB ID : 5U8T / pdb_00005u8t
EMDB ID : EMD-8519
Title : Structure of Eukaryotic CMG Helicase at a Replication Fork and Implications
Authors : Li, B.; Georgescu, R.; Yuan, Z.; Santos, R.; Sun, J.; Zhang, D.; Yurieva, O.;
Li, H.; O'Donnell, M.E.
Deposited on : 2016-12-15
Resolution : 4.90 Å(reported)

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

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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
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

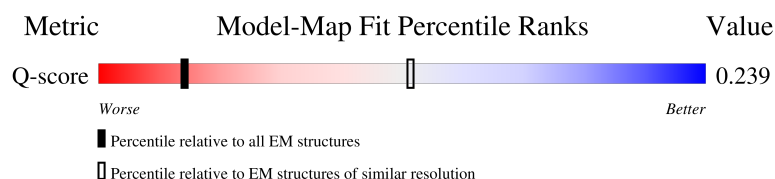
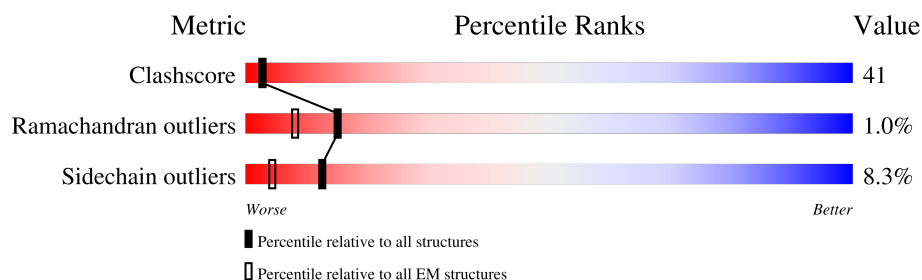
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.90 Å.

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



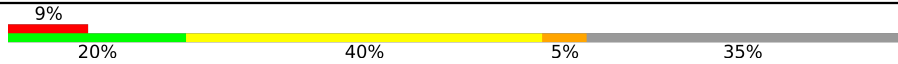
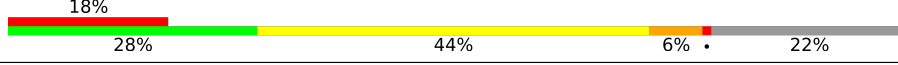
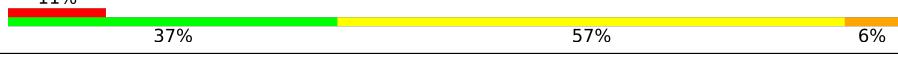
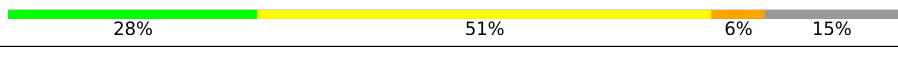
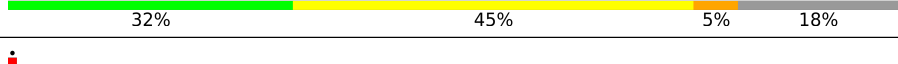
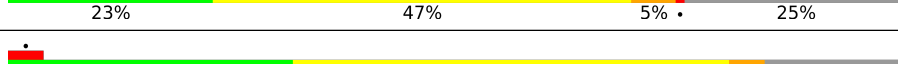
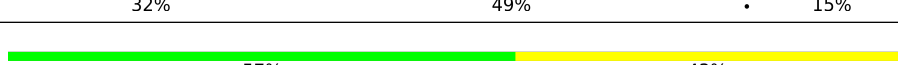
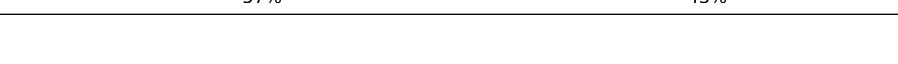
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	1274 (4.40 - 5.40)

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	2	868	 5% 22% 39% 6% 33%
2	3	971	 5% 21% 34% 5% 39%
3	4	933	 12% 25% 41% 5% 28%
4	5	775	 9% 24% 47% 6% 22%

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Mol	Chain	Length	Quality of chain
5	6	1017	
6	7	845	
7	A	208	
8	B	213	
9	C	194	
10	D	294	
11	E	650	
12	F	14	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	ANP	2	901	-	-	X	-
13	ANP	3	1001	-	-	X	-
13	ANP	5	801	-	-	X	-

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 40788 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA replication licensing factor MCM2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	583	Total	C	N	O	S	0	0
			4591	2899	818	858	16		

- Molecule 2 is a protein called DNA replication licensing factor MCM3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	3	589	Total	C	N	O	S	0	0
			4624	2915	824	872	13		

- Molecule 3 is a protein called DNA replication licensing factor MCM4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	4	672	Total	C	N	O	S	0	0
			5318	3340	929	1021	28		

- Molecule 4 is a protein called Minichromosome maintenance protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	5	602	Total	C	N	O	S	0	0
			4740	2980	815	921	24		

- Molecule 5 is a protein called DNA replication licensing factor MCM6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	6	661	Total	C	N	O	S	0	0
			5142	3247	905	967	23		

- Molecule 6 is a protein called DNA replication licensing factor MCM7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	7	660	Total	C	N	O	S	0	0
			5201	3278	903	991	29		

- Molecule 7 is a protein called DNA replication complex GINS protein PSF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A	208	Total	C	N	O	S	0	0
			1696	1065	290	331	10		

- Molecule 8 is a protein called DNA replication complex GINS protein PSF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	B	181	Total	C	N	O	S	0	0
			1513	978	261	270	4		

- Molecule 9 is a protein called DNA replication complex GINS protein PSF3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	C	159	Total	C	N	O	S	0	0
			1288	843	207	232	6		

- Molecule 10 is a protein called DNA replication complex GINS protein SLD5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	D	221	Total	C	N	O	S	0	0
			1820	1159	300	348	13		

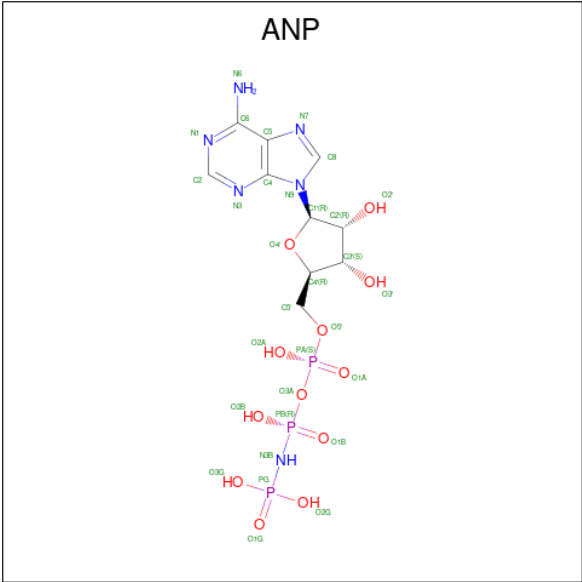
- Molecule 11 is a protein called Cell division control protein 45.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	E	553	Total	C	N	O	S	0	0
			4482	2862	763	844	13		

- Molecule 12 is a DNA chain called DNA (5'-D(P*TP*TP*TP*TP*TP*TP*TP*TP*T
P*TP*TP*TP*T)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
12	F	14	Total	C	N	O	P	0	0
			280	140	28	98	14		

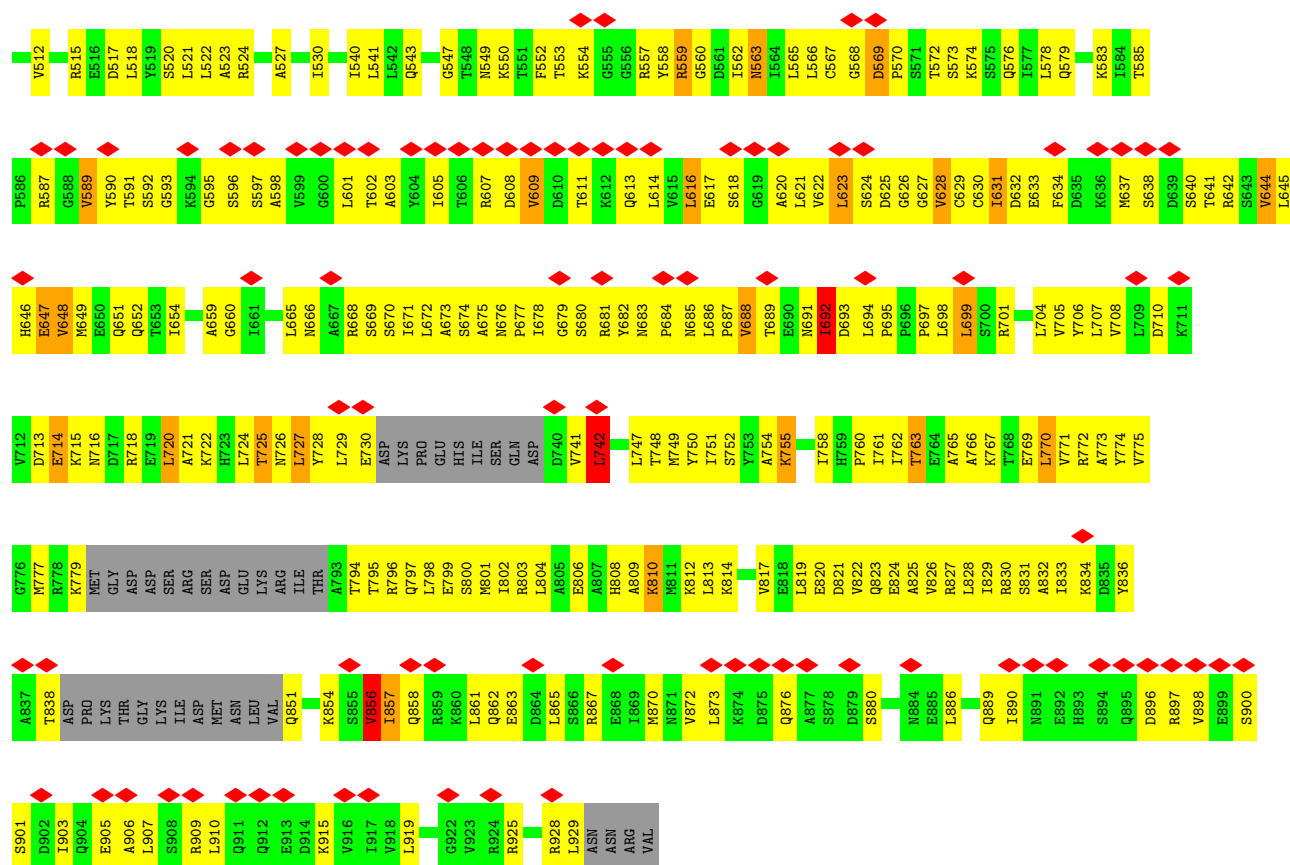
- Molecule 13 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).



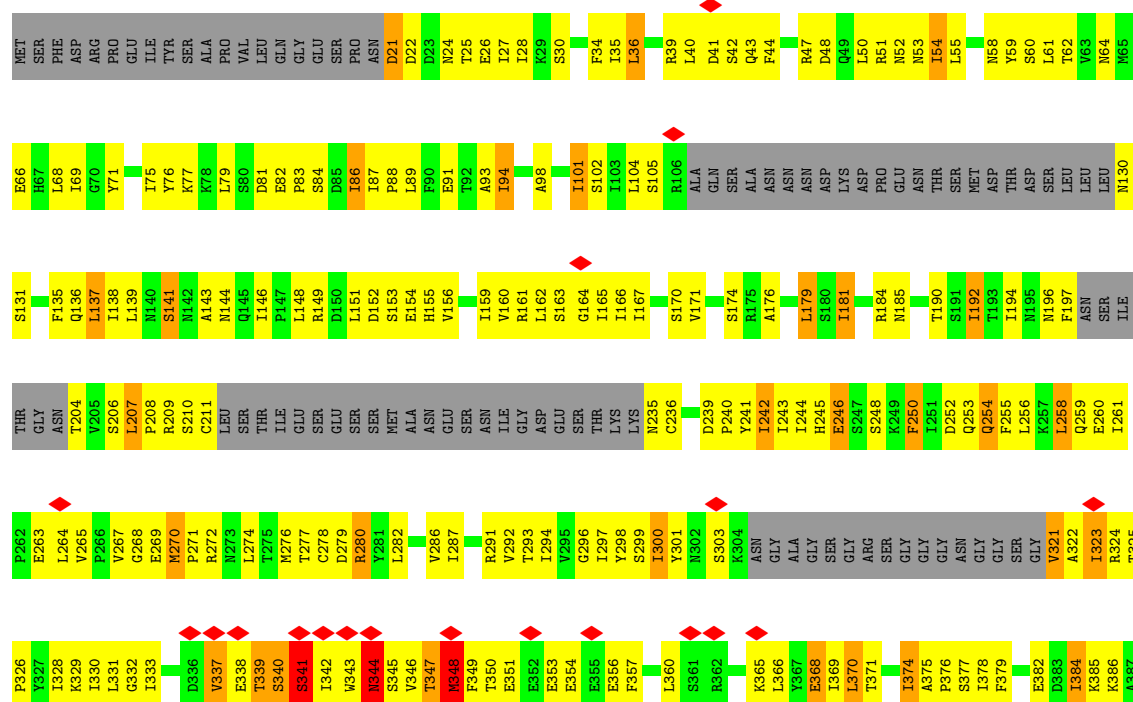
Mol	Chain	Residues	Atoms					AltConf
13	2	1	Total	C	N	O	P	0
			31	10	6	12	3	
13	3	1	Total	C	N	O	P	0
			31	10	6	12	3	
13	5	1	Total	C	N	O	P	0
			31	10	6	12	3	

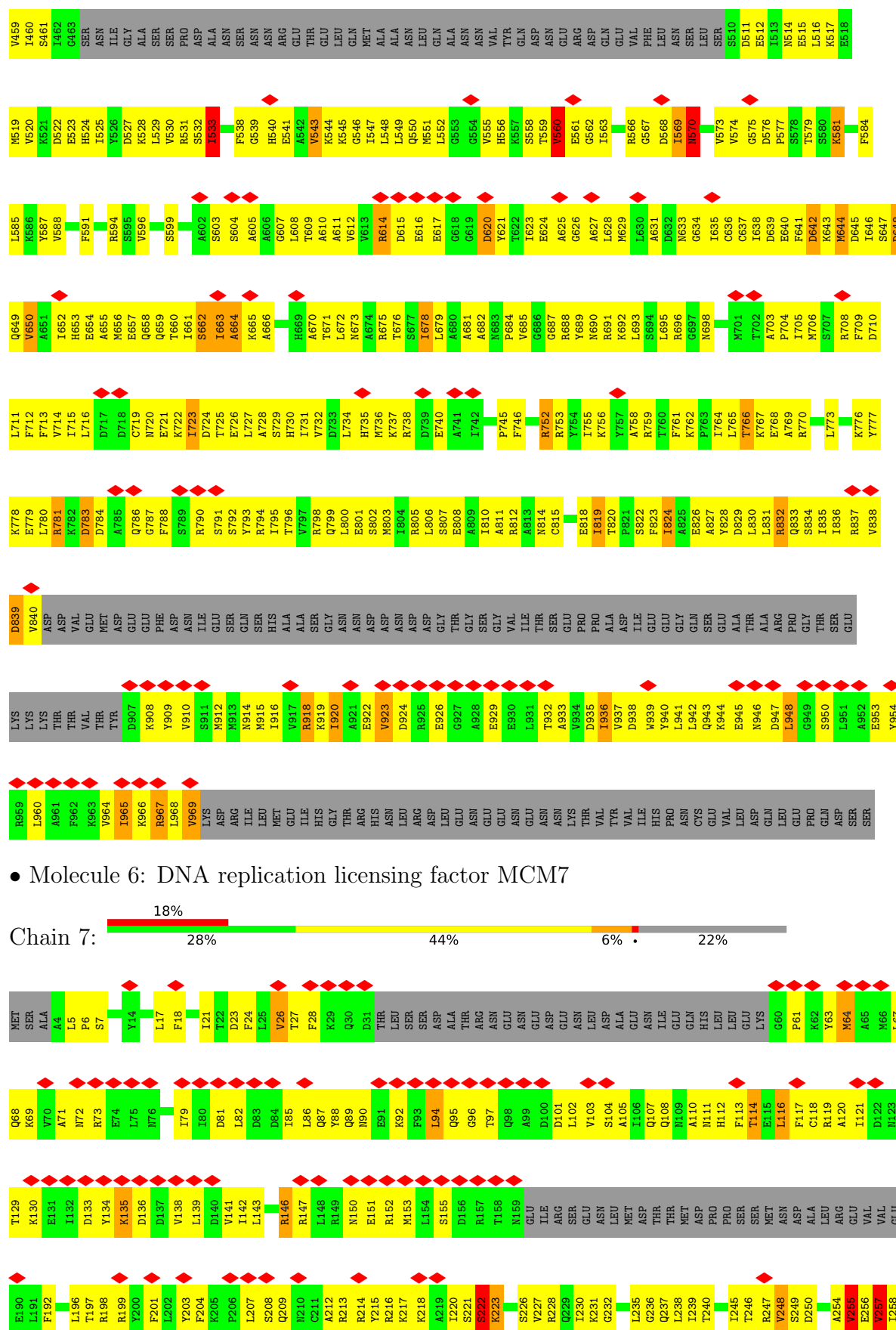


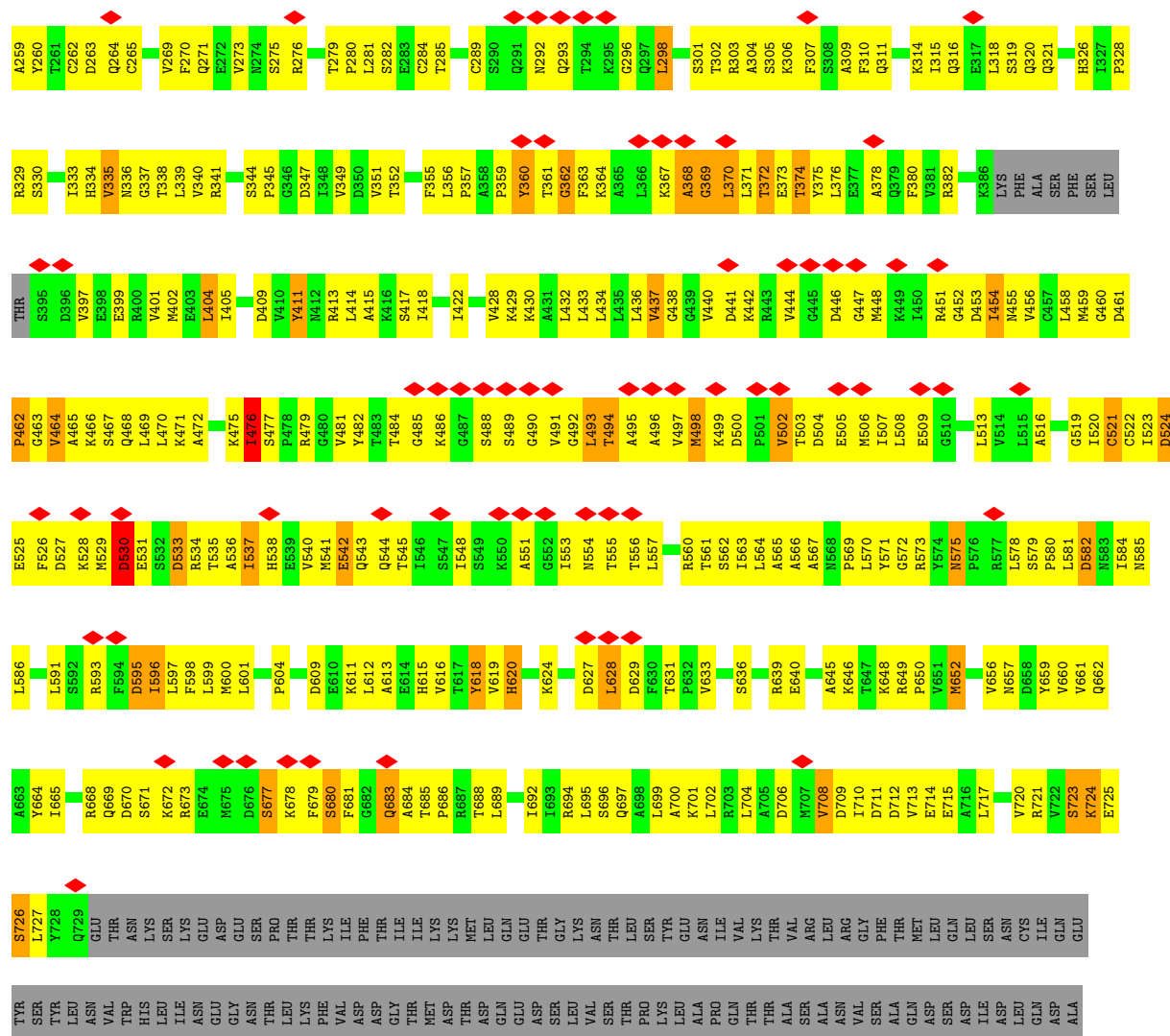
• Molecule 2: DNA replication licensing factor MCM3



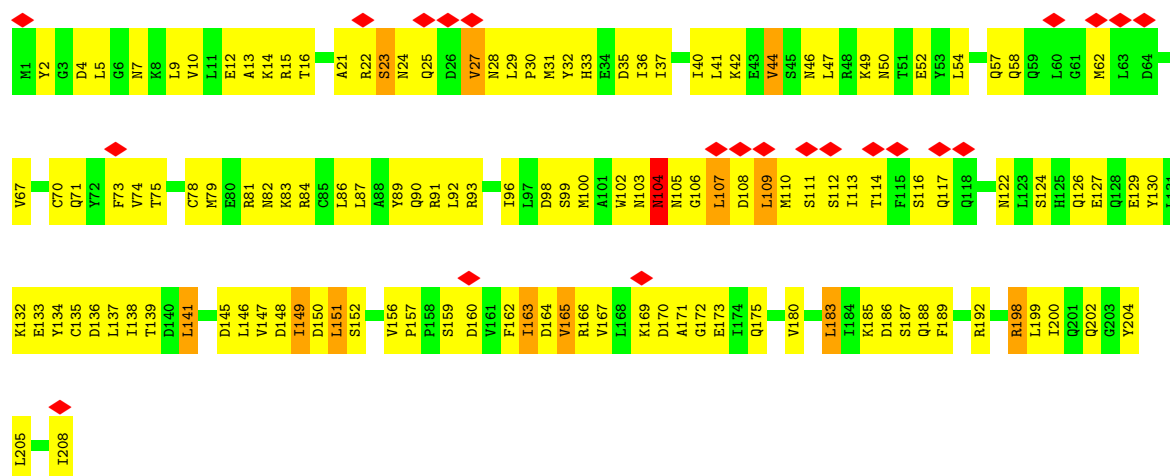
• Molecule 4: Minichromosome maintenance protein 5

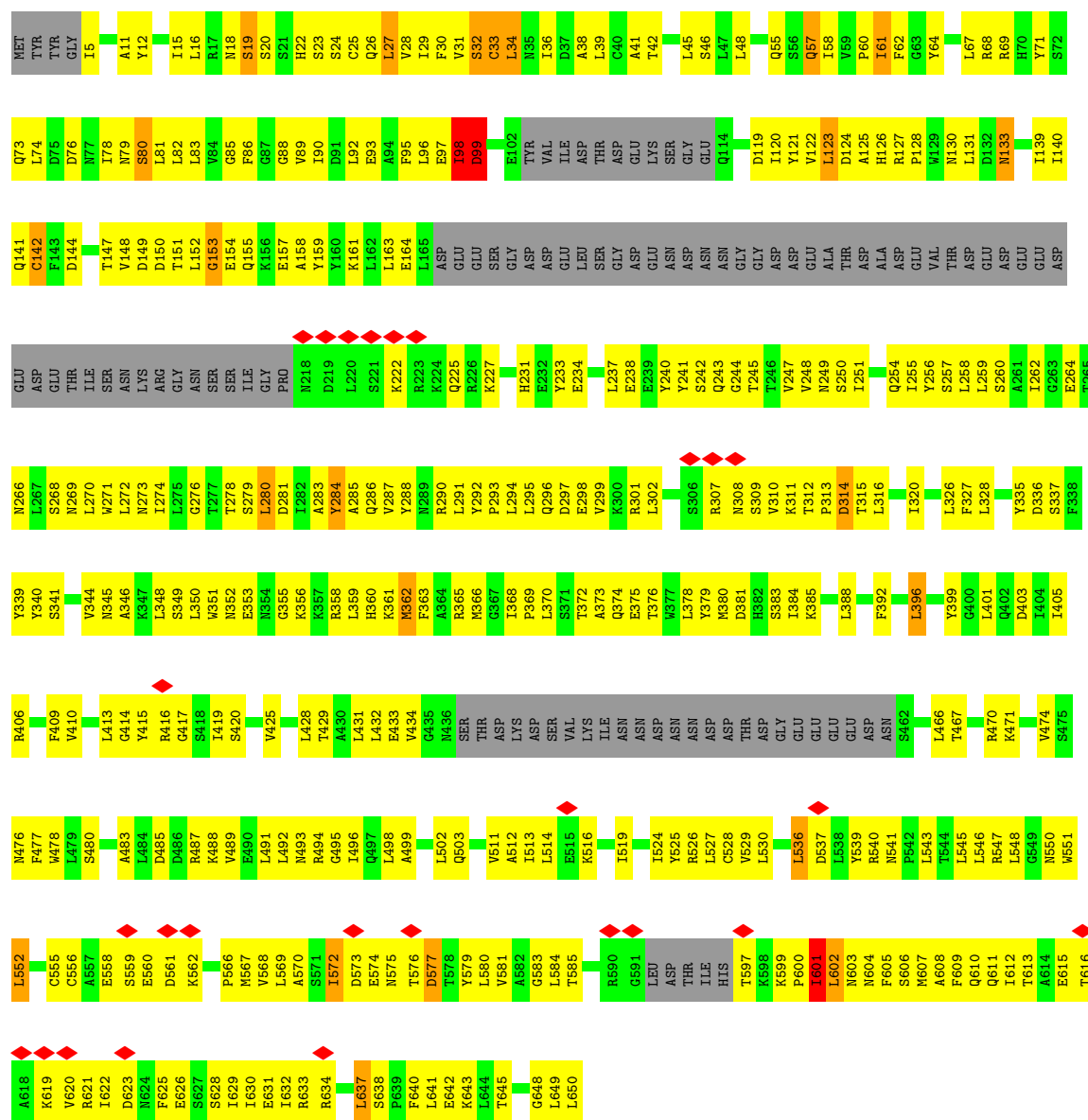




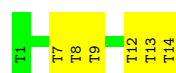


• Molecule 7: DNA replication complex GINS protein PSF1





- Molecule 12: DNA (5'-D(P*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*T)-3')



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	395443	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	10	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.103	Depositor
Minimum map value	-0.032	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	332.8, 332.8, 332.8	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3, 1.3, 1.3	Depositor

5 Model quality

5.1 Standard geometry

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

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	2	0.49	1/4668 (0.0%)	1.03	11/6306 (0.2%)
2	3	0.47	1/4702 (0.0%)	1.02	29/6374 (0.5%)
3	4	0.44	0/5388	1.02	25/7273 (0.3%)
4	5	0.47	0/4805	1.06	31/6489 (0.5%)
5	6	0.51	1/5218 (0.0%)	1.11	25/7039 (0.4%)
6	7	0.47	0/5281	1.03	24/7136 (0.3%)
7	A	0.51	0/1718	1.06	6/2314 (0.3%)
8	B	0.47	0/1545	1.00	9/2092 (0.4%)
9	C	0.46	0/1320	0.94	3/1784 (0.2%)
10	D	0.48	0/1853	1.11	17/2500 (0.7%)
11	E	0.46	0/4563	0.98	10/6173 (0.2%)
12	F	0.51	0/307	0.67	0/472
All	All	0.47	3/41368 (0.0%)	1.03	190/55952 (0.3%)

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	2	0	2
2	3	0	5
3	4	0	3
4	5	0	1
5	6	0	1
6	7	0	5
7	A	0	2
10	D	0	1
All	All	0	20

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	6	664	ALA	CA-CB	-5.97	1.44	1.53
2	3	122	ILE	CA-CB	5.90	1.57	1.53
1	2	633	LYS	CE-NZ	5.48	1.65	1.49

All (190) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	6	839	ASP	N-CA-C	17.44	129.97	111.14
11	E	19	SER	N-CA-C	17.18	129.70	111.14
6	7	263	ASP	N-CA-C	15.70	128.09	111.14
5	6	533	ILE	N-CA-C	13.41	122.94	110.74
1	2	846	VAL	N-CA-C	12.89	122.79	110.42
11	E	133	ASN	N-CA-C	12.32	124.45	111.14
7	A	21	ALA	N-CA-C	12.21	124.14	111.07
10	D	173	ASP	N-CA-C	11.57	123.64	111.14
4	5	576	HIS	N-CA-C	11.49	123.78	111.03
5	6	923	VAL	N-CA-C	10.61	123.57	112.96
3	4	428	ARG	N-CA-C	10.36	122.33	111.14
2	3	122	ILE	CA-C-N	-10.00	110.08	120.38
2	3	122	ILE	C-N-CA	-10.00	110.08	120.38
6	7	362	GLY	N-CA-C	9.77	122.01	112.04
9	C	90	THR	N-CA-C	9.69	121.61	111.14
6	7	411	TYR	N-CA-C	8.55	120.22	111.07
2	3	424	ASN	N-CA-C	8.45	123.92	112.68
4	5	444	SER	N-CA-C	8.41	123.55	109.76
4	5	564	ARG	N-CA-C	-8.35	101.71	112.23
4	5	207	LEU	CA-C-N	8.34	128.10	119.76
4	5	207	LEU	C-N-CA	8.34	128.10	119.76
1	2	775	TYR	CA-C-N	8.13	127.89	119.76
1	2	775	TYR	C-N-CA	8.13	127.89	119.76
6	7	94	LEU	N-CA-C	8.05	119.68	111.07
2	3	151	HIS	CA-C-N	8.03	127.69	119.82
2	3	151	HIS	C-N-CA	8.03	127.69	119.82
1	2	658	ASN	N-CA-C	7.85	123.12	112.68
3	4	647	GLU	N-CA-C	7.59	119.63	111.36
2	3	490	MET	N-CA-C	7.54	122.89	112.04
3	4	240	ASN	N-CA-C	7.45	121.67	111.39
10	D	260	ILE	N-CA-C	7.43	117.13	108.96
4	5	597	GLU	N-CA-C	-7.42	103.69	112.89
2	3	184	GLY	N-CA-C	7.37	120.84	110.38
10	D	260	ILE	CA-C-N	7.28	127.71	119.92
10	D	260	ILE	C-N-CA	7.28	127.71	119.92
5	6	171	SER	N-CA-C	7.27	119.00	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	4	763	THR	CB-CA-C	-7.21	107.20	115.79
5	6	663	ILE	N-CA-C	7.20	119.34	107.24
3	4	714	GLU	N-CA-C	7.18	120.53	111.69
6	7	369	GLY	N-CA-C	7.12	133.96	113.30
1	2	433	ASN	N-CA-C	7.04	119.39	110.24
5	6	368	ILE	CA-C-N	7.02	128.61	119.84
5	6	368	ILE	C-N-CA	7.02	128.61	119.84
7	A	198	ARG	N-CA-C	7.01	119.96	111.40
8	B	184	PHE	N-CA-C	6.85	118.40	111.07
2	3	326	VAL	N-CA-C	6.82	123.53	109.34
4	5	330	ILE	N-CA-C	6.74	117.34	107.37
1	2	594	GLY	N-CA-C	-6.73	103.46	112.14
4	5	81	ASP	N-CA-C	6.69	118.45	111.03
3	4	714	GLU	CA-C-N	6.67	133.70	121.70
3	4	714	GLU	C-N-CA	6.67	133.70	121.70
3	4	559	ARG	CB-CA-C	-6.58	107.20	115.89
1	2	660	THR	N-CA-C	-6.55	104.22	111.82
4	5	181	ILE	N-CA-C	6.55	117.24	108.27
4	5	561	ASN	N-CA-C	6.54	118.74	110.24
2	3	325	THR	N-CA-C	6.51	121.59	112.93
2	3	265	ALA	CA-C-N	6.48	125.91	118.85
2	3	265	ALA	C-N-CA	6.48	125.91	118.85
6	7	677	SER	N-CA-C	6.47	118.87	111.11
5	6	664	ALA	N-CA-C	6.39	119.20	108.02
4	5	374	ILE	N-CA-C	6.37	117.12	110.62
5	6	333	CYS	CA-C-N	6.32	127.75	119.84
5	6	333	CYS	C-N-CA	6.32	127.75	119.84
6	7	372	THR	N-CA-C	6.27	118.64	111.11
5	6	404	VAL	CA-C-N	6.23	126.41	120.31
5	6	404	VAL	C-N-CA	6.23	126.41	120.31
6	7	94	LEU	CA-C-N	6.21	132.87	121.70
6	7	94	LEU	C-N-CA	6.21	132.87	121.70
1	2	376	ASN	N-CA-C	6.18	116.40	108.24
6	7	726	SER	N-CA-C	-6.13	105.76	113.18
8	B	115	LEU	CA-C-N	6.12	125.81	119.56
8	B	115	LEU	C-N-CA	6.12	125.81	119.56
10	D	266	GLU	N-CA-C	6.12	118.68	110.35
4	5	325	THR	CA-C-N	6.11	125.87	119.76
4	5	325	THR	C-N-CA	6.11	125.87	119.76
3	4	755	LYS	N-CA-C	6.11	120.81	112.68
4	5	593	GLU	N-CA-C	6.08	118.61	110.35
2	3	499	LYS	N-CA-C	6.07	118.43	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	6	620	ASP	N-CA-C	6.02	116.91	108.00
3	4	202	LYS	CA-C-N	6.02	132.54	121.70
3	4	202	LYS	C-N-CA	6.02	132.54	121.70
10	D	253	LYS	CA-C-N	-5.99	112.35	119.84
10	D	253	LYS	C-N-CA	-5.99	112.35	119.84
10	D	258	VAL	N-CA-C	-5.99	96.88	109.34
2	3	192	VAL	N-CA-C	5.96	116.75	109.30
3	4	742	LEU	N-CA-C	5.95	119.42	108.94
6	7	628	LEU	N-CA-C	5.94	119.59	111.39
2	3	163	ALA	CA-C-N	5.93	132.38	121.70
2	3	163	ALA	C-N-CA	5.93	132.38	121.70
3	4	628	VAL	N-CA-C	5.92	116.81	108.17
3	4	448	SER	CA-C-N	5.90	132.32	121.70
3	4	448	SER	C-N-CA	5.90	132.32	121.70
10	D	267	VAL	N-CA-C	5.90	121.61	109.34
4	5	400	LEU	CA-C-N	5.89	126.19	119.83
4	5	400	LEU	C-N-CA	5.89	126.19	119.83
6	7	542	GLU	N-CA-C	-5.89	105.86	113.16
5	6	645	ASP	CB-CA-C	-5.88	108.10	116.34
5	6	766	THR	N-CA-C	-5.87	106.16	113.38
2	3	368	ALA	CA-C-N	5.82	125.02	118.97
2	3	368	ALA	C-N-CA	5.82	125.02	118.97
2	3	472	ILE	N-CA-C	5.80	116.35	107.77
7	A	157	PRO	CA-C-N	5.79	126.24	119.99
7	A	157	PRO	C-N-CA	5.79	126.24	119.99
4	5	394	GLY	N-CA-C	-5.76	105.51	112.48
8	B	28	PHE	CA-C-N	5.76	125.69	119.76
8	B	28	PHE	C-N-CA	5.76	125.69	119.76
8	B	108	HIS	CA-C-N	5.75	125.42	119.56
8	B	108	HIS	C-N-CA	5.75	125.42	119.56
1	2	412	ALA	CB-CA-C	-5.74	109.98	116.63
6	7	575	ASN	CA-C-N	5.72	125.84	119.32
6	7	575	ASN	C-N-CA	5.72	125.84	119.32
2	3	153	TRP	CB-CA-C	-5.69	109.02	115.79
3	4	421	ASP	CB-CA-C	-5.69	110.00	116.54
5	6	645	ASP	N-CA-C	5.66	116.38	108.00
4	5	344	ASN	N-CA-C	5.65	122.83	110.80
11	E	98	ILE	CA-C-N	5.64	131.86	121.70
11	E	98	ILE	C-N-CA	5.64	131.86	121.70
5	6	570	ASN	N-CA-C	5.64	118.40	108.75
10	D	200	LYS	CA-C-N	5.64	131.86	121.70
10	D	200	LYS	C-N-CA	5.64	131.86	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	3	246	GLY	N-CA-C	-5.62	107.57	115.32
3	4	447	ASN	N-CA-C	5.58	118.94	111.24
2	3	305	GLY	N-CA-C	-5.58	108.04	115.40
2	3	668	ILE	CA-C-N	5.58	125.19	119.56
2	3	668	ILE	C-N-CA	5.58	125.19	119.56
6	7	530	ASP	CB-CA-C	-5.57	108.54	115.89
2	3	670	GLN	CB-CA-C	-5.54	109.70	117.23
6	7	146	ARG	N-CA-C	-5.53	104.89	111.03
6	7	275	SER	CB-CA-C	-5.53	108.59	115.89
11	E	153	GLY	N-CA-C	-5.52	106.12	115.34
10	D	291	VAL	N-CA-C	5.52	115.83	108.27
2	3	166	LEU	N-CA-C	5.50	117.79	110.53
3	4	685	ASN	CB-CA-C	-5.50	110.25	116.63
6	7	560	ARG	N-CA-C	-5.50	106.16	112.92
5	6	355	ASP	CA-C-N	5.47	131.56	121.70
5	6	355	ASP	C-N-CA	5.47	131.56	121.70
6	7	133	ASP	CB-CA-C	-5.46	109.29	115.79
11	E	638	SER	CA-C-N	-5.45	114.06	119.56
11	E	638	SER	C-N-CA	-5.45	114.06	119.56
4	5	254	GLN	N-CA-C	5.43	118.02	111.40
5	6	652	ILE	N-CA-C	-5.39	106.60	112.80
6	7	64	MET	N-CA-C	5.39	119.95	112.45
2	3	137	ASP	N-CA-C	-5.36	103.46	110.53
4	5	374	ILE	CA-C-N	-5.36	115.64	122.98
4	5	374	ILE	C-N-CA	-5.36	115.64	122.98
1	2	428	GLY	N-CA-C	5.35	121.46	112.85
2	3	123	PRO	N-CA-C	5.34	117.21	110.70
4	5	611	ALA	CA-C-N	5.33	125.31	120.03
4	5	611	ALA	C-N-CA	5.33	125.31	120.03
6	7	618	TYR	N-CA-C	-5.33	106.61	113.01
4	5	507	ALA	CB-CA-C	-5.33	110.45	116.63
10	D	197	SER	N-CA-C	5.33	119.71	112.04
8	B	119	TRP	N-CA-C	5.32	117.50	111.11
6	7	684	ALA	N-CA-C	-5.30	104.71	110.91
9	C	91	ASP	CA-C-N	5.29	125.35	119.32
9	C	91	ASP	C-N-CA	5.29	125.35	119.32
4	5	185	ASN	N-CA-C	5.28	119.48	112.72
2	3	208	ARG	CB-CA-C	-5.28	108.92	115.89
4	5	86	ILE	N-CA-C	5.27	116.17	111.90
3	4	659	ALA	CB-CA-C	-5.26	110.53	116.63
6	7	551	ALA	CB-CA-C	-5.24	110.55	116.63
5	6	568	ASP	CB-CA-C	-5.23	109.01	116.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	156	VAL	CA-C-N	5.22	125.76	120.38
7	A	156	VAL	C-N-CA	5.22	125.76	120.38
10	D	255	CYS	N-CA-C	5.21	116.73	108.96
5	6	335	ASN	CA-C-N	5.18	139.44	127.00
5	6	335	ASN	C-N-CA	5.18	139.44	127.00
5	6	620	ASP	CB-CA-C	-5.18	109.09	116.34
3	4	896	ASP	N-CA-C	-5.16	106.76	113.16
3	4	692	ILE	N-CA-C	-5.16	106.87	112.80
1	2	636	ILE	N-CA-C	5.16	115.46	107.78
4	5	615	SER	CA-C-N	5.16	125.20	119.32
4	5	615	SER	C-N-CA	5.16	125.20	119.32
10	D	172	THR	N-CA-C	-5.13	107.03	113.28
3	4	602	THR	N-CA-C	5.11	116.73	108.26
8	B	113	SER	CB-CA-C	-5.11	109.19	116.34
4	5	280	ARG	CB-CA-C	-5.10	110.71	116.63
4	5	250	PHE	N-CA-C	5.08	116.53	108.96
10	D	204	GLU	N-CA-C	5.08	116.50	111.07
5	6	737	LYS	N-CA-C	-5.07	105.46	111.69
11	E	599	LYS	CA-C-N	5.06	124.56	119.19
11	E	599	LYS	C-N-CA	5.06	124.56	119.19
11	E	88	GLY	N-CA-C	-5.05	108.71	115.32
3	4	585	THR	CA-C-N	5.04	124.48	119.24
3	4	585	THR	C-N-CA	5.04	124.48	119.24
3	4	863	GLU	N-CA-C	-5.03	105.88	111.36
6	7	476	ILE	N-CA-C	5.03	115.88	111.56
2	3	280	ASP	CB-CA-C	-5.02	110.40	117.23
10	D	224	TRP	N-CA-C	-5.02	107.16	113.28
4	5	323	ILE	N-CA-C	5.01	119.76	109.34

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	2	355	SER	Peptide
1	2	633	LYS	Peptide
2	3	163	ALA	Peptide
2	3	172	THR	Peptide
2	3	428	LEU	Peptide
2	3	437	SER	Peptide
2	3	498	ALA	Peptide
3	4	245	ALA	Peptide
3	4	374	ILE	Peptide

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Mol	Chain	Res	Type	Group
3	4	448	SER	Peptide
4	5	348	MET	Peptide
5	6	560	VAL	Peptide
6	7	257	VAL	Peptide
6	7	360	TYR	Peptide
6	7	368	ALA	Peptide
6	7	680	SER	Peptide
6	7	683	GLN	Peptide
7	A	104	ASN	Peptide
7	A	159	SER	Peptide
10	D	200	LYS	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	4591	0	4639	443	0
2	3	4624	0	4689	383	0
3	4	5318	0	5390	441	0
4	5	4740	0	4798	450	0
5	6	5142	0	5093	516	0
6	7	5201	0	5276	438	0
7	A	1696	0	1698	148	0
8	B	1513	0	1558	128	0
9	C	1288	0	1298	94	0
10	D	1820	0	1824	209	0
11	E	4482	0	4499	377	0
12	F	280	0	169	8	0
13	2	31	0	13	9	0
13	3	31	0	13	10	0
13	5	31	0	13	9	0
All	All	40788	0	40970	3322	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 41.

