



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 05:44 PM UTC

PDB ID : 3JC6 / pdb_00003jc6
EMDB ID : EMD-6534
Title : Structure of the eukaryotic replicative CMG helicase and pumpjack motion
Authors : Li, H.; Bai, L.; Yuan, Z.; Sun, J.; Georgescu, R.E.; Liu, J.; O'Donnell, M.E.
Deposited on : 2015-11-24
Resolution : 3.70 Å(reported)
Based on initial model : 2Q9Q

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

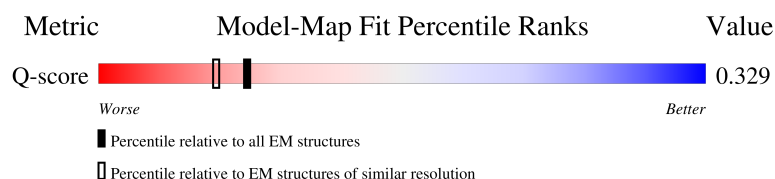
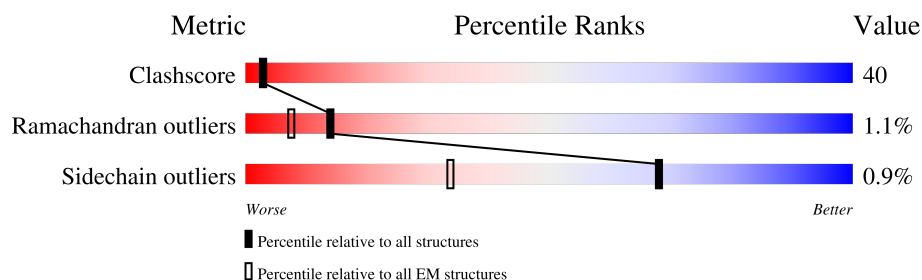
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 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	11569 (3.20 - 4.20)

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	 16% 11% 72%
2	3	971	 13% 13% 72%
3	4	933	 13% 15% 71%
4	5	775	 15% 17% 67%

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Mol	Chain	Length	Quality of chain
5	6	1017	14%12%74%
6	7	845	5%19%17%62%
7	E	672	8%42%38%18%
8	D	294	35%38%25%
9	B	213	38%46%15%
10	A	208	15%40%56%
11	C	194	39%42%18%

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 23732 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	241	Total	C	N	O	S	0	0
			1911	1214	338	354	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	3	269	Total	C	N	O	S	0	0
			2130	1354	368	404	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	4	275	Total	C	N	O	S	0	0
			2203	1391	382	413	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	5	254	Total	C	N	O	S	0	0
			2028	1284	347	388	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	6	267	Total	C	N	O	S	0	0
			2049	1296	366	381	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	7	325	Total	C	N	O	S	0	0
			2611	1653	455	491	12		

- Molecule 7 is a protein called Cell division control protein 45.

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

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	651	ASP	-	expression tag	UNP Q08032
E	652	TYR	-	expression tag	UNP Q08032
E	653	LYS	-	expression tag	UNP Q08032
E	654	ASP	-	expression tag	UNP Q08032
E	655	HIS	-	expression tag	UNP Q08032
E	656	ASP	-	expression tag	UNP Q08032
E	657	GLY	-	expression tag	UNP Q08032
E	658	ASP	-	expression tag	UNP Q08032
E	659	TYR	-	expression tag	UNP Q08032
E	660	LYS	-	expression tag	UNP Q08032
E	661	ASP	-	expression tag	UNP Q08032
E	662	HIS	-	expression tag	UNP Q08032
E	663	ASP	-	expression tag	UNP Q08032
E	664	ILE	-	expression tag	UNP Q08032
E	665	ASP	-	expression tag	UNP Q08032
E	666	TYR	-	expression tag	UNP Q08032
E	667	LYS	-	expression tag	UNP Q08032
E	668	ASP	-	expression tag	UNP Q08032
E	669	ASP	-	expression tag	UNP Q08032
E	670	ASP	-	expression tag	UNP Q08032
E	671	ASP	-	expression tag	UNP Q08032
E	672	LYS	-	expression tag	UNP Q08032

- Molecule 8 is a protein called DNA replication complex GINS protein SLD5.

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

- Molecule 9 is a protein called DNA replication complex GINS protein PSF2.

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

- Molecule 10 is a protein called DNA replication complex GINS protein PSF1.

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

- Molecule 11 is a protein called DNA replication complex GINS protein PSF3.

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

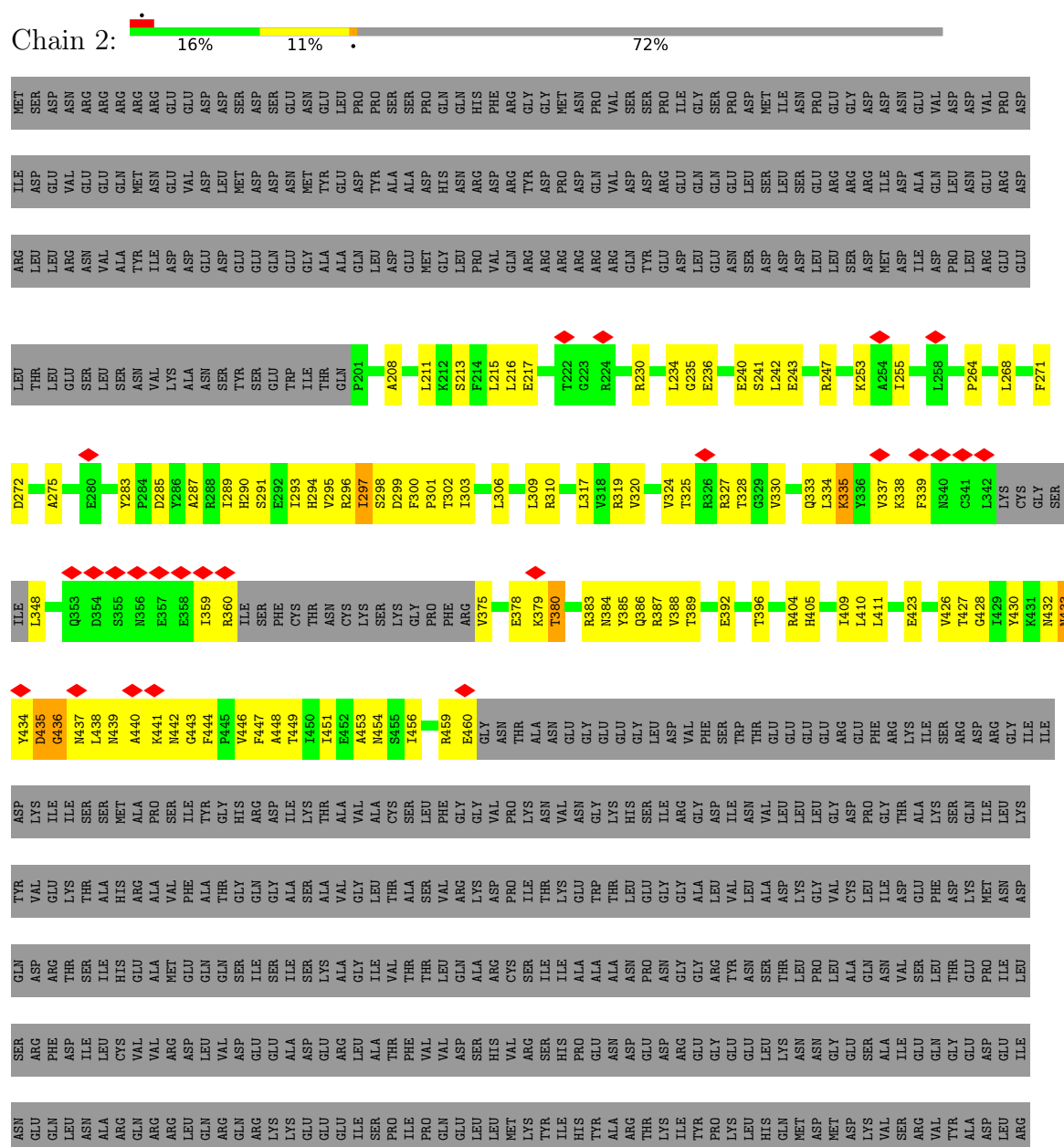
- Molecule 12 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
12	7	1	Total	Zn	0
			1	1	

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: DNA replication licensing factor MCM2



- Molecule 2: DNA replication licensing factor MCM3

[illegible]

VAL	LEU	SER	LEU	LEU	ILE	SER	GLY	ILE	ILE	ALA	ARG	LEU	MET	GLN	THR	GLY	ILE	PHE	GLU	GLU	SER	LYS	TRP	PRO	VAL	ALA	SER	LEU	PHE	ARG	ILE	ASN	GLU	GLY	LEU	PRO	GLU	GLY	LYS	PHE	SER	ALA	GLN	GLY	TRP	LEU	ALA	GLY	LEU	LYS	ILE	MET	SER	ASP	ASN	ASN	LEU	MET
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- Molecule 3: DNA replication licensing factor MCM4



MET	GLN	GLN	SER	SER	SER	PRO	THR	LYS	GLU	ASP	ASN	ASN	SER	SER	SER	PRO	PRO	VAL	VAL	ASN	ASN	ASP	SER	SER	GLN	LEU	SER	SER	PRO	ALA	PRO	LEU	PHE	TYR	SER	SER	SER	SER	SER	GLN	GLY	ASP	ASP	ILE	TYR	GLY	ARG	ASN	ASN	SER	SER	GLN	ASN	LEU	SER	SER	GLN	GLY	GLY
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ASN	ILE	ARG	ALA	ALA	ILE	GLY	SER	SER	PRO	LEU	ASN	PHE	PRO	SER	SER	SER	GLN	ARG	GLN	ASN	ASP	VAL	PHE	GLN	SER	SER	GLY	GLN	ARG	GLY	GLY	ILE	ILE	ARG	SER	SER	SER	ALA	ALA	ALA	GLY	ARG	SER	ARG	ARG	TYR	HIS	SER	ASP	LEU	ARG	SER	ASP	ARG	ALA	LEU	PRO	THR	SER	SER
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SER	SER	LEU	GLY	ARG	ASN	GLY	GLN	ASN	ASN	ARG	VAL	HIS	MET	ARG	ARG	ASN	ASP	ILE	THR	SER	ASP	LEU	SER	SER	PRO	PRO	ARG	ARG	ILE	VAL	ASP	PHE	ASP	ASP	THR	THR	SER	GLY	VAL	ASN	THR	THR	LEU	ASP	THR	THR	SER	SER	SER	SER	ALA	PRO	PRO	PRO	SER	SER	ALA	SER	GLU	GLU	PRO	L177	L180
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G182	T183	T184		F197		S200	P201	X202	Y203	K204	P205	ARG	ARG	LYS	ILE	LEU	ASP	GLU	ARG	GLU	GLU	PHE	ASN	ASN	THR	THR	ASP	GLU	GLU	GLU	LEU	Y225	Y226	Y227	K228	Q229		M233	R234	E235	L236	G237	T238	S239	M240	L241	M242	L243	L244	L245	R246	N247	L248	L249	A250		T254	E255		L261
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[illegible]

S335	S336	S337	S338	S339	M342	K343	V344	A345	F346	F347	K348	V351	C352	D353	H354	S355	M356	A357	I360	D361	R362	G363	V364	R370	C371	E372	R373	I374	D375	C376	M377	E378	P379	M382	I385	H386	N387	R388	A392	Q395	K398	L399	Q400	E401	T402	F403	D404	F405	V406
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P407	D408	G409	Q410	T411	P412	H413	S414	L415	S416	L417	C418	V419	Y420	D421	E422	L423	V424	D425	R426	R428	A429	G430	L433	E434	V435	T436	G437	T438	F439	R440	S441	I442	P443	I444	R445	A446	M447	S448	R449	Q450	R451	V452	L453	H455	V456	K457	K458	V459	S470	ASP	LVS
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ARG LEU ASP VAL ASP THR SER THR THR ILE GLU GLN GLU LEU MET GLN ASN LYS VAL ASP HIS ASN GLU VAL GLU GLU ASP ARG ILE THR THR ASP GLN GLN ASP LEU ALA LYS ILE ARG GLU VAL VAL ALA ALA ALA ARG GLU ASP TYR SER LEU LEU LEU LEU PRO SER ILE TYR THR

LEU GLU ASP VAL LYS GLY ILE LEU LEU GLN PHE GLY GLY THR THR LYS THR PHE THR THR LYS GLY ARG TYR ARG ARG ASP ASP ILE ASN GLN LEU LEU LEU CYS GLY ASP ASP PRO SER SER SER LYS SER GLN ILE LEU LEU LEU GLN TYR VAL HIS LYS ILE ILE THR THR PRO ARG GLY VAL TYR THR THR

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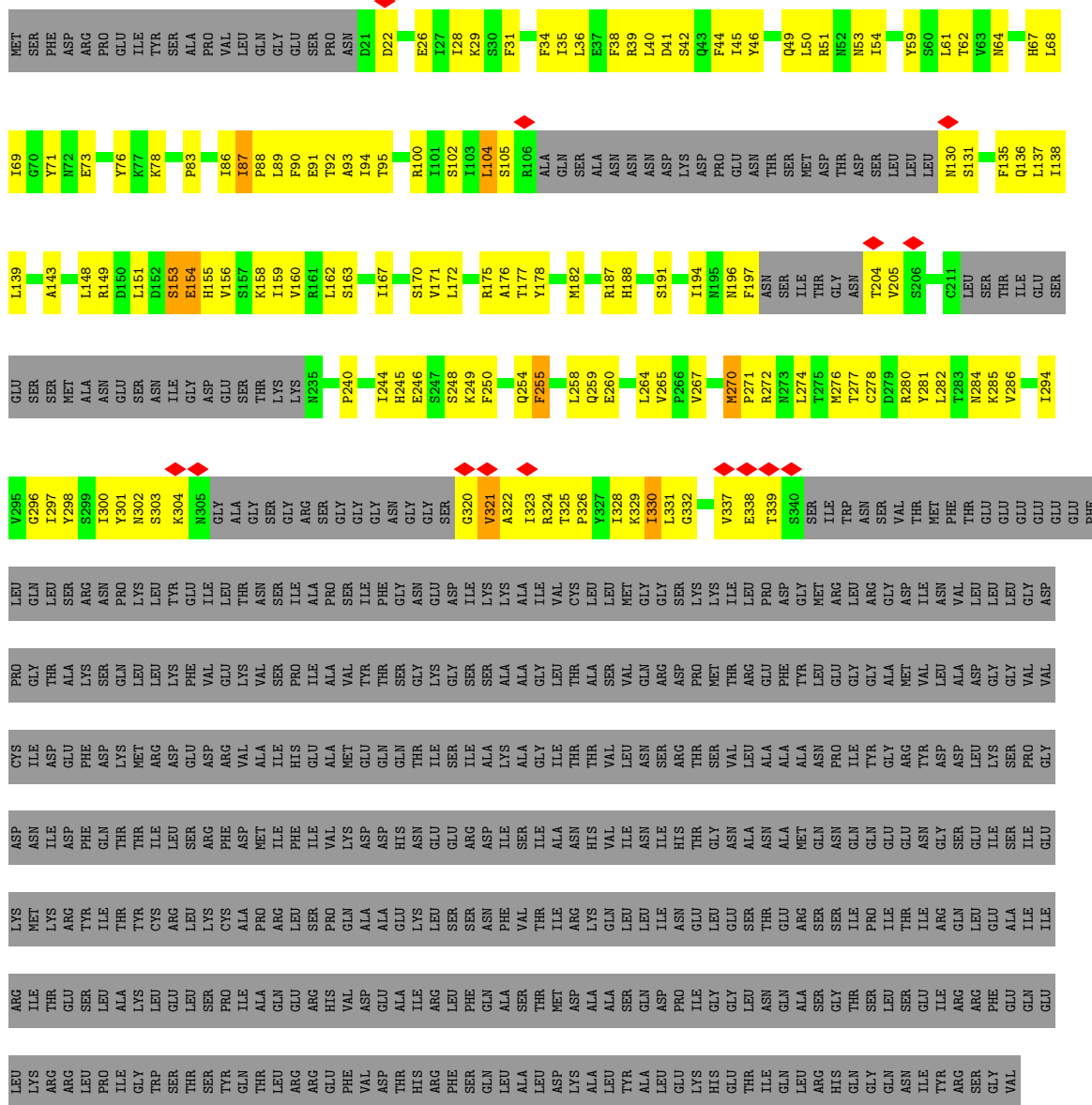
THR	ILE	SER	ILE	ALA	LYS	ALA	GLY	ILE	THR	THR	LEU	ASN	ALA	ARG	SER	SER	ILE	LEU	ALA	ALA	ASN	PRO	GLY	SER	ARG	TYR	ASN	PRO	ASN	LEU	PRO	VAL	THR	GLU	ASN	ILE	ASP	LEU	PRO	PRO	LEU	LEU	SER	ARG	PHE	ASP	LEU	VAL	TYR	LEU	VAL	LEU	ASP	LYS	VAL
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ASP	GLU	LYS	LYS	ASN	ASP	ARG	GLU	LEU	ALA	LYS	HIS	LEU	THR	ASN	LEU	TYR	LEU	LEU	GLU	ASP	LYS	PRO	PRO	GLU	ILE	ILE	SER	GLN	ASP	ASP	ASP	VAL	LEU	PRO	VAL	GLU	PHE	LEU	THR	MET	ILE	TYR	SER	SER	TYR	ALA	LYS	GLU	HIS	ILE	ILE	PRO	HIS	PRO	ILE	ILE	THR	GLU	GLA	ALA	ALA	LYS	THR	GLU	LEU	VAL	PC
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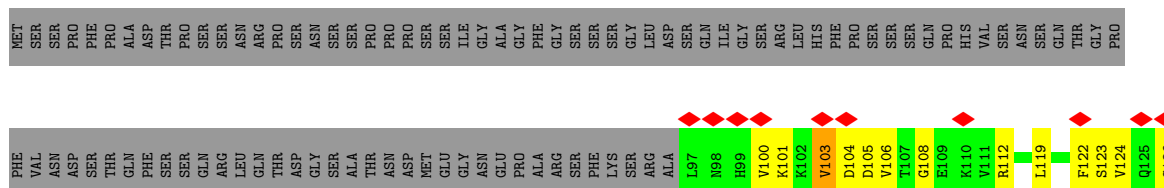
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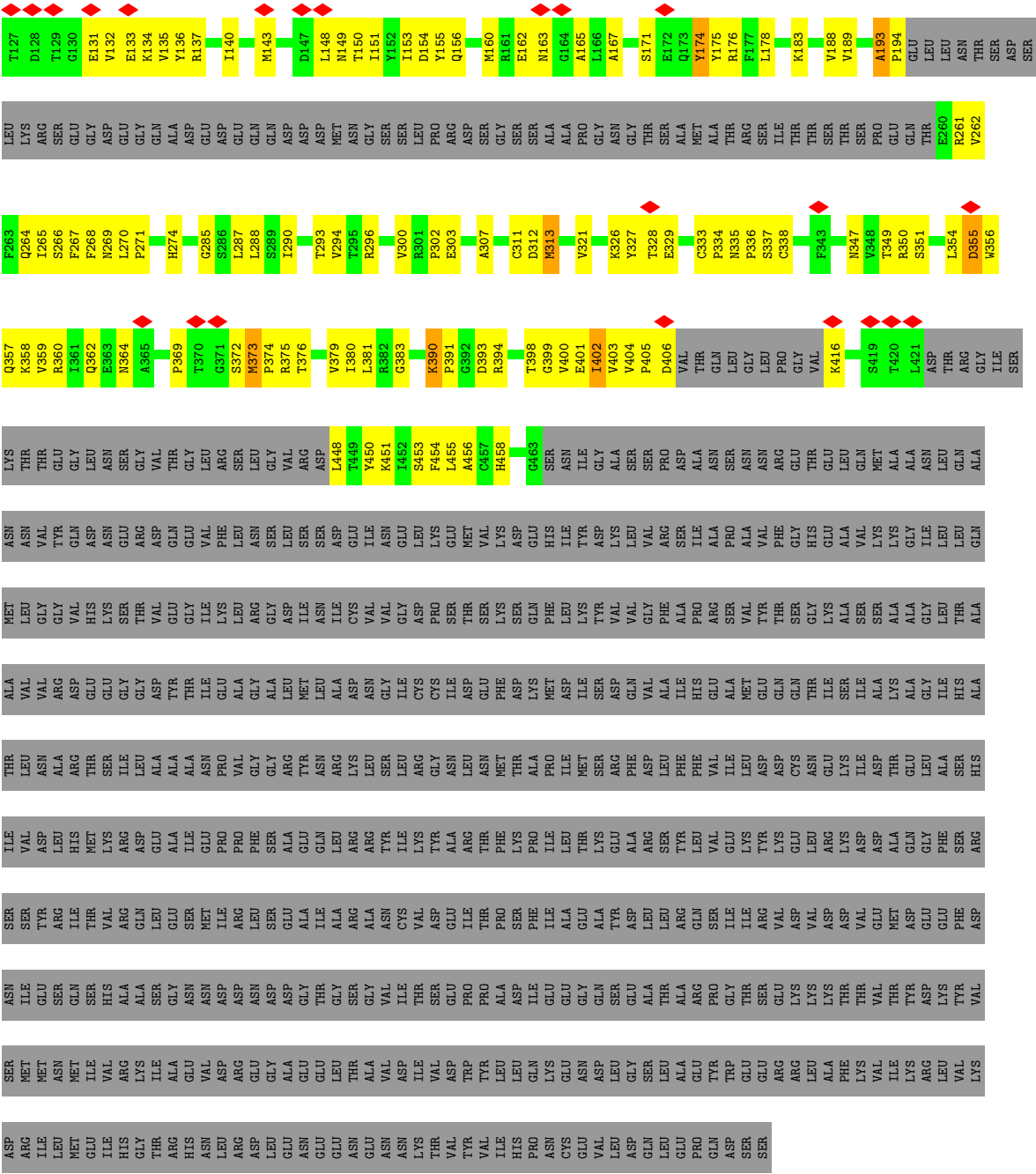
ILE LYS ASP TYR THR ASP PRO LYS THR GLY LYS ILE ASP MET ASN LEU VAL GLN THR LYS GLY SER LEU GLN GLU ASP LEU SER ARG GLU ILE MET ASN VAL LEU LYS ASP GLN ALA SER ASP ASP SER MET SER PHE ASN GLN LEU ILE LYS GLN ILE ILE ASN THR

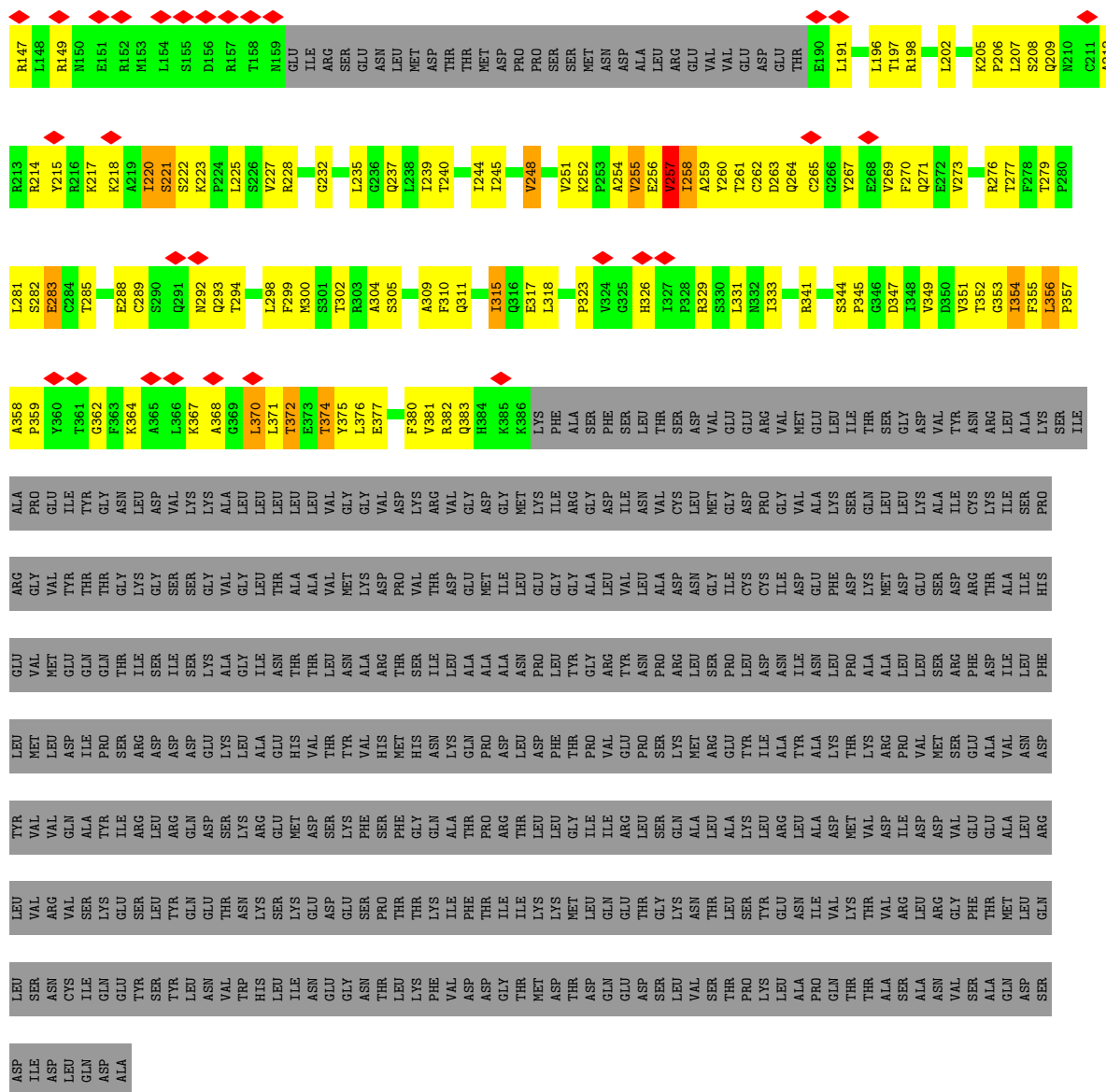
Chain 5: 15% 17% . 67%



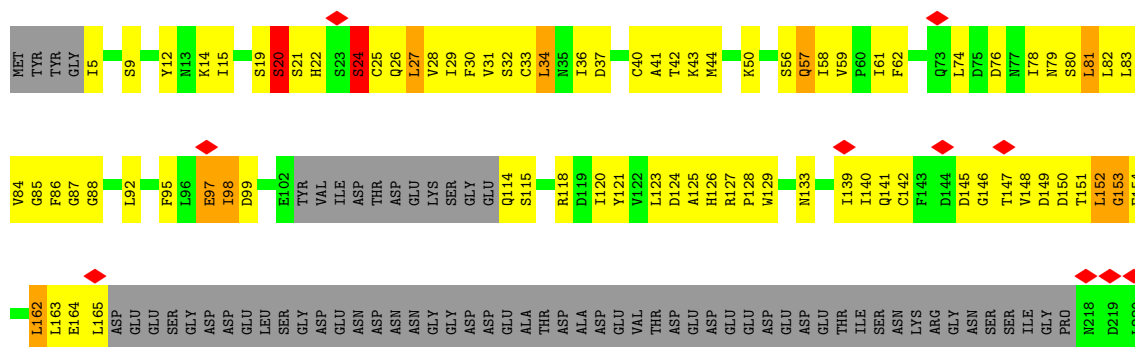
Chain 6: 14% 12% 74%

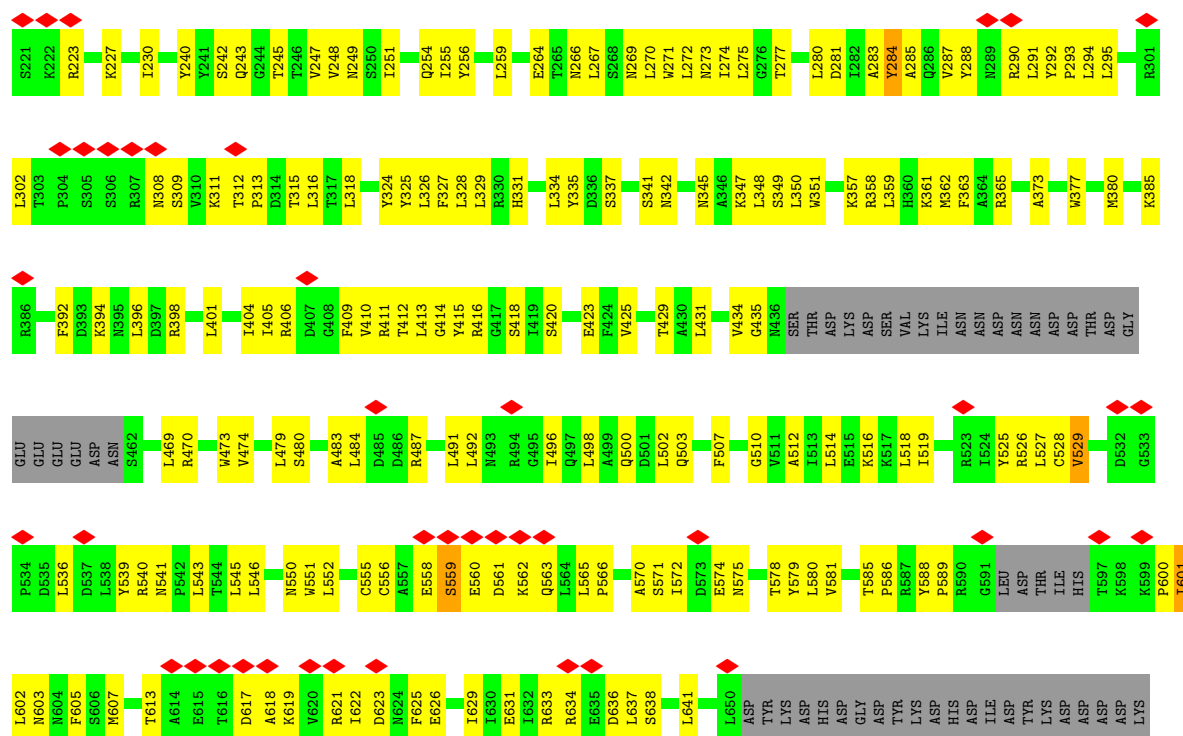




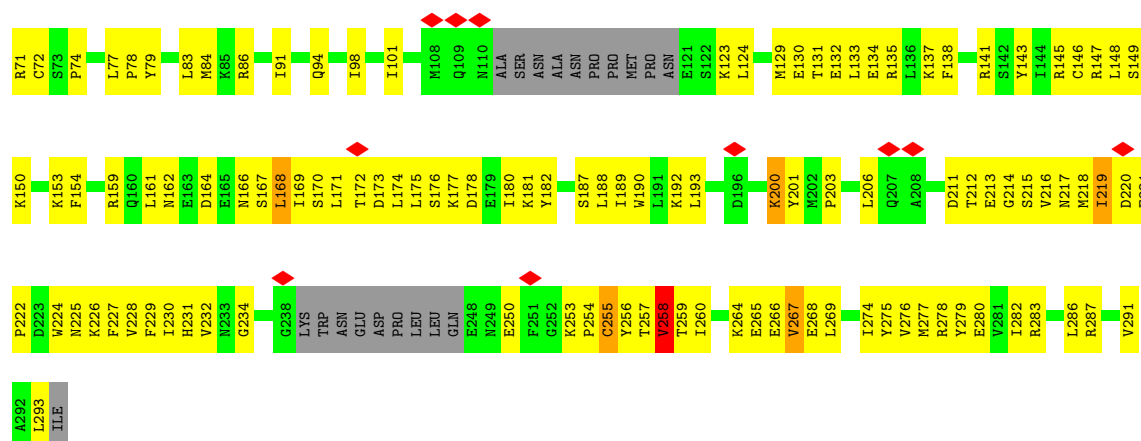
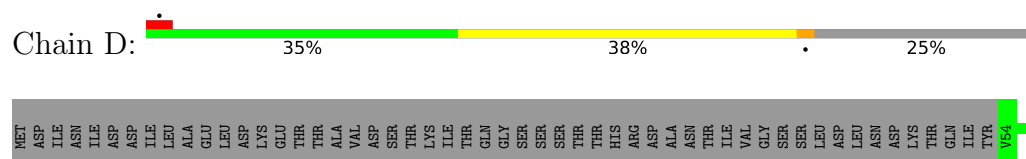


