Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 03:34 PM EST

PDB ID	:	3JC6
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:

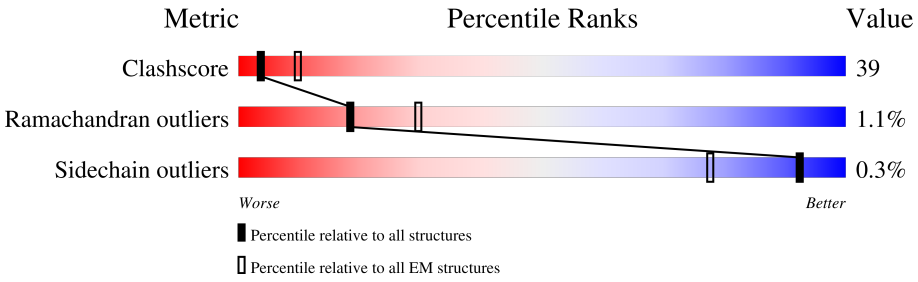
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 <=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% 12% 72%
2	3	971	14% 13% 72%
3	4	933	14% 15% 71%
4	5	775	16% 17% 67%
5	6	1017	14% 12% 74%
6	7	845	5% 20% 18% 62%
7	E	672	8% 43% 38% 18%
8	D	294	36% 37% 25%

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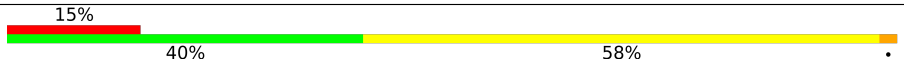
Mol	Chain	Length	Quality of chain
9	B	213	
10	A	208	
11	C	194	

2 Entry composition (i)

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
			Total	C	N	O	S		
1	2	241	1911	1214	338	354	5	0	0

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

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

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

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

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

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

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

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

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

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

- 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 (three-letter code: ZN) (formula: Zn).

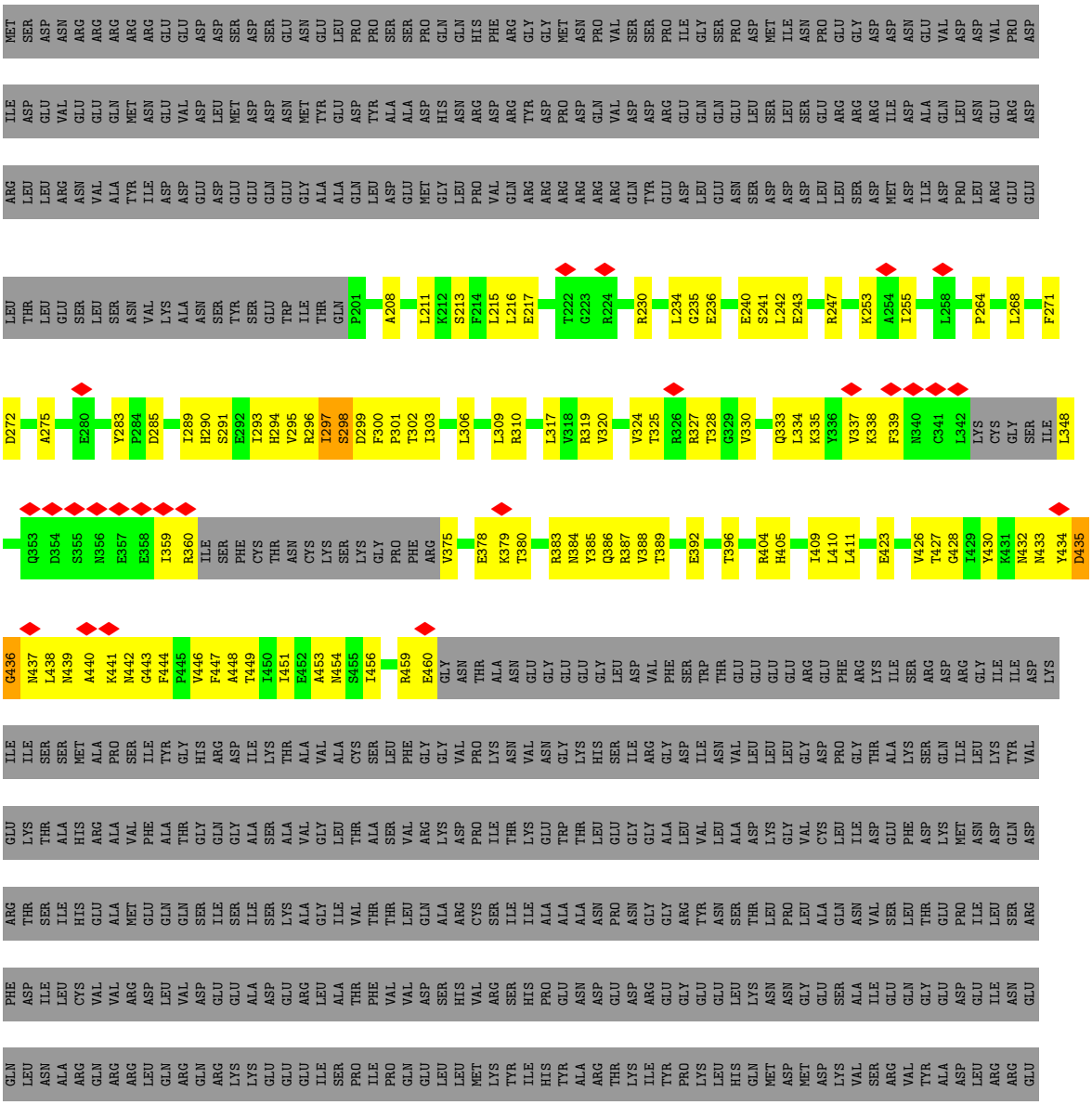
Mol	Chain	Residues	Atoms		AltConf
12	7	1	Total	Zn	0
			1	1	

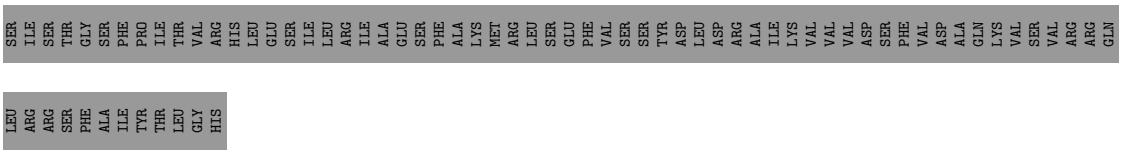
3 Residue-property plots (i)