All (3322) 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)
10:D:260:ILE:CG1	10:D:266:GLU:CD	1.87	1.46
10:D:260:ILE:HG13	10:D:266:GLU:CG	1.46	1.45
10:D:260:ILE:HG12	10:D:266:GLU:CD	1.38	1.42
6:7:221:SER:CA	6:7:222:SER:HB2	1.40	1.39
10:D:260:ILE:CG1	10:D:266:GLU:OE2	1.74	1.35
10:D:260:ILE:CD1	10:D:266:GLU:OE2	1.78	1.30
4:5:341:SER:O	4:5:345:SER:HB2	1.28	1.30
4:5:623:SER:O	4:5:627:VAL:HG13	1.27	1.30
6:7:221:SER:HA	6:7:222:SER:CB	1.58	1.29
6:7:490:GLY:O	6:7:494:THR:HG22	1.33	1.20
10:D:260:ILE:CG2	10:D:265:GLU:HA	1.71	1.18
7:A:108:ASP:HB3	7:A:109:LEU:CB	1.74	1.17
1:2:632:SER:HB2	4:5:442:LYS:HB3	1.25	1.15
11:E:540:ARG:NH2	11:E:574:GLU:HB2	1.61	1.15
7:A:108:ASP:CB	7:A:109:LEU:HB3	1.77	1.14
3:4:623:LEU:HD22	5:6:370:THR:HG21	1.23	1.13
3:4:623:LEU:HD22	5:6:370:THR:CG2	1.77	1.12
10:D:260:ILE:HD11	10:D:266:GLU:OE2	1.42	1.12
10:D:258:VAL:HB	10:D:259:THR:HA	1.24	1.11
1:2:846:VAL:O	1:2:853:VAL:HG21	1.46	1.11
3:4:332:VAL:HB	3:4:429:ALA:HA	1.27	1.11
10:D:260:ILE:HG12	10:D:266:GLU:OE2	1.40	1.07
11:E:579:TYR:CE2	11:E:634:ARG:HB3	1.89	1.07
10:D:260:ILE:CG1	10:D:266:GLU:CG	2.28	1.06
10:D:260:ILE:HG23	10:D:265:GLU:C	1.81	1.05
11:E:576:THR:O	11:E:577:ASP:CG	1.99	1.05
6:7:221:SER:N	6:7:222:SER:HB2	1.69	1.05
6:7:221:SER:CA	6:7:222:SER:CB	2.25	1.05
3:4:624:SER:O	3:4:626:GLY:O	1.75	1.04
10:D:260:ILE:HG21	10:D:265:GLU:HA	1.38	1.04
6:7:472:ALA:O	6:7:476:ILE:HD13	1.57	1.04
5:6:418:SER:HG	5:6:448:LEU:N	1.58	1.01
1:2:608:GLU:HB3	1:2:611:LYS:HD3	1.42	1.00
3:4:727:LEU:N	3:4:728:TYR:HB3	1.77	1.00
4:5:143:ALA:HA	11:E:379:TYR:HE2	1.23	1.00
6:7:221:SER:HA	6:7:222:SER:HB2	1.02	1.00
3:4:449:ARG:HG3	3:4:450:GLN:H	1.23	0.99
4:5:477:VAL:HB	4:5:519:VAL:HA	1.40	0.99
11:E:5:ILE:N	11:E:142:CYS:HG	1.61	0.98
3:4:432:ARG:NH2	6:7:557:LEU:HB3	1.77	0.98
3:4:589:VAL:HG21	3:4:624:SER:OG	1.62	0.97
5:6:100:VAL:HG23	5:6:101:LYS:CG	1.94	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:778:LEU:HG	4:5:577:THR:CG2	1.94	0.97
4:5:196:ASN:HB3	4:5:197:PHE:HD1	1.30	0.97
3:4:202:LYS:HB3	3:4:203:TYR:HB3	1.47	0.97
4:5:448:GLY:HA2	4:5:486:ARG:HH12	1.27	0.96
1:2:540:LEU:HA	1:2:648:ALA:HB3	1.48	0.95
5:6:790:ARG:NH2	5:6:839:ASP:O	1.99	0.95
2:3:25:VAL:O	2:3:29:GLN:HG2	1.66	0.95
6:7:220:ILE:C	6:7:222:SER:HB2	1.92	0.95
11:E:15:ILE:O	11:E:19:SER:OG	1.83	0.95
5:6:653:HIS:HA	5:6:656:MET:HG2	1.49	0.94
6:7:470:LEU:HD21	6:7:564:LEU:HD22	1.49	0.94
1:2:842:VAL:O	1:2:846:VAL:HG23	1.67	0.93
6:7:489:SER:O	6:7:493:LEU:HG	1.68	0.93
10:D:260:ILE:HG13	10:D:266:GLU:HG3	0.96	0.93
10:D:260:ILE:CG1	10:D:266:GLU:HG3	1.92	0.93
5:6:558:SER:HB3	5:6:559:THR:HA	1.51	0.92
6:7:94:LEU:HB2	6:7:95:GLN:HB2	1.52	0.92
4:5:482:PHE:HB3	4:5:523:ALA:HB2	1.51	0.91
3:4:623:LEU:CD2	5:6:370:THR:HG21	2.00	0.91
1:2:502:ALA:HB1	1:2:505:ILE:HB	1.51	0.91
5:6:304:LEU:HD11	5:6:307:ALA:HB2	1.52	0.91
6:7:489:SER:O	6:7:493:LEU:CD2	2.18	0.91
6:7:459:MET:HB2	6:7:597:LEU:HD21	1.53	0.91
2:3:533:ILE:HG22	2:3:535:LEU:H	1.35	0.91
10:D:260:ILE:HG13	10:D:266:GLU:CD	1.73	0.90
2:3:192:VAL:HB	6:7:329:ARG:HH12	1.36	0.90
5:6:167:ALA:O	5:6:171:SER:OG	1.89	0.89
10:D:260:ILE:CG2	10:D:265:GLU:CA	2.50	0.89
10:D:260:ILE:HG23	10:D:265:GLU:CA	2.02	0.89
3:4:689:THR:HG1	3:4:851:GLN:N	1.70	0.89
6:7:118:CYS:SG	6:7:198:ARG:NH2	2.45	0.89
4:5:664:ALA:HA	4:5:676:HIS:HE1	1.36	0.89
8:B:7:LEU:N	8:B:8:GLN:HA	1.85	0.89
6:7:490:GLY:O	6:7:494:THR:CG2	2.21	0.88
6:7:472:ALA:O	6:7:476:ILE:CD1	2.22	0.88
4:5:369:ILE:HG23	4:5:594:ILE:HD11	1.56	0.88
1:2:634:ALA:O	4:5:448:GLY:N	2.07	0.87
1:2:384:ASN:HB2	1:2:415:VAL:HG21	1.57	0.87
11:E:540:ARG:HH21	11:E:574:GLU:HB2	1.37	0.87
1:2:580:VAL:HG22	1:2:591:LEU:HG	1.57	0.86
6:7:459:MET:HB3	6:7:599:LEU:HA	1.55	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:276:MET:HG2	4:5:328:ILE:HB	1.56	0.86
5:6:646:ILE:HA	5:6:649:GLN:HG2	1.54	0.86
6:7:256:GLU:HA	6:7:273:VAL:HG21	1.57	0.86
10:D:260:ILE:HG23	10:D:265:GLU:HA	1.57	0.86
3:4:804:LEU:HD21	3:4:828:LEU:HD12	1.57	0.86
11:E:579:TYR:O	11:E:581:VAL:HG23	1.76	0.86
2:3:104:ARG:NH1	9:C:90:THR:HG23	1.90	0.86
6:7:466:LYS:HA	6:7:469:LEU:HD13	1.57	0.85
6:7:520:ILE:HA	6:7:562:SER:HB2	1.57	0.85
10:D:67:TRP:HE1	10:D:142:SER:HB3	1.41	0.85
10:D:123:LYS:HE3	11:E:20:SER:HB3	1.56	0.85
3:4:629:CYS:HB3	3:4:671:ILE:HG12	1.57	0.85
4:5:413:LEU:HD13	4:5:553:ILE:HG13	1.58	0.85
1:2:574:VAL:HG22	1:2:595:ALA:HB2	1.57	0.85
3:4:243:LEU:HD22	3:4:305:PRO:HA	1.59	0.85
5:6:689:TYR:HA	5:6:690:ASN:HB2	1.58	0.85
5:6:720:ASN:O	5:6:724:ASP:N	2.10	0.85
6:7:315:ILE:HD13	6:7:333:ILE:HD12	1.59	0.85
11:E:83:LEU:HD21	11:E:86:PHE:HB2	1.58	0.84
5:6:693:LEU:HD13	5:6:698:ASN:HA	1.58	0.84
10:D:79:TYR:HA	10:D:147:ARG:HH12	1.43	0.84
3:4:713:ASP:HB2	3:4:716:ASN:HB2	1.56	0.84
10:D:250:GLU:HA	10:D:256:TYR:HB3	1.59	0.84
2:3:176:LEU:HD23	2:3:177:ASN:HB2	1.60	0.84
1:2:325:THR:HG21	1:2:391:GLN:HB3	1.60	0.84
1:2:611:LYS:HE2	5:6:650:VAL:HG21	1.59	0.84
4:5:649:THR:H	4:5:652:GLN:HG3	1.43	0.83
8:B:11:PHE:HB2	8:B:179:ASN:HD21	1.41	0.83
1:2:262:LYS:HE2	1:2:263:CYS:SG	2.17	0.83
5:6:802:SER:HA	5:6:805:ARG:HG2	1.58	0.83
3:4:726:ASN:C	3:4:727:LEU:HG	2.03	0.83
5:6:570:ASN:HD21	5:6:678:ILE:H	1.24	0.83
3:4:332:VAL:CB	3:4:429:ALA:HA	2.07	0.83
1:2:428:GLY:HA3	1:2:453:ALA:HA	1.60	0.83
11:E:33:CYS:SG	11:E:34:LEU:N	2.50	0.83
3:4:563:ASN:ND2	3:4:649:MET:SD	2.52	0.83
6:7:440:VAL:HG11	6:7:649:ARG:HA	1.58	0.83
2:3:389:VAL:HG12	2:3:390:GLU:H	1.44	0.83
4:5:39:ARG:HG2	4:5:41:ASP:H	1.42	0.83
3:4:248:LEU:HB2	3:4:258:TYR:HB2	1.60	0.82
5:6:795:ILE:HG22	5:6:799:GLN:HG3	1.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:533:ILE:HG21	5:6:548:LEU:HD11	1.60	0.82
6:7:461:ASP:HB3	6:7:569:PRO:HD2	1.61	0.82
8:B:71:VAL:HB	8:B:75:ILE:HD11	1.59	0.82
11:E:502:LEU:HD13	11:E:547:ARG:HH22	1.44	0.82
3:4:771:VAL:HG13	5:6:728:ALA:HB1	1.59	0.82
10:D:220:ASP:HB3	10:D:221:GLU:HG2	1.60	0.82
6:7:489:SER:O	6:7:493:LEU:CG	2.28	0.82
1:2:571:ALA:HB3	5:6:664:ALA:HB3	1.61	0.82
2:3:172:THR:O	2:3:175:HIS:ND1	2.13	0.82
3:4:587:ARG:HD3	3:4:623:LEU:O	1.80	0.82
6:7:504:ASP:HB3	6:7:505:GLU:HB3	1.62	0.82
5:6:326:LYS:H	5:6:327:TYR:HA	1.45	0.81
3:4:342:MET:HB3	3:4:360:ILE:HD13	1.63	0.81
3:4:448:SER:HB3	3:4:449:ARG:HB3	1.60	0.81
6:7:670:ASP:HA	6:7:673:ARG:HG2	1.60	0.81
11:E:344:VAL:HG13	11:E:348:LEU:HD12	1.59	0.81
2:3:519:VAL:HG22	2:3:534:ALA:HB2	1.62	0.81
4:5:143:ALA:HA	11:E:379:TYR:CE2	2.11	0.81
5:6:791:SER:HB3	5:6:835:ILE:HG22	1.63	0.81
5:6:100:VAL:HG23	5:6:101:LYS:HG2	1.61	0.81
1:2:294:HIS:O	1:2:296:ARG:NH1	2.14	0.81
3:4:234:ARG:HB3	3:4:280:MET:HE1	1.63	0.81
3:4:589:VAL:CG2	3:4:624:SER:OG	2.28	0.81
5:6:525:ILE:HA	5:6:528:LYS:HB2	1.62	0.81
11:E:604:ASN:HB2	11:E:650:LEU:HD23	1.63	0.80
3:4:338:VAL:HB	5:6:452:ILE:HD11	1.62	0.80
4:5:261:ILE:HD11	4:5:264:LEU:HG	1.61	0.80
10:D:132:GLU:HG2	10:D:135:ARG:HH12	1.46	0.80
11:E:26:GLN:HB3	11:E:78:ILE:HA	1.63	0.80
1:2:610:ASP:OD2	1:2:651:ASN:ND2	2.15	0.80
1:2:684:ARG:HB3	1:2:685:ASP:HB3	1.63	0.80
4:5:184:ARG:HH11	4:5:240:PRO:HA	1.46	0.80
5:6:796:THR:HG22	5:6:798:ARG:H	1.46	0.80
7:A:145:ASP:HA	7:A:146:LEU:HB3	1.64	0.80
10:D:230:ILE:HD12	10:D:291:VAL:HG21	1.62	0.80
6:7:490:GLY:HA2	6:7:493:LEU:HD11	1.63	0.80
6:7:228:ARG:HH12	6:7:326:HIS:HB3	1.45	0.80
1:2:641:GLN:HB3	1:2:643:ARG:HH12	1.46	0.79
5:6:603:SER:H	5:6:604:SER:HA	1.48	0.79
1:2:792:ASP:O	1:2:859:ARG:NH1	2.16	0.79
2:3:437:SER:HA	2:3:440:VAL:H	1.45	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:D:216:VAL:HG13	10:D:217:ASN:HA	1.65	0.79
11:E:29:ILE:HD13	11:E:31:VAL:HG23	1.65	0.79
4:5:138:ILE:HG12	4:5:282:LEU:HD21	1.63	0.79
11:E:363:PHE:HA	11:E:366:MET:HB2	1.63	0.79
1:2:338:LYS:HD2	1:2:379:LYS:HB3	1.63	0.79
2:3:405:ILE:HG23	2:3:545:LEU:HB2	1.64	0.79
3:4:449:ARG:HG3	3:4:450:GLN:N	1.97	0.79
6:7:143:LEU:HD21	6:7:197:THR:HG22	1.65	0.79
6:7:493:LEU:HD21	6:7:533:ASP:CG	2.07	0.79
10:D:256:TYR:HB2	10:D:257:THR:HG23	1.65	0.79
2:3:665:GLU:HG2	2:3:666:ARG:HG3	1.64	0.78
11:E:572:ILE:HG12	11:E:577:ASP:HA	1.64	0.78
6:7:289:CYS:HB3	6:7:296:GLY:HA3	1.63	0.78
11:E:540:ARG:HH22	11:E:574:GLU:HB2	1.49	0.78
10:D:216:VAL:HG22	10:D:219:ILE:HG13	1.66	0.78
11:E:61:ILE:H	11:E:61:ILE:HD12	1.48	0.78
11:E:337:SER:O	11:E:341:SER:OG	2.01	0.78
2:3:177:ASN:ND2	4:5:246:GLU:O	2.17	0.78
6:7:677:SER:O	6:7:680:SER:HB3	1.83	0.78
11:E:288:TYR:OH	11:E:406:ARG:NH1	2.16	0.78
1:2:846:VAL:O	1:2:853:VAL:CG2	2.29	0.78
2:3:138:ASP:CG	2:3:140:PRO:HD2	2.08	0.78
2:3:382:LEU:HD12	2:3:385:LEU:HD12	1.66	0.78
11:E:26:GLN:HG3	11:E:78:ILE:HG13	1.66	0.78
3:4:798:LEU:HA	3:4:801:MET:HB2	1.63	0.78
7:A:79:MET:HB3	10:D:206:LEU:HD11	1.66	0.78
5:6:112:ARG:HH22	5:6:183:LYS:HG3	1.47	0.78
11:E:572:ILE:HD13	11:E:579:TYR:H	1.48	0.78
3:4:512:VAL:HG12	3:4:518:LEU:HD12	1.66	0.78
5:6:151:ILE:O	5:6:266:SER:OG	2.00	0.78
1:2:538:ASN:HB2	1:2:677:PHE:HA	1.64	0.77
3:4:721:ALA:O	3:4:725:THR:N	2.17	0.77
11:E:335:TYR:HB2	11:E:373:ALA:HB1	1.66	0.77
3:4:432:ARG:HH22	6:7:557:LEU:HB3	1.49	0.77
4:5:656:ILE:HA	4:5:659:ILE:HD12	1.64	0.77
5:6:765:LEU:HD12	5:6:819:ILE:HB	1.66	0.77
10:D:232:VAL:HB	10:D:271:ILE:HA	1.67	0.77
1:2:501:MET:HG2	1:2:516:ALA:HB2	1.67	0.77
3:4:433:ILE:HD13	3:4:469:VAL:HA	1.67	0.77
5:6:100:VAL:HG23	5:6:101:LYS:HG3	1.66	0.77
8:B:168:LEU:HB2	10:D:276:VAL:HB	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:275:ASP:N	2:3:275:ASP:OD1	2.16	0.77
1:2:632:SER:HB2	4:5:442:LYS:CB	2.12	0.77
3:4:303:VAL:HG12	3:4:305:PRO:HD3	1.65	0.77
3:4:623:LEU:HD22	5:6:370:THR:HG23	1.67	0.77
5:6:533:ILE:O	5:6:587:TYR:CZ	2.38	0.77
5:6:794:ARG:H	5:6:795:ILE:HA	1.48	0.77
6:7:68:GLN:O	6:7:72:ASN:N	2.18	0.77
2:3:261:MET:HB2	2:3:264:MET:HG2	1.66	0.77
4:5:579:ASN:HB2	4:5:582:ALA:HB3	1.65	0.77
11:E:315:THR:N	11:E:316:LEU:HB3	2.00	0.77
1:2:813:ILE:HD12	1:2:841:VAL:HG21	1.65	0.77
1:2:231:ILE:HG23	1:2:279:THR:HG23	1.66	0.76
6:7:368:ALA:H	6:7:370:LEU:HD22	1.48	0.76
1:2:338:LYS:H	1:2:380:THR:HG22	1.49	0.76
1:2:569:GLN:HB2	1:2:612:MET:HA	1.66	0.76
3:4:315:ARG:NH1	6:7:250:ASP:OD1	2.18	0.76
4:5:414:LEU:HD13	4:5:422:LYS:HB2	1.66	0.76
10:D:260:ILE:HG22	10:D:264:LYS:O	1.85	0.76
1:2:777:LYS:H	1:2:828:PHE:HA	1.51	0.76
1:2:523:VAL:HG12	1:2:525:LYS:HB3	1.67	0.76
1:2:672:PRO:HA	4:5:418:PRO:HG3	1.66	0.76
5:6:117:GLN:O	5:6:121:ASP:N	2.19	0.76
5:6:530:VAL:HA	5:6:533:ILE:HD11	1.67	0.76
11:E:150:ASP:HB3	11:E:152:LEU:HB2	1.67	0.76
2:3:272:ARG:HD2	4:5:171:VAL:HG13	1.67	0.76
4:5:287:ILE:HD11	4:5:342:ILE:HG23	1.68	0.76
2:3:437:SER:HB3	2:3:438:SER:HA	1.67	0.76
2:3:435:ARG:NH1	2:3:477:LYS:O	2.18	0.76
6:7:490:GLY:C	6:7:494:THR:HG22	2.11	0.76
4:5:578:GLY:O	4:5:579:ASN:C	2.28	0.76
5:6:773:LEU:HD12	5:6:824:ILE:HG21	1.66	0.76
1:2:422:GLU:OE2	1:2:562:ARG:NH1	2.19	0.75
2:3:189:THR:HA	2:3:256:ILE:HD12	1.68	0.75
2:3:428:LEU:HB3	2:3:429:ALA:HA	1.68	0.75
3:4:928:ARG:HB2	5:6:946:ASN:HB2	1.68	0.75
8:B:21:GLU:HA	8:B:73:LEU:HD23	1.66	0.75
11:E:92:LEU:HA	11:E:95:PHE:HB3	1.68	0.75
6:7:220:ILE:C	6:7:222:SER:CB	2.60	0.75
3:4:830:ARG:O	3:4:834:LYS:N	2.19	0.75
1:2:790:TYR:OH	1:2:794:ARG:NH2	2.19	0.75
2:3:195:LYS:HE3	6:7:369:GLY:HA3	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:448:ALA:HA	5:6:301:ARG:HD3	1.69	0.74
5:6:828:TYR:OH	5:6:832:ARG:NH2	2.21	0.74
3:4:252:LYS:HG2	3:4:253:GLN:HA	1.67	0.74
5:6:162:GLU:HG3	5:6:165:ALA:HB3	1.69	0.74
2:3:113:GLY:HA2	2:3:116:VAL:HB	1.68	0.74
5:6:819:ILE:HG22	5:6:820:THR:H	1.53	0.74
10:D:76:LEU:HD11	10:D:147:ARG:HE	1.52	0.74
3:4:598:ALA:HA	3:4:644:VAL:HG22	1.68	0.74
5:6:533:ILE:O	5:6:587:TYR:CE1	2.40	0.74
7:A:84:ARG:HH22	10:D:217:ASN:HB3	1.53	0.74
8:B:25:ILE:HD12	8:B:87:ILE:HD13	1.70	0.74
1:2:692:ASP:OD2	5:6:781:ARG:NH2	2.20	0.74
11:E:576:THR:O	11:E:577:ASP:CB	2.34	0.74
1:2:286:TYR:HA	1:2:289:ILE:HB	1.70	0.74
3:4:726:ASN:O	3:4:727:LEU:HG	1.86	0.74
5:6:792:SER:HA	5:6:793:TYR:HB2	1.69	0.74
1:2:268:LEU:HA	1:2:271:PHE:HB3	1.70	0.74
1:2:398:PRO:HG2	1:2:401:ARG:HD2	1.69	0.74
5:6:628:LEU:HG	5:6:631:ALA:HB3	1.69	0.74
5:6:720:ASN:HB3	5:6:723:ILE:HB	1.68	0.74
6:7:220:ILE:HB	6:7:222:SER:OG	1.87	0.73
6:7:255:VAL:HG23	6:7:258:ILE:HG13	1.69	0.73
3:4:725:THR:HG23	6:7:657:ASN:HD21	1.51	0.73
11:E:576:THR:O	11:E:577:ASP:OD2	2.04	0.73
2:3:156:SER:HB2	2:3:325:THR:HG22	1.69	0.73
4:5:66:GLU:HA	4:5:69:ILE:HG22	1.69	0.73
5:6:570:ASN:HD21	5:6:678:ILE:N	1.85	0.73
6:7:256:GLU:HG3	6:7:257:VAL:HG22	1.69	0.73
6:7:645:ALA:HB1	6:7:701:LYS:HB3	1.70	0.73
1:2:659:SER:HA	3:4:928:ARG:HH22	1.53	0.73
6:7:476:ILE:HD12	6:7:476:ILE:N	2.03	0.73
10:D:258:VAL:CB	10:D:259:THR:HA	2.06	0.73
1:2:384:ASN:OD1	1:2:384:ASN:N	2.14	0.73
2:3:276:VAL:HG22	2:3:321:ILE:HB	1.69	0.73
11:E:81:LEU:HB3	11:E:120:ILE:HG13	1.71	0.73
3:4:862:GLN:HA	3:4:865:LEU:HB2	1.71	0.73
11:E:159:TYR:O	11:E:163:LEU:N	2.15	0.73
11:E:579:TYR:HB2	11:E:632:ILE:O	1.87	0.73
2:3:214:TYR:HA	2:3:227:THR:HG21	1.70	0.73
2:3:298:PHE:HD1	2:3:321:ILE:HG12	1.52	0.73
1:2:488:SER:HA	1:2:493:ILE:HD13	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:254:THR:HB	3:4:257:LEU:HB3	1.70	0.73
5:6:288:LEU:H	5:6:399:GLY:H	1.37	0.73
2:3:394:GLU:O	2:3:395:ASN:ND2	2.14	0.72
6:7:258:ILE:H	6:7:305:SER:HA	1.51	0.72
8:B:17:GLN:OE1	9:C:190:TRP:NE1	2.19	0.72
3:4:557:ARG:HH22	3:4:652:GLN:HB3	1.53	0.72
4:5:43:GLN:HB3	9:C:192:PHE:CZ	2.23	0.72
5:6:137:ARG:NH2	5:6:192:TYR:OH	2.22	0.72
1:2:780:GLN:HE22	4:5:573:ILE:HG22	1.53	0.72
3:4:557:ARG:HE	3:4:668:ARG:HH21	1.37	0.72
4:5:379:PHE:HB3	4:5:568:ILE:HD13	1.70	0.72
7:A:149:ILE:HA	7:A:150:ASP:HB2	1.71	0.72
1:2:533:ILE:HD13	4:5:576:HIS:CE1	2.25	0.72
11:E:25:CYS:HB3	11:E:26:GLN:HA	1.69	0.72
11:E:392:PHE:HA	11:E:396:LEU:HD23	1.72	0.72
3:4:543:GLN:HA	3:4:562:ILE:HD11	1.71	0.72
8:B:5:ALA:O	8:B:8:GLN:HB3	1.88	0.72
8:B:184:PHE:O	8:B:188:ILE:HD12	1.90	0.72
5:6:511:ASP:OD1	5:6:514:ASN:ND2	2.22	0.72
5:6:810:ILE:HD11	5:6:827:ALA:HB2	1.69	0.72
1:2:778:LEU:HG	4:5:577:THR:HG21	1.71	0.72
2:3:554:ASN:HB2	2:3:557:ARG:HB2	1.71	0.72
3:4:572:THR:HG21	3:4:708:VAL:HG21	1.71	0.72
8:B:119:TRP:HE1	8:B:174:SER:HB2	1.53	0.72
3:4:234:ARG:HB2	3:4:291:TYR:HE2	1.55	0.71
5:6:294:VAL:HB	5:6:391:PRO:HA	1.72	0.71
5:6:695:LEU:H	5:6:838:VAL:HG13	1.54	0.71
11:E:19:SER:O	11:E:25:CYS:SG	2.48	0.71
3:4:428:ARG:O	3:4:429:ALA:HB2	1.87	0.71
3:4:765:ALA:HB1	3:4:819:LEU:HD12	1.71	0.71
5:6:944:LYS:HD2	5:6:957:GLU:HB3	1.70	0.71
1:2:422:GLU:HG3	1:2:598:LEU:HD11	1.71	0.71
1:2:856:GLN:HE22	1:2:859:ARG:HH21	1.37	0.71
2:3:190:SER:O	2:3:254:GLN:NE2	2.21	0.71
3:4:601:LEU:HG	3:4:620:ALA:HB3	1.72	0.71
4:5:138:ILE:HG23	4:5:332:GLY:HA3	1.72	0.71
1:2:546:GLY:HA3	5:6:796:THR:HG23	1.73	0.71
4:5:588:GLU:O	4:5:593:GLU:N	2.23	0.71
1:2:614:ASP:OD1	1:2:617:ARG:NH1	2.24	0.71
11:E:29:ILE:HA	11:E:82:LEU:HB3	1.72	0.71
6:7:334:HIS:N	6:7:376:LEU:O	2.22	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:656:ARG:NH1	5:6:793:TYR:O	2.23	0.71
2:3:193:ARG:HD2	6:7:371:LEU:HG	1.73	0.71
3:4:364:VAL:HB	3:4:366:GLN:HE22	1.56	0.71
4:5:196:ASN:HB3	4:5:197:PHE:CD1	2.21	0.71
4:5:412:VAL:HG22	4:5:552:MET:HB2	1.72	0.71
9:C:118:LYS:HD2	9:C:118:LYS:O	1.91	0.71
5:6:603:SER:HB3	5:6:607:GLY:HA2	1.72	0.70
11:E:498:LEU:O	11:E:502:LEU:HG	1.90	0.70
2:3:292:VAL:HG11	2:3:326:VAL:HG13	1.72	0.70
3:4:758:ILE:HD13	3:4:813:LEU:HA	1.73	0.70
5:6:609:THR:HG23	5:6:663:ILE:HG12	1.73	0.70
1:2:572:SER:C	5:6:664:ALA:HB2	2.16	0.70
1:2:675:SER:OG	1:2:806:THR:OG1	2.09	0.70
2:3:39:ARG:HH22	2:3:132:LEU:HD11	1.56	0.70
4:5:298:TYR:HA	4:5:328:ILE:HG12	1.73	0.70
11:E:269:ASN:O	11:E:273:ASN:ND2	2.23	0.70
1:2:542:LEU:HD23	1:2:682:VAL:HG13	1.73	0.70
3:4:524:ARG:HG3	3:4:742:LEU:HD23	1.73	0.70
5:6:653:HIS:CD2	5:6:705:ILE:HA	2.27	0.70
3:4:646:HIS:HA	3:4:701:ARG:HH22	1.56	0.70
5:6:695:LEU:HA	5:6:698:ASN:HB2	1.73	0.70
5:6:937:VAL:HG12	5:6:941:LEU:HD21	1.72	0.70
11:E:637:LEU:HA	11:E:640:PHE:HB3	1.72	0.70
1:2:780:GLN:NE2	4:5:573:ILE:O	2.25	0.70
4:5:384:ILE:HG13	4:5:554:PHE:HD2	1.55	0.70
2:3:450:ARG:O	2:3:456:ARG:NH1	2.25	0.70
9:C:55:ALA:HB2	9:C:74:LEU:HD11	1.72	0.70
1:2:675:SER:HG	1:2:806:THR:HG1	1.37	0.70
4:5:422:LYS:NZ	13:5:801:ANP:O2B	2.25	0.70
6:7:221:SER:HA	6:7:222:SER:HB3	1.70	0.70
4:5:455:ARG:HA	4:5:462:PHE:HA	1.72	0.69
2:3:440:VAL:HG12	2:3:461:ALA:HB3	1.74	0.69
3:4:634:PHE:HA	3:4:637:MET:HG2	1.74	0.69
5:6:533:ILE:CG2	5:6:548:LEU:HD11	2.22	0.69
6:7:432:LEU:HD11	6:7:469:LEU:HD23	1.75	0.69
7:A:199:LEU:HB2	7:A:205:LEU:HG	1.72	0.69
2:3:193:ARG:NH2	2:3:452:THR:OG1	2.21	0.69
5:6:566:ARG:NH2	5:6:655:ALA:O	2.21	0.69
2:3:259:GLN:HG3	2:3:273:SER:HB3	1.74	0.69
6:7:82:LEU:HA	6:7:85:ILE:HD12	1.75	0.69
6:7:357:PRO:HA	6:7:374:THR:HA	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:108:ASP:HB3	7:A:109:LEU:HB3	0.83	0.69
8:B:52:LEU:HD13	10:D:125:PRO:HB2	1.72	0.69
10:D:266:GLU:HB3	10:D:268:GLU:HG3	1.74	0.69
4:5:414:LEU:HB2	4:5:522:ALA:HA	1.73	0.69
4:5:434:PRO:HA	4:5:600:LYS:HE2	1.74	0.69
5:6:297:THR:HA	5:6:359:VAL:HG12	1.75	0.69
6:7:271:GLN:NE2	6:7:279:THR:O	2.24	0.69
1:2:218:TYR:HB3	1:2:227:TYR:HE2	1.57	0.69
1:2:442:ASN:OD1	1:2:443:GLY:N	2.24	0.69
5:6:953:GLU:O	5:6:957:GLU:HG2	1.93	0.69
11:E:45:LEU:HD21	11:E:82:LEU:HD11	1.74	0.69
2:3:33:ASP:HB2	2:3:39:ARG:HH11	1.58	0.69
3:4:876:GLN:NE2	3:4:880:SER:O	2.26	0.69
4:5:83:PRO:O	4:5:87:ILE:HG13	1.92	0.69
6:7:662:GLN:HA	6:7:665:ILE:HD12	1.74	0.69
10:D:143:TYR:OH	10:D:147:ARG:NH1	2.25	0.69
10:D:260:ILE:HG23	10:D:266:GLU:N	2.08	0.69
11:E:270:LEU:O	11:E:274:ILE:HG13	1.92	0.69
1:2:404:ARG:NH2	5:6:297:THR:OG1	2.25	0.69
2:3:209:PHE:O	6:7:7:SER:OG	2.08	0.69
2:3:413:THR:HB	2:3:415:LYS:HE2	1.75	0.69
5:6:625:ALA:HB3	5:6:626:GLY:HA2	1.75	0.69
6:7:139:LEU:HA	6:7:142:ILE:HB	1.74	0.69
6:7:680:SER:HB2	6:7:681:PHE:HA	1.74	0.69
1:2:550:SER:N	13:2:901:ANP:O1A	2.25	0.69
2:3:223:THR:HG21	4:5:245:HIS:H	1.58	0.69
4:5:469:MET:HE1	4:5:477:VAL:HG13	1.73	0.69
7:A:188:GLN:HG3	11:E:58:ILE:HD12	1.74	0.69
1:2:571:ALA:CB	5:6:664:ALA:HB3	2.23	0.69
3:4:824:GLU:HA	3:4:827:ARG:HB3	1.75	0.69
4:5:55:LEU:HB3	9:C:137:HIS:HB3	1.73	0.69
5:6:612:VAL:HG23	5:6:623:ILE:HA	1.75	0.69
11:E:576:THR:C	11:E:577:ASP:CG	2.59	0.69
1:2:547:THR:O	13:2:901:ANP:O2A	2.11	0.68
1:2:706:SER:OG	1:2:706:SER:O	2.11	0.68
2:3:229:ALA:CB	6:7:370:LEU:HD21	2.24	0.68
4:5:547:LEU:HD22	4:5:553:ILE:HG12	1.73	0.68
5:6:284:ILE:HA	5:6:401:GLU:HB3	1.75	0.68
5:6:361:ILE:HD12	5:6:397:PHE:HE2	1.57	0.68
11:E:577:ASP:HB2	11:E:633:ARG:HE	1.58	0.68
1:2:638:THR:H	4:5:445:SER:H	1.40	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:806:THR:H	1:2:809:HIS:HB2	1.57	0.68
2:3:23:ASP:OD1	2:3:26:ARG:NH2	2.26	0.68
2:3:257:THR:HA	2:3:275:ASP:HA	1.75	0.68
4:5:282:LEU:HD22	4:5:333:ILE:HG22	1.75	0.68
7:A:200:ILE:HD11	7:A:208:ILE:HD11	1.75	0.68
1:2:541:LEU:N	1:2:648:ALA:O	2.22	0.68
2:3:48:TYR:HB3	2:3:92:LEU:HD11	1.76	0.68
3:4:607:ARG:HG2	3:4:609:VAL:H	1.57	0.68
3:4:692:ILE:HD11	3:4:705:VAL:HG11	1.75	0.68
4:5:341:SER:O	4:5:345:SER:CB	2.24	0.68
4:5:623:SER:O	4:5:627:VAL:CG1	2.23	0.68
2:3:347:ILE:O	2:3:351:ASN:ND2	2.27	0.68
5:6:738:ARG:HD3	5:6:740:GLU:H	1.59	0.68
7:A:147:VAL:H	7:A:148:ASP:HA	1.59	0.68
3:4:623:LEU:HB3	5:6:370:THR:HG21	1.76	0.68
5:6:522:ASP:HB2	5:6:525:ILE:HG23	1.74	0.68
11:E:316:LEU:HD11	11:E:414:GLY:N	2.09	0.68
1:2:339:PHE:HA	1:2:378:GLU:HB3	1.75	0.68
2:3:163:ALA:H	2:3:164:HIS:HB2	1.58	0.68
2:3:406:LEU:HD12	2:3:514:ALA:HB3	1.75	0.68
10:D:232:VAL:HG21	10:D:269:LEU:HD12	1.76	0.68
10:D:258:VAL:HB	10:D:259:THR:CA	2.14	0.68
3:4:718:ARG:HG3	6:7:661:VAL:HG11	1.74	0.68
6:7:466:LYS:HD2	6:7:566:ALA:HB1	1.75	0.68
11:E:85:GLY:N	11:E:123:LEU:O	2.26	0.68
2:3:687:ARG:HB3	6:7:604:PRO:HB3	1.76	0.68
7:A:46:ASN:O	7:A:50:ASN:ND2	2.27	0.68
11:E:381:ASP:HB2	11:E:384:ILE:HG13	1.76	0.68
1:2:824:ARG:NH2	1:2:833:ASP:OD1	2.27	0.67
2:3:101:ASP:HA	2:3:104:ARG:HH21	1.59	0.67
3:4:683:ASN:HD21	3:4:686:LEU:HD22	1.59	0.67
4:5:370:LEU:HD12	4:5:599:MET:HE1	1.76	0.67
11:E:140:ILE:HA	11:E:141:GLN:HB3	1.75	0.67
1:2:328:THR:O	1:2:386:GLN:NE2	2.26	0.67
6:7:434:LEU:HD13	6:7:695:LEU:HD22	1.76	0.67
7:A:71:GLN:HA	7:A:74:VAL:HB	1.76	0.67
11:E:31:VAL:HG22	11:E:42:THR:HG21	1.74	0.67
3:4:524:ARG:HG3	3:4:742:LEU:CD2	2.24	0.67
6:7:104:SER:OG	6:7:216:ARG:NE	2.27	0.67
6:7:256:GLU:N	6:7:306:LYS:O	2.22	0.67
2:3:25:VAL:CG2	2:3:124:PRO:HB2	2.25	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:461:ASP:HB2	6:7:462:PRO:HA	1.77	0.67
3:4:873:LEU:HD22	5:6:942:LEU:HG	1.76	0.67
4:5:255:PHE:HA	4:5:277:THR:HG22	1.76	0.67
4:5:413:LEU:HD11	4:5:550:PHE:CD2	2.29	0.67
5:6:805:ARG:HA	5:6:808:GLU:CD	2.20	0.67
6:7:208:SER:HB2	6:7:209:GLN:HA	1.76	0.67
11:E:540:ARG:NH2	11:E:574:GLU:CB	2.50	0.67
2:3:429:ALA:H	2:3:469:VAL:H	1.43	0.67
5:6:396:LYS:HB3	5:6:460:ILE:HG22	1.76	0.67
8:B:10:THR:HA	8:B:182:ARG:HH11	1.60	0.67
8:B:112:PHE:O	8:B:152:ARG:NH1	2.26	0.67
2:3:199:SER:HB3	2:3:212:ARG:HB3	1.76	0.67
3:4:589:VAL:HG21	3:4:624:SER:CB	2.25	0.67
5:6:400:VAL:HG23	5:6:455:LEU:O	1.94	0.67
10:D:83:LEU:O	10:D:87:LEU:HG	1.95	0.67
1:2:423:GLU:HB2	1:2:459:ARG:HD3	1.77	0.67
2:3:183:GLU:OE1	2:3:183:GLU:N	2.23	0.67
3:4:714:GLU:H	3:4:715:LYS:HB3	1.58	0.67
5:6:381:LEU:HB3	5:6:386:VAL:HA	1.77	0.67
5:6:533:ILE:O	5:6:587:TYR:OH	2.13	0.67
6:7:26:VAL:H	6:7:63:TYR:HB2	1.59	0.67
3:4:647:GLU:O	3:4:651:GLN:HB2	1.95	0.67
6:7:458:LEU:HB2	6:7:566:ALA:HA	1.77	0.67
2:3:30:GLU:O	2:3:34:THR:OG1	2.13	0.66
3:4:521:LEU:HD11	3:4:741:VAL:O	1.96	0.66
3:4:607:ARG:HA	3:4:614:LEU:HA	1.75	0.66
5:6:122:PHE:HB2	5:6:124:VAL:HB	1.78	0.66
8:B:10:THR:OG1	8:B:179:ASN:OD1	2.13	0.66
2:3:192:VAL:HB	6:7:329:ARG:NH1	2.07	0.66
2:3:701:THR:O	2:3:704:THR:OG1	2.13	0.66
6:7:668:ARG:HD2	6:7:672:LYS:HZ1	1.58	0.66
7:A:149:ILE:HD11	10:D:141:ARG:HG2	1.76	0.66
1:2:653:ASN:ND2	1:2:666:ASN:O	2.28	0.66
1:2:660:THR:OG1	3:4:928:ARG:NH1	2.28	0.66
3:4:302:LYS:NZ	3:4:421:ASP:OD2	2.28	0.66
3:4:527:ALA:HB1	3:4:530:ILE:HD13	1.77	0.66
4:5:453:VAL:HG21	4:5:509:ILE:HD11	1.77	0.66
6:7:318:LEU:HD23	6:7:321:GLN:HG3	1.77	0.66
2:3:339:ARG:HB2	2:3:340:GLN:HA	1.77	0.66
2:3:706:ILE:O	2:3:710:THR:OG1	2.13	0.66
3:4:354:HIS:CD2	3:4:356:MET:HG2	2.31	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:426:LEU:HD21	4:5:520:LEU:HD22	1.78	0.66
6:7:656:VAL:O	6:7:660:VAL:HG23	1.96	0.66
8:B:7:LEU:H	8:B:8:GLN:HA	1.61	0.66
10:D:218:MET:HA	10:D:220:ASP:N	2.10	0.66
1:2:325:THR:OG1	1:2:389:THR:O	2.12	0.66
2:3:451:GLU:HG3	2:3:452:THR:HG23	1.76	0.66
3:4:701:ARG:HA	3:4:796:ARG:HH21	1.61	0.66
4:5:562:GLU:HB3	4:5:563:GLU:HG3	1.76	0.66
7:A:7:ASN:HA	7:A:10:VAL:HG12	1.78	0.66
8:B:12:SER:HB3	8:B:15:GLU:HG3	1.76	0.66
1:2:234:LEU:HB3	1:2:237:MET:HB3	1.78	0.66
2:3:116:VAL:HG12	2:3:117:GLU:HG3	1.77	0.66
5:6:355:ASP:HB3	5:6:356:TRP:HA	1.77	0.66
11:E:360:HIS:HA	11:E:363:PHE:HD2	1.61	0.66
4:5:571:HIS:O	4:5:581:ASN:ND2	2.29	0.66
1:2:484:PHE:CE1	1:2:766:TYR:HA	2.30	0.66
2:3:439:GLY:HA3	2:3:442:LEU:HD22	1.78	0.66
3:4:714:GLU:N	3:4:715:LYS:HB3	2.11	0.66
4:5:321:VAL:N	4:5:323:ILE:HG13	2.11	0.66
4:5:649:THR:N	4:5:652:GLN:HG3	2.09	0.66
5:6:533:ILE:HG12	5:6:548:LEU:HD11	1.77	0.66
1:2:567:THR:HG23	1:2:568:GLY:N	2.10	0.66
2:3:156:SER:O	2:3:324:ASN:ND2	2.28	0.66
8:B:52:LEU:HD11	10:D:129:MET:HB2	1.78	0.66
11:E:621:ARG:HB2	11:E:631:GLU:HB2	1.78	0.66
2:3:367:LEU:HD12	2:3:378:LYS:HB3	1.78	0.65
6:7:69:LYS:HA	6:7:72:ASN:HB2	1.78	0.65
10:D:94:GLN:HA	10:D:97:LEU:HB3	1.78	0.65
1:2:539:VAL:HB	1:2:647:ILE:HA	1.79	0.65
4:5:377:SER:OG	4:5:424:GLN:NE2	2.27	0.65
4:5:451:ALA:HB2	4:5:470:VAL:HG21	1.78	0.65
4:5:606:CYS:O	4:5:665:LYS:NZ	2.29	0.65
5:6:171:SER:O	5:6:286:SER:HB2	1.96	0.65
5:6:561:GLU:N	5:6:562:GLY:HA3	2.10	0.65
3:4:617:GLU:HG2	5:6:373:MET:HE1	1.78	0.65
6:7:496:ALA:O	6:7:508:LEU:HG	1.95	0.65
1:2:632:SER:CB	4:5:442:LYS:HB3	2.16	0.65
1:2:789:VAL:HG13	1:2:863:ILE:HD12	1.78	0.65
7:A:138:ILE:HD12	7:A:141:LEU:HD23	1.77	0.65
11:E:131:LEU:O	11:E:155:GLN:NE2	2.29	0.65
3:4:589:VAL:HB	3:4:629:CYS:HA	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:662:SER:HB3	5:6:671:THR:HG22	1.78	0.65
10:D:200:LYS:H	10:D:201:TYR:HB2	1.61	0.65
11:E:73:GLN:HG2	11:E:74:LEU:HG	1.77	0.65
1:2:803:PHE:HB3	1:2:805:ILE:H	1.61	0.65
6:7:21:ILE:HG21	6:7:117:PHE:HA	1.77	0.65
5:6:122:PHE:HA	5:6:123:SER:HB2	1.78	0.65
1:2:436:GLY:N	1:2:437:ASN:HA	2.11	0.65
1:2:481:GLU:HA	1:2:484:PHE:HB3	1.79	0.65
2:3:314:LEU:HD23	4:5:253:GLN:HE22	1.62	0.65
3:4:572:THR:HB	3:4:574:LYS:HE3	1.79	0.65
6:7:368:ALA:N	6:7:370:LEU:HD22	2.11	0.65
10:D:159:ARG:HA	10:D:162:ASN:HB3	1.78	0.65
11:E:362:MET:HE1	11:E:396:LEU:HD22	1.79	0.65
1:2:317:LEU:HA	1:2:429:ILE:HG22	1.79	0.65
1:2:334:LEU:HA	1:2:382:TYR:CD1	2.32	0.65
3:4:613:GLN:HG3	5:6:360:ARG:HH22	1.62	0.65
4:5:53:ASN:HB3	4:5:58:ASN:HB3	1.79	0.65
4:5:62:THR:HA	4:5:138:ILE:O	1.97	0.65
4:5:481:GLU:HG2	4:5:484:LYS:HB2	1.79	0.65
5:6:348:VAL:O	5:6:351:SER:OG	2.14	0.65
11:E:526:ARG:HB2	11:E:567:MET:SD	2.37	0.65
1:2:685:ASP:O	5:6:794:ARG:NE	2.25	0.65
3:4:907:LEU:HD23	3:4:910:LEU:HD12	1.78	0.65
4:5:664:ALA:HA	4:5:676:HIS:CE1	2.26	0.65
5:6:783:ASP:OD1	5:6:783:ASP:N	2.27	0.65
6:7:513:LEU:HA	6:7:561:THR:HG21	1.79	0.65
2:3:47:VAL:HG12	2:3:51:ASN:HD21	1.63	0.64
2:3:471:CYS:HA	2:3:513:ILE:O	1.97	0.64
3:4:201:PHE:HB2	3:4:202:LYS:HA	1.79	0.64
4:5:181:ILE:HG21	4:5:241:TYR:HB3	1.78	0.64
5:6:143:MET:HE2	5:6:150:THR:H	1.61	0.64
11:E:489:VAL:O	11:E:493:ASN:ND2	2.29	0.64
5:6:174:TYR:CE2	5:6:178:LEU:HD11	2.33	0.64
5:6:605:ALA:O	5:6:607:GLY:HA3	1.96	0.64
6:7:531:GLU:HA	6:7:534:ARG:HB2	1.78	0.64
6:7:575:ASN:HB3	6:7:578:LEU:HD22	1.79	0.64
9:C:104:PHE:O	9:C:108:ALA:N	2.28	0.64
9:C:105:PHE:HZ	9:C:127:LEU:HD22	1.62	0.64
11:E:285:ALA:HB1	11:E:288:TYR:HB3	1.79	0.64
11:E:611:GLN:HG3	11:E:649:LEU:HD21	1.78	0.64
6:7:311:GLN:O	6:7:335:VAL:HB	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:165:ILE:HG12	4:5:291:ARG:HA	1.79	0.64
4:5:356:GLU:O	4:5:360:LEU:HG	1.98	0.64
5:6:964:VAL:HA	5:6:967:ARG:HB3	1.79	0.64
7:A:167:VAL:HG21	7:A:183:LEU:HD12	1.79	0.64
10:D:199:LEU:HD13	10:D:202:MET:HE3	1.79	0.64
11:E:292:TYR:O	11:E:296:GLN:N	2.28	0.64
2:3:139:VAL:N	2:3:140:PRO:HD2	2.12	0.64
3:4:332:VAL:HB	3:4:429:ALA:CA	2.18	0.64
3:4:461:VAL:HG12	3:4:463:VAL:H	1.63	0.64
3:4:649:MET:HG3	3:4:701:ARG:HD3	1.78	0.64
4:5:366:LEU:HA	4:5:369:ILE:HG22	1.79	0.64
4:5:464:LEU:HD23	4:5:466:GLY:H	1.61	0.64
2:3:139:VAL:N	2:3:140:PRO:CD	2.58	0.64
3:4:271:ILE:O	3:4:275:THR:HG23	1.97	0.64
4:5:343:TRP:O	4:5:344:ASN:HB3	1.96	0.64
4:5:378:ILE:HA	13:5:801:ANP:HN61	1.62	0.64
10:D:59:ASP:OD2	10:D:90:ARG:NH1	2.30	0.64
3:4:183:THR:HG21	3:4:267:GLU:HG3	1.80	0.64
4:5:375:ALA:HB3	4:5:385:LYS:HE3	1.80	0.64
6:7:23:ASP:O	6:7:27:THR:OG1	2.16	0.64
8:B:163:LEU:HB3	8:B:189:MET:HE1	1.79	0.64
2:3:292:VAL:HG11	2:3:326:VAL:CG1	2.27	0.64
10:D:123:LYS:HD3	11:E:22:HIS:NE2	2.13	0.64
3:4:241:LEU:HD22	3:4:303:VAL:HG22	1.79	0.64
3:4:574:LYS:NZ	3:4:675:ALA:O	2.23	0.64
3:4:682:TYR:O	3:4:691:ASN:ND2	2.31	0.64
4:5:368:GLU:O	4:5:371:THR:OG1	2.12	0.64
4:5:254:GLN:HB3	4:5:278:CYS:HB2	1.80	0.63
11:E:24:SER:HB2	11:E:25:CYS:HB2	1.80	0.63
2:3:433:THR:HG23	4:5:503:SER:HB3	1.81	0.63
2:3:524:ASP:HA	2:3:532:ASN:HD21	1.63	0.63
3:4:289:LEU:HB3	3:4:293:LEU:HD21	1.80	0.63
3:4:443:PRO:HB2	3:4:453:LEU:HD22	1.80	0.63
5:6:304:LEU:HA	5:6:353:PHE:CE1	2.32	0.63
1:2:575:GLY:N	5:6:664:ALA:HB1	2.13	0.63
2:3:49:ASN:OD1	2:3:50:SER:N	2.32	0.63
3:4:727:LEU:N	3:4:728:TYR:CB	2.58	0.63
5:6:119:LEU:HD11	5:6:188:VAL:HG21	1.81	0.63
5:6:355:ASP:OD2	5:6:383:GLY:N	2.31	0.63
6:7:108:GLN:OE1	6:7:237:GLN:NE2	2.31	0.63
6:7:147:ARG:HH21	6:7:197:THR:HG23	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:489:SER:O	6:7:493:LEU:HD23	1.97	0.63
4:5:440:SER:HA	4:5:480:ASP:HB2	1.80	0.63
3:4:419:VAL:HB	3:4:423:LEU:HB2	1.81	0.63
4:5:144:ASN:HD22	11:E:375:GLU:HA	1.63	0.63
2:3:53:ALA:HA	6:7:218:LYS:HD2	1.80	0.63
3:4:830:ARG:HA	3:4:833:ILE:HB	1.81	0.63
4:5:343:TRP:O	4:5:344:ASN:CB	2.47	0.63
4:5:639:GLU:HB2	4:5:641:THR:HG23	1.81	0.63
5:6:523:GLU:OE1	5:6:524:HIS:ND1	2.31	0.63
5:6:708:ARG:HD3	5:6:798:ARG:HD3	1.80	0.63
6:7:411:TYR:CD1	6:7:433:LEU:HD23	2.34	0.63
6:7:417:SER:HB3	6:7:633:VAL:HB	1.81	0.63
1:2:309:LEU:O	1:2:310:ARG:NH1	2.31	0.63
2:3:564:HIS:HA	2:3:567:ARG:HG2	1.81	0.63
3:4:771:VAL:HG22	5:6:732:VAL:HG21	1.80	0.63
7:A:109:LEU:HG	7:A:111:SER:HB3	1.80	0.63
10:D:224:TRP:O	10:D:280:GLU:N	2.31	0.63
1:2:612:MET:O	1:2:617:ARG:NH2	2.32	0.63
1:2:630:SER:HA	4:5:445:SER:HB2	1.81	0.63
10:D:269:LEU:HD13	10:D:275:TYR:CD2	2.34	0.63
1:2:320:VAL:HB	1:2:426:VAL:HG23	1.79	0.63
1:2:573:ALA:HB2	5:6:663:ILE:O	1.99	0.63
2:3:434:GLY:N	2:3:473:ASP:O	2.32	0.63
5:6:533:ILE:HG21	5:6:548:LEU:CD1	2.28	0.63
5:6:560:VAL:HB	5:6:561:GLU:HA	1.81	0.63
6:7:541:MET:HB2	6:7:593:ARG:HH11	1.64	0.63
8:B:11:PHE:HB2	8:B:179:ASN:ND2	2.12	0.63
1:2:704:VAL:HG13	5:6:766:THR:HG23	1.81	0.62
2:3:171:LEU:HD23	2:3:172:THR:H	1.64	0.62
3:4:324:LYS:O	3:4:438:THR:HA	1.99	0.62
5:6:581:LYS:NZ	5:6:682:ALA:O	2.32	0.62
7:A:31:MET:O	7:A:93:ARG:NH2	2.31	0.62
1:2:581:ARG:NH1	1:2:592:GLU:OE2	2.32	0.62
2:3:706:ILE:HG21	6:7:620:HIS:HE2	1.64	0.62
6:7:265:CYS:N	6:7:289:CYS:SG	2.66	0.62
6:7:543:GLN:HG3	6:7:544:GLN:H	1.65	0.62
8:B:165:GLU:OE1	8:B:165:GLU:N	2.30	0.62
10:D:73:SER:OG	10:D:150:LYS:NZ	2.31	0.62
1:2:335:LYS:HB2	1:2:381:VAL:O	2.00	0.62
2:3:360:PHE:HD1	2:3:715:VAL:HG11	1.64	0.62
5:6:653:HIS:CD2	5:6:656:MET:HB2	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:E:351:TRP:HB2	11:E:511:VAL:HG13	1.81	0.62
1:2:641:GLN:HB3	1:2:643:ARG:NH1	2.14	0.62
2:3:100:LEU:HB3	2:3:111:TRP:HZ3	1.65	0.62
6:7:513:LEU:HD13	6:7:540:VAL:HG21	1.80	0.62
11:E:30:PHE:CE2	11:E:81:LEU:HD21	2.35	0.62
3:4:628:VAL:HA	3:4:670:SER:O	1.99	0.62
5:6:610:ALA:HB3	5:6:663:ILE:HG21	1.80	0.62
10:D:143:TYR:O	10:D:147:ARG:HG3	1.99	0.62
1:2:438:LEU:HD13	5:6:301:ARG:HH12	1.63	0.62
3:4:236:LEU:HB3	3:4:238:THR:HG23	1.80	0.62
4:5:349:PHE:CD2	4:5:351:GLU:HA	2.34	0.62
5:6:614:ARG:NH2	12:F:12:DT:O4'	2.32	0.62
10:D:200:LYS:HB2	10:D:201:TYR:CG	2.35	0.62
2:3:168:PRO:HG2	2:3:260:GLU:HB3	1.82	0.62
3:4:695:PRO:HB2	3:4:697:PRO:HG2	1.82	0.62
5:6:831:LEU:O	5:6:835:ILE:HG13	1.99	0.62
11:E:285:ALA:HB3	11:E:286:GLN:HA	1.82	0.62
11:E:292:TYR:HB2	11:E:293:PRO:HD3	1.82	0.62
2:3:138:ASP:CB	2:3:140:PRO:HD2	2.30	0.62
3:4:400:GLN:HG3	6:7:508:LEU:HB2	1.81	0.62
3:4:428:ARG:O	3:4:429:ALA:CB	2.47	0.62
3:4:758:ILE:HD11	3:4:813:LEU:HD23	1.81	0.62
4:5:136:GLN:HB2	4:5:280:ARG:HE	1.65	0.62
5:6:576:ASP:O	5:6:579:THR:OG1	2.09	0.62
5:6:703:ALA:HA	5:6:706:MET:HB3	1.81	0.62
7:A:100:MET:HG2	7:A:117:GLN:HE21	1.64	0.62
9:C:170:GLU:O	9:C:174:LYS:N	2.33	0.62
11:E:312:THR:OG1	11:E:314:ASP:O	2.18	0.62
1:2:414:LEU:HD22	1:2:455:SER:HA	1.81	0.62
3:4:418:CYS:O	3:4:419:VAL:HG22	2.00	0.62
5:6:941:LEU:HD22	5:6:958:ARG:HH21	1.65	0.62
11:E:575:ASN:O	11:E:576:THR:OG1	2.07	0.62
1:2:622:GLU:HG3	1:2:626:GLN:NE2	2.15	0.62
2:3:100:LEU:HB3	2:3:111:TRP:CZ3	2.35	0.62
3:4:547:GLY:HA3	3:4:560:GLY:HA2	1.81	0.62
4:5:410:ILE:O	4:5:411:ASN:ND2	2.31	0.62
5:6:796:THR:HG22	5:6:798:ARG:N	2.14	0.62
7:A:37:ILE:O	7:A:41:LEU:HG	2.00	0.62
8:B:195:ILE:HG22	9:C:109:ILE:HD13	1.81	0.62
2:3:414:ALA:HA	13:3:1001:ANP:H5'1	1.82	0.61
5:6:399:GLY:HA2	5:6:454:PHE:CZ	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:662:SER:HA	5:6:671:THR:HA	1.82	0.61
3:4:549:ASN:OD1	3:4:559:ARG:NH2	2.33	0.61
7:A:138:ILE:HA	7:A:141:LEU:HD23	1.82	0.61
11:E:530:LEU:HD22	11:E:536:LEU:HD11	1.81	0.61
3:4:722:LYS:HA	3:4:725:THR:HB	1.80	0.61
3:4:727:LEU:H	3:4:728:TYR:HB3	1.65	0.61
4:5:347:THR:HB	4:5:349:PHE:HA	1.81	0.61
6:7:459:MET:HG3	6:7:460:GLY:H	1.64	0.61
8:B:13:PRO:HA	8:B:16:ILE:HG12	1.81	0.61
8:B:192:LEU:O	8:B:195:ILE:HG13	2.00	0.61
6:7:415:ALA:HA	6:7:418:ILE:HD12	1.81	0.61
7:A:150:ASP:OD1	7:A:198:ARG:NH2	2.34	0.61
10:D:74:PRO:HG3	10:D:279:TYR:CG	2.36	0.61
11:E:413:LEU:HD23	11:E:416:ARG:HD2	1.81	0.61
4:5:64:ASN:HD21	4:5:66:GLU:HB2	1.65	0.61
5:6:540:HIS:HD2	5:6:715:ILE:HG21	1.66	0.61
11:E:336:ASP:HA	11:E:339:TYR:HB3	1.82	0.61
11:E:551:TRP:HE3	11:E:552:LEU:HD12	1.65	0.61
1:2:853:VAL:HA	1:2:856:GLN:HB3	1.82	0.61
3:4:396:VAL:HA	3:4:418:CYS:HA	1.82	0.61
10:D:260:ILE:HG12	10:D:266:GLU:OE1	1.96	0.61
2:3:254:GLN:HE21	2:3:256:ILE:HD11	1.64	0.61
4:5:51:ARG:HA	4:5:54:ILE:HG12	1.83	0.61
4:5:553:ILE:H	4:5:553:ILE:HD12	1.66	0.61
5:6:919:LYS:HD2	5:6:936:ILE:HB	1.82	0.61
11:E:12:TYR:CE1	11:E:48:LEU:HD21	2.36	0.61
11:E:316:LEU:HD21	11:E:413:LEU:O	2.00	0.61
1:2:479:GLU:O	1:2:482:ARG:HG2	2.01	0.61
1:2:543:GLY:N	1:2:650:ALA:O	2.33	0.61
2:3:301:LEU:H	2:3:319:THR:HG22	1.66	0.61
2:3:356:LYS:HB2	2:3:359:ILE:HG23	1.83	0.61
5:6:189:VAL:O	5:6:193:ALA:N	2.33	0.61
5:6:940:TYR:OH	5:6:957:GLU:OE1	2.19	0.61
9:C:82:THR:HA	9:C:85:MET:HG2	1.81	0.61
11:E:33:CYS:SG	11:E:62:PHE:HA	2.40	0.61
11:E:68:ARG:HB2	11:E:95:PHE:CE2	2.35	0.61
1:2:296:ARG:O	1:2:455:SER:OG	2.08	0.61
3:4:822:VAL:HA	3:4:825:ALA:HB3	1.83	0.61
6:7:82:LEU:HB3	6:7:207:LEU:HD23	1.83	0.61
11:E:243:GLN:N	11:E:607:MET:SD	2.74	0.61
11:E:577:ASP:HB2	11:E:633:ARG:NE	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:299:ASP:HB3	1:2:319:ARG:NH1	2.16	0.61
2:3:244:GLU:O	2:3:248:SER:OG	2.16	0.61
2:3:409:GLY:O	2:3:415:LYS:NZ	2.34	0.61
3:4:518:LEU:HG	3:4:522:LEU:HG	1.83	0.61
4:5:349:PHE:HD2	4:5:351:GLU:HA	1.65	0.61
7:A:198:ARG:O	7:A:202:GLN:HB2	2.01	0.61
9:C:162:THR:N	9:C:163:SER:HA	2.14	0.61
4:5:339:THR:O	4:5:341:SER:OG	2.17	0.60
5:6:690:ASN:HB3	5:6:693:LEU:HD12	1.83	0.60
2:3:554:ASN:O	2:3:558:ASP:N	2.34	0.60
3:4:826:VAL:HA	3:4:829:ILE:HD12	1.81	0.60
5:6:943:GLN:HA	5:6:946:ASN:HD21	1.66	0.60
6:7:228:ARG:NH1	6:7:326:HIS:HB3	2.15	0.60
2:3:210:HIS:HB3	6:7:5:LEU:HD21	1.83	0.60
6:7:369:GLY:H	6:7:371:LEU:HB2	1.66	0.60
6:7:440:VAL:HG23	6:7:697:GLN:HB3	1.81	0.60
11:E:311:LYS:N	11:E:312:THR:HA	2.16	0.60
1:2:564:VAL:HG11	1:2:595:ALA:HB1	1.83	0.60
1:2:793:LEU:HD11	1:2:863:ILE:HG21	1.83	0.60
2:3:105:GLU:OE1	2:3:105:GLU:N	2.34	0.60
2:3:402:ASP:OD1	2:3:402:ASP:N	2.29	0.60
13:3:1001:ANP:O2B	13:3:1001:ANP:O3G	2.20	0.60
7:A:22:ARG:HB3	7:A:23:SER:HA	1.83	0.60
7:A:67:VAL:HG21	9:C:25:PRO:HD2	1.83	0.60
11:E:431:LEU:O	11:E:476:ASN:ND2	2.33	0.60
2:3:53:ALA:O	6:7:217:LYS:NZ	2.32	0.60
3:4:608:ASP:OD2	3:4:611:THR:OG1	2.18	0.60
3:4:725:THR:O	3:4:728:TYR:HB2	2.01	0.60
4:5:144:ASN:ND2	11:E:374:GLN:O	2.35	0.60
9:C:107:LEU:O	9:C:110:LYS:N	2.32	0.60
1:2:625:GLU:CD	13:5:801:ANP:HNB1	2.09	0.60
1:2:783:MET:HB3	4:5:573:ILE:HG21	1.81	0.60
3:4:517:ASP:O	3:4:521:LEU:N	2.26	0.60
4:5:675:ARG:HA	4:5:678:ASP:HB2	1.84	0.60
5:6:725:THR:HA	5:6:728:ALA:HB3	1.84	0.60
6:7:664:TYR:CG	6:7:689:LEU:HD13	2.36	0.60
11:E:346:ALA:HB2	11:E:555:CYS:HA	1.84	0.60
11:E:583:GLY:N	11:E:628:SER:O	2.27	0.60
1:2:275:ALA:O	1:2:279:THR:N	2.33	0.60
1:2:611:LYS:N	1:2:611:LYS:HD2	2.17	0.60
2:3:303:ALA:HB1	2:3:307:ASN:HB2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:137:LEU:HD11	4:5:139:LEU:HD23	1.82	0.60
11:E:92:LEU:O	11:E:96:LEU:N	2.34	0.60
11:E:567:MET:HB2	11:E:584:LEU:HB2	1.83	0.60
2:3:161:PHE:HB3	2:3:162:GLY:HA3	1.84	0.60
2:3:229:ALA:O	2:3:230:ILE:HG23	2.01	0.60
11:E:512:ALA:O	11:E:516:LYS:HG3	2.02	0.60
4:5:338:GLU:HG2	4:5:340:SER:OG	2.01	0.60
1:2:283:TYR:O	1:2:285:ASP:N	2.33	0.60
3:4:755:LYS:HA	3:4:810:LYS:HD3	1.82	0.60
4:5:66:GLU:OE1	4:5:66:GLU:N	2.35	0.60
5:6:304:LEU:HD12	5:6:353:PHE:HE1	1.67	0.60
11:E:346:ALA:HB1	11:E:558:GLU:HG3	1.83	0.60
1:2:778:LEU:HG	4:5:577:THR:HG22	1.83	0.59
2:3:553:ILE:HG22	4:5:630:ARG:HH11	1.67	0.59
5:6:357:GLN:HE21	5:6:381:LEU:HD12	1.66	0.59
6:7:113:PHE:O	6:7:117:PHE:HB3	2.00	0.59
11:E:227:LYS:O	11:E:231:HIS:ND1	2.30	0.59
1:2:306:LEU:HD11	1:2:406:ARG:HG2	1.84	0.59
1:2:803:PHE:HB3	1:2:805:ILE:HD12	1.83	0.59
3:4:642:ARG:HA	3:4:645:LEU:HB2	1.85	0.59
3:4:758:ILE:CD1	3:4:813:LEU:HA	2.31	0.59
5:6:910:VAL:O	5:6:914:ASN:HB2	2.02	0.59
6:7:490:GLY:HA2	6:7:493:LEU:CD1	2.32	0.59
8:B:25:ILE:HD11	8:B:73:LEU:HA	1.84	0.59
2:3:200:VAL:HB	2:3:244:GLU:HB2	1.83	0.59
2:3:372:TYR:OH	2:3:564:HIS:HB3	2.02	0.59
6:7:495:ALA:HB3	6:7:557:LEU:HD21	1.84	0.59
6:7:521:CYS:N	6:7:562:SER:O	2.27	0.59
7:A:47:LEU:HD22	7:A:79:MET:SD	2.42	0.59
8:B:132:ASP:OD1	8:B:132:ASP:N	2.31	0.59
11:E:574:GLU:O	11:E:575:ASN:HB2	2.01	0.59
2:3:25:VAL:HG22	2:3:124:PRO:HB2	1.85	0.59
2:3:228:PRO:HB2	2:3:229:ALA:HB2	1.85	0.59
3:4:260:GLN:HG2	6:7:135:LYS:HZ1	1.67	0.59
4:5:136:GLN:HA	4:5:280:ARG:HH21	1.66	0.59
5:6:616:GLU:N	5:6:617:GLU:HA	2.17	0.59
6:7:364:LYS:O	6:7:367:LYS:N	2.36	0.59
11:E:148:VAL:HG13	11:E:150:ASP:HB2	1.84	0.59
1:2:328:THR:HG22	1:2:387:ARG:O	2.02	0.59
1:2:659:SER:HA	3:4:928:ARG:NH2	2.18	0.59
2:3:368:ALA:HB1	2:3:371:ILE:HB	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:686:LEU:HD12	3:4:687:PRO:HD2	1.84	0.59
5:6:400:VAL:CG2	5:6:455:LEU:O	2.49	0.59
6:7:444:VAL:HG22	6:7:448:MET:H	1.68	0.59
7:A:150:ASP:HB2	10:D:141:ARG:HH21	1.68	0.59
10:D:231:HIS:O	10:D:292:ALA:N	2.35	0.59
11:E:434:VAL:O	11:E:476:ASN:ND2	2.34	0.59
2:3:229:ALA:CB	6:7:370:LEU:CD2	2.81	0.59
3:4:234:ARG:HB2	3:4:291:TYR:CE2	2.36	0.59
4:5:298:TYR:HD1	4:5:328:ILE:HD11	1.67	0.59
4:5:633:LEU:HD12	4:5:648:ILE:HG13	1.85	0.59
10:D:70:GLU:O	10:D:150:LYS:NZ	2.35	0.59
11:E:541:ASN:HD21	11:E:543:LEU:HB2	1.66	0.59
2:3:408:VAL:HA	2:3:516:ALA:O	2.03	0.59
3:4:605:ILE:HG13	3:4:616:LEU:HD12	1.84	0.59
3:4:886:LEU:O	3:4:890:ILE:HG12	2.03	0.59
6:7:128:PRO:HD2	6:7:129:THR:HA	1.84	0.59
10:D:77:LEU:O	10:D:147:ARG:NH2	2.36	0.59
1:2:633:LYS:HD2	12:F:12:DT:P	2.43	0.59
8:B:122:LEU:O	8:B:126:LEU:HG	2.03	0.59
10:D:59:ASP:HB3	10:D:87:LEU:HD21	1.85	0.59
1:2:605:LEU:HD23	1:2:647:ILE:HB	1.83	0.59
3:4:435:VAL:HA	3:4:466:VAL:HG22	1.84	0.59
5:6:307:ALA:HA	5:6:351:SER:HB3	1.84	0.59
5:6:795:ILE:CG2	5:6:799:GLN:HG3	2.30	0.59
5:6:806:LEU:HD13	5:6:827:ALA:HB1	1.85	0.59
6:7:380:PHE:HE2	6:7:382:ARG:HB2	1.68	0.59
11:E:327:PHE:N	11:E:341:SER:OG	2.32	0.59
2:3:186:VAL:O	2:3:289:GLY:N	2.28	0.58
2:3:679:ILE:HB	2:3:705:LEU:HD13	1.85	0.58
5:6:182:GLN:HG2	5:6:265:ILE:HD13	1.85	0.58
5:6:723:ILE:O	5:6:727:LEU:HG	2.03	0.58
6:7:284:CYS:SG	6:7:289:CYS:HB2	2.42	0.58
6:7:650:PRO:HA	6:7:706:ASP:HA	1.85	0.58
8:B:59:ALA:HB1	8:B:60:LEU:HB2	1.84	0.58
11:E:540:ARG:HH22	11:E:574:GLU:CB	2.13	0.58
5:6:689:TYR:HD2	5:6:716:LEU:HD12	1.68	0.58
6:7:282:SER:HA	6:7:298:LEU:HD11	1.85	0.58
7:A:5:LEU:HD11	7:A:36:ILE:HD11	1.86	0.58
2:3:428:LEU:HB3	2:3:429:ALA:CA	2.33	0.58
4:5:301:TYR:CE1	4:5:303:SER:HB3	2.39	0.58
4:5:374:ILE:HA	4:5:428:PHE:CE2	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:714:VAL:HB	5:6:837:ARG:HD3	1.84	0.58
5:6:765:LEU:HB2	5:6:819:ILE:HD13	1.85	0.58
6:7:465:ALA:HB1	6:7:468:GLN:HG2	1.83	0.58
1:2:499:SER:HB2	1:2:509:ARG:HH22	1.68	0.58
1:2:661:LEU:HB3	1:2:662:PRO:HD2	1.84	0.58
2:3:43:ARG:O	2:3:47:VAL:HG23	2.02	0.58
2:3:196:LEU:HD23	6:7:370:LEU:HB2	1.85	0.58
4:5:176:ALA:HA	4:5:250:PHE:CD1	2.39	0.58
4:5:342:ILE:HG13	4:5:342:ILE:O	2.03	0.58
5:6:610:ALA:HA	5:6:624:GLU:HG2	1.85	0.58
6:7:71:ALA:HB1	6:7:129:THR:HG21	1.86	0.58
8:B:113:SER:O	8:B:172:ASN:ND2	2.27	0.58
1:2:506:TYR:HB2	1:2:698:PHE:CE2	2.39	0.58
1:2:549:LYS:HA	1:2:552:ILE:HD12	1.84	0.58
2:3:200:VAL:HG21	2:3:247:TYR:CD2	2.39	0.58
3:4:348:LYS:O	3:4:383:SER:N	2.24	0.58
3:4:705:VAL:H	3:4:832:ALA:HB2	1.68	0.58
4:5:235:ASN:HA	4:5:236:CYS:C	2.29	0.58
4:5:485:MET:HE3	4:5:490:ARG:HA	1.86	0.58
5:6:914:ASN:O	5:6:918:ARG:HB2	2.04	0.58
6:7:142:ILE:O	6:7:146:ARG:HG2	2.04	0.58
2:3:228:PRO:CB	2:3:229:ALA:HB2	2.33	0.58
3:4:601:LEU:HB3	3:4:621:LEU:HG	1.86	0.58
6:7:203:TYR:OH	6:7:338:THR:N	2.37	0.58
9:C:178:LYS:O	9:C:182:GLU:HG2	2.04	0.58
11:E:579:TYR:CD1	11:E:637:LEU:HD21	2.39	0.58
2:3:32:LEU:HG	2:3:132:LEU:HD22	1.85	0.58
3:4:280:MET:O	3:4:284:ILE:HG12	2.04	0.58
3:4:348:LYS:N	3:4:383:SER:O	2.35	0.58
4:5:136:GLN:NE2	4:5:279:ASP:O	2.33	0.58
4:5:321:VAL:CA	4:5:323:ILE:HG13	2.34	0.58
6:7:68:GLN:HG2	6:7:72:ASN:HD21	1.69	0.58
8:B:120:LEU:HB2	8:B:176:LEU:HD13	1.85	0.58
10:D:138:PHE:HA	10:D:141:ARG:HH11	1.68	0.58
1:2:534:ARG:HH11	1:2:815:ARG:HH22	1.52	0.58
7:A:136:ASP:O	7:A:139:THR:OG1	2.20	0.58
10:D:62:ASP:HA	10:D:65:LYS:HB3	1.86	0.58
4:5:76:TYR:HA	4:5:79:LEU:HB3	1.85	0.58
4:5:673:GLN:HB2	4:5:676:HIS:HB2	1.85	0.58
5:6:533:ILE:CG1	5:6:548:LEU:HD11	2.32	0.58
5:6:545:LYS:O	5:6:549:LEU:HG	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:558:SER:HB3	5:6:559:THR:CA	2.31	0.58
6:7:259:ALA:HB3	6:7:304:ALA:HB1	1.86	0.58
6:7:664:TYR:CD1	6:7:689:LEU:HD13	2.38	0.58
9:C:3:TYR:HE1	10:D:218:MET:HG3	1.69	0.58
10:D:60:PHE:HA	10:D:63:LEU:HB3	1.84	0.58
11:E:24:SER:HB3	11:E:55:GLN:OE1	2.03	0.58
1:2:524:PRO:HB2	1:2:525:LYS:HA	1.85	0.58
13:3:1001:ANP:O5'	4:5:651:ARG:NH1	2.36	0.58
3:4:777:MET:SD	3:4:830:ARG:NE	2.77	0.58
5:6:326:LYS:N	5:6:327:TYR:HA	2.12	0.58
10:D:144:ILE:HG13	10:D:145:ARG:N	2.19	0.58
10:D:211:ASP:HB2	10:D:219:ILE:HD11	1.86	0.58
2:3:371:ILE:HA	13:3:1001:ANP:N6	2.18	0.57
3:4:568:GLY:HA3	3:4:708:VAL:HB	1.86	0.57
4:5:571:HIS:O	4:5:575:ILE:HG13	2.04	0.57
3:4:554:LYS:NZ	5:6:752:ARG:HH22	2.02	0.57
5:6:550:GLN:HG2	5:6:569:ILE:HG23	1.86	0.57
6:7:534:ARG:HH21	6:7:586:LEU:HD23	1.67	0.57
9:C:132:ALA:HA	9:C:135:LEU:HB2	1.86	0.57
11:E:30:PHE:HD1	11:E:61:ILE:HD11	1.69	0.57
11:E:30:PHE:HE2	11:E:81:LEU:HD21	1.69	0.57
11:E:642:GLU:O	11:E:645:THR:OG1	2.22	0.57
1:2:300:PHE:O	1:2:302:THR:OG1	2.15	0.57
1:2:546:GLY:CA	5:6:796:THR:HG23	2.34	0.57
1:2:656:ARG:NH1	5:6:792:SER:HB2	2.19	0.57
2:3:378:LYS:HA	2:3:381:ILE:HD12	1.85	0.57
3:4:402:THR:O	3:4:405:PHE:N	2.34	0.57
4:5:654:GLU:O	4:5:657:ILE:HB	2.05	0.57
5:6:168:MET:O	5:6:171:SER:HB2	2.03	0.57
7:A:106:GLY:H	7:A:107:LEU:HD22	1.69	0.57
10:D:257:THR:H	10:D:269:LEU:HB2	1.68	0.57
11:E:5:ILE:N	11:E:142:CYS:SG	2.74	0.57
2:3:291:ARG:HB2	2:3:329:LEU:HG	1.85	0.57
3:4:447:ASN:O	3:4:450:GLN:HB2	2.04	0.57
5:6:966:LYS:HA	5:6:969:VAL:HG12	1.85	0.57
1:2:573:ALA:HB3	5:6:670:ALA:H	1.67	0.57
3:4:367:GLU:OE1	3:4:367:GLU:N	2.36	0.57
4:5:148:LEU:HD23	4:5:260:GLU:HB3	1.85	0.57
4:5:375:ALA:HB1	4:5:378:ILE:H	1.70	0.57
4:5:407:ARG:CZ	4:5:658:ARG:HH12	2.18	0.57
4:5:486:ARG:NH2	4:5:489:ASP:OD2	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:124:VAL:HG11	5:6:132:VAL:HG23	1.86	0.57
6:7:612:LEU:O	6:7:616:VAL:HG23	2.04	0.57
9:C:50:LEU:O	9:C:54:LEU:HG	2.05	0.57
11:E:29:ILE:HG22	11:E:82:LEU:HD13	1.85	0.57
11:E:81:LEU:N	11:E:119:ASP:O	2.38	0.57
1:2:302:THR:O	1:2:303:ILE:HG22	2.04	0.57
5:6:765:LEU:HD22	5:6:770:ARG:HB3	1.87	0.57
6:7:374:THR:OG1	6:7:375:TYR:N	2.36	0.57
8:B:92:TRP:CD2	8:B:116:PRO:HG2	2.40	0.57
1:2:763:LEU:O	1:2:766:TYR:HB3	2.04	0.57
2:3:40:ASP:OD1	2:3:41:SER:N	2.33	0.57
3:4:900:SER:HA	3:4:903:ILE:HD12	1.87	0.57
4:5:22:ASP:O	4:5:26:GLU:HG2	2.05	0.57
4:5:66:GLU:OE1	4:5:141:SER:OG	2.21	0.57
5:6:365:ALA:HA	5:6:368:ILE:HG12	1.85	0.57
6:7:689:LEU:O	6:7:692:ILE:HG22	2.04	0.57
7:A:170:ASP:HB3	7:A:204:TYR:CD1	2.40	0.57
9:C:86:ASN:HA	9:C:89:LYS:HD3	1.85	0.57
10:D:57:GLN:N	10:D:57:GLN:OE1	2.38	0.57
10:D:132:GLU:HA	10:D:135:ARG:NH2	2.18	0.57
10:D:132:GLU:HA	10:D:135:ARG:HH22	1.70	0.57
11:E:556:CYS:O	11:E:560:GLU:HG2	2.03	0.57
3:4:418:CYS:SG	3:4:419:VAL:N	2.78	0.57
3:4:726:ASN:C	3:4:728:TYR:HB3	2.29	0.57
6:7:411:TYR:HD1	6:7:702:LEU:CD1	2.18	0.57
11:E:249:ASN:HB2	11:E:254:GLN:HE22	1.70	0.57
11:E:287:VAL:HG13	11:E:290:ARG:HH11	1.69	0.57
1:2:686:LEU:HG	5:6:788:PHE:CE1	2.40	0.57
3:4:388:ARG:HH22	5:6:176:ARG:HD2	1.69	0.57
3:4:623:LEU:CD2	5:6:370:THR:CG2	2.66	0.57
3:4:688:VAL:HG11	3:4:836:TYR:HD1	1.69	0.57
3:4:748:THR:HA	3:4:751:ILE:HD12	1.86	0.57
5:6:696:ARG:HD2	5:6:706:MET:SD	2.43	0.57
6:7:302:THR:O	6:7:305:SER:OG	2.22	0.57
6:7:479:ARG:HG3	6:7:516:ALA:HB1	1.86	0.57
1:2:238:ASN:HD21	11:E:370:LEU:HB2	1.70	0.57
1:2:422:GLU:OE1	1:2:458:ARG:NE	2.37	0.57
1:2:591:LEU:HB3	4:5:270:MET:HE1	1.87	0.57
2:3:326:VAL:O	2:3:326:VAL:HG12	2.02	0.57
5:6:268:PHE:HB3	5:6:458:HIS:CE1	2.40	0.57
5:6:636:CYS:HB3	5:6:678:ILE:HD13	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:720:VAL:O	6:7:723:SER:OG	2.23	0.57
11:E:64:TYR:HB2	11:E:625:PHE:HA	1.87	0.57
11:E:149:ASP:N	11:E:150:ASP:HA	2.19	0.57
1:2:569:GLN:HB2	1:2:612:MET:HG2	1.87	0.56
1:2:578:ALA:O	1:2:631:ILE:HG21	2.04	0.56
2:3:491:GLU:HB2	2:3:542:ARG:NE	2.20	0.56
2:3:716:ARG:HH12	2:3:722:ASN:HB3	1.70	0.56
3:4:349:CYS:SG	3:4:382:MET:HA	2.45	0.56
3:4:365:ILE:O	5:6:420:THR:OG1	2.22	0.56
3:4:395:GLN:HB2	3:4:424:VAL:HG13	1.87	0.56
4:5:323:ILE:O	4:5:323:ILE:HG22	2.04	0.56
4:5:439:THR:HA	4:5:444:SER:CB	2.34	0.56
5:6:418:SER:HA	5:6:448:LEU:HG	1.87	0.56
5:6:908:LYS:HB3	5:6:960:LEU:HD21	1.86	0.56
6:7:481:VAL:HG22	6:7:516:ALA:HB3	1.85	0.56
10:D:92:SER:HA	10:D:95:SER:HB3	1.87	0.56
11:E:244:GLY:HA3	11:E:602:LEU:HB3	1.87	0.56
1:2:568:GLY:HA2	1:2:606:ILE:HG23	1.86	0.56
3:4:557:ARG:NH2	3:4:652:GLN:HB3	2.18	0.56
3:4:798:LEU:HG	5:6:735:HIS:CE1	2.40	0.56
5:6:801:GLU:OE2	5:6:805:ARG:NE	2.36	0.56
5:6:919:LYS:NZ	5:6:929:GLU:OE2	2.33	0.56
1:2:233:THR:O	1:2:237:MET:N	2.31	0.56
1:2:295:VAL:O	1:2:454:ASN:ND2	2.39	0.56
1:2:334:LEU:HA	1:2:382:TYR:HD1	1.68	0.56
1:2:637:VAL:HA	4:5:447:ALA:HB2	1.86	0.56
1:2:805:ILE:HA	1:2:809:HIS:ND1	2.21	0.56
1:2:837:ALA:O	1:2:841:VAL:HG23	2.04	0.56
2:3:669:PRO:O	2:3:720:THR:HA	2.05	0.56
4:5:47:ARG:HD3	8:B:146:GLN:HG2	1.85	0.56
4:5:559:ASP:HB2	4:5:561:ASN:ND2	2.20	0.56
4:5:571:HIS:ND1	4:5:575:ILE:HD11	2.21	0.56
5:6:261:ARG:HD2	5:6:263:PHE:HE1	1.70	0.56
5:6:403:VAL:CG1	5:6:450:TYR:HB3	2.35	0.56
5:6:517:LYS:HA	5:6:520:VAL:HG22	1.86	0.56
6:7:646:LYS:HA	6:7:701:LYS:HE3	1.86	0.56
7:A:27:VAL:HG13	7:A:28:ASN:H	1.70	0.56
11:E:12:TYR:HE1	11:E:48:LEU:HD21	1.68	0.56
11:E:425:VAL:HA	11:E:428:LEU:HD12	1.87	0.56
1:2:240:GLU:HB3	1:2:290:HIS:ND1	2.20	0.56
3:4:929:LEU:HB2	5:6:947:ASP:HB3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:364:ASN:HB3	5:6:394:ARG:HD3	1.86	0.56
11:E:536:LEU:HB3	11:E:573:ASP:HB2	1.88	0.56
11:E:559:SER:HA	11:E:560:GLU:HB3	1.87	0.56
1:2:856:GLN:HE22	1:2:859:ARG:NH2	2.01	0.56
2:3:156:SER:CB	2:3:325:THR:HG22	2.35	0.56
3:4:774:TYR:HB2	3:4:801:MET:HE1	1.88	0.56
4:5:156:VAL:HG22	4:5:298:TYR:HD2	1.71	0.56
4:5:371:THR:O	4:5:385:LYS:HE2	2.06	0.56
5:6:944:LYS:O	5:6:948:LEU:HD13	2.06	0.56
7:A:96:ILE:O	7:A:99:SER:OG	2.22	0.56
10:D:269:LEU:HA	10:D:275:TYR:CE2	2.41	0.56
10:D:286:LEU:HD11	10:D:293:LEU:HD11	1.86	0.56
11:E:12:TYR:O	11:E:15:ILE:HG22	2.05	0.56
11:E:81:LEU:O	11:E:121:TYR:N	2.36	0.56
2:3:197:ILE:HD11	2:3:251:ILE:HB	1.87	0.56
4:5:264:LEU:HB2	4:5:265:VAL:HG22	1.88	0.56
5:6:638:ILE:HG21	5:6:644:MET:HE2	1.87	0.56
6:7:215:TYR:HE1	6:7:217:LYS:HD3	1.71	0.56
9:C:165:PHE:O	9:C:168:LYS:HG2	2.06	0.56
3:4:578:LEU:HD21	3:4:672:LEU:HD22	1.87	0.56
4:5:417:ASP:O	4:5:420:THR:OG1	2.21	0.56
5:6:706:MET:HE2	5:6:793:TYR:CZ	2.41	0.56
6:7:147:ARG:HA	6:7:150:ASN:HB3	1.88	0.56
6:7:545:THR:HG23	6:7:556:THR:HB	1.88	0.56
11:E:86:PHE:CE1	11:E:625:PHE:HB2	2.40	0.56
11:E:161:LYS:HB3	11:E:233:TYR:CE2	2.40	0.56
1:2:573:ALA:HB3	5:6:670:ALA:N	2.21	0.56
2:3:294:VAL:HG22	2:3:326:VAL:HG22	1.87	0.56
2:3:296:GLY:HA2	2:3:324:ASN:HB2	1.88	0.56
2:3:712:HIS:ND1	2:3:725:ASP:OD1	2.39	0.56
3:4:509:ILE:HD11	3:4:749:MET:HE2	1.88	0.56
3:4:590:TYR:HA	3:4:630:CYS:O	2.06	0.56
4:5:343:TRP:C	4:5:345:SER:HA	2.31	0.56
6:7:436:LEU:HD23	6:7:477:SER:HB2	1.87	0.56
9:C:112:ILE:HG23	9:C:113:MET:HE2	1.88	0.56
11:E:474:VAL:O	11:E:477:PHE:HB3	2.06	0.56
11:E:566:PRO:HB2	11:E:605:PHE:CE2	2.41	0.56
2:3:216:ASP:OD1	2:3:217:ALA:N	2.39	0.56
2:3:389:VAL:HG22	2:3:714:LYS:HE3	1.88	0.56
3:4:613:GLN:HB3	5:6:360:ARG:HH12	1.71	0.56
4:5:256:LEU:H	4:5:256:LEU:HD12	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:829:ASP:HA	5:6:832:ARG:HB3	1.88	0.56
6:7:456:VAL:O	6:7:564:LEU:HG	2.05	0.56
10:D:74:PRO:HG3	10:D:279:TYR:CD2	2.41	0.56
10:D:260:ILE:CG2	10:D:261:PRO:HD2	2.36	0.56
11:E:231:HIS:HA	11:E:234:GLU:HB2	1.88	0.56
11:E:254:GLN:OE1	11:E:254:GLN:N	2.39	0.56
11:E:315:THR:H	11:E:316:LEU:HB3	1.67	0.56
11:E:546:LEU:O	11:E:550:ASN:HB2	2.05	0.56
1:2:285:ASP:O	1:2:286:TYR:HB2	2.06	0.56
1:2:296:ARG:HH21	1:2:413:ASP:HB2	1.71	0.56
2:3:474:GLU:HG3	4:5:491:VAL:CG1	2.35	0.56
3:4:758:ILE:HG22	3:4:760:PRO:HD3	1.88	0.56
4:5:40:LEU:O	11:E:416:ARG:NH2	2.39	0.56
4:5:375:ALA:HB1	4:5:378:ILE:HB	1.88	0.56
7:A:50:ASN:O	7:A:54:LEU:HG	2.05	0.56
8:B:11:PHE:HE1	10:D:71:ARG:HB2	1.69	0.56
8:B:137:PRO:HA	8:B:141:LEU:HD13	1.88	0.56
8:B:193:ARG:CZ	10:D:225:ASN:HB3	2.36	0.56
9:C:135:LEU:HD13	9:C:176:ILE:HD11	1.88	0.56
2:3:176:LEU:HD12	2:3:298:PHE:HE2	1.71	0.55
2:3:200:VAL:HG23	2:3:248:SER:HB3	1.88	0.55
2:3:438:SER:OG	12:F:9:DT:OP2	2.09	0.55
3:4:506:LEU:HD23	3:4:509:ILE:HD12	1.89	0.55
6:7:367:LYS:HA	6:7:368:ALA:HB3	1.86	0.55
8:B:140:GLU:O	8:B:144:LYS:HG2	2.05	0.55
11:E:543:LEU:HA	11:E:546:LEU:HB3	1.87	0.55
1:2:435:ASP:N	1:2:436:GLY:HA3	2.21	0.55
1:2:690:GLU:HA	1:2:693:GLU:CD	2.31	0.55
2:3:491:GLU:HB2	2:3:542:ARG:CZ	2.37	0.55
3:4:304:ARG:NH2	3:4:422:GLU:OE1	2.39	0.55
4:5:321:VAL:HA	4:5:323:ILE:HG13	1.88	0.55
7:A:104:ASN:O	7:A:104:ASN:ND2	2.35	0.55
11:E:308:ASN:HA	11:E:309:SER:HB2	1.87	0.55
2:3:108:ARG:HA	2:3:111:TRP:HB3	1.89	0.55
2:3:227:THR:N	2:3:228:PRO:HD2	2.21	0.55
2:3:379:LYS:O	2:3:383:LEU:HG	2.07	0.55
3:4:321:ASP:OD1	3:4:321:ASP:N	2.35	0.55
4:5:407:ARG:HD2	4:5:497:MET:O	2.06	0.55
7:A:2:TYR:OH	7:A:75:THR:HA	2.04	0.55
10:D:216:VAL:CG1	10:D:217:ASN:HA	2.37	0.55