• Molecule 7: Cell division control protein 45

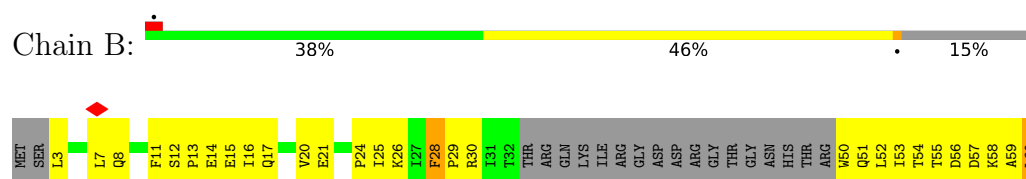


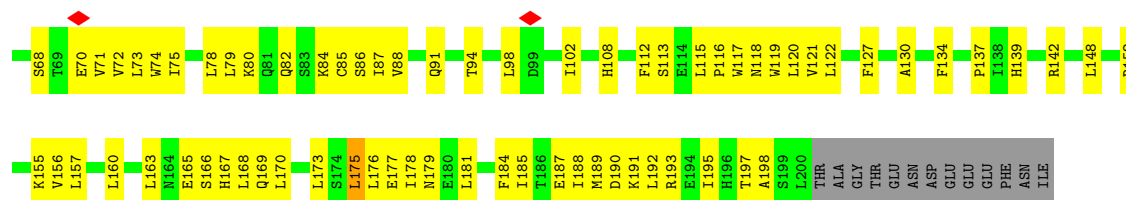


• Molecule 8: DNA replication complex GINS protein SLD5

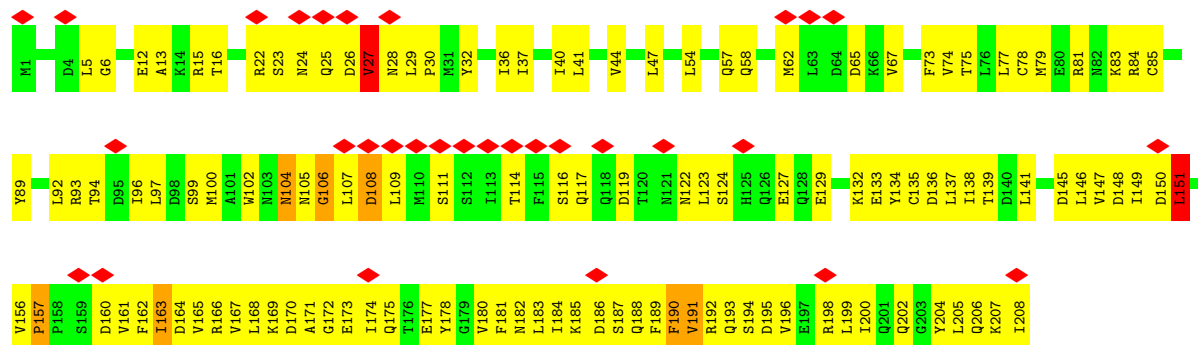


• Molecule 9: DNA replication complex GINS protein PSF2

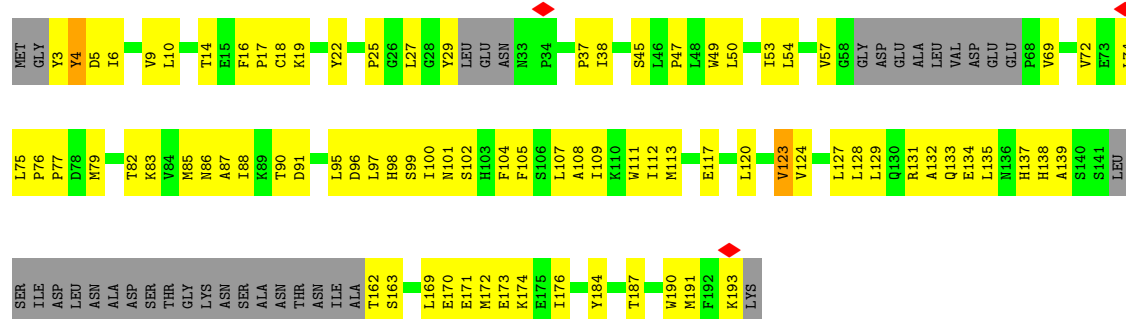




• Molecule 10: DNA replication complex GINS protein PSF1



• Molecule 11: DNA replication complex GINS protein PSF3



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	469818	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	CTFFIND4	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	49505	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.155	Depositor
Minimum map value	-0.084	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.02	Depositor
Map size ($\text{\AA}$)	258.56, 258.56, 258.56	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.01, 1.01, 1.01	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.54	0/1946	1.00	6/2633 (0.2%)
2	3	0.63	0/2179	1.11	18/2963 (0.6%)
3	4	0.49	0/2240	1.09	17/3029 (0.6%)
4	5	0.66	0/2057	1.21	13/2781 (0.5%)
5	6	0.51	0/2081	1.08	13/2813 (0.5%)
6	7	0.53	0/2657	1.02	14/3592 (0.4%)
7	E	0.49	0/4563	0.93	10/6173 (0.2%)
8	D	0.54	0/1853	1.00	5/2500 (0.2%)
9	B	0.58	0/1545	1.02	6/2092 (0.3%)
10	A	0.52	1/1718 (0.1%)	1.01	10/2314 (0.4%)
11	C	0.56	0/1320	0.90	1/1784 (0.1%)
All	All	0.55	1/24159 (0.0%)	1.03	113/32674 (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
2	3	0	2
3	4	0	5
5	6	0	3
6	7	0	4
7	E	0	1
8	D	0	2
10	A	0	4
All	All	0	21

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	27	VAL	CA-CB	5.84	1.62	1.54

All (113) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	5	325	THR	CA-C-N	19.01	140.37	119.83
4	5	325	THR	C-N-CA	19.01	140.37	119.83
3	4	378	GLU	CA-C-N	14.66	134.51	119.56
3	4	378	GLU	C-N-CA	14.66	134.51	119.56
5	6	333	CYS	CA-C-N	13.09	136.20	119.84
5	6	333	CYS	C-N-CA	13.09	136.20	119.84
6	7	94	LEU	N-CA-C	11.46	123.86	111.36
5	6	373	MET	CA-C-N	9.20	129.28	119.90
5	6	373	MET	C-N-CA	9.20	129.28	119.90
10	A	156	VAL	CA-C-N	9.17	129.83	120.38
10	A	156	VAL	C-N-CA	9.17	129.83	120.38
4	5	87	ILE	CA-C-N	-8.08	111.40	119.56
4	5	87	ILE	C-N-CA	-8.08	111.40	119.56
2	3	153	TRP	CB-CA-C	-8.03	106.24	115.79
8	D	267	VAL	N-CA-C	7.83	118.42	110.82
6	7	374	THR	CB-CA-C	-7.56	106.79	115.79
6	7	356	LEU	CA-C-N	7.41	128.00	120.14
6	7	356	LEU	C-N-CA	7.41	128.00	120.14
1	2	433	ASN	N-CA-C	7.37	119.82	110.24
1	2	335	LYS	CB-CA-C	-7.14	108.33	116.54
5	6	193	ALA	N-CA-C	7.14	116.53	108.25
2	3	163	ALA	CA-C-N	6.90	134.11	121.70
2	3	163	ALA	C-N-CA	6.90	134.11	121.70
3	4	318	ASN	CA-C-N	6.89	127.03	119.87
3	4	318	ASN	C-N-CA	6.89	127.03	119.87
8	D	258	VAL	CA-C-N	6.87	134.06	121.70
8	D	258	VAL	C-N-CA	6.87	134.06	121.70
7	E	541	ASN	CA-C-N	6.81	127.08	119.32
7	E	541	ASN	C-N-CA	6.81	127.08	119.32
3	4	421	ASP	CB-CA-C	-6.76	108.77	116.54
6	7	374	THR	N-CA-C	6.65	121.56	109.32
10	A	108	ASP	CA-C-N	6.60	133.59	121.70
10	A	108	ASP	C-N-CA	6.60	133.59	121.70
9	B	113	SER	CB-CA-C	-6.53	107.20	116.34
6	7	326	HIS	CB-CA-C	-6.51	108.04	115.79
2	3	123	PRO	N-CA-C	6.47	118.60	110.70
4	5	286	VAL	N-CA-C	6.46	117.34	107.77
3	4	339	ILE	CA-C-N	6.45	126.21	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	4	339	ILE	C-N-CA	6.45	126.21	119.76
5	6	390	LYS	CA-C-N	6.40	126.62	119.90
5	6	390	LYS	C-N-CA	6.40	126.62	119.90
3	4	448	SER	CA-C-N	6.36	133.16	121.70
3	4	448	SER	C-N-CA	6.36	133.16	121.70
5	6	174	TYR	N-CA-C	6.34	118.72	111.11
6	7	372	THR	N-CA-C	6.32	118.98	111.33
4	5	143	ALA	CB-CA-C	-6.29	109.31	116.54
2	3	122	ILE	CA-C-N	-6.28	113.91	120.38
2	3	122	ILE	C-N-CA	-6.28	113.91	120.38
2	3	137	ASP	N-CA-C	6.27	118.63	108.41
8	D	253	LYS	CA-C-N	-6.26	112.02	118.85
8	D	253	LYS	C-N-CA	-6.26	112.02	118.85
7	E	284	TYR	CB-CA-C	-6.23	108.38	115.79
9	B	113	SER	N-CA-C	6.16	117.11	108.00
1	2	287	ALA	N-CA-C	-6.13	104.51	112.23
2	3	280	ASP	CB-CA-C	-6.11	109.54	116.63
6	7	267	TYR	CB-CA-C	-6.10	107.80	116.34
4	5	270	MET	CA-C-N	6.10	125.86	119.76
4	5	270	MET	C-N-CA	6.10	125.86	119.76
7	E	59	VAL	N-CA-C	6.10	114.68	107.73
7	E	435	GLY	N-CA-C	-6.07	106.94	115.32
4	5	330	ILE	N-CA-C	6.02	116.28	107.37
3	4	373	ARG	N-CA-C	5.99	123.55	110.80
3	4	202	LYS	CA-C-N	5.90	132.32	121.70
3	4	202	LYS	C-N-CA	5.90	132.32	121.70
5	6	355	ASP	CA-C-N	5.83	132.20	121.70
5	6	355	ASP	C-N-CA	5.83	132.20	121.70
3	4	421	ASP	N-CA-C	5.76	117.07	108.31
3	4	288	ASN	CB-CA-C	-5.76	109.95	116.63
2	3	166	LEU	N-CA-C	5.72	118.57	110.50
10	A	190	PHE	CA-C-N	5.70	130.92	123.06
10	A	190	PHE	C-N-CA	5.70	130.92	123.06
4	5	39	ARG	N-CA-C	5.70	118.16	108.02
11	C	4	TYR	N-CA-C	5.67	118.40	111.82
4	5	163	SER	N-CA-C	5.66	117.65	108.26
9	B	28	PHE	CA-C-N	5.62	125.38	119.76
9	B	28	PHE	C-N-CA	5.62	125.38	119.76
10	A	151	LEU	N-CA-C	-5.60	104.81	111.69
2	3	159	GLY	CA-C-N	5.58	131.74	121.70
2	3	159	GLY	C-N-CA	5.58	131.74	121.70
2	3	316	GLY	N-CA-C	5.57	118.72	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	E	559	SER	CA-C-N	5.57	131.72	121.70
7	E	559	SER	C-N-CA	5.57	131.72	121.70
5	6	313	MET	N-CA-C	5.55	122.62	110.80
4	5	255	PHE	N-CA-C	5.51	117.36	110.91
3	4	376	CYS	CA-C-N	5.47	131.56	121.70
3	4	376	CYS	C-N-CA	5.47	131.56	121.70
2	3	220	THR	CB-CA-C	-5.46	110.26	116.54
2	3	265	ALA	CA-C-N	5.45	124.79	118.85
2	3	265	ALA	C-N-CA	5.45	124.79	118.85
10	A	157	PRO	N-CA-C	5.43	117.32	110.70
6	7	220	ILE	N-CA-C	5.37	116.11	107.73
6	7	257	VAL	CA-C-N	5.37	131.37	121.70
6	7	257	VAL	C-N-CA	5.37	131.37	121.70
7	E	292	TYR	CA-C-N	-5.30	113.45	118.97
7	E	292	TYR	C-N-CA	-5.30	113.45	118.97
2	3	270	LEU	CA-C-N	5.28	125.04	119.76
2	3	270	LEU	C-N-CA	5.28	125.04	119.76
3	4	243	LEU	CB-CA-C	-5.22	109.00	115.89
6	7	255	VAL	N-CA-C	5.21	115.78	108.17
9	B	108	HIS	CA-C-N	5.21	124.88	119.56
9	B	108	HIS	C-N-CA	5.21	124.88	119.56
10	A	22	ARG	N-CA-C	5.13	116.95	111.36
6	7	94	LEU	CA-C-N	5.13	130.93	121.70
6	7	94	LEU	C-N-CA	5.13	130.93	121.70
1	2	380	THR	CA-C-N	-5.09	116.02	122.43
1	2	380	THR	C-N-CA	-5.09	116.02	122.43
10	A	191	VAL	N-CA-C	5.08	115.80	108.48
1	2	436	GLY	N-CA-C	5.07	128.01	113.30
7	E	153	GLY	N-CA-C	-5.06	107.77	115.66
4	5	240	PRO	CA-C-O	-5.05	117.57	121.31
5	6	270	LEU	CA-C-N	5.03	125.05	119.32
5	6	270	LEU	C-N-CA	5.03	125.05	119.32
2	3	221	LEU	N-CA-C	-5.02	105.39	112.12

There are no chirality outliers.

All (21) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	3	163	ALA	Peptide
2	3	165	ALA	Peptide
3	4	202	LYS	Peptide
3	4	245	ALA	Peptide

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Mol	Chain	Res	Type	Group
3	4	372	GLU	Peptide
3	4	377	ASN	Peptide
3	4	448	SER	Peptide
5	6	103	VAL	Peptide
5	6	313	MET	Peptide
5	6	334	PRO	Peptide
6	7	221	SER	Peptide
6	7	257	VAL	Peptide
6	7	283	GLU	Peptide
6	7	359	PRO	Peptide
10	A	104	ASN	Peptide
10	A	105	ASN	Peptide
10	A	106	GLY	Peptide
10	A	160	ASP	Peptide
8	D	200	LYS	Peptide
8	D	258	VAL	Peptide
7	E	97	GLU	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	1911	0	1908	129	0
2	3	2130	0	2105	175	0
3	4	2203	0	2188	202	0
4	5	2028	0	2055	176	0
5	6	2049	0	1959	134	0
6	7	2611	0	2623	168	0
7	E	4482	0	4497	331	0
8	D	1820	0	1823	219	0
9	B	1513	0	1558	151	0
10	A	1696	0	1698	312	0
11	C	1288	0	1298	103	0
12	7	1	0	0	0	0
All	All	23732	0	23712	1885	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 40.

All (1885) 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)
4:5:197:PHE:CE2	4:5:329:LYS:HG2	1.19	1.65
6:7:17:LEU:HD11	6:7:102:LEU:CD2	1.37	1.55
5:6:290:ILE:HD13	5:6:454:PHE:CZ	1.40	1.51
9:B:187:GLU:CD	11:C:176:ILE:HG22	1.07	1.46
3:4:342:MET:HB3	3:4:360:ILE:CD1	1.45	1.46
9:B:187:GLU:OE2	11:C:176:ILE:CG2	1.65	1.43
10:A:149:ILE:HG23	10:A:151:LEU:N	1.23	1.43
9:B:187:GLU:CD	11:C:176:ILE:CG2	1.94	1.40
10:A:149:ILE:CG2	10:A:151:LEU:N	1.85	1.39
8:D:141:ARG:NH2	10:A:147:VAL:HG12	1.06	1.38
10:A:149:ILE:HG21	10:A:151:LEU:CB	1.55	1.36
4:5:197:PHE:CE2	4:5:329:LYS:CG	2.05	1.36
1:2:234:LEU:HD12	1:2:234:LEU:O	1.18	1.34
8:D:161:LEU:O	8:D:169:ILE:CD1	1.74	1.34
3:4:433:ILE:HG12	3:4:469:VAL:O	1.27	1.33
2:3:234:GLU:OE2	2:3:240:LYS:HA	1.27	1.33
8:D:141:ARG:NH2	10:A:147:VAL:CG1	1.91	1.33
5:6:290:ILE:CD1	5:6:454:PHE:CZ	2.12	1.33
6:7:259:ALA:HB2	6:7:270:PHE:CD1	1.64	1.32
10:A:170:ASP:OD2	10:A:204:TYR:HA	1.16	1.31
10:A:175:GLN:HE22	10:A:199:LEU:CD2	1.41	1.31
4:5:197:PHE:HZ	4:5:329:LYS:NZ	1.29	1.30
2:3:122:ILE:HG21	2:3:221:LEU:CD1	1.62	1.28
4:5:197:PHE:CZ	4:5:329:LYS:CE	2.16	1.28
10:A:168:LEU:CD2	10:A:206:GLN:CB	2.12	1.28
10:A:149:ILE:HG23	10:A:151:LEU:CA	1.64	1.27
4:5:197:PHE:CZ	4:5:329:LYS:NZ	2.01	1.27
10:A:169:LYS:HG3	10:A:185:LYS:CE	1.64	1.27
2:3:312:ASN:O	2:3:313:THR:HG23	1.21	1.26
10:A:149:ILE:CG2	10:A:151:LEU:HB3	1.66	1.26
6:7:17:LEU:CD1	6:7:102:LEU:HD21	1.64	1.26
10:A:168:LEU:HD21	10:A:206:GLN:CB	1.65	1.26
3:4:243:LEU:HD23	3:4:244:ASP:N	1.51	1.25
3:4:433:ILE:CG1	3:4:469:VAL:O	1.85	1.25
4:5:197:PHE:CZ	4:5:329:LYS:HE3	1.71	1.25
7:E:600:PRO:O	7:E:601:ILE:HG13	1.35	1.24
7:E:34:LEU:O	7:E:34:LEU:HD13	1.34	1.24
7:E:326:LEU:HD21	7:E:337:SER:OG	1.32	1.23
10:A:149:ILE:CG2	10:A:151:LEU:CB	2.15	1.23
8:D:229:PHE:HD1	8:D:276:VAL:CG2	1.50	1.23