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

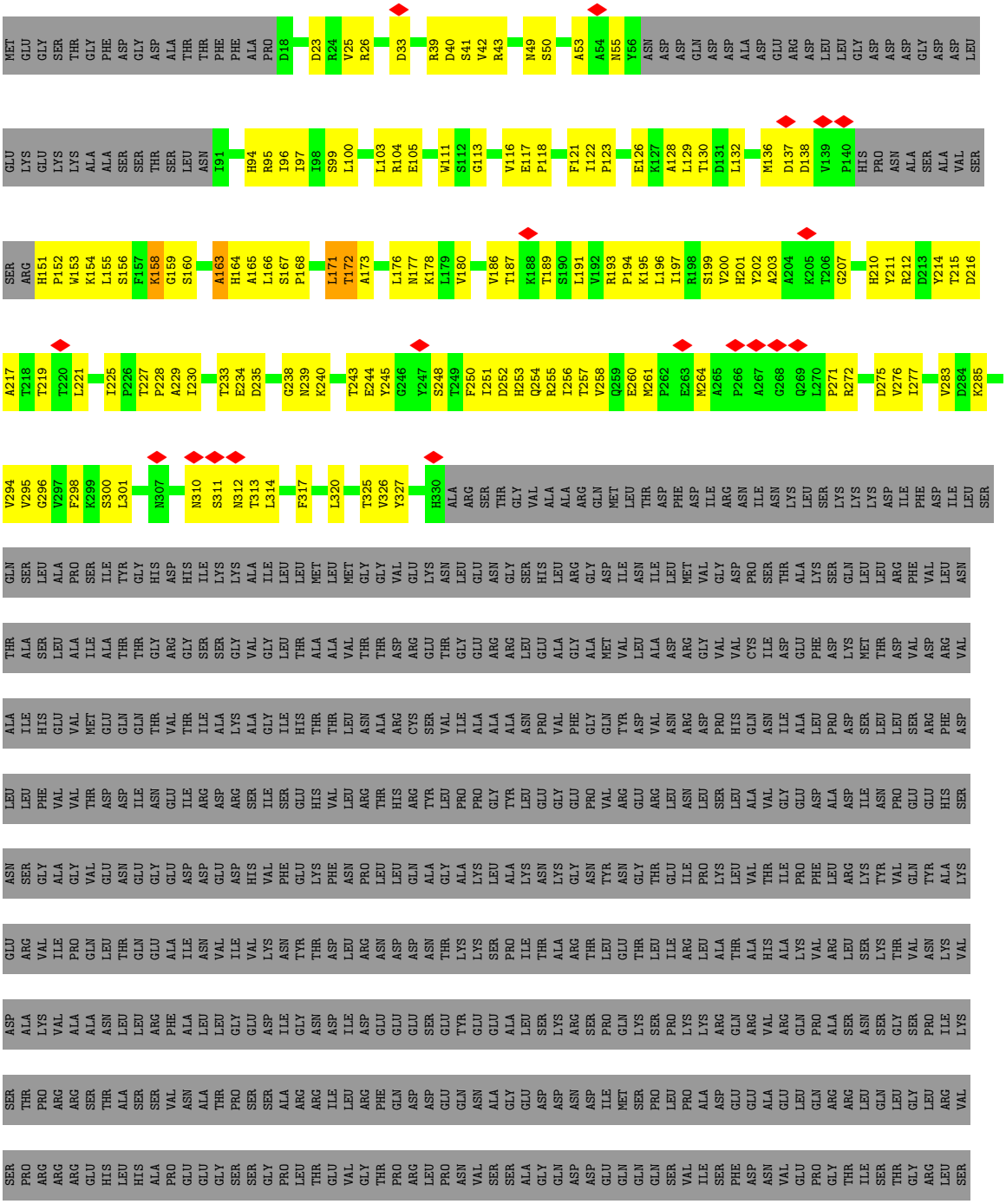
Chain 2:

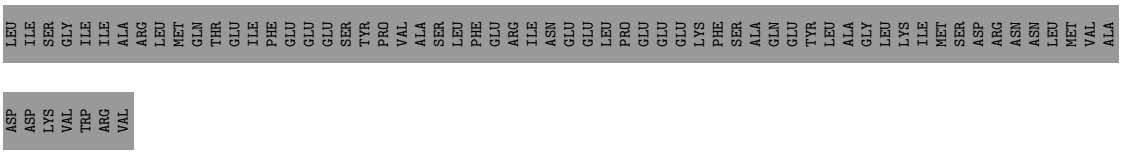




• Molecule 2: DNA replication licensing factor MCM3

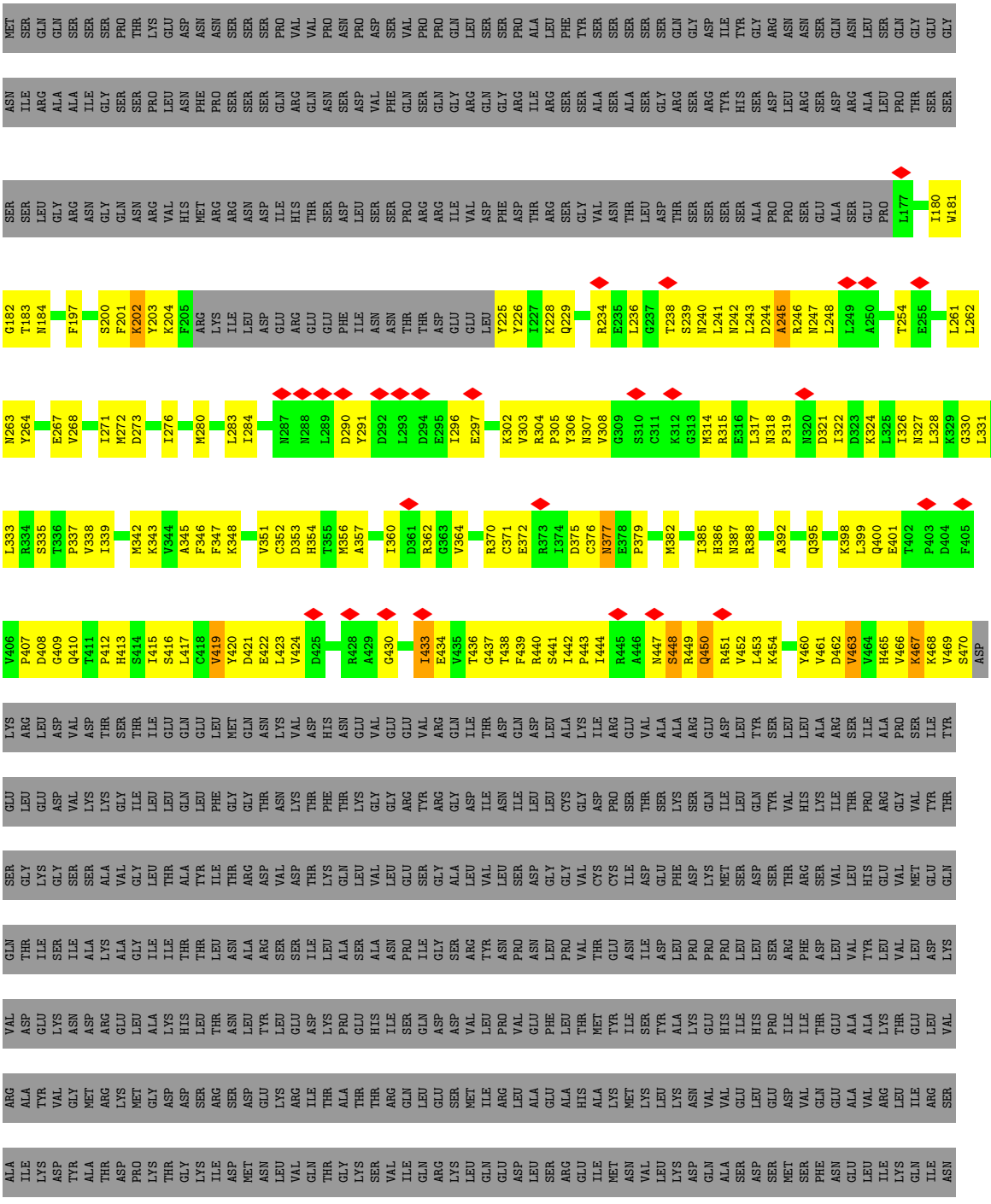
Chain 3:

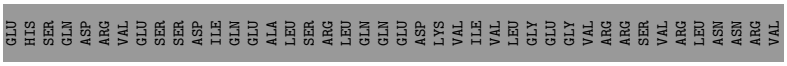




• Molecule 3: DNA replication licensing factor MCM4

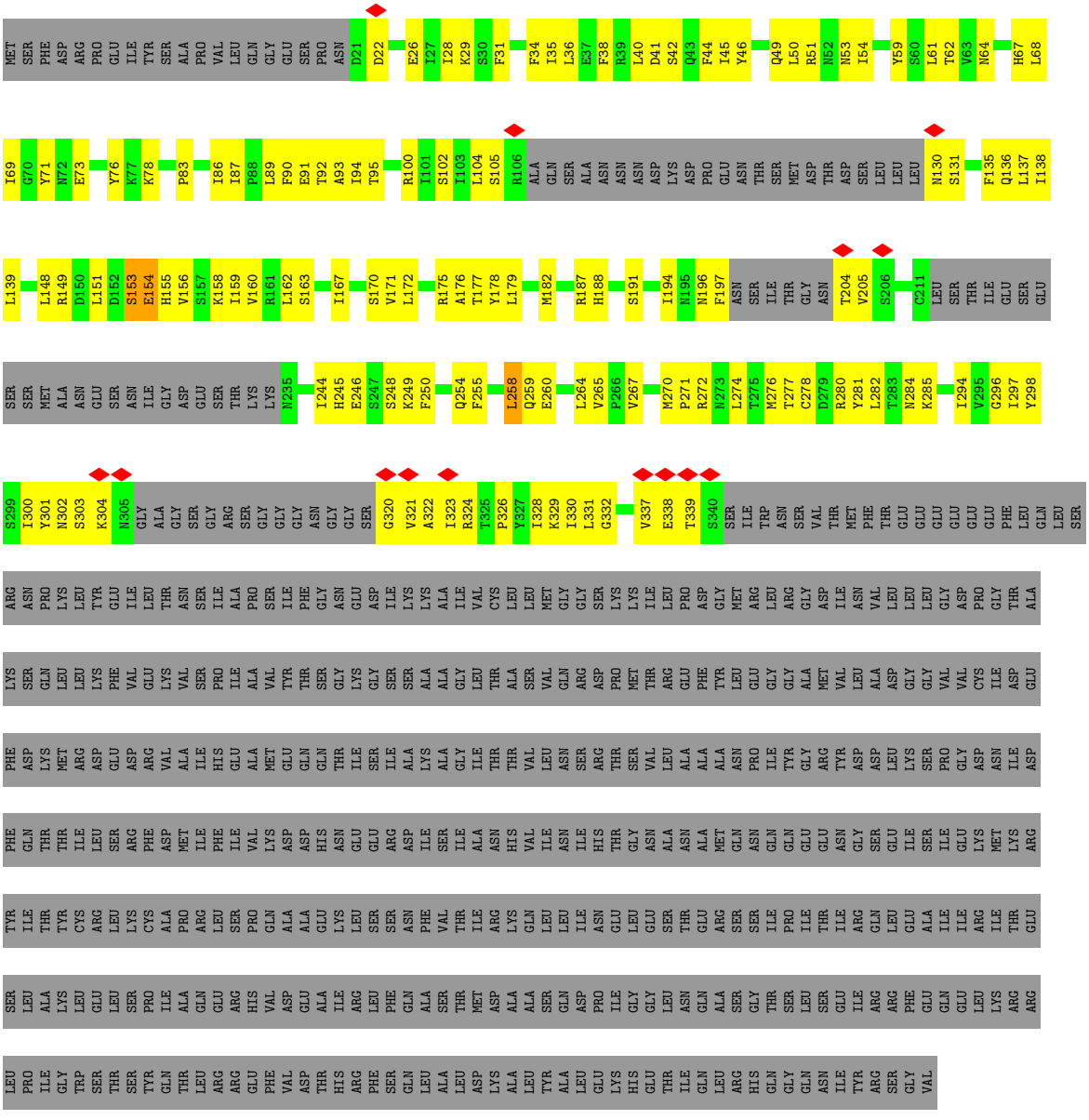
Chain 4:





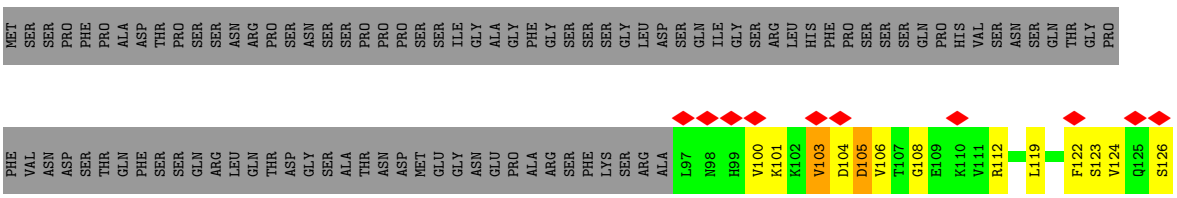
• Molecule 4: Minichromosome maintenance protein 5

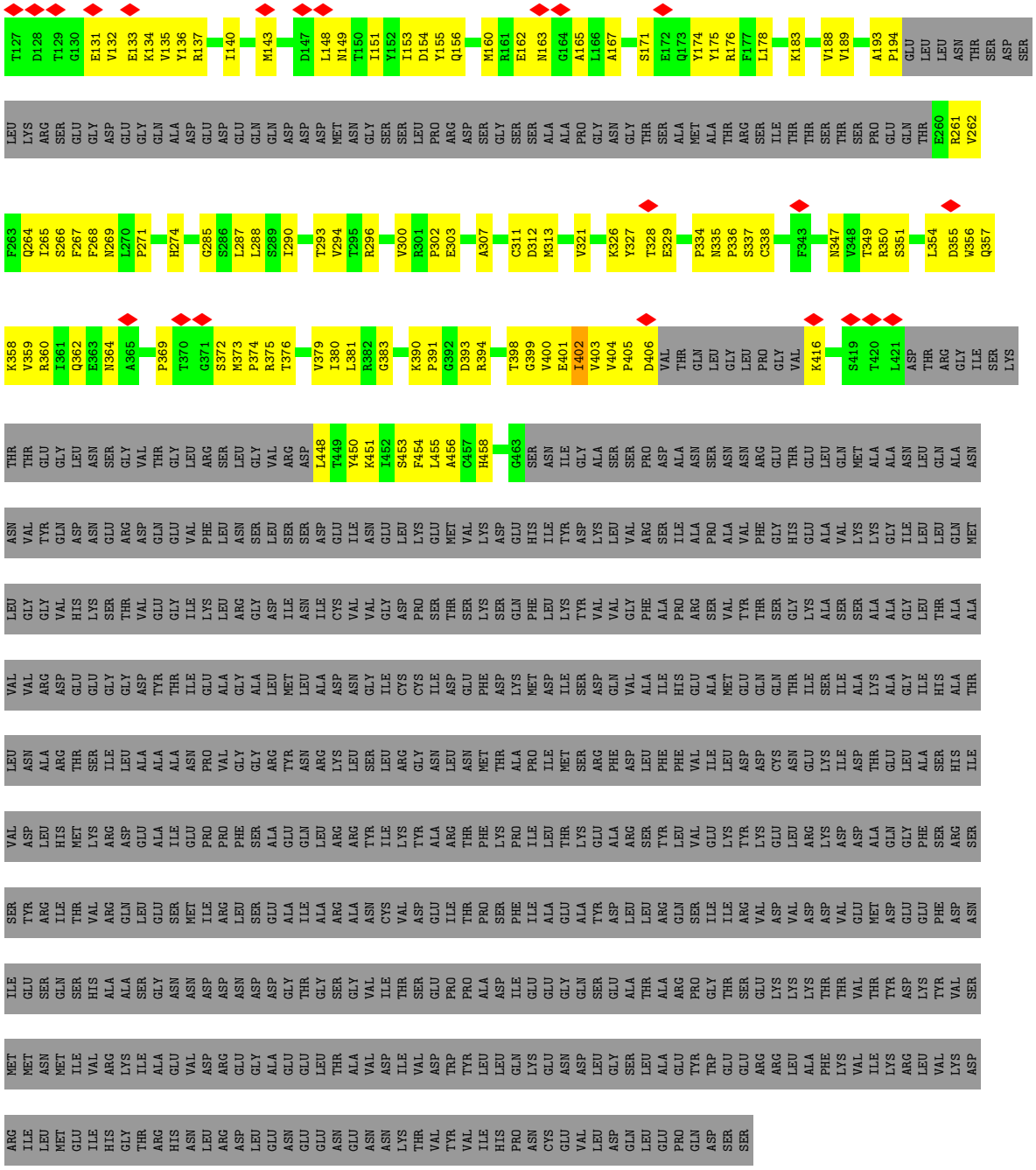
Chain 5:



• Molecule 5: DNA replication licensing factor MCM6

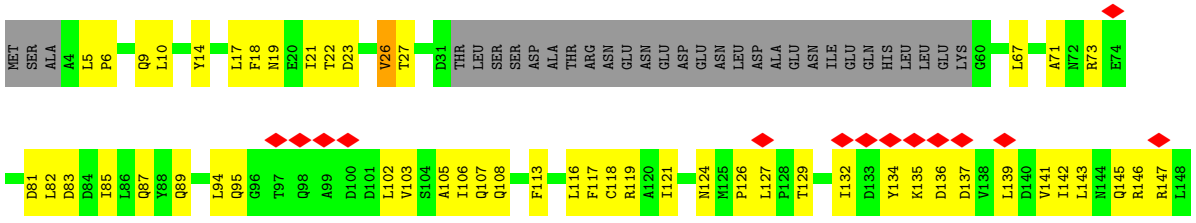
Chain 6:

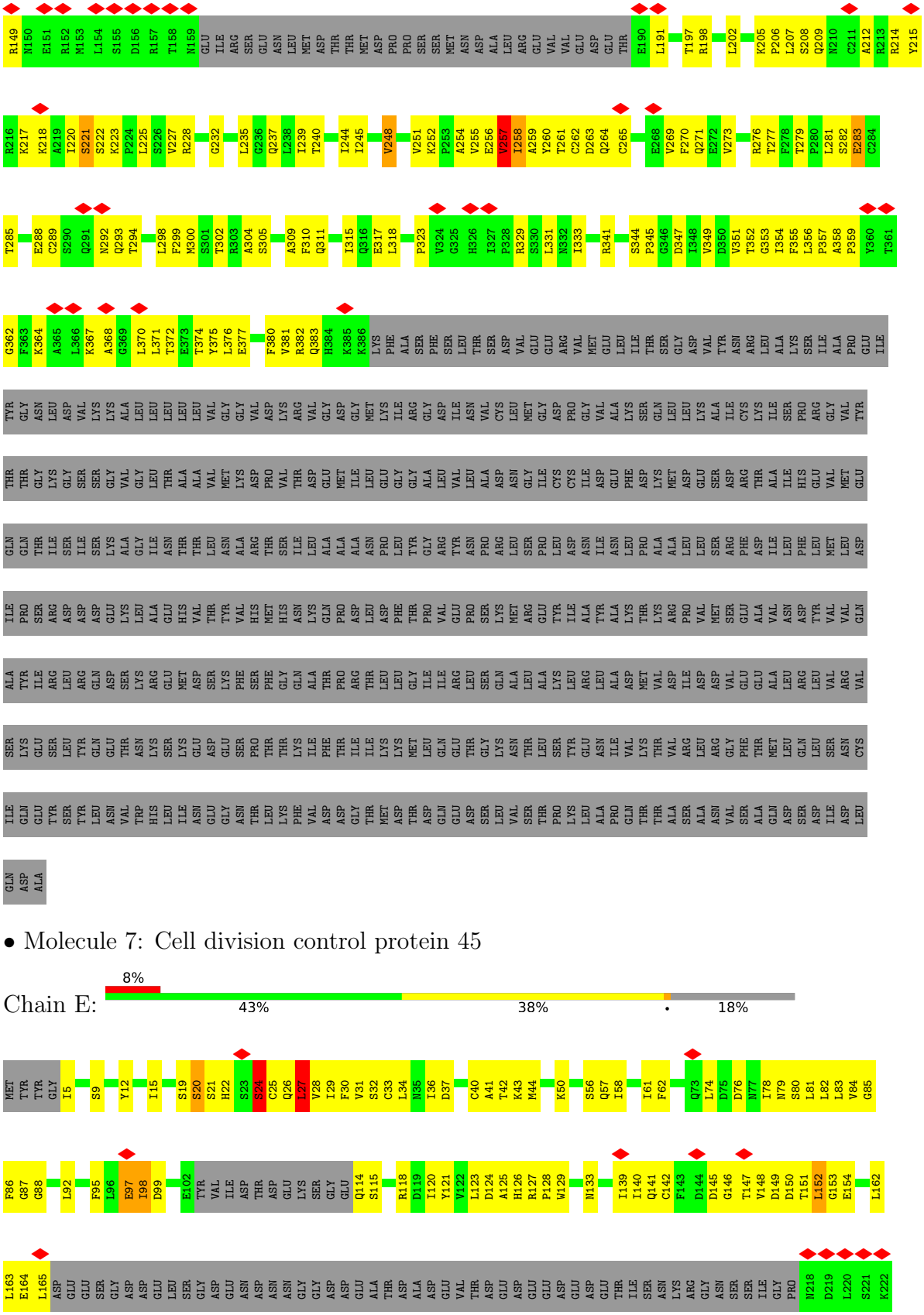




• Molecule 6: DNA replication licensing factor MCM7

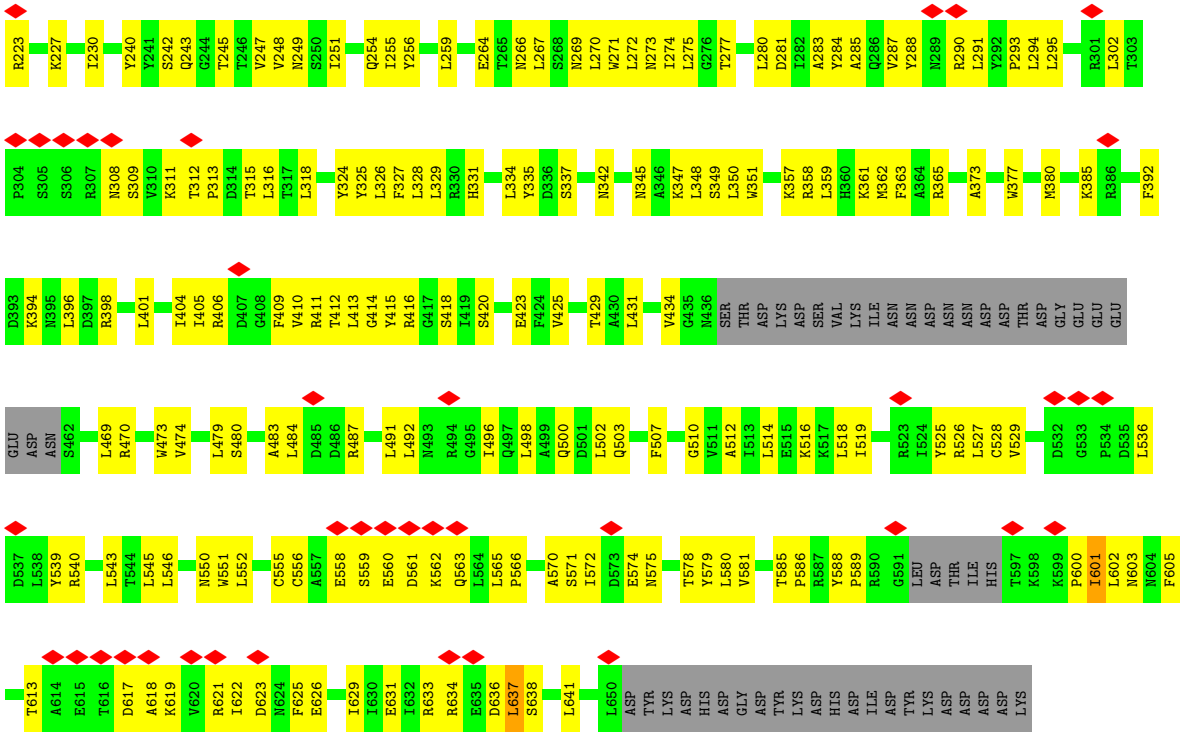
Chain 7:





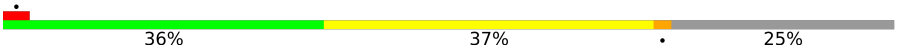
• Molecule 7: Cell division control protein 45