11:E:151:THR:HB	11:E:153:GLY:N	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:567:THR:HG23	1:2:568:GLY:H	1.72	0.55
2:3:46:GLN:HA	2:3:49:ASN:HD21	1.70	0.55
2:3:163:ALA:N	2:3:164:HIS:HB2	2.21	0.55
2:3:195:LYS:NZ	2:3:218:THR:OG1	2.39	0.55
3:4:204:LYS:HA	3:4:205:PHE:C	2.31	0.55
3:4:574:LYS:HD3	3:4:674:SER:HB2	1.87	0.55
4:5:287:ILE:HD11	4:5:342:ILE:CG2	2.34	0.55
5:6:124:VAL:CG2	5:6:132:VAL:HA	2.36	0.55
5:6:134:LYS:HB3	5:6:137:ARG:H	1.70	0.55
5:6:155:TYR:CE1	5:6:167:ALA:HB1	2.42	0.55
2:3:462:MET:HE3	2:3:489:VAL:HG21	1.87	0.55
3:4:330:GLY:C	3:4:432:ARG:HA	2.32	0.55
3:4:385:ILE:HG22	3:4:388:ARG:H	1.71	0.55
4:5:25:THR:HA	4:5:28:ILE:HD12	1.87	0.55
4:5:28:ILE:HG23	4:5:93:ALA:HB2	1.87	0.55
4:5:555:ILE:HG22	4:5:557:LYS:HD3	1.88	0.55
6:7:24:PHE:HE1	6:7:85:ILE:HA	1.71	0.55
6:7:143:LEU:HA	6:7:146:ARG:HB2	1.89	0.55
6:7:461:ASP:OD2	6:7:573:ARG:HA	2.07	0.55
7:A:42:LYS:O	7:A:46:ASN:HB2	2.07	0.55
10:D:69:ASN:HA	10:D:293:LEU:HD22	1.89	0.55
1:2:432:ASN:HB2	1:2:447:PHE:HB3	1.89	0.55
1:2:581:ARG:NH2	5:6:621:TYR:HB3	2.22	0.55
4:5:428:PHE:O	4:5:432:VAL:HG23	2.07	0.55
5:6:290:ILE:HD13	5:6:454:PHE:CZ	2.42	0.55
6:7:470:LEU:HD13	6:7:522:CYS:HB3	1.88	0.55
8:B:124:ARG:HD3	9:C:190:TRP:CH2	2.41	0.55
10:D:200:LYS:N	10:D:201:TYR:HB2	2.22	0.55
11:E:574:GLU:O	11:E:575:ASN:CB	2.54	0.55
2:3:483:ARG:HD3	2:3:539:LEU:HD11	1.87	0.55
3:4:332:VAL:HG13	3:4:397:ILE:HG21	1.89	0.55
3:4:919:LEU:HD13	3:4:925:ARG:HD2	1.89	0.55
5:6:105:ASP:O	5:6:108:GLY:N	2.40	0.55
5:6:288:LEU:H	5:6:399:GLY:N	2.05	0.55
5:6:551:MET:HA	5:6:635:ILE:HD11	1.89	0.55
5:6:768:GLU:OE1	5:6:768:GLU:N	2.35	0.55
5:6:777:TYR:CZ	5:6:781:ARG:HD2	2.42	0.55
10:D:84:MET:O	10:D:87:LEU:HB2	2.07	0.55
1:2:207:ILE:HG22	1:2:211:LEU:HD23	1.88	0.55
1:2:256:LEU:HD23	1:2:259:PHE:HD2	1.72	0.55
1:2:567:THR:O	1:2:606:ILE:HG23	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:176:LEU:HD22	4:5:250:PHE:HD2	1.72	0.55
3:4:245:ALA:HB3	3:4:306:TYR:O	2.05	0.55
4:5:412:VAL:C	4:5:413:LEU:HD12	2.32	0.55
6:7:134:TYR:HB2	6:7:141:VAL:HG12	1.89	0.55
7:A:170:ASP:HB3	7:A:204:TYR:HD1	1.70	0.55
11:E:360:HIS:HA	11:E:363:PHE:CD2	2.40	0.55
1:2:276:MET:O	1:2:280:GLU:N	2.40	0.55
1:2:571:ALA:O	5:6:663:ILE:HA	2.07	0.55
1:2:702:SER:O	5:6:559:THR:HG21	2.06	0.55
2:3:372:TYR:CZ	2:3:564:HIS:HB3	2.41	0.55
3:4:417:LEU:HB2	3:4:463:VAL:HG11	1.88	0.55
3:4:449:ARG:C	3:4:451:ARG:H	2.15	0.55
3:4:550:LYS:HE2	3:4:558:TYR:HD2	1.71	0.55
5:6:274:HIS:CG	5:6:288:LEU:HD11	2.42	0.55
5:6:610:ALA:H	5:6:663:ILE:HD13	1.72	0.55
6:7:482:TYR:HA	6:7:522:CYS:HB2	1.89	0.55
6:7:499:LYS:NZ	6:7:500:ASP:O	2.36	0.55
8:B:120:LEU:HD11	8:B:177:GLU:HG3	1.89	0.55
11:E:22:HIS:HA	11:E:23:SER:C	2.30	0.55
11:E:433:GLU:OE1	11:E:433:GLU:N	2.34	0.55
1:2:766:TYR:OH	1:2:823:MET:O	2.25	0.55
3:4:453:LEU:H	6:7:280:PRO:HD3	1.71	0.55
3:4:547:GLY:O	3:4:810:LYS:NZ	2.40	0.55
3:4:596:SER:O	3:4:641:THR:OG1	2.25	0.55
3:4:638:SER:OG	3:4:641:THR:OG1	2.15	0.55
3:4:646:HIS:HA	3:4:701:ARG:NH2	2.21	0.55
5:6:923:VAL:HA	5:6:926:GLU:HG2	1.88	0.55
6:7:68:GLN:HG2	6:7:72:ASN:ND2	2.21	0.55
6:7:422:ILE:HD13	6:7:469:LEU:HD11	1.88	0.55
6:7:533:ASP:N	6:7:533:ASP:OD1	2.39	0.55
7:A:90:GLN:HA	7:A:93:ARG:HB3	1.88	0.55
10:D:83:LEU:O	10:D:83:LEU:HD23	2.07	0.55
1:2:553:LEU:HD12	1:2:554:LYS:N	2.22	0.54
2:3:254:GLN:NE2	2:3:256:ILE:HD11	2.21	0.54
2:3:517:ASN:ND2	13:3:1001:ANP:O1G	2.31	0.54
6:7:318:LEU:HG	6:7:320:GLN:HG2	1.88	0.54
6:7:724:LYS:C	6:7:726:SER:H	2.15	0.54
10:D:137:LYS:HG2	10:D:141:ARG:NH1	2.21	0.54
11:E:81:LEU:HD22	11:E:82:LEU:H	1.73	0.54
2:3:25:VAL:HG23	2:3:124:PRO:HB2	1.89	0.54
2:3:201:HIS:HB3	2:3:241:LEU:HB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:667:VAL:HG11	2:3:719:LYS:NZ	2.21	0.54
5:6:803:MET:HA	5:6:806:LEU:HD12	1.87	0.54
5:6:839:ASP:O	5:6:840:VAL:C	2.51	0.54
1:2:631:ILE:HG13	4:5:445:SER:O	2.07	0.54
2:3:667:VAL:HG11	2:3:719:LYS:HZ1	1.73	0.54
13:3:1001:ANP:O2B	13:3:1001:ANP:O2A	2.25	0.54
3:4:183:THR:OG1	6:7:303:ARG:NH2	2.41	0.54
3:4:330:GLY:HA2	3:4:403:PRO:HD2	1.89	0.54
4:5:64:ASN:ND2	4:5:66:GLU:HB2	2.21	0.54
4:5:390:CYS:O	4:5:662:SER:HB2	2.07	0.54
6:7:475:LYS:C	6:7:476:ILE:HD12	2.32	0.54
7:A:13:ALA:HA	7:A:16:THR:HG22	1.89	0.54
1:2:519:LEU:HD13	1:2:556:VAL:HG13	1.88	0.54
3:4:889:GLN:O	3:4:897:ARG:NH1	2.41	0.54
4:5:685:GLN:O	4:5:688:THR:OG1	2.25	0.54
5:6:796:THR:O	5:6:799:GLN:HG2	2.07	0.54
6:7:245:ILE:HG12	6:7:347:ASP:O	2.07	0.54
6:7:260:TYR:CD1	6:7:298:LEU:HD13	2.43	0.54
7:A:33:HIS:HB3	7:A:36:ILE:HG22	1.88	0.54
7:A:109:LEU:HD23	7:A:109:LEU:O	2.07	0.54
7:A:162:PHE:HD1	7:A:192:ARG:HA	1.73	0.54
11:E:355:GLY:HA2	11:E:358:ARG:HB3	1.88	0.54
1:2:324:VAL:HG23	1:2:422:GLU:O	2.07	0.54
1:2:696:ALA:HA	1:2:699:VAL:HB	1.89	0.54
2:3:559:ARG:O	2:3:562:SER:OG	2.20	0.54
3:4:181:TRP:CG	3:4:182:GLY:H	2.25	0.54
3:4:773:ALA:O	3:4:777:MET:HG2	2.07	0.54
5:6:637:CYS:HA	5:6:679:LEU:O	2.06	0.54
6:7:595:ASP:HB3	6:7:694:ARG:NH1	2.23	0.54
8:B:121:VAL:HG22	8:B:176:LEU:HD12	1.89	0.54
9:C:97:LEU:O	9:C:100:ILE:HG12	2.07	0.54
10:D:212:THR:N	10:D:213:GLU:HA	2.21	0.54
1:2:639:THR:HA	4:5:445:SER:HB3	1.89	0.54
4:5:382:GLU:OE1	4:5:382:GLU:N	2.38	0.54
13:5:801:ANP:O2B	13:5:801:ANP:O3G	2.26	0.54
5:6:152:TYR:HB3	5:6:268:PHE:HE2	1.71	0.54
5:6:574:VAL:HG12	5:6:684:PRO:HG3	1.89	0.54
5:6:796:THR:HG22	5:6:798:ARG:HB3	1.89	0.54
6:7:147:ARG:NH2	6:7:192:PHE:HB2	2.23	0.54
12:F:7:DT:C6	12:F:7:DT:H5'	2.43	0.54
2:3:371:ILE:HA	13:3:1001:ANP:HN61	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:433:THR:O	2:3:433:THR:OG1	2.26	0.54
6:7:103:VAL:HG11	6:7:207:LEU:HD21	1.89	0.54
7:A:29:LEU:HD23	7:A:93:ARG:HD3	1.88	0.54
10:D:144:ILE:O	10:D:148:LEU:HG	2.08	0.54
11:E:83:LEU:HB3	11:E:122:VAL:HG22	1.90	0.54
11:E:327:PHE:CE2	11:E:503:GLN:HG3	2.43	0.54
1:2:289:ILE:HG22	1:2:290:HIS:CE1	2.43	0.54
1:2:419:LYS:NZ	1:2:598:LEU:HD12	2.23	0.54
4:5:488:GLU:HG2	4:5:489:ASP:N	2.23	0.54
4:5:554:PHE:HZ	4:5:683:LEU:O	1.90	0.54
5:6:283:LYS:HD2	5:6:288:LEU:HD22	1.90	0.54
5:6:796:THR:CG2	5:6:798:ARG:HB3	2.38	0.54
6:7:203:TYR:OH	6:7:339:LEU:N	2.33	0.54
7:A:102:TRP:HB3	10:D:145:ARG:NH2	2.22	0.54
10:D:132:GLU:HG2	10:D:135:ARG:NH1	2.18	0.54
10:D:176:SER:HB3	10:D:179:GLU:HG3	1.89	0.54
10:D:257:THR:O	10:D:268:GLU:HB3	2.08	0.54
10:D:264:LYS:HG2	10:D:265:GLU:H	1.72	0.54
11:E:5:ILE:HG12	11:E:142:CYS:SG	2.48	0.54
1:2:333:GLN:HB2	1:2:385:TYR:HB2	1.90	0.54
3:4:432:ARG:HH12	6:7:555:THR:HB	1.73	0.54
3:4:521:LEU:O	3:4:524:ARG:HG2	2.08	0.54
4:5:479:ILE:CG2	4:5:482:PHE:HB2	2.38	0.54
5:6:648:ASP:OD1	5:6:648:ASP:N	2.29	0.54
5:6:727:LEU:O	5:6:731:ILE:HB	2.08	0.54
5:6:833:GLN:O	5:6:837:ARG:N	2.41	0.54
5:6:834:SER:HA	5:6:837:ARG:HB2	1.90	0.54
6:7:460:GLY:HA3	6:7:600:MET:O	2.08	0.54
10:D:171:LEU:HB2	10:D:173:ASP:H	1.71	0.54
11:E:499:ALA:HA	11:E:502:LEU:HD12	1.90	0.54
1:2:229:ALA:O	1:2:233:THR:OG1	2.14	0.54
1:2:493:ILE:HG13	1:2:494:ILE:N	2.23	0.54
1:2:790:TYR:HH	1:2:794:ARG:HH21	1.49	0.54
1:2:842:VAL:C	1:2:846:VAL:HG23	2.32	0.54
3:4:333:LEU:HD21	3:4:400:GLN:HG2	1.89	0.54
4:5:414:LEU:HD11	4:5:425:LEU:HD22	1.90	0.54
4:5:482:PHE:HB3	4:5:523:ALA:CB	2.32	0.54
5:6:538:PHE:HB2	5:6:730:HIS:ND1	2.22	0.54
5:6:773:LEU:HD21	5:6:800:LEU:HD11	1.91	0.54
6:7:668:ARG:HH22	6:7:686:PRO:HD3	1.73	0.54
8:B:54:THR:HG22	10:D:132:GLU:HG3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:103:GLN:O	8:B:107:THR:HG22	2.07	0.54
11:E:613:THR:HG22	11:E:620:VAL:HG11	1.90	0.54
1:2:328:THR:HG23	1:2:329:GLY:O	2.08	0.53
1:2:631:ILE:N	4:5:445:SER:O	2.41	0.53
2:3:260:GLU:CD	2:3:272:ARG:H	2.16	0.53
3:4:225:TYR:N	3:4:228:LYS:HB2	2.23	0.53
3:4:393:ASP:OD1	5:6:281:SER:N	2.40	0.53
4:5:59:TYR:HD1	4:5:135:PHE:HE1	1.57	0.53
5:6:147:ASP:OD2	5:6:261:ARG:NH2	2.41	0.53
5:6:941:LEU:HA	5:6:944:LYS:HD3	1.90	0.53
6:7:498:MET:HG3	6:7:498:MET:O	2.08	0.53
7:A:47:LEU:HD21	7:A:75:THR:HB	1.90	0.53
7:A:189:PHE:CE1	11:E:57:GLN:HB2	2.43	0.53
11:E:362:MET:HE3	11:E:399:TYR:HE2	1.72	0.53
11:E:558:GLU:HB2	11:E:559:SER:C	2.33	0.53
1:2:778:LEU:CG	4:5:577:THR:CG2	2.78	0.53
2:3:292:VAL:HG12	2:3:294:VAL:HG23	1.90	0.53
4:5:55:LEU:HD22	9:C:137:HIS:CG	2.43	0.53
4:5:349:PHE:CZ	4:5:354:GLU:HG3	2.43	0.53
5:6:276:ILE:HD13	5:6:375:ARG:O	2.08	0.53
7:A:89:TYR:OH	7:A:93:ARG:NH2	2.42	0.53
9:C:15:GLU:HB3	9:C:45:SER:HB2	1.90	0.53
10:D:257:THR:H	10:D:269:LEU:CB	2.20	0.53
1:2:549:LYS:NZ	13:2:901:ANP:O3G	2.35	0.53
2:3:199:SER:HB2	2:3:214:TYR:CE2	2.44	0.53
2:3:225:ILE:HD12	2:3:225:ILE:H	1.73	0.53
5:6:402:ILE:HG13	5:6:453:SER:OG	2.09	0.53
5:6:551:MET:O	5:6:759:ARG:NH1	2.41	0.53
5:6:810:ILE:O	5:6:814:ASN:ND2	2.40	0.53
6:7:677:SER:O	6:7:678:LYS:C	2.49	0.53
7:A:145:ASP:HA	7:A:146:LEU:CB	2.38	0.53
8:B:50:TRP:N	8:B:51:GLN:OE1	2.41	0.53
8:B:165:GLU:HG3	8:B:193:ARG:HA	1.88	0.53
9:C:26:GLY:H	9:C:36:ARG:HG3	1.74	0.53
9:C:165:PHE:CE2	9:C:169:LEU:HD11	2.43	0.53
11:E:126:HIS:CD2	11:E:247:VAL:HG22	2.44	0.53
2:3:527:ARG:HD3	2:3:531:GLN:HB2	1.91	0.53
3:4:179:ILE:HD11	3:4:184:ASN:HB2	1.89	0.53
4:5:439:THR:HA	4:5:444:SER:OG	2.09	0.53
5:6:168:MET:HA	5:6:171:SER:HB2	1.91	0.53
6:7:111:ASN:HB2	6:7:356:LEU:HD11	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:213:ARG:C	6:7:215:TYR:HB3	2.34	0.53
11:E:259:LEU:HG	11:E:264:GLU:HB2	1.90	0.53
11:E:607:MET:O	11:E:611:GLN:HG2	2.08	0.53
13:2:901:ANP:O3G	5:6:704:PRO:HB3	2.08	0.53
13:2:901:ANP:HNB1	5:6:653:HIS:HE1	1.56	0.53
2:3:403:ILE:HG22	2:3:405:ILE:HD11	1.91	0.53
2:3:412:SER:OG	4:5:649:THR:HB	2.08	0.53
3:4:202:LYS:CB	3:4:203:TYR:HB3	2.30	0.53
3:4:277:LYS:O	3:4:281:VAL:HG23	2.07	0.53
4:5:209:ARG:HA	4:5:241:TYR:CE2	2.42	0.53
4:5:496:ALA:HB1	4:5:515:SER:OG	2.08	0.53
4:5:568:ILE:O	4:5:572:VAL:HG23	2.09	0.53
5:6:794:ARG:N	5:6:795:ILE:HA	2.22	0.53
6:7:463:GLY:C	6:7:465:ALA:H	2.17	0.53
10:D:228:VAL:O	10:D:276:VAL:HG13	2.08	0.53
11:E:433:GLU:HB3	11:E:541:ASN:ND2	2.24	0.53
11:E:605:PHE:HA	11:E:608:ALA:HB3	1.89	0.53
1:2:533:ILE:CD1	4:5:576:HIS:CE1	2.92	0.53
4:5:392:LEU:HB3	4:5:603:ILE:HD13	1.91	0.53
5:6:552:LEU:HD23	5:6:812:ARG:HB2	1.90	0.53
5:6:729:SER:OG	5:6:730:HIS:N	2.42	0.53
11:E:76:ASP:H	11:E:78:ILE:HD13	1.72	0.53
11:E:97:GLU:HA	11:E:98:ILE:O	2.09	0.53
11:E:579:TYR:HE2	11:E:634:ARG:HB3	1.66	0.53
1:2:428:GLY:HA3	1:2:452:GLU:O	2.08	0.53
2:3:303:ALA:CB	2:3:307:ASN:HB2	2.39	0.53
2:3:682:ASN:O	2:3:686:LEU:HG	2.09	0.53
3:4:335:SER:HB3	3:4:395:GLN:HE22	1.74	0.53
4:5:411:ASN:HA	4:5:519:VAL:O	2.09	0.53
5:6:140:ILE:HA	5:6:143:MET:HB3	1.89	0.53
5:6:355:ASP:HB3	5:6:356:TRP:CA	2.38	0.53
6:7:135:LYS:HA	6:7:136:ASP:C	2.33	0.53
11:E:349:SER:HA	11:E:351:TRP:CZ3	2.44	0.53
1:2:839:LYS:HD3	1:2:864:TYR:HA	1.91	0.53
2:3:156:SER:CA	2:3:325:THR:HG22	2.39	0.53
2:3:223:THR:CG2	4:5:245:HIS:H	2.20	0.53
2:3:314:LEU:HD23	4:5:253:GLN:NE2	2.24	0.53
2:3:518:PRO:HG3	2:3:524:ASP:HB2	1.90	0.53
3:4:267:GLU:O	3:4:270:SER:OG	2.23	0.53
3:4:802:ILE:O	3:4:806:GLU:N	2.31	0.53
4:5:77:LYS:HZ3	11:E:383:SER:H	1.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:548:SER:HB2	4:5:649:THR:HG21	1.90	0.53
5:6:362:GLN:HG3	5:6:376:THR:HG21	1.91	0.53
5:6:529:LEU:O	5:6:533:ILE:HG13	2.09	0.53
6:7:88:TYR:O	6:7:92:LYS:HG2	2.09	0.53
7:A:129:GLU:HA	7:A:132:LYS:HE3	1.91	0.53
8:B:97:GLU:O	8:B:100:ARG:HG2	2.08	0.53
11:E:93:GLU:HG3	11:E:98:ILE:HG22	1.90	0.53
1:2:585:ILE:HG12	1:2:586:THR:HG23	1.91	0.53
2:3:176:LEU:HA	2:3:298:PHE:HD2	1.73	0.53
2:3:386:MET:HB3	2:3:714:LYS:HD2	1.90	0.53
4:5:170:SER:HB3	4:5:254:GLN:O	2.08	0.53
4:5:365:LYS:O	4:5:369:ILE:N	2.37	0.53
4:5:626:PHE:CD2	4:5:653:LEU:HD12	2.43	0.53
5:6:625:ALA:HB1	5:6:629:MET:HB2	1.90	0.53
5:6:640:GLU:HA	5:6:682:ALA:HA	1.91	0.53
5:6:784:ASP:OD2	5:6:795:ILE:HG12	2.08	0.53
6:7:660:VAL:HG12	6:7:689:LEU:HD11	1.91	0.53
7:A:44:VAL:O	7:A:79:MET:HE1	2.09	0.53
7:A:79:MET:HE3	10:D:203:PRO:HG2	1.89	0.53
8:B:51:GLN:H	8:B:53:ILE:HD12	1.74	0.53
11:E:34:LEU:HD21	11:E:543:LEU:HD11	1.90	0.53
1:2:519:LEU:HG	1:2:767:ILE:HD13	1.91	0.53
3:4:448:SER:CB	3:4:449:ARG:HB3	2.35	0.53
4:5:439:THR:O	4:5:479:ILE:HA	2.09	0.53
4:5:545:THR:O	4:5:548:SER:OG	2.19	0.53
5:6:654:GLU:HB2	5:6:661:ILE:HG12	1.91	0.53
7:A:81:ARG:HD3	9:C:49:TRP:CD2	2.44	0.53
8:B:16:ILE:O	8:B:20:VAL:HG12	2.08	0.53
11:E:11:ALA:HB1	11:E:121:TYR:HE1	1.72	0.53
11:E:257:SER:HA	11:E:260:SER:HB3	1.91	0.53
11:E:271:TRP:HA	11:E:274:ILE:HD12	1.91	0.53
1:2:484:PHE:HA	1:2:487:ILE:HD12	1.91	0.52
1:2:541:LEU:HA	1:2:681:CYS:HB2	1.91	0.52
1:2:578:ALA:O	1:2:631:ILE:HD13	2.09	0.52
2:3:306:MET:HB3	4:5:206:SER:HA	1.91	0.52
3:4:794:THR:HG22	3:4:797:GLN:HG2	1.90	0.52
4:5:209:ARG:HA	4:5:241:TYR:HE2	1.74	0.52
4:5:321:VAL:HG23	4:5:322:ALA:HA	1.91	0.52
6:7:116:LEU:O	6:7:119:ARG:HG2	2.09	0.52
6:7:257:VAL:HA	6:7:258:ILE:HB	1.90	0.52
8:B:195:ILE:HD11	9:C:125:SER:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:C:20:PHE:CD1	9:C:72:VAL:HG22	2.44	0.52
11:E:298:GLU:HA	11:E:301:ARG:HB2	1.91	0.52
1:2:553:LEU:CD2	1:2:607:ASP:HB3	2.39	0.52
3:4:679:GLY:HA3	3:4:681:ARG:O	2.08	0.52
3:4:823:GLN:OE1	3:4:823:GLN:N	2.39	0.52
4:5:448:GLY:HA2	4:5:486:ARG:NH1	2.11	0.52
6:7:333:ILE:HG12	6:7:376:LEU:HB3	1.91	0.52
11:E:98:ILE:N	11:E:99:ASP:HB3	2.24	0.52
11:E:494:ARG:O	11:E:498:LEU:HG	2.08	0.52
1:2:778:LEU:HD13	1:2:783:MET:HG2	1.91	0.52
2:3:475:PHE:HE1	2:3:486:ILE:HD13	1.74	0.52
3:4:411:THR:OG1	6:7:507:ILE:HD13	2.09	0.52
3:4:928:ARG:CB	5:6:946:ASN:HB2	2.38	0.52
5:6:126:SER:H	5:6:131:GLU:HG3	1.74	0.52
6:7:721:ARG:O	6:7:725:GLU:HG2	2.10	0.52
8:B:185:ILE:H	8:B:185:ILE:HD12	1.73	0.52
9:C:47:PRO:HD2	9:C:50:LEU:HD21	1.92	0.52
10:D:144:ILE:HG13	10:D:145:ARG:H	1.73	0.52
10:D:195:ASN:HA	10:D:199:LEU:HD12	1.91	0.52
1:2:216:LEU:HD12	1:2:217:GLU:HB3	1.91	0.52
2:3:201:HIS:HA	2:3:242:THR:O	2.08	0.52
3:4:315:ARG:N	3:4:401:GLU:OE1	2.43	0.52
4:5:441:GLY:HA3	4:5:442:LYS:C	2.35	0.52
4:5:482:PHE:CB	4:5:523:ALA:HB2	2.32	0.52
5:6:284:ILE:N	5:6:401:GLU:OE1	2.42	0.52
5:6:308:SER:CB	5:6:350:ARG:HB2	2.40	0.52
5:6:530:VAL:O	5:6:533:ILE:HD12	2.09	0.52
5:6:634:GLY:H	5:6:676:THR:HG22	1.74	0.52
11:E:316:LEU:HD21	11:E:413:LEU:C	2.34	0.52
1:2:271:PHE:CE2	1:2:295:VAL:HG11	2.45	0.52
1:2:335:LYS:HE3	1:2:383:ARG:HD2	1.92	0.52
1:2:538:ASN:HB3	1:2:677:PHE:HD1	1.74	0.52
2:3:490:MET:HE1	2:3:543:PHE:CD1	2.45	0.52
3:4:826:VAL:O	3:4:830:ARG:HG2	2.09	0.52
4:5:409:ASP:O	4:5:410:ILE:HG12	2.10	0.52
5:6:118:PHE:HB2	5:6:161:ARG:HD3	1.91	0.52
5:6:556:HIS:H	5:6:567:GLY:HA2	1.75	0.52
5:6:608:LEU:HD23	5:6:628:LEU:HD13	1.89	0.52
5:6:936:ILE:HA	5:6:939:TRP:HE1	1.74	0.52
6:7:249:SER:O	6:7:311:GLN:HG3	2.10	0.52
6:7:437:VAL:HG21	6:7:702:LEU:HD21	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:495:ALA:CB	6:7:557:LEU:HD21	2.40	0.52
6:7:680:SER:CB	6:7:681:PHE:HA	2.38	0.52
1:2:424:VAL:HG23	1:2:458:ARG:HA	1.91	0.52
1:2:516:ALA:HA	1:2:519:LEU:HB3	1.91	0.52
1:2:596:LEU:HD12	1:2:629:ILE:HD11	1.90	0.52
2:3:176:LEU:HD12	2:3:298:PHE:CE2	2.45	0.52
2:3:223:THR:HG21	4:5:244:ILE:HA	1.90	0.52
2:3:661:GLN:HA	2:3:664:LYS:HD3	1.90	0.52
3:4:332:VAL:CG1	3:4:429:ALA:HA	2.39	0.52
3:4:399:LEU:HB3	3:4:415:ILE:HB	1.91	0.52
3:4:578:LEU:HD13	3:4:630:CYS:HB3	1.92	0.52
3:4:828:LEU:O	3:4:831:SER:OG	2.25	0.52
3:4:925:ARG:HH21	3:4:928:ARG:HD3	1.74	0.52
6:7:609:ASP:HA	6:7:612:LEU:HB3	1.92	0.52
7:A:175:GLN:HB3	7:A:180:VAL:HA	1.91	0.52
8:B:120:LEU:HD13	8:B:176:LEU:HD22	1.91	0.52
9:C:186:ASP:OD1	9:C:189:ARG:NH2	2.42	0.52
10:D:169:ILE:HG22	10:D:170:SER:H	1.73	0.52
1:2:479:GLU:H	1:2:479:GLU:CD	2.17	0.52
1:2:641:GLN:NE2	4:5:263:GLU:HA	2.24	0.52
2:3:685:ASP:O	2:3:689:ASP:HB2	2.10	0.52
3:4:336:THR:O	3:4:395:GLN:NE2	2.36	0.52
3:4:347:PHE:CE1	3:4:384:LEU:HD12	2.43	0.52
4:5:629:ILE:HG22	4:5:648:ILE:HD11	1.91	0.52
5:6:118:PHE:O	5:6:123:SER:OG	2.26	0.52
5:6:540:HIS:CD2	5:6:715:ILE:HG21	2.44	0.52
5:6:560:VAL:HB	5:6:561:GLU:CA	2.40	0.52
6:7:235:LEU:HD22	6:7:357:PRO:HD3	1.91	0.52
6:7:404:LEU:HD11	6:7:414:LEU:HD21	1.92	0.52
8:B:115:LEU:HD11	8:B:152:ARG:CZ	2.39	0.52
11:E:405:ILE:H	11:E:405:ILE:HD12	1.75	0.52
1:2:306:LEU:HD22	1:2:392:GLU:HB2	1.90	0.52
1:2:780:GLN:NE2	4:5:573:ILE:HG22	2.24	0.52
2:3:278:LEU:HB3	2:3:282:LEU:HB2	1.92	0.52
3:4:387:ASN:HD21	5:6:402:ILE:HG22	1.75	0.52
4:5:572:VAL:HA	4:5:575:ILE:HD12	1.92	0.52
5:6:103:VAL:HB	5:6:104:ASP:HB2	1.91	0.52
7:A:2:TYR:CE2	7:A:78:CYS:HB2	2.44	0.52
9:C:3:TYR:CG	9:C:4:TYR:N	2.78	0.52
11:E:67:LEU:HD12	11:E:86:PHE:HD2	1.75	0.52
1:2:243:GLU:OE2	1:2:298:SER:HB3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:264:PRO:HA	1:2:267:MET:HE2	1.92	0.52
3:4:446:ALA:O	3:4:447:ASN:OD1	2.27	0.52
3:4:633:GLU:OE2	3:4:676:ASN:HB2	2.10	0.52
5:6:755:ILE:O	5:6:759:ARG:N	2.42	0.52
6:7:316:GLN:HG2	6:7:330:SER:HB3	1.92	0.52
10:D:168:LEU:HD21	10:D:173:ASP:OD2	2.09	0.52
11:E:327:PHE:CE2	11:E:328:LEU:HG	2.45	0.52
2:3:491:GLU:OE2	2:3:700:ARG:NH1	2.43	0.52
2:3:566:LEU:HD13	4:5:619:ALA:HB1	1.92	0.52
4:5:252:ASP:OD1	4:5:253:GLN:N	2.42	0.52
4:5:398:LYS:HZ1	4:5:613:ARG:HD2	1.72	0.52
4:5:560:HIS:ND1	4:5:560:HIS:N	2.56	0.52
4:5:662:SER:OG	4:5:663:LEU:N	2.44	0.52
8:B:18:PHE:CE1	10:D:135:ARG:HG2	2.45	0.52
8:B:119:TRP:HZ2	8:B:177:GLU:OE2	1.93	0.52
10:D:161:LEU:HD21	10:D:169:ILE:HA	1.92	0.52
1:2:433:ASN:HB2	1:2:434:TYR:HB3	1.91	0.51
4:5:632:GLN:O	4:5:636:ASN:HB2	2.09	0.51
5:6:143:MET:HE2	5:6:150:THR:O	2.10	0.51
5:6:519:MET:O	5:6:525:ILE:HG21	2.10	0.51
6:7:428:VAL:HA	6:7:598:PHE:CE2	2.45	0.51
11:E:38:ALA:O	11:E:42:THR:N	2.31	0.51
1:2:632:SER:HA	4:5:443:GLY:H	1.74	0.51
3:4:410:GLN:HE21	6:7:345:PRO:HG3	1.76	0.51
3:4:461:VAL:O	3:4:463:VAL:HG22	2.10	0.51
4:5:347:THR:OG1	4:5:348:MET:HA	2.10	0.51
6:7:248:VAL:HG11	6:7:345:PRO:HD3	1.92	0.51
8:B:112:PHE:HB3	8:B:152:ARG:NH1	2.25	0.51
8:B:197:THR:HG22	10:D:263:LEU:HD23	1.91	0.51
11:E:155:GLN:HA	11:E:158:ALA:HB3	1.93	0.51
11:E:157:GLU:O	11:E:161:LYS:HB2	2.10	0.51
11:E:561:ASP:HB3	11:E:562:LYS:HG2	1.92	0.51
2:3:20:VAL:O	2:3:24:ARG:HG2	2.11	0.51
6:7:362:GLY:HA2	6:7:363:PHE:CD2	2.46	0.51
6:7:516:ALA:O	6:7:561:THR:HG22	2.10	0.51
11:E:619:LYS:HD2	11:E:633:ARG:HG3	1.93	0.51
1:2:454:ASN:ND2	1:2:454:ASN:O	2.40	0.51
1:2:484:PHE:CZ	1:2:766:TYR:HA	2.44	0.51
1:2:660:THR:HG21	5:6:947:ASP:HB2	1.93	0.51
1:2:686:LEU:HG	5:6:788:PHE:CZ	2.45	0.51
1:2:794:ARG:HH11	4:5:560:HIS:HA	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:277:LYS:HA	3:4:301:TYR:HD2	1.76	0.51
5:6:570:ASN:ND2	5:6:678:ILE:H	2.02	0.51
9:C:16:PHE:HZ	9:C:107:LEU:HD21	1.75	0.51
1:2:474:PHE:HZ	1:2:561:HIS:HA	1.76	0.51
1:2:477:THR:HG22	1:2:478:GLU:H	1.74	0.51
1:2:550:SER:HB2	13:2:901:ANP:O1A	2.10	0.51
2:3:686:LEU:O	2:3:690:ASP:N	2.40	0.51
3:4:203:TYR:CG	3:4:204:LYS:N	2.77	0.51
3:4:329:LYS:HB2	3:4:402:THR:HG22	1.93	0.51
4:5:253:GLN:HE21	4:5:277:THR:HB	1.75	0.51
4:5:338:GLU:N	4:5:339:THR:HA	2.26	0.51
6:7:579:SER:O	6:7:582:ASP:HB2	2.10	0.51
6:7:659:TYR:CG	6:7:710:ILE:HD11	2.45	0.51
7:A:166:ARG:HG3	7:A:188:GLN:HB3	1.92	0.51
11:E:125:ALA:HB1	11:E:248:VAL:H	1.75	0.51
1:2:253:LYS:HE2	1:2:253:LYS:HA	1.92	0.51
1:2:544:ASP:OD2	1:2:547:THR:OG1	2.27	0.51
1:2:816:ILE:O	1:2:819:SER:OG	2.28	0.51
3:4:319:PRO:HB3	6:7:307:PHE:HB2	1.91	0.51
4:5:136:GLN:CB	4:5:280:ARG:HE	2.24	0.51
4:5:441:GLY:HA3	4:5:443:GLY:N	2.25	0.51
4:5:631:LYS:HE3	4:5:635:ILE:HD11	1.91	0.51
6:7:490:GLY:O	6:7:494:THR:N	2.41	0.51
8:B:61:ASN:OD1	8:B:62:ASN:N	2.44	0.51
9:C:20:PHE:HE1	9:C:46:LEU:HD11	1.75	0.51
1:2:496:LYS:HG2	1:2:758:ILE:HG13	1.93	0.51
1:2:497:ILE:HD13	1:2:823:MET:HE2	1.92	0.51
1:2:628:SER:HB2	1:2:640:LEU:O	2.10	0.51
1:2:796:GLU:HB2	1:2:859:ARG:HE	1.76	0.51
2:3:472:ILE:HD13	2:3:475:PHE:CD1	2.46	0.51
2:3:556:ILE:H	2:3:556:ILE:HD12	1.75	0.51
3:4:547:GLY:HA2	3:4:806:GLU:HG3	1.93	0.51
3:4:720:LEU:O	3:4:724:LEU:HG	2.10	0.51
4:5:407:ARG:HD3	4:5:498:GLU:HA	1.92	0.51
5:6:656:MET:HG3	5:6:709:PHE:CE1	2.46	0.51
6:7:619:VAL:HG12	6:7:620:HIS:ND1	2.26	0.51
7:A:58:GLN:HA	7:A:62:MET:HB2	1.92	0.51
11:E:30:PHE:CD1	11:E:61:ILE:HD11	2.45	0.51
1:2:260:LEU:HA	1:2:264:PRO:HB3	1.92	0.51
1:2:695:LEU:O	1:2:699:VAL:HG23	2.09	0.51
1:2:838:ILE:O	1:2:842:VAL:HG23	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:330:GLY:O	3:4:432:ARG:HA	2.10	0.51
4:5:239:ASP:N	4:5:239:ASP:OD1	2.43	0.51
4:5:377:SER:HB3	4:5:378:ILE:HD12	1.93	0.51
6:7:584:ILE:HG22	6:7:586:LEU:H	1.76	0.51
7:A:35:ASP:OD1	7:A:35:ASP:N	2.43	0.51
7:A:173:GLU:HB3	7:A:183:LEU:H	1.74	0.51
8:B:187:GLU:CD	9:C:176:ILE:HG22	2.36	0.51
1:2:566:ALA:O	1:2:572:SER:HB2	2.10	0.51
1:2:566:ALA:C	1:2:572:SER:HB2	2.35	0.51
1:2:579:SER:HA	1:2:633:LYS:HE3	1.93	0.51
1:2:778:LEU:CD1	4:5:577:THR:HG23	2.41	0.51
2:3:216:ASP:O	2:3:219:THR:HG22	2.11	0.51
2:3:483:ARG:HA	2:3:486:ILE:HD12	1.92	0.51
2:3:533:ILE:CG2	2:3:540:LEU:HD11	2.40	0.51
3:4:861:LEU:O	3:4:865:LEU:HG	2.10	0.51
3:4:919:LEU:HB2	3:4:925:ARG:HB2	1.93	0.51
5:6:920:ILE:HB	5:6:924:ASP:HB3	1.92	0.51
6:7:255:VAL:CG2	6:7:258:ILE:HG13	2.40	0.51
7:A:49:LYS:O	7:A:52:GLU:HG2	2.10	0.51
8:B:11:PHE:CE1	10:D:71:ARG:HB2	2.45	0.51
10:D:78:PRO:HA	10:D:174:LEU:HD12	1.93	0.51
3:4:692:ILE:HG21	3:4:699:LEU:HD13	1.91	0.51
4:5:184:ARG:HD2	4:5:240:PRO:HA	1.91	0.51
4:5:439:THR:HA	4:5:444:SER:HB2	1.92	0.51
5:6:179:PRO:O	5:6:183:LYS:HG2	2.11	0.51
5:6:303:GLU:HB2	5:6:354:LEU:HG	1.92	0.51
6:7:340:VAL:HG13	6:7:341:ARG:HG3	1.92	0.51
6:7:536:ALA:O	6:7:540:VAL:HG23	2.10	0.51
8:B:191:LYS:HG3	9:C:172:MET:HE1	1.93	0.51
10:D:260:ILE:CG2	10:D:264:LYS:O	2.56	0.51
11:E:339:TYR:O	11:E:350:LEU:HD13	2.11	0.51
11:E:600:PRO:O	11:E:601:ILE:HG13	2.11	0.51
2:3:104:ARG:NH2	9:C:86:ASN:HB2	2.25	0.50
2:3:198:ARG:O	2:3:248:SER:HB2	2.11	0.50
2:3:671:LEU:HD11	2:3:676:ILE:HD11	1.93	0.50
3:4:200:SER:HB3	3:4:202:LYS:HB2	1.92	0.50
3:4:579:GLN:O	3:4:583:LYS:NZ	2.29	0.50
3:4:682:TYR:CZ	3:4:707:LEU:HD21	2.46	0.50
4:5:104:LEU:HD22	4:5:105:SER:H	1.76	0.50
4:5:276:MET:HE2	4:5:328:ILE:HD12	1.92	0.50
6:7:256:GLU:O	6:7:306:LYS:HB3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:170:ASP:OD2	7:A:204:TYR:HA	2.10	0.50
11:E:514:LEU:HD11	11:E:555:CYS:SG	2.51	0.50
1:2:264:PRO:HG3	1:2:317:LEU:N	2.26	0.50
3:4:261:LEU:HB2	3:4:268:VAL:HG11	1.93	0.50
4:5:101:ILE:HG23	8:B:150:GLU:OE2	2.11	0.50
4:5:153:SER:OG	4:5:154:GLU:N	2.44	0.50
4:5:287:ILE:HG12	4:5:342:ILE:HD13	1.92	0.50
5:6:149:ASN:HB3	5:6:262:VAL:O	2.11	0.50
6:7:428:VAL:HA	6:7:598:PHE:CD2	2.46	0.50
6:7:440:VAL:HG21	6:7:650:PRO:HD2	1.93	0.50
6:7:685:THR:HB	6:7:686:PRO:HD2	1.93	0.50
7:A:107:LEU:HD21	7:A:152:SER:C	2.36	0.50
8:B:107:THR:HG23	8:B:108:HIS:ND1	2.26	0.50
8:B:134:PHE:HB2	8:B:137:PRO:HG3	1.91	0.50
11:E:345:ASN:ND2	11:E:555:CYS:HB2	2.27	0.50
2:3:495:VAL:HG23	2:3:508:ALA:HB2	1.94	0.50
3:4:750:TYR:CE1	3:4:754:ALA:HB2	2.47	0.50
3:4:766:ALA:O	3:4:770:LEU:HB3	2.11	0.50
4:5:679:GLU:O	4:5:683:LEU:HB2	2.11	0.50
5:6:653:HIS:HA	5:6:656:MET:CG	2.31	0.50
6:7:89:GLN:HA	6:7:92:LYS:HB2	1.94	0.50
6:7:227:VAL:HG13	6:7:230:ILE:HD12	1.93	0.50
8:B:193:ARG:HD2	10:D:278:ARG:NE	2.25	0.50
11:E:612:ILE:HG21	11:E:640:PHE:CD1	2.46	0.50
1:2:301:PRO:HA	1:2:302:THR:OG1	2.10	0.50
1:2:586:THR:HA	4:5:457:PRO:HB2	1.93	0.50
2:3:258:VAL:O	2:3:273:SER:HA	2.11	0.50
2:3:347:ILE:HA	2:3:350:ILE:HD13	1.93	0.50
3:4:346:PHE:H	3:4:389:CYS:HB3	1.77	0.50
3:4:566:LEU:HA	3:4:706:TYR:HB2	1.92	0.50
5:6:109:GLU:O	5:6:112:ARG:HB3	2.10	0.50
5:6:533:ILE:HG22	5:6:587:TYR:CE2	2.47	0.50
5:6:819:ILE:HA	5:6:823:PHE:HD2	1.76	0.50
5:6:834:SER:HA	5:6:837:ARG:HD2	1.92	0.50
5:6:945:GLU:O	5:6:948:LEU:HD22	2.11	0.50
6:7:481:VAL:CG2	6:7:516:ALA:HB3	2.41	0.50
6:7:493:LEU:HD22	6:7:533:ASP:HB3	1.92	0.50
11:E:5:ILE:N	11:E:142:CYS:O	2.44	0.50
11:E:315:THR:N	11:E:316:LEU:CB	2.73	0.50
1:2:256:LEU:HD23	1:2:259:PHE:CD2	2.47	0.50
2:3:562:SER:O	2:3:566:LEU:HG	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:440:VAL:HG22	6:7:701:LYS:HD2	1.93	0.50
7:A:32:TYR:CA	7:A:93:ARG:HH12	2.24	0.50
8:B:124:ARG:HD3	9:C:190:TRP:CZ3	2.47	0.50
10:D:202:MET:HE2	10:D:207:GLN:HA	1.92	0.50
10:D:269:LEU:HD13	10:D:275:TYR:HD2	1.75	0.50
11:E:18:ASN:O	11:E:79:ASN:ND2	2.34	0.50
11:E:128:PRO:HB2	11:E:240:TYR:CZ	2.47	0.50
11:E:158:ALA:HB1	11:E:237:LEU:HD22	1.93	0.50
1:2:302:THR:OG1	1:2:319:ARG:HB3	2.12	0.50
1:2:706:SER:O	5:6:762:LYS:NZ	2.45	0.50
2:3:400:ARG:O	2:3:707:ARG:NE	2.39	0.50
3:4:291:TYR:HB2	3:4:296:ILE:HG12	1.93	0.50
5:6:170:ILE:O	5:6:174:TYR:HB2	2.11	0.50
5:6:377:LEU:HD11	5:6:454:PHE:HB2	1.93	0.50
5:6:776:LYS:HA	5:6:779:GLU:HG2	1.94	0.50
7:A:4:ASP:N	7:A:4:ASP:OD1	2.43	0.50
7:A:113:ILE:H	7:A:113:ILE:HD12	1.77	0.50
7:A:124:SER:OG	7:A:127:GLU:HG2	2.12	0.50
8:B:173:LEU:HD23	8:B:178:ILE:HG12	1.94	0.50
11:E:42:THR:O	11:E:46:SER:N	2.32	0.50
1:2:632:SER:HA	4:5:443:GLY:N	2.27	0.50
3:4:330:GLY:HA3	3:4:400:GLN:O	2.12	0.50
3:4:812:LYS:HE3	3:4:814:LYS:HG3	1.93	0.50
4:5:181:ILE:HG12	4:5:243:ILE:HA	1.93	0.50
4:5:384:ILE:HD13	4:5:414:LEU:HD23	1.93	0.50
6:7:541:MET:HE1	6:7:563:ILE:HG21	1.94	0.50
6:7:581:LEU:HB2	6:7:681:PHE:CZ	2.47	0.50
8:B:54:THR:CG2	10:D:132:GLU:HG3	2.42	0.50
11:E:144:ASP:OD2	11:E:148:VAL:HB	2.12	0.50
11:E:603:ASN:OD1	11:E:605:PHE:N	2.36	0.50
11:E:609:PHE:O	11:E:613:THR:HG23	2.12	0.50
1:2:778:LEU:HD12	4:5:577:THR:HG23	1.93	0.50
1:2:782:ASP:OD1	1:2:782:ASP:N	2.38	0.50
2:3:41:SER:HA	2:3:44:SER:HB3	1.93	0.50
2:3:237:GLU:O	2:3:239:ASN:N	2.44	0.50
4:5:537:GLY:C	4:5:539:ASN:H	2.19	0.50
11:E:238:GLU:O	11:E:242:SER:OG	2.29	0.50
11:E:615:GLU:HG2	11:E:616:THR:H	1.77	0.50
1:2:767:ILE:HG13	1:2:768:HIS:N	2.26	0.50
2:3:111:TRP:CZ2	9:C:90:THR:HG22	2.47	0.50
2:3:196:LEU:HA	2:3:250:PHE:CD1	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:313:THR:HA	4:5:301:TYR:CD1	2.47	0.50
3:4:314:MET:SD	3:4:415:ILE:HA	2.52	0.50
3:4:592:SER:OG	3:4:593:GLY:N	2.45	0.50
4:5:71:TYR:HD1	11:E:415:TYR:HE1	1.59	0.50
4:5:659:ILE:O	4:5:662:SER:OG	2.18	0.50
6:7:352:THR:OG1	6:7:380:PHE:HB3	2.11	0.50
10:D:191:LEU:HA	10:D:194:VAL:HG12	1.94	0.50
10:D:254:PRO:HG2	10:D:270:THR:HG21	1.94	0.50
11:E:537:ASP:HA	11:E:540:ARG:HG3	1.94	0.50
1:2:246:TYR:CE2	1:2:300:PHE:HD1	2.30	0.49
1:2:256:LEU:HA	1:2:259:PHE:CD2	2.46	0.49
1:2:641:GLN:HE22	4:5:263:GLU:HA	1.76	0.49
2:3:374:HIS:HB2	2:3:378:LYS:NZ	2.26	0.49
3:4:264:TYR:HE2	6:7:135:LYS:HE2	1.76	0.49
3:4:613:GLN:CG	5:6:360:ARG:HH22	2.25	0.49
4:5:166:ILE:HD11	4:5:256:LEU:HD23	1.94	0.49
5:6:134:LYS:N	5:6:135:VAL:HA	2.27	0.49
5:6:641:PHE:CD1	5:6:682:ALA:HB2	2.47	0.49
6:7:493:LEU:HD21	6:7:533:ASP:CB	2.42	0.49
7:A:82:ASN:O	7:A:86:LEU:HG	2.12	0.49
11:E:67:LEU:HD11	11:E:83:LEU:HD11	1.94	0.49
11:E:83:LEU:N	11:E:121:TYR:O	2.45	0.49
11:E:559:SER:HB2	11:E:560:GLU:C	2.37	0.49
2:3:47:VAL:HG12	2:3:51:ASN:ND2	2.26	0.49
2:3:113:GLY:HA3	2:3:121:PHE:CE2	2.47	0.49
2:3:226:PRO:C	2:3:228:PRO:HD2	2.37	0.49
2:3:300:SER:HB2	4:5:250:PHE:CE2	2.46	0.49
2:3:409:GLY:O	2:3:518:PRO:HD3	2.12	0.49
3:4:506:LEU:O	3:4:509:ILE:HB	2.12	0.49
3:4:747:LEU:O	3:4:751:ILE:HG13	2.12	0.49
3:4:872:VAL:O	3:4:876:GLN:N	2.35	0.49
4:5:396:SER:HB3	4:5:661:GLU:CD	2.36	0.49
4:5:628:THR:O	4:5:632:GLN:HB2	2.10	0.49
6:7:446:ASP:HB2	6:7:447:GLY:HA2	1.92	0.49
7:A:100:MET:HE2	7:A:117:GLN:HG2	1.94	0.49
10:D:151:ILE:O	10:D:155:SER:N	2.45	0.49
11:E:124:ASP:OD1	11:E:125:ALA:N	2.45	0.49
2:3:359:ILE:O	2:3:363:LEU:HG	2.12	0.49
3:4:198:LEU:HG	3:4:227:ILE:HD11	1.94	0.49
5:6:527:ASP:OD2	5:6:531:ARG:NH1	2.45	0.49
5:6:801:GLU:CD	5:6:805:ARG:HH21	2.21	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:523:ILE:HG21	6:7:526:PHE:HD1	1.77	0.49
6:7:581:LEU:HB2	6:7:681:PHE:HZ	1.77	0.49
6:7:711:ASP:HA	6:7:714:GLU:HB3	1.93	0.49
9:C:165:PHE:CZ	9:C:169:LEU:HD11	2.47	0.49
10:D:60:PHE:HE1	10:D:139:VAL:HG21	1.78	0.49
11:E:258:LEU:O	11:E:262:ILE:HG13	2.11	0.49
1:2:226:VAL:O	1:2:230:ARG:HG2	2.11	0.49
1:2:272:ASP:OD1	1:2:273:LEU:N	2.46	0.49
1:2:588:GLU:H	1:2:588:GLU:CD	2.19	0.49
2:3:130:THR:HG22	2:3:153:TRP:CD1	2.47	0.49
4:5:491:VAL:HA	4:5:494:HIS:HB2	1.93	0.49
5:6:765:LEU:CD2	5:6:770:ARG:HB3	2.42	0.49
10:D:56:PRO:HA	10:D:90:ARG:HH12	1.78	0.49
10:D:103:MET:HA	10:D:106:LEU:HD13	1.93	0.49
11:E:67:LEU:HD12	11:E:86:PHE:CD2	2.47	0.49
1:2:636:ILE:HG23	4:5:446:ALA:HB3	1.94	0.49
1:2:810:LEU:O	1:2:813:ILE:HG12	2.11	0.49
1:2:858:ARG:HA	1:2:861:PHE:CE2	2.47	0.49
2:3:300:SER:HB2	4:5:250:PHE:HE2	1.78	0.49
2:3:702:LEU:O	2:3:705:LEU:N	2.43	0.49
3:4:341:ASP:HB3	3:4:343:LYS:HZ1	1.77	0.49
3:4:362:ARG:O	3:4:364:VAL:HG22	2.12	0.49
3:4:365:ILE:HB	5:6:419:SER:HA	1.94	0.49
4:5:413:LEU:HD11	4:5:550:PHE:CG	2.47	0.49
5:6:560:VAL:HB	5:6:561:GLU:HG3	1.93	0.49
5:6:695:LEU:O	5:6:695:LEU:HD23	2.12	0.49
5:6:793:TYR:CD2	5:6:795:ILE:HG23	2.48	0.49
6:7:112:HIS:CE1	6:7:116:LEU:HD13	2.47	0.49
7:A:130:TYR:CD2	10:D:193:LEU:HD22	2.47	0.49
8:B:142:ARG:NH1	11:E:314:ASP:OD2	2.45	0.49
11:E:69:ARG:O	11:E:73:GLN:HB2	2.12	0.49
1:2:234:LEU:HA	1:2:235:GLY:C	2.37	0.49
1:2:603:VAL:HG22	1:2:645:SER:HB2	1.93	0.49
3:4:666:ASN:HD22	3:4:668:ARG:NH2	2.10	0.49
6:7:73:ARG:HA	6:7:199:ARG:HH22	1.78	0.49
6:7:128:PRO:CD	6:7:129:THR:HA	2.42	0.49
7:A:192:ARG:H	11:E:55:GLN:HE21	1.61	0.49
11:E:256:TYR:OH	11:E:298:GLU:OE1	2.22	0.49
11:E:290:ARG:C	11:E:293:PRO:HD2	2.37	0.49
1:2:232:ARG:HA	1:2:283:TYR:CE2	2.47	0.49
1:2:582:LYS:HA	1:2:589:TRP:HA	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:41:SER:O	2:3:45:ILE:HG12	2.12	0.49
2:3:50:SER:HA	2:3:53:ALA:HB3	1.95	0.49
2:3:53:ALA:HA	6:7:218:LYS:CD	2.42	0.49
2:3:252:ASP:OD1	2:3:253:HIS:N	2.46	0.49
3:4:416:SER:OG	3:4:459:THR:O	2.26	0.49
3:4:456:LEU:HG	6:7:254:ALA:HA	1.94	0.49
3:4:644:VAL:O	3:4:648:VAL:HG23	2.12	0.49
4:5:620:GLU:O	4:5:623:SER:OG	2.22	0.49
4:5:625:ASN:O	4:5:629:ILE:HG13	2.12	0.49
5:6:126:SER:O	5:6:132:VAL:HB	2.12	0.49
5:6:290:ILE:HD13	5:6:454:PHE:CE1	2.48	0.49
5:6:385:SER:HA	5:6:388:ARG:HE	1.78	0.49
5:6:939:TRP:O	5:6:942:LEU:HB3	2.13	0.49
5:6:965:ILE:O	5:6:969:VAL:HB	2.13	0.49
6:7:269:VAL:HG21	6:7:285:THR:HB	1.93	0.49
6:7:669:GLN:O	6:7:673:ARG:N	2.36	0.49
10:D:67:TRP:HD1	10:D:143:TYR:HB2	1.78	0.49
11:E:467:THR:O	11:E:471:LYS:HB2	2.12	0.49
11:E:620:VAL:HG13	11:E:630:ILE:HD12	1.94	0.49
3:4:331:LEU:HB2	3:4:430:GLY:HA2	1.94	0.49
4:5:91:GLU:OE2	4:5:137:LEU:N	2.46	0.49
4:5:600:LYS:O	4:5:604:THR:HG23	2.13	0.49
5:6:641:PHE:HD1	5:6:682:ALA:HB2	1.77	0.49
6:7:21:ILE:HD13	6:7:117:PHE:HA	1.95	0.49
6:7:262:CYS:HA	6:7:298:LEU:HB3	1.93	0.49
6:7:488:SER:OG	6:7:492:GLY:O	2.30	0.49
9:C:162:THR:HG21	9:C:166:LEU:HD13	1.93	0.49
11:E:278:THR:HA	11:E:281:ASP:CG	2.38	0.49
11:E:291:LEU:HD23	11:E:294:LEU:HD12	1.95	0.49
1:2:326:ARG:NH2	1:2:389:THR:HG21	2.28	0.49
1:2:442:ASN:OD1	1:2:444:PHE:N	2.41	0.49
1:2:770:ALA:O	1:2:774:ILE:HG22	2.13	0.49
2:3:277:ILE:HD12	2:3:320:LEU:HD11	1.95	0.49
4:5:379:PHE:HD2	4:5:568:ILE:HB	1.77	0.49
4:5:450:THR:HG21	4:5:492:ALA:HB3	1.95	0.49
6:7:146:ARG:HH22	6:7:304:ALA:HA	1.78	0.49
6:7:220:ILE:O	6:7:222:SER:CB	2.60	0.49
7:A:130:TYR:CG	10:D:193:LEU:HD22	2.48	0.49
7:A:192:ARG:H	11:E:55:GLN:NE2	2.10	0.49
8:B:157:LEU:HD21	9:C:137:HIS:NE2	2.28	0.49
1:2:636:ILE:HG12	1:2:638:THR:HG23	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:705:ARG:HB2	5:6:559:THR:HB	1.94	0.49
2:3:476:ASP:OD2	2:3:517:ASN:N	2.46	0.49
3:4:754:ALA:O	3:4:758:ILE:HD12	2.13	0.49
5:6:831:LEU:HB3	5:6:835:ILE:HD11	1.95	0.49
6:7:228:ARG:HH12	6:7:326:HIS:CB	2.22	0.49
6:7:648:LYS:HE2	6:7:704:LEU:HD22	1.95	0.49
7:A:126:GLN:OE1	10:D:197:SER:OG	2.22	0.49
8:B:193:ARG:NH1	10:D:225:ASN:HB3	2.28	0.49
1:2:402:LEU:HD11	3:4:660:GLY:HA2	1.95	0.48
1:2:850:LYS:HG3	1:2:852:SER:H	1.78	0.48
2:3:193:ARG:HH22	2:3:452:THR:HG1	1.51	0.48
4:5:578:GLY:O	4:5:580:ALA:N	2.45	0.48
5:6:269:ASN:H	5:6:396:LYS:HE2	1.78	0.48
5:6:649:GLN:HB3	5:6:705:ILE:HD13	1.95	0.48
5:6:777:TYR:HD1	5:6:780:LEU:HD13	1.78	0.48
6:7:151:GLU:O	6:7:155:SER:N	2.45	0.48
6:7:437:VAL:HG12	6:7:701:LYS:HZ1	1.78	0.48
7:A:9:LEU:HD21	7:A:89:TYR:HB2	1.94	0.48
11:E:12:TYR:O	11:E:16:LEU:HG	2.13	0.48
11:E:351:TRP:HB3	11:E:511:VAL:HG22	1.95	0.48
2:3:480:ASP:OD1	2:3:480:ASP:N	2.45	0.48
4:5:627:VAL:O	4:5:631:LYS:HB2	2.12	0.48
6:7:204:PHE:O	6:7:380:PHE:HB2	2.12	0.48
6:7:217:LYS:O	6:7:220:ILE:HG12	2.12	0.48
6:7:484:THR:HA	6:7:524:ASP:H	1.77	0.48
8:B:14:GLU:O	8:B:17:GLN:HG2	2.12	0.48
8:B:30:ARG:NH1	8:B:66:MET:HE1	2.28	0.48
10:D:60:PHE:HD1	10:D:63:LEU:HD23	1.77	0.48
11:E:31:VAL:HG11	11:E:477:PHE:CZ	2.47	0.48
11:E:34:LEU:HD21	11:E:432:LEU:HB3	1.95	0.48
1:2:607:ASP:HA	1:2:649:ALA:O	2.14	0.48
2:3:176:LEU:HD22	4:5:250:PHE:CD2	2.48	0.48
4:5:652:GLN:O	4:5:656:ILE:HG13	2.14	0.48
6:7:61:PRO:HG2	6:7:64:MET:HE2	1.95	0.48
6:7:255:VAL:HG23	6:7:258:ILE:CG1	2.40	0.48
6:7:618:TYR:HE2	6:7:624:LYS:O	1.96	0.48
6:7:628:LEU:N	6:7:629:ASP:HA	2.28	0.48
10:D:54:VAL:HA	10:D:86:ARG:HH12	1.78	0.48
11:E:124:ASP:CG	11:E:126:HIS:HD1	2.21	0.48
1:2:572:SER:HB3	5:6:662:SER:HB2	1.95	0.48
1:2:595:ALA:O	1:2:598:LEU:HB3	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:258:TYR:CZ	3:4:308:VAL:HG12	2.48	0.48
3:4:308:VAL:HG21	3:4:325:LEU:HD12	1.94	0.48
4:5:21:ASP:O	4:5:25:THR:N	2.47	0.48
4:5:568:ILE:HD12	4:5:571:HIS:HB3	1.96	0.48
5:6:727:LEU:HA	5:6:731:ILE:HG13	1.95	0.48
5:6:732:VAL:O	5:6:736:MET:HG2	2.13	0.48
9:C:88:ILE:HD12	9:C:127:LEU:HD12	1.95	0.48
9:C:112:ILE:C	9:C:113:MET:HE2	2.38	0.48
11:E:545:LEU:HA	11:E:548:LEU:HB3	1.95	0.48
1:2:444:PHE:HB3	1:2:445:PRO:HD2	1.95	0.48
2:3:360:PHE:CD1	2:3:715:VAL:HG11	2.46	0.48
2:3:671:LEU:HA	2:3:721:VAL:HB	1.94	0.48
4:5:91:GLU:HA	4:5:94:ILE:HG13	1.95	0.48
4:5:636:ASN:CG	4:5:643:ARG:HH22	2.21	0.48
6:7:380:PHE:CE2	6:7:382:ARG:HB2	2.47	0.48
6:7:520:ILE:HG13	6:7:562:SER:HB2	1.95	0.48
6:7:596:ILE:HG23	6:7:723:SER:HB3	1.94	0.48
8:B:92:TRP:CE2	8:B:116:PRO:HG2	2.48	0.48
1:2:409:ILE:HB	1:2:452:GLU:HG2	1.96	0.48
1:2:525:LYS:HZ1	4:5:576:HIS:C	2.21	0.48
2:3:95:ARG:NH2	2:3:281:ASP:OD1	2.47	0.48
2:3:487:HIS:HB3	2:3:542:ARG:HH21	1.79	0.48
2:3:494:THR:HA	2:3:508:ALA:H	1.78	0.48
4:5:349:PHE:CE2	4:5:353:GLU:HB2	2.48	0.48
5:6:807:SER:HB2	5:6:819:ILE:HG21	1.96	0.48
6:7:226:SER:HB2	6:7:321:GLN:HB3	1.95	0.48
6:7:228:ARG:HH22	6:7:326:HIS:HB3	1.78	0.48
7:A:188:GLN:HG2	11:E:478:TRP:CH2	2.48	0.48
8:B:167:HIS:NE2	10:D:267:VAL:HG11	2.28	0.48
11:E:25:CYS:H	11:E:26:GLN:CA	2.26	0.48
11:E:327:PHE:CZ	11:E:328:LEU:HG	2.48	0.48
1:2:829:VAL:HG13	1:2:833:ASP:HB2	1.96	0.48
3:4:713:ASP:HB2	3:4:716:ASN:CB	2.38	0.48
4:5:407:ARG:CD	4:5:498:GLU:HA	2.44	0.48
5:6:399:GLY:C	5:6:400:VAL:CG2	2.85	0.48
5:6:516:LEU:O	5:6:520:VAL:HG13	2.14	0.48
5:6:546:GLY:O	5:6:550:GLN:N	2.46	0.48
5:6:560:VAL:CB	5:6:561:GLU:HA	2.43	0.48
6:7:359:PRO:HA	6:7:360:TYR:HA	1.66	0.48
6:7:530:ASP:O	6:7:534:ARG:NH1	2.43	0.48
6:7:535:THR:HA	6:7:538:HIS:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:D:70:GLU:O	10:D:73:SER:OG	2.22	0.48
10:D:231:HIS:HA	10:D:274:ILE:HG22	1.95	0.48
11:E:307:ARG:HD3	11:E:308:ASN:H	1.78	0.48
2:3:340:GLN:HB3	2:3:661:GLN:HE22	1.78	0.48
2:3:340:GLN:HG2	2:3:341:MET:H	1.78	0.48
2:3:712:HIS:CD2	2:3:728:VAL:HG21	2.48	0.48
3:4:314:MET:HE2	3:4:413:HIS:CE1	2.49	0.48
3:4:803:ARG:HA	3:4:806:GLU:HG2	1.94	0.48
4:5:165:ILE:N	4:5:259:GLN:O	2.29	0.48
4:5:374:ILE:HG21	4:5:388:ILE:HD13	1.96	0.48
4:5:409:ASP:C	4:5:410:ILE:HG12	2.39	0.48
5:6:289:SER:HA	5:6:397:PHE:O	2.14	0.48
6:7:458:LEU:HD22	6:7:600:MET:HE3	1.96	0.48
6:7:696:SER:HA	6:7:699:LEU:HB2	1.96	0.48
7:A:14:LYS:HA	9:C:6:ILE:HD13	1.96	0.48
9:C:18:CYS:HB3	9:C:72:VAL:CG1	2.44	0.48
11:E:24:SER:O	11:E:26:GLN:NE2	2.47	0.48
11:E:57:GLN:OE1	11:E:58:ILE:N	2.47	0.48
1:2:640:LEU:HA	1:2:640:LEU:HD23	1.51	0.48
3:4:443:PRO:HD3	3:4:457:TYR:CE2	2.49	0.48
3:4:572:THR:HG23	3:4:708:VAL:HG11	1.95	0.48
3:4:686:LEU:HD23	3:4:691:ASN:CG	2.39	0.48
4:5:413:LEU:HG	4:5:521:ALA:HB3	1.96	0.48
5:6:777:TYR:CG	5:6:800:LEU:HD13	2.49	0.48
10:D:54:VAL:HA	10:D:86:ARG:NH1	2.28	0.48
10:D:133:LEU:O	10:D:136:LEU:N	2.46	0.48
11:E:613:THR:HG21	11:E:622:ILE:HD11	1.94	0.48
1:2:626:GLN:HA	4:5:427:LYS:HZ1	1.79	0.48
2:3:246:GLY:N	6:7:236:GLY:HA3	2.29	0.48
2:3:347:ILE:HD11	2:3:662:TYR:CZ	2.49	0.48
2:3:372:TYR:H	13:3:1001:ANP:HN62	1.62	0.48
2:3:470:VAL:HB	2:3:512:VAL:HG13	1.95	0.48
3:4:324:LYS:NZ	6:7:138:VAL:HG11	2.29	0.48
3:4:354:HIS:HD2	3:4:356:MET:HG2	1.76	0.48
3:4:592:SER:HA	3:4:632:ASP:HB2	1.96	0.48
5:6:596:VAL:HG21	5:6:631:ALA:HB2	1.95	0.48
5:6:616:GLU:CB	5:6:620:ASP:HA	2.43	0.48
5:6:918:ARG:HD3	5:6:918:ARG:HA	1.71	0.48
6:7:21:ILE:HG12	6:7:117:PHE:HD1	1.78	0.48
6:7:227:VAL:HA	6:7:230:ILE:HG13	1.95	0.48
7:A:109:LEU:O	7:A:110:MET:C	2.56	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:50:TRP:N	8:B:51:GLN:HA	2.28	0.48
1:2:580:VAL:HG12	1:2:589:TRP:HB3	1.96	0.47
1:2:696:ALA:HB1	5:6:800:LEU:HD22	1.95	0.47
2:3:132:LEU:O	2:3:135:SER:OG	2.21	0.47
2:3:200:VAL:HG21	2:3:247:TYR:CE2	2.49	0.47
2:3:255:ARG:O	2:3:256:ILE:HD13	2.14	0.47
3:4:249:LEU:HA	3:4:250:ALA:HA	1.61	0.47
5:6:143:MET:HE1	5:6:148:LEU:HB2	1.96	0.47
5:6:819:ILE:O	5:6:820:THR:HG23	2.14	0.47
6:7:257:VAL:H	6:7:273:VAL:CG2	2.25	0.47
8:B:60:LEU:HB3	8:B:63:MET:HG2	1.95	0.47
8:B:118:ASN:OD1	8:B:118:ASN:N	2.47	0.47
11:E:480:SER:HA	11:E:483:ALA:HB3	1.96	0.47
1:2:408:VAL:HA	1:2:451:ILE:O	2.14	0.47
1:2:660:THR:OG1	5:6:947:ASP:HA	2.14	0.47
1:2:785:LYS:HG3	1:2:788:ARG:HH21	1.78	0.47
2:3:101:ASP:OD2	9:C:86:ASN:ND2	2.48	0.47
2:3:533:ILE:HG21	2:3:540:LEU:HD11	1.96	0.47
3:4:633:GLU:N	3:4:674:SER:O	2.38	0.47
3:4:867:ARG:HD2	3:4:870:MET:HE3	1.96	0.47
4:5:294:ILE:HG12	4:5:333:ILE:HG13	1.96	0.47
4:5:371:THR:HG21	4:5:386:LYS:HG2	1.96	0.47
4:5:540:ILE:HG22	4:5:546:ILE:HD13	1.96	0.47
5:6:591:PHE:CE1	5:6:752:ARG:HG3	2.49	0.47
5:6:731:ILE:HG22	5:6:735:HIS:CD2	2.49	0.47
10:D:269:LEU:HA	10:D:275:TYR:HE2	1.76	0.47
11:E:29:ILE:HD11	11:E:58:ILE:HG23	1.96	0.47
11:E:60:PRO:HG3	11:E:478:TRP:NE1	2.29	0.47
11:E:268:SER:O	11:E:271:TRP:N	2.48	0.47
1:2:264:PRO:HD2	1:2:315:SER:O	2.14	0.47
1:2:585:ILE:HG23	1:2:586:THR:H	1.78	0.47
2:3:21:PHE:O	2:3:25:VAL:HG23	2.13	0.47
2:3:25:VAL:CG2	2:3:124:PRO:CB	2.92	0.47
2:3:172:THR:OG1	2:3:173:ALA:HA	2.14	0.47
3:4:228:LYS:HA	3:4:231:ASN:HB2	1.95	0.47
3:4:330:GLY:HA2	3:4:403:PRO:CD	2.43	0.47
3:4:386:HIS:CE1	5:6:405:PRO:HD3	2.48	0.47
5:6:726:GLU:C	5:6:729:SER:H	2.23	0.47
6:7:567:ALA:O	6:7:569:PRO:HD3	2.14	0.47
8:B:56:ASP:OD1	8:B:56:ASP:N	2.35	0.47
10:D:79:TYR:CE2	10:D:81:HIS:HB3	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:338:LYS:O	1:2:378:GLU:N	2.26	0.47
1:2:379:LYS:NZ	4:5:82:GLU:OE2	2.46	0.47
1:2:525:LYS:HE3	4:5:576:HIS:O	2.13	0.47
1:2:525:LYS:HE2	4:5:576:HIS:ND1	2.30	0.47
2:3:234:GLU:OE1	2:3:240:LYS:HD2	2.14	0.47
2:3:405:ILE:HB	2:3:513:ILE:HG12	1.96	0.47
3:4:631:ILE:O	3:4:674:SER:N	2.48	0.47
3:4:775:VAL:O	3:4:779:LYS:N	2.45	0.47
4:5:21:ASP:N	4:5:21:ASP:OD1	2.47	0.47
4:5:253:GLN:HE21	4:5:277:THR:CB	2.27	0.47
5:6:659:GLN:HG3	5:6:675:ARG:HA	1.96	0.47
6:7:529:MET:HE2	6:7:533:ASP:HB2	1.96	0.47
6:7:650:PRO:HG3	6:7:700:ALA:HB3	1.95	0.47
7:A:110:MET:N	7:A:111:SER:HA	2.27	0.47
7:A:175:GLN:CB	7:A:180:VAL:HA	2.44	0.47
9:C:172:MET:O	9:C:176:ILE:HG23	2.14	0.47
10:D:260:ILE:HG23	10:D:261:PRO:HD2	1.97	0.47
11:E:370:LEU:O	11:E:374:GLN:HG2	2.15	0.47
1:2:550:SER:OG	13:2:901:ANP:O1G	2.26	0.47
3:4:854:LYS:HE2	3:4:857:ILE:HD11	1.97	0.47
4:5:382:GLU:HA	4:5:385:LYS:HB3	1.97	0.47
4:5:422:LYS:HA	4:5:425:LEU:HB3	1.95	0.47
5:6:614:ARG:CZ	5:6:614:ARG:HB3	2.44	0.47
5:6:665:LYS:HD3	5:6:665:LYS:HA	1.72	0.47
5:6:732:VAL:HG13	5:6:736:MET:HE3	1.96	0.47
5:6:761:PHE:HB2	5:6:812:ARG:HE	1.79	0.47
5:6:776:LYS:O	5:6:780:LEU:N	2.47	0.47
6:7:87:GLN:O	6:7:90:ASN:HB2	2.15	0.47
6:7:107:GLN:HA	6:7:238:LEU:HB3	1.96	0.47
6:7:114:THR:HG23	6:7:204:PHE:HE2	1.79	0.47
7:A:185:LYS:HD2	7:A:186:ASP:N	2.29	0.47
1:2:645:SER:C	1:2:646:ILE:HG13	2.40	0.47
1:2:828:PHE:CE2	11:E:516:LYS:HG2	2.49	0.47
2:3:260:GLU:OE1	2:3:260:GLU:N	2.40	0.47
2:3:317:PHE:HE2	4:5:176:ALA:HB2	1.80	0.47
2:3:389:VAL:HG21	2:3:669:PRO:HD2	1.95	0.47
3:4:727:LEU:HA	3:4:728:TYR:C	2.40	0.47
3:4:796:ARG:O	3:4:799:GLU:HB3	2.15	0.47
3:4:820:GLU:HG3	3:4:823:GLN:CD	2.39	0.47
4:5:566:ILE:O	4:5:570:ASN:HB2	2.15	0.47
4:5:635:ILE:HA	4:5:638:LEU:HG	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:126:SER:HB3	5:6:131:GLU:HB3	1.96	0.47
5:6:298:SER:O	5:6:357:GLN:HB2	2.15	0.47
6:7:18:PHE:CE1	6:7:120:ALA:HB2	2.50	0.47
6:7:455:ASN:HA	6:7:563:ILE:O	2.13	0.47
9:C:7:ASP:HA	9:C:10:LEU:HB3	1.95	0.47
9:C:58:GLY:HA3	9:C:69:VAL:O	2.15	0.47
11:E:280:LEU:O	11:E:283:ALA:N	2.42	0.47
11:E:359:LEU:O	11:E:362:MET:HB2	2.15	0.47
11:E:519:ILE:HA	11:E:528:CYS:SG	2.55	0.47
1:2:232:ARG:HG3	1:2:283:TYR:OH	2.14	0.47
1:2:325:THR:O	1:2:326:ARG:C	2.58	0.47
1:2:432:ASN:OD1	1:2:432:ASN:N	2.48	0.47
1:2:435:ASP:HB3	1:2:447:PHE:HE1	1.79	0.47
1:2:676:ARG:HH12	4:5:418:PRO:HB2	1.79	0.47
1:2:796:GLU:O	1:2:799:SER:HB2	2.14	0.47
2:3:200:VAL:HG21	2:3:247:TYR:HD2	1.80	0.47
2:3:201:HIS:NE2	2:3:232:PRO:HD2	2.29	0.47
2:3:662:TYR:HE1	2:3:666:ARG:HD2	1.79	0.47
3:4:330:GLY:O	3:4:399:LEU:HD11	2.15	0.47
4:5:22:ASP:HA	4:5:25:THR:HB	1.95	0.47
4:5:149:ARG:NH2	4:5:269:GLU:OE1	2.48	0.47
4:5:299:SER:OG	4:5:300:ILE:N	2.48	0.47
4:5:382:GLU:O	4:5:386:LYS:HG3	2.15	0.47
4:5:594:ILE:HD13	4:5:599:MET:HE1	1.96	0.47
5:6:313:MET:HA	5:6:314:CYS:HA	1.62	0.47
5:6:368:ILE:HG21	5:6:374:PRO:HB3	1.97	0.47
5:6:603:SER:N	5:6:604:SER:HA	2.17	0.47
5:6:753:ARG:HA	5:6:756:LYS:HE2	1.96	0.47
5:6:943:GLN:HA	5:6:946:ASN:ND2	2.29	0.47
5:6:945:GLU:HA	5:6:948:LEU:HD13	1.97	0.47
6:7:519:GLY:O	6:7:562:SER:N	2.39	0.47
6:7:645:ALA:HB1	6:7:701:LYS:CB	2.44	0.47
7:A:14:LYS:HZ1	9:C:171:GLU:CD	2.22	0.47
7:A:23:SER:N	7:A:24:ASN:HA	2.29	0.47
10:D:137:LYS:HG2	10:D:141:ARG:HH12	1.80	0.47
11:E:28:VAL:HG12	11:E:29:ILE:O	2.15	0.47
11:E:32:SER:HA	11:E:33:CYS:HA	1.41	0.47
11:E:41:ALA:HB1	11:E:255:ILE:HD12	1.95	0.47
11:E:89:VAL:O	11:E:130:ASN:ND2	2.48	0.47
11:E:222:LYS:HA	11:E:225:GLN:HB3	1.97	0.47
11:E:264:GLU:N	11:E:264:GLU:OE1	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:E:284:TYR:HB2	11:E:285:ALA:H	1.56	0.47
11:E:372:THR:HG23	11:E:375:GLU:OE1	2.15	0.47
11:E:566:PRO:HB2	11:E:605:PHE:HE2	1.76	0.47
1:2:567:THR:HG22	1:2:572:SER:HB2	1.96	0.47
2:3:233:THR:C	2:3:234:GLU:HG2	2.40	0.47
3:4:629:CYS:SG	3:4:630:CYS:N	2.87	0.47
3:4:689:THR:OG1	3:4:851:GLN:N	2.40	0.47
4:5:98:ALA:O	4:5:102:SER:N	2.42	0.47
4:5:379:PHE:CD2	4:5:568:ILE:HB	2.49	0.47
4:5:473:ASP:HA	4:5:517:THR:HG22	1.95	0.47
4:5:575:ILE:HG13	4:5:581:ASN:HD22	1.78	0.47
5:6:371:GLY:HA3	6:7:554:ASN:OD1	2.15	0.47
5:6:608:LEU:HA	5:6:627:ALA:HB3	1.96	0.47
5:6:711:LEU:HB3	5:6:713:PHE:CE1	2.50	0.47
6:7:441:ASP:H	6:7:452:GLY:HA2	1.78	0.47
6:7:485:GLY:H	6:7:525:GLU:HB2	1.80	0.47
8:B:94:THR:O	8:B:98:LEU:HG	2.15	0.47
9:C:101:ASN:HD22	9:C:104:PHE:HB2	1.79	0.47
11:E:419:ILE:HG22	11:E:420:SER:O	2.14	0.47
11:E:489:VAL:HG12	11:E:493:ASN:HD21	1.79	0.47
1:2:580:VAL:HG21	4:5:446:ALA:HB1	1.95	0.47
2:3:407:MET:HE3	2:3:549:VAL:HG21	1.97	0.47
3:4:433:ILE:HG21	3:4:468:LYS:C	2.40	0.47
4:5:344:ASN:N	4:5:345:SER:HA	2.29	0.47
4:5:353:GLU:O	4:5:357:PHE:N	2.43	0.47
4:5:514:ASN:OD1	4:5:516:ARG:NH2	2.48	0.47
5:6:122:PHE:HA	5:6:123:SER:CB	2.45	0.47
5:6:529:LEU:O	5:6:533:ILE:CG1	2.62	0.47
5:6:656:MET:SD	5:6:678:ILE:HG13	2.55	0.47
5:6:964:VAL:HG13	5:6:967:ARG:NE	2.30	0.47
6:7:476:ILE:CD1	6:7:476:ILE:N	2.73	0.47
6:7:489:SER:O	6:7:493:LEU:HD21	2.13	0.47
7:A:103:ASN:OD1	7:A:104:ASN:N	2.44	0.47
8:B:184:PHE:O	8:B:188:ILE:CD1	2.63	0.47
11:E:140:ILE:HB	11:E:141:GLN:C	2.40	0.47
1:2:323:VAL:HG23	1:2:393:ALA:HB2	1.97	0.47
2:3:101:ASP:OD1	2:3:104:ARG:NH2	2.48	0.47
2:3:389:VAL:HG12	2:3:390:GLU:N	2.23	0.47
3:4:258:TYR:OH	3:4:308:VAL:HG12	2.15	0.47
3:4:618:SER:HB3	3:4:622:VAL:HB	1.95	0.47
4:5:166:ILE:HG12	4:5:258:LEU:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:384:ILE:HG13	4:5:554:PHE:CD2	2.43	0.47
4:5:565:ASP:O	4:5:568:ILE:N	2.48	0.47
5:6:174:TYR:O	5:6:178:LEU:HD12	2.15	0.47
5:6:363:GLU:HB3	5:6:374:PRO:HB2	1.96	0.47
5:6:660:THR:HG22	5:6:673:ASN:HA	1.96	0.47
5:6:758:ALA:HA	5:6:761:PHE:CE2	2.49	0.47
6:7:454:ILE:HG22	6:7:456:VAL:HG23	1.96	0.47
8:B:151:ILE:O	8:B:154:ILE:HG13	2.14	0.47
10:D:159:ARG:NH2	10:D:187:SER:OG	2.48	0.47
11:E:158:ALA:HB2	11:E:237:LEU:HD13	1.97	0.47
11:E:641:LEU:O	11:E:645:THR:HG23	2.15	0.47
1:2:270:ILE:O	1:2:274:VAL:HG23	2.15	0.46
1:2:337:VAL:HB	1:2:351:PHE:H	1.79	0.46
1:2:550:SER:HB3	5:6:657:GLU:CD	2.40	0.46
2:3:104:ARG:HH22	9:C:86:ASN:HB2	1.79	0.46
3:4:794:THR:HG23	3:4:796:ARG:H	1.79	0.46
3:4:910:LEU:O	3:4:915:LYS:N	2.32	0.46
4:5:184:ARG:HH21	4:5:242:ILE:HD11	1.80	0.46
5:6:288:LEU:O	5:6:399:GLY:N	2.48	0.46
5:6:713:PHE:HA	5:6:834:SER:OG	2.16	0.46
5:6:777:TYR:O	5:6:780:LEU:HB3	2.14	0.46
6:7:459:MET:HG3	6:7:460:GLY:N	2.30	0.46
7:A:27:VAL:HG11	7:A:100:MET:CE	2.45	0.46
7:A:151:LEU:O	10:D:145:ARG:NH1	2.48	0.46
10:D:200:LYS:C	10:D:202:MET:H	2.23	0.46
10:D:260:ILE:HD12	10:D:260:ILE:H	1.80	0.46
11:E:164:GLU:OE1	11:E:164:GLU:N	2.46	0.46
1:2:549:LYS:HG3	1:2:550:SER:H	1.81	0.46
3:4:666:ASN:HD22	3:4:668:ARG:HH22	1.61	0.46
4:5:659:ILE:C	4:5:662:SER:HG	2.17	0.46
5:6:130:GLY:CA	5:6:131:GLU:HB3	2.45	0.46
5:6:361:ILE:HD12	5:6:397:PHE:CE2	2.45	0.46
6:7:318:LEU:O	6:7:319:SER:OG	2.31	0.46
8:B:7:LEU:HD22	8:B:10:THR:HG23	1.98	0.46
10:D:212:THR:H	10:D:213:GLU:HA	1.79	0.46
10:D:237:ASP:OD2	10:D:248:GLU:N	2.48	0.46
2:3:151:HIS:CG	2:3:152:PRO:HD2	2.50	0.46
3:4:573:SER:HA	3:4:576:GLN:HG2	1.96	0.46
3:4:613:GLN:OE1	5:6:360:ARG:NH1	2.49	0.46
3:4:646:HIS:HE1	3:4:698:LEU:HD13	1.79	0.46
5:6:689:TYR:CD2	5:6:716:LEU:HD12	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:727:LEU:HB3	5:6:731:ILE:HD12	1.97	0.46
5:6:794:ARG:HB2	5:6:795:ILE:C	2.41	0.46
7:A:98:ASP:O	7:A:102:TRP:HD1	1.98	0.46
8:B:92:TRP:CH2	8:B:93:LEU:HD12	2.50	0.46
9:C:16:PHE:CZ	9:C:107:LEU:HD21	2.50	0.46
10:D:268:GLU:O	10:D:269:LEU:HD22	2.16	0.46
11:E:320:ILE:HG22	11:E:409:PHE:HD1	1.80	0.46
1:2:296:ARG:HD2	1:2:414:LEU:HD21	1.97	0.46
1:2:487:ILE:O	1:2:493:ILE:HG21	2.15	0.46
2:3:174:GLN:H	2:3:174:GLN:CD	2.24	0.46
2:3:490:MET:HB2	2:3:542:ARG:HD2	1.97	0.46
2:3:680:VAL:HG13	6:7:613:ALA:HB3	1.96	0.46
3:4:181:TRP:CD1	3:4:182:GLY:H	2.33	0.46
3:4:572:THR:CG2	3:4:708:VAL:HG11	2.45	0.46
4:5:50:LEU:HD11	4:5:135:PHE:CZ	2.51	0.46
4:5:176:ALA:HA	4:5:250:PHE:CE1	2.51	0.46
4:5:360:LEU:HB3	4:5:366:LEU:HD22	1.97	0.46
4:5:660:THR:HG22	4:5:677:VAL:HG13	1.98	0.46
5:6:186:ARG:O	5:6:190:ARG:HB2	2.16	0.46
5:6:658:GLN:C	5:6:660:THR:H	2.22	0.46
5:6:689:TYR:HB3	5:6:691:ARG:HD3	1.97	0.46
5:6:706:MET:HE2	5:6:793:TYR:CE1	2.49	0.46
5:6:950:SER:HB2	5:6:953:GLU:HG2	1.98	0.46
6:7:467:SER:O	6:7:471:LYS:HB2	2.14	0.46
6:7:537:ILE:HG23	6:7:541:MET:HE2	1.98	0.46
6:7:669:GLN:O	6:7:673:ARG:HG2	2.16	0.46
6:7:714:GLU:HA	6:7:717:LEU:HB2	1.96	0.46
7:A:105:ASN:ND2	7:A:110:MET:SD	2.88	0.46
7:A:171:ALA:HA	7:A:172:GLY:HA3	1.68	0.46
8:B:30:ARG:HD3	8:B:66:MET:HE3	1.98	0.46
11:E:155:GLN:HA	11:E:158:ALA:CB	2.46	0.46
11:E:234:GLU:O	11:E:238:GLU:HB2	2.16	0.46
11:E:376:THR:HG22	11:E:378:LEU:H	1.80	0.46
1:2:428:GLY:CA	1:2:453:ALA:HA	2.37	0.46
2:3:384:MET:HA	2:3:403:ILE:HD13	1.98	0.46
3:4:447:ASN:N	3:4:448:SER:HA	2.29	0.46
3:4:570:PRO:HD3	3:4:680:SER:HB2	1.97	0.46
4:5:375:ALA:CB	4:5:378:ILE:HB	2.45	0.46
4:5:425:LEU:O	4:5:429:VAL:HG23	2.16	0.46
4:5:493:ILE:O	4:5:497:MET:HG3	2.16	0.46
5:6:122:PHE:CB	5:6:124:VAL:HB	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:357:GLN:HG2	5:6:386:VAL:HG23	1.96	0.46
8:B:18:PHE:HE1	10:D:135:ARG:HG2	1.80	0.46
8:B:184:PHE:CZ	9:C:132:ALA:HB1	2.50	0.46
10:D:195:ASN:HA	10:D:199:LEU:HB2	1.97	0.46
10:D:255:CYS:HB2	10:D:270:THR:HG22	1.98	0.46
11:E:120:ILE:HB	11:E:139:ILE:O	2.15	0.46
3:4:566:LEU:HG	3:4:672:LEU:HD21	1.97	0.46
5:6:397:PHE:HD1	5:6:459:VAL:HG22	1.80	0.46
7:A:67:VAL:O	7:A:70:CYS:HB2	2.15	0.46
7:A:187:SER:OG	11:E:57:GLN:NE2	2.43	0.46
8:B:184:PHE:CE1	8:B:188:ILE:HD11	2.51	0.46
10:D:135:ARG:CZ	10:D:135:ARG:HB3	2.46	0.46
10:D:257:THR:O	10:D:269:LEU:HB2	2.15	0.46
10:D:266:GLU:CD	10:D:266:GLU:H	2.23	0.46
11:E:353:GLU:O	11:E:356:LYS:HB3	2.16	0.46
11:E:466:LEU:O	11:E:470:ARG:HG3	2.16	0.46
1:2:210:GLU:O	1:2:213:SER:HB3	2.15	0.46
1:2:812:SER:O	1:2:816:ILE:HG13	2.16	0.46
1:2:813:ILE:HD12	1:2:841:VAL:CG2	2.42	0.46
5:6:801:GLU:OE1	5:6:805:ARG:NH2	2.44	0.46
5:6:909:TYR:HA	5:6:912:MET:HB2	1.98	0.46
7:A:102:TRP:CZ3	7:A:151:LEU:HD23	2.51	0.46
7:A:133:GLU:O	7:A:136:ASP:HB2	2.15	0.46
9:C:53:ILE:HG12	9:C:54:LEU:N	2.31	0.46
10:D:162:ASN:HA	10:D:169:ILE:HG23	1.98	0.46
11:E:140:ILE:HA	11:E:141:GLN:CB	2.43	0.46
3:4:428:ARG:HE	5:6:369:PRO:CG	2.29	0.46
3:4:563:ASN:OD1	3:4:563:ASN:N	2.47	0.46
4:5:353:GLU:O	4:5:356:GLU:HG2	2.15	0.46
4:5:409:ASP:O	4:5:518:SER:HB2	2.16	0.46
4:5:439:THR:H	4:5:478:CYS:HB2	1.80	0.46
5:6:302:PRO:HB2	5:6:353:PHE:CD2	2.50	0.46
5:6:356:TRP:CZ3	5:6:380:ILE:HB	2.51	0.46
5:6:730:HIS:CE1	5:6:734:LEU:HD21	2.51	0.46
5:6:767:LYS:HG2	5:6:769:ALA:H	1.81	0.46
5:6:811:ALA:O	5:6:815:CYS:N	2.49	0.46
11:E:358:ARG:O	11:E:361:LYS:HB3	2.15	0.46
11:E:625:PHE:CE1	11:E:626:GLU:HB2	2.51	0.46
1:2:533:ILE:HD13	4:5:576:HIS:NE2	2.30	0.46
1:2:856:GLN:NE2	1:2:859:ARG:HH21	2.09	0.46
2:3:29:GLN:O	2:3:32:LEU:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:566:LEU:HB3	4:5:619:ALA:HB1	1.98	0.46
3:4:397:ILE:HB	3:4:417:LEU:HD11	1.98	0.46
3:4:593:GLY:C	3:4:595:GLY:H	2.22	0.46
3:4:821:ASP:OD1	3:4:822:VAL:HG23	2.16	0.46
4:5:411:ASN:ND2	4:5:519:VAL:HB	2.30	0.46