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:169:LYS:HD3	10:A:185:LYS:NZ	1.54	1.23
2:3:122:ILE:CG2	2:3:221:LEU:CD1	2.18	1.22
8:D:259:THR:HG22	8:D:269:LEU:CD2	1.67	1.22
10:A:173:GLU:CB	10:A:182:ASN:HA	1.69	1.21
7:E:81:LEU:HD13	7:E:82:LEU:N	1.54	1.20
8:D:259:THR:CG2	8:D:269:LEU:HD23	1.71	1.20
10:A:168:LEU:CD2	10:A:206:GLN:HB2	1.68	1.20
11:C:83:LYS:O	11:C:86:ASN:OD1	1.55	1.19
1:2:444:PHE:CE2	5:6:380:ILE:HD13	1.78	1.19
10:A:169:LYS:HA	10:A:185:LYS:HD3	1.26	1.18
2:3:189:THR:HA	2:3:256:ILE:CD1	1.72	1.18
10:A:167:VAL:HG23	10:A:187:SER:O	1.42	1.18
6:7:126:PRO:O	6:7:129:THR:HG22	1.40	1.18
9:B:187:GLU:OE2	11:C:176:ILE:HG22	1.04	1.18
8:D:141:ARG:CZ	10:A:147:VAL:CG1	2.22	1.17
8:D:229:PHE:CD1	8:D:276:VAL:HG21	1.78	1.17
10:A:175:GLN:NE2	10:A:199:LEU:HD22	1.59	1.17
7:E:266:ASN:HB2	7:E:269:ASN:ND2	1.58	1.17
7:E:33:CYS:SG	7:E:61:ILE:O	2.04	1.15
1:2:410:LEU:O	1:2:411:LEU:HD12	1.44	1.15
9:B:188:ILE:O	9:B:192:LEU:HD13	1.47	1.15
3:4:433:ILE:HD13	3:4:469:VAL:N	1.61	1.15
4:5:197:PHE:HE2	4:5:329:LYS:CG	1.45	1.14
3:4:243:LEU:CD2	3:4:244:ASP:H	1.59	1.14
5:6:290:ILE:HD13	5:6:454:PHE:CE1	1.83	1.14
7:E:57:GLN:HG2	10:A:189:PHE:CE1	1.80	1.14
8:D:229:PHE:CD1	8:D:276:VAL:CG2	2.30	1.13
8:D:259:THR:CG2	8:D:269:LEU:CD2	2.26	1.12
2:3:234:GLU:OE1	2:3:238:GLY:O	1.67	1.12
4:5:276:MET:HE1	4:5:294:ILE:HD12	1.32	1.12
8:D:211:ASP:OD2	8:D:213:GLU:HB3	1.47	1.12
2:3:122:ILE:HG23	2:3:123:PRO:HD3	1.16	1.11
2:3:312:ASN:O	2:3:313:THR:CG2	1.97	1.11
8:D:141:ARG:NH2	10:A:148:ASP:O	1.83	1.11
11:C:173:GLU:O	11:C:176:ILE:HG13	1.50	1.11
5:6:290:ILE:CD1	5:6:454:PHE:CE1	2.33	1.11
10:A:169:LYS:CD	10:A:185:LYS:HZ3	1.64	1.11
2:3:189:THR:CA	2:3:256:ILE:HD12	1.81	1.10
4:5:276:MET:SD	4:5:294:ILE:HD13	1.90	1.10
1:2:444:PHE:CE2	5:6:380:ILE:CD1	2.33	1.10
10:A:149:ILE:CG2	10:A:151:LEU:CA	2.25	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:282:ILE:HD13	8:D:286:LEU:HD11	1.22	1.09
10:A:168:LEU:CD2	10:A:206:GLN:HB3	1.80	1.09
8:D:161:LEU:O	8:D:169:ILE:HD12	1.45	1.09
3:4:370:ARG:CB	3:4:371:CYS:SG	2.40	1.09
7:E:81:LEU:HD12	7:E:120:ILE:HG23	1.32	1.09
10:A:149:ILE:HG22	10:A:151:LEU:H	1.16	1.09
2:3:186:VAL:HG13	2:3:256:ILE:CG2	1.84	1.08
3:4:342:MET:CB	3:4:360:ILE:CD1	2.30	1.08
10:A:169:LYS:CD	10:A:185:LYS:NZ	2.14	1.08
5:6:136:TYR:O	5:6:140:ILE:HD12	1.52	1.07
2:3:195:LYS:NZ	2:3:216:ASP:OD2	1.86	1.07
7:E:57:GLN:CG	10:A:189:PHE:CE1	2.37	1.06
2:3:122:ILE:CG2	2:3:221:LEU:HD12	1.83	1.06
10:A:168:LEU:HD21	10:A:206:GLN:HB3	1.11	1.06
10:A:169:LYS:HG3	10:A:185:LYS:HE2	1.07	1.06
6:7:259:ALA:HB2	6:7:270:PHE:CE1	1.88	1.06
4:5:196:ASN:HB3	4:5:197:PHE:HD1	1.12	1.05
8:D:134:GLU:OE1	10:A:161:VAL:HG11	1.56	1.05
9:B:118:ASN:OD1	9:B:122:LEU:HD12	1.57	1.05
1:2:442:ASN:OD1	1:2:443:GLY:N	1.90	1.04
4:5:104:LEU:HD13	4:5:105:SER:N	1.72	1.04
7:E:57:GLN:NE2	10:A:189:PHE:CZ	2.23	1.04
10:A:108:ASP:HB3	10:A:109:LEU:HB3	1.39	1.04
2:3:122:ILE:HG21	2:3:221:LEU:HD11	1.35	1.04
3:4:433:ILE:HD13	3:4:469:VAL:CA	1.87	1.04
8:D:229:PHE:CE1	8:D:276:VAL:HG21	1.93	1.04
7:E:345:ASN:OD1	7:E:507:PHE:HE1	1.40	1.04
4:5:258:LEU:HD21	4:5:294:ILE:HD12	1.39	1.03
8:D:229:PHE:HD1	8:D:276:VAL:HG22	1.18	1.03
10:A:173:GLU:HB3	10:A:182:ASN:HA	1.38	1.03
7:E:33:CYS:SG	7:E:62:PHE:HA	1.98	1.03
8:D:141:ARG:CZ	10:A:147:VAL:HG11	1.88	1.03
8:D:259:THR:HG23	8:D:269:LEU:HD23	1.36	1.03
9:B:187:GLU:OE1	11:C:176:ILE:HG22	1.59	1.03
3:4:433:ILE:CD1	3:4:469:VAL:O	2.07	1.02
7:E:326:LEU:CD2	7:E:337:SER:OG	2.07	1.02
1:2:234:LEU:HD21	1:2:241:SER:O	1.57	1.02
4:5:276:MET:SD	4:5:294:ILE:CD1	2.47	1.02
8:D:269:LEU:HD11	8:D:277:MET:HE1	1.42	1.02
3:4:342:MET:HB3	3:4:360:ILE:HD11	1.08	1.02
3:4:370:ARG:HB2	3:4:371:CYS:SG	1.98	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:B:188:ILE:HG22	9:B:192:LEU:HD13	1.37	1.02
11:C:83:LYS:HA	11:C:86:ASN:ND2	1.74	1.02
4:5:197:PHE:CD2	4:5:329:LYS:HG2	1.94	1.01
7:E:22:HIS:CE1	10:A:192:ARG:NH2	2.28	1.01
8:D:256:TYR:HB2	8:D:257:THR:HG22	1.38	1.01
3:4:469:VAL:HG12	3:4:470:SER:H	1.24	1.01
8:D:141:ARG:CZ	10:A:147:VAL:HG12	1.87	1.01
2:3:197:ILE:HD12	2:3:251:ILE:HG13	1.38	1.00
7:E:57:GLN:HG2	10:A:189:PHE:CD1	1.95	1.00
1:2:234:LEU:O	1:2:234:LEU:CD1	2.08	1.00
6:7:207:LEU:HD12	6:7:207:LEU:O	1.61	1.00
8:D:137:LYS:O	8:D:141:ARG:NH1	1.94	1.00
10:A:108:ASP:O	10:A:198:ARG:NH1	1.95	1.00
10:A:175:GLN:HG2	10:A:183:LEU:HD21	1.44	1.00
4:5:138:ILE:HG23	4:5:332:GLY:HA3	1.41	1.00
10:A:164:ASP:OD1	10:A:190:PHE:HD1	1.43	1.00
10:A:175:GLN:NE2	10:A:199:LEU:CD2	2.19	0.99
8:D:254:PRO:O	8:D:255:CYS:SG	2.20	0.99
2:3:122:ILE:CG2	2:3:123:PRO:HD3	1.92	0.99
7:E:15:ILE:HD13	7:E:121:TYR:CE2	1.97	0.99
5:6:404:VAL:HG23	5:6:453:SER:OG	1.62	0.99
2:3:122:ILE:HG23	2:3:123:PRO:CD	1.92	0.99
7:E:22:HIS:HE1	10:A:192:ARG:NH2	1.61	0.98
10:A:168:LEU:HD23	10:A:206:GLN:HB2	1.44	0.98
2:3:189:THR:HA	2:3:256:ILE:HD12	1.01	0.98
9:B:191:LYS:HE2	11:C:172:MET:HE1	1.45	0.98
10:A:175:GLN:HG2	10:A:183:LEU:CD2	1.94	0.98
8:D:169:ILE:HG22	8:D:170:SER:H	1.29	0.98
3:4:243:LEU:HD23	3:4:244:ASP:H	0.83	0.97
8:D:268:GLU:O	8:D:269:LEU:HD22	1.64	0.97
5:6:354:LEU:HD13	5:6:355:ASP:OD2	1.61	0.97
7:E:15:ILE:HD13	7:E:121:TYR:HE2	1.29	0.97
6:7:370:LEU:O	6:7:370:LEU:HD13	1.64	0.97
8:D:70:GLU:O	8:D:150:LYS:NZ	1.97	0.97
10:A:165:VAL:HG21	10:A:205:LEU:HD13	1.47	0.97
3:4:433:ILE:CD1	3:4:469:VAL:C	2.37	0.97
2:3:122:ILE:HG23	2:3:221:LEU:HD12	1.47	0.97
6:7:17:LEU:CD1	6:7:102:LEU:CD2	2.33	0.96
11:C:83:LYS:HA	11:C:86:ASN:HD21	1.30	0.96
9:B:188:ILE:CG2	9:B:192:LEU:CD1	2.43	0.96
8:D:141:ARG:HH21	10:A:147:VAL:HG12	1.25	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:327:ARG:HH11	1:2:386:GLN:NE2	1.63	0.96
9:B:25:ILE:CD1	9:B:87:ILE:HD11	1.95	0.95
10:A:169:LYS:CG	10:A:185:LYS:HZ3	1.78	0.95
3:4:433:ILE:CD1	3:4:469:VAL:CA	2.44	0.95
6:7:126:PRO:O	6:7:129:THR:CG2	2.14	0.95
1:2:444:PHE:HE2	5:6:380:ILE:HD13	1.21	0.95
2:3:234:GLU:OE2	2:3:240:LYS:CA	2.15	0.94
1:2:325:THR:OG1	1:2:389:THR:OG1	1.80	0.94
8:D:282:ILE:CD1	8:D:286:LEU:HD11	1.96	0.94
10:A:149:ILE:CG2	10:A:151:LEU:H	1.62	0.94
4:5:276:MET:CE	4:5:294:ILE:CD1	2.45	0.94
4:5:276:MET:HE1	4:5:294:ILE:CD1	1.95	0.94
10:A:149:ILE:HG22	10:A:151:LEU:HD12	1.49	0.94
7:E:43:LYS:HG2	7:E:484:LEU:CD2	1.97	0.93
4:5:40:LEU:HG	4:5:40:LEU:O	1.66	0.93
8:D:137:LYS:C	8:D:141:ARG:HH11	1.76	0.93
7:E:74:LEU:HD13	10:A:182:ASN:HB3	1.49	0.93
9:B:188:ILE:CG2	9:B:192:LEU:HD13	1.96	0.93
9:B:139:HIS:H	9:B:142:ARG:HH11	0.97	0.93
4:5:196:ASN:HB3	4:5:197:PHE:CD1	2.01	0.93
6:7:17:LEU:HD11	6:7:102:LEU:HD23	1.49	0.93
10:A:170:ASP:OD2	10:A:204:TYR:CA	2.13	0.93
7:E:57:GLN:NE2	10:A:189:PHE:CE1	2.37	0.93
1:2:216:LEU:HD12	1:2:217:GLU:N	1.84	0.93
10:A:175:GLN:HE22	10:A:199:LEU:HD22	0.79	0.93
3:4:467:LYS:HG3	3:4:468:LYS:HB2	1.51	0.92
10:A:169:LYS:HD3	10:A:185:LYS:HZ3	1.11	0.92
9:B:195:ILE:HG22	11:C:109:ILE:HD13	1.50	0.92
6:7:147:ARG:HH12	6:7:191:LEU:HD21	1.34	0.92
1:2:327:ARG:HH11	1:2:386:GLN:HE22	1.09	0.92
7:E:74:LEU:HD21	10:A:173:GLU:CD	1.95	0.92
4:5:197:PHE:CE1	4:5:329:LYS:HE3	2.05	0.92
11:C:134:GLU:OE2	11:C:138:HIS:CD2	2.23	0.92
7:E:266:ASN:HB2	7:E:269:ASN:HD22	1.29	0.91
10:A:167:VAL:HG11	10:A:185:LYS:HA	1.52	0.91
4:5:276:MET:CE	4:5:294:ILE:HD13	2.01	0.91
8:D:256:TYR:HB2	8:D:257:THR:CG2	1.99	0.91
8:D:162:ASN:OD1	8:D:169:ILE:HG21	1.70	0.91
10:A:168:LEU:HD23	10:A:206:GLN:CB	1.98	0.91
3:4:370:ARG:HA	3:4:371:CYS:SG	2.11	0.91
10:A:149:ILE:HG22	10:A:151:LEU:CD1	2.00	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:141:ARG:HH22	10:A:147:VAL:HG12	1.32	0.90
1:2:410:LEU:C	1:2:411:LEU:HD12	1.96	0.90
9:B:191:LYS:CE	11:C:172:MET:HE1	2.01	0.90
5:6:400:VAL:HG23	5:6:455:LEU:HB3	1.52	0.90
9:B:25:ILE:HD12	9:B:87:ILE:HD11	1.52	0.90
10:A:169:LYS:CA	10:A:185:LYS:HD3	2.01	0.90
3:4:433:ILE:HD13	3:4:468:LYS:C	1.95	0.90
7:E:342:ASN:OD1	7:E:551:TRP:HD1	1.54	0.90
10:A:93:ARG:O	10:A:97:LEU:HG	1.69	0.90
7:E:30:PHE:CE2	7:E:81:LEU:HD21	2.06	0.90
2:3:186:VAL:CG1	2:3:256:ILE:HG21	2.02	0.90
10:A:175:GLN:OE1	10:A:199:LEU:HD11	1.72	0.90
3:4:267:GLU:O	3:4:271:ILE:HD12	1.72	0.90
7:E:22:HIS:HE1	10:A:192:ARG:HH21	1.17	0.90
7:E:316:LEU:HD11	7:E:414:GLY:N	1.87	0.90
6:7:260:TYR:CD1	6:7:298:LEU:HD13	2.07	0.89
9:B:191:LYS:HE2	11:C:172:MET:CE	2.01	0.89
8:D:141:ARG:HE	10:A:149:ILE:HG12	1.37	0.89
3:4:284:ILE:HG23	3:4:290:ASP:HB2	1.55	0.89
1:2:241:SER:OG	1:2:296:ARG:HG2	1.73	0.89
7:E:57:GLN:NE2	10:A:187:SER:OG	2.06	0.89
10:A:200:ILE:CD1	10:A:208:ILE:HD11	2.03	0.89
10:A:147:VAL:HB	10:A:149:ILE:HG13	1.56	0.88
5:6:266:SER:HB2	5:6:458:HIS:HB2	1.54	0.88
7:E:83:LEU:HD21	7:E:86:PHE:HB2	1.54	0.88
7:E:316:LEU:HD11	7:E:413:LEU:C	1.97	0.88
2:3:33:ASP:HB2	2:3:39:ARG:HH11	1.37	0.88
3:4:467:LYS:CG	3:4:468:LYS:HB2	2.04	0.88
10:A:169:LYS:CG	10:A:185:LYS:HE2	2.01	0.88
9:B:139:HIS:H	9:B:142:ARG:NH1	1.72	0.87
5:6:288:LEU:H	5:6:399:GLY:HA3	1.39	0.87
3:4:438:THR:HG22	3:4:462:ASP:HB3	1.53	0.87
3:4:370:ARG:CA	3:4:371:CYS:SG	2.63	0.87
8:D:282:ILE:CD1	8:D:286:LEU:CD1	2.52	0.87
10:A:106:GLY:H	10:A:107:LEU:HB2	1.38	0.87
1:2:234:LEU:CD2	1:2:241:SER:O	2.23	0.87
3:4:417:LEU:HD13	3:4:463:VAL:HG21	1.57	0.87
7:E:57:GLN:CG	10:A:189:PHE:HE1	1.86	0.87
8:D:282:ILE:HD13	8:D:286:LEU:CD1	2.04	0.86
9:B:188:ILE:HG23	9:B:192:LEU:CD1	2.05	0.86
1:2:442:ASN:OD1	1:2:444:PHE:N	2.07	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:259:ALA:CB	6:7:270:PHE:CE1	2.59	0.86
7:E:22:HIS:HA	7:E:24:SER:N	1.90	0.86
10:A:149:ILE:HG23	10:A:150:ASP:C	2.00	0.86
10:A:173:GLU:HB2	10:A:182:ASN:HA	1.55	0.86
8:D:256:TYR:HD1	8:D:257:THR:HG23	1.41	0.86
3:4:342:MET:HB3	3:4:360:ILE:HD13	1.55	0.86
10:A:164:ASP:OD1	10:A:190:PHE:CD1	2.29	0.86
5:6:290:ILE:HD13	5:6:454:PHE:CE2	2.08	0.86
8:D:162:ASN:HA	8:D:169:ILE:HD12	1.56	0.85
9:B:187:GLU:OE2	11:C:176:ILE:HG23	1.72	0.85
6:7:260:TYR:CE1	6:7:298:LEU:HD22	2.11	0.85
10:A:169:LYS:CG	10:A:185:LYS:NZ	2.36	0.85
5:6:290:ILE:HD11	5:6:454:PHE:CE1	2.12	0.85
7:E:325:TYR:CZ	7:E:406:ARG:HD2	2.11	0.85
7:E:342:ASN:OD1	7:E:551:TRP:CD1	2.30	0.84
7:E:22:HIS:CE1	10:A:192:ARG:HH21	1.90	0.84
8:D:141:ARG:NE	10:A:149:ILE:HG12	1.91	0.84
10:A:147:VAL:HG21	10:A:149:ILE:HD11	1.59	0.84
4:5:94:ILE:HD11	4:5:135:PHE:HB2	1.59	0.84
7:E:76:ASP:OD2	10:A:180:VAL:HG21	1.78	0.84
10:A:147:VAL:HG21	10:A:149:ILE:CD1	2.08	0.84
8:D:137:LYS:CD	8:D:141:ARG:NH2	2.30	0.84
10:A:177:GLU:HG2	10:A:178:TYR:HD2	1.41	0.84
10:A:168:LEU:CG	10:A:206:GLN:HB2	2.06	0.84
2:3:195:LYS:CE	2:3:216:ASP:OD2	2.26	0.84
7:E:22:HIS:CD2	8:D:123:LYS:NZ	2.45	0.83
10:A:23:SER:OG	10:A:24:ASN:C	2.21	0.83
2:3:104:ARG:NH1	11:C:86:ASN:O	2.09	0.83
2:3:197:ILE:CD1	2:3:251:ILE:HG13	2.07	0.83
8:D:161:LEU:O	8:D:169:ILE:HD11	1.74	0.83
8:D:169:ILE:HG22	8:D:170:SER:N	1.90	0.83
9:B:71:VAL:HB	9:B:75:ILE:HD11	1.60	0.83
10:A:169:LYS:HG3	10:A:185:LYS:NZ	1.93	0.83
2:3:123:PRO:HD3	2:3:221:LEU:HD12	1.57	0.83
7:E:22:HIS:HA	7:E:24:SER:H	1.39	0.83
9:B:163:LEU:HD22	9:B:189:MET:HE1	1.58	0.83
10:A:173:GLU:CB	10:A:182:ASN:CA	2.55	0.83
7:E:22:HIS:CD2	8:D:123:LYS:HZ2	1.96	0.83
2:3:166:LEU:HD12	2:3:166:LEU:O	1.78	0.83
4:5:197:PHE:CE2	4:5:329:LYS:CE	2.62	0.83
7:E:43:LYS:HG2	7:E:484:LEU:HD21	1.61	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:259:GLN:HE21	4:5:271:PRO:HG2	1.44	0.83
2:3:312:ASN:C	2:3:313:THR:HG23	2.04	0.82
6:7:71:ALA:HB1	6:7:129:THR:HG21	1.60	0.82
4:5:258:LEU:CD2	4:5:294:ILE:CD1	2.56	0.82
4:5:90:PHE:HD2	4:5:137:LEU:CD2	1.91	0.82
11:C:18:CYS:HB3	11:C:72:VAL:HG11	1.61	0.82
9:B:118:ASN:OD1	9:B:122:LEU:CD1	2.27	0.82
9:B:118:ASN:ND2	9:B:122:LEU:HD11	1.94	0.82
3:4:449:ARG:HG3	3:4:450:GLN:H	1.42	0.82
10:A:169:LYS:CG	10:A:185:LYS:CE	2.54	0.82
7:E:74:LEU:HD12	10:A:184:ILE:HD11	1.61	0.82
4:5:258:LEU:HD21	4:5:294:ILE:CD1	2.09	0.82
3:4:342:MET:CB	3:4:360:ILE:HD13	2.07	0.82
7:E:345:ASN:OD1	7:E:507:PHE:CE1	2.31	0.82
7:E:34:LEU:O	7:E:34:LEU:CD1	2.25	0.82
1:2:392:GLU:OE2	1:2:396:THR:OG1	1.95	0.81
6:7:357:PRO:HA	6:7:374:THR:HA	1.62	0.81
8:D:190:TRP:HZ3	10:A:94:THR:HG1	1.28	0.81
1:2:306:LEU:HD21	1:2:405:HIS:HA	1.62	0.81
7:E:74:LEU:CD2	10:A:173:GLU:OE2	2.28	0.81
7:E:74:LEU:CD2	10:A:173:GLU:CD	2.53	0.81
7:E:81:LEU:HD13	7:E:81:LEU:C	2.05	0.81
7:E:24:SER:CB	7:E:25:CYS:HA	2.10	0.81
9:B:188:ILE:HG22	9:B:192:LEU:CD1	2.08	0.81
2:3:186:VAL:CG1	2:3:256:ILE:CG2	2.58	0.81
2:3:200:VAL:HG12	2:3:244:GLU:HB2	1.63	0.81
4:5:136:GLN:HB2	4:5:280:ARG:HE	1.45	0.81
9:B:173:LEU:HD12	9:B:177:GLU:OE1	1.80	0.81
4:5:258:LEU:CD2	4:5:294:ILE:HD12	2.11	0.81
3:4:433:ILE:HD13	3:4:469:VAL:C	2.04	0.81
11:C:104:PHE:H	11:C:170:GLU:CD	1.88	0.80
7:E:37:ASP:OD2	7:E:251:ILE:HG12	1.81	0.80
8:D:169:ILE:CG2	8:D:170:SER:H	1.95	0.80
4:5:137:LEU:HD12	4:5:137:LEU:O	1.80	0.80
8:D:211:ASP:OD2	8:D:213:GLU:CB	2.29	0.80
2:3:171:LEU:O	2:3:172:THR:HG22	1.82	0.80
10:A:58:GLN:HA	10:A:62:MET:HB2	1.61	0.80
2:3:159:GLY:HA2	2:3:160:SER:HB2	1.61	0.80
3:4:315:ARG:HH12	6:7:251:VAL:H	1.29	0.80
5:6:379:VAL:HG22	5:6:454:PHE:HB3	1.64	0.80
1:2:327:ARG:NH1	1:2:386:GLN:HE22	1.80	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:258:ILE:HD13	6:7:305:SER:HB3	1.61	0.80
7:E:325:TYR:CE1	7:E:406:ARG:HD2	2.17	0.80
4:5:104:LEU:HD13	4:5:104:LEU:C	2.06	0.80
1:2:444:PHE:CZ	5:6:380:ILE:HD11	2.17	0.80
4:5:196:ASN:CB	4:5:197:PHE:HD1	1.94	0.80
7:E:74:LEU:HD21	10:A:173:GLU:OE2	1.82	0.80
10:A:104:ASN:OD1	10:A:104:ASN:O	2.00	0.79
3:4:433:ILE:HD13	3:4:469:VAL:O	1.82	0.79
8:D:231:HIS:HA	8:D:274:ILE:HG22	1.64	0.79
10:A:173:GLU:HB3	10:A:182:ASN:CA	2.12	0.79
4:5:175:ARG:NH2	4:5:196:ASN:OD1	2.16	0.79
2:3:176:LEU:HA	2:3:298:PHE:HD2	1.48	0.79
10:A:166:ARG:HH22	10:A:207:LYS:CE	1.95	0.79
7:E:43:LYS:HG2	7:E:484:LEU:HD23	1.64	0.79
11:C:83:LYS:O	11:C:86:ASN:CG	2.24	0.79
6:7:17:LEU:HD11	6:7:102:LEU:HD21	0.80	0.79
1:2:299:ASP:HB3	1:2:319:ARG:NH1	1.97	0.78
9:B:117:TRP:CZ2	9:B:175:LEU:HD22	2.19	0.78
10:A:177:GLU:HG2	10:A:178:TYR:CD2	2.19	0.78
4:5:258:LEU:HD21	4:5:276:MET:HE1	1.65	0.78
10:A:108:ASP:OD2	10:A:177:GLU:HG3	1.83	0.78
10:A:149:ILE:HG21	10:A:151:LEU:HB3	0.80	0.78
8:D:189:ILE:HD13	10:A:133:GLU:CD	2.08	0.78
7:E:410:VAL:HG22	7:E:420:SER:HA	1.63	0.78
8:D:282:ILE:HD12	8:D:286:LEU:HD13	1.65	0.78
10:A:145:ASP:HA	10:A:146:LEU:HB3	1.65	0.78
9:B:188:ILE:O	9:B:192:LEU:CD1	2.29	0.78
8:D:229:PHE:CD1	8:D:276:VAL:HG22	2.11	0.77
11:C:104:PHE:N	11:C:170:GLU:OE2	2.16	0.77
2:3:122:ILE:CG2	2:3:123:PRO:CD	2.56	0.77
10:A:169:LYS:HD3	10:A:185:LYS:HZ1	1.44	0.77
1:2:306:LEU:HD23	1:2:392:GLU:HB2	1.67	0.77
2:3:216:ASP:OD1	2:3:217:ALA:N	2.16	0.77
10:A:175:GLN:O	10:A:180:VAL:HA	1.85	0.77
2:3:53:ALA:O	6:7:217:LYS:NZ	2.17	0.77
9:B:188:ILE:HD13	11:C:132:ALA:HB2	1.65	0.77
1:2:335:LYS:HE3	1:2:383:ARG:HD2	1.66	0.77
2:3:186:VAL:HG13	2:3:256:ILE:HG22	1.65	0.77
7:E:600:PRO:C	7:E:601:ILE:HG13	2.09	0.77
10:A:147:VAL:H	10:A:148:ASP:HA	1.49	0.77
3:4:284:ILE:HG13	3:4:297:GLU:OE2	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:137:LYS:CD	8:D:141:ARG:HH22	1.96	0.76
10:A:27:VAL:HG13	10:A:28:ASN:H	1.50	0.76
6:7:358:ALA:HB2	6:7:375:TYR:HE2	1.48	0.76
11:C:117:GLU:OE2	11:C:120:LEU:HD23	1.85	0.76
3:4:202:LYS:HB3	3:4:203:TYR:HB3	1.68	0.76
5:6:175:TYR:HA	5:6:178:LEU:HD13	1.67	0.76
6:7:94:LEU:HB2	6:7:95:GLN:HB2	1.66	0.76
8:D:137:LYS:CE	8:D:141:ARG:HH22	1.99	0.76
8:D:145:ARG:NH1	10:A:102:TRP:CE3	2.54	0.76
10:A:147:VAL:CB	10:A:149:ILE:HG13	2.15	0.76
10:A:165:VAL:CG2	10:A:205:LEU:HD13	2.16	0.76
3:4:201:PHE:HB2	3:4:202:LYS:HA	1.66	0.76
8:D:141:ARG:HH21	10:A:148:ASP:C	1.93	0.76
1:2:235:GLY:HA2	1:2:283:TYR:HE2	1.50	0.76
7:E:74:LEU:HD21	10:A:173:GLU:OE1	1.85	0.76
8:D:279:TYR:CE1	8:D:286:LEU:CD2	2.69	0.76
9:B:163:LEU:HD22	9:B:189:MET:CE	2.16	0.76
3:4:433:ILE:CD1	3:4:468:LYS:C	2.59	0.75
4:5:36:LEU:HD11	4:5:100:ARG:HH22	1.50	0.75
10:A:163:ILE:HG22	10:A:164:ASP:H	1.49	0.75
2:3:166:LEU:HD12	2:3:166:LEU:C	2.11	0.75
3:4:338:VAL:HG23	5:6:375:ARG:HH12	1.52	0.75
3:4:438:THR:CG2	3:4:462:ASP:HB3	2.15	0.75
7:E:491:LEU:C	7:E:491:LEU:HD12	2.11	0.75
2:3:252:ASP:OD1	2:3:253:HIS:N	2.19	0.75
6:7:315:ILE:HD13	6:7:333:ILE:HD12	1.67	0.75
6:7:235:LEU:HD22	6:7:357:PRO:HD3	1.68	0.75
10:A:32:TYR:HB2	10:A:93:ARG:HH12	1.52	0.75
3:4:243:LEU:HD23	3:4:244:ASP:CA	2.16	0.75
4:5:90:PHE:CD2	4:5:137:LEU:HD22	2.22	0.75
10:A:108:ASP:OD1	10:A:198:ARG:HD3	1.85	0.74
5:6:404:VAL:CG2	5:6:453:SER:OG	2.35	0.74
9:B:157:LEU:HD11	11:C:137:HIS:CD2	2.22	0.74
9:B:157:LEU:HD11	11:C:137:HIS:HD2	1.52	0.74
8:D:256:TYR:CD1	8:D:257:THR:HG23	2.21	0.74
2:3:172:THR:O	2:3:172:THR:HG23	1.87	0.74
5:6:134:LYS:H	5:6:135:VAL:HA	1.53	0.74
7:E:22:HIS:HD2	8:D:123:LYS:NZ	1.83	0.74
8:D:229:PHE:HA	8:D:276:VAL:HG22	1.68	0.74
1:2:300:PHE:N	1:2:319:ARG:HH11	1.86	0.74
4:5:90:PHE:HD2	4:5:137:LEU:HD22	1.52	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:74:LEU:CD1	10:A:184:ILE:HD11	2.18	0.74
10:A:23:SER:H	10:A:24:ASN:HA	1.53	0.74
9:B:134:PHE:HB2	9:B:137:PRO:HB3	1.68	0.73
7:E:377:TRP:NE1	7:E:385:LYS:HZ2	1.85	0.73
10:A:165:VAL:HG21	10:A:205:LEU:CD1	2.18	0.73
2:3:122:ILE:HG21	2:3:221:LEU:HD13	1.67	0.73
4:5:197:PHE:CE2	4:5:329:LYS:CD	2.70	0.73
4:5:137:LEU:HD12	4:5:137:LEU:C	2.13	0.73
8:D:259:THR:HG22	8:D:269:LEU:HD21	1.65	0.73
2:3:33:ASP:HB2	2:3:39:ARG:NH1	2.02	0.73
4:5:182:MET:HE3	4:5:187:ARG:HG3	1.70	0.73
2:3:99:SER:HA	2:3:158:LYS:HB3	1.71	0.73
5:6:335:ASN:H	5:6:338:CYS:H	1.37	0.73
7:E:57:GLN:CD	10:A:189:PHE:CE1	2.66	0.73
10:A:175:GLN:CD	10:A:199:LEU:CD1	2.62	0.73
5:6:303:GLU:HG3	5:6:356:TRP:CD1	2.24	0.73
7:E:28:VAL:O	7:E:81:LEU:HD22	1.89	0.73
3:4:362:ARG:HH11	6:7:299:PHE:HD2	1.38	0.72
5:6:124:VAL:HG23	5:6:134:LYS:O	1.89	0.72
6:7:298:LEU:HD12	6:7:298:LEU:O	1.89	0.72
9:B:168:LEU:HD11	9:B:189:MET:HE3	1.71	0.72
8:D:216:VAL:CG1	8:D:217:ASN:HA	2.19	0.72
7:E:469:LEU:HD11	7:E:540:ARG:HD3	1.69	0.72
8:D:130:GLU:OE2	10:A:192:ARG:NH1	2.21	0.72
1:2:446:VAL:HG21	5:6:356:TRP:HZ2	1.53	0.72
2:3:234:GLU:OE1	2:3:239:ASN:O	2.08	0.72
10:A:168:LEU:HG	10:A:206:GLN:HB2	1.70	0.72
3:4:330:GLY:C	3:4:399:LEU:HD11	2.15	0.72
5:6:149:ASN:HB3	5:6:262:VAL:O	1.89	0.72
8:D:161:LEU:C	8:D:169:ILE:HD12	2.14	0.72
7:E:345:ASN:CB	7:E:551:TRP:HE1	2.03	0.71
3:4:338:VAL:H	5:6:375:ARG:NH1	1.88	0.71
3:4:417:LEU:HD22	3:4:463:VAL:HG11	1.71	0.71
4:5:258:LEU:CD2	4:5:276:MET:SD	2.78	0.71
1:2:442:ASN:ND2	1:2:444:PHE:O	2.23	0.71
3:4:244:ASP:HB2	3:4:247:ASN:HD21	1.54	0.71
3:4:261:LEU:HB2	3:4:268:VAL:HG11	1.71	0.71
1:2:339:PHE:HA	1:2:378:GLU:HB3	1.72	0.71
7:E:318:LEU:HA	7:E:411:ARG:HA	1.72	0.71
7:E:347:LYS:HD2	7:E:401:LEU:HD23	1.72	0.71
7:E:81:LEU:HD13	7:E:82:LEU:CA	2.20	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:166:ARG:O	10:A:168:LEU:CD2	2.39	0.71
1:2:387:ARG:HH12	4:5:323:ILE:HD11	1.55	0.71
4:5:153:SER:OG	4:5:154:GLU:N	2.20	0.71
8:D:224:TRP:CZ3	8:D:283:ARG:HD3	2.26	0.70
2:3:96:ILE:HD13	2:3:129:LEU:HD11	1.72	0.70
2:3:234:GLU:OE1	2:3:238:GLY:C	2.34	0.70
4:5:71:TYR:HD1	7:E:415:TYR:HE1	1.39	0.70
5:6:356:TRP:HZ3	5:6:358:LYS:HB2	1.55	0.70
7:E:559:SER:HA	7:E:560:GLU:HB3	1.73	0.70
2:3:191:LEU:HG	6:7:329:ARG:NH1	2.06	0.70
8:D:211:ASP:CG	8:D:213:GLU:CB	2.65	0.70
8:D:259:THR:HG22	8:D:269:LEU:HD22	1.70	0.70
9:B:188:ILE:CG2	9:B:192:LEU:HD11	2.20	0.70
7:E:526:ARG:HH11	7:E:565:LEU:HB2	1.57	0.70
1:2:241:SER:OG	1:2:296:ARG:CG	2.39	0.70
3:4:304:ARG:HH12	3:4:423:LEU:HD21	1.56	0.70
8:D:141:ARG:NE	10:A:147:VAL:HG11	2.05	0.70
8:D:161:LEU:O	8:D:169:ILE:HD13	1.88	0.70
8:D:211:ASP:OD1	8:D:213:GLU:CB	2.39	0.70
3:4:328:LEU:HD11	3:4:461:VAL:HG21	1.73	0.70
5:6:119:LEU:HD11	5:6:188:VAL:HG21	1.74	0.69
10:A:175:GLN:CD	10:A:199:LEU:HD11	2.16	0.69
3:4:330:GLY:O	3:4:399:LEU:CD1	2.40	0.69
3:4:433:ILE:HG21	3:4:468:LYS:H	1.58	0.69
7:E:266:ASN:CB	7:E:269:ASN:ND2	2.48	0.69
7:E:345:ASN:CG	7:E:507:PHE:HE1	2.01	0.69
8:D:211:ASP:OD1	8:D:213:GLU:HB2	1.92	0.69
2:3:186:VAL:HG11	2:3:256:ILE:HG21	1.72	0.69
3:4:236:LEU:HB3	3:4:238:THR:HG23	1.74	0.69
4:5:258:LEU:HD23	4:5:294:ILE:HD11	1.74	0.69
5:6:379:VAL:HG22	5:6:454:PHE:HD2	1.57	0.69
7:E:125:ALA:HB1	7:E:247:VAL:HG13	1.74	0.69
7:E:349:SER:HA	7:E:351:TRP:CZ3	2.26	0.69
8:D:269:LEU:CD1	8:D:277:MET:HE1	2.21	0.69
4:5:170:SER:HB3	4:5:255:PHE:HB2	1.73	0.69
4:5:258:LEU:HD21	4:5:276:MET:CE	2.21	0.69
8:D:145:ARG:NH1	10:A:102:TRP:HE3	1.89	0.69
8:D:282:ILE:HD12	8:D:286:LEU:CD1	2.19	0.69
1:2:444:PHE:CZ	5:6:380:ILE:CD1	2.75	0.69
10:A:149:ILE:CG2	10:A:151:LEU:HD12	2.22	0.69
2:3:197:ILE:CD1	2:3:251:ILE:CG1	2.71	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:433:ILE:CD1	3:4:469:VAL:HA	2.23	0.69
6:7:118:CYS:SG	6:7:198:ARG:NH2	2.66	0.69
8:D:137:LYS:HE2	8:D:141:ARG:HH22	1.58	0.69
5:6:290:ILE:HD12	5:6:454:PHE:CZ	2.25	0.69
10:A:26:ASP:O	10:A:27:VAL:HG12	1.93	0.69
10:A:175:GLN:HG3	10:A:181:PHE:HB2	1.73	0.69
7:E:84:VAL:HG22	7:E:123:LEU:HD12	1.73	0.69
2:3:195:LYS:HE2	2:3:216:ASP:OD2	1.94	0.68
2:3:43:ARG:HH12	2:3:137:ASP:HB3	1.58	0.68
3:4:433:ILE:HD11	3:4:469:VAL:CA	2.22	0.68
3:4:433:ILE:HD11	3:4:469:VAL:HA	1.75	0.68
8:D:131:THR:HG23	10:A:161:VAL:CG2	2.23	0.68
5:6:379:VAL:HG22	5:6:454:PHE:CD2	2.28	0.68
6:7:259:ALA:CB	6:7:270:PHE:CD1	2.60	0.68
8:D:145:ARG:HH12	10:A:102:TRP:HE3	1.41	0.68
10:A:167:VAL:CG1	10:A:185:LYS:HA	2.23	0.68
10:A:169:LYS:CD	10:A:185:LYS:HZ1	1.97	0.68
1:2:375:VAL:HG11	4:5:324:ARG:HH22	1.58	0.68
2:3:189:THR:CA	2:3:256:ILE:CD1	2.54	0.68
7:E:285:ALA:HB1	7:E:288:TYR:HB3	1.76	0.68
7:E:434:VAL:HG13	7:E:498:LEU:HD13	1.75	0.68
9:B:118:ASN:CG	9:B:122:LEU:CD1	2.66	0.68
1:2:236:GLU:OE2	7:E:361:LYS:HB2	1.92	0.68
2:3:130:THR:HG22	2:3:153:TRP:HD1	1.59	0.68
2:3:216:ASP:CG	2:3:217:ALA:H	2.02	0.68
9:B:17:GLN:HA	9:B:20:VAL:HG12	1.76	0.68
10:A:166:ARG:O	10:A:168:LEU:HD22	1.94	0.68
10:A:175:GLN:HG3	10:A:181:PHE:HD2	1.58	0.68
3:4:304:ARG:NH1	3:4:423:LEU:HD21	2.07	0.68
7:E:315:THR:N	7:E:316:LEU:HB3	2.09	0.68
9:B:118:ASN:HD21	9:B:122:LEU:HD11	1.57	0.68
10:A:163:ILE:HD11	10:A:193:GLN:CD	2.19	0.68
2:3:118:PRO:O	2:3:122:ILE:HG22	1.94	0.67
8:D:282:ILE:O	8:D:286:LEU:HD13	1.94	0.67
10:A:149:ILE:CG2	10:A:151:LEU:CD1	2.71	0.67
3:4:330:GLY:O	3:4:399:LEU:HD11	1.94	0.67
4:5:87:ILE:HD13	4:5:331:LEU:HD21	1.74	0.67
9:B:94:THR:O	9:B:98:LEU:HG	1.94	0.67
7:E:345:ASN:HA	7:E:350:LEU:HD12	1.75	0.67
8:D:211:ASP:OD1	8:D:216:VAL:HG22	1.94	0.67
5:6:267:PHE:HD2	5:6:287:LEU:HD21	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:137:LYS:HD3	8:D:141:ARG:NH2	2.07	0.67
10:A:145:ASP:HB3	10:A:147:VAL:HG23	1.77	0.67
2:3:272:ARG:HD2	4:5:171:VAL:HG13	1.76	0.67
3:4:330:GLY:C	3:4:399:LEU:CD1	2.68	0.67
7:E:308:ASN:HA	7:E:309:SER:HB2	1.77	0.67
8:D:141:ARG:HE	10:A:149:ILE:CG1	2.07	0.67
8:D:230:ILE:HD11	8:D:277:MET:HE3	1.75	0.67
3:4:395:GLN:HB2	3:4:424:VAL:HG13	1.75	0.67
3:4:417:LEU:HD12	3:4:417:LEU:O	1.95	0.67
7:E:79:ASN:O	7:E:118:ARG:HA	1.93	0.67
2:3:122:ILE:CG2	2:3:221:LEU:HD11	2.06	0.67
2:3:197:ILE:HD12	2:3:251:ILE:CG1	2.20	0.67
7:E:29:ILE:HG22	7:E:82:LEU:HB3	1.77	0.67
7:E:249:ASN:HB2	7:E:254:GLN:HE22	1.58	0.67
8:D:211:ASP:CG	8:D:213:GLU:HB3	2.20	0.67
8:D:267:VAL:HG11	9:B:167:HIS:CE1	2.30	0.67
10:A:81:ARG:NH1	11:C:9:VAL:O	2.28	0.67
3:4:342:MET:CB	3:4:360:ILE:HD11	2.04	0.66
4:5:71:TYR:HD1	7:E:415:TYR:CE1	2.12	0.66
3:4:469:VAL:HG12	3:4:470:SER:N	2.04	0.66
7:E:15:ILE:CD1	7:E:121:TYR:HE2	2.05	0.66
10:A:29:LEU:HD11	10:A:96:ILE:HG12	1.77	0.66
11:C:18:CYS:HB3	11:C:72:VAL:CG1	2.25	0.66
2:3:317:PHE:HE2	4:5:176:ALA:HB2	1.60	0.66
3:4:433:ILE:HD11	3:4:469:VAL:C	2.19	0.66
10:A:108:ASP:OD2	10:A:177:GLU:CG	2.42	0.66
1:2:242:LEU:HD13	1:2:275:ALA:HB1	1.77	0.66
3:4:180:ILE:O	3:4:180:ILE:HD12	1.95	0.66
8:D:162:ASN:CA	8:D:169:ILE:HD12	2.25	0.66
9:B:7:LEU:N	9:B:8:GLN:HA	2.10	0.66
1:2:436:GLY:N	1:2:437:ASN:HA	2.10	0.66
4:5:264:LEU:HB2	4:5:265:VAL:HG22	1.77	0.66
9:B:112:PHE:HB3	9:B:152:ARG:NH1	2.10	0.66
2:3:191:LEU:HG	6:7:329:ARG:HH12	1.59	0.66
2:3:171:LEU:O	2:3:172:THR:CG2	2.44	0.66
2:3:193:ARG:CD	6:7:371:LEU:HD11	2.26	0.66
3:4:243:LEU:CG	3:4:244:ASP:H	2.08	0.66
9:B:139:HIS:N	9:B:142:ARG:HH11	1.82	0.66
3:4:233:MET:HE3	3:4:239:SER:HA	1.77	0.66
6:7:135:LYS:HB2	6:7:141:VAL:HG11	1.77	0.66
4:5:258:LEU:CD2	4:5:294:ILE:HD11	2.24	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:194:PRO:O	6:7:371:LEU:HD12	1.97	0.65
7:E:151:THR:HA	7:E:152:LEU:HB3	1.76	0.65
2:3:163:ALA:HB3	2:3:164:HIS:CG	2.31	0.65
11:C:86:ASN:OD1	11:C:87:ALA:N	2.29	0.65
3:4:398:LYS:NZ	3:4:400:GLN:OE1	2.29	0.65
6:7:260:TYR:HE1	6:7:298:LEU:HD22	1.62	0.65
11:C:101:ASN:HB2	11:C:102:SER:C	2.21	0.65
1:2:213:SER:OG	1:2:217:GLU:OE2	2.11	0.65
9:B:57:ASP:OD1	9:B:58:LYS:N	2.28	0.65
5:6:112:ARG:HH22	5:6:183:LYS:HG3	1.60	0.65
7:E:621:ARG:HB3	7:E:623:ASP:OD2	1.96	0.65
10:A:93:ARG:O	10:A:97:LEU:CG	2.44	0.65
10:A:108:ASP:HA	10:A:198:ARG:HH11	1.62	0.65
2:3:197:ILE:HD11	2:3:251:ILE:HB	1.79	0.65
4:5:36:LEU:HD11	4:5:100:ARG:NH2	2.11	0.65
7:E:34:LEU:HD13	7:E:34:LEU:C	2.18	0.65
10:A:67:VAL:HG11	11:C:25:PRO:HD2	1.78	0.65
1:2:327:ARG:HH12	4:5:272:ARG:NH2	1.94	0.65
2:3:116:VAL:HG12	2:3:117:GLU:HG3	1.78	0.65
3:4:370:ARG:HD3	3:4:379:PRO:HA	1.79	0.65
1:2:300:PHE:O	1:2:302:THR:OG1	2.10	0.65
7:E:267:LEU:HD21	7:E:302:LEU:HD13	1.79	0.65
11:C:134:GLU:OE2	11:C:138:HIS:HD2	1.79	0.65
2:3:229:ALA:HB1	6:7:370:LEU:HD23	1.79	0.65
4:5:296:GLY:HA2	4:5:331:LEU:H	1.60	0.65
7:E:540:ARG:HH22	7:E:574:GLU:HB2	1.61	0.65
10:A:173:GLU:HB2	10:A:182:ASN:CA	2.21	0.65
5:6:400:VAL:HG23	5:6:455:LEU:CB	2.24	0.64
7:E:331:HIS:ND1	7:E:496:ILE:HD13	2.12	0.64
3:4:437:GLY:HA3	3:4:463:VAL:HA	1.80	0.64
7:E:92:LEU:HA	7:E:95:PHE:HB3	1.78	0.64
2:3:186:VAL:HG13	2:3:256:ILE:HG21	1.61	0.64
6:7:333:ILE:HG12	6:7:376:LEU:HB3	1.78	0.64
7:E:585:THR:HG22	7:E:603:ASN:HB2	1.79	0.64
3:4:371:CYS:HB2	3:4:377:ASN:H	1.63	0.64
4:5:94:ILE:CD1	4:5:135:PHE:HB2	2.28	0.64
7:E:561:ASP:HB3	7:E:562:LYS:HG2	1.80	0.64
9:B:188:ILE:O	9:B:188:ILE:HG22	1.97	0.64
1:2:294:HIS:O	1:2:296:ARG:NH1	2.30	0.64
3:4:330:GLY:CA	3:4:399:LEU:HD11	2.26	0.64
6:7:258:ILE:HD13	6:7:305:SER:CB	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:224:TRP:HZ3	8:D:283:ARG:HD3	1.63	0.64
3:4:371:CYS:HB2	3:4:377:ASN:N	2.13	0.64
4:5:59:TYR:HD1	4:5:135:PHE:HE1	1.44	0.64
10:A:166:ARG:NH2	10:A:207:LYS:CE	2.61	0.64
7:E:31:VAL:HG22	7:E:42:THR:HG21	1.80	0.64
2:3:187:THR:O	2:3:257:THR:OG1	2.12	0.64
4:5:259:GLN:HE21	4:5:271:PRO:CG	2.10	0.64
6:7:82:LEU:HD23	6:7:85:ILE:HD12	1.80	0.63
3:4:315:ARG:NH1	6:7:251:VAL:HG12	2.12	0.63
5:6:335:ASN:H	5:6:337:SER:HA	1.64	0.63
5:6:379:VAL:CG2	5:6:454:PHE:HD2	2.10	0.63
7:E:588:TYR:OH	7:E:601:ILE:HG21	1.98	0.63
8:D:212:THR:N	8:D:213:GLU:HA	2.13	0.63
3:4:386:HIS:CE1	5:6:405:PRO:HD3	2.33	0.63
7:E:29:ILE:HD11	7:E:58:ILE:HG12	1.81	0.63
8:D:200:LYS:HB2	8:D:201:TYR:HB2	1.81	0.63
8:D:206:LEU:HB3	10:A:83:LYS:NZ	2.12	0.63
1:2:327:ARG:HD2	1:2:386:GLN:NE2	2.13	0.63
1:2:334:LEU:HD13	4:5:322:ALA:HB3	1.79	0.63
6:7:331:LEU:HD11	6:7:355:PHE:HE1	1.63	0.63
4:5:156:VAL:HG22	4:5:298:TYR:HE2	1.63	0.63
6:7:126:PRO:C	6:7:129:THR:HG22	2.21	0.63
6:7:276:ARG:HG3	6:7:277:THR:HG23	1.80	0.63
10:A:177:GLU:CG	10:A:178:TYR:CD2	2.81	0.63
6:7:269:VAL:HG21	6:7:285:THR:HB	1.80	0.63
7:E:33:CYS:HG	7:E:61:ILE:C	1.94	0.63
1:2:216:LEU:HD12	1:2:217:GLU:HB3	1.79	0.63
4:5:156:VAL:HG22	4:5:298:TYR:CE2	2.33	0.63
10:A:173:GLU:CG	10:A:182:ASN:HA	2.28	0.63
4:5:167:ILE:HD11	4:5:259:GLN:HB2	1.79	0.63
6:7:208:SER:HB2	6:7:209:GLN:HA	1.80	0.63
8:D:178:ASP:HA	8:D:181:LYS:NZ	2.14	0.63
3:4:370:ARG:HB3	3:4:371:CYS:SG	2.35	0.63
7:E:266:ASN:HD22	7:E:269:ASN:HD21	1.46	0.63
7:E:401:LEU:HB3	7:E:404:ILE:HD11	1.80	0.63
7:E:413:LEU:HD23	7:E:416:ARG:HD2	1.81	0.63
7:E:516:LYS:HE2	7:E:518:LEU:HD11	1.80	0.63
9:B:157:LEU:HD21	11:C:137:HIS:NE2	2.13	0.63
10:A:161:VAL:O	10:A:161:VAL:HG12	1.99	0.63