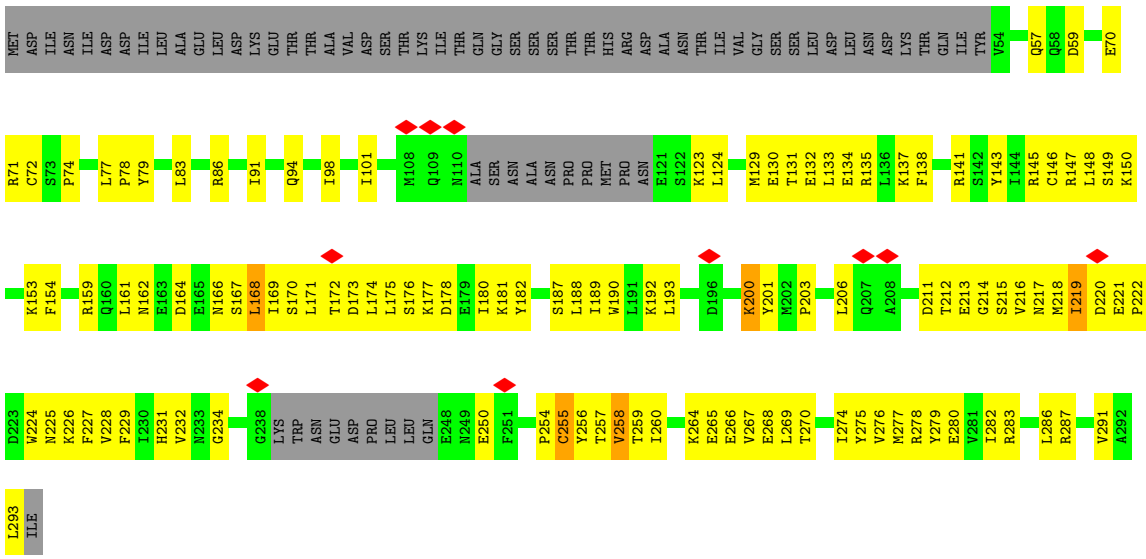
Chain E:



• Molecule 8: DNA replication complex GINS protein SLD5

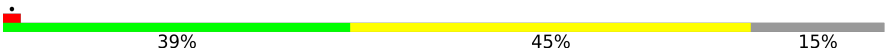
Chain D:

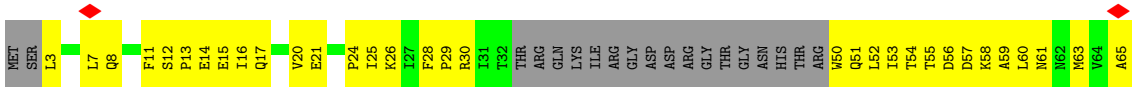


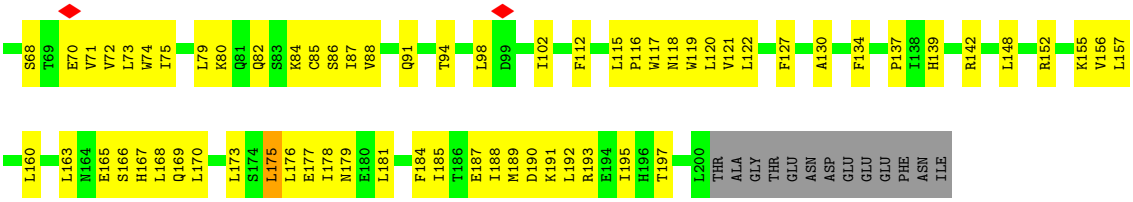


• Molecule 9: DNA replication complex GINS protein PSF2

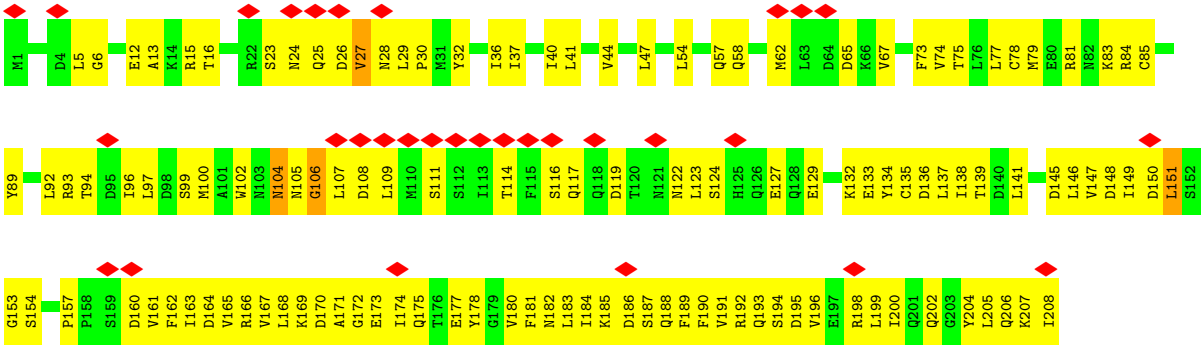
Chain B:



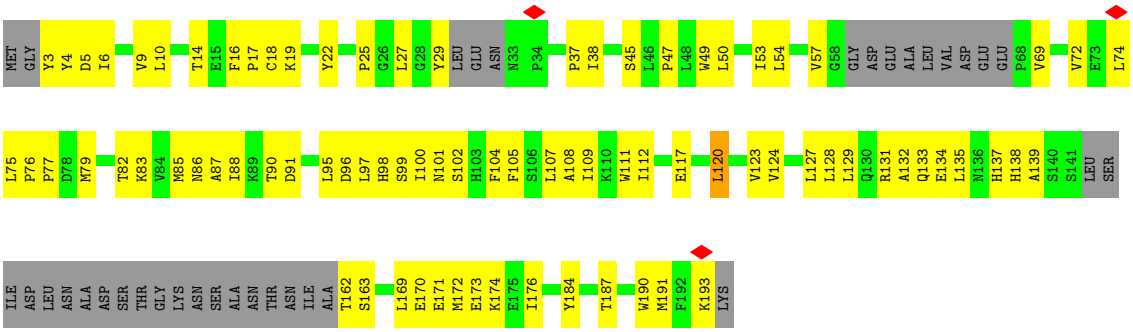




• Molecule 10: DNA replication complex GINS protein PSF1



• Molecule 11: DNA replication complex GINS protein PSF3



4 Experimental information (i)

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 ($e^-/Å^2$)	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 (Å)	258.56, 258.56, 258.56	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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	0.41	0/1946	0.66	1/2633 (0.0%)
2	3	0.46	0/2179	0.70	1/2963 (0.0%)
3	4	0.38	0/2240	0.67	0/3029
4	5	0.50	0/2057	0.73	2/2781 (0.1%)
5	6	0.39	0/2081	0.66	1/2813 (0.0%)
6	7	0.41	0/2657	0.66	1/3592 (0.0%)
7	E	0.39	0/4563	0.63	2/6173 (0.0%)
8	D	0.43	0/1853	0.64	0/2500
9	B	0.44	0/1545	0.69	0/2092
10	A	0.39	0/1718	0.65	0/2314
11	C	0.46	0/1320	0.64	1/1784 (0.1%)
All	All	0.42	0/24159	0.66	9/32674 (0.0%)

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

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	E	27	LEU	CA-CB-CG	7.97	133.63	115.30
4	5	258	LEU	CA-CB-CG	7.60	132.78	115.30
2	3	171	LEU	CA-CB-CG	7.21	131.88	115.30
5	6	105	ASP	CB-CG-OD1	6.55	124.20	118.30
1	2	436	GLY	N-CA-C	5.96	128.01	113.10
11	C	120	LEU	CA-CB-CG	5.77	128.58	115.30
6	7	127	LEU	CA-CB-CG	5.51	127.98	115.30
7	E	637	LEU	CA-CB-CG	5.47	127.88	115.30
4	5	179	LEU	CA-CB-CG	5.08	126.97	115.30

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
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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	1911	0	1908	126	0
2	3	2130	0	2105	172	0
3	4	2203	0	2188	198	0
4	5	2028	0	2055	177	0
5	6	2049	0	1959	132	0
6	7	2611	0	2623	165	0
7	E	4482	0	4497	322	0
8	D	1820	0	1823	214	0
9	B	1513	0	1558	150	0
10	A	1696	0	1698	310	0
11	C	1288	0	1298	104	0
12	7	1	0	0	0	0
All	All	23732	0	23712	1852	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 39.