4:5:412:VAL:HB	4:5:520:LEU:HG	1.97	0.46
5:6:566:ARG:HA	5:6:567:GLY:HA3	1.73	0.46
6:7:143:LEU:O	6:7:146:ARG:HB2	2.16	0.46
6:7:493:LEU:HD11	6:7:533:ASP:HA	1.98	0.46
6:7:656:VAL:HG11	6:7:708:VAL:O	2.16	0.46
8:B:198:ALA:HB1	9:C:113:MET:SD	2.56	0.46
9:C:46:LEU:HB3	9:C:50:LEU:HD11	1.98	0.46
11:E:130:ASN:OD1	11:E:131:LEU:N	2.48	0.46
11:E:133:ASN:O	11:E:140:ILE:CD1	2.64	0.46
11:E:256:TYR:HB2	11:E:273:ASN:OD1	2.16	0.46
11:E:524:ILE:HB	11:E:525:TYR:HD2	1.80	0.46
1:2:519:LEU:HD21	1:2:559:THR:HG21	1.98	0.46
2:3:520:PHE:HB3	2:3:527:ARG:HH22	1.80	0.46
3:4:419:VAL:HG23	3:4:420:TYR:N	2.31	0.46
3:4:550:LYS:HE2	3:4:558:TYR:CD2	2.49	0.46
3:4:603:ALA:HA	3:4:617:GLU:O	2.16	0.46
4:5:41:ASP:HA	4:5:42:SER:HA	1.66	0.46
4:5:136:GLN:CD	4:5:280:ARG:HB2	2.41	0.46
4:5:420:THR:N	13:5:801:ANP:O2A	2.49	0.46
4:5:496:ALA:HB2	4:5:502:ILE:HG12	1.98	0.46
4:5:578:GLY:O	4:5:579:ASN:OD1	2.35	0.46
5:6:714:VAL:HB	5:6:837:ARG:HB3	1.98	0.46
6:7:26:VAL:H	6:7:63:TYR:CB	2.28	0.46
8:B:97:GLU:OE2	8:B:101:LYS:NZ	2.39	0.46
10:D:75:GLU:OE1	10:D:222:PRO:HA	2.16	0.46
11:E:26:GLN:CB	11:E:78:ILE:HA	2.39	0.46
11:E:28:VAL:HG13	11:E:57:GLN:O	2.15	0.46
11:E:133:ASN:O	11:E:142:CYS:HB3	2.16	0.46
11:E:150:ASP:N	11:E:151:THR:HA	2.31	0.46
1:2:494:ILE:O	1:2:498:ILE:HG13	2.16	0.45
1:2:520:PHE:CE2	1:2:822:LYS:HB3	2.50	0.45
1:2:569:GLN:C	1:2:571:ALA:HA	2.42	0.45
1:2:657:TYR:HE2	1:2:660:THR:HG22	1.81	0.45
2:3:435:ARG:HA	2:3:436:GLY:HA3	1.54	0.45
2:3:565:VAL:O	2:3:568:THR:HB	2.16	0.45
3:4:199:MET:H	3:4:227:ILE:HG12	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:467:LYS:HG3	3:4:468:LYS:HB2	1.97	0.45
4:5:68:LEU:HD21	4:5:76:TYR:HB2	1.98	0.45
4:5:300:ILE:HD13	4:5:326:PRO:HA	1.97	0.45
5:6:270:LEU:H	5:6:396:LYS:NZ	2.14	0.45
5:6:532:SER:HB2	5:6:746:PHE:HB2	1.96	0.45
5:6:555:VAL:HG13	5:6:808:GLU:HG2	1.97	0.45
6:7:411:TYR:HD1	6:7:702:LEU:HD13	1.82	0.45
6:7:422:ILE:HD13	6:7:469:LEU:CD1	2.46	0.45
7:A:130:TYR:HB2	10:D:193:LEU:HD13	1.98	0.45
7:A:163:ILE:HG22	7:A:164:ASP:H	1.80	0.45
7:A:185:LYS:HD2	7:A:186:ASP:H	1.80	0.45
11:E:81:LEU:HB3	11:E:120:ILE:HA	1.98	0.45
11:E:349:SER:HB3	11:E:352:ASN:ND2	2.31	0.45
11:E:483:ALA:HA	11:E:491:LEU:HD11	1.97	0.45
11:E:637:LEU:O	11:E:641:LEU:HG	2.16	0.45
1:2:432:ASN:HA	1:2:448:ALA:O	2.16	0.45
1:2:520:PHE:CD1	1:2:823:MET:HG2	2.52	0.45
1:2:778:LEU:H	4:5:577:THR:HG21	1.81	0.45
2:3:28:PHE:O	2:3:31:PHE:HB3	2.16	0.45
3:4:257:LEU:HD12	3:4:260:GLN:HB2	1.97	0.45
3:4:336:THR:O	5:6:375:ARG:NH1	2.49	0.45
3:4:375:ASP:HA	3:4:376:CYS:C	2.42	0.45
3:4:410:GLN:OE1	3:4:411:THR:HG22	2.16	0.45
4:5:479:ILE:O	4:5:522:ALA:HB3	2.16	0.45
5:6:558:SER:CB	5:6:559:THR:HA	2.28	0.45
5:6:941:LEU:HD13	5:6:958:ARG:NH2	2.31	0.45
8:B:24:PRO:HB2	8:B:70:GLU:OE2	2.15	0.45
9:C:105:PHE:CZ	9:C:127:LEU:HD22	2.48	0.45
1:2:624:MET:HG2	1:2:646:ILE:CD1	2.47	0.45
1:2:828:PHE:CZ	11:E:516:LYS:HG2	2.52	0.45
3:4:779:LYS:HA	3:4:779:LYS:HD2	1.71	0.45
3:4:821:ASP:OD1	3:4:821:ASP:N	2.47	0.45
4:5:143:ALA:HB3	4:5:161:ARG:CD	2.46	0.45
4:5:146:ILE:HD12	4:5:160:VAL:HG13	1.99	0.45
5:6:777:TYR:CD1	5:6:780:LEU:HD13	2.51	0.45
5:6:956:GLU:O	5:6:960:LEU:HB2	2.16	0.45
6:7:203:TYR:HE2	6:7:338:THR:HB	1.81	0.45
6:7:273:VAL:O	6:7:273:VAL:HG12	2.16	0.45
6:7:334:HIS:O	6:7:378:ALA:N	2.46	0.45
6:7:451:ARG:HA	6:7:452:GLY:HA3	1.64	0.45
7:A:127:GLU:CD	10:D:193:LEU:HD11	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:199:LEU:CB	7:A:205:LEU:HG	2.45	0.45
8:B:32:THR:C	8:B:62:ASN:HB2	2.40	0.45
8:B:167:HIS:NE2	10:D:267:VAL:CG1	2.79	0.45
10:D:230:ILE:HA	10:D:293:LEU:HA	1.97	0.45
11:E:25:CYS:H	11:E:26:GLN:CB	2.30	0.45
11:E:288:TYR:HA	11:E:291:LEU:HB2	1.98	0.45
11:E:493:ASN:HA	11:E:496:ILE:HD12	1.99	0.45
11:E:536:LEU:HD13	11:E:536:LEU:HA	1.78	0.45
12:F:12:DT:H1'	12:F:13:DT:OP2	2.15	0.45
1:2:400:GLY:H	5:6:629:MET:HE3	1.82	0.45
1:2:788:ARG:O	1:2:791:ALA:HB3	2.16	0.45
1:2:839:LYS:HD2	1:2:839:LYS:HA	1.61	0.45
2:3:533:ILE:O	2:3:534:ALA:HB3	2.16	0.45
3:4:373:ARG:HD3	3:4:373:ARG:HA	1.54	0.45
4:5:149:ARG:NH1	4:5:272:ARG:HG3	2.32	0.45
4:5:398:LYS:NZ	4:5:613:ARG:HD2	2.31	0.45
4:5:442:LYS:O	4:5:449:LEU:HD12	2.17	0.45
4:5:497:MET:HG2	4:5:519:VAL:HG21	1.99	0.45
5:6:791:SER:CB	5:6:835:ILE:HG22	2.41	0.45
6:7:87:GLN:OE1	6:7:214:ARG:NH1	2.49	0.45
6:7:498:MET:HE3	6:7:509:GLU:HB3	1.98	0.45
6:7:677:SER:O	6:7:680:SER:N	2.49	0.45
7:A:135:CYS:O	7:A:139:THR:HG23	2.17	0.45
9:C:6:ILE:HG13	9:C:7:ASP:N	2.32	0.45
10:D:83:LEU:O	10:D:86:ARG:HG2	2.16	0.45
10:D:215:SER:HA	10:D:216:VAL:HA	1.55	0.45
1:2:216:LEU:HD12	1:2:217:GLU:N	2.31	0.45
1:2:288:ARG:HH21	11:E:384:ILE:HG12	1.82	0.45
1:2:419:LYS:HG3	1:2:420:PRO:HD2	1.99	0.45
2:3:96:ILE:HD13	2:3:129:LEU:HD11	1.99	0.45
2:3:363:LEU:HD22	2:3:656:LEU:HD12	1.97	0.45
2:3:436:GLY:O	4:5:506:LYS:HG2	2.17	0.45
3:4:397:ILE:O	3:4:417:LEU:HG	2.17	0.45
3:4:434:GLU:HB3	3:4:467:LYS:O	2.16	0.45
4:5:413:LEU:HB2	4:5:553:ILE:HA	1.99	0.45
4:5:629:ILE:HG22	4:5:648:ILE:CD1	2.47	0.45
5:6:547:ILE:O	5:6:550:GLN:HB2	2.17	0.45
5:6:941:LEU:HA	5:6:944:LYS:CD	2.47	0.45
6:7:67:LEU:HD11	6:7:121:ILE:HG23	1.99	0.45
6:7:677:SER:C	6:7:680:SER:HB3	2.41	0.45
7:A:84:ARG:HH12	10:D:217:ASN:CB	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:E:259:LEU:HD21	11:E:269:ASN:HD22	1.81	0.45
11:E:561:ASP:HB3	11:E:562:LYS:CG	2.47	0.45
11:E:607:MET:O	11:E:610:GLN:HB2	2.17	0.45
1:2:206:THR:HA	1:2:209:ARG:HD3	1.99	0.45
1:2:253:LYS:HA	1:2:253:LYS:CE	2.44	0.45
1:2:614:ASP:HA	1:2:617:ARG:NH1	2.31	0.45
1:2:803:PHE:HB2	1:2:804:PRO:HA	1.98	0.45
2:3:43:ARG:HD3	2:3:136:MET:HE2	1.98	0.45
2:3:377:ILE:O	2:3:381:ILE:HG13	2.16	0.45
2:3:466:ASP:HA	2:3:510:CYS:SG	2.57	0.45
2:3:706:ILE:HD13	6:7:620:HIS:CE1	2.52	0.45
3:4:567:CYS:HB3	3:4:675:ALA:HB3	1.99	0.45
3:4:634:PHE:CZ	3:4:642:ARG:HG2	2.52	0.45
3:4:749:MET:O	3:4:752:SER:OG	2.28	0.45
4:5:44:PHE:HB2	4:5:47:ARG:HB3	1.98	0.45
4:5:411:ASN:HB3	4:5:550:PHE:CD1	2.52	0.45
4:5:585:ASN:O	4:5:589:GLU:HG2	2.16	0.45
5:6:112:ARG:HH22	5:6:183:LYS:CG	2.25	0.45
5:6:611:ALA:N	5:6:624:GLU:HG2	2.32	0.45
5:6:823:PHE:O	5:6:826:GLU:HB2	2.17	0.45
10:D:274:ILE:HG13	10:D:274:ILE:O	2.16	0.45
11:E:29:ILE:CD1	11:E:31:VAL:HG23	2.42	0.45
11:E:97:GLU:HA	11:E:98:ILE:C	2.42	0.45
11:E:125:ALA:HB2	11:E:249:ASN:O	2.16	0.45
11:E:147:THR:OG1	11:E:148:VAL:N	2.50	0.45
11:E:414:GLY:O	11:E:417:GLY:N	2.37	0.45
1:2:571:ALA:HB3	5:6:664:ALA:O	2.16	0.45
1:2:574:VAL:C	1:2:576:LEU:H	2.23	0.45
1:2:581:ARG:HH22	5:6:621:TYR:HB3	1.79	0.45
1:2:667:VAL:HG22	1:2:669:LEU:H	1.82	0.45
2:3:405:ILE:HD13	2:3:513:ILE:HD11	1.99	0.45
3:4:202:LYS:HB3	3:4:203:TYR:CB	2.32	0.45
3:4:348:LYS:HG2	3:4:354:HIS:O	2.17	0.45
4:5:68:LEU:CD2	4:5:76:TYR:HB2	2.47	0.45
4:5:369:ILE:HD11	4:5:592:SER:C	2.42	0.45
4:5:568:ILE:O	4:5:571:HIS:HB3	2.17	0.45
5:6:721:GLU:OE1	5:6:721:GLU:N	2.42	0.45
7:A:135:CYS:O	7:A:138:ILE:HG22	2.17	0.45
7:A:165:VAL:HG11	7:A:205:LEU:HD22	1.99	0.45
9:C:79:MET:HE2	9:C:79:MET:HB3	1.71	0.45
11:E:286:GLN:NE2	11:E:597:THR:HG21	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:E:310:VAL:HG13	11:E:311:LYS:HD2	1.98	0.45
1:2:203:VAL:O	1:2:206:THR:OG1	2.24	0.45
1:2:339:PHE:HD1	1:2:341:CYS:H	1.65	0.45
1:2:693:GLU:H	1:2:693:GLU:HG3	1.65	0.45
2:3:410:ASP:OD1	2:3:522:GLN:HA	2.17	0.45
4:5:91:GLU:HA	4:5:94:ILE:CG1	2.46	0.45
5:6:610:ALA:H	5:6:663:ILE:HG21	1.81	0.45
7:A:84:ARG:HD3	7:A:84:ARG:HA	1.75	0.45
8:B:107:THR:HG23	8:B:108:HIS:CE1	2.52	0.45
9:C:20:PHE:HA	9:C:72:VAL:HA	1.98	0.45
9:C:101:ASN:HB2	9:C:102:SER:C	2.42	0.45
10:D:262:ASP:OD1	10:D:263:LEU:N	2.49	0.45
11:E:585:THR:HB	11:E:601:ILE:HD11	1.99	0.45
1:2:481:GLU:O	1:2:485:ARG:HG2	2.17	0.45
1:2:586:THR:O	1:2:586:THR:OG1	2.34	0.45
2:3:39:ARG:NH2	2:3:132:LEU:HD11	2.29	0.45
2:3:245:TYR:C	6:7:236:GLY:HA3	2.41	0.45
3:4:191:THR:HG23	3:4:192:THR:HG23	1.98	0.45
3:4:688:VAL:HG22	3:4:838:THR:HG22	1.99	0.45
4:5:353:GLU:HB3	4:5:357:PHE:CE2	2.52	0.45
4:5:455:ARG:HH11	4:5:460:ARG:HD2	1.81	0.45
5:6:786:GLN:HG3	5:6:787:GLY:HA2	1.99	0.45
6:7:404:LEU:HD21	6:7:414:LEU:HD11	1.98	0.45
8:B:169:GLN:HG2	10:D:275:TYR:CE1	2.52	0.45
9:C:76:PRO:HA	9:C:77:PRO:HD3	1.81	0.45
10:D:220:ASP:HA	10:D:222:PRO:HD2	1.98	0.45
11:E:15:ILE:HD13	11:E:121:TYR:HE2	1.82	0.45
11:E:495:GLY:HA2	11:E:498:LEU:HB2	1.99	0.45
1:2:609:PHE:CZ	1:2:648:ALA:HB1	2.52	0.45
2:3:674:GLU:HB3	2:3:723:LYS:HB2	1.99	0.45
3:4:624:SER:O	3:4:625:ASP:C	2.59	0.45
3:4:631:ILE:H	3:4:673:ALA:HA	1.82	0.45
3:4:761:ILE:O	3:4:817:VAL:HG12	2.17	0.45
3:4:769:GLU:OE1	3:4:823:GLN:NE2	2.50	0.45
4:5:179:LEU:HD22	4:5:243:ILE:HG12	1.99	0.45
5:6:650:VAL:HA	5:6:653:HIS:HB3	1.99	0.45
5:6:665:LYS:NZ	12:F:14:DT:OP1	2.36	0.45
11:E:248:VAL:HG12	11:E:249:ASN:CG	2.42	0.45
11:E:615:GLU:OE1	11:E:643:LYS:HB3	2.16	0.45
11:E:622:ILE:O	11:E:622:ILE:HG22	2.17	0.45
1:2:656:ARG:HB2	5:6:794:ARG:HH22	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:229:ALA:HB1	6:7:370:LEU:CD2	2.46	0.44
2:3:474:GLU:HG3	4:5:491:VAL:HG11	1.98	0.44
2:3:497:ILE:O	2:3:503:HIS:HA	2.17	0.44
3:4:264:TYR:CE2	6:7:135:LYS:HE2	2.52	0.44
4:5:420:THR:HG23	4:5:556:VAL:HG11	2.00	0.44
5:6:168:MET:O	5:6:171:SER:N	2.48	0.44
5:6:293:THR:HG23	5:6:392:GLY:HA2	1.98	0.44
5:6:362:GLN:HA	5:6:376:THR:HG21	1.98	0.44
6:7:411:TYR:HD1	6:7:702:LEU:HD12	1.83	0.44
7:A:105:ASN:HB3	7:A:110:MET:SD	2.56	0.44
7:A:134:TYR:O	7:A:137:LEU:HB3	2.18	0.44
8:B:51:GLN:N	8:B:52:LEU:HA	2.32	0.44
10:D:161:LEU:HD21	10:D:168:LEU:O	2.17	0.44
11:E:34:LEU:HD11	11:E:543:LEU:HG	1.99	0.44
11:E:154:GLU:CD	11:E:240:TYR:HB2	2.42	0.44
11:E:163:LEU:HA	11:E:164:GLU:HA	1.70	0.44
1:2:208:ALA:HA	1:2:211:LEU:HG	1.99	0.44
1:2:327:ARG:HE	1:2:420:PRO:HD3	1.83	0.44
1:2:480:GLU:HB3	1:2:765:LYS:HE2	1.98	0.44
1:2:850:LYS:HG3	1:2:851:VAL:N	2.31	0.44
2:3:24:ARG:CZ	2:3:121:PHE:HE1	2.30	0.44
2:3:245:TYR:CZ	6:7:357:PRO:HG2	2.53	0.44
2:3:524:ASP:OD1	2:3:532:ASN:ND2	2.50	0.44
3:4:677:PRO:HB3	3:4:682:TYR:HB3	1.99	0.44
3:4:767:LYS:O	3:4:771:VAL:HB	2.17	0.44
3:4:854:LYS:HB3	3:4:857:ILE:HD11	1.99	0.44
4:5:156:VAL:HG22	4:5:298:TYR:CD2	2.50	0.44
4:5:374:ILE:HD13	4:5:388:ILE:HB	1.99	0.44
5:6:169:ALA:O	5:6:173:GLN:HB2	2.18	0.44
6:7:18:PHE:CZ	6:7:120:ALA:HB2	2.52	0.44
6:7:355:PHE:CZ	6:7:374:THR:HG21	2.52	0.44
6:7:451:ARG:HB2	6:7:453:ASP:N	2.32	0.44
7:A:108:ASP:H	7:A:109:LEU:C	2.26	0.44
11:E:131:LEU:HD22	11:E:237:LEU:HD11	1.98	0.44
11:E:577:ASP:O	11:E:633:ARG:HA	2.17	0.44
1:2:286:TYR:HA	1:2:289:ILE:CB	2.45	0.44
2:3:169:ARG:NH2	2:3:272:ARG:HH12	2.15	0.44
3:4:388:ARG:NH2	5:6:176:ARG:HD2	2.32	0.44
3:4:718:ARG:O	3:4:722:LYS:HG2	2.17	0.44
4:5:184:ARG:NH1	4:5:239:ASP:O	2.51	0.44
4:5:286:VAL:HG11	4:5:292:VAL:HG11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:345:SER:OG	4:5:346:VAL:N	2.51	0.44
4:5:402:ASP:O	4:5:404:MET:N	2.51	0.44
4:5:477:VAL:HG11	4:5:519:VAL:HG22	2.00	0.44
5:6:134:LYS:CB	5:6:137:ARG:H	2.29	0.44
5:6:142:PHE:HA	5:6:145:ILE:HG12	1.99	0.44
5:6:794:ARG:HD3	5:6:794:ARG:HA	1.78	0.44
6:7:228:ARG:HD3	6:7:228:ARG:HA	1.77	0.44
6:7:247:ARG:CZ	6:7:502:VAL:HG21	2.47	0.44
6:7:362:GLY:HA2	6:7:363:PHE:CG	2.52	0.44
6:7:472:ALA:O	6:7:476:ILE:HD12	2.13	0.44
6:7:543:GLN:CG	6:7:544:GLN:H	2.28	0.44
6:7:571:TYR:HA	6:7:572:GLY:HA2	1.70	0.44
7:A:30:PRO:C	7:A:122:ASN:HD21	2.23	0.44
8:B:102:ILE:HG22	8:B:148:LEU:HG	1.99	0.44
9:C:33:ASN:HB3	9:C:34:PRO:HD3	1.99	0.44
10:D:66:SER:O	10:D:70:GLU:HB2	2.18	0.44
10:D:200:LYS:HB2	10:D:201:TYR:CD2	2.53	0.44
10:D:286:LEU:HD21	10:D:293:LEU:HD11	1.98	0.44
11:E:27:LEU:HA	11:E:80:SER:O	2.17	0.44
2:3:33:ASP:HB2	2:3:39:ARG:NH1	2.31	0.44
2:3:115:LEU:HA	2:3:179:LEU:HB3	1.99	0.44
2:3:138:ASP:OD2	2:3:140:PRO:HD2	2.17	0.44
3:4:627:GLY:O	3:4:669:SER:HB2	2.18	0.44
3:4:630:CYS:C	3:4:631:ILE:HG12	2.42	0.44
3:4:728:TYR:CG	3:4:729:LEU:N	2.83	0.44
4:5:296:GLY:HA2	4:5:331:LEU:H	1.81	0.44
5:6:575:GLY:HA3	5:6:715:ILE:O	2.18	0.44
5:6:662:SER:HB3	5:6:670:ALA:O	2.18	0.44
5:6:787:GLY:O	5:6:790:ARG:HB2	2.17	0.44
5:6:948:LEU:CD1	5:6:954:TYR:HA	2.48	0.44
6:7:260:TYR:HD1	6:7:298:LEU:HD13	1.81	0.44
6:7:374:THR:O	6:7:375:TYR:HB3	2.17	0.44
6:7:493:LEU:CD2	6:7:533:ASP:HB3	2.48	0.44
6:7:498:MET:O	6:7:499:LYS:C	2.60	0.44
6:7:595:ASP:OD1	6:7:595:ASP:N	2.44	0.44
7:A:167:VAL:HG13	7:A:170:ASP:HB2	2.00	0.44
1:2:342:LEU:HD11	1:2:376:ASN:HD21	1.82	0.44
1:2:547:THR:HG21	1:2:683:VAL:HB	1.99	0.44
1:2:551:GLN:OE1	5:6:563:ILE:HG21	2.18	0.44
1:2:567:THR:O	1:2:606:ILE:HA	2.18	0.44
1:2:826:SER:C	1:2:828:PHE:H	2.25	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:21:PHE:CE1	2:3:124:PRO:HD3	2.52	0.44
3:4:376:CYS:HA	3:4:377:ASN:C	2.42	0.44
3:4:431:ASP:HB3	3:4:433:ILE:CD1	2.48	0.44
4:5:34:PHE:HA	4:5:71:TYR:CZ	2.53	0.44
4:5:331:LEU:HA	4:5:332:GLY:HA2	1.61	0.44
5:6:124:VAL:HG21	5:6:133:GLU:H	1.82	0.44
5:6:512:GLU:O	5:6:516:LEU:HG	2.18	0.44
5:6:561:GLU:N	5:6:562:GLY:CA	2.79	0.44
5:6:585:LEU:HA	5:6:585:LEU:HD23	1.55	0.44
5:6:655:ALA:O	5:6:659:GLN:HA	2.18	0.44
5:6:758:ALA:HA	5:6:761:PHE:CD2	2.53	0.44
5:6:806:LEU:HB3	5:6:827:ALA:HB1	1.99	0.44
6:7:476:ILE:O	6:7:639:ARG:HD3	2.17	0.44
6:7:486:LYS:NZ	6:7:530:ASP:OD2	2.33	0.44
7:A:36:ILE:O	7:A:40:ILE:HG13	2.17	0.44
7:A:92:LEU:O	7:A:96:ILE:HG22	2.17	0.44
10:D:146:CYS:O	10:D:149:SER:OG	2.31	0.44
10:D:151:ILE:HA	10:D:158:LEU:HD11	1.99	0.44
11:E:240:TYR:C	11:E:242:SER:H	2.26	0.44
1:2:437:ASN:O	1:2:437:ASN:ND2	2.35	0.44
1:2:625:GLU:OE1	13:5:801:ANP:N3B	2.50	0.44
2:3:154:LYS:HD3	2:3:154:LYS:HA	1.61	0.44
3:4:710:ASP:OD1	6:7:672:LYS:NZ	2.35	0.44
3:4:833:ILE:HA	3:4:836:TYR:CD2	2.52	0.44
4:5:264:LEU:HA	4:5:265:VAL:HA	1.79	0.44
4:5:385:LYS:HA	4:5:388:ILE:HD12	1.98	0.44
4:5:498:GLU:OE1	4:5:498:GLU:N	2.51	0.44
5:6:581:LYS:HD3	5:6:681:ALA:HB1	1.99	0.44
5:6:807:SER:HA	5:6:810:ILE:HB	1.99	0.44
6:7:235:LEU:HD23	6:7:235:LEU:HA	1.68	0.44
6:7:240:THR:HA	6:7:352:THR:HG22	1.99	0.44
6:7:309:ALA:O	6:7:336:ASN:HA	2.18	0.44
7:A:12:GLU:O	7:A:15:ARG:HG2	2.18	0.44
9:C:52:ARG:HG3	9:C:114:LEU:HD13	2.00	0.44
11:E:541:ASN:ND2	11:E:543:LEU:HB2	2.32	0.44
1:2:271:PHE:CE2	1:2:295:VAL:HG21	2.52	0.44
1:2:395:GLY:HA2	5:6:672:LEU:HA	1.99	0.44
1:2:856:GLN:NE2	1:2:856:GLN:O	2.50	0.44
2:3:414:ALA:H	13:3:1001:ANP:H5'2	1.83	0.44
2:3:558:ASP:OD2	4:5:627:VAL:HA	2.18	0.44
3:4:331:LEU:CD1	6:7:553:ILE:HG12	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:455:SER:HB3	6:7:276:ARG:O	2.18	0.44
3:4:597:SER:HB2	3:4:640:SER:OG	2.17	0.44
3:4:862:GLN:NE2	3:4:909:ARG:HB3	2.33	0.44
4:5:338:GLU:HG2	4:5:340:SER:HG	1.82	0.44
4:5:412:VAL:O	4:5:521:ALA:N	2.35	0.44
5:6:175:TYR:HA	5:6:178:LEU:HD13	2.00	0.44
5:6:793:TYR:HB3	5:6:795:ILE:HA	1.99	0.44
6:7:362:GLY:HA2	6:7:363:PHE:CB	2.47	0.44
7:A:83:LYS:HE2	10:D:206:LEU:HB3	2.00	0.44
8:B:7:LEU:HD11	8:B:12:SER:HB2	1.98	0.44
8:B:108:HIS:O	8:B:155:LYS:NZ	2.29	0.44
8:B:182:ARG:N	8:B:183:PRO:HD2	2.33	0.44
9:C:75:LEU:HG	9:C:76:PRO:HD2	2.00	0.44
10:D:220:ASP:HA	10:D:221:GLU:HA	1.56	0.44
1:2:341:CYS:N	1:2:342:LEU:HA	2.32	0.44
1:2:591:LEU:HB3	4:5:270:MET:CE	2.47	0.44
2:3:127:LYS:O	2:3:131:ASP:HB2	2.18	0.44
2:3:139:VAL:HB	2:3:140:PRO:HD3	1.98	0.44
3:4:331:LEU:HD13	6:7:553:ILE:HG12	2.00	0.44
3:4:512:VAL:HG13	3:4:515:ARG:NH1	2.32	0.44
3:4:682:TYR:HB2	3:4:691:ASN:ND2	2.32	0.44
3:4:688:VAL:HG11	3:4:836:TYR:HA	1.99	0.44
4:5:677:VAL:HG12	4:5:681:ILE:CD1	2.48	0.44
5:6:178:LEU:N	5:6:179:PRO:HD2	2.33	0.44
5:6:559:THR:O	5:6:559:THR:OG1	2.32	0.44
5:6:584:PHE:O	5:6:587:TYR:HB3	2.17	0.44
5:6:937:VAL:O	5:6:941:LEU:HG	2.17	0.44
8:B:176:LEU:HD21	9:C:191:MET:HE2	2.00	0.44
10:D:63:LEU:HD11	10:D:140:ILE:HG22	2.00	0.44
11:E:433:GLU:H	11:E:433:GLU:CD	2.24	0.44
1:2:485:ARG:NH1	1:2:825:LEU:HD23	2.33	0.44
1:2:538:ASN:CB	1:2:677:PHE:HA	2.41	0.44
1:2:767:ILE:O	1:2:771:ARG:HG3	2.18	0.44
2:3:48:TYR:HD2	2:3:92:LEU:HG	1.83	0.44
2:3:411:PRO:HB3	13:3:1001:ANP:O2G	2.18	0.44
3:4:395:GLN:HG2	3:4:396:VAL:H	1.83	0.44
3:4:568:GLY:O	3:4:677:PRO:HD2	2.18	0.44
4:5:86:ILE:O	4:5:89:LEU:N	2.50	0.44
5:6:710:ASP:HA	5:6:711:LEU:HA	1.39	0.44
6:7:24:PHE:HD1	6:7:88:TYR:CD2	2.36	0.44
6:7:335:VAL:HG11	6:7:340:VAL:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:490:GLY:C	6:7:494:THR:CG2	2.85	0.44
7:A:33:HIS:O	7:A:37:ILE:HG12	2.18	0.44
7:A:149:ILE:HG23	7:A:151:LEU:N	2.33	0.44
8:B:18:PHE:O	8:B:22:ASN:ND2	2.51	0.44
8:B:57:ASP:OD1	8:B:58:LYS:N	2.51	0.44
8:B:185:ILE:HG22	8:B:189:MET:HG2	1.98	0.44
9:C:27:LEU:CD2	9:C:29:TYR:H	2.31	0.44
10:D:125:PRO:HA	10:D:128:CYS:HB3	2.00	0.44
10:D:229:PHE:HD1	10:D:276:VAL:HG21	1.82	0.44
11:E:26:GLN:O	11:E:79:ASN:N	2.51	0.44
11:E:34:LEU:HD11	11:E:543:LEU:CG	2.48	0.44
11:E:540:ARG:HH22	11:E:574:GLU:CA	2.31	0.44
1:2:246:TYR:CE2	1:2:300:PHE:CD1	3.06	0.43
1:2:246:TYR:OH	1:2:257:ALA:HB1	2.18	0.43
1:2:563:ALA:HA	1:2:603:VAL:O	2.17	0.43
2:3:372:TYR:OH	2:3:560:SER:O	2.24	0.43
2:3:420:ARG:O	2:3:423:LEU:HB3	2.17	0.43
2:3:475:PHE:CE1	2:3:486:ILE:HD13	2.53	0.43
3:4:345:ALA:HA	3:4:389:CYS:HB3	1.98	0.43
3:4:349:CYS:HB2	3:4:351:VAL:O	2.17	0.43
3:4:824:GLU:HA	3:4:827:ARG:CB	2.44	0.43
4:5:342:ILE:HA	4:5:343:TRP:HA	1.57	0.43
4:5:438:TYR:HA	4:5:478:CYS:HB2	1.99	0.43
4:5:531:ASP:OD2	4:5:539:ASN:ND2	2.51	0.43
4:5:640:SER:O	4:5:640:SER:OG	2.30	0.43
5:6:417:PRO:O	5:6:448:LEU:N	2.50	0.43
5:6:819:ILE:HG22	5:6:820:THR:N	2.26	0.43
5:6:830:LEU:HA	5:6:833:GLN:OE1	2.18	0.43
6:7:152:ARG:HH21	6:7:153:MET:HE1	1.81	0.43
6:7:203:TYR:CE2	6:7:339:LEU:HG	2.53	0.43
6:7:292:ASN:OD1	6:7:293:GLN:HB2	2.18	0.43
6:7:493:LEU:CD2	6:7:533:ASP:CG	2.84	0.43
9:C:112:ILE:HG23	9:C:113:MET:CE	2.47	0.43
9:C:139:ALA:HB1	9:C:184:TYR:CZ	2.53	0.43
11:E:25:CYS:N	11:E:26:GLN:HA	2.33	0.43
1:2:774:ILE:HG12	1:2:825:LEU:HA	1.99	0.43
2:3:98:ILE:HB	2:3:157:PHE:HD1	1.83	0.43
2:3:167:SER:HB3	2:3:168:PRO:HD2	2.00	0.43
2:3:244:GLU:HB3	2:3:247:TYR:HB3	2.01	0.43
3:4:437:GLY:CA	3:4:464:VAL:H	2.31	0.43
3:4:670:SER:C	3:4:671:ILE:HG13	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:909:ARG:CZ	5:6:685:VAL:HB	2.48	0.43
4:5:329:LYS:HD2	4:5:329:LYS:HA	1.79	0.43
4:5:617:GLN:O	4:5:620:GLU:HG2	2.18	0.43
5:6:117:GLN:CD	5:6:161:ARG:HH21	2.26	0.43
5:6:400:VAL:CG2	5:6:455:LEU:C	2.91	0.43
5:6:594:ARG:HD2	5:6:633:ASN:O	2.17	0.43
5:6:695:LEU:HA	5:6:698:ASN:CB	2.44	0.43
6:7:370:LEU:HD22	6:7:370:LEU:HA	1.69	0.43
7:A:110:MET:SD	7:A:113:ILE:HG13	2.58	0.43
10:D:70:GLU:OE2	10:D:147:ARG:HG2	2.18	0.43
11:E:38:ALA:HA	11:E:251:ILE:HD11	1.99	0.43
11:E:340:TYR:HB3	11:E:503:GLN:HE21	1.83	0.43
11:E:384:ILE:O	11:E:388:LEU:HB2	2.18	0.43
11:E:429:THR:HA	11:E:432:LEU:CD1	2.48	0.43
1:2:506:TYR:OH	1:2:694:ARG:HD3	2.18	0.43
2:3:279:ASP:H	2:3:282:LEU:HD12	1.83	0.43
2:3:368:ALA:CB	2:3:378:LYS:HE3	2.48	0.43
2:3:449:ASP:HA	2:3:454:GLU:O	2.18	0.43
3:4:521:LEU:HD11	3:4:741:VAL:HB	2.00	0.43
3:4:774:TYR:CG	3:4:798:LEU:HD22	2.54	0.43
4:5:176:ALA:CB	4:5:194:ILE:HG21	2.48	0.43
4:5:577:THR:HG23	4:5:577:THR:O	2.18	0.43
4:5:652:GLN:HE21	4:5:652:GLN:HB3	1.67	0.43
5:6:266:SER:HB2	5:6:458:HIS:CD2	2.53	0.43
5:6:399:GLY:O	5:6:400:VAL:HG23	2.18	0.43
6:7:201:PHE:CZ	6:7:337:GLY:HA2	2.53	0.43
10:D:69:ASN:O	10:D:73:SER:HB3	2.18	0.43
10:D:154:PHE:O	10:D:158:LEU:HG	2.18	0.43
11:E:79:ASN:OD1	11:E:80:SER:OG	2.23	0.43
11:E:131:LEU:HD21	11:E:240:TYR:HD2	1.83	0.43
11:E:251:ILE:O	11:E:255:ILE:HG13	2.18	0.43
11:E:558:GLU:N	11:E:559:SER:HA	2.32	0.43
11:E:575:ASN:C	11:E:576:THR:HG23	2.42	0.43
1:2:204:SER:O	1:2:207:ILE:HB	2.18	0.43
1:2:339:PHE:CD2	1:2:376:ASN:HB3	2.53	0.43
2:3:122:ILE:O	2:3:126:GLU:HB2	2.19	0.43
2:3:695:SER:HB3	2:3:696:PRO:HA	2.00	0.43
3:4:351:VAL:HA	3:4:352:CYS:HA	1.55	0.43
5:6:194:PRO:O	5:6:261:ARG:NE	2.51	0.43
5:6:533:ILE:HG12	5:6:548:LEU:HD21	1.99	0.43
5:6:689:TYR:HB2	5:6:716:LEU:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:146:ARG:HH12	6:7:304:ALA:HA	1.84	0.43
6:7:484:THR:OG1	6:7:485:GLY:N	2.50	0.43
9:C:180:SER:O	9:C:183:SER:OG	2.15	0.43
10:D:168:LEU:HD11	10:D:173:ASP:CG	2.43	0.43
10:D:205:GLU:OE1	10:D:205:GLU:N	2.46	0.43
11:E:25:CYS:H	11:E:26:GLN:HA	1.83	0.43
11:E:285:ALA:HB3	11:E:286:GLN:CA	2.47	0.43
1:2:577:THR:OG1	5:6:666:ALA:HB2	2.18	0.43
2:3:138:ASP:HB3	2:3:140:PRO:HD2	2.00	0.43
2:3:227:THR:N	2:3:228:PRO:CD	2.81	0.43
2:3:374:HIS:O	2:3:378:LYS:HG2	2.19	0.43
2:3:520:PHE:HB3	2:3:527:ARG:NH2	2.32	0.43
3:4:239:SER:OG	3:4:240:ASN:N	2.41	0.43
5:6:122:PHE:CD1	5:6:124:VAL:HB	2.54	0.43
5:6:122:PHE:CG	5:6:124:VAL:HB	2.54	0.43
5:6:532:SER:HB3	5:6:745:PRO:HG2	1.99	0.43
5:6:729:SER:HG	5:6:730:HIS:H	1.64	0.43
6:7:101:ASP:OD2	6:7:105:ALA:N	2.51	0.43
6:7:541:MET:HB2	6:7:593:ARG:HD3	2.00	0.43
7:A:29:LEU:HD23	7:A:93:ARG:CD	2.49	0.43
7:A:73:PHE:CE2	9:C:53:ILE:HG13	2.54	0.43
7:A:108:ASP:CB	7:A:109:LEU:CB	2.62	0.43
9:C:109:ILE:HA	9:C:112:ILE:HG22	2.00	0.43
9:C:131:ARG:HD3	9:C:131:ARG:HA	1.71	0.43
11:E:276:GLY:O	11:E:279:SER:HB3	2.19	0.43
11:E:286:GLN:HA	11:E:286:GLN:OE1	2.18	0.43
11:E:328:LEU:HD11	11:E:499:ALA:HB3	2.01	0.43
11:E:388:LEU:HG	11:E:392:PHE:CZ	2.53	0.43
1:2:213:SER:HA	1:2:217:GLU:OE1	2.17	0.43
1:2:334:LEU:HA	1:2:382:TYR:CE1	2.53	0.43
1:2:520:PHE:CE1	1:2:823:MET:HG2	2.53	0.43
1:2:535:GLY:C	1:2:815:ARG:HD2	2.43	0.43
2:3:317:PHE:CE2	4:5:176:ALA:HB2	2.54	0.43
2:3:518:PRO:CG	2:3:524:ASP:HB2	2.49	0.43
4:5:207:LEU:HA	4:5:208:PRO:HD2	1.81	0.43
4:5:413:LEU:HD12	4:5:413:LEU:N	2.34	0.43
5:6:173:GLN:O	5:6:176:ARG:HB3	2.19	0.43
6:7:147:ARG:HH22	6:7:192:PHE:HB2	1.83	0.43
7:A:2:TYR:HH	7:A:75:THR:HA	1.82	0.43
11:E:579:TYR:CD1	11:E:637:LEU:CD2	3.02	0.43
1:2:271:PHE:HE2	1:2:295:VAL:HG11	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:628:SER:OG	1:2:629:ILE:N	2.51	0.43
2:3:216:ASP:OD2	2:3:218:THR:OG1	2.36	0.43
2:3:400:ARG:HE	2:3:707:ARG:NH2	2.17	0.43
3:4:443:PRO:HD3	3:4:457:TYR:CZ	2.54	0.43
4:5:130:ASN:HA	4:5:131:SER:HA	1.79	0.43
4:5:375:ALA:HA	4:5:376:PRO:HD2	1.89	0.43
4:5:397:LYS:NZ	4:5:399:ILE:HD11	2.34	0.43
5:6:541:GLU:O	5:6:544:LYS:HG2	2.19	0.43
5:6:915:MET:HA	5:6:918:ARG:HB2	2.01	0.43
6:7:441:ASP:OD1	6:7:442:LYS:N	2.51	0.43
6:7:470:LEU:HD23	6:7:470:LEU:HA	1.62	0.43
6:7:689:LEU:HD12	6:7:692:ILE:HG21	2.00	0.43
7:A:7:ASN:HA	7:A:10:VAL:CG1	2.48	0.43
7:A:87:LEU:HD23	10:D:198:ILE:HD11	2.00	0.43
7:A:105:ASN:HA	7:A:106:GLY:HA3	1.71	0.43
8:B:77:LEU:HD21	8:B:129:LYS:HE3	1.99	0.43
11:E:126:HIS:O	11:E:127:ARG:NH1	2.46	0.43
11:E:487:ARG:HG3	11:E:488:LYS:N	2.33	0.43
1:2:685:ASP:OD1	1:2:685:ASP:N	2.50	0.43
2:3:195:LYS:HA	6:7:371:LEU:HA	2.00	0.43
2:3:342:LEU:HD21	2:3:661:GLN:HE21	1.84	0.43
2:3:439:GLY:HA3	2:3:442:LEU:HB2	2.00	0.43
2:3:689:ASP:O	2:3:692:THR:OG1	2.35	0.43
3:4:239:SER:OG	3:4:301:TYR:HA	2.18	0.43
3:4:579:GLN:HG3	6:7:542:GLU:HG3	2.01	0.43
3:4:714:GLU:HG3	3:4:718:ARG:HH12	1.84	0.43
3:4:858:GLN:OE1	3:4:906:ALA:HB2	2.19	0.43
4:5:149:ARG:HG3	4:5:265:VAL:O	2.18	0.43
4:5:386:LYS:NZ	4:5:679:GLU:OE2	2.52	0.43
4:5:430:GLU:OE1	4:5:431:LYS:HG2	2.18	0.43
5:6:399:GLY:C	5:6:400:VAL:HG22	2.43	0.43
5:6:912:MET:HB3	5:6:964:VAL:HG21	2.00	0.43
6:7:269:VAL:HG21	6:7:285:THR:CB	2.49	0.43
6:7:372:THR:O	6:7:373:GLU:HB3	2.17	0.43
6:7:411:TYR:OH	6:7:430:LYS:HG3	2.18	0.43
6:7:442:LYS:HA	6:7:442:LYS:HD2	1.80	0.43
7:A:41:LEU:HA	7:A:44:VAL:HG12	2.01	0.43
7:A:102:TRP:CE3	7:A:151:LEU:HD23	2.54	0.43
7:A:199:LEU:HA	7:A:202:GLN:CB	2.48	0.43
8:B:165:GLU:HA	8:B:166:SER:HA	1.49	0.43
8:B:181:LEU:HD13	8:B:185:ILE:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:E:268:SER:O	11:E:272:LEU:HG	2.18	0.43
11:E:316:LEU:HD11	11:E:414:GLY:CA	2.49	0.43
1:2:307:ARG:NH1	1:2:398:PRO:HG3	2.33	0.43
1:2:600:ASP:HB3	4:5:268:GLY:HA2	1.99	0.43
1:2:778:LEU:HA	1:2:829:VAL:HB	2.01	0.43
2:3:276:VAL:HG21	2:3:294:VAL:HG11	2.00	0.43
2:3:298:PHE:CD1	2:3:321:ILE:HG12	2.43	0.43
2:3:490:MET:HE1	2:3:543:PHE:CE1	2.53	0.43
4:5:166:ILE:HA	4:5:258:LEU:HA	2.01	0.43
4:5:300:ILE:HG22	4:5:324:ARG:HB2	2.00	0.43
4:5:347:THR:CB	4:5:349:PHE:HA	2.47	0.43
5:6:261:ARG:HD2	5:6:263:PHE:CE1	2.50	0.43
5:6:284:ILE:HG13	5:6:402:ILE:HA	2.01	0.43
5:6:403:VAL:HG11	5:6:450:TYR:HB3	2.01	0.43
6:7:192:PHE:HB3	6:7:196:LEU:HD13	2.00	0.43
9:C:181:HIS:ND1	9:C:185:LYS:HD2	2.34	0.43
11:E:291:LEU:O	11:E:295:LEU:HG	2.18	0.43
1:2:202:ASN:O	1:2:205:ARG:HB3	2.18	0.43
1:2:670:THR:OG1	1:2:672:PRO:HD2	2.19	0.43
1:2:783:MET:SD	1:2:834:LEU:HD11	2.58	0.43
2:3:464:LEU:HD12	2:3:464:LEU:HA	1.89	0.43
3:4:282:SER:O	3:4:285:VAL:HG22	2.18	0.43
3:4:332:VAL:O	3:4:429:ALA:HB1	2.18	0.43
3:4:363:GLY:O	3:4:364:VAL:HG13	2.18	0.43
3:4:501:ILE:HG21	3:4:506:LEU:HD21	2.01	0.43
3:4:559:ARG:HB3	3:4:560:GLY:H	1.58	0.43
3:4:683:ASN:ND2	3:4:686:LEU:HD22	2.31	0.43
4:5:36:LEU:HD22	4:5:47:ARG:CZ	2.49	0.43
4:5:559:ASP:HB2	4:5:561:ASN:HD21	1.83	0.43
4:5:571:HIS:HA	4:5:581:ASN:HD21	1.84	0.43
5:6:599:SER:HA	5:6:639:ASP:H	1.83	0.43
6:7:24:PHE:CE1	6:7:85:ILE:HA	2.53	0.43
6:7:463:GLY:C	6:7:465:ALA:N	2.77	0.43
6:7:528:LYS:HD2	6:7:528:LYS:N	2.34	0.43
8:B:147:ASP:O	8:B:150:GLU:HB3	2.19	0.43
9:C:29:TYR:HE2	9:C:44:LEU:HD13	1.83	0.43
10:D:256:TYR:HD1	10:D:257:THR:OG1	2.02	0.43
11:E:316:LEU:HD11	11:E:413:LEU:C	2.43	0.43
11:E:536:LEU:HA	11:E:539:TYR:HD2	1.84	0.43
1:2:311:GLU:OE1	1:2:311:GLU:N	2.42	0.42
1:2:497:ILE:H	1:2:497:ILE:HG13	1.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:347:ILE:HG12	2:3:351:ASN:HD21	1.84	0.42
2:3:487:HIS:NE2	2:3:539:LEU:HG	2.34	0.42
2:3:504:THR:HG21	6:7:328:PRO:HB2	2.01	0.42
2:3:555:GLU:HA	2:3:558:ASP:HB3	2.00	0.42
3:4:257:LEU:HA	3:4:260:GLN:HB2	2.00	0.42
3:4:508:LYS:O	3:4:512:VAL:HG23	2.19	0.42
3:4:714:GLU:OE2	6:7:665:ILE:HG21	2.18	0.42
4:5:50:LEU:HD12	4:5:50:LEU:HA	1.73	0.42
4:5:151:LEU:HA	4:5:155:HIS:NE2	2.33	0.42
4:5:179:LEU:HD12	4:5:192:ILE:HB	2.00	0.42
4:5:421:ALA:HA	13:5:801:ANP:C5'	2.49	0.42
4:5:486:ARG:O	4:5:490:ARG:HB2	2.19	0.42
5:6:287:LEU:HG	5:6:398:THR:CG2	2.49	0.42
5:6:764:ILE:O	5:6:818:GLU:HA	2.19	0.42
6:7:209:GLN:HB3	6:7:212:ALA:HB2	2.01	0.42
7:A:91:ARG:HA	10:D:190:TRP:HH2	1.83	0.42
8:B:112:PHE:HD1	8:B:152:ARG:HG3	1.84	0.42
8:B:149:ARG:NH1	8:B:153:GLN:OE1	2.52	0.42
10:D:273:SER:HB3	10:D:275:TYR:CE1	2.53	0.42
11:E:266:ASN:HB2	11:E:269:ASN:ND2	2.33	0.42
11:E:285:ALA:CB	11:E:288:TYR:HB3	2.47	0.42
1:2:400:GLY:HA2	5:6:629:MET:HE3	2.01	0.42
1:2:631:ILE:HB	1:2:633:LYS:HE2	2.02	0.42
1:2:638:THR:H	4:5:445:SER:N	2.13	0.42
2:3:94:HIS:HB3	2:3:153:TRP:CE3	2.54	0.42
2:3:553:ILE:O	2:3:553:ILE:HG13	2.19	0.42
2:3:662:TYR:CE1	2:3:666:ARG:HD2	2.54	0.42
3:4:276:ILE:HA	3:4:279:CYS:HB2	2.01	0.42
3:4:311:CYS:HB3	3:4:326:ILE:HG23	2.01	0.42
3:4:630:CYS:HA	3:4:672:LEU:O	2.19	0.42
4:5:176:ALA:HA	4:5:250:PHE:HD1	1.82	0.42
5:6:144:LYS:HE2	5:6:194:PRO:HD2	2.01	0.42
5:6:328:THR:HA	5:6:329:GLU:HA	1.80	0.42
5:6:948:LEU:HD11	5:6:954:TYR:HA	2.01	0.42
6:7:333:ILE:HD13	6:7:376:LEU:HD23	2.01	0.42
6:7:422:ILE:O	6:7:422:ILE:HG13	2.18	0.42
6:7:493:LEU:CD2	6:7:533:ASP:CB	2.97	0.42
7:A:114:THR:C	7:A:116:SER:H	2.27	0.42
9:C:84:VAL:O	9:C:88:ILE:HG23	2.19	0.42
10:D:136:LEU:O	10:D:139:VAL:HB	2.19	0.42
10:D:218:MET:HA	10:D:219:ILE:C	2.43	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:D:285:LEU:HD22	10:D:290:LYS:HD2	2.00	0.42
11:E:288:TYR:HA	11:E:291:LEU:CG	2.49	0.42
11:E:295:LEU:O	11:E:299:VAL:HG23	2.19	0.42
11:E:580:LEU:HD11	11:E:629:ILE:HD11	2.01	0.42
1:2:534:ARG:HH11	1:2:815:ARG:NH2	2.17	0.42
1:2:574:VAL:C	5:6:664:ALA:HB1	2.44	0.42
1:2:585:ILE:HG23	1:2:586:THR:N	2.35	0.42
2:3:310:ASN:HA	2:3:311:SER:HA	1.52	0.42
2:3:431:ALA:HB2	2:3:471:CYS:HB2	2.01	0.42
3:4:401:GLU:HG2	3:4:413:HIS:O	2.19	0.42
3:4:552:PHE:HB3	3:4:553:THR:H	1.62	0.42
3:4:800:SER:HA	3:4:803:ARG:HB2	2.01	0.42
4:5:166:ILE:HG13	4:5:292:VAL:HG21	2.01	0.42
5:6:122:PHE:HB2	5:6:124:VAL:CB	2.48	0.42
5:6:292:GLY:O	5:6:394:ARG:HA	2.19	0.42
5:6:915:MET:HE2	5:6:915:MET:HB3	1.90	0.42
6:7:302:THR:C	6:7:305:SER:HG	2.26	0.42
6:7:652:MET:HB2	6:7:652:MET:HE3	1.69	0.42
7:A:47:LEU:HD21	7:A:75:THR:CB	2.48	0.42
8:B:55:THR:OG1	10:D:132:GLU:OE2	2.22	0.42
9:C:174:LYS:O	9:C:177:TYR:HB3	2.19	0.42
10:D:257:THR:HB	10:D:258:VAL:O	2.19	0.42
11:E:81:LEU:HD12	11:E:120:ILE:HG23	2.00	0.42
11:E:274:ILE:HG23	11:E:409:PHE:HD2	1.84	0.42
11:E:540:ARG:O	11:E:580:LEU:HD13	2.19	0.42
1:2:236:GLU:OE2	11:E:361:LYS:HB2	2.20	0.42
1:2:258:LEU:HD12	1:2:261:ALA:HB3	1.99	0.42
1:2:446:VAL:HG13	5:6:301:ARG:HD2	2.01	0.42
1:2:693:GLU:HG2	5:6:778:LYS:HD3	2.01	0.42
1:2:806:THR:HG22	1:2:807:VAL:H	1.85	0.42
2:3:100:LEU:HD21	2:3:157:PHE:CG	2.54	0.42
2:3:437:SER:HA	2:3:440:VAL:N	2.24	0.42
3:4:324:LYS:HZ1	6:7:138:VAL:HG11	1.83	0.42
3:4:572:THR:O	3:4:572:THR:HG22	2.19	0.42
3:4:714:GLU:OE2	6:7:665:ILE:HD13	2.18	0.42
4:5:393:MET:HE2	4:5:666:LEU:HA	2.01	0.42
4:5:395:GLY:N	4:5:409:ASP:HB2	2.35	0.42
5:6:944:LYS:NZ	5:6:957:GLU:O	2.51	0.42
6:7:231:LYS:HG2	6:7:232:GLY:N	2.35	0.42
6:7:499:LYS:HD2	6:7:506:MET:H	1.85	0.42
6:7:580:PRO:HG2	6:7:679:PHE:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:D:214:GLY:HA2	10:D:215:SER:HA	1.45	0.42
11:E:348:LEU:HD21	11:E:401:LEU:HD21	2.01	0.42
1:2:246:TYR:CD2	1:2:300:PHE:HD1	2.37	0.42
1:2:564:VAL:HG21	1:2:595:ALA:O	2.19	0.42
2:3:300:SER:OG	4:5:245:HIS:ND1	2.44	0.42
2:3:527:ARG:HG2	2:3:528:ASP:N	2.35	0.42
3:4:266:GLN:OE1	3:4:440:ARG:NH2	2.53	0.42
3:4:328:LEU:O	3:4:435:VAL:N	2.52	0.42
3:4:704:LEU:HD12	3:4:704:LEU:HA	1.89	0.42
3:4:704:LEU:HD12	3:4:832:ALA:HB2	2.01	0.42
4:5:143:ALA:HB3	4:5:161:ARG:HD3	2.01	0.42
4:5:388:ILE:HD11	4:5:425:LEU:HD11	2.02	0.42
4:5:392:LEU:HD23	4:5:392:LEU:HA	1.77	0.42
4:5:411:ASN:HB2	4:5:550:PHE:HA	2.01	0.42
4:5:579:ASN:O	4:5:583:MET:HG2	2.19	0.42
5:6:124:VAL:HG22	5:6:132:VAL:HA	2.00	0.42
5:6:530:VAL:HA	5:6:533:ILE:CD1	2.43	0.42
5:6:625:ALA:HB3	5:6:626:GLY:CA	2.45	0.42
5:6:956:GLU:HB2	5:6:960:LEU:HD13	2.02	0.42
6:7:134:TYR:HB2	6:7:141:VAL:CG1	2.48	0.42
6:7:528:LYS:C	6:7:530:ASP:H	2.26	0.42
11:E:25:CYS:CB	11:E:26:GLN:HA	2.34	0.42
1:2:540:LEU:HD23	1:2:680:LEU:HG	2.02	0.42
3:4:243:LEU:HD13	3:4:303:VAL:HG13	2.02	0.42
3:4:281:VAL:HG22	3:4:297:GLU:CG	2.49	0.42
3:4:343:LYS:C	3:4:360:ILE:HD12	2.45	0.42
5:6:563:ILE:H	5:6:563:ILE:HD12	1.84	0.42
6:7:17:LEU:HD21	6:7:113:PHE:CE1	2.54	0.42
6:7:107:GLN:HB2	6:7:238:LEU:O	2.19	0.42
7:A:134:TYR:HE1	10:D:186:HIS:ND1	2.18	0.42
10:D:123:LYS:O	10:D:126:LEU:HB3	2.20	0.42
1:2:574:VAL:HB	5:6:666:ALA:HA	2.01	0.42
2:3:493:GLN:NE2	2:3:509:ARG:HA	2.35	0.42
2:3:716:ARG:NH1	2:3:722:ASN:HB3	2.32	0.42
3:4:318:ASN:OD1	6:7:341:ARG:NH1	2.46	0.42
3:4:337:PRO:HA	5:6:375:ARG:HH11	1.84	0.42
4:5:244:ILE:O	4:5:248:SER:OG	2.36	0.42
4:5:484:LYS:HD2	4:5:484:LYS:N	2.34	0.42
4:5:618:ALA:O	4:5:622:LEU:HG	2.19	0.42
5:6:711:LEU:HD12	5:6:712:PHE:H	1.84	0.42
5:6:802:SER:O	5:6:806:LEU:HG	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:129:THR:OG1	6:7:130:LYS:N	2.52	0.42
6:7:310:PHE:HE1	6:7:334:HIS:CG	2.38	0.42
6:7:361:THR:OG1	6:7:362:GLY:N	2.53	0.42
8:B:15:GLU:O	8:B:18:PHE:HB3	2.19	0.42
10:D:218:MET:HG2	10:D:220:ASP:HB2	2.01	0.42
11:E:148:VAL:CG1	11:E:150:ASP:HB2	2.48	0.42
1:2:279:THR:O	1:2:283:TYR:N	2.49	0.42
1:2:569:GLN:HA	1:2:571:ALA:CB	2.50	0.42
1:2:572:SER:HA	5:6:662:SER:C	2.45	0.42
1:2:631:ILE:HB	1:2:632:SER:H	1.60	0.42
2:3:156:SER:OG	2:3:157:PHE:N	2.53	0.42
2:3:485:ALA:O	2:3:488:GLU:HB3	2.20	0.42
3:4:243:LEU:HD21	3:4:245:ALA:HB2	2.02	0.42
3:4:501:ILE:HD11	3:4:752:SER:OG	2.19	0.42
3:4:856:VAL:HG23	3:4:857:ILE:H	1.82	0.42
4:5:40:LEU:HA	4:5:40:LEU:HD12	1.79	0.42
4:5:349:PHE:HE2	4:5:354:GLU:H	1.68	0.42
5:6:133:GLU:HA	5:6:134:LYS:HA	1.72	0.42
5:6:194:PRO:HG2	5:6:261:ARG:NH2	2.35	0.42
5:6:512:GLU:O	5:6:515:GLU:HB3	2.19	0.42
8:B:26:LYS:HB2	8:B:88:VAL:HG11	2.01	0.42
9:C:182:GLU:HA	9:C:185:LYS:HB2	2.01	0.42
11:E:410:VAL:HA	11:E:420:SER:HA	2.02	0.42
11:E:513:ILE:HG12	11:E:516:LYS:HZ1	1.84	0.42
11:E:572:ILE:HD12	11:E:572:ILE:HA	1.86	0.42
1:2:289:ILE:HD12	1:2:289:ILE:HG23	1.80	0.42
1:2:520:PHE:CD1	1:2:823:MET:HE3	2.55	0.42
1:2:856:GLN:OE1	1:2:859:ARG:HD3	2.20	0.42
2:3:214:TYR:HD1	2:3:227:THR:HG22	1.84	0.42
2:3:706:ILE:HG21	6:7:620:HIS:NE2	2.31	0.42
3:4:248:LEU:HB3	3:4:254:THR:O	2.19	0.42
3:4:467:LYS:HA	3:4:468:LYS:HA	1.85	0.42
3:4:522:LEU:HB2	3:4:541:LEU:HD11	2.02	0.42
3:4:830:ARG:HB3	3:4:834:LYS:HE2	2.01	0.42
4:5:347:THR:CB	4:5:348:MET:HA	2.49	0.42
4:5:444:SER:HA	4:5:445:SER:HA	1.77	0.42
5:6:543:VAL:HG23	5:6:713:PHE:HB3	2.02	0.42
6:7:81:ASP:OD1	6:7:81:ASP:N	2.44	0.42
6:7:82:LEU:HD23	6:7:85:ILE:HD12	2.01	0.42
6:7:139:LEU:CA	6:7:142:ILE:HB	2.47	0.42
7:A:37:ILE:HA	7:A:40:ILE:HD12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:57:GLN:HG2	7:A:62:MET:HG2	2.01	0.42
10:D:286:LEU:HD21	10:D:293:LEU:HD21	2.02	0.42
11:E:131:LEU:HD13	11:E:237:LEU:HD21	2.01	0.42
11:E:150:ASP:CB	11:E:152:LEU:HB2	2.42	0.42
11:E:280:LEU:H	11:E:280:LEU:HG	1.54	0.42
11:E:283:ALA:HB1	11:E:284:TYR:CE2	2.55	0.42
11:E:327:PHE:CZ	11:E:503:GLN:HG3	2.55	0.42
11:E:524:ILE:HD13	11:E:648:GLY:HA3	2.02	0.42
11:E:545:LEU:HD22	11:E:580:LEU:HD23	2.02	0.42
11:E:619:LYS:HB3	11:E:633:ARG:CG	2.50	0.42
1:2:218:TYR:HD2	1:2:227:TYR:CE2	2.37	0.42
1:2:423:GLU:OE1	1:2:423:GLU:N	2.52	0.42
1:2:569:GLN:CD	1:2:616:ASP:HB2	2.45	0.42
1:2:790:TYR:HA	1:2:793:LEU:HB2	2.02	0.42
1:2:830:SER:N	1:2:833:ASP:OD2	2.41	0.42
2:3:122:ILE:HG22	2:3:123:PRO:HD3	2.02	0.42
2:3:228:PRO:HA	2:3:229:ALA:HA	1.75	0.42
2:3:687:ARG:HE	6:7:604:PRO:HA	1.85	0.42
3:4:245:ALA:H	3:4:247:ASN:CG	2.28	0.42
3:4:909:ARG:NH2	5:6:685:VAL:HB	2.35	0.42
4:5:258:LEU:HD21	4:5:276:MET:SD	2.60	0.42
4:5:339:THR:O	4:5:340:SER:C	2.63	0.42
4:5:413:LEU:HD22	4:5:553:ILE:HG23	2.00	0.42
4:5:566:ILE:H	4:5:566:ILE:HG13	1.72	0.42
5:6:173:GLN:N	5:6:173:GLN:OE1	2.53	0.42
5:6:585:LEU:HA	5:6:588:VAL:HG23	2.01	0.42
5:6:642:ASP:OD1	5:6:642:ASP:N	2.51	0.42
5:6:767:LYS:HB3	5:6:767:LYS:HE3	1.76	0.42
5:6:834:SER:O	5:6:838:VAL:HG23	2.20	0.42
5:6:919:LYS:HB2	5:6:939:TRP:HZ2	1.84	0.42
5:6:932:THR:OG1	5:6:933:ALA:N	2.53	0.42
7:A:22:ARG:N	7:A:23:SER:HA	2.35	0.42
7:A:91:ARG:NH2	10:D:218:MET:HE1	2.35	0.42
7:A:145:ASP:CA	7:A:146:LEU:HB3	2.42	0.42
7:A:169:LYS:HA	7:A:185:LYS:HD3	2.02	0.42
11:E:575:ASN:O	11:E:576:THR:CB	2.68	0.42
3:4:434:GLU:O	3:4:466:VAL:HG13	2.20	0.41
3:4:626:GLY:N	3:4:668:ARG:O	2.48	0.41
3:4:795:THR:O	3:4:799:GLU:HB2	2.20	0.41
3:4:808:HIS:ND1	3:4:808:HIS:O	2.53	0.41
4:5:181:ILE:HG23	4:5:242:ILE:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:337:VAL:HA	4:5:338:GLU:HA	1.70	0.41
6:7:214:ARG:N	6:7:215:TYR:HA	2.34	0.41
6:7:314:LYS:C	6:7:315:ILE:HD12	2.45	0.41
6:7:401:VAL:HG12	6:7:405:ILE:HG13	2.02	0.41
8:B:184:PHE:HB2	9:C:180:SER:OG	2.20	0.41
10:D:76:LEU:HD11	10:D:147:ARG:NE	2.25	0.41
11:E:36:ILE:HG23	11:E:39:LEU:HD12	2.02	0.41
11:E:579:TYR:CZ	11:E:634:ARG:HB3	2.49	0.41
1:2:273:LEU:O	1:2:277:GLU:HG2	2.20	0.41
1:2:523:VAL:O	1:2:535:GLY:HA3	2.21	0.41
1:2:544:ASP:H	1:2:549:LYS:HE2	1.85	0.41
1:2:626:GLN:HG3	1:2:628:SER:N	2.35	0.41
1:2:640:LEU:HD21	4:5:271:PRO:HD3	2.02	0.41
2:3:211:TYR:CE1	6:7:6:PRO:HG2	2.56	0.41
2:3:234:GLU:H	2:3:241:LEU:HD12	1.85	0.41
2:3:687:ARG:HB3	6:7:604:PRO:CB	2.47	0.41
3:4:191:THR:HB	3:4:275:THR:HG22	2.02	0.41
3:4:342:MET:HG3	5:6:417:PRO:HG3	2.02	0.41
3:4:410:GLN:HE21	6:7:345:PRO:CG	2.33	0.41
3:4:633:GLU:HA	3:4:675:ALA:HA	2.01	0.41
5:6:126:SER:O	5:6:130:GLY:HA3	2.19	0.41
5:6:533:ILE:HG22	5:6:587:TYR:CZ	2.55	0.41
6:7:28:PHE:O	6:7:61:PRO:HB3	2.20	0.41
6:7:399:GLU:HA	6:7:402:MET:HB2	2.02	0.41
6:7:709:ASP:HB2	6:7:712:ASP:HB2	2.01	0.41
8:B:15:GLU:O	8:B:18:PHE:N	2.53	0.41
8:B:119:TRP:CD1	8:B:119:TRP:H	2.38	0.41
8:B:124:ARG:HD2	9:C:191:MET:O	2.19	0.41
1:2:532:SER:C	1:2:533:ILE:HG13	2.46	0.41
1:2:846:VAL:HG13	1:2:856:GLN:HG3	2.02	0.41
2:3:672:THR:OG1	2:3:721:VAL:O	2.23	0.41
2:3:675:ALA:HB1	2:3:726:ALA:HB2	2.01	0.41
2:3:687:ARG:CG	2:3:697:ILE:HG21	2.50	0.41
2:3:704:THR:O	2:3:708:LEU:HD13	2.20	0.41
3:4:449:ARG:CG	3:4:450:GLN:N	2.77	0.41
3:4:449:ARG:O	3:4:451:ARG:N	2.50	0.41
3:4:682:TYR:HB2	3:4:691:ASN:CG	2.44	0.41
3:4:726:ASN:C	3:4:728:TYR:CB	2.93	0.41
4:5:87:ILE:N	4:5:88:PRO:HD2	2.35	0.41
4:5:408:GLY:HA2	4:5:409:ASP:HA	1.44	0.41
5:6:556:HIS:ND1	5:6:556:HIS:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:836:ILE:HA	5:6:839:ASP:HB2	2.02	0.41
6:7:428:VAL:O	6:7:432:LEU:HG	2.21	0.41
8:B:144:LYS:O	8:B:148:LEU:HB2	2.20	0.41
8:B:152:ARG:O	8:B:156:VAL:HG23	2.20	0.41
9:C:22:TYR:CD2	9:C:71:PHE:HD1	2.38	0.41
9:C:27:LEU:HD12	9:C:35:GLY:HA3	2.02	0.41
10:D:260:ILE:HA	10:D:261:PRO:HD3	1.60	0.41
11:E:36:ILE:HD11	11:E:429:THR:HG22	2.02	0.41
1:2:335:LYS:HA	1:2:353:GLN:O	2.19	0.41
1:2:404:ARG:NH2	5:6:298:SER:O	2.53	0.41
1:2:476:TRP:CG	1:2:769:TYR:HD1	2.39	0.41
2:3:462:MET:SD	2:3:470:VAL:HG21	2.60	0.41
3:4:437:GLY:HA3	3:4:464:VAL:H	1.86	0.41
3:4:506:LEU:HA	3:4:509:ILE:HD12	2.02	0.41
3:4:598:ALA:HB2	3:4:640:SER:O	2.20	0.41
3:4:621:LEU:HD23	3:4:621:LEU:HA	1.92	0.41
3:4:692:ILE:HG21	3:4:699:LEU:CD1	2.51	0.41
3:4:729:LEU:HB3	3:4:730:GLU:CD	2.45	0.41
4:5:297:ILE:N	4:5:328:ILE:HG23	2.36	0.41
5:6:279:ILE:HG21	5:6:452:ILE:HD13	2.02	0.41
5:6:711:LEU:CD2	5:6:834:SER:HB2	2.51	0.41
5:6:945:GLU:HA	5:6:948:LEU:CD1	2.50	0.41
6:7:82:LEU:CB	6:7:207:LEU:HD23	2.48	0.41
6:7:264:GLN:CD	6:7:296:GLY:HA2	2.46	0.41
6:7:570:LEU:HB2	6:7:585:ASN:HD21	1.85	0.41
8:B:26:LYS:O	8:B:88:VAL:HG12	2.20	0.41
8:B:126:LEU:O	8:B:130:ALA:N	2.54	0.41
9:C:98:HIS:HA	9:C:102:SER:HB2	2.02	0.41
9:C:127:LEU:HD23	9:C:131:ARG:HG2	2.01	0.41
10:D:67:TRP:O	10:D:70:GLU:HB3	2.20	0.41
11:E:36:ILE:HB	11:E:279:SER:OG	2.21	0.41
11:E:369:PRO:HD2	11:E:372:THR:HB	2.01	0.41
12:F:7:DT:H5'	12:F:7:DT:H6	1.85	0.41
1:2:327:ARG:NH2	4:5:269:GLU:OE1	2.54	0.41
1:2:780:GLN:NE2	4:5:577:THR:O	2.42	0.41
2:3:31:PHE:HZ	2:3:38:TYR:HE2	1.68	0.41
2:3:257:THR:HB	2:3:273:SER:HB2	2.03	0.41
2:3:350:ILE:HG23	2:3:659:TYR:HD1	1.85	0.41
3:4:225:TYR:HA	3:4:226:TYR:HA	1.67	0.41
3:4:252:LYS:CG	3:4:253:GLN:HA	2.46	0.41
3:4:314:MET:HA	3:4:317:LEU:HG	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:761:ILE:HG22	3:4:763:THR:H	1.86	0.41
5:6:154:ASP:OD2	5:6:156:GLN:HB3	2.20	0.41
5:6:159:SER:O	5:6:164:GLY:N	2.54	0.41
5:6:398:THR:OG1	5:6:458:HIS:HB3	2.20	0.41
6:7:203:TYR:CZ	6:7:339:LEU:HG	2.56	0.41
6:7:409:ASP:O	6:7:413:ARG:HB3	2.20	0.41
6:7:453:ASP:OD1	6:7:562:SER:HA	2.20	0.41
6:7:470:LEU:HD22	6:7:522:CYS:SG	2.60	0.41
6:7:713:VAL:HG12	6:7:717:LEU:CD1	2.50	0.41
7:A:110:MET:HG2	7:A:112:SER:N	2.35	0.41
10:D:188:LEU:O	10:D:192:LYS:HG2	2.20	0.41
1:2:249:LEU:HG	1:2:257:ALA:HB2	2.03	0.41
1:2:506:TYR:HD2	1:2:695:LEU:HD12	1.85	0.41
1:2:562:ARG:HD2	1:2:600:ASP:O	2.20	0.41
1:2:621:HIS:CD2	1:2:673:ILE:HG13	2.55	0.41
1:2:693:GLU:HG2	5:6:778:LYS:HZ2	1.85	0.41
2:3:118:PRO:O	2:3:122:ILE:HG22	2.20	0.41
2:3:300:SER:O	4:5:245:HIS:ND1	2.54	0.41
2:3:437:SER:O	4:5:506:LYS:HA	2.21	0.41
2:3:500:ALA:H	2:3:501:GLY:HA3	1.86	0.41
3:4:272:MET:HB3	3:4:303:VAL:HG21	2.02	0.41
3:4:319:PRO:O	3:4:322:ILE:HG23	2.21	0.41
3:4:754:ALA:O	3:4:810:LYS:HG2	2.20	0.41
4:5:455:ARG:HG3	4:5:462:PHE:CD1	2.55	0.41
4:5:490:ARG:NH1	4:5:541:ASP:OD2	2.54	0.41
4:5:660:THR:CG2	4:5:677:VAL:HG13	2.51	0.41
5:6:102:LYS:HE2	5:6:102:LYS:HB2	1.90	0.41
5:6:403:VAL:HG12	5:6:404:VAL:N	2.36	0.41
6:7:201:PHE:CE2	6:7:337:GLY:HA2	2.55	0.41
6:7:438:GLY:HA2	6:7:454:ILE:HG13	2.01	0.41
6:7:495:ALA:O	6:7:548:ILE:HG21	2.20	0.41
8:B:51:GLN:HB2	8:B:52:LEU:C	2.45	0.41
10:D:175:LEU:HB2	10:D:180:ILE:HG23	2.02	0.41
11:E:30:PHE:HD1	11:E:61:ILE:CD1	2.33	0.41
11:E:283:ALA:C	11:E:284:TYR:CG	2.98	0.41
11:E:285:ALA:CA	11:E:288:TYR:HB3	2.51	0.41
11:E:288:TYR:HA	11:E:291:LEU:HG	2.01	0.41
1:2:433:ASN:HB2	1:2:434:TYR:HD2	1.86	0.41
1:2:445:PRO:HG3	5:6:304:LEU:HB3	2.01	0.41
1:2:479:GLU:OE1	1:2:479:GLU:N	2.45	0.41
1:2:567:THR:CG2	1:2:568:GLY:N	2.77	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:624:MET:HE3	1:2:624:MET:HB2	1.54	0.41
2:3:43:ARG:HD2	2:3:43:ARG:HA	1.84	0.41
2:3:110:PHE:O	2:3:114:ILE:HG13	2.20	0.41
2:3:488:GLU:HG3	2:3:494:THR:O	2.20	0.41
2:3:545:LEU:HD13	2:3:547:PHE:CZ	2.56	0.41
2:3:653:ILE:O	2:3:656:LEU:HB3	2.20	0.41
2:3:714:LYS:O	2:3:717:LEU:HD12	2.20	0.41
3:4:540:ILE:O	3:4:543:GLN:HB3	2.20	0.41
3:4:683:ASN:HA	3:4:684:PRO:HD3	1.94	0.41
3:4:901:SER:O	3:4:905:GLU:HG2	2.21	0.41
4:5:27:ILE:O	4:5:30:SER:HB3	2.20	0.41
4:5:286:VAL:CG1	4:5:292:VAL:HG11	2.51	0.41
4:5:343:TRP:CE3	4:5:344:ASN:HB3	2.56	0.41
5:6:539:GLY:O	5:6:544:LYS:HE3	2.20	0.41
6:7:523:ILE:HD13	6:7:526:PHE:CE1	2.56	0.41
7:A:138:ILE:HD12	7:A:138:ILE:HA	1.97	0.41
10:D:87:LEU:O	10:D:90:ARG:N	2.54	0.41
10:D:94:GLN:O	10:D:98:ILE:HG23	2.20	0.41
11:E:561:ASP:HA	11:E:562:LYS:HA	1.76	0.41
1:2:660:THR:O	1:2:850:LYS:HB2	2.20	0.41
2:3:35:PHE:CE2	2:3:102:ASP:HB3	2.55	0.41
2:3:102:ASP:O	2:3:105:GLU:HB2	2.21	0.41
5:6:266:SER:HB2	5:6:458:HIS:HD2	1.85	0.41
5:6:577:PRO:HD2	5:6:687:GLY:O	2.21	0.41
6:7:611:LYS:O	6:7:615:HIS:HB2	2.21	0.41
7:A:145:ASP:HB3	7:A:147:VAL:HG23	2.01	0.41
8:B:160:LEU:HD21	8:B:184:PHE:HE2	1.86	0.41
11:E:297:ASP:O	11:E:301:ARG:N	2.54	0.41
11:E:431:LEU:H	11:E:431:LEU:HG	1.62	0.41
11:E:569:LEU:O	11:E:581:VAL:HA	2.20	0.41
11:E:577:ASP:OD2	11:E:633:ARG:NH2	2.53	0.41
1:2:240:GLU:HB3	1:2:290:HIS:CE1	2.56	0.41
1:2:311:GLU:HG3	5:6:353:PHE:C	2.46	0.41
1:2:439:ASN:O	1:2:442:ASN:N	2.39	0.41
1:2:505:ILE:O	13:2:901:ANP:N6	2.24	0.41
1:2:802:SER:HA	1:2:803:PHE:HA	1.66	0.41
2:3:356:LYS:HB2	2:3:359:ILE:CG2	2.48	0.41
2:3:375:ASP:O	2:3:379:LYS:HG3	2.21	0.41
2:3:528:ASP:O	2:3:532:ASN:HB2	2.21	0.41
2:3:716:ARG:HH22	2:3:724:VAL:HB	1.86	0.41
3:4:569:ASP:HB3	6:7:683:GLN:OE1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:52:ASN:OD1	9:C:140:SER:HB3	2.21	0.41
4:5:349:PHE:O	4:5:350:THR:OG1	2.38	0.41
4:5:422:LYS:NZ	13:5:801:ANP:O3G	2.54	0.41
4:5:483:ASP:HB3	4:5:484:LYS:HD2	2.02	0.41
4:5:557:LYS:HA	4:5:557:LYS:HD2	1.79	0.41
4:5:559:ASP:HB2	4:5:561:ASN:CG	2.46	0.41
4:5:601:ARG:HA	4:5:601:ARG:HD2	1.82	0.41
5:6:656:MET:HG3	5:6:709:PHE:HE1	1.84	0.41
5:6:722:LYS:O	5:6:725:THR:OG1	2.29	0.41
6:7:89:GLN:HG3	6:7:102:LEU:HD12	2.03	0.41
6:7:110:ALA:HB2	6:7:238:LEU:N	2.35	0.41
6:7:246:THR:HG21	6:7:316:GLN:NE2	2.36	0.41
6:7:429:LYS:HA	6:7:432:LEU:HD12	2.02	0.41
6:7:464:VAL:HG11	6:7:600:MET:SD	2.61	0.41
6:7:486:LYS:HA	6:7:486:LYS:HD3	1.90	0.41
6:7:564:LEU:HD23	6:7:565:ALA:N	2.36	0.41
6:7:650:PRO:HB3	6:7:706:ASP:HA	2.03	0.41
6:7:668:ARG:HH22	6:7:686:PRO:CD	2.33	0.41
6:7:688:THR:O	6:7:692:ILE:HB	2.21	0.41
6:7:699:LEU:HD13	6:7:715:GLU:HB3	2.01	0.41
7:A:30:PRO:O	7:A:122:ASN:ND2	2.42	0.41
7:A:31:MET:HG2	7:A:32:TYR:N	2.36	0.41
7:A:102:TRP:CD1	8:B:3:LEU:HG	2.56	0.41
9:C:95:LEU:O	9:C:131:ARG:NH2	2.54	0.41
9:C:172:MET:HG3	9:C:173:GLU:N	2.36	0.41
10:D:135:ARG:O	10:D:139:VAL:HG23	2.20	0.41
10:D:199:LEU:C	10:D:202:MET:HB2	2.46	0.41
1:2:759:PRO:HG2	1:2:762:LEU:HD12	2.02	0.41
1:2:803:PHE:HB3	1:2:805:ILE:N	2.30	0.41
2:3:410:ASP:O	2:3:413:THR:OG1	2.29	0.41
3:4:388:ARG:NH2	5:6:176:ARG:HB2	2.36	0.41
3:4:565:LEU:HD23	3:4:566:LEU:N	2.35	0.41
4:5:163:SER:OG	4:5:164:GLY:N	2.54	0.41
4:5:270:MET:HE2	4:5:270:MET:HB2	1.65	0.41
4:5:494:HIS:HB3	4:5:549:ARG:NE	2.36	0.41
4:5:564:ARG:O	4:5:568:ILE:HG22	2.20	0.41
5:6:395:CYS:SG	5:6:461:SER:HA	2.62	0.41
5:6:836:ILE:O	5:6:839:ASP:HB2	2.20	0.41
6:7:217:LYS:HG3	6:7:218:LYS:H	1.86	0.41
6:7:499:LYS:NZ	6:7:504:ASP:OD1	2.35	0.41
6:7:660:VAL:HG22	6:7:713:VAL:HG11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:32:TYR:CB	7:A:124:SER:HB3	2.51	0.41
7:A:46:ASN:OD1	7:A:50:ASN:ND2	2.52	0.41
7:A:87:LEU:HD13	9:C:4:TYR:OH	2.21	0.41
8:B:79:LEU:O	8:B:83:SER:N	2.54	0.41
8:B:182:ARG:HA	10:D:229:PHE:HE2	1.86	0.41
11:E:34:LEU:HD22	11:E:34:LEU:O	2.20	0.41
11:E:60:PRO:HG3	11:E:478:TRP:HE1	1.85	0.41
11:E:240:TYR:O	11:E:241:TYR:HB3	2.21	0.41
11:E:356:LYS:O	11:E:360:HIS:ND1	2.45	0.41
11:E:368:ILE:HA	11:E:369:PRO:HD3	1.92	0.41
1:2:553:LEU:HD21	1:2:607:ASP:HB3	2.03	0.40
1:2:778:LEU:CD1	4:5:577:THR:CG2	2.99	0.40
2:3:197:ILE:O	2:3:214:TYR:HB2	2.21	0.40
2:3:315:ILE:HG22	4:5:255:PHE:CZ	2.56	0.40
2:3:519:VAL:HB	2:3:527:ARG:HH12	1.86	0.40
2:3:527:ARG:NH1	2:3:531:GLN:O	2.54	0.40
2:3:654:PRO:HA	2:3:657:ARG:CZ	2.51	0.40
3:4:312:LYS:O	3:4:316:GLU:HB3	2.22	0.40
4:5:378:ILE:HA	13:5:801:ANP:N6	2.30	0.40
5:6:654:GLU:CD	5:6:661:ILE:HG23	2.46	0.40
5:6:738:ARG:HD3	5:6:738:ARG:HA	1.91	0.40
6:7:71:ALA:CB	6:7:129:THR:HG21	2.51	0.40
6:7:222:SER:HB3	6:7:223:LYS:H	1.67	0.40
6:7:451:ARG:HB2	6:7:453:ASP:H	1.86	0.40
10:D:143:TYR:CZ	10:D:147:ARG:HD2	2.56	0.40
11:E:127:ARG:O	11:E:245:THR:HA	2.20	0.40
11:E:380:MET:HB2	11:E:385:LYS:HE2	2.02	0.40
12:F:8:DT:H6	12:F:8:DT:H2'	1.68	0.40
1:2:243:GLU:HA	1:2:296:ARG:HB2	2.02	0.40
1:2:587:LYS:HE3	1:2:587:LYS:HB2	1.93	0.40
1:2:676:ARG:HA	1:2:676:ARG:HD3	1.75	0.40
1:2:783:MET:SD	1:2:783:MET:N	2.94	0.40
3:4:228:LYS:HA	3:4:231:ASN:HD22	1.86	0.40
3:4:273:ASP:CG	3:4:302:LYS:HA	2.46	0.40
3:4:280:MET:HE3	3:4:280:MET:HB3	1.88	0.40
3:4:370:ARG:HD2	3:4:378:GLU:O	2.21	0.40
3:4:419:VAL:HG21	3:4:423:LEU:C	2.46	0.40
4:5:60:SER:HA	4:5:136:GLN:O	2.22	0.40
4:5:153:SER:O	4:5:156:VAL:HG23	2.21	0.40
4:5:413:LEU:HD23	4:5:415:LEU:CD2	2.52	0.40
5:6:124:VAL:HG23	5:6:134:LYS:C	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:311:CYS:HA	5:6:312:ASP:CB	2.50	0.40
5:6:360:ARG:HA	5:6:378:ASP:HA	2.04	0.40
5:6:544:LYS:HE2	5:6:584:PHE:HE1	1.85	0.40
5:6:641:PHE:H	5:6:682:ALA:HB2	1.86	0.40
6:7:110:ALA:CB	6:7:238:LEU:HB2	2.51	0.40
6:7:368:ALA:HA	6:7:369:GLY:HA2	1.79	0.40
6:7:523:ILE:O	6:7:566:ALA:N	2.36	0.40
6:7:544:GLN:O	6:7:545:THR:OG1	2.24	0.40
6:7:700:ALA:O	6:7:704:LEU:N	2.54	0.40
7:A:150:ASP:O	10:D:141:ARG:NE	2.52	0.40
8:B:166:SER:HB3	10:D:227:PHE:HE1	1.86	0.40
10:D:69:ASN:OD1	10:D:293:LEU:HD13	2.22	0.40
10:D:150:LYS:HA	10:D:153:LYS:HE2	2.02	0.40
11:E:64:TYR:OH	11:E:90:ILE:HB	2.21	0.40
1:2:247:ARG:HH11	1:2:247:ARG:HA	1.86	0.40
1:2:266:GLU:H	1:2:266:GLU:CD	2.28	0.40
1:2:606:ILE:HG22	1:2:609:PHE:HE1	1.86	0.40
1:2:803:PHE:CB	1:2:805:ILE:H	2.29	0.40
1:2:806:THR:H	1:2:809:HIS:CB	2.30	0.40
2:3:245:TYR:CD2	6:7:356:LEU:HD22	2.56	0.40
2:3:406:LEU:HD13	2:3:543:PHE:CE2	2.57	0.40
2:3:469:VAL:HA	2:3:511:SER:O	2.21	0.40
3:4:345:ALA:N	3:4:360:ILE:HG13	2.36	0.40
3:4:442:ILE:HG22	3:4:443:PRO:O	2.20	0.40
3:4:557:ARG:HE	3:4:668:ARG:NH2	2.10	0.40
3:4:678:ILE:HD11	3:4:693:ASP:HA	2.02	0.40
3:4:898:VAL:O	3:4:903:ILE:HD11	2.22	0.40
4:5:86:ILE:O	4:5:87:ILE:C	2.64	0.40
4:5:437:VAL:HG23	4:5:472:ALA:HB2	2.03	0.40
5:6:640:GLU:HB3	5:6:643:LYS:HG2	2.04	0.40
6:7:96:GLY:HA3	6:7:97:THR:HA	1.92	0.40
6:7:397:VAL:HG12	6:7:640:GLU:HG2	2.02	0.40
6:7:495:ALA:O	6:7:548:ILE:HG12	2.20	0.40
6:7:724:LYS:C	6:7:726:SER:N	2.80	0.40
8:B:18:PHE:HE1	10:D:135:ARG:CG	2.35	0.40
8:B:66:MET:HE2	8:B:66:MET:HA	2.03	0.40
11:E:71:TYR:CD2	11:E:96:LEU:HD13	2.55	0.40
1:2:514:ALA:HB1	1:2:679:ILE:HG21	2.03	0.40
13:2:901:ANP:HNB1	5:6:653:HIS:CE1	2.36	0.40
2:3:288:PRO:O	2:3:464:LEU:HD11	2.22	0.40
2:3:372:TYR:CZ	2:3:561:ILE:HA	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:384:MET:HE2	2:3:384:MET:HB3	1.73	0.40
3:4:243:LEU:CG	3:4:244:ASP:H	2.34	0.40
3:4:505:ASP:HA	3:4:508:LYS:HB3	2.02	0.40
3:4:865:LEU:HD21	3:4:903:ILE:HG23	2.03	0.40
4:5:24:ASN:O	4:5:28:ILE:HG13	2.21	0.40
4:5:94:ILE:HD12	4:5:135:PHE:HD2	1.87	0.40
5:6:548:LEU:O	5:6:552:LEU:HD13	2.21	0.40
5:6:585:LEU:HD21	5:6:679:LEU:CD2	2.51	0.40
5:6:610:ALA:N	5:6:663:ILE:HD13	2.35	0.40
6:7:81:ASP:O	6:7:85:ILE:HG13	2.21	0.40
6:7:220:ILE:O	6:7:222:SER:HB2	2.17	0.40
6:7:259:ALA:HB2	6:7:270:PHE:CE1	2.56	0.40
6:7:459:MET:CB	6:7:597:LEU:HD21	2.38	0.40
8:B:95:THR:HG23	8:B:96:LYS:H	1.86	0.40
8:B:198:ALA:HB1	9:C:113:MET:CE	2.52	0.40
11:E:28:VAL:CG2	11:E:57:GLN:HB3	2.51	0.40
11:E:313:PRO:HA	11:E:415:TYR:CE2	2.57	0.40
1:2:284:PRO:HD2	11:E:365:ARG:HD3	2.03	0.40
1:2:359:ILE:HA	1:2:360:ARG:HA	1.79	0.40
1:2:691:ALA:O	1:2:694:ARG:HB3	2.20	0.40
2:3:53:ALA:CA	6:7:218:LYS:HD2	2.51	0.40
2:3:130:THR:HG22	2:3:153:TRP:HD1	1.86	0.40
2:3:687:ARG:HG3	2:3:697:ILE:HG21	2.03	0.40
3:4:408:ASP:HA	3:4:409:GLY:HA2	1.66	0.40
3:4:520:SER:O	3:4:523:ALA:HB3	2.22	0.40
3:4:760:PRO:HB2	3:4:809:ALA:HB1	2.03	0.40
4:5:370:LEU:HD23	4:5:666:LEU:HD22	2.03	0.40
4:5:605:TYR:HE2	4:5:668:LEU:HD11	1.87	0.40
5:6:152:TYR:HB3	5:6:268:PHE:CE2	2.55	0.40
6:7:139:LEU:HA	6:7:142:ILE:CB	2.49	0.40
6:7:360:TYR:CE2	6:7:363:PHE:HB2	2.57	0.40
6:7:441:ASP:N	6:7:452:GLY:HA2	2.37	0.40
6:7:650:PRO:CA	6:7:706:ASP:HA	2.50	0.40
7:A:47:LEU:C	7:A:47:LEU:HD23	2.47	0.40
7:A:106:GLY:N	7:A:107:LEU:HD22	2.36	0.40
7:A:199:LEU:HA	7:A:202:GLN:HB3	2.03	0.40
8:B:166:SER:HB3	10:D:227:PHE:CE1	2.57	0.40
9:C:38:ILE:HD13	9:C:38:ILE:HG21	1.86	0.40
10:D:98:ILE:HG22	10:D:129:MET:HG2	2.03	0.40
11:E:527:LEU:HD12	11:E:568:VAL:HB	2.04	0.40
11:E:570:ALA:HB2	11:E:581:VAL:HG22	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	2	573/868 (66%)	502 (88%)	63 (11%)	8 (1%)	9	39
2	3	579/971 (60%)	525 (91%)	52 (9%)	2 (0%)	36	71
3	4	660/933 (71%)	577 (87%)	72 (11%)	11 (2%)	7	35
4	5	590/775 (76%)	537 (91%)	48 (8%)	5 (1%)	16	52
5	6	649/1017 (64%)	571 (88%)	72 (11%)	6 (1%)	14	49
6	7	652/845 (77%)	566 (87%)	76 (12%)	10 (2%)	8	38
7	A	206/208 (99%)	185 (90%)	20 (10%)	1 (0%)	24	63
8	B	177/213 (83%)	156 (88%)	21 (12%)	0	100	100
9	C	151/194 (78%)	140 (93%)	11 (7%)	0	100	100
10	D	215/294 (73%)	193 (90%)	19 (9%)	3 (1%)	9	39
11	E	543/650 (84%)	488 (90%)	50 (9%)	5 (1%)	14	49
All	All	4995/6968 (72%)	4440 (89%)	504 (10%)	51 (1%)	15	47