10:A:173:GLU:HA	10:A:183:LEU:HB2	1.80	0.63
7:E:24:SER:HB2	7:E:25:CYS:HA	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:C:27:LEU:HD12	11:C:38:ILE:HG12	1.81	0.62
6:7:260:TYR:HA	6:7:300:MET:HA	1.81	0.62
10:A:175:GLN:HG3	10:A:181:PHE:CD2	2.34	0.62
1:2:302:THR:O	1:2:303:ILE:HG22	1.98	0.62
2:3:105:GLU:OE1	2:3:105:GLU:N	2.33	0.62
4:5:31:PHE:CD2	4:5:90:PHE:HD1	2.17	0.62
4:5:197:PHE:HE2	4:5:329:LYS:HG3	1.58	0.62
6:7:106:ILE:HA	6:7:113:PHE:CE2	2.34	0.62
7:E:281:ASP:OD2	7:E:406:ARG:NH1	2.30	0.62
4:5:40:LEU:O	4:5:40:LEU:CG	2.43	0.62
6:7:258:ILE:HG22	6:7:258:ILE:O	2.00	0.62
8:D:268:GLU:C	8:D:269:LEU:HD22	2.25	0.62
9:B:115:LEU:HD13	9:B:119:TRP:HE1	1.64	0.62
3:4:243:LEU:HD23	3:4:244:ASP:C	2.25	0.62
4:5:156:VAL:HA	4:5:298:TYR:HD2	1.64	0.62
7:E:32:SER:OG	7:E:84:VAL:O	2.17	0.62
11:C:77:PRO:HB2	11:C:79:MET:HG2	1.81	0.62
1:2:216:LEU:HD12	1:2:217:GLU:H	1.65	0.62
1:2:446:VAL:HG22	5:6:356:TRP:HE1	1.64	0.62
10:A:163:ILE:HD11	10:A:193:GLN:NE2	2.15	0.62
2:3:234:GLU:OE1	2:3:239:ASN:C	2.43	0.62
4:5:62:THR:HG22	4:5:138:ILE:HB	1.82	0.62
8:D:220:ASP:HB3	8:D:221:GLU:HG2	1.82	0.62
11:C:162:THR:N	11:C:163:SER:HA	2.15	0.62
7:E:150:ASP:H	7:E:151:THR:HA	1.63	0.61
8:D:266:GLU:HB3	8:D:268:GLU:HG3	1.81	0.61
8:D:267:VAL:N	8:D:268:GLU:HA	2.15	0.61
10:A:29:LEU:HB2	10:A:119:ASP:OD2	2.00	0.61
5:6:290:ILE:CD1	5:6:454:PHE:HZ	2.03	0.61
8:D:131:THR:HG23	10:A:161:VAL:HG21	1.82	0.61
3:4:449:ARG:O	3:4:451:ARG:N	2.33	0.61
3:4:450:GLN:HB3	3:4:452:VAL:HG22	1.80	0.61
9:B:115:LEU:HD11	9:B:152:ARG:NH1	2.14	0.61
2:3:104:ARG:HH22	11:C:86:ASN:HB2	1.65	0.61
2:3:314:LEU:HD12	2:3:314:LEU:N	2.16	0.61
6:7:220:ILE:O	6:7:220:ILE:HG13	2.00	0.61
6:7:367:LYS:HG2	6:7:371:LEU:CD2	2.30	0.61
10:A:169:LYS:H	10:A:185:LYS:CD	2.12	0.61
1:2:444:PHE:CE2	5:6:380:ILE:HD11	2.28	0.61
2:3:122:ILE:HG13	2:3:155:LEU:HD12	1.82	0.61
2:3:234:GLU:CD	2:3:239:ASN:O	2.44	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:177:THR:O	4:5:194:ILE:HG22	2.00	0.61
8:D:129:MET:SD	9:B:54:THR:HA	2.41	0.61
4:5:282:LEU:HA	4:5:285:LYS:HE2	1.81	0.61
5:6:399:GLY:HA2	5:6:454:PHE:CZ	2.36	0.61
9:B:28:PHE:HE1	9:B:68:SER:HB2	1.65	0.61
10:A:108:ASP:OD2	10:A:177:GLU:CD	2.44	0.61
3:4:338:VAL:H	5:6:375:ARG:HH12	1.48	0.61
8:D:162:ASN:HA	8:D:169:ILE:HG23	1.80	0.61
1:2:447:PHE:HB2	5:6:302:PRO:HG2	1.81	0.61
2:3:301:LEU:HD21	2:3:320:LEU:HD21	1.83	0.61
10:A:175:GLN:CG	10:A:181:PHE:HB2	2.31	0.61
1:2:283:TYR:O	1:2:285:ASP:N	2.30	0.61
3:4:243:LEU:CD2	3:4:245:ALA:N	2.64	0.61
4:5:69:ILE:HD11	4:5:73:GLU:HG2	1.82	0.61
5:6:122:PHE:HA	5:6:123:SER:HB2	1.81	0.61
5:6:296:ARG:HH12	5:6:360:ARG:NH1	1.98	0.61
9:B:188:ILE:O	9:B:188:ILE:CG2	2.48	0.61
10:A:12:GLU:O	10:A:15:ARG:HG2	2.01	0.61
1:2:338:LYS:HB3	1:2:379:LYS:O	2.01	0.60
6:7:262:CYS:SG	6:7:263:ASP:N	2.70	0.60
7:E:586:PRO:HD2	7:E:601:ILE:HD13	1.83	0.60
8:D:124:LEU:HD21	9:B:84:LYS:HD3	1.83	0.60
10:A:54:LEU:HD23	10:A:57:GLN:OE1	2.00	0.60
7:E:33:CYS:SG	7:E:62:PHE:CA	2.84	0.60
4:5:197:PHE:CE2	4:5:329:LYS:HE3	2.30	0.60
4:5:258:LEU:HD23	4:5:276:MET:SD	2.41	0.60
7:E:81:LEU:C	7:E:81:LEU:CD1	2.71	0.60
1:2:442:ASN:CG	1:2:444:PHE:H	2.09	0.60
2:3:25:VAL:HG13	2:3:128:ALA:HB2	1.83	0.60
9:B:50:TRP:N	9:B:51:GLN:OE1	2.33	0.60
3:4:315:ARG:NH1	6:7:251:VAL:H	1.99	0.60
4:5:244:ILE:O	4:5:248:SER:OG	2.20	0.60
7:E:526:ARG:NH1	7:E:565:LEU:HB2	2.14	0.60
8:D:177:LYS:O	8:D:181:LYS:NZ	2.35	0.60
8:D:218:MET:HA	8:D:220:ASP:N	2.16	0.60
11:C:82:THR:HA	11:C:85:MET:HG2	1.82	0.60
4:5:104:LEU:C	4:5:104:LEU:CD1	2.74	0.60
6:7:23:ASP:O	6:7:27:THR:OG1	2.20	0.60
6:7:136:ASP:CG	6:7:137:ASP:N	2.57	0.60
7:E:22:HIS:CD2	8:D:123:LYS:HZ1	2.20	0.60
10:A:149:ILE:HG21	10:A:151:LEU:CG	2.29	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:398:LYS:HZ3	3:4:414:SER:HB2	1.66	0.60
5:6:124:VAL:CG2	5:6:134:LYS:O	2.49	0.60
6:7:244:ILE:HD11	6:7:318:LEU:HD12	1.83	0.60
7:E:15:ILE:O	7:E:19:SER:OG	2.05	0.60
7:E:392:PHE:HA	7:E:396:LEU:HD23	1.82	0.60
8:D:231:HIS:CA	8:D:274:ILE:HG22	2.31	0.60
6:7:81:ASP:HA	6:7:205:LYS:HG2	1.82	0.60
7:E:147:THR:HG22	7:E:249:ASN:HD22	1.67	0.60
4:5:178:TYR:CE1	4:5:191:SER:HB2	2.36	0.59
4:5:276:MET:CE	4:5:294:ILE:HD12	2.11	0.59
6:7:146:ARG:HH22	6:7:304:ALA:HB2	1.66	0.59
1:2:272:ASP:HB2	1:2:293:ILE:O	2.02	0.59
1:2:409:ILE:HG22	1:2:411:LEU:CD1	2.32	0.59
4:5:40:LEU:HD22	4:5:45:ILE:HD11	1.85	0.59
1:2:230:ARG:NH1	1:2:243:GLU:OE1	2.36	0.59
1:2:264:PRO:HG3	1:2:317:LEU:H	1.67	0.59
2:3:272:ARG:HG2	4:5:171:VAL:HG22	1.84	0.59
6:7:260:TYR:CE2	6:7:281:LEU:HD11	2.37	0.59
7:E:272:LEU:HD21	7:E:484:LEU:HD11	1.82	0.59
8:D:225:ASN:HB3	9:B:193:ARG:CZ	2.32	0.59
10:A:175:GLN:HE22	10:A:199:LEU:HD21	1.54	0.59
1:2:306:LEU:CD2	1:2:392:GLU:HB2	2.32	0.59
3:4:303:VAL:HG12	3:4:305:PRO:HD3	1.84	0.59
7:E:348:LEU:HD11	7:E:401:LEU:HD11	1.84	0.59
3:4:342:MET:HB2	3:4:360:ILE:HD13	1.82	0.59
8:D:143:TYR:CE2	8:D:147:ARG:HD2	2.38	0.59
9:B:59:ALA:HB1	9:B:60:LEU:HB2	1.84	0.59
1:2:302:THR:OG1	1:2:303:ILE:N	2.35	0.59
4:5:276:MET:HG2	4:5:328:ILE:HB	1.83	0.59
2:3:95:ARG:HB3	2:3:154:LYS:HB2	1.84	0.59
7:E:25:CYS:SG	7:E:27:LEU:HD12	2.43	0.59
7:E:50:LYS:HG2	10:A:190:PHE:CZ	2.37	0.59
7:E:556:CYS:O	7:E:560:GLU:HG2	2.02	0.59
9:B:160:LEU:HD23	11:C:133:GLN:HE22	1.68	0.59
10:A:175:GLN:NE2	10:A:199:LEU:HD21	2.14	0.59
7:E:57:GLN:HG3	10:A:189:PHE:HE1	1.66	0.59
7:E:474:VAL:HG12	10:A:186:ASP:HB3	1.84	0.59
2:3:300:SER:O	4:5:245:HIS:ND1	2.34	0.59
4:5:331:LEU:HD12	4:5:331:LEU:O	2.03	0.59
10:A:173:GLU:HG3	10:A:182:ASN:OD1	2.03	0.59
2:3:23:ASP:OD1	2:3:26:ARG:NH2	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:71:ARG:NH1	9:B:11:PHE:CD1	2.71	0.59
8:D:79:TYR:HB3	8:D:173:ASP:O	2.02	0.58
10:A:175:GLN:CG	10:A:183:LEU:HD21	2.27	0.58
3:4:321:ASP:HB2	3:4:324:LYS:HD2	1.84	0.58
4:5:35:ILE:HD11	4:5:94:ILE:HG22	1.85	0.58
8:D:259:THR:CG2	8:D:269:LEU:HD22	2.27	0.58
11:C:27:LEU:HD23	11:C:29:TYR:H	1.67	0.58
2:3:176:LEU:HA	2:3:298:PHE:CD2	2.36	0.58
7:E:491:LEU:HD12	7:E:492:LEU:N	2.18	0.58
8:D:203:PRO:HB2	8:D:206:LEU:HB2	1.86	0.58
8:D:282:ILE:CD1	8:D:286:LEU:HD13	2.28	0.58
1:2:268:LEU:HD21	1:2:297:ILE:HD11	1.85	0.58
7:E:15:ILE:HD12	7:E:80:SER:HB2	1.85	0.58
8:D:134:GLU:OE1	10:A:161:VAL:CG1	2.44	0.58
3:4:438:THR:HG22	3:4:462:ASP:CB	2.32	0.58
3:4:443:PRO:HB2	3:4:453:LEU:HD22	1.85	0.58
5:6:143:MET:HE2	5:6:150:THR:H	1.69	0.58
8:D:57:GLN:HG3	9:B:56:ASP:O	2.04	0.58
9:B:168:LEU:HD11	9:B:189:MET:CE	2.33	0.58
10:A:185:LYS:HG3	10:A:186:ASP:OD1	2.03	0.58
3:4:225:TYR:N	3:4:229:GLN:H	2.02	0.58
6:7:255:VAL:HG13	6:7:273:VAL:HG11	1.85	0.58
7:E:626:GLU:HB3	7:E:629:ILE:HG22	1.85	0.58
7:E:637:LEU:O	7:E:641:LEU:HG	2.03	0.58
10:A:13:ALA:O	10:A:16:THR:HG22	2.04	0.58
4:5:139:LEU:O	4:5:139:LEU:HD12	2.04	0.58
6:7:9:GLN:O	6:7:10:LEU:HD23	2.04	0.58
9:B:118:ASN:CG	9:B:122:LEU:HD11	2.29	0.58
1:2:303:ILE:HA	1:2:319:ARG:HD2	1.86	0.58
1:2:384:ASN:N	1:2:384:ASN:OD1	2.34	0.58
2:3:189:THR:HG23	2:3:256:ILE:CD1	2.32	0.58
3:4:243:LEU:CD2	3:4:244:ASP:N	2.36	0.58
3:4:401:GLU:HG2	3:4:413:HIS:H	1.69	0.58
7:E:57:GLN:OE1	7:E:58:ILE:N	2.37	0.58
10:A:29:LEU:HD21	10:A:96:ILE:HG21	1.85	0.58
5:6:400:VAL:HG21	5:6:455:LEU:HG	1.86	0.58
7:E:267:LEU:CD2	7:E:302:LEU:HD13	2.34	0.58
1:2:446:VAL:HG21	5:6:356:TRP:CZ2	2.37	0.57
6:7:256:GLU:HG3	6:7:257:VAL:HG22	1.86	0.57
9:B:52:LEU:HD12	9:B:53:ILE:H	1.68	0.57
3:4:461:VAL:HG12	3:4:463:VAL:H	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:133:ASN:O	7:E:140:ILE:HD11	2.04	0.57
8:D:229:PHE:HE1	8:D:276:VAL:HG21	1.63	0.57
6:7:214:ARG:N	6:7:215:TYR:HA	2.19	0.57
8:D:178:ASP:HA	8:D:181:LYS:HZ1	1.70	0.57
10:A:175:GLN:OE1	10:A:199:LEU:HD21	2.05	0.57
2:3:245:TYR:CD2	6:7:356:LEU:HD22	2.39	0.57
3:4:339:ILE:HG21	5:6:416:LYS:NZ	2.19	0.57
4:5:278:CYS:SG	4:5:330:ILE:HD12	2.45	0.57
7:E:313:PRO:HG3	7:E:415:TYR:OH	2.03	0.57
11:C:47:PRO:HB2	11:C:49:TRP:CD1	2.40	0.57
3:4:440:ARG:HH11	3:4:440:ARG:HG3	1.69	0.57
7:E:487:ARG:HB2	11:C:193:LYS:NZ	2.20	0.57
3:4:315:ARG:HH22	6:7:311:GLN:HE22	1.52	0.57
5:6:124:VAL:HG11	5:6:132:VAL:HG23	1.86	0.57
9:B:50:TRP:N	9:B:51:GLN:HA	2.20	0.57
11:C:88:ILE:HB	11:C:127:LEU:HD12	1.87	0.57
2:3:177:ASN:ND2	4:5:246:GLU:O	2.38	0.57
9:B:198:ALA:HB3	11:C:113:MET:HE3	1.85	0.57
2:3:261:MET:HE3	2:3:262:PRO:HD2	1.85	0.57
4:5:170:SER:O	4:5:254:GLN:NE2	2.37	0.57
2:3:186:VAL:HG22	2:3:258:VAL:HG22	1.85	0.57
3:4:343:LYS:NZ	3:4:392:ALA:HB3	2.20	0.57
6:7:67:LEU:HD22	6:7:126:PRO:HD2	1.87	0.57
6:7:207:LEU:HD11	6:7:220:ILE:HG22	1.85	0.57
8:D:254:PRO:C	8:D:255:CYS:SG	2.88	0.57
8:D:269:LEU:HD11	8:D:277:MET:CE	2.27	0.57
10:A:6:GLY:HA3	10:A:85:CYS:SG	2.45	0.57
10:A:163:ILE:HG21	10:A:208:ILE:HG23	1.87	0.57
10:A:202:GLN:HE21	10:A:204:TYR:HE2	1.53	0.57
11:C:25:PRO:HA	11:C:37:PRO:HA	1.86	0.57
3:4:338:VAL:N	5:6:375:ARG:HH12	2.02	0.56
3:4:339:ILE:HG21	5:6:416:LYS:HZ2	1.70	0.56
6:7:207:LEU:CD1	6:7:220:ILE:HG22	2.35	0.56
7:E:474:VAL:HG12	10:A:186:ASP:CB	2.35	0.56
9:B:193:ARG:HH11	9:B:197:THR:HG21	1.70	0.56
1:2:438:LEU:C	1:2:440:ALA:H	2.12	0.56
7:E:74:LEU:HD22	10:A:173:GLU:CD	2.30	0.56
7:E:81:LEU:CD1	7:E:82:LEU:N	2.48	0.56
8:D:279:TYR:CE1	8:D:286:LEU:HD22	2.40	0.56
9:B:160:LEU:O	11:C:133:GLN:NE2	2.37	0.56
2:3:171:LEU:C	2:3:172:THR:HG22	2.30	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:255:ARG:O	2:3:256:ILE:HD13	2.05	0.56
4:5:178:TYR:HD2	4:5:249:LYS:HZ3	1.51	0.56
4:5:197:PHE:HZ	4:5:329:LYS:HZ2	0.60	0.56
6:7:136:ASP:CG	6:7:137:ASP:H	2.12	0.56
6:7:142:ILE:O	6:7:146:ARG:HG2	2.05	0.56
6:7:223:LYS:O	6:7:225:LEU:N	2.39	0.56
7:E:121:TYR:CD1	7:E:141:GLN:HG3	2.40	0.56
9:B:12:SER:HB3	9:B:15:GLU:HG3	1.87	0.56
10:A:166:ARG:HH12	10:A:207:LYS:HE2	1.70	0.56
8:D:137:LYS:HG3	10:A:147:VAL:CG1	2.35	0.56
10:A:202:GLN:NE2	10:A:204:TYR:CE2	2.73	0.56
2:3:126:GLU:OE1	2:3:155:LEU:HG	2.05	0.56
2:3:261:MET:HB2	2:3:264:MET:HG2	1.87	0.56
3:4:337:PRO:HA	5:6:375:ARG:NH1	2.20	0.56
9:B:121:VAL:HG22	9:B:176:LEU:HD12	1.88	0.56
9:B:193:ARG:HG2	9:B:197:THR:HG23	1.88	0.56
3:4:243:LEU:HD23	3:4:245:ALA:N	2.21	0.56
3:4:419:VAL:HA	3:4:463:VAL:HG23	1.88	0.56
6:7:136:ASP:OD1	6:7:137:ASP:N	2.39	0.56
10:A:149:ILE:HA	10:A:150:ASP:HB2	1.86	0.56
3:4:319:PRO:HG2	6:7:309:ALA:HA	1.87	0.56
7:E:281:ASP:OD2	7:E:288:TYR:CE2	2.59	0.56
7:E:380:MET:HB2	7:E:385:LYS:HE2	1.87	0.56
10:A:165:VAL:O	10:A:188:GLN:HA	2.06	0.56
3:4:364:VAL:HG21	6:7:299:PHE:CZ	2.40	0.56
10:A:169:LYS:N	10:A:185:LYS:NZ	2.54	0.56
8:D:74:PRO:HB3	8:D:226:LYS:HD2	1.88	0.56
8:D:137:LYS:C	8:D:141:ARG:NH1	2.32	0.56
2:3:39:ARG:HH12	2:3:132:LEU:HD11	1.70	0.56
2:3:113:GLY:HA3	2:3:121:PHE:CE2	2.41	0.56
7:E:345:ASN:HB2	7:E:551:TRP:HE1	1.70	0.56
3:4:203:TYR:CG	3:4:204:LYS:N	2.73	0.55
3:4:352:CYS:SG	5:6:103:VAL:HG22	2.46	0.55
4:5:197:PHE:CE2	4:5:329:LYS:NZ	2.71	0.55
8:D:267:VAL:HB	8:D:268:GLU:O	2.06	0.55
1:2:208:ALA:HA	1:2:211:LEU:HG	1.88	0.55
1:2:215:LEU:HD21	1:2:275:ALA:HA	1.88	0.55
3:4:433:ILE:CG2	3:4:469:VAL:O	2.54	0.55
10:A:200:ILE:HD12	10:A:208:ILE:HD11	1.87	0.55
7:E:324:TYR:CE1	7:E:405:ILE:HG13	2.41	0.55
10:A:172:GLY:H	10:A:174:ILE:HG23	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:135:ARG:NH1	9:B:74:TRP:NE1	2.54	0.55
8:D:278:ARG:HE	9:B:193:ARG:HD2	1.72	0.55
9:B:184:PHE:HD2	9:B:185:ILE:HD12	1.70	0.55
1:2:338:LYS:H	1:2:380:THR:HG22	1.72	0.55
3:4:449:ARG:C	3:4:451:ARG:H	2.14	0.55
8:D:190:TRP:HZ3	10:A:94:THR:OG1	1.87	0.55
9:B:160:LEU:HD11	9:B:185:ILE:HD11	1.89	0.55
11:C:134:GLU:O	11:C:137:HIS:HB2	2.06	0.55
4:5:197:PHE:HE2	4:5:329:LYS:HG2	0.76	0.55
7:E:272:LEU:CD2	7:E:484:LEU:HD11	2.37	0.55
8:D:132:GLU:HB2	9:B:74:TRP:CH2	2.42	0.55
10:A:164:ASP:O	10:A:207:LYS:O	2.25	0.55
7:E:313:PRO:O	7:E:316:LEU:CD2	2.55	0.55
2:3:100:LEU:HB3	2:3:111:TRP:CZ3	2.40	0.55
4:5:31:PHE:CG	4:5:90:PHE:HD1	2.25	0.55
7:E:619:LYS:HG2	7:E:636:ASP:OD2	2.07	0.55
8:D:216:VAL:HG13	8:D:217:ASN:HA	1.89	0.55
10:A:173:GLU:HB3	10:A:182:ASN:C	2.31	0.55
2:3:227:THR:N	2:3:228:PRO:HD2	2.22	0.55
6:7:362:GLY:CA	6:7:364:LYS:HG3	2.37	0.55
7:E:114:GLN:HG2	7:E:115:SER:H	1.72	0.55
7:E:313:PRO:O	7:E:316:LEU:HD22	2.07	0.55
11:C:105:PHE:HD2	11:C:170:GLU:OE1	1.90	0.55
2:3:42:VAL:HG22	2:3:96:ILE:HG12	1.89	0.55
3:4:370:ARG:HA	3:4:371:CYS:HG	1.70	0.55
7:E:580:LEU:HD11	7:E:629:ILE:HD11	1.89	0.55
8:D:162:ASN:HA	8:D:169:ILE:CG2	2.37	0.55
10:A:84:ARG:HD2	11:C:3:TYR:N	2.22	0.55
10:A:108:ASP:HB3	10:A:109:LEU:CB	2.26	0.55
2:3:201:HIS:ND1	2:3:243:THR:HA	2.22	0.54
3:4:244:ASP:HB2	3:4:247:ASN:ND2	2.20	0.54
6:7:298:LEU:HD12	6:7:298:LEU:C	2.32	0.54
10:A:108:ASP:CG	10:A:198:ARG:HD3	2.31	0.54
3:4:342:MET:C	3:4:360:ILE:HD12	2.32	0.54
4:5:38:PHE:CZ	4:5:67:HIS:HB3	2.42	0.54
4:5:41:ASP:HB2	7:E:416:ARG:HH22	1.72	0.54
4:5:91:GLU:O	4:5:94:ILE:HG13	2.07	0.54
4:5:258:LEU:HD21	4:5:276:MET:SD	2.46	0.54
11:C:16:PHE:HZ	11:C:107:LEU:HD21	1.72	0.54
1:2:438:LEU:O	1:2:440:ALA:N	2.39	0.54
2:3:43:ARG:NH1	2:3:137:ASP:HB3	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:312:ASN:HB3	4:5:302:ASN:HB2	1.88	0.54
6:7:257:VAL:HG23	6:7:257:VAL:O	2.07	0.54
7:E:74:LEU:HD13	10:A:182:ASN:CB	2.31	0.54
8:D:211:ASP:OD1	8:D:213:GLU:HA	2.06	0.54
3:4:449:ARG:CG	3:4:450:GLN:H	2.14	0.54
6:7:143:LEU:HD21	6:7:197:THR:HG22	1.89	0.54
7:E:312:THR:HB	9:B:139:HIS:CD2	2.42	0.54
8:D:206:LEU:HB3	10:A:83:LYS:HZ2	1.69	0.54
8:D:216:VAL:HG12	8:D:217:ASN:HA	1.89	0.54
10:A:167:VAL:C	10:A:168:LEU:HD22	2.32	0.54
11:C:83:LYS:CA	11:C:86:ASN:ND2	2.61	0.54
4:5:153:SER:O	4:5:155:HIS:N	2.34	0.54
7:E:85:GLY:N	7:E:123:LEU:O	2.28	0.54
3:4:468:LYS:HG3	3:4:469:VAL:HG23	1.89	0.54
6:7:353:GLY:HA3	6:7:377:GLU:O	2.07	0.54
10:A:166:ARG:NH2	10:A:207:LYS:HE3	2.22	0.54
8:D:72:CYS:SG	8:D:293:LEU:HD23	2.48	0.54
10:A:163:ILE:CD1	10:A:193:GLN:NE2	2.70	0.54
10:A:200:ILE:HD13	10:A:208:ILE:HD11	1.87	0.54
2:3:171:LEU:HD21	2:3:298:PHE:CZ	2.43	0.54
6:7:245:ILE:HA	6:7:315:ILE:HG13	1.89	0.54
1:2:339:PHE:HA	1:2:378:GLU:CB	2.37	0.54
2:3:276:VAL:HG11	2:3:294:VAL:HG11	1.88	0.54
5:6:294:VAL:HG13	5:6:359:VAL:HB	1.89	0.54
8:D:94:GLN:OE1	9:B:55:THR:CG2	2.56	0.54
11:C:5:ASP:OD1	11:C:6:ILE:N	2.41	0.54
2:3:100:LEU:HB2	2:3:159:GLY:HA2	1.89	0.54
6:7:244:ILE:HD11	6:7:318:LEU:CD1	2.38	0.54
7:E:140:ILE:HD13	7:E:142:CYS:HB3	1.90	0.54
8:D:79:TYR:HD1	8:D:147:ARG:HH12	1.55	0.54
10:A:37:ILE:O	10:A:41:LEU:HG	2.07	0.54
2:3:314:LEU:N	2:3:314:LEU:CD1	2.71	0.53
3:4:338:VAL:N	5:6:375:ARG:NH1	2.56	0.53
5:6:154:ASP:OD2	5:6:156:GLN:HB3	2.08	0.53
8:D:225:ASN:OD1	8:D:278:ARG:HD3	2.08	0.53
10:A:175:GLN:CD	10:A:199:LEU:CD2	2.82	0.53
3:4:387:ASN:ND2	5:6:402:ILE:HG22	2.23	0.53
7:E:579:TYR:CE2	7:E:634:ARG:HB3	2.43	0.53
7:E:588:TYR:OH	7:E:601:ILE:CG2	2.56	0.53
10:A:166:ARG:HH22	10:A:207:LYS:HE2	1.70	0.53
10:A:177:GLU:C	10:A:178:TYR:CD2	2.86	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:309:LEU:O	1:2:310:ARG:NH1	2.34	0.53
4:5:40:LEU:O	4:5:41:ASP:HB2	2.08	0.53
7:E:81:LEU:HD13	7:E:82:LEU:C	2.32	0.53
7:E:154:GLU:OE2	7:E:240:TYR:HB2	2.08	0.53
8:D:91:ILE:HD13	10:A:147:VAL:O	2.08	0.53
8:D:211:ASP:CG	8:D:213:GLU:HA	2.33	0.53
10:A:102:TRP:HZ3	10:A:151:LEU:HD23	1.73	0.53
1:2:404:ARG:NH2	5:6:357:GLN:OE1	2.26	0.53
7:E:288:TYR:HA	7:E:291:LEU:HB2	1.89	0.53
10:A:149:ILE:HG23	10:A:151:LEU:HA	1.79	0.53
4:5:204:THR:HG22	4:5:205:VAL:HG23	1.91	0.53
7:E:558:GLU:N	7:E:559:SER:HA	2.24	0.53
7:E:586:PRO:CG	7:E:601:ILE:HD13	2.38	0.53
8:D:231:HIS:CB	8:D:274:ILE:HG22	2.38	0.53
10:A:27:VAL:HG13	10:A:28:ASN:N	2.22	0.53
3:4:245:ALA:HB3	3:4:306:TYR:O	2.08	0.53
3:4:400:GLN:HE21	3:4:412:PRO:HG2	1.73	0.53
5:6:362:GLN:HB2	5:6:376:THR:HG22	1.90	0.53
10:A:169:LYS:N	10:A:185:LYS:HD3	2.24	0.53
4:5:104:LEU:HD13	4:5:105:SER:CA	2.37	0.53
9:B:115:LEU:HD11	9:B:152:ARG:CZ	2.38	0.53
1:2:327:ARG:HD2	1:2:386:GLN:HE22	1.74	0.53
5:6:369:PRO:C	5:6:372:SER:OG	2.52	0.53
7:E:151:THR:HB	7:E:153:GLY:N	2.24	0.53
7:E:287:VAL:O	7:E:290:ARG:HG2	2.08	0.53
8:D:259:THR:HG21	8:D:268:GLU:HB3	1.90	0.53
3:4:318:ASN:O	3:4:321:ASP:OD1	2.27	0.53
7:E:290:ARG:O	7:E:293:PRO:HD2	2.09	0.53
6:7:73:ARG:HH21	6:7:132:ILE:HA	1.74	0.53
8:D:258:VAL:HG13	8:D:260:ILE:HG13	1.90	0.53
4:5:138:ILE:CG2	4:5:332:GLY:HA3	2.28	0.52
6:7:71:ALA:CB	6:7:129:THR:HG21	2.35	0.52
6:7:367:LYS:HG2	6:7:371:LEU:HD23	1.91	0.52
7:E:586:PRO:HD2	7:E:601:ILE:CD1	2.39	0.52
8:D:141:ARG:CD	10:A:149:ILE:HG12	2.39	0.52
10:A:170:ASP:HB3	10:A:204:TYR:CD1	2.44	0.52
1:2:387:ARG:NH1	4:5:323:ILE:HD11	2.22	0.52
3:4:315:ARG:HH22	6:7:311:GLN:NE2	2.06	0.52
3:4:448:SER:H	3:4:449:ARG:HB3	1.73	0.52
7:E:139:ILE:HG13	7:E:140:ILE:HG23	1.91	0.52
8:D:159:ARG:HH21	8:D:187:SER:HB2	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:433:ILE:CD1	3:4:468:LYS:O	2.57	0.52
4:5:255:PHE:HA	4:5:276:MET:O	2.09	0.52
6:7:261:THR:N	6:7:299:PHE:O	2.37	0.52
6:7:370:LEU:HD13	6:7:370:LEU:C	2.31	0.52
7:E:86:PHE:CE1	7:E:625:PHE:HB2	2.43	0.52
7:E:536:LEU:HD12	7:E:571:SER:HB2	1.91	0.52
8:D:94:GLN:OE1	9:B:55:THR:HG23	2.09	0.52
10:A:169:LYS:N	10:A:185:LYS:HZ3	2.06	0.52
10:A:172:GLY:HA2	10:A:183:LEU:HB2	1.90	0.52
1:2:253:LYS:HB3	1:2:255:ILE:HG22	1.90	0.52
1:2:327:ARG:HB2	1:2:388:VAL:HG22	1.91	0.52
3:4:291:TYR:HB3	3:4:296:ILE:HG21	1.91	0.52
4:5:49:GLN:NE2	4:5:53:ASN:OD1	2.42	0.52
7:E:401:LEU:HB3	7:E:404:ILE:CD1	2.39	0.52
7:E:420:SER:HB2	7:E:423:GLU:HG2	1.91	0.52
10:A:149:ILE:CG2	10:A:151:LEU:CG	2.83	0.52
11:C:105:PHE:CE1	11:C:128:LEU:HB2	2.45	0.52
3:4:354:HIS:CD2	3:4:356:MET:HG2	2.45	0.52
1:2:241:SER:HG	1:2:296:ARG:HG2	1.70	0.52
2:3:250:PHE:HB2	6:7:232:GLY:O	2.09	0.52
3:4:326:ILE:HD12	3:4:439:PHE:HB2	1.92	0.52
7:E:124:ASP:OD1	7:E:126:HIS:ND1	2.42	0.52
11:C:25:PRO:HG3	11:C:37:PRO:HB3	1.91	0.52
1:2:216:LEU:CD1	1:2:217:GLU:OE1	2.58	0.52
3:4:331:LEU:HB2	3:4:430:GLY:HA2	1.90	0.52
3:4:433:ILE:HG12	3:4:469:VAL:C	2.23	0.52
6:7:18:PHE:CE1	6:7:119:ARG:NH1	2.78	0.52
6:7:265:CYS:SG	6:7:288:GLU:HB3	2.50	0.52
7:E:149:ASP:HB3	7:E:150:ASP:HA	1.91	0.52
9:B:112:PHE:O	9:B:152:ARG:NH1	2.39	0.52
1:2:333:GLN:HB2	1:2:385:TYR:HB2	1.92	0.52
2:3:166:LEU:C	2:3:166:LEU:CD1	2.83	0.52
6:7:209:GLN:HB3	6:7:212:ALA:HB2	1.92	0.52
6:7:221:SER:HA	6:7:223:LYS:N	2.24	0.52
7:E:25:CYS:HB3	7:E:26:GLN:HA	1.92	0.52
7:E:512:ALA:O	7:E:516:LYS:NZ	2.36	0.52
1:2:235:GLY:HA2	1:2:283:TYR:CE2	2.38	0.52
5:6:174:TYR:HB3	5:6:285:GLY:O	2.10	0.52
7:E:5:ILE:HG12	7:E:142:CYS:SG	2.50	0.52
7:E:150:ASP:HB3	7:E:151:THR:C	2.35	0.52
10:A:30:PRO:O	10:A:122:ASN:ND2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:266:ASN:O	7:E:269:ASN:HB2	2.10	0.52
7:E:311:LYS:N	7:E:312:THR:HA	2.25	0.52
8:D:193:LEU:HD11	10:A:127:GLU:OE2	2.10	0.52
8:D:216:VAL:HG13	8:D:217:ASN:CA	2.40	0.52
9:B:167:HIS:O	9:B:168:LEU:HD12	2.09	0.52
9:B:187:GLU:CD	11:C:176:ILE:HG21	2.19	0.52
10:A:47:LEU:HD11	10:A:78:CYS:HB3	1.91	0.52
10:A:173:GLU:CB	10:A:183:LEU:N	2.73	0.52
2:3:189:THR:CB	2:3:256:ILE:HD12	2.38	0.51
3:4:307:ASN:H	3:4:436:THR:HG21	1.75	0.51
4:5:149:ARG:HD3	4:5:260:GLU:OE2	2.10	0.51
7:E:519:ILE:HA	7:E:528:CYS:SG	2.50	0.51
8:D:200:LYS:H	8:D:201:TYR:C	2.18	0.51
10:A:177:GLU:CG	10:A:178:TYR:CE2	2.92	0.51
4:5:71:TYR:CD1	7:E:415:TYR:HE1	2.23	0.51
6:7:374:THR:OG1	6:7:375:TYR:N	2.35	0.51
7:E:566:PRO:HB2	7:E:605:PHE:HE2	1.75	0.51
9:B:112:PHE:HB3	9:B:152:ARG:HH12	1.75	0.51
2:3:168:PRO:HG2	2:3:260:GLU:HB3	1.91	0.51
2:3:257:THR:HA	2:3:275:ASP:HA	1.91	0.51
4:5:196:ASN:CB	4:5:197:PHE:CD1	2.79	0.51
5:6:167:ALA:O	5:6:171:SER:OG	2.19	0.51
6:7:108:GLN:OE1	6:7:237:GLN:NE2	2.38	0.51
6:7:244:ILE:CD1	6:7:318:LEU:HD12	2.41	0.51
8:D:214:GLY:HA2	8:D:216:VAL:HA	1.92	0.51
10:A:177:GLU:HG3	10:A:178:TYR:HE2	1.75	0.51
9:B:14:GLU:C	9:B:14:GLU:CD	2.79	0.51
10:A:32:TYR:HA	10:A:93:ARG:HH22	1.74	0.51
10:A:135:CYS:HA	10:A:138:ILE:HG22	1.93	0.51
10:A:173:GLU:O	10:A:173:GLU:HG2	2.10	0.51
11:C:138:HIS:ND1	11:C:162:THR:O	2.43	0.51
2:3:113:GLY:HA3	2:3:121:PHE:HE2	1.74	0.51
4:5:136:GLN:HE22	4:5:282:LEU:HG	1.75	0.51
7:E:57:GLN:HG2	10:A:189:PHE:HE1	1.49	0.51
7:E:613:THR:HG21	7:E:622:ILE:HD11	1.93	0.51
8:D:231:HIS:HB2	8:D:274:ILE:HG22	1.93	0.51
7:E:148:VAL:HG12	7:E:152:LEU:HD22	1.93	0.51
2:3:122:ILE:HG23	2:3:221:LEU:CD1	2.11	0.51
3:4:342:MET:HB3	3:4:360:ILE:HD12	1.72	0.51
7:E:572:ILE:HD13	7:E:579:TYR:H	1.76	0.51
9:B:51:GLN:H	9:B:52:LEU:HA	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:27:VAL:HG11	10:A:100:MET:HE1	1.93	0.51
1:2:236:GLU:OE1	7:E:357:LYS:HB3	2.11	0.51
7:E:318:LEU:C	7:E:318:LEU:HD12	2.36	0.51
10:A:77:LEU:HD11	11:C:53:ILE:HD11	1.92	0.51
10:A:77:LEU:HD21	11:C:53:ILE:HD11	1.93	0.51
11:C:72:VAL:HG12	11:C:74:LEU:H	1.76	0.51
8:D:225:ASN:HB3	9:B:193:ARG:NH1	2.25	0.51
9:B:24:PRO:HB2	9:B:70:GLU:OE2	2.10	0.51
1:2:423:GLU:HB2	1:2:459:ARG:HD3	1.93	0.50
7:E:41:ALA:HB1	7:E:255:ILE:HD12	1.93	0.50
10:A:163:ILE:HG22	10:A:164:ASP:N	2.22	0.50
11:C:129:LEU:HD23	11:C:129:LEU:C	2.36	0.50
1:2:294:HIS:CD2	1:2:296:ARG:HH12	2.29	0.50
3:4:197:PHE:HZ	3:4:247:ASN:HB3	1.76	0.50
4:5:69:ILE:HD12	4:5:73:GLU:HA	1.93	0.50
8:D:279:TYR:CE1	8:D:286:LEU:HD21	2.46	0.50
10:A:177:GLU:HG3	10:A:178:TYR:CE2	2.45	0.50
1:2:320:VAL:HG21	1:2:451:ILE:HD13	1.93	0.50
2:3:100:LEU:HB3	2:3:111:TRP:HZ3	1.75	0.50
3:4:319:PRO:HG2	6:7:309:ALA:CA	2.41	0.50
3:4:345:ALA:O	3:4:357:ALA:HB1	2.11	0.50
5:6:274:HIS:ND1	5:6:288:LEU:HD11	2.26	0.50
8:D:266:GLU:CB	8:D:268:GLU:HG3	2.41	0.50
8:D:279:TYR:HE1	8:D:286:LEU:CD2	2.20	0.50
10:A:109:LEU:HG	10:A:111:SER:HB3	1.94	0.50
10:A:162:PHE:HD1	10:A:192:ARG:HA	1.75	0.50
1:2:459:ARG:HA	1:2:460:GLU:HB2	1.92	0.50
8:D:98:ILE:HA	8:D:101:ILE:HG22	1.93	0.50
8:D:146:CYS:O	8:D:149:SER:OG	2.16	0.50
10:A:100:MET:SD	10:A:117:GLN:HG2	2.52	0.50
6:7:362:GLY:HA3	6:7:364:LYS:NZ	2.27	0.50
6:7:371:LEU:O	6:7:371:LEU:HG	2.11	0.50
1:2:435:ASP:N	1:2:436:GLY:HA3	2.26	0.50
3:4:352:CYS:N	3:4:353:ASP:HA	2.27	0.50
5:6:335:ASN:N	5:6:338:CYS:H	2.07	0.50
10:A:23:SER:OG	10:A:24:ASN:CA	2.59	0.50
10:A:134:TYR:O	10:A:137:LEU:HB3	2.12	0.50
4:5:34:PHE:HD1	4:5:71:TYR:CD2	2.30	0.50
5:6:143:MET:HE1	5:6:148:LEU:HB2	1.94	0.50
5:6:194:PRO:O	5:6:261:ARG:NH2	2.44	0.50
7:E:324:TYR:HD2	7:E:329:LEU:HD13	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:124:SER:OG	10:A:127:GLU:HG2	2.12	0.50
2:3:97:ILE:HA	2:3:156:SER:OG	2.11	0.49
3:4:322:ILE:HA	3:4:439:PHE:HD2	1.77	0.49
3:4:407:PRO:HG2	3:4:410:GLN:HB3	1.94	0.49
4:5:158:LYS:O	4:5:160:VAL:HG23	2.12	0.49
4:5:249:LYS:C	4:5:250:PHE:HD1	2.19	0.49
8:D:218:MET:HA	8:D:219:ILE:C	2.36	0.49
1:2:306:LEU:CD2	1:2:404:ARG:O	2.60	0.49
2:3:275:ASP:N	2:3:275:ASP:OD1	2.38	0.49
7:E:249:ASN:HB2	7:E:254:GLN:NE2	2.26	0.49
3:4:335:SER:HB3	3:4:395:GLN:NE2	2.27	0.49
6:7:116:LEU:O	6:7:119:ARG:HG2	2.13	0.49
6:7:354:ILE:O	6:7:376:LEU:HD12	2.12	0.49
7:E:335:TYR:HB2	7:E:373:ALA:HB1	1.94	0.49
9:B:188:ILE:HD13	11:C:132:ALA:CB	2.39	0.49
10:A:166:ARG:HH22	10:A:207:LYS:CD	2.26	0.49
6:7:357:PRO:HB3	6:7:372:THR:HB	1.94	0.49
9:B:60:LEU:HD12	9:B:61:ASN:H	1.78	0.49
3:4:346:PHE:CE2	3:4:348:LYS:HG3	2.47	0.49
9:B:14:GLU:HG2	9:B:17:GLN:HE21	1.78	0.49
9:B:121:VAL:HG13	11:C:190:TRP:CH2	2.46	0.49
1:2:430:TYR:OH	1:2:449:THR:HG22	2.13	0.49
3:4:242:ASN:HA	3:4:304:ARG:HB2	1.95	0.49
6:7:260:TYR:CG	6:7:298:LEU:HD13	2.48	0.49
8:D:59:ASP:HA	8:D:83:LEU:HD11	1.94	0.49
10:A:106:GLY:N	10:A:107:LEU:HB2	2.19	0.49
1:2:435:ASP:HB3	1:2:447:PHE:HD1	1.77	0.49
2:3:199:SER:HB3	2:3:212:ARG:HB3	1.94	0.49
2:3:314:LEU:CD2	4:5:277:THR:HG21	2.43	0.49
7:E:256:TYR:HB2	7:E:273:ASN:OD1	2.13	0.49
7:E:271:TRP:O	7:E:275:LEU:HG	2.12	0.49
10:A:41:LEU:HA	10:A:44:VAL:HG12	1.94	0.49
1:2:216:LEU:HD12	1:2:217:GLU:CB	2.43	0.49
1:2:325:THR:OG1	1:2:389:THR:O	2.31	0.49
3:4:438:THR:CG2	3:4:462:ASP:CB	2.89	0.49
5:6:288:LEU:O	5:6:290:ILE:HD12	2.12	0.49
6:7:255:VAL:HG23	6:7:258:ILE:HG12	1.94	0.49
11:C:117:GLU:CD	11:C:120:LEU:HD23	2.37	0.49
1:2:306:LEU:HD23	1:2:404:ARG:O	2.12	0.49
4:5:259:GLN:NE2	4:5:271:PRO:HG2	2.19	0.49
9:B:160:LEU:HD23	11:C:133:GLN:NE2	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:108:ASP:H	10:A:109:LEU:C	2.21	0.49
10:A:175:GLN:CD	10:A:199:LEU:HD21	2.38	0.49
3:4:241:LEU:HD23	3:4:243:LEU:H	1.79	0.48
3:4:448:SER:HB3	3:4:449:ARG:HB3	1.94	0.48
4:5:87:ILE:HD12	4:5:297:ILE:HD11	1.94	0.48
6:7:102:LEU:O	6:7:105:ALA:N	2.46	0.48
6:7:362:GLY:HA2	6:7:364:LYS:HG3	1.93	0.48
7:E:431:LEU:HD22	7:E:479:LEU:HD23	1.95	0.48
8:D:216:VAL:CG1	8:D:218:MET:H	2.26	0.48
9:B:25:ILE:CD1	9:B:87:ILE:CD1	2.80	0.48
10:A:135:CYS:O	10:A:139:THR:HG23	2.13	0.48
3:4:239:SER:OG	3:4:240:ASN:N	2.40	0.48
4:5:338:GLU:N	4:5:339:THR:HA	2.28	0.48
6:7:258:ILE:H	6:7:305:SER:CB	2.25	0.48
7:E:127:ARG:NH2	7:E:147:THR:OG1	2.41	0.48
7:E:147:THR:HG22	7:E:249:ASN:ND2	2.26	0.48
7:E:324:TYR:HE1	7:E:405:ILE:HG13	1.77	0.48
7:E:328:LEU:H	7:E:423:GLU:CD	2.21	0.48
7:E:529:VAL:HG23	7:E:570:ALA:HB3	1.95	0.48
7:E:546:LEU:O	7:E:550:ASN:HB2	2.12	0.48
7:E:613:THR:O	7:E:617:ASP:HB3	2.12	0.48
9:B:160:LEU:HD21	9:B:184:PHE:HE2	1.79	0.48
10:A:169:LYS:N	10:A:185:LYS:CD	2.76	0.48
4:5:40:LEU:CD2	4:5:45:ILE:HD11	2.43	0.48
5:6:153:ILE:HD11	5:6:267:PHE:CD1	2.48	0.48
6:7:17:LEU:O	6:7:21:ILE:HG13	2.13	0.48
7:E:510:GLY:HA3	7:E:551:TRP:HZ3	1.77	0.48
7:E:575:ASN:O	7:E:578:THR:HG23	2.13	0.48
9:B:29:PRO:O	9:B:65:ALA:HA	2.14	0.48
10:A:23:SER:HG	10:A:24:ASN:C	2.20	0.48
1:2:264:PRO:HG3	1:2:317:LEU:N	2.28	0.48
1:2:335:LYS:HG3	1:2:383:ARG:HB3	1.95	0.48
3:4:448:SER:HB3	3:4:449:ARG:CB	2.43	0.48
7:E:316:LEU:CD1	7:E:414:GLY:N	2.68	0.48
7:E:586:PRO:CD	7:E:601:ILE:HD13	2.43	0.48
8:D:130:GLU:CD	10:A:192:ARG:NH1	2.71	0.48
8:D:164:ASP:O	8:D:169:ILE:HD11	2.13	0.48
11:C:187:THR:O	11:C:191:MET:HG2	2.13	0.48
2:3:172:THR:O	2:3:172:THR:CG2	2.57	0.48
3:4:306:TYR:HB3	3:4:465:HIS:CD2	2.48	0.48
3:4:440:ARG:HG3	3:4:440:ARG:NH1	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:260:TYR:CZ	6:7:269:VAL:HB	2.48	0.48
7:E:150:ASP:H	7:E:152:LEU:HB3	1.78	0.48
7:E:431:LEU:HD13	7:E:480:SER:HA	1.96	0.48
8:D:141:ARG:NE	10:A:149:ILE:CG1	2.70	0.48
9:B:116:PRO:O	9:B:117:TRP:HB3	2.12	0.48
9:B:177:GLU:O	9:B:181:LEU:HG	2.12	0.48
10:A:175:GLN:CD	10:A:199:LEU:HD13	2.38	0.48
1:2:427:THR:OG1	1:2:454:ASN:HB3	2.12	0.48
2:3:163:ALA:HB2	11:C:91:ASP:OD2	2.14	0.48
4:5:90:PHE:CD2	4:5:137:LEU:CD2	2.80	0.48
5:6:379:VAL:CG2	5:6:454:PHE:CD2	2.93	0.48
6:7:237:GLN:O	6:7:239:ILE:HG23	2.12	0.48
9:B:160:LEU:O	9:B:163:LEU:HG	2.12	0.48
10:A:178:TYR:OH	10:A:198:ARG:NE	2.47	0.48
7:E:24:SER:HB2	7:E:25:CYS:CA	2.42	0.48
7:E:34:LEU:CD1	7:E:34:LEU:C	2.83	0.48
7:E:539:TYR:HB3	7:E:545:LEU:HD11	1.95	0.48
9:B:21:GLU:HA	9:B:73:LEU:HD23	1.95	0.48
9:B:51:GLN:N	9:B:52:LEU:HA	2.28	0.48
10:A:23:SER:OG	10:A:25:GLN:N	2.46	0.48
1:2:327:ARG:HH12	4:5:272:ARG:HH21	1.60	0.48
3:4:202:LYS:CB	3:4:203:TYR:HB3	2.39	0.48
5:6:154:ASP:OD1	5:6:269:ASN:HB3	2.14	0.48
7:E:147:THR:HB	7:E:248:VAL:HG11	1.95	0.48
7:E:259:LEU:CD2	7:E:264:GLU:O	2.62	0.48
7:E:335:TYR:HD1	7:E:363:PHE:HE2	1.59	0.48
7:E:558:GLU:H	7:E:560:GLU:CB	2.27	0.48
7:E:558:GLU:OE1	7:E:560:GLU:HB2	2.14	0.48
9:B:30:ARG:NH2	9:B:86:SER:OG	2.46	0.48
9:B:80:LYS:HE3	9:B:130:ALA:HA	1.96	0.48
1:2:327:ARG:NH1	1:2:386:GLN:NE2	2.44	0.48
2:3:151:HIS:CG	2:3:152:PRO:HD2	2.48	0.48
2:3:216:ASP:CG	2:3:217:ALA:N	2.67	0.48
5:6:105:ASP:O	5:6:108:GLY:N	2.41	0.48
7:E:34:LEU:O	7:E:543:LEU:HD11	2.12	0.48
7:E:88:GLY:HA3	7:E:124:ASP:OD2	2.13	0.48
8:D:79:TYR:HD1	8:D:147:ARG:NH1	2.12	0.48
9:B:191:LYS:HD3	9:B:191:LYS:HA	1.59	0.48
10:A:173:GLU:CB	10:A:183:LEU:H	2.27	0.48
10:A:175:GLN:CB	10:A:181:PHE:HB2	2.44	0.48
1:2:216:LEU:CD1	1:2:217:GLU:HB3	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:426:VAL:HG12	1:2:456:ILE:HD13	1.95	0.48
5:6:406:ASP:HB2	5:6:451:LYS:HZ2	1.79	0.48
6:7:26:VAL:HG13	6:7:64:MET:HE2	1.95	0.48
7:E:154:GLU:CD	7:E:240:TYR:HB2	2.38	0.48