All (1852) 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
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:HG22	1.07	1.41
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
9:B:187:GLU:CD	11:C:176:ILE:CG2	1.94	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
4:5:276:MET:HE1	4:5:294:ILE:CD1	1.82	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:5:276:MET:HE1	4:5:294:ILE:HD12	1.36	1.03
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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
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
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
3:4:433:ILE:CD1	3:4:469:VAL:C	2.37	0.92
3:4:467:LYS:HG3	3:4:468:LYS:HB2	1.51	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
9:B:191:LYS:HE2	11:C:172:MET:HE3	1.51	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
8:D:141:ARG:HH22	10:A:147:VAL:HG12	1.32	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
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
8:D:137:LYS:C	8:D:141:ARG:HH11	1.76	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
7:E:74:LEU:HD21	10:A:173:GLU:CD	1.95	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
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: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
1:2:410:LEU:C	1:2:411:LEU:HD12	1.96	0.85
8:D:162:ASN:HA	8:D:169:ILE:HD12	1.56	0.85
3:4:433:ILE:HD13	3:4:468:LYS:C	1.95	0.85
9:B:187:GLU:OE2	11:C:176:ILE:HG23	1.72	0.85
9:B:163:LEU:HD22	9:B:189:MET:HE1	1.57	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
7:E:316:LEU:HD11	7:E:413:LEU:C	1.97	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
4:5:259:GLN:HE21	4:5:271:PRO:HG2	1.44	0.83
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
10:A:149:ILE:HG23	10:A:150:ASP:C	2.00	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
10:A:23:SER:OG	10:A:24:ASN:C	2.21	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
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
2:3:312:ASN:C	2:3:313:THR:HG23	2.04	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:74:LEU:CD2	10:A:173:GLU:CD	2.53	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:81:LEU:HD13	7:E:81:LEU:C	2.05	0.77
10:A:147:VAL:H	10:A:148:ASP:HA	1.49	0.77
9:B:168:LEU:HD11	9:B:189:MET:HE3	1.67	0.77
3:4:284:ILE:HG13	3:4:297:GLU:OE2	1.85	0.76
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
3:4:433:ILE:HD13	3:4:469:VAL:C	2.04	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
11:C:104:PHE:H	11:C:170:GLU:CD	1.88	0.76
9:B:163:LEU:HD22	9:B:189:MET:CE	2.16	0.76
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
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
2:3:252:ASP:OD1	2:3:253:HIS:N	2.19	0.75
4:5:104:LEU:HD13	4:5:104:LEU:C	2.06	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
4:5:276:MET:CE	4:5:294:ILE:HD12	2.11	0.75
10:A:108:ASP:OD1	10:A:198:ARG:HD3	1.85	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
11:C:83:LYS:O	11:C:86:ASN:CG	2.24	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:189:ILE:HD13	10:A:133:GLU:CD	2.08	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
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
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
4:5:153:SER:OG	4:5:154:GLU:N	2.20	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
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
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
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
7:E:600:PRO:C	7:E:601:ILE:HG13	2.09	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
5:6:149:ASN:HB3	5:6:262:VAL:O	1.89	0.72
8:D:269:LEU:HD11	8:D:277:MET:HE3	1.71	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:141:ARG:HH21	10:A:148:ASP:C	1.93	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
3:4:433:ILE:CD1	3:4:468:LYS:C	2.59	0.71
7:E:81:LEU:HD13	7:E:82:LEU:CA	2.20	0.71
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
2:3:166:LEU:HD12	2:3:166:LEU:C	2.11	0.71
7:E:491:LEU:C	7:E:491:LEU:HD12	2.11	0.70
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
4:5:258:LEU:HD21	4:5:276:MET:CE	2.21	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: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
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
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
4:5:170:SER:HB3	4:5:255:PHE:HB2	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
7:E:57:GLN:CD	10:A:189:PHE:CE1	2.66	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
10:A:175:GLN:CD	10:A:199:LEU:CD1	2.62	0.68
4:5:137:LEU:HD12	4:5:137:LEU:C	2.13	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:4:330:GLY:C	3:4:399:LEU:HD11	2.15	0.67
5:6:267:PHE:HD2	5:6:287:LEU:HD21	1.59	0.67
8:D:137:LYS:HD3	8:D:141:ARG:NH2	2.07	0.67
8:D:161:LEU:C	8:D:169:ILE:HD12	2.14	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
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
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:234:GLU:OE1	2:3:238:GLY:C	2.34	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
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
8:D:211:ASP:CG	8:D:213:GLU:CB	2.65	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
10:A:67:VAL:HG11	11:C:25:PRO:HD2	1.78	0.65
10:A:175:GLN:CD	10:A:199:LEU:HD11	2.16	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
7:E:345:ASN:CG	7:E:507:PHE:HE1	2.01	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
8:D:269:LEU:HD11	8:D:277:MET:CE	2.27	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
9:B:118:ASN:CG	9:B:122:LEU:CD1	2.66	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
6:7:276: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
2:3:216:ASP:CG	2:3:217:ALA:H	2.02	0.63
6:7:269:VAL:HG21	6:7:285:THR:HB	1.80	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:163:ILE:HD11	10:A:193:GLN:CD	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
3:4:330:GLY:C	3:4:399:LEU:CD1	2.68	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
9:B:115:LEU:HD13	9:B:119:TRP:HE1	1.64	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
3:4:433:ILE:HD11	3:4:469:VAL:C	2.19	0.62
10:A:163:ILE:HD11	10:A:193:GLN:NE2	2.15	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
11:C:101:ASN:HB2	11:C:102:SER:C	2.21	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
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:34:LEU:HD13	7:E:34:LEU:C	2.18	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
6:7:23:ASP:O	6:7:27:THR:OG1	2.20	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)
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
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
5:6:143:MET:HE3	5:6:148:LEU:HB2	1.85	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
8:D:71:ARG:NH1	9:B:11:PHE:CD1	2.71	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:81:LEU:CD1	7:E:82:LEU:N	2.48	0.58
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
6:7:126:PRO:C	6:7:129:THR:HG22	2.21	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
1:2:213:SER:OG	1:2:217:GLU:OE2	2.11	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
6:7:374:THR:OG1	6:7:375:TYR:N	2.35	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
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
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
8:D:268:GLU:C	8:D:269:LEU:HD22	2.25	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:B:52:LEU:HD12	9:B:53:ILE:H	1.68	0.57
9:B:191:LYS:CE	11:C:172:MET:CE	2.80	0.57
3:4:461:VAL:HG12	3:4:463:VAL:H	1.70	0.57
6:7:136:ASP:CG	6:7:137:ASP:N	2.57	0.57
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:81:LEU:C	7:E:81:LEU:CD1	2.71	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
2:3:234:GLU:OE1	2:3:239:ASN:C	2.43	0.57
3:4:243:LEU:HD23	3:4:244:ASP:C	2.25	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:191:LYS:CE	11:C:172:MET:HE3	2.30	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
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
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
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
2:3:234:GLU:CD	2:3:239:ASN:O	2.44	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
6:7:142: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:108:ASP:OD2	10:A:177:GLU:CD	2.44	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
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
1:2:442:ASN:CG	1:2:444:PHE:H	2.09	0.55
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
4:5:104:LEU:C	4:5:104:LEU:CD1	2.74	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
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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:216:VAL:HG12	8:D:217:ASN:HA	1.89	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
3:4:333:LEU:HD12	3:4:398:LYS:HZ2	1.73	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:211:ASP:CG	8:D:213:GLU:HB3	2.20	0.53
8:D:225:ASN:OD1	8:D:278:ARG:HD3	2.08	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
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: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
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
6:7:136:ASP:CG	6:7:137:ASP:H	2.12	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
9:B:118:ASN:CG	9:B:122:LEU:HD11	2.29	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
1:2:438:LEU:C	1:2:440:ALA:H	2.12	0.53
3:4:239:SER:OG	3:4:240:ASN:N	2.40	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
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:206:LEU:HB3	10:A:83:LYS:HZ2	1.71	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:94:GLN:OE1	9:B:55:THR:HG23	2.09	0.52
9:B:187:GLU:CD	11:C:176:ILE:HG21	2.19	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
5:6:369:PRO:C	5:6:372:SER:HG	2.13	0.52
7:E:124:ASP:OD1	7:E:126:HIS:ND1	2.42	0.52
8:D:254:PRO:C	8:D:255:CYS:SG	2.88	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
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
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:74:LEU:HD22	10:A:173:GLU:CD	2.30	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