All (51) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	4	429	ALA
4	5	596	ILE
6	7	26	VAL
6	7	222	SER
6	7	464	VAL
11	E	577	ASP
11	E	601	ILE
2	3	389	VAL
3	4	419	VAL
3	4	433	ILE

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Mol	Chain	Res	Type
4	5	410	ILE
5	6	402	ILE
5	6	560	VAL
5	6	569	ILE
5	6	819	ILE
1	2	533	ILE
1	2	656	ARG
3	4	450	GLN
3	4	609	VAL
4	5	340	SER
10	D	219	ILE
1	2	291	SER
1	2	585	ILE
1	2	631	ILE
2	3	440	VAL
3	4	857	ILE
4	5	267	VAL
4	5	341	SER
5	6	106	VAL
5	6	321	VAL
6	7	502	VAL
7	A	27	VAL
10	D	210	ASN
3	4	373	ARG
6	7	255	VAL
6	7	374	THR
11	E	602	LEU
1	2	297	ILE
6	7	248	VAL
6	7	257	VAL
11	E	98	ILE
3	4	364	VAL
1	2	842	VAL
3	4	463	VAL
3	4	856	VAL
6	7	708	VAL
10	D	258	VAL
1	2	303	ILE
3	4	694	LEU
6	7	462	PRO
11	E	99	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	2	502/770 (65%)	451 (90%)	51 (10%)	7	23
2	3	512/835 (61%)	467 (91%)	45 (9%)	9	29
3	4	599/848 (71%)	560 (94%)	39 (6%)	15	37
4	5	542/688 (79%)	478 (88%)	64 (12%)	5	19
5	6	539/886 (61%)	487 (90%)	52 (10%)	8	25
6	7	582/753 (77%)	534 (92%)	48 (8%)	10	31
7	A	193/193 (100%)	180 (93%)	13 (7%)	15	37
8	B	171/198 (86%)	161 (94%)	10 (6%)	18	40
9	C	144/173 (83%)	134 (93%)	10 (7%)	14	36
10	D	213/279 (76%)	203 (95%)	10 (5%)	23	45
11	E	499/586 (85%)	470 (94%)	29 (6%)	18	40
All	All	4496/6209 (72%)	4125 (92%)	371 (8%)	12	30