7:E:243:GLN:HE21	7:E:602:LEU:HD21	1.78	0.48
8:D:234:GLY:O	8:D:256:TYR:OH	2.29	0.48
10:A:65:ASP:OD2	10:A:67:VAL:HB	2.13	0.48
2:3:317:PHE:CE2	4:5:176:ALA:HB2	2.46	0.47
3:4:234:ARG:HD2	3:4:283:LEU:HD21	1.96	0.47
7:E:227:LYS:HD3	7:E:230:ILE:HD12	1.96	0.47
8:D:216:VAL:CG1	8:D:219:ILE:HB	2.44	0.47
3:4:315:ARG:HH12	6:7:251:VAL:N	2.06	0.47
3:4:338:VAL:HG23	5:6:375:ARG:NH1	2.24	0.47
6:7:18:PHE:HA	6:7:21:ILE:HD12	1.97	0.47
6:7:21:ILE:HD13	6:7:117:PHE:HA	1.95	0.47
7:E:28:VAL:O	7:E:81:LEU:CD2	2.62	0.47
8:D:72:CYS:SG	8:D:228:VAL:HB	2.54	0.47
8:D:189:ILE:CD1	10:A:133:GLU:CD	2.82	0.47
8:D:211:ASP:HB2	8:D:219:ILE:HD11	1.96	0.47
10:A:175:GLN:NE2	10:A:199:LEU:CD1	2.77	0.47
1:2:327:ARG:HH22	4:5:272:ARG:HH21	1.62	0.47
2:3:137:ASP:HA	2:3:138:ASP:HA	1.59	0.47
2:3:202:TYR:CE2	6:7:14:TYR:HD2	2.31	0.47
5:6:162:GLU:HG3	5:6:165:ALA:HB3	1.97	0.47
5:6:349:THR:HG23	5:6:350:ARG:NH1	2.28	0.47
6:7:103:VAL:O	6:7:107:GLN:HG2	2.14	0.47
7:E:163:LEU:HA	7:E:164:GLU:HA	1.57	0.47
8:D:83:LEU:O	8:D:86:ARG:HG2	2.14	0.47
8:D:259:THR:OG1	8:D:260:ILE:N	2.47	0.47
2:3:94:HIS:HB3	2:3:153:TRP:CE3	2.49	0.47
2:3:151:HIS:ND1	2:3:152:PRO:HD2	2.29	0.47
4:5:86:ILE:O	4:5:89:LEU:N	2.43	0.47
6:7:228:ARG:NH1	6:7:323:PRO:HD2	2.29	0.47
7:E:328:LEU:HD23	7:E:423:GLU:OE1	2.14	0.47
8:D:94:GLN:HE21	8:D:133:LEU:HG	1.80	0.47
11:C:123:VAL:HG12	11:C:124:VAL:N	2.29	0.47
3:4:321:ASP:OD1	3:4:321:ASP:O	2.32	0.47
5:6:134:LYS:HG2	5:6:137:ARG:HG3	1.96	0.47
8:D:137:LYS:O	8:D:141:ARG:HG3	2.15	0.47
9:B:25:ILE:HD11	9:B:87:ILE:HD11	1.90	0.47
1:2:428:GLY:HA3	1:2:453:ALA:HA	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:28:ILE:HG12	4:5:93:ALA:HB2	1.97	0.47
5:6:335:ASN:N	5:6:337:SER:HA	2.29	0.47
8:D:211:ASP:OD1	8:D:213:GLU:CA	2.62	0.47
10:A:5:LEU:HD11	10:A:36:ILE:HD11	1.96	0.47
10:A:183:LEU:C	10:A:184:ILE:HG12	2.39	0.47
1:2:339:PHE:HZ	1:2:348:LEU:HB2	1.80	0.47
1:2:442:ASN:CG	1:2:444:PHE:O	2.57	0.47
2:3:178:LYS:O	2:3:180:VAL:HG23	2.14	0.47
6:7:264:GLN:HB2	6:7:289:CYS:SG	2.55	0.47
7:E:121:TYR:CE1	7:E:141:GLN:CG	2.98	0.47
7:E:337:SER:O	7:E:341:SER:OG	2.32	0.47
9:B:53:ILE:H	9:B:53:ILE:HD12	1.80	0.47
9:B:191:LYS:CD	11:C:172:MET:HE1	2.43	0.47
10:A:147:VAL:CG1	10:A:149:ILE:HG13	2.45	0.47
3:4:375:ASP:HA	3:4:376:CYS:O	2.15	0.47
4:5:22:ASP:O	4:5:26:GLU:HG2	2.15	0.47
5:6:390:LYS:HA	5:6:391:PRO:HD3	1.78	0.47
9:B:72:VAL:O	9:B:75:ILE:HG12	2.15	0.47
10:A:47:LEU:HD22	10:A:79:MET:SD	2.54	0.47
1:2:409:ILE:HG22	1:2:411:LEU:HD11	1.97	0.47
5:6:328:THR:HA	5:6:329:GLU:HA	1.62	0.47
6:7:221:SER:HA	6:7:222:SER:C	2.40	0.47
7:E:558:GLU:O	7:E:589:PRO:HB3	2.15	0.47
7:E:634:ARG:HA	7:E:637:LEU:HD23	1.96	0.47
9:B:102:ILE:HG23	9:B:148:LEU:HD12	1.97	0.47
10:A:168:LEU:HD21	10:A:206:GLN:CG	2.40	0.47
11:C:135:LEU:HD11	11:C:169:LEU:HD21	1.96	0.47
3:4:331:LEU:O	3:4:399:LEU:HD12	2.15	0.47
4:5:303:SER:O	4:5:303:SER:OG	2.18	0.47
1:2:404:ARG:NH1	5:6:300:VAL:HG23	2.31	0.46
5:6:355:ASP:HB3	5:6:356:TRP:HA	1.97	0.46
6:7:18:PHE:CZ	6:7:119:ARG:NH1	2.83	0.46
7:E:243:GLN:HG2	7:E:602:LEU:HD23	1.97	0.46
7:E:469:LEU:HD21	7:E:473:TRP:CZ2	2.49	0.46
7:E:474:VAL:CG1	10:A:186:ASP:CB	2.93	0.46
7:E:491:LEU:C	7:E:491:LEU:CD1	2.82	0.46
7:E:586:PRO:HG2	7:E:601:ILE:HD13	1.97	0.46
1:2:334:LEU:HD11	4:5:324:ARG:NE	2.29	0.46
3:4:441:SER:C	3:4:442:ILE:HD12	2.41	0.46
4:5:270:MET:SD	4:5:271:PRO:HD2	2.55	0.46
5:6:326:LYS:H	5:6:327:TYR:HA	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:403:VAL:HG11	5:6:450:TYR:HB3	1.96	0.46
7:E:563:GLN:O	7:E:565:LEU:HG	2.16	0.46
10:A:185:LYS:HG3	10:A:186:ASP:CG	2.40	0.46
11:C:139:ALA:HB1	11:C:184:TYR:CE2	2.51	0.46
1:2:433:ASN:HB2	1:2:434:TYR:HB3	1.97	0.46
2:3:260:GLU:OE2	2:3:271:PRO:HA	2.14	0.46
3:4:245:ALA:HA	3:4:246:ARG:HA	1.61	0.46
4:5:59:TYR:CD1	4:5:135:PHE:HE1	2.28	0.46
4:5:274:LEU:HD12	4:5:328:ILE:HD11	1.96	0.46
5:6:354:LEU:CD1	5:6:355:ASP:OD2	2.50	0.46
6:7:19:ASN:O	6:7:22:THR:OG1	2.26	0.46
6:7:206:PRO:HG3	6:7:352:THR:HG21	1.98	0.46
6:7:227:VAL:HB	6:7:317:GLU:OE2	2.16	0.46
8:D:145:ARG:HH22	10:A:102:TRP:HB3	1.79	0.46
8:D:258:VAL:HA	8:D:259:THR:OG1	2.14	0.46
11:C:101:ASN:H	11:C:102:SER:HA	1.81	0.46
2:3:197:ILE:CD1	2:3:251:ILE:HB	2.44	0.46
4:5:130:ASN:HA	4:5:131:SER:HA	1.68	0.46
5:6:356:TRP:HB2	5:6:381:LEU:O	2.15	0.46
7:E:29:ILE:CG1	7:E:58:ILE:HG12	2.44	0.46
8:D:226:LYS:HG3	9:B:190:ASP:OD2	2.14	0.46
9:B:157:LEU:HD23	9:B:157:LEU:O	2.16	0.46
10:A:167:VAL:HG11	10:A:185:LYS:CA	2.33	0.46
3:4:422:GLU:H	3:4:422:GLU:CD	2.23	0.46
4:5:148:LEU:CD2	4:5:260:GLU:HB3	2.45	0.46
7:E:527:LEU:HD23	7:E:528:CYS:N	2.30	0.46
8:D:168:LEU:HD11	8:D:171:LEU:HD12	1.96	0.46
8:D:227:PHE:HD2	9:B:190:ASP:OD1	1.98	0.46
8:D:275:TYR:CE1	9:B:169:GLN:HA	2.50	0.46
11:C:22:TYR:OH	11:C:69:VAL:HB	2.14	0.46
11:C:88:ILE:HG22	11:C:95:LEU:HD13	1.98	0.46
1:2:240:GLU:O	1:2:293:ILE:HG23	2.16	0.46
3:4:444:ILE:HD11	3:4:454:LYS:HD2	1.97	0.46
5:6:303:GLU:HG3	5:6:356:TRP:HD1	1.79	0.46
7:E:15:ILE:CD1	7:E:80:SER:HB2	2.45	0.46
7:E:29:ILE:CD1	7:E:58:ILE:HG12	2.44	0.46
7:E:345:ASN:CG	7:E:507:PHE:CE1	2.87	0.46
9:B:13:PRO:O	9:B:16:ILE:HG12	2.16	0.46
9:B:84:LYS:HE3	9:B:84:LYS:HB3	1.77	0.46
10:A:73:PHE:CZ	11:C:57:VAL:HG21	2.51	0.46
10:A:161:VAL:O	10:A:193:GLN:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:171:ALA:HA	10:A:172:GLY:HA3	1.61	0.46
10:A:189:PHE:HB3	10:A:191:VAL:HG23	1.98	0.46
1:2:359:ILE:HA	1:2:360:ARG:HA	1.65	0.46
3:4:388:ARG:HH22	5:6:176:ARG:HB2	1.81	0.46
6:7:135:LYS:HB2	6:7:141:VAL:CG1	2.46	0.46
6:7:380:PHE:HE2	6:7:382:ARG:HB2	1.80	0.46
9:B:184:PHE:CE1	9:B:188:ILE:HD12	2.50	0.46
10:A:138:ILE:HD12	10:A:141:LEU:HB2	1.96	0.46
11:C:50:LEU:O	11:C:54:LEU:HG	2.16	0.46
2:3:166:LEU:HD13	2:3:167:SER:O	2.16	0.46
3:4:234:ARG:HB3	3:4:280:MET:HE1	1.97	0.46
5:6:134:LYS:N	5:6:135:VAL:HA	2.21	0.46
6:7:135:LYS:HA	6:7:136:ASP:C	2.41	0.46
7:E:127:ARG:HG3	7:E:248:VAL:HG23	1.98	0.46
7:E:618:ALA:HB1	7:E:636:ASP:HB3	1.97	0.46
8:D:282:ILE:O	8:D:286:LEU:CD1	2.64	0.46
10:A:129:GLU:HA	10:A:132:LYS:HE3	1.98	0.46
1:2:294:HIS:CD2	1:2:296:ARG:NH1	2.84	0.46
2:3:189:THR:HG23	2:3:256:ILE:HD11	1.97	0.46
3:4:375:ASP:HA	3:4:376:CYS:C	2.41	0.46
7:E:15:ILE:HB	7:E:121:TYR:CE2	2.50	0.46
4:5:54:ILE:HG22	4:5:135:PHE:CZ	2.51	0.46
8:D:79:TYR:CE1	8:D:176:SER:HB2	2.51	0.46
9:B:112:PHE:CE1	9:B:156:VAL:HG22	2.51	0.46
2:3:55:ASN:O	6:7:217:LYS:HD2	2.16	0.45
3:4:419:VAL:O	3:4:420:TYR:CG	2.68	0.45
4:5:68:LEU:CD2	4:5:76:TYR:HB2	2.46	0.45
4:5:138:ILE:HG12	4:5:282:LEU:HD21	1.97	0.45
7:E:240:TYR:C	7:E:242:SER:H	2.25	0.45
7:E:401:LEU:O	7:E:404:ILE:HG13	2.16	0.45
7:E:570:ALA:HB2	7:E:581:VAL:HG22	1.98	0.45
8:D:211:ASP:CG	8:D:213:GLU:CA	2.89	0.45
9:B:29:PRO:HG2	9:B:63:MET:HB3	1.98	0.45
11:C:172:MET:HG3	11:C:173:GLU:N	2.31	0.45
1:2:387:ARG:HH12	4:5:323:ILE:CD1	2.28	0.45
2:3:199:SER:HB2	2:3:214:TYR:CE2	2.51	0.45
2:3:234:GLU:OE2	2:3:240:LYS:HD2	2.16	0.45
4:5:151:LEU:HA	4:5:155:HIS:NE2	2.32	0.45
5:6:398:THR:O	5:6:456:ALA:HA	2.17	0.45
7:E:15:ILE:HD13	7:E:121:TYR:CD2	2.48	0.45
8:D:257:THR:O	8:D:269:LEU:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:216:LEU:HD12	1:2:217:GLU:CA	2.43	0.45
1:2:435:ASP:HB3	1:2:447:PHE:CD1	2.51	0.45
4:5:83:PRO:HB2	4:5:297:ILE:CD1	2.46	0.45
5:6:122:PHE:HB2	5:6:124:VAL:N	2.32	0.45
7:E:277:THR:HG21	7:E:295:LEU:HD11	1.98	0.45
8:D:229:PHE:CD2	9:B:178:ILE:HG23	2.52	0.45
2:3:254:GLN:NE2	2:3:256:ILE:HD11	2.31	0.45
3:4:438:THR:HG23	3:4:438:THR:O	2.15	0.45
5:6:264:GLN:CD	5:6:383:GLY:HA2	2.40	0.45
6:7:67:LEU:HD11	6:7:121:ILE:HG23	1.97	0.45
7:E:242:SER:HB2	7:E:607:MET:HE3	1.99	0.45
7:E:272:LEU:HD21	7:E:484:LEU:HD21	1.98	0.45
8:D:71:ARG:NH1	9:B:11:PHE:HD1	2.14	0.45
8:D:224:TRP:HB3	8:D:280:GLU:HB2	1.98	0.45
9:B:188:ILE:CD1	11:C:132:ALA:HB2	2.39	0.45
10:A:166:ARG:HH22	10:A:207:LYS:HD3	1.81	0.45
3:4:466:VAL:HG12	3:4:467:LYS:N	2.31	0.45
6:7:207:LEU:O	6:7:207:LEU:CD1	2.50	0.45
6:7:349:VAL:HG21	6:7:381:VAL:HG13	1.99	0.45
10:A:114:THR:C	10:A:116:SER:H	2.25	0.45
10:A:169:LYS:HA	10:A:185:LYS:CD	2.19	0.45
11:C:131:ARG:HD3	11:C:131:ARG:HA	1.71	0.45
9:B:115:LEU:HD22	9:B:119:TRP:CD1	2.52	0.45
2:3:104:ARG:NH2	11:C:86:ASN:HB2	2.32	0.45
2:3:277:ILE:HD12	2:3:320:LEU:HD13	1.98	0.45
6:7:83:ASP:O	6:7:87:GLN:HG2	2.16	0.45
7:E:36:ILE:HD12	7:E:425:VAL:HG13	1.98	0.45
8:D:148:LEU:HD22	8:D:182:TYR:CD2	2.51	0.45
10:A:93:ARG:HG3	10:A:97:LEU:HD11	1.98	0.45
3:4:180:ILE:CD1	3:4:183:THR:HB	2.47	0.45
3:4:343:LYS:HZ1	3:4:392:ALA:HB3	1.80	0.45
4:5:50:LEU:HD13	4:5:61:LEU:HD12	1.98	0.45
4:5:337:VAL:HA	4:5:338:GLU:HA	1.77	0.45
6:7:282:SER:O	6:7:298:LEU:HD21	2.16	0.45
7:E:345:ASN:CB	7:E:551:TRP:NE1	2.75	0.45
8:D:224:TRP:O	8:D:280:GLU:N	2.50	0.45
10:A:188:GLN:O	10:A:188:GLN:HG3	2.15	0.45
2:3:166:LEU:HD11	2:3:171:LEU:HD12	1.99	0.45
2:3:294:VAL:HG12	2:3:295:VAL:O	2.16	0.45
4:5:31:PHE:CG	4:5:90:PHE:CD1	3.04	0.45
5:6:400:VAL:CG2	5:6:455:LEU:HG	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:43:LYS:CG	7:E:484:LEU:HD23	2.42	0.45
7:E:269:ASN:O	7:E:272:LEU:HB2	2.16	0.45
1:2:432:ASN:HA	1:2:448:ALA:O	2.17	0.45
2:3:122:ILE:HG22	2:3:123:PRO:CD	2.46	0.45
3:4:302:LYS:HD2	3:4:304:ARG:HH21	1.82	0.45
7:E:280:LEU:O	7:E:283:ALA:N	2.48	0.45
8:D:174:LEU:HG	8:D:175:LEU:HD12	1.99	0.45
8:D:232:VAL:HA	8:D:291:VAL:HG23	1.99	0.45
10:A:123:LEU:HD21	10:A:127:GLU:HB2	1.99	0.45
3:4:351:VAL:HA	3:4:352:CYS:HA	1.56	0.44
4:5:264:LEU:HA	4:5:265:VAL:HA	1.67	0.44
6:7:215:TYR:HE1	6:7:217:LYS:HD3	1.82	0.44
6:7:217:LYS:HG3	6:7:218:LYS:H	1.82	0.44
7:E:74:LEU:CD2	10:A:173:GLU:OE1	2.61	0.44
1:2:300:PHE:H	1:2:319:ARG:HH11	1.59	0.44
2:3:94:HIS:HB3	2:3:153:TRP:CZ3	2.52	0.44
2:3:163:ALA:HB3	2:3:164:HIS:ND1	2.31	0.44
2:3:257:THR:HG22	2:3:275:ASP:HB3	1.99	0.44
4:5:62:THR:HA	4:5:138:ILE:O	2.17	0.44
9:B:78:LEU:HD23	9:B:78:LEU:C	2.42	0.44
2:3:153:TRP:HB3	2:3:154:LYS:H	1.65	0.44
2:3:163:ALA:H	2:3:164:HIS:HB2	1.83	0.44
2:3:255:ARG:NH2	2:3:275:ASP:OD2	2.49	0.44
5:6:403:VAL:CG1	5:6:450:TYR:HB3	2.48	0.44
6:7:331:LEU:HD11	6:7:355:PHE:CE1	2.48	0.44
7:E:19:SER:O	7:E:20:SER:C	2.59	0.44
10:A:57:GLN:HE21	10:A:62:MET:HE3	1.82	0.44
2:3:189:THR:HG23	2:3:256:ILE:HD12	1.98	0.44
3:4:416:SER:O	3:4:460:TYR:HB2	2.18	0.44
5:6:156:GLN:O	5:6:160:MET:HG2	2.17	0.44
7:E:316:LEU:HD12	7:E:412:THR:O	2.18	0.44
7:E:380:MET:HB2	7:E:385:LYS:CE	2.48	0.44
7:E:483:ALA:HA	7:E:491:LEU:HD11	1.99	0.44
7:E:637:LEU:HD12	7:E:638:SER:N	2.32	0.44
8:D:79:TYR:HB2	8:D:147:ARG:HH22	1.81	0.44
9:B:11:PHE:HB2	9:B:179:ASN:ND2	2.32	0.44
11:C:112:ILE:HG23	11:C:113:MET:HE2	1.99	0.44
1:2:264:PRO:HG3	1:2:317:LEU:HB2	1.98	0.44
2:3:158:LYS:HA	2:3:327:TYR:OH	2.17	0.44
2:3:235:ASP:HB2	6:7:5:LEU:HD13	2.00	0.44
7:E:32:SER:HA	7:E:33:CYS:HA	1.28	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:327:PHE:CE2	7:E:503:GLN:HG3	2.53	0.44
7:E:619:LYS:HB3	7:E:633:ARG:HG2	1.99	0.44
10:A:47:LEU:HD21	10:A:75:THR:HB	1.99	0.44
10:A:102:TRP:NE1	10:A:134:TYR:OH	2.50	0.44
10:A:136:ASP:O	10:A:139:THR:OG1	2.36	0.44
10:A:182:ASN:O	10:A:184:ILE:HG12	2.17	0.44
11:C:105:PHE:HE1	11:C:128:LEU:HB2	1.81	0.44
3:4:201:PHE:CB	3:4:202:LYS:HA	2.35	0.44
7:E:43:LYS:CG	7:E:484:LEU:CD2	2.84	0.44
7:E:148:VAL:HG12	7:E:152:LEU:CD2	2.47	0.44
7:E:326:LEU:HD22	7:E:329:LEU:HD12	1.99	0.44
8:D:275:TYR:HD1	9:B:168:LEU:O	2.00	0.44
10:A:167:VAL:CG2	10:A:187:SER:O	2.37	0.44
2:3:200:VAL:HB	2:3:248:SER:HB3	1.99	0.44
2:3:310:ASN:HA	2:3:311:SER:HA	1.68	0.44
3:4:200:SER:HB3	3:4:202:LYS:HB2	2.00	0.44
6:7:293:GLN:HA	6:7:294:THR:HA	1.64	0.44
6:7:362:GLY:HA3	6:7:364:LYS:HZ2	1.82	0.44
9:B:134:PHE:O	9:B:137:PRO:HD3	2.17	0.44
9:B:165:GLU:HA	9:B:166:SER:HA	1.34	0.44
9:B:187:GLU:O	9:B:190:ASP:N	2.50	0.44
1:2:301:PRO:HD3	1:2:319:ARG:NH1	2.33	0.44
5:6:336:PRO:HA	5:6:337:SER:HA	1.48	0.44
5:6:379:VAL:HA	5:6:454:PHE:O	2.17	0.44
6:7:134:TYR:HB2	6:7:141:VAL:HG12	2.00	0.44
7:E:318:LEU:HD12	7:E:318:LEU:O	2.18	0.44
11:C:104:PHE:HB3	11:C:170:GLU:OE1	2.18	0.44
3:4:225:TYR:N	3:4:228:LYS:HB2	2.33	0.44
3:4:467:LYS:CG	3:4:468:LYS:CB	2.88	0.44
4:5:172:LEU:HD11	4:5:284:ASN:HD21	1.83	0.44
4:5:182:MET:HA	4:5:188:HIS:O	2.17	0.44
6:7:67:LEU:CD2	6:7:126:PRO:HD2	2.47	0.44
6:7:118:CYS:SG	6:7:202:LEU:HB2	2.58	0.44
8:D:216:VAL:HG11	8:D:219:ILE:HB	1.99	0.44
8:D:282:ILE:C	8:D:286:LEU:HD13	2.42	0.44
2:3:314:LEU:CD1	2:3:314:LEU:H	2.30	0.43
5:6:364:ASN:HB3	5:6:394:ARG:HD3	1.99	0.43
6:7:222:SER:O	6:7:222:SER:OG	2.33	0.43
6:7:240:THR:HG23	6:7:352:THR:HG22	1.99	0.43
7:E:291:LEU:HD23	7:E:294:LEU:HD12	2.00	0.43
7:E:561:ASP:HB3	7:E:562:LYS:CG	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:36:ILE:O	10:A:40:ILE:HG13	2.18	0.43
1:2:271:PHE:CE2	1:2:295:VAL:HG11	2.52	0.43
4:5:159:ILE:H	4:5:159:ILE:HG13	1.63	0.43
4:5:160:VAL:HG12	4:5:162:LEU:HD23	1.99	0.43
5:6:356:TRP:CZ3	5:6:358:LYS:HB2	2.44	0.43
6:7:17:LEU:CG	6:7:102:LEU:HD21	2.39	0.43
9:B:175:LEU:HA	9:B:178:ILE:HD12	2.00	0.43
10:A:169:LYS:H	10:A:185:LYS:NZ	2.14	0.43
11:C:19:LYS:O	11:C:72:VAL:HG13	2.18	0.43
11:C:97:LEU:HG	11:C:131:ARG:HH22	1.83	0.43
1:2:303:ILE:HG13	1:2:319:ARG:HH21	1.83	0.43
2:3:49:ASN:OD1	2:3:50:SER:N	2.52	0.43
4:5:301:TYR:CE1	4:5:303:SER:HB3	2.54	0.43
5:6:100:VAL:HA	5:6:101:LYS:HA	1.49	0.43
5:6:307:ALA:HA	5:6:351:SER:HB3	2.01	0.43
7:E:514:LEU:HD11	7:E:555:CYS:SG	2.57	0.43
11:C:16:PHE:O	11:C:45:SER:HA	2.19	0.43
2:3:295:VAL:HG12	2:3:296:GLY:N	2.34	0.43
3:4:347:PHE:HB3	3:4:382:MET:SD	2.58	0.43
6:7:254:ALA:HB2	6:7:310:PHE:HB2	1.99	0.43
7:E:22:HIS:CA	7:E:24:SER:N	2.73	0.43
8:D:206:LEU:HD22	10:A:83:LYS:HD2	2.01	0.43
9:B:51:GLN:HB2	9:B:52:LEU:HA	2.01	0.43
10:A:192:ARG:HD2	10:A:194:SER:OG	2.18	0.43
2:3:189:THR:CG2	2:3:256:ILE:CD1	2.97	0.43
2:3:237:GLU:H	2:3:237:GLU:CD	2.25	0.43
3:4:317:LEU:O	6:7:341:ARG:NH2	2.52	0.43
3:4:322:ILE:HD13	6:7:302:THR:HB	1.99	0.43
6:7:367:LYS:HG2	6:7:371:LEU:HD22	2.00	0.43
7:E:349:SER:HA	7:E:351:TRP:CH2	2.54	0.43
7:E:365:ARG:HH12	7:E:398:ARG:CD	2.32	0.43
9:B:155:LYS:HE3	9:B:155:LYS:HB2	1.76	0.43
9:B:165:GLU:H	9:B:165:GLU:CD	2.26	0.43
10:A:175:GLN:OE1	10:A:199:LEU:CD1	2.51	0.43
2:3:156:SER:O	2:3:325:THR:CG2	2.67	0.43
5:6:347:ASN:OD1	5:6:349:THR:HG22	2.17	0.43
7:E:22:HIS:HD2	8:D:123:LYS:HZ2	1.43	0.43
7:E:40:CYS:O	7:E:44:MET:HG2	2.18	0.43
7:E:74:LEU:HD11	10:A:184:ILE:HD11	2.00	0.43
7:E:377:TRP:NE1	7:E:385:LYS:NZ	2.61	0.43
8:D:266:GLU:H	8:D:266:GLU:CD	2.27	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:162:PHE:CE1	10:A:192:ARG:HB3	2.53	0.43
11:C:76:PRO:HA	11:C:77:PRO:HD3	1.81	0.43
3:4:385:ILE:HG22	3:4:388:ARG:H	1.84	0.43
4:5:300:ILE:HD13	4:5:326:PRO:HA	2.01	0.43
7:E:98:ILE:N	7:E:99:ASP:HB3	2.34	0.43
7:E:324:TYR:C	7:E:326:LEU:N	2.75	0.43
9:B:184:PHE:CZ	11:C:132:ALA:HB1	2.53	0.43
2:3:210:HIS:HB3	6:7:5:LEU:HD21	2.01	0.43
2:3:215:THR:HB	2:3:219:THR:HG21	1.99	0.43
6:7:145:GLN:O	6:7:149:ARG:HG2	2.18	0.43
6:7:349:VAL:HB	6:7:383:GLN:HG2	2.01	0.43
7:E:36:ILE:HD11	7:E:429:THR:HG23	2.01	0.43
7:E:525:TYR:HE1	7:E:527:LEU:HD12	1.82	0.43
9:B:185:ILE:O	9:B:189:MET:HG2	2.19	0.43
3:4:314:MET:HG2	3:4:415:ILE:HG12	2.00	0.43
3:4:466:VAL:O	3:4:467:LYS:HB2	2.19	0.43
5:6:122:PHE:HB2	5:6:124:VAL:HG23	2.01	0.43
5:6:155:TYR:CD2	5:6:271:PRO:HD3	2.54	0.43
6:7:281:LEU:HB2	6:7:283:GLU:OE2	2.18	0.43
7:E:223:ARG:O	7:E:227:LYS:HG2	2.19	0.43
7:E:359:LEU:O	7:E:362:MET:HB2	2.19	0.43
8:D:256:TYR:CD1	8:D:257:THR:CG2	2.98	0.43
9:B:181:LEU:HD13	9:B:185:ILE:HD13	2.00	0.43
10:A:151:LEU:H	10:A:151:LEU:HD13	1.83	0.43
10:A:161:VAL:O	10:A:161:VAL:CG1	2.65	0.43
10:A:175:GLN:NE2	10:A:199:LEU:HD13	2.34	0.43
11:C:98:HIS:HA	11:C:102:SER:HB2	2.01	0.43
11:C:104:PHE:O	11:C:108:ALA:N	2.42	0.43
2:3:189:THR:CG2	2:3:256:ILE:HD12	2.49	0.43
6:7:292:ASN:OD1	6:7:293:GLN:HB2	2.19	0.43
7:E:345:ASN:ND2	7:E:507:PHE:CE1	2.87	0.43
8:D:137:LYS:HE2	8:D:141:ARG:NH2	2.28	0.43
8:D:215:SER:HA	8:D:216:VAL:HA	1.66	0.43
10:A:23:SER:N	10:A:24:ASN:HA	2.26	0.43
2:3:236:THR:HA	2:3:237:GLU:C	2.44	0.42
5:6:133:GLU:HA	5:6:134:LYS:HA	1.72	0.42
5:6:151:ILE:HD11	5:6:265:ILE:HG23	2.01	0.42
7:E:74:LEU:HD22	10:A:173:GLU:OE2	2.15	0.42
10:A:169:LYS:HE2	10:A:169:LYS:HB2	1.88	0.42
3:4:388:ARG:HH22	5:6:176:ARG:HD2	1.83	0.42
3:4:419:VAL:HG23	3:4:424:VAL:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:266:ASN:HD22	7:E:269:ASN:ND2	2.16	0.42
7:E:413:LEU:HD12	7:E:413:LEU:HA	1.66	0.42
8:D:214:GLY:HA2	8:D:215:SER:HA	1.32	0.42
9:B:25:ILE:HD11	9:B:87:ILE:CD1	2.48	0.42
3:4:319:PRO:HG2	6:7:309:ALA:HB2	2.01	0.42
3:4:354:HIS:NE2	3:4:356:MET:HG2	2.34	0.42
4:5:59:TYR:HB2	4:5:281:TYR:OH	2.18	0.42
4:5:244:ILE:CG2	4:5:246:GLU:HG2	2.49	0.42
5:6:189:VAL:O	5:6:193:ALA:N	2.51	0.42
5:6:335:ASN:H	5:6:338:CYS:N	2.12	0.42
6:7:196:LEU:HD23	6:7:196:LEU:C	2.45	0.42
7:E:561:ASP:HA	7:E:562:LYS:HA	1.80	0.42
9:B:127:PHE:CE1	9:B:134:PHE:HE2	2.36	0.42
3:4:314:MET:SD	3:4:317:LEU:HD12	2.60	0.42
3:4:343:LYS:HD3	3:4:343:LYS:HA	1.76	0.42
6:7:139:LEU:HA	6:7:142:ILE:HG13	2.02	0.42
7:E:416:ARG:NH1	7:E:416:ARG:HG3	2.34	0.42
10:A:93:ARG:O	10:A:97:LEU:CD1	2.68	0.42
1:2:330:VAL:CG2	4:5:272:ARG:HH12	2.33	0.42
2:3:211:TYR:CZ	6:7:6:PRO:HG2	2.55	0.42
3:4:184:ASN:HB3	6:7:145:GLN:HE22	1.83	0.42
3:4:248:LEU:HB3	3:4:254:THR:O	2.19	0.42
4:5:92:THR:HA	4:5:95:THR:HG22	2.00	0.42
5:6:103:VAL:HA	5:6:104:ASP:HA	1.77	0.42
5:6:153:ILE:HD11	5:6:267:PHE:CE1	2.55	0.42
5:6:162:GLU:O	5:6:163:ASN:HB2	2.20	0.42
6:7:89:GLN:NE2	6:7:102:LEU:H	2.18	0.42
7:E:9:SER:O	7:E:12:TYR:HB3	2.19	0.42
7:E:626:GLU:HB3	7:E:629:ILE:CG2	2.49	0.42
11:C:3:TYR:CG	11:C:4:TYR:N	2.88	0.42
11:C:47:PRO:HB2	11:C:49:TRP:NE1	2.35	0.42
3:4:327:ASN:HB3	3:4:434:GLU:OE2	2.19	0.42
3:4:387:ASN:OD1	5:6:402:ILE:HA	2.19	0.42
4:5:46:TYR:OH	4:5:64:ASN:N	2.27	0.42
4:5:54:ILE:HD13	4:5:102:SER:HB3	2.01	0.42
4:5:331:LEU:HA	4:5:332:GLY:HA2	1.60	0.42
7:E:164:GLU:CD	7:E:164:GLU:H	2.28	0.42
7:E:283:ALA:O	7:E:284:TYR:CG	2.73	0.42
7:E:334:LEU:O	7:E:337:SER:HB3	2.20	0.42
7:E:365:ARG:HH12	7:E:398:ARG:NE	2.17	0.42
11:C:134:GLU:OE2	11:C:138:HIS:NE2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:438:LEU:C	1:2:440:ALA:N	2.77	0.42
2:3:111:TRP:CZ2	11:C:90:THR:HG22	2.55	0.42
2:3:196:LEU:HG	2:3:214:TYR:HD2	1.84	0.42
2:3:203:ALA:HB3	2:3:207:GLY:O	2.20	0.42
3:4:273:ASP:O	3:4:276:ILE:HG13	2.20	0.42
5:6:268:PHE:HD1	5:6:269:ASN:HB2	1.85	0.42
5:6:293:THR:HG23	5:6:393:ASP:N	2.35	0.42
5:6:373:MET:HA	5:6:374:PRO:HD2	1.82	0.42
6:7:128:PRO:HB2	6:7:129:THR:C	2.44	0.42
7:E:470:ARG:O	7:E:474:VAL:HG23	2.19	0.42
7:E:536:LEU:HA	7:E:539:TYR:HD2	1.85	0.42
7:E:551:TRP:CE3	7:E:552:LEU:HD12	2.54	0.42
8:D:166:ASN:HA	8:D:167:SER:HA	1.65	0.42
8:D:264:LYS:HG2	8:D:265:GLU:N	2.35	0.42
10:A:192:ARG:CD	10:A:194:SER:OG	2.67	0.42
1:2:441:LYS:HE3	1:2:441:LYS:HB3	1.76	0.42
1:2:442:ASN:CG	1:2:443:GLY:N	2.71	0.42
4:5:41:ASP:HA	4:5:42:SER:HA	1.76	0.42
4:5:78:LYS:HB3	4:5:78:LYS:HE2	1.76	0.42
4:5:178:TYR:HE1	4:5:191:SER:HB2	1.84	0.42
6:7:344:SER:HB2	6:7:347:ASP:OD2	2.19	0.42
7:E:34:LEU:HD12	7:E:543:LEU:HD21	1.62	0.42
7:E:151:THR:HB	7:E:152:LEU:C	2.45	0.42
8:D:138:PHE:CZ	10:A:157:PRO:HG3	2.54	0.42
8:D:153:LYS:HE3	8:D:154:PHE:CE1	2.54	0.42
8:D:216:VAL:HG13	8:D:218:MET:N	2.35	0.42
9:B:51:GLN:HB2	9:B:53:ILE:HD12	2.00	0.42
9:B:163:LEU:HD13	9:B:189:MET:HE2	2.02	0.42
9:B:170:LEU:HD23	9:B:170:LEU:HA	1.95	0.42
10:A:178:TYR:CE2	10:A:195:ASP:OD1	2.73	0.42
1:2:234:LEU:HD22	1:2:241:SER:O	2.16	0.42
5:6:455:LEU:HD12	5:6:456:ALA:H	1.84	0.42
6:7:26:VAL:HG21	6:7:124:ASN:HB2	2.02	0.42
7:E:328:LEU:CD1	7:E:500:GLN:HG2	2.50	0.42
10:A:54:LEU:CD2	10:A:57:GLN:OE1	2.68	0.42
3:4:302:LYS:HE2	3:4:302:LYS:HB3	1.90	0.42
4:5:170:SER:HB3	4:5:254:GLN:O	2.20	0.42
7:E:56:SER:H	10:A:190:PHE:HB3	1.84	0.42
7:E:392:PHE:O	7:E:396:LEU:HB2	2.20	0.42
10:A:13:ALA:HB1	10:A:92:LEU:HD23	2.00	0.42
10:A:173:GLU:HB3	10:A:183:LEU:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:C:10:LEU:HD12	11:C:10:LEU:HA	1.80	0.42
2:3:40:ASP:OD1	2:3:41:SER:N	2.53	0.41
4:5:136:GLN:HE22	4:5:282:LEU:CD1	2.33	0.41
5:6:290:ILE:HD12	5:6:454:PHE:HZ	1.75	0.41
5:6:356:TRP:HZ3	5:6:358:LYS:CB	2.29	0.41
5:6:399:GLY:O	5:6:400:VAL:C	2.63	0.41
7:E:140:ILE:HA	7:E:141:GLN:HB3	2.02	0.41
7:E:256:TYR:CD1	7:E:273:ASN:ND2	2.85	0.41
7:E:394:LYS:HB2	7:E:394:LYS:HE3	1.84	0.41
8:D:138:PHE:CE2	10:A:157:PRO:HG3	2.55	0.41
8:D:260:ILE:HG12	8:D:266:GLU:OE2	2.19	0.41
3:4:315:ARG:NH2	6:7:311:GLN:HE22	2.14	0.41
5:6:126:SER:HB3	5:6:131:GLU:HB3	2.02	0.41
5:6:154:ASP:OD1	5:6:155:TYR:N	2.53	0.41
7:E:97:GLU:HG3	7:E:97:GLU:O	2.20	0.41
7:E:124:ASP:OD1	7:E:125:ALA:N	2.53	0.41
8:D:257:THR:O	8:D:259:THR:HG23	2.21	0.41
10:A:167:VAL:HG21	10:A:184:ILE:O	2.20	0.41
11:C:96:ASP:OD2	11:C:99:SER:HB3	2.19	0.41
11:C:97:LEU:O	11:C:100:ILE:HG12	2.20	0.41
2:3:252:ASP:OD2	2:3:283:VAL:HG11	2.20	0.41
2:3:311:SER:OG	4:5:304:LYS:NZ	2.53	0.41
3:4:318:ASN:HA	3:4:319:PRO:HD3	1.81	0.41
3:4:408:ASP:HA	3:4:409:GLY:HA2	1.87	0.41
4:5:44:PHE:N	4:5:44:PHE:CD1	2.88	0.41
5:6:274:HIS:CG	5:6:288:LEU:HD11	2.55	0.41
6:7:248:VAL:HG11	6:7:345:PRO:HD3	2.02	0.41
7:E:502:LEU:HA	7:E:502:LEU:HD23	1.69	0.41
8:D:212:THR:HB	8:D:213:GLU:C	2.45	0.41
8:D:258:VAL:CG1	8:D:260:ILE:HG13	2.50	0.41
9:B:184:PHE:CD2	9:B:185:ILE:HD12	2.54	0.41
10:A:74:VAL:O	10:A:77:LEU:HB2	2.20	0.41
11:C:18:CYS:SG	11:C:74:LEU:HA	2.61	0.41
4:5:137:LEU:C	4:5:137:LEU:CD1	2.84	0.41
6:7:367:LYS:HA	6:7:368:ALA:HB3	2.03	0.41
7:E:12:TYR:HA	7:E:15:ILE:HG22	2.02	0.41
7:E:88:GLY:HA2	7:E:129:TRP:CE3	2.54	0.41
8:D:171:LEU:HB3	8:D:172:THR:H	1.51	0.41
9:B:82:GLN:HB3	9:B:84:LYS:HG3	2.02	0.41
11:C:17:PRO:O	11:C:75:LEU:HB3	2.21	0.41
1:2:247:ARG:HH12	1:2:301:PRO:HD2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:330:VAL:HG21	4:5:272:ARG:HH12	1.86	0.41
3:4:263:ASN:HD22	3:4:324:LYS:HE3	1.86	0.41
3:4:302:LYS:NZ	3:4:421:ASP:OD2	2.54	0.41
5:6:136:TYR:O	5:6:140:ILE:CD1	2.43	0.41
7:E:26:GLN:O	7:E:78:ILE:HG23	2.20	0.41
9:B:26:LYS:HB2	9:B:88:VAL:HG11	2.03	0.41
9:B:54:THR:HB	9:B:57:ASP:OD2	2.20	0.41
9:B:79:LEU:HB2	9:B:85:CYS:SG	2.61	0.41
10:A:151:LEU:H	10:A:151:LEU:CD1	2.33	0.41
11:C:108:ALA:O	11:C:112:ILE:HG22	2.20	0.41
2:3:197:ILE:O	2:3:214:TYR:HB2	2.21	0.41
3:4:181:TRP:CG	3:4:182:GLY:N	2.89	0.41
3:4:183:THR:HG23	3:4:264:TYR:HB3	2.02	0.41
3:4:262:LEU:HD13	3:4:308:VAL:HB	2.01	0.41
3:4:433:ILE:O	3:4:434:GLU:HB2	2.20	0.41
4:5:34:PHE:CZ	4:5:46:TYR:HE2	2.39	0.41
4:5:297:ILE:HG22	4:5:298:TYR:N	2.36	0.41
4:5:320:GLY:HA2	4:5:321:VAL:HA	1.71	0.41
7:E:559:SER:HA	7:E:560:GLU:CB	2.45	0.41
8:D:250:GLU:HG3	8:D:256:TYR:HD2	1.85	0.41
10:A:192:ARG:O	10:A:196:VAL:HG23	2.20	0.41
1:2:289:ILE:HG22	1:2:290:HIS:ND1	2.35	0.41
2:3:172:THR:HA	2:3:173:ALA:HA	1.81	0.41
7:E:87:GLY:O	7:E:133:ASN:ND2	2.51	0.41
7:E:295:LEU:HB3	7:E:409:PHE:HE2	1.85	0.41
8:D:200:LYS:HB2	8:D:201:TYR:CB	2.49	0.41
8:D:222:PRO:O	8:D:224:TRP:CD1	2.73	0.41
9:B:120:LEU:HD13	9:B:176:LEU:HD22	2.02	0.41
10:A:89:TYR:O	10:A:92:LEU:HB3	2.20	0.41
10:A:150:ASP:OD1	10:A:198:ARG:CZ	2.69	0.41
3:4:181:TRP:CG	3:4:182:GLY:H	2.38	0.41
3:4:225:TYR:HA	3:4:226:TYR:HA	1.79	0.41
4:5:86:ILE:C	4:5:88:PRO:HD2	2.46	0.41
7:E:43:LYS:CG	7:E:484:LEU:HD21	2.41	0.41
7:E:81:LEU:HB3	7:E:120:ILE:HG13	2.03	0.41
7:E:269:ASN:HA	7:E:272:LEU:HD12	2.01	0.41
7:E:621:ARG:HB2	7:E:631:GLU:HB2	2.03	0.41
1:2:337:VAL:HA	1:2:380:THR:HG22	2.03	0.41
1:2:433:ASN:HA	1:2:434:TYR:HA	1.81	0.41
2:3:132:LEU:O	2:3:136:MET:HG2	2.21	0.41
2:3:254:GLN:HE21	2:3:256:ILE:HD11	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:304:ARG:NH2	3:4:422:GLU:OE1	2.54	0.41
3:4:346:PHE:CE2	3:4:388:ARG:HD3	2.55	0.41
4:5:51:ARG:O	4:5:54:ILE:HG13	2.21	0.41
4:5:69:ILE:HD13	4:5:76:TYR:CD2	2.55	0.41
4:5:296:GLY:HA3	4:5:329:LYS:O	2.21	0.41
5:6:132:VAL:HG22	5:6:133:GLU:CD	2.46	0.41
5:6:174:TYR:CE2	5:6:178:LEU:HD11	2.56	0.41
5:6:448:LEU:HD12	5:6:448:LEU:O	2.20	0.41
7:E:15:ILE:HB	7:E:121:TYR:CZ	2.55	0.41
7:E:97:GLU:HA	7:E:98:ILE:O	2.21	0.41
7:E:128:PRO:HB2	7:E:240:TYR:CZ	2.56	0.41
7:E:280:LEU:HD11	7:E:285:ALA:O	2.21	0.41
7:E:316:LEU:CD1	7:E:412:THR:O	2.68	0.41
7:E:525:TYR:CE1	7:E:527:LEU:HD12	2.55	0.41
8:D:176:SER:O	8:D:180:ILE:HG23	2.21	0.41
8:D:188:LEU:O	8:D:192:LYS:HG2	2.20	0.41
10:A:132:LYS:HA	10:A:135:CYS:SG	2.61	0.41
11:C:14:THR:HG21	11:C:107:LEU:HD12	2.03	0.41
1:2:299:ASP:C	1:2:319:ARG:HH11	2.29	0.41
2:3:193:ARG:CG	6:7:371:LEU:HD11	2.51	0.41
2:3:234:GLU:CD	2:3:239:ASN:C	2.89	0.41
3:4:272:MET:HB3	3:4:303:VAL:HG21	2.02	0.41
3:4:304:ARG:HH12	3:4:423:LEU:CD2	2.30	0.41
3:4:434:GLU:O	3:4:467:LYS:O	2.39	0.41
4:5:321:VAL:HA	4:5:322:ALA:HA	1.84	0.41
5:6:311:CYS:HA	5:6:312:ASP:CB	2.51	0.41
6:7:135:LYS:HD2	6:7:136:ASP:O	2.21	0.41
6:7:252:LYS:HE3	6:7:252:LYS:HB3	1.84	0.41
7:E:14:LYS:HZ3	7:E:141:GLN:CD	2.22	0.41
7:E:412:THR:HG22	7:E:418:SER:OG	2.21	0.41
7:E:558:GLU:H	7:E:560:GLU:HB2	1.86	0.41
8:D:260:ILE:H	8:D:266:GLU:HG3	1.85	0.41
8:D:287:ARG:HE	8:D:287:ARG:HB2	1.70	0.41
9:B:14:GLU:O	9:B:17:GLN:HG2	2.20	0.41
9:B:112:PHE:O	9:B:152:ARG:NH2	2.53	0.41
11:C:16:PHE:CZ	11:C:107:LEU:HD21	2.55	0.41
2:3:95:ARG:NH2	2:3:154:LYS:HG3	2.36	0.40
3:4:449:ARG:HG3	3:4:450:GLN:N	2.22	0.40
4:5:29:LYS:HA	4:5:29:LYS:HD3	1.87	0.40
5:6:134:LYS:HG2	5:6:137:ARG:CG	2.52	0.40
5:6:401:GLU:O	5:6:402:ILE:HG12	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:326:LEU:HD23	7:E:326:LEU:C	2.46	0.40
9:B:91:GLN:OE1	9:B:91:GLN:N	2.34	0.40
10:A:36:ILE:HD12	10:A:36:ILE:HA	1.97	0.40
10:A:99:SER:O	10:A:102:TRP:HB2	2.20	0.40
10:A:108:ASP:OD1	10:A:198:ARG:CD	2.64	0.40
1:2:324:VAL:HG13	1:2:388:VAL:CG1	2.51	0.40
1:2:328:THR:HG22	1:2:387:ARG:H	1.86	0.40
2:3:189:THR:HA	2:3:256:ILE:HD13	1.83	0.40
6:7:271:GLN:NE2	6:7:279:THR:O	2.32	0.40
7:E:121:TYR:CE1	7:E:141:GLN:HG3	2.57	0.40
7:E:162:LEU:HD22	7:E:165:LEU:HD23	2.03	0.40
8:D:220:ASP:HA	8:D:221:GLU:HA	1.66	0.40
9:B:24:PRO:HA	9:B:72:VAL:HA	2.01	0.40
9:B:187:GLU:OE1	11:C:176:ILE:CG2	2.40	0.40
10:A:138:ILE:HD12	10:A:138:ILE:HA	1.85	0.40
10:A:165:VAL:HG13	10:A:205:LEU:HB3	1.46	0.40
11:C:100:ILE:HG13	11:C:101:ASN:ND2	2.36	0.40
5:6:296:ARG:NH1	5:6:360:ARG:CZ	2.84	0.40
7:E:148:VAL:CG1	7:E:152:LEU:HD22	2.52	0.40
7:E:270:LEU:O	7:E:274:ILE:HG13	2.22	0.40
7:E:572:ILE:HG21	7:E:579:TYR:CZ	2.56	0.40
7:E:634:ARG:HA	7:E:637:LEU:CD2	2.51	0.40
8:D:84:MET:HE1	8:D:143:TYR:CD2	2.57	0.40
8:D:275:TYR:HE1	9:B:169:GLN:CB	2.34	0.40
2:3:103:LEU:HA	2:3:103:LEU:HD23	1.79	0.40
2:3:285:LYS:HD3	2:3:285:LYS:HA	1.86	0.40
3:4:280:MET:O	3:4:284:ILE:HG12	2.21	0.40
6:7:333:ILE:HD13	6:7:351:VAL:HG11	2.03	0.40
7:E:127:ARG:O	7:E:245:THR:HA	2.22	0.40
7:E:145:ASP:HA	7:E:146:GLY:HA2	1.68	0.40
7:E:358:ARG:O	7:E:362:MET:HG3	2.22	0.40
8:D:77:LEU:HB3	8:D:78:PRO:HD2	2.04	0.40
8:D:282:ILE:H	8:D:282:ILE:HG13	1.73	0.40
9:B:3:LEU:HD12	10:A:99:SER:N	2.36	0.40
9:B:112:PHE:CE1	9:B:156:VAL:CG2	3.05	0.40
11:C:74:LEU:HD22	11:C:111:TRP:HZ3	1.86	0.40
1:2:410:LEU:C	1:2:411:LEU:CD1	2.81	0.40
3:4:447:ASN:HA	3:4:448:SER:HA	1.90	0.40
4:5:46:TYR:O	4:5:49:GLN:N	2.55	0.40
6:7:258:ILE:H	6:7:305:SER:HB2	1.85	0.40
11:C:171:GLU:O	11:C:174:LYS:HB3	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	2	235/868 (27%)	205 (87%)	25 (11%)	5 (2%)	5	31
2	3	263/971 (27%)	236 (90%)	22 (8%)	5 (2%)	6	33
3	4	271/933 (29%)	230 (85%)	36 (13%)	5 (2%)	6	34
4	5	244/775 (32%)	222 (91%)	19 (8%)	3 (1%)	10	40
5	6	259/1017 (26%)	229 (88%)	27 (10%)	3 (1%)	10	40
6	7	319/845 (38%)	270 (85%)	45 (14%)	4 (1%)	9	38
7	E	543/672 (81%)	491 (90%)	47 (9%)	5 (1%)	14	45
8	D	215/294 (73%)	197 (92%)	16 (7%)	2 (1%)	14	45
9	B	177/213 (83%)	163 (92%)	14 (8%)	0	100	100
10	A	206/208 (99%)	180 (87%)	25 (12%)	1 (0%)	24	56
11	C	151/194 (78%)	144 (95%)	7 (5%)	0	100	100
All	All	2883/6990 (41%)	2567 (89%)	283 (10%)	33 (1%)	14	42