2:3:171:LEU:C	2:3:172:THR:HG22	2.30	0.52
2:3:225:ILE:HD11	4:5:182:MET:HE1	1.91	0.52
5:6:174:TYR:HB3	5:6:285:GLY:O	2.10	0.52
6:7:207:LEU:O	6:7:222:SER:OG	2.22	0.52
7:E:5:ILE:HG12	7:E:142:CYS:SG	2.50	0.52
10:A:30:PRO:O	10:A:122:ASN:ND2	2.43	0.52
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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
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
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:137:LYS:C	8:D:141:ARG:NH1	2.32	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
9:B:187:GLU:OE1	11:C:176:ILE:CG2	2.40	0.51
1:2:236:GLU:OE1	7:E:357:LYS:HB3	2.11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
3:4:449:ARG:C	3:4:451:ARG:H	2.14	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
9:B:191:LYS:CD	11:C:172:MET:HE1	2.42	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
6:7:371:LEU:O	6:7:371:LEU:HG	2.11	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
10:A:173:GLU:HB3	10:A:182:ASN:C	2.31	0.50
6:7:362:GLY:HA3	6:7:364:LYS:NZ	2.27	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
6:7:298:LEU:HD12	6:7:298:LEU:C	2.32	0.50
10:A:23:SER:OG	10:A:24:ASN:CA	2.59	0.50
10:A:108:ASP:CG	10:A:198:ARG:HD3	2.31	0.50
10:A:134:TYR:O	10:A:137:LEU:HB3	2.12	0.50
3:4:342:MET:C	3:4:360:ILE:HD12	2.32	0.50
4:5:34:PHE:HD1	4:5:71:TYR:CD2	2.30	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
10:A:167:VAL:C	10:A:168:LEU:HD22	2.32	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:81:LEU:HD13	7:E:82:LEU:C	2.32	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
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
10:A:177:GLU:C	10:A:178:TYR:CD2	2.86	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:211:ASP:CG	8:D:213:GLU:HA	2.33	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
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: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
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: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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
7:E:5:ILE:N	7:E:142:CYS:HG	2.10	0.48
9:B:160:LEU:O	9:B:163:LEU:HG	2.12	0.48
10:A:175:GLN:OE1	10:A:199:LEU:CD1	2.51	0.48
10:A:178:TYR:OH	10:A:198:ARG:NE	2.47	0.48
4:5:276:MET:HE1	4:5:294:ILE:HD13	1.65	0.48
5:6:369:PRO:C	5:6:372:SER:OG	2.52	0.48
7:E:24:SER:HB2	7:E:25:CYS:CA	2.42	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
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
1:2:426:VAL:HG12	1:2:456:ILE:HD13	1.95	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
6:7:370:LEU:HD13	6:7:370:LEU:C	2.31	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
3:4:433:ILE:HG12	3:4:469:VAL:C	2.23	0.47
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
1:2:339:PHE:HZ	1:2:348:LEU:HB2	1.80	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:150:ASP:HB3	7:E:151:THR:C	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:B:53:ILE:H	9:B:53:ILE:HD12	1.80	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
8:D:189:ILE:CD1	10:A:133:GLU:CD	2.82	0.47
8:D:200:LYS:H	8:D:201:TYR:C	2.18	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
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: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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:270:THR:HG1	8:D:275:TYR:HE2	1.60	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
3:4:339:ILE:HG21	5:6:416:LYS:HZ1	1.81	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
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
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
10:A:188:GLN:HG3	10:A:188:GLN:O	2.15	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
5:6:134:LYS:N	5:6:135:VAL:HA	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
11:C:129:LEU:HD23	11:C:129:LEU:C	2.36	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
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: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
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
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
2:3:166:LEU:C	2:3:166:LEU:CD1	2.83	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
5:6:406:ASP:HB2	5:6:451:LYS:HZ2	1.81	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
6:7:67:LEU:HD11	6:7:121:ILE:HG23	1.97	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
7:E:318:LEU:C	7:E:318:LEU:HD12	2.36	0.45
7:E:377:TRP:NE1	7:E:385:LYS:NZ	2.61	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
4:5:249:LYS:C	4:5:250:PHE:HD1	2.19	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
8:D:218:MET:HA	8:D:219:ILE:C	2.36	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
2:3:166:LEU:HD11	2:3:171:LEU:HD12	1.99	0.45
2:3:216:ASP:CG	2:3:217:ALA:N	2.67	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
4:5:182:MET:HE3	4:5:187:ARG:HG3	1.99	0.45
5:6:400:VAL:CG2	5:6:455:LEU:HG	2.47	0.45
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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:491:LEU:C	7:E:491:LEU:CD1	2.82	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
10:A:175:GLN:CD	10:A:199:LEU:CD2	2.82	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
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: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
11:C:117:GLU:CD	11:C:120:LEU:HD23	2.37	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
10:A:175:GLN:CD	10:A:199:LEU:HD21	2.38	0.44
2:3:200:VAL:HB	2:3:248:SER:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
10:A:108:ASP:H	10:A:109:LEU:C	2.21	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
7:E:328:LEU:H	7:E:423:GLU:CD	2.21	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
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:OG	6:7:222:SER:O	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
8:D:130:GLU:CD	10:A:192:ARG:NH1	2.71	0.43
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:34:LEU:CD1	7:E:34:LEU:C	2.83	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
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
10:A:162:PHE:CE1	10:A:192:ARG:HB3	2.53	0.43
10:A:183:LEU:C	10:A:184:ILE:HG12	2.39	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
9:B:184:PHE:CZ	11:C:132:ALA:HB1	2.53	0.43
9:B:191:LYS:HE2	11:C:172:MET:HE1	1.94	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:154:GLU:CD	7:E:240:TYR:HB2	2.38	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
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
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
4:5:163:SER:O	4:5:163:SER:OG	2.37	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:2:442:ASN:CG	1:2:444:PHE:O	2.57	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
1:2:298:SER:OG	1:2:299:ASP:N	2.50	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: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
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
6:7:221:SER:HA	6:7:222:SER:C	2.40	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:102:TRP:NE1	10:A:134:TYR:OH	2.50	0.42
10:A:192:ARG:CD	10:A:194:SER:OG	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:441:LYS:HE3	1:2:441:LYS:HB3	1.76	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
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: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
10:A:175:GLN:CD	10:A:199:LEU:HD13	2.38	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:345:ASN:CG	7:E:507:PHE:CE1	2.87	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
10:A:185:LYS:HG3	10:A:186:ASP:CG	2.40	0.42
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
3:4:422:GLU:H	3:4:422:GLU:CD	2.23	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
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
4:5:137:LEU:C	4:5:137:LEU:CD1	2.84	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
9:B:191:LYS:CE	11:C:172:MET:HE1	2.49	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:258:VAL:CG1	8:D:260:ILE:HG13	2.50	0.41
9:B:14:GLU:C	9:B:14:GLU:CD	2.79	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
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
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
3:4:441:SER:C	3:4:442:ILE:HD12	2.41	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
6:7:135:LYS:HA	6:7:136:ASP:C	2.41	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
3:4:375:ASP:HA	3:4:376:CYS:C	2.41	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
3:4:225:TYR:HA	3:4:226:TYR:HA	1.79	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
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
5:6:167:ALA:O	5:6:171:SER:OG	2.19	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:240:TYR:C	7:E:242:SER:H	2.25	0.41
7:E:280:LEU:HD11	7:E:285:ALA:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
8:D:211:ASP:CG	8:D:213:GLU:CA	2.89	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
2:3:193:ARG:CG	6:7:371:LEU:HD11	2.51	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: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
5:6:264:GLN:CD	5:6:383:GLY:HA2	2.40	0.40
5:6:401:GLU:O	5:6:402:ILE:HG12	2.21	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
10:A:114:THR:C	10:A:116:SER:H	2.25	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:275:TYR:HE1	9:B:169:GLN:CB	2.34	0.40
10:A:153:GLY:O	10:A:154:SER:OG	2.37	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
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%)	7	38
2	3	263/971 (27%)	236 (90%)	22 (8%)	5 (2%)	8	40
3	4	271/933 (29%)	230 (85%)	36 (13%)	5 (2%)	8	41
4	5	244/775 (32%)	222 (91%)	19 (8%)	3 (1%)	13	48
5	6	259/1017 (26%)	229 (88%)	27 (10%)	3 (1%)	13	48
6	7	319/845 (38%)	270 (85%)	45 (14%)	4 (1%)	12	47
7	E	543/672 (81%)	491 (90%)	47 (9%)	5 (1%)	17	54
8	D	215/294 (73%)	197 (92%)	16 (7%)	2 (1%)	17	54
9	B	177/213 (83%)	163 (92%)	14 (8%)	0	100	100
10	A	206/208 (99%)	180 (87%)	25 (12%)	1 (0%)	29	66
11	C	151/194 (78%)	144 (95%)	7 (5%)	0	100	100
All	All	2883/6990 (41%)	2567 (89%)	283 (10%)	33 (1%)	18	50