All (371) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	2	211	LEU
1	2	234	LEU
1	2	247	ARG
1	2	253	LYS
1	2	263	CYS
1	2	297	ILE
1	2	298	SER
1	2	314	LEU
1	2	384	ASN
1	2	391	GLN
1	2	432	ASN
1	2	437	ASN
1	2	441	LYS
1	2	446	VAL
1	2	473	VAL

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Mol	Chain	Res	Type
1	2	497	ILE
1	2	501	MET
1	2	511	ILE
1	2	533	ILE
1	2	538	ASN
1	2	549	LYS
1	2	567	THR
1	2	577	THR
1	2	590	THR
1	2	610	ASP
1	2	624	MET
1	2	628	SER
1	2	629	ILE
1	2	630	SER
1	2	631	ILE
1	2	633	LYS
1	2	636	ILE
1	2	639	THR
1	2	640	LEU
1	2	646	ILE
1	2	651	ASN
1	2	686	LEU
1	2	705	ARG
1	2	706	SER
1	2	760	GLN
1	2	763	LEU
1	2	782	ASP
1	2	783	MET
1	2	787	SER
1	2	793	LEU
1	2	802	SER
1	2	805	ILE
1	2	806	THR
1	2	807	VAL
1	2	850	LYS
1	2	860	SER
2	3	137	ASP
2	3	154	LYS
2	3	169	ARG
2	3	170	THR
2	3	171	LEU
2	3	172	THR