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	2	291	SER
3	4	450	GLN
6	7	26	VAL
7	E	601	ILE
3	4	419	VAL
5	6	402	ILE
1	2	435	ASP
1	2	439	ASN
2	3	230	ILE
3	4	467	LYS

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Mol	Chain	Res	Type
5	6	106	VAL
7	E	20	SER
7	E	21	SER
1	2	298	SER
2	3	158	LYS
2	3	172	THR
2	3	233	THR
4	5	153	SER
4	5	154	GLU
4	5	267	VAL
5	6	321	VAL
6	7	257	VAL
7	E	24	SER
8	D	219	ILE
8	D	255	CYS
10	A	27	VAL
1	2	297	ILE
7	E	98	ILE
6	7	258	ILE
3	4	433	ILE
3	4	463	VAL
6	7	248	VAL
2	3	326	VAL

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	206/770 (27%)	206 (100%)	0	100	100
2	3	236/835 (28%)	236 (100%)	0	100	100
3	4	249/848 (29%)	248 (100%)	1 (0%)	84	81
4	5	241/688 (35%)	239 (99%)	2 (1%)	73	76
5	6	207/886 (23%)	207 (100%)	0	100	100
6	7	295/753 (39%)	291 (99%)	4 (1%)	59	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	E	499/607 (82%)	490 (98%)	9 (2%)	51	67
8	D	213/279 (76%)	211 (99%)	2 (1%)	70	75
9	B	171/198 (86%)	169 (99%)	2 (1%)	63	72
10	A	193/193 (100%)	191 (99%)	2 (1%)	68	74
11	C	144/173 (83%)	143 (99%)	1 (1%)	76	77
All	All	2654/6230 (43%)	2631 (99%)	23 (1%)	68	75