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Mol	Chain	Res	Type
2	3	188	LYS
2	3	190	SER
2	3	227	THR
2	3	230	ILE
2	3	234	GLU
2	3	275	ASP
2	3	291	ARG
2	3	300	SER
2	3	329	LEU
2	3	346	ASP
2	3	350	ILE
2	3	362	ILE
2	3	384	MET
2	3	395	ASN
2	3	402	ASP
2	3	423	LEU
2	3	438	SER
2	3	464	LEU
2	3	469	VAL
2	3	473	ASP
2	3	497	ILE
2	3	506	LEU
2	3	513	ILE
2	3	519	VAL
2	3	535	LEU
2	3	541	SER
2	3	542	ARG
2	3	546	LEU
2	3	553	ILE
2	3	563	GLU
2	3	565	VAL
2	3	656	LEU
2	3	657	ARG
2	3	665	GLU
2	3	667	VAL
2	3	668	ILE
2	3	691	ASN
2	3	732	LEU
2	3	733	LEU
3	4	243	LEU
3	4	252	LYS
3	4	261	LEU

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Mol	Chain	Res	Type
3	4	271	ILE
3	4	279	CYS
3	4	311	CYS
3	4	314	MET
3	4	321	ASP
3	4	324	LYS
3	4	371	CYS
3	4	389	CYS
3	4	416	SER
3	4	449	ARG
3	4	451	ARG
3	4	463	VAL
3	4	502	THR
3	4	563	ASN
3	4	569	ASP
3	4	589	VAL
3	4	591	THR
3	4	616	LEU
3	4	623	LEU
3	4	631	ILE
3	4	644	VAL
3	4	648	VAL
3	4	654	ILE
3	4	665	LEU
3	4	688	VAL
3	4	692	ILE
3	4	699	LEU
3	4	720	LEU
3	4	725	THR
3	4	727	LEU
3	4	742	LEU
3	4	762	ILE
3	4	770	LEU
3	4	772	ARG
3	4	810	LYS
3	4	856	VAL
4	5	21	ASP
4	5	35	ILE
4	5	36	LEU
4	5	48	ASP
4	5	54	ILE
4	5	61	LEU

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Mol	Chain	Res	Type
4	5	75	ILE
4	5	84	SER
4	5	94	ILE
4	5	101	ILE
4	5	137	LEU
4	5	141	SER
4	5	152	ASP
4	5	159	ILE
4	5	162	LEU
4	5	167	ILE
4	5	174	SER
4	5	179	LEU
4	5	190	THR
4	5	192	ILE
4	5	204	THR
4	5	210	SER
4	5	211	CYS
4	5	242	ILE
4	5	246	GLU
4	5	258	LEU
4	5	270	MET
4	5	274	LEU
4	5	293	THR
4	5	300	ILE
4	5	321	VAL
4	5	337	VAL
4	5	339	THR
4	5	341	SER
4	5	344	ASN
4	5	347	THR
4	5	348	MET
4	5	368	GLU
4	5	370	LEU
4	5	384	ILE
4	5	404	MET
4	5	410	ILE
4	5	426	LEU
4	5	430	GLU
4	5	435	ILE
4	5	439	THR
4	5	444	SER
4	5	449	LEU

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Mol	Chain	Res	Type
4	5	454	GLN
4	5	462	PHE
4	5	479	ILE
4	5	511	THR
4	5	526	ILE
4	5	560	HIS
4	5	563	GLU
4	5	594	ILE
4	5	595	SER
4	5	598	LYS
4	5	640	SER
4	5	642	GLU
4	5	650	ILE
4	5	652	GLN
4	5	668	LEU
4	5	681	ILE
5	6	101	LYS
5	6	106	VAL
5	6	124	VAL
5	6	140	ILE
5	6	148	LEU
5	6	153	ILE
5	6	178	LEU
5	6	266	SER
5	6	354	LEU
5	6	361	ILE
5	6	364	ASN
5	6	376	THR
5	6	377	LEU
5	6	400	VAL
5	6	404	VAL
5	6	533	ILE
5	6	543	VAL
5	6	560	VAL
5	6	570	ASN
5	6	573	VAL
5	6	581	LYS
5	6	614	ARG
5	6	615	ASP
5	6	642	ASP
5	6	644	MET
5	6	647	SER

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Mol	Chain	Res	Type
5	6	648	ASP
5	6	650	VAL
5	6	662	SER
5	6	678	ILE
5	6	688	ARG
5	6	692	LYS
5	6	719	CYS
5	6	723	ILE
5	6	752	ARG
5	6	781	ARG
5	6	783	ASP
5	6	822	SER
5	6	824	ILE
5	6	832	ARG
5	6	916	ILE
5	6	918	ARG
5	6	920	ILE
5	6	922	GLU
5	6	935	ASP
5	6	936	ILE
5	6	938	ASP
5	6	948	LEU
5	6	965	ILE
5	6	967	ARG
5	6	968	LEU
5	6	969	VAL
6	7	79	ILE
6	7	86	LEU
6	7	114	THR
6	7	116	LEU
6	7	127	LEU
6	7	135	LYS
6	7	222	SER
6	7	223	LYS
6	7	239	ILE
6	7	255	VAL
6	7	281	LEU
6	7	298	LEU
6	7	301	SER
6	7	335	VAL
6	7	344	SER
6	7	349	VAL

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Mol	Chain	Res	Type
6	7	351	VAL
6	7	370	LEU
6	7	404	LEU
6	7	437	VAL
6	7	454	ILE
6	7	476	ILE
6	7	491	VAL
6	7	493	LEU
6	7	494	THR
6	7	497	VAL
6	7	498	MET
6	7	503	THR
6	7	521	CYS
6	7	524	ASP
6	7	527	ASP
6	7	530	ASP
6	7	533	ASP
6	7	537	ILE
6	7	582	ASP
6	7	591	LEU
6	7	595	ASP
6	7	596	ILE
6	7	601	LEU
6	7	620	HIS
6	7	627	ASP
6	7	631	THR
6	7	636	SER
6	7	652	MET
6	7	671	SER
6	7	723	SER
6	7	724	LYS
6	7	727	LEU
7	A	23	SER
7	A	25	GLN
7	A	44	VAL
7	A	104	ASN
7	A	107	LEU
7	A	109	LEU
7	A	141	LEU
7	A	149	ILE
7	A	151	LEU
7	A	160	ASP

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Mol	Chain	Res	Type
7	A	163	ILE
7	A	165	VAL
7	A	183	LEU
8	B	20	VAL
8	B	31	ILE
8	B	54	THR
8	B	87	ILE
8	B	95	THR
8	B	118	ASN
8	B	160	LEU
8	B	166	SER
8	B	175	LEU
8	B	189	MET
9	C	24	ILE
9	C	53	ILE
9	C	79	MET
9	C	88	ILE
9	C	95	LEU
9	C	109	ILE
9	C	112	ILE
9	C	120	LEU
9	C	125	SER
9	C	163	SER
10	D	75	GLU
10	D	124	LEU
10	D	127	LEU
10	D	129	MET
10	D	188	LEU
10	D	257	THR
10	D	259	THR
10	D	260	ILE
10	D	269	LEU
10	D	289	ASP
11	E	27	LEU
11	E	32	SER
11	E	33	CYS
11	E	34	LEU
11	E	57	GLN
11	E	61	ILE
11	E	80	SER
11	E	99	ASP
11	E	123	LEU

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Mol	Chain	Res	Type
11	E	142	CYS
11	E	250	SER
11	E	280	LEU
11	E	284	TYR
11	E	302	LEU
11	E	314	ASP
11	E	326	LEU
11	E	362	MET
11	E	396	LEU
11	E	403	ASP
11	E	485	ASP
11	E	492	LEU
11	E	529	VAL
11	E	536	LEU
11	E	552	LEU
11	E	572	ILE
11	E	601	ILE
11	E	606	SER
11	E	623	ASP
11	E	637	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such sidechains are listed below:

Mol	Chain	Res	Type
1	2	238	ASN
1	2	376	ASN
1	2	626	GLN
1	2	641	GLN
1	2	651	ASN
1	2	780	GLN
1	2	856	GLN
2	3	51	ASN
2	3	312	ASN
2	3	330	HIS
2	3	349	ASN
2	3	351	ASN
2	3	417	GLN
2	3	507	ASN
2	3	532	ASN
2	3	661	GLN
2	3	677	ASN
3	4	260	GLN

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Mol	Chain	Res	Type
3	4	287	ASN
3	4	400	GLN
3	4	797	GLN
3	4	876	GLN
3	4	889	GLN
3	4	911	GLN
4	5	49	GLN
4	5	140	ASN
4	5	195	ASN
4	5	253	GLN
4	5	302	ASN
4	5	372	ASN
4	5	411	ASN
4	5	454	GLN
4	5	499	GLN
4	5	500	GLN
4	5	561	ASN
4	5	570	ASN
4	5	581	ASN
4	5	590	ASN
4	5	625	ASN
4	5	676	HIS
5	6	458	HIS
5	6	570	ASN
5	6	649	GLN
5	6	653	HIS
5	6	683	ASN
5	6	698	ASN
5	6	735	HIS
6	7	90	ASN
6	7	455	ASN
6	7	468	GLN
6	7	543	GLN
6	7	615	HIS
6	7	657	ASN
6	7	683	GLN
7	A	7	ASN
8	B	81	GLN
8	B	128	ASN
9	C	33	ASN
9	C	101	ASN
10	D	100	ASN

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Mol	Chain	Res	Type
10	D	110	ASN
11	E	7	GLN
11	E	26	GLN
11	E	269	ASN
11	E	286	GLN
11	E	308	ASN
11	E	342	ASN
11	E	493	ASN
11	E	563	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](#)

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
13	ANP	5	801	-	33,33,33	1.54	5 (15%)	45,52,52	0.80	1 (2%)
13	ANP	2	901	-	33,33,33	1.99	6 (18%)	45,52,52	0.87	3 (6%)
13	ANP	3	1001	-	33,33,33	2.09	6 (18%)	45,52,52	0.83	2 (4%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	ANP	5	801	-	-	7/18/38/38	0/3/3/3
13	ANP	2	901	-	-	8/18/38/38	0/3/3/3
13	ANP	3	1001	-	-	12/18/38/38	0/3/3/3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	2	901	ANP	PG-O1G	7.88	1.58	1.46
13	3	1001	ANP	PG-O1G	7.81	1.58	1.46
13	3	1001	ANP	PB-O1B	6.82	1.56	1.46
13	5	801	ANP	PB-O1B	6.61	1.56	1.46
13	2	901	ANP	PB-O1B	6.10	1.55	1.46
13	3	1001	ANP	PB-O2B	-2.98	1.48	1.56
13	2	901	ANP	PB-O3A	-2.93	1.55	1.59
13	5	801	ANP	PB-O3A	-2.84	1.55	1.59
13	3	1001	ANP	PG-O2G	-2.77	1.49	1.56
13	3	1001	ANP	PB-O3A	-2.74	1.55	1.59
13	5	801	ANP	PG-O1G	2.58	1.50	1.46
13	5	801	ANP	PB-O2B	-2.52	1.50	1.56
13	2	901	ANP	PG-O2G	-2.46	1.50	1.56
13	3	1001	ANP	PG-N3B	2.45	1.69	1.63
13	2	901	ANP	PB-O2B	-2.45	1.50	1.56
13	2	901	ANP	PG-N3B	2.43	1.69	1.63
13	5	801	ANP	PG-N3B	2.19	1.69	1.63

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	2	901	ANP	O1B-PB-N3B	-3.13	107.17	111.77
13	3	1001	ANP	O3G-PG-O1G	-2.63	106.85	113.45
13	3	1001	ANP	O1G-PG-N3B	-2.62	107.92	111.77
13	5	801	ANP	O3A-PA-O1A	-2.45	103.34	110.70
13	2	901	ANP	O3G-PG-O1G	-2.25	107.81	113.45
13	2	901	ANP	O3A-PB-N3B	2.03	112.21	106.59

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	2	901	ANP	PB-N3B-PG-O1G
13	2	901	ANP	C5'-O5'-PA-O1A
13	2	901	ANP	C5'-O5'-PA-O2A
13	2	901	ANP	C5'-O5'-PA-O3A
13	2	901	ANP	O4'-C1'-N9-C8
13	2	901	ANP	O4'-C1'-N9-C4
13	3	1001	ANP	PB-N3B-PG-O1G
13	3	1001	ANP	PG-N3B-PB-O1B
13	3	1001	ANP	PA-O3A-PB-O2B
13	3	1001	ANP	C5'-O5'-PA-O2A
13	3	1001	ANP	C5'-O5'-PA-O3A
13	3	1001	ANP	O4'-C1'-N9-C8
13	3	1001	ANP	O4'-C1'-N9-C4
13	5	801	ANP	PG-N3B-PB-O1B
13	5	801	ANP	C5'-O5'-PA-O3A
13	5	801	ANP	O4'-C1'-N9-C8
13	5	801	ANP	O4'-C1'-N9-C4
13	2	901	ANP	O4'-C4'-C5'-O5'
13	5	801	ANP	C4'-C5'-O5'-PA
13	5	801	ANP	O4'-C4'-C5'-O5'
13	3	1001	ANP	O4'-C4'-C5'-O5'
13	3	1001	ANP	PB-O3A-PA-O2A
13	2	901	ANP	C3'-C4'-C5'-O5'
13	3	1001	ANP	PB-O3A-PA-O1A
13	3	1001	ANP	PA-O3A-PB-O1B
13	3	1001	ANP	C3'-C4'-C5'-O5'
13	5	801	ANP	C3'-C4'-C5'-O5'

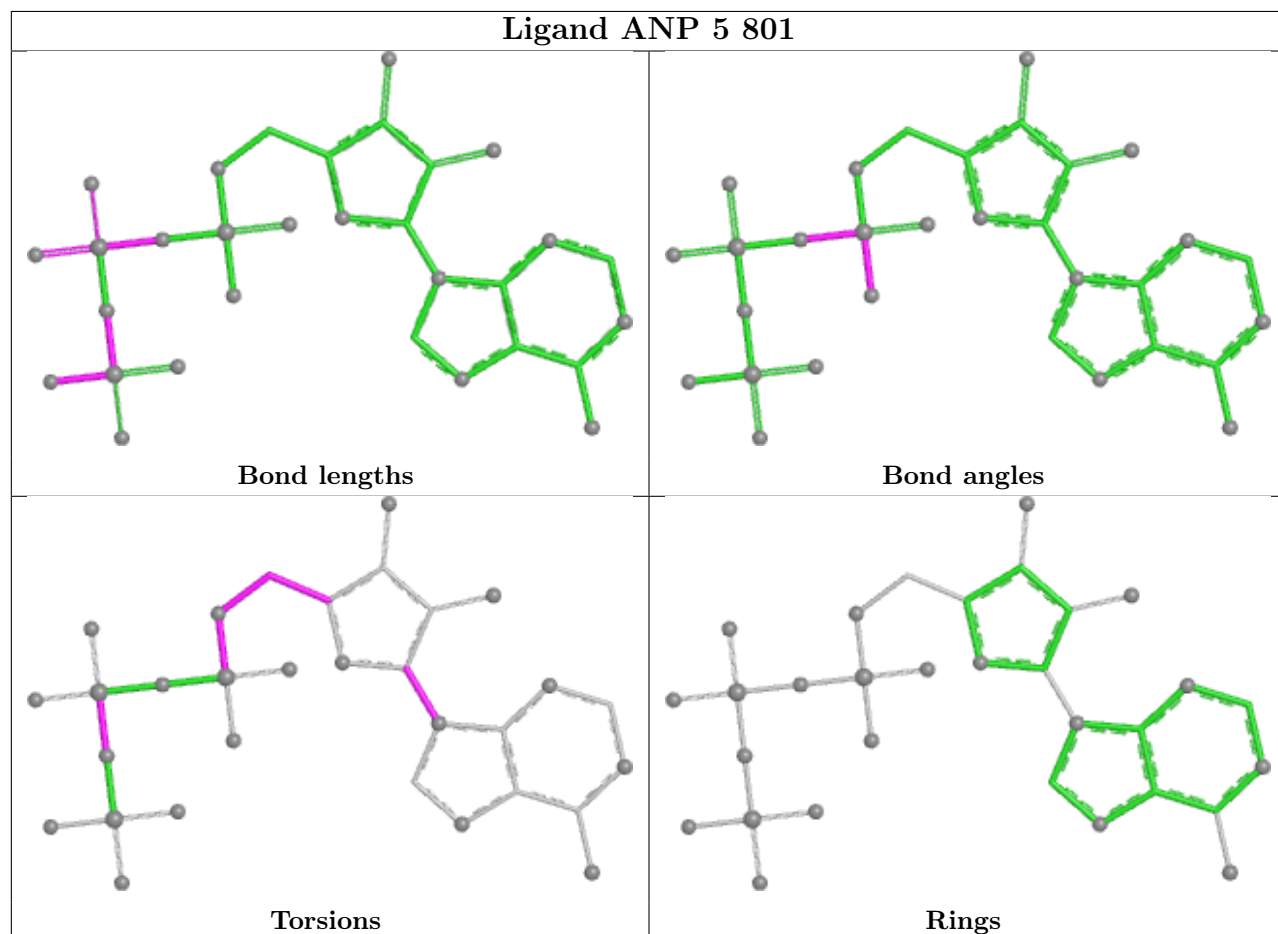
There are no ring outliers.

3 monomers are involved in 28 short contacts:

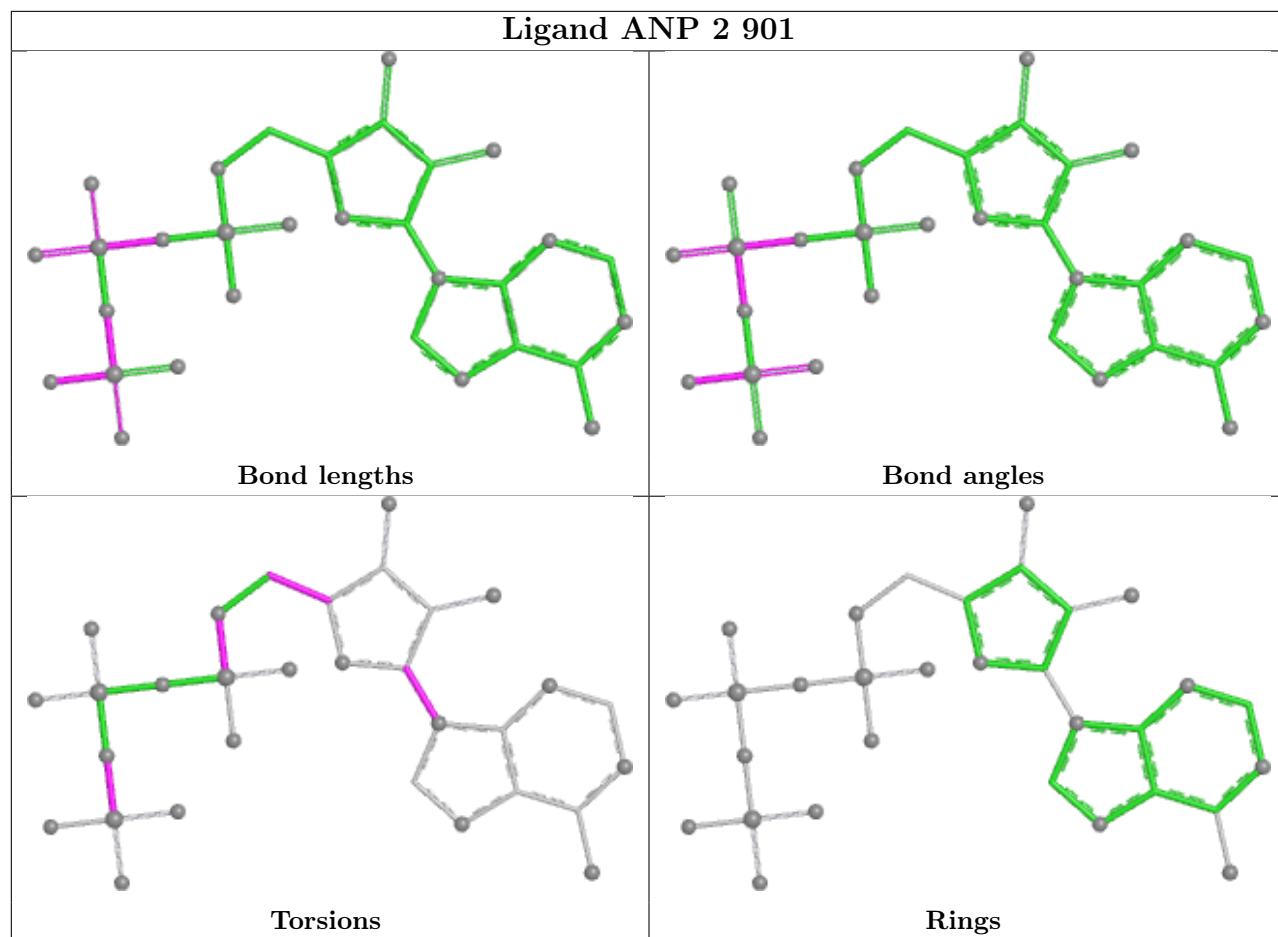
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	5	801	ANP	9	0
13	2	901	ANP	9	0
13	3	1001	ANP	10	0

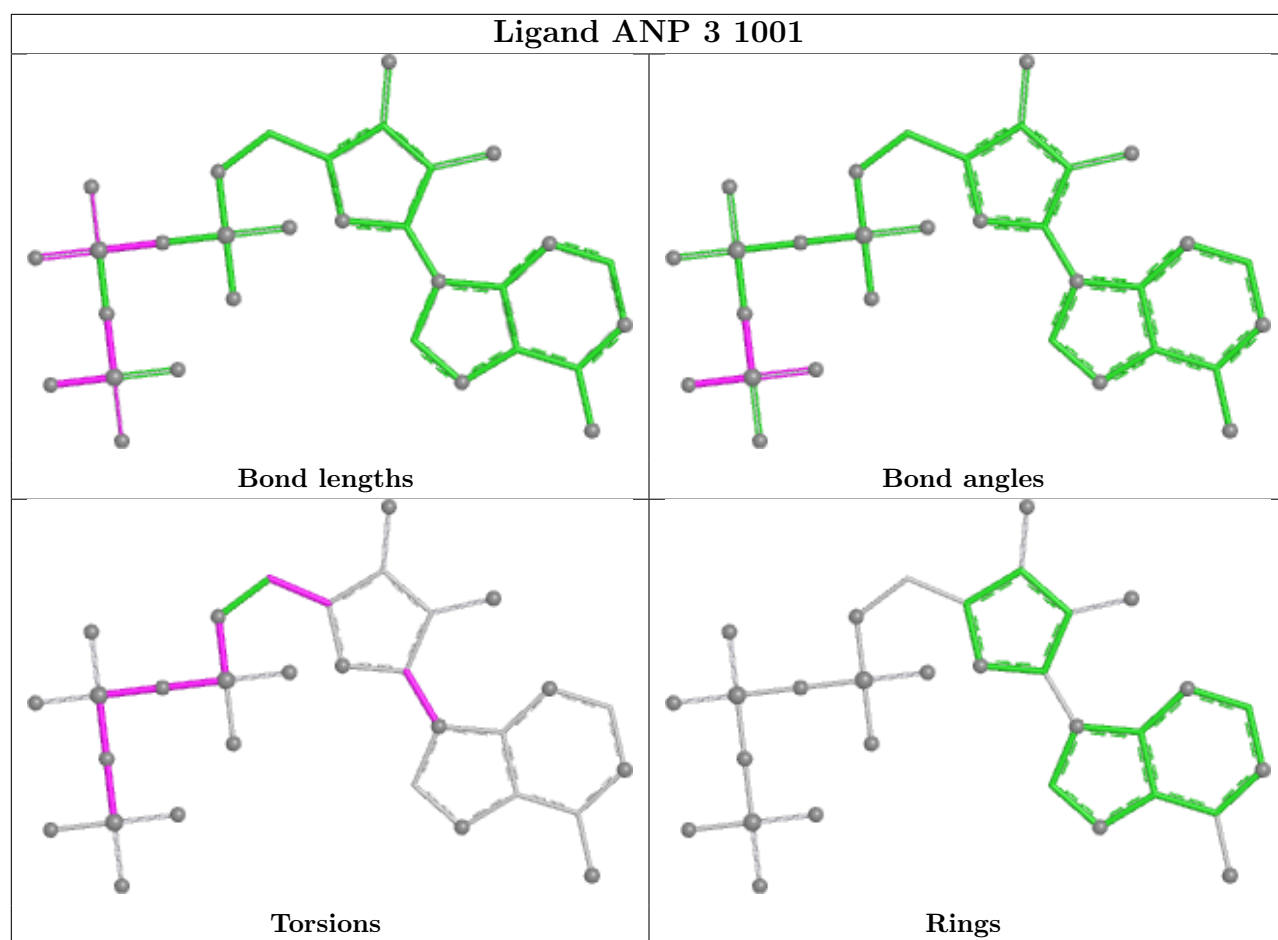
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



Ligand ANP 2 901





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.

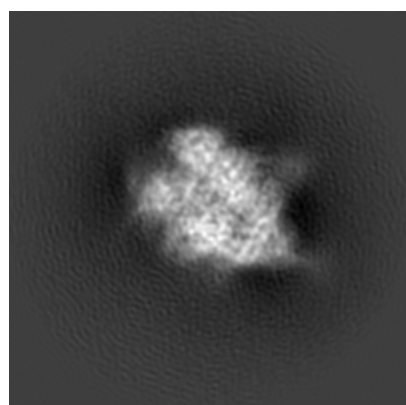
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8519. These allow visual inspection of the internal detail of the map and identification of artifacts.

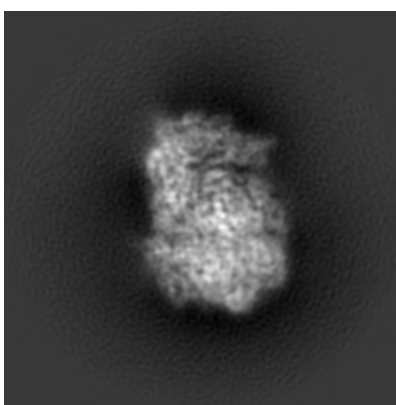
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

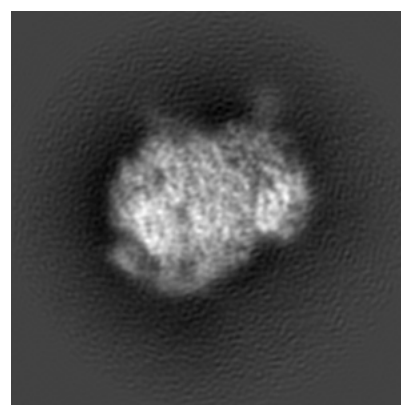
6.1.1 Primary map



X



Y

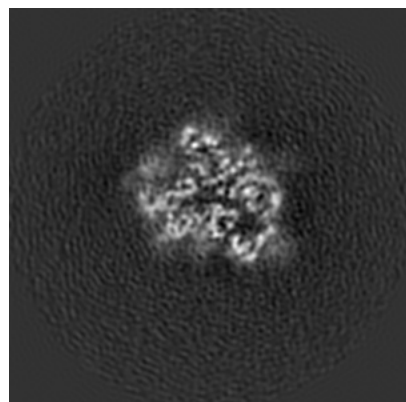


Z

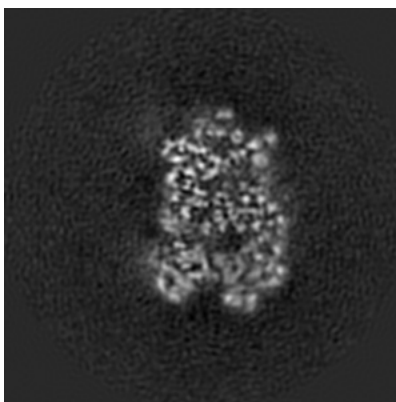
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

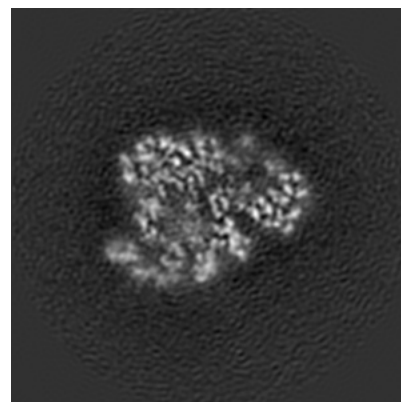
6.2.1 Primary map



X Index: 128



Y Index: 128

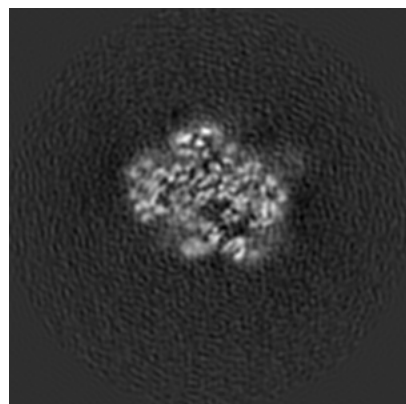


Z Index: 128

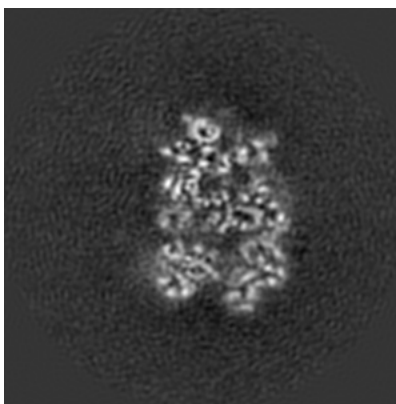
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

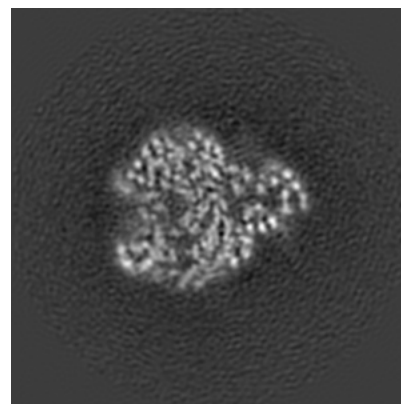
6.3.1 Primary map



X Index: 121



Y Index: 125

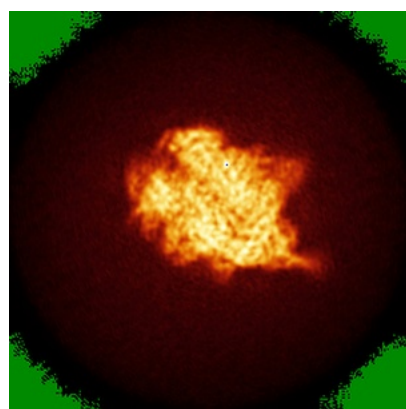


Z Index: 137

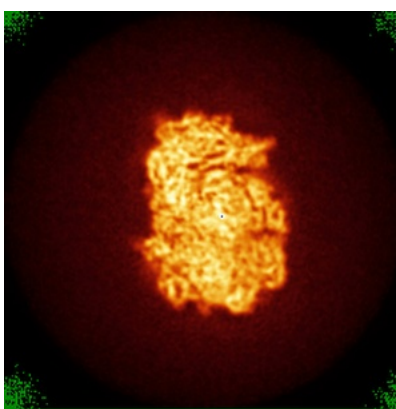
The images above show the largest variance slices of the map in three orthogonal directions.

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

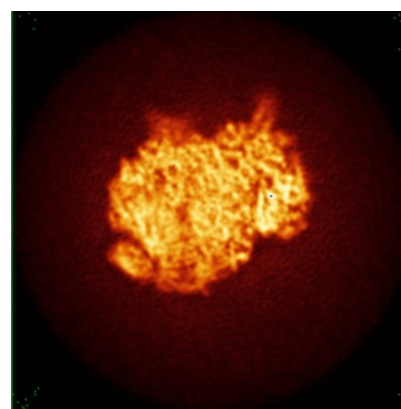
6.4.1 Primary map



X



Y

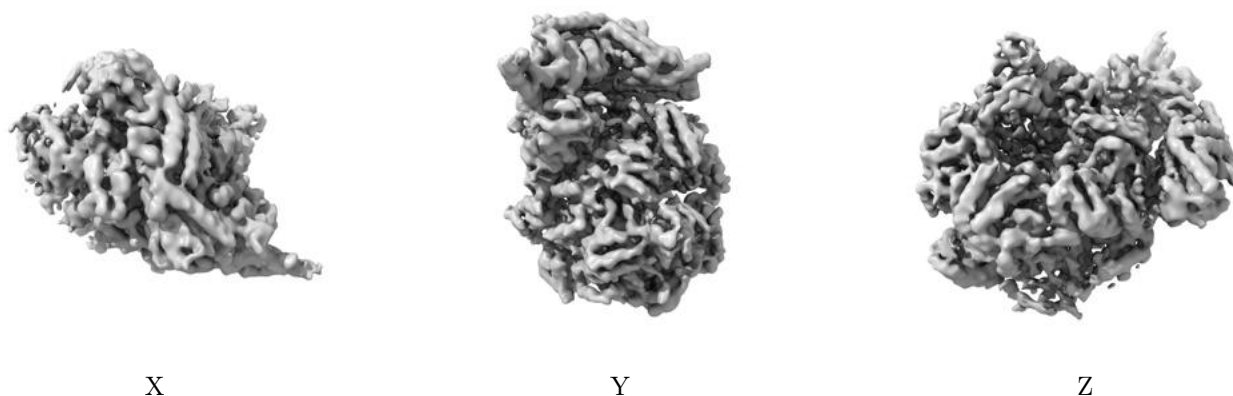


Z

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 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

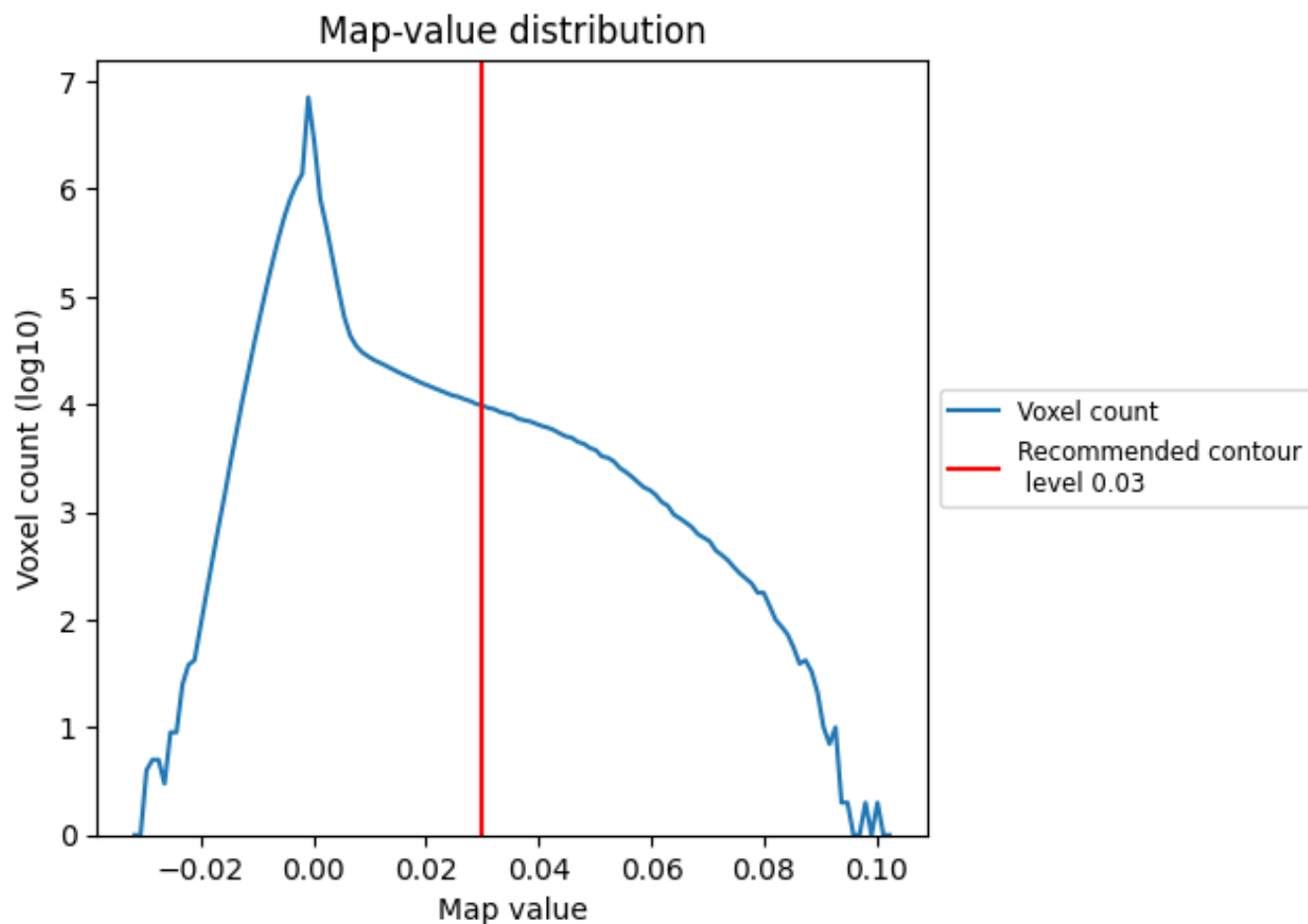
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

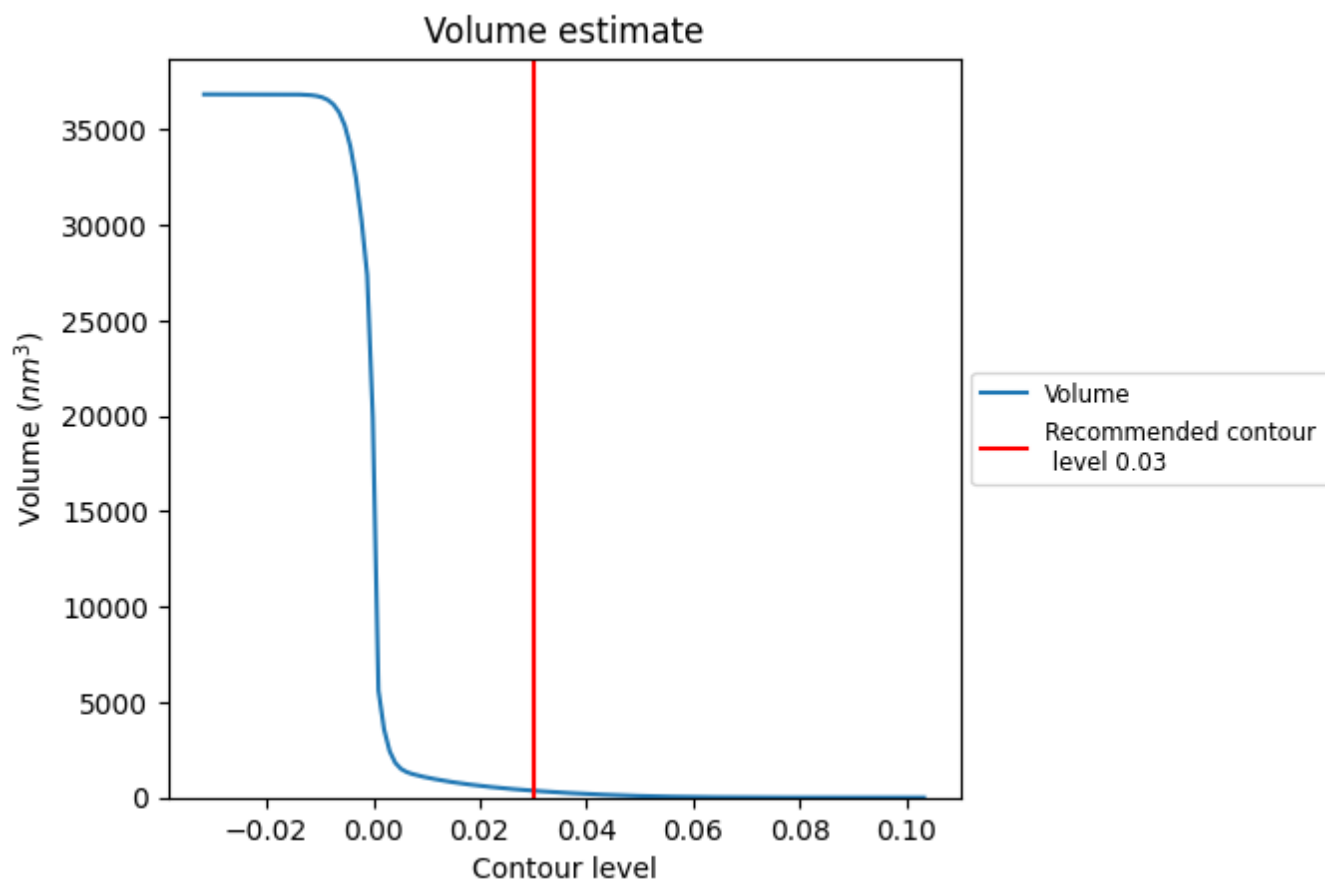
This section contains the results of statistical analysis of the map.

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.

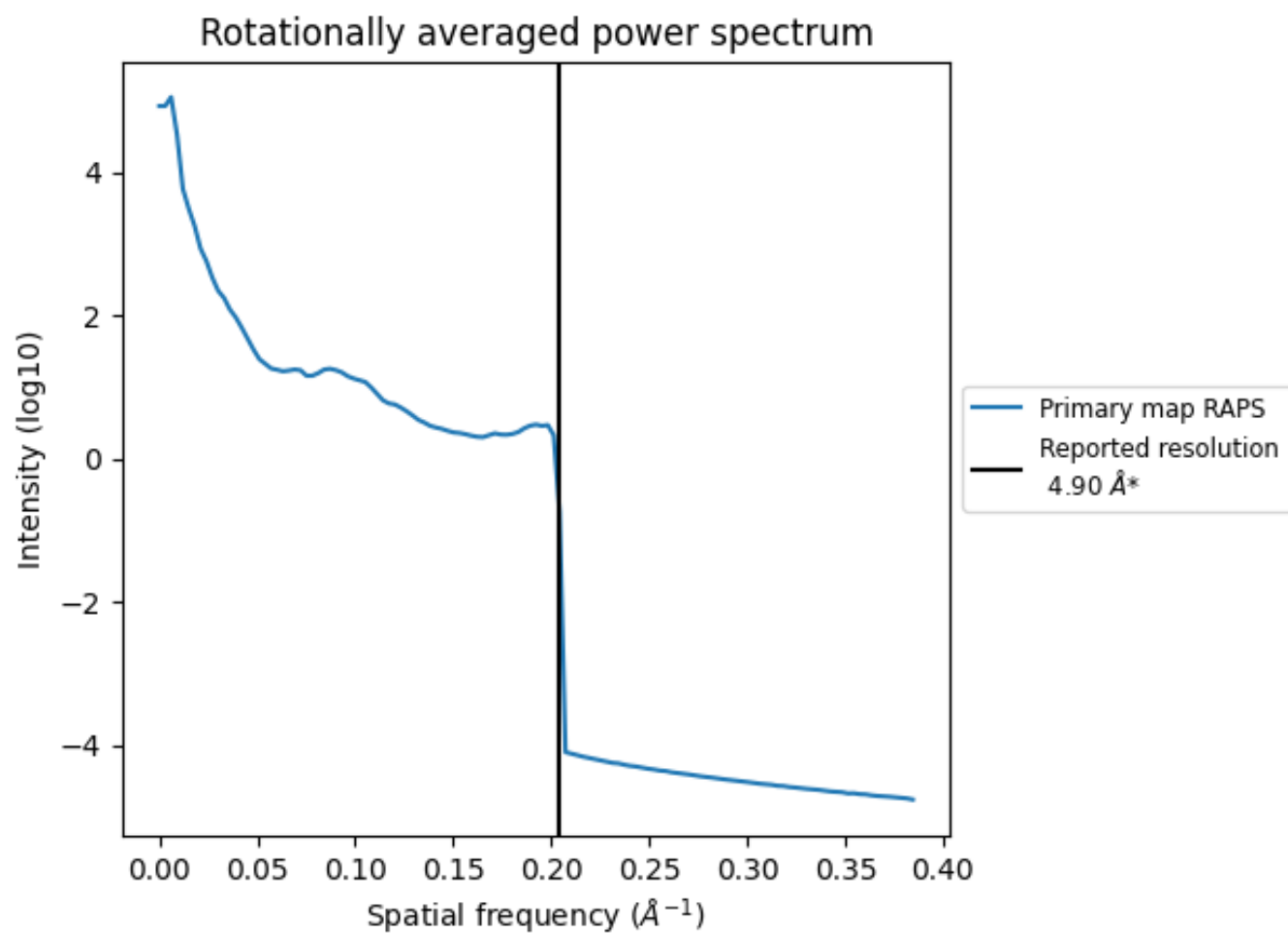
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 361 nm³; this corresponds to an approximate mass of 326 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 0.204 $\text{\AA}^{-1}$

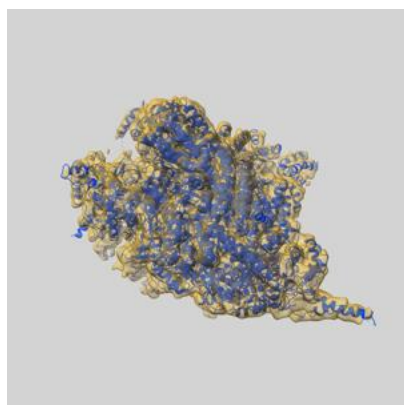
8 Fourier-Shell correlation

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

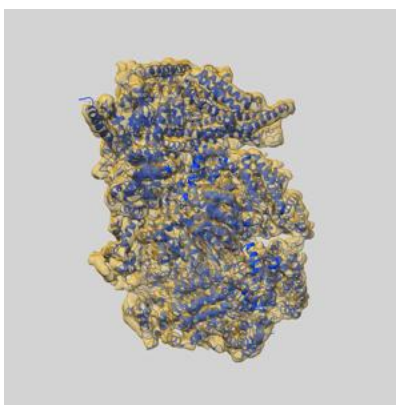
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-8519 and PDB model 5U8T. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

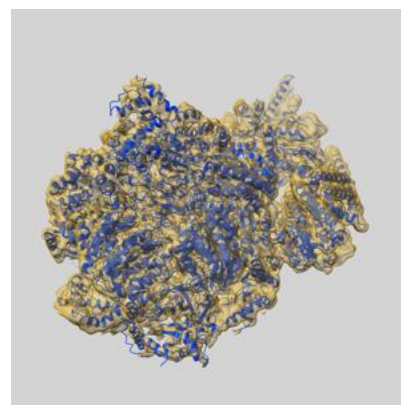
9.1 Map-model overlay [i](#)



X



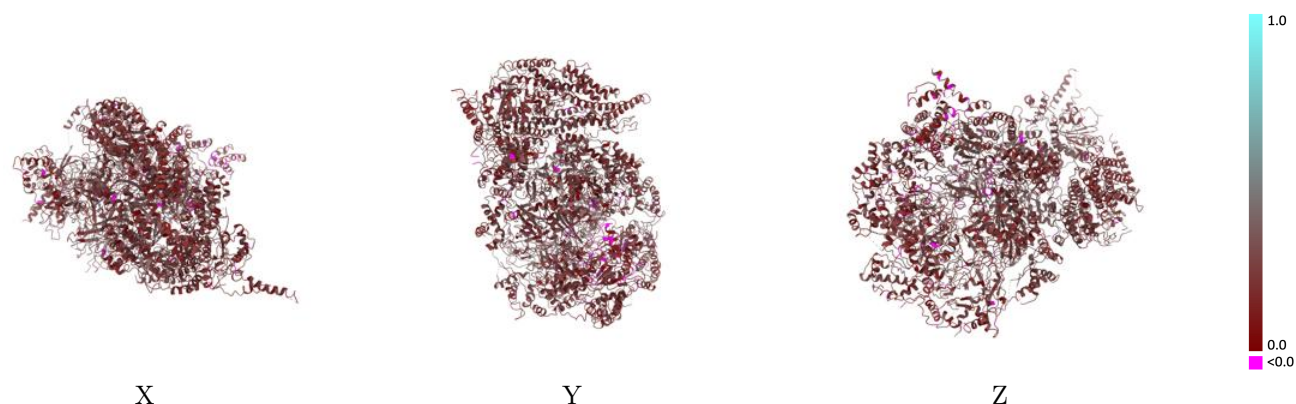
Y



Z

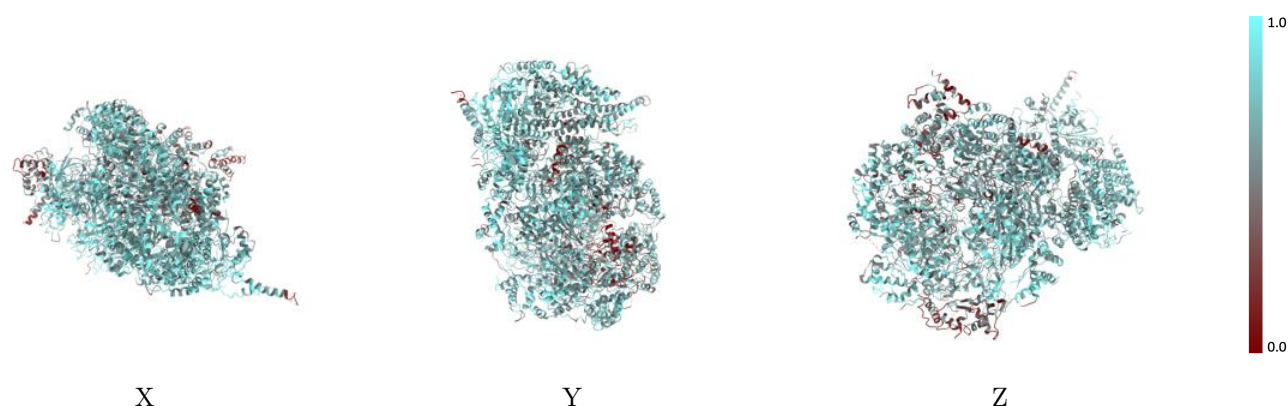
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



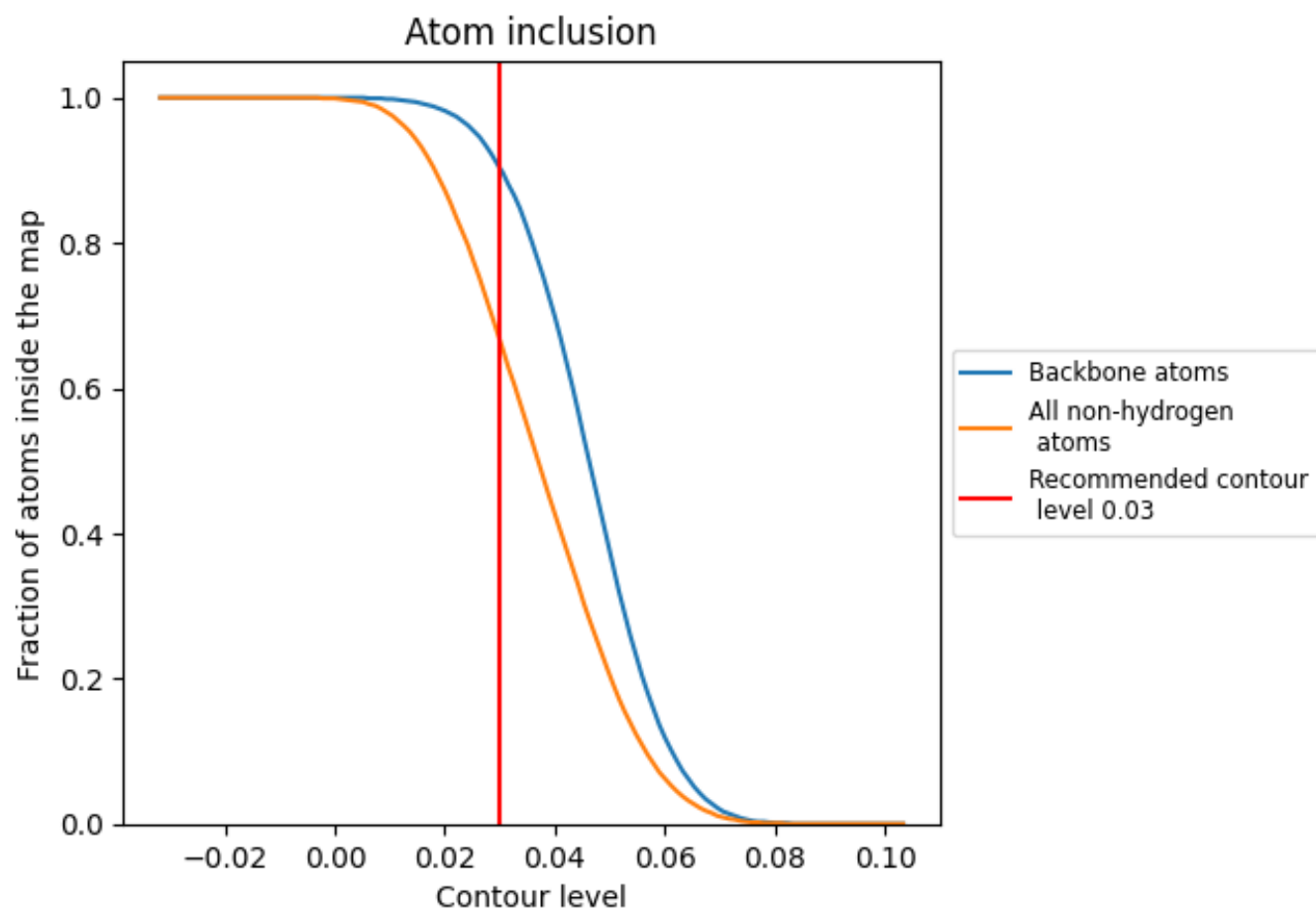
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 67% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6670	0.2390
2	0.6860	0.2540
3	0.6920	0.2550
4	0.6430	0.2080
5	0.6430	0.2580
6	0.6510	0.2250
7	0.5680	0.2290
A	0.6480	0.2140
B	0.7350	0.2550
C	0.7400	0.2550
D	0.7520	0.2420
E	0.7310	0.2430
F	0.7610	0.3030