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	4	293	LEU
4	5	104	LEU
4	5	321	VAL
6	7	86	LEU
6	7	315	ILE
6	7	354	ILE
6	7	370	LEU
7	E	20	SER
7	E	24	SER
7	E	27	LEU
7	E	34	LEU
7	E	57	GLN
7	E	81	LEU
7	E	152	LEU
7	E	162	LEU
7	E	529	VAL
8	D	168	LEU
8	D	258	VAL
9	B	60	LEU
9	B	175	LEU
10	A	151	LEU
10	A	163	ILE
11	C	123	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	2	386	GLN
1	2	439	ASN

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Mol	Chain	Res	Type
2	3	29	GLN
2	3	239	ASN
2	3	310	ASN
3	4	231	ASN
3	4	247	ASN
3	4	410	GLN
3	4	413	HIS
4	5	49	GLN
4	5	53	ASN
4	5	58	ASN
4	5	136	GLN
4	5	253	GLN
4	5	259	GLN
4	5	284	ASN
5	6	139	GLN
5	6	364	ASN
6	7	87	GLN
6	7	90	ASN
6	7	311	GLN
7	E	22	HIS
7	E	26	GLN
7	E	243	GLN
7	E	249	ASN
7	E	266	ASN
7	E	273	ASN
7	E	286	GLN
7	E	289	ASN
7	E	521	HIS
7	E	550	ASN
7	E	563	GLN
7	E	575	ASN
7	E	604	ASN
7	E	624	ASN
8	D	109	GLN
8	D	110	ASN
8	D	231	HIS
9	B	17	GLN
9	B	128	ASN
9	B	139	HIS
9	B	146	GLN
9	B	167	HIS
10	A	50	ASN

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Mol	Chain	Res	Type
10	A	104	ASN
10	A	175	GLN
10	A	188	GLN
10	A	202	GLN
11	C	41	ASN
11	C	101	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

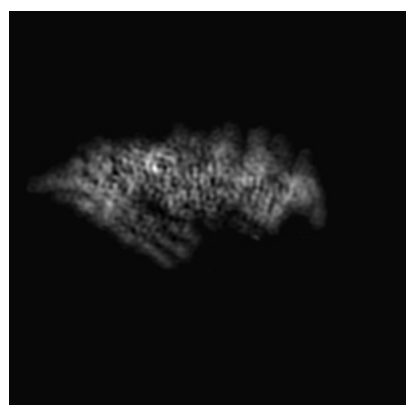
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6534. These allow visual inspection of the internal detail of the map and identification of artifacts.

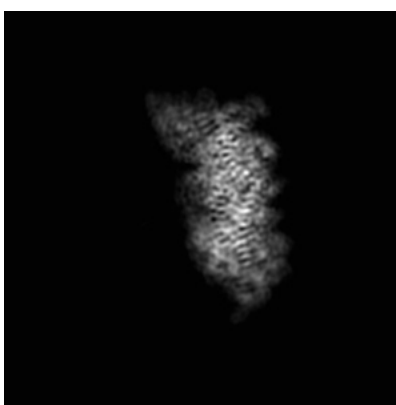
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

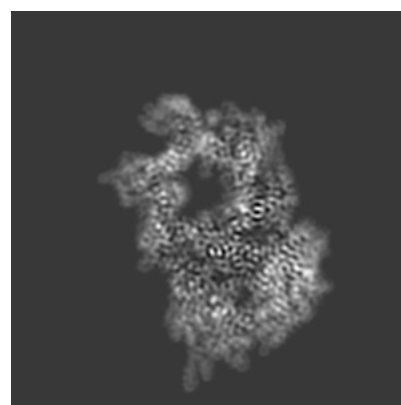
6.1.1 Primary map



X



Y

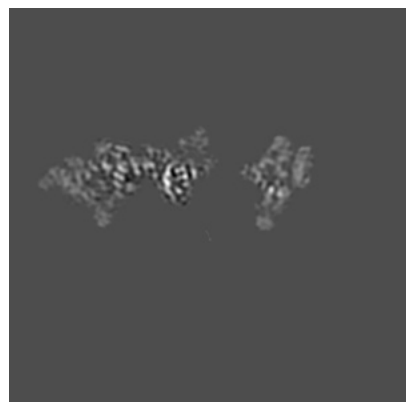


Z

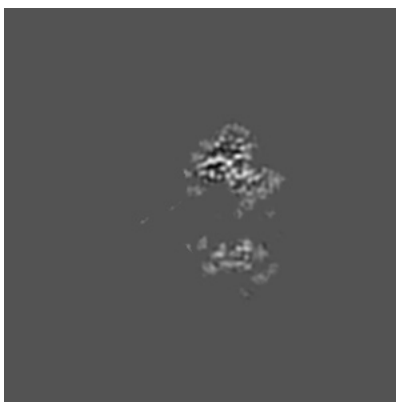
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

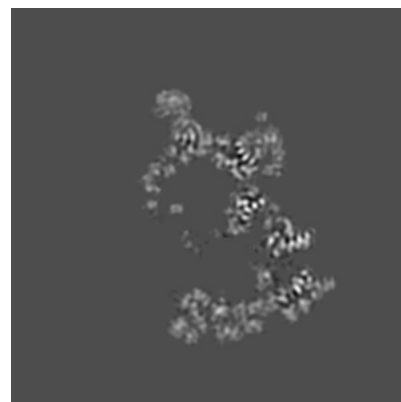
6.2.1 Primary map



X Index: 128



Y Index: 128

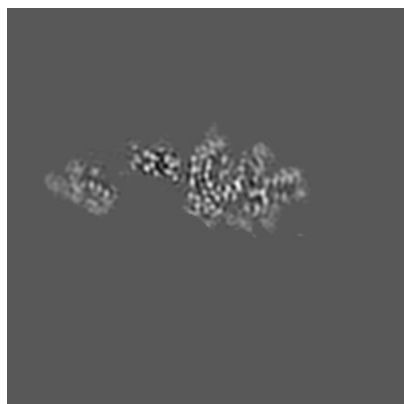


Z Index: 128

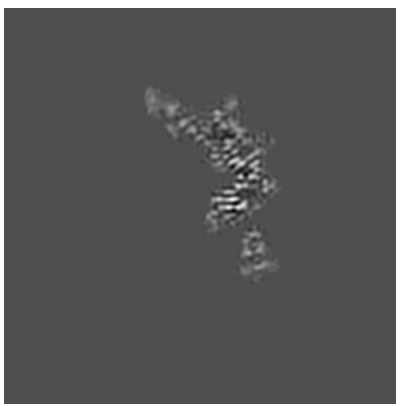
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

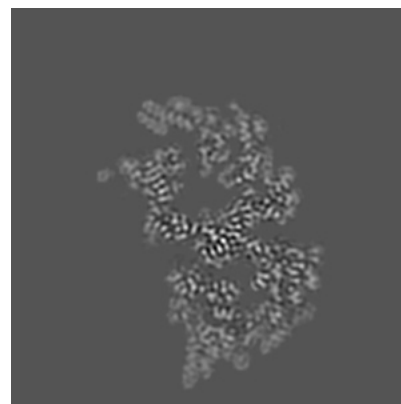
6.3.1 Primary map



X Index: 149



Y Index: 101

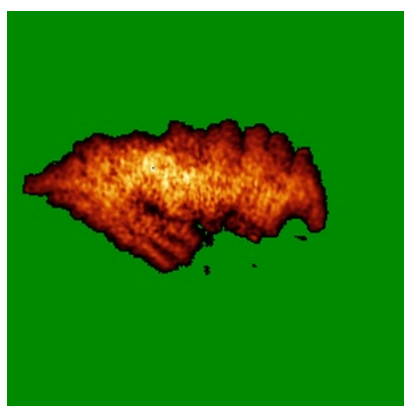


Z Index: 147

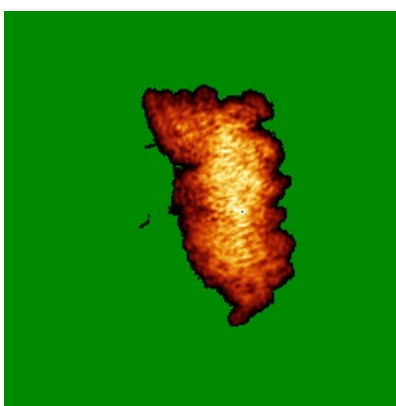
The images above show the largest variance slices of the map in three orthogonal directions.

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

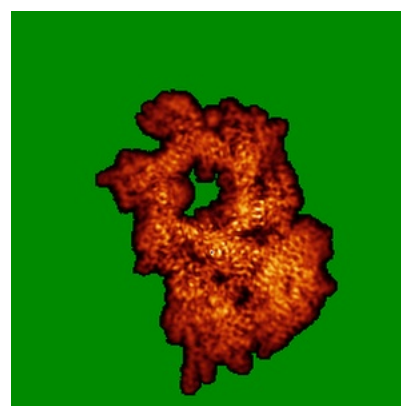
6.4.1 Primary map



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

This section was not generated.

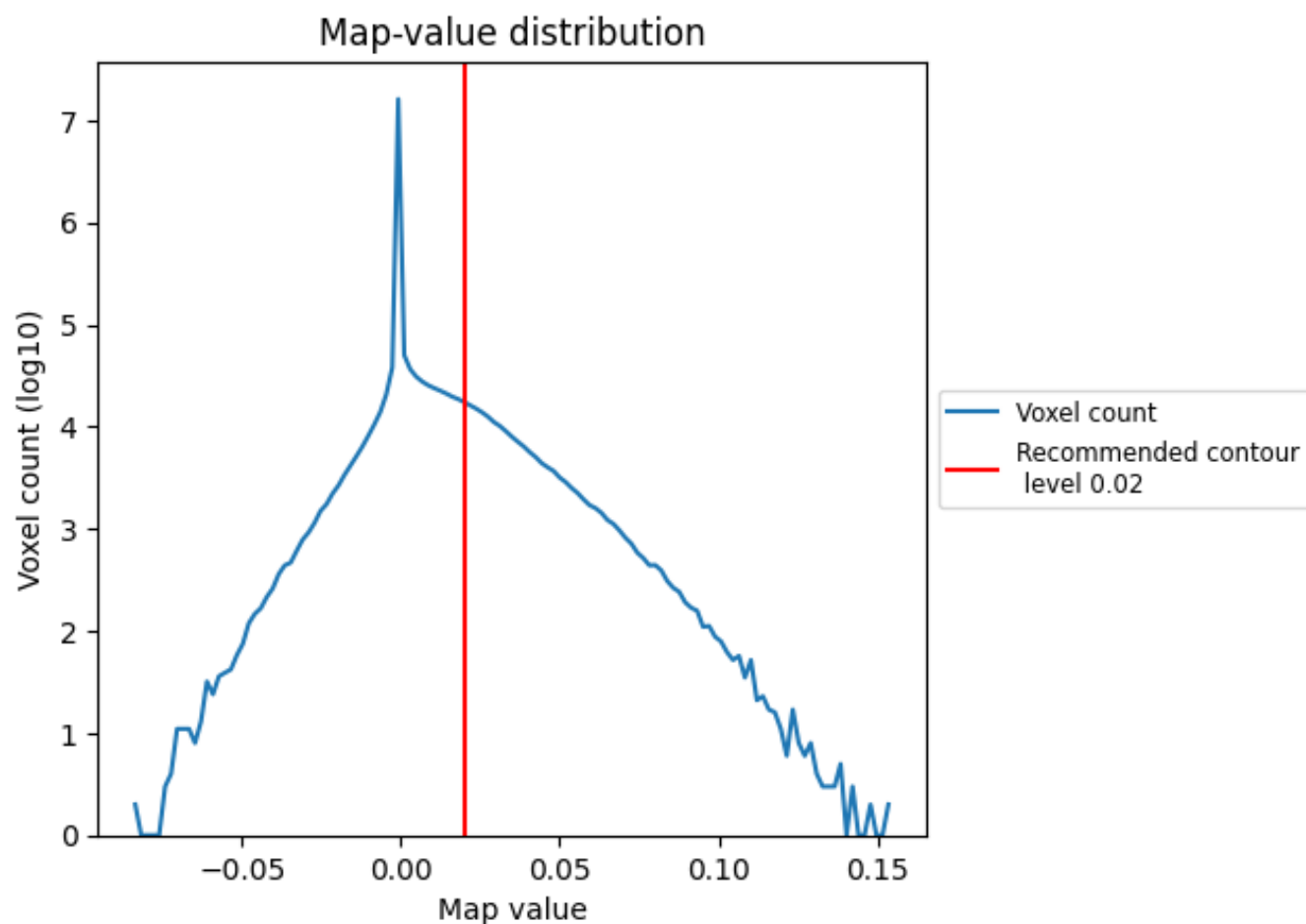
6.6 Mask visualisation

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

7 Map analysis [i](#)

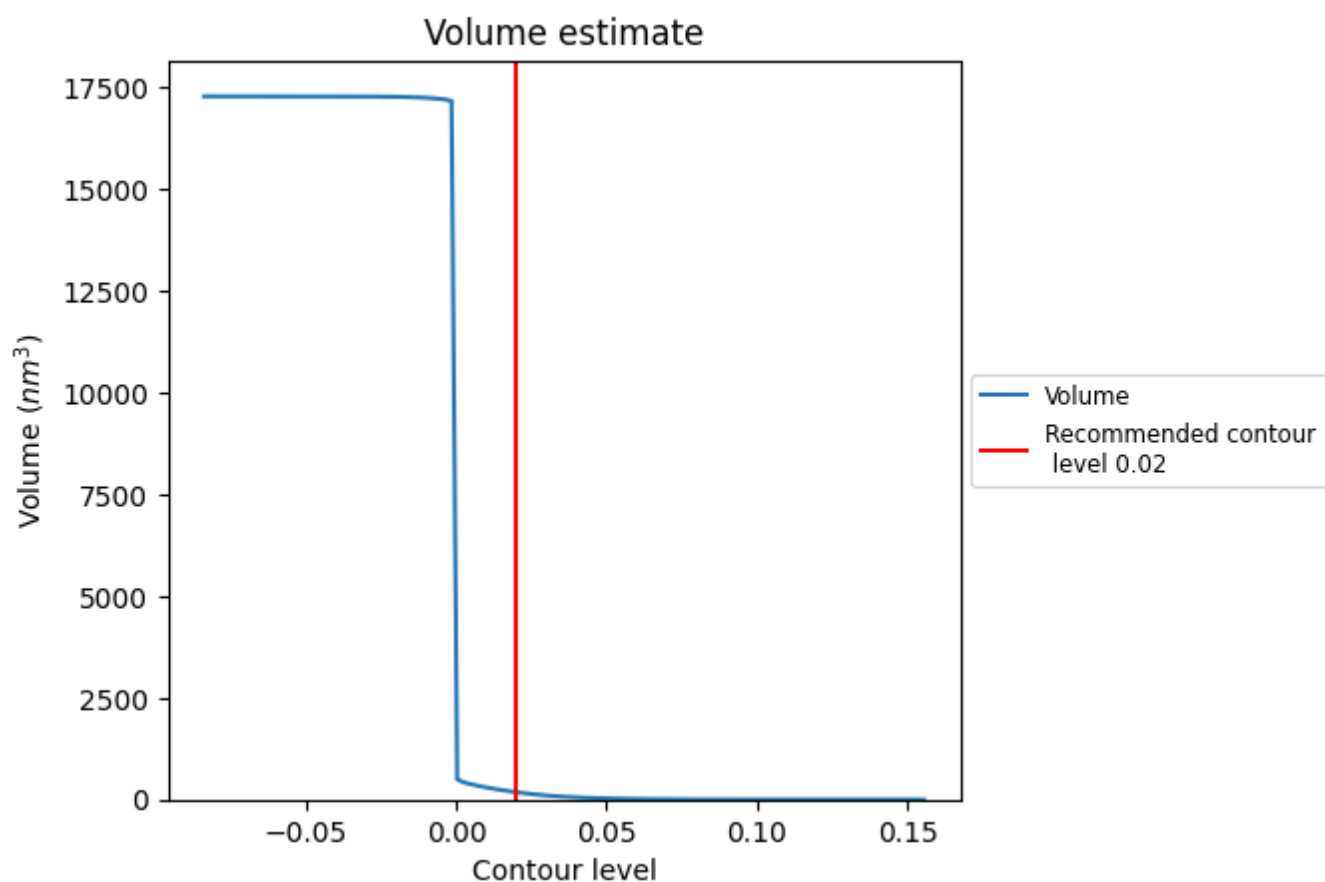
This section contains the results of statistical analysis of the map.

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.

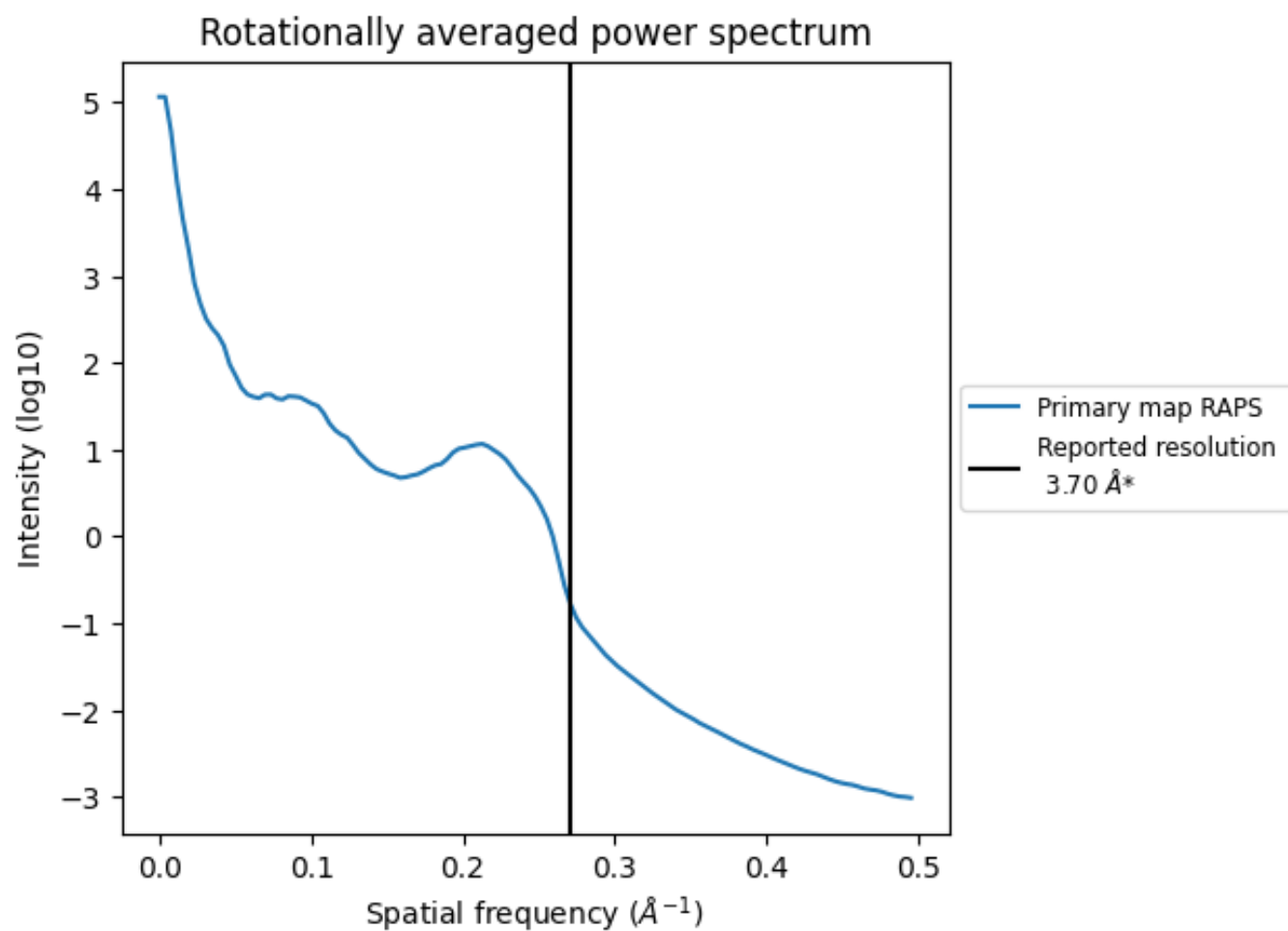
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 181 nm³; this corresponds to an approximate mass of 164 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 0.270 Å⁻¹

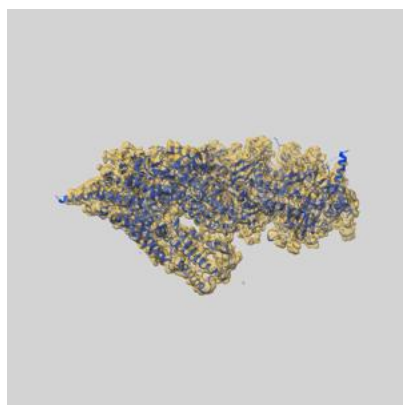
8 Fourier-Shell correlation ⓘ

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

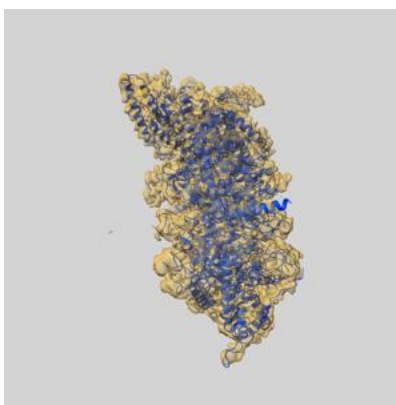
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-6534 and PDB model 3JC6. Per-residue inclusion information can be found in section [3](#) on page [7](#).

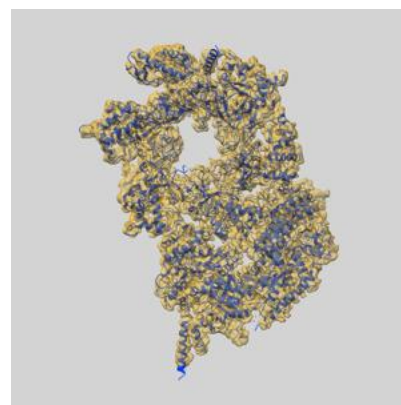
9.1 Map-model overlay [i](#)



X



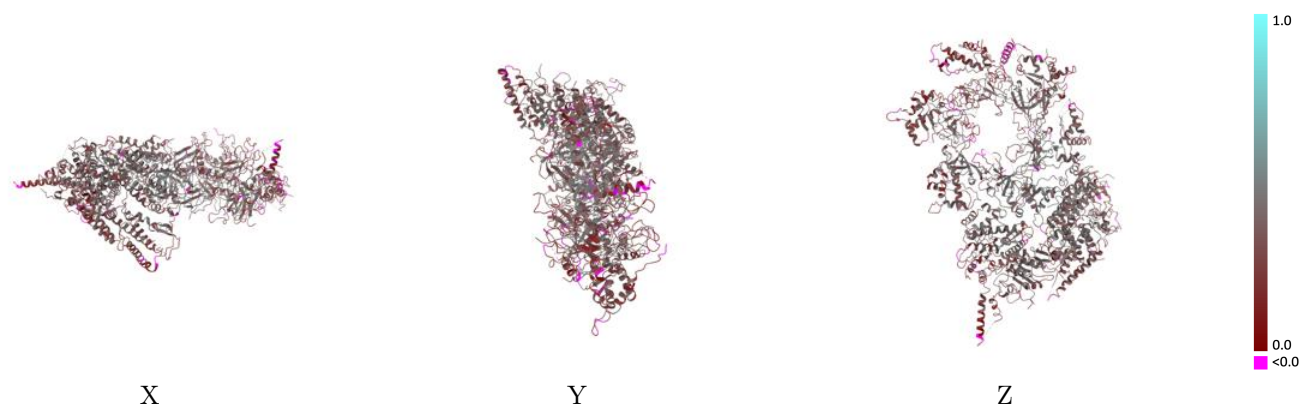
Y



Z

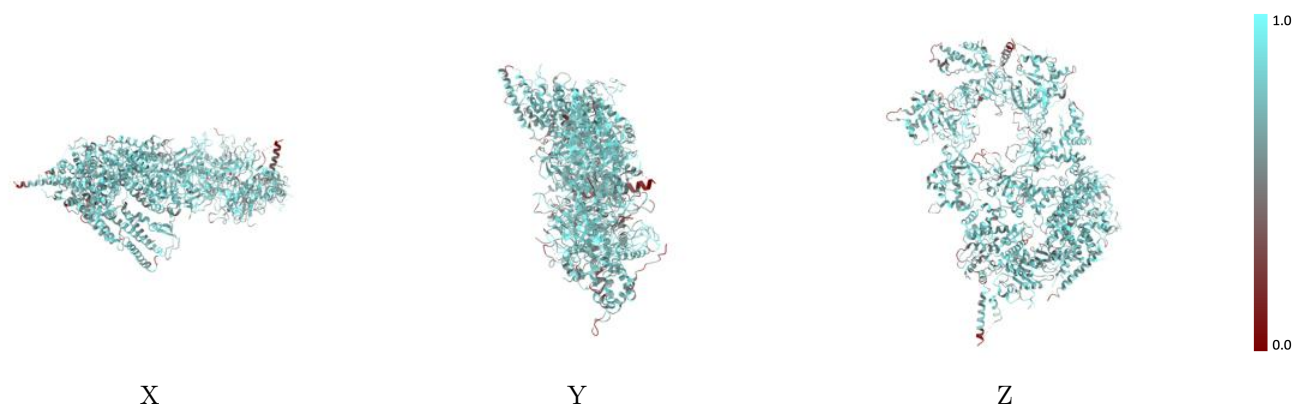
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



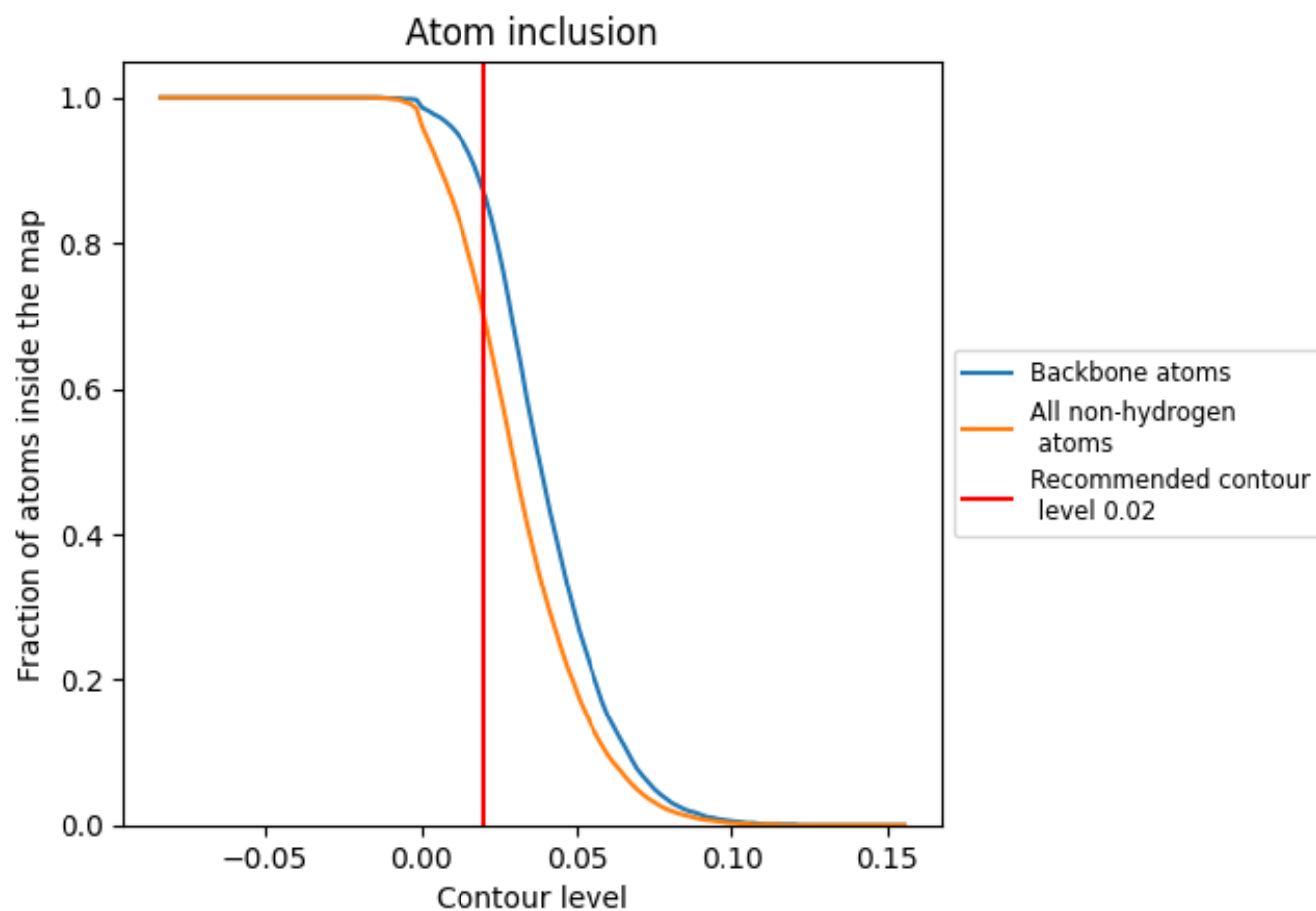
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).

9.4 Atom inclusion ⓘ



At the recommended contour level, 87% of all backbone atoms, 71% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7060	0.3290
2	0.7000	0.3380
3	0.7450	0.3680
4	0.6760	0.2630
5	0.7680	0.4160
6	0.6790	0.2950
7	0.6520	0.2910
A	0.6490	0.2820
B	0.7470	0.3740
C	0.7680	0.3830
D	0.7240	0.3260
E	0.7000	0.3270

1.0

0.0

<0.0