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
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

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Mol	Chain	Res	Type
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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	2	206/770 (27%)	206 (100%)	0	100	100
2	3	236/835 (28%)	236 (100%)	0	100	100
3	4	249/848 (29%)	249 (100%)	0	100	100
4	5	241/688 (35%)	241 (100%)	0	100	100
5	6	207/886 (23%)	207 (100%)	0	100	100
6	7	295/753 (39%)	295 (100%)	0	100	100
7	E	499/607 (82%)	495 (99%)	4 (1%)	81	89
8	D	213/279 (76%)	212 (100%)	1 (0%)	88	94
9	B	171/198 (86%)	170 (99%)	1 (1%)	86	93
10	A	193/193 (100%)	192 (100%)	1 (0%)	88	94
11	C	144/173 (83%)	144 (100%)	0	100	100
All	All	2654/6230 (43%)	2647 (100%)	7 (0%)	92	96

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	E	20	SER

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Mol	Chain	Res	Type
7	E	24	SER
7	E	27	LEU
7	E	152	LEU
8	D	168	LEU
9	B	175	LEU
10	A	151	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	2	238	ASN
1	2	386	GLN
1	2	439	ASN
2	3	29	GLN
3	4	184	ASN
3	4	231	ASN
4	5	49	GLN
4	5	53	ASN
4	5	58	ASN
4	5	253	GLN
4	5	259	GLN
6	7	76	ASN
6	7	87	GLN
6	7	89	GLN
6	7	145	GLN
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	550	ASN
8	D	110	ASN
9	B	62	ASN
9	B	146	GLN
9	B	167	HIS
9	B	179	ASN
10	A	104	ASN
10	A	175	GLN
10	A	202	GLN
11	C	41	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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 (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

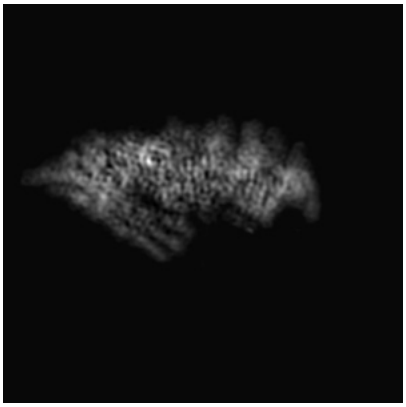
6 Map visualisation

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.

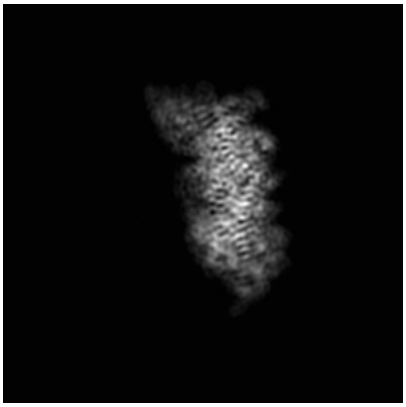
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

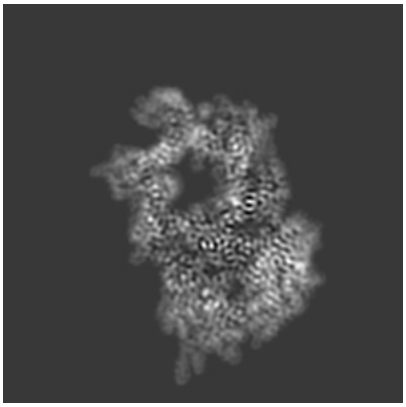
6.1.1 Primary map



X



Y

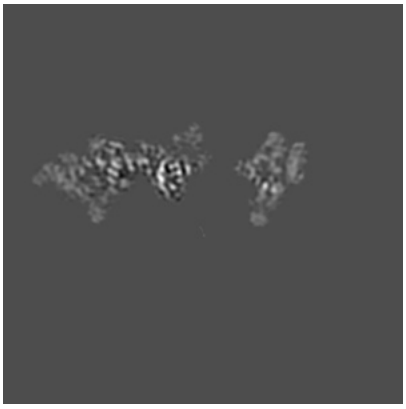


Z

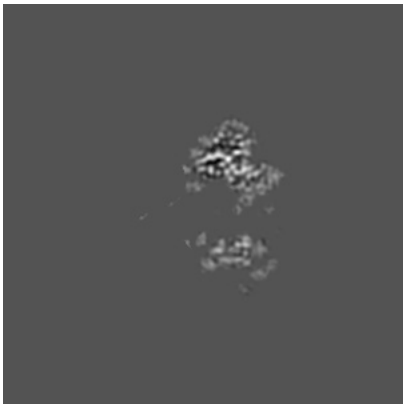
The images above show the map projected in three orthogonal directions.

6.2 Central slices

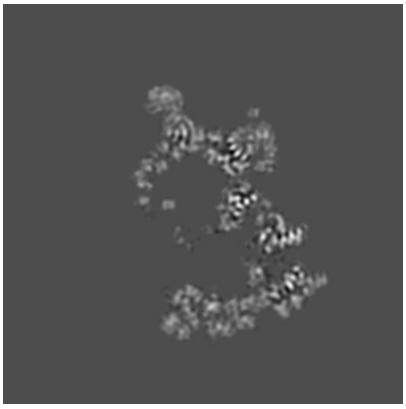
6.2.1 Primary map



X Index: 128



Y Index: 128

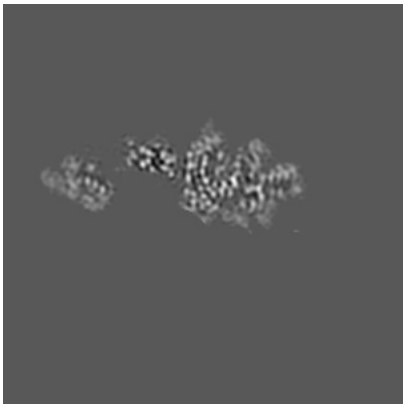


Z Index: 128

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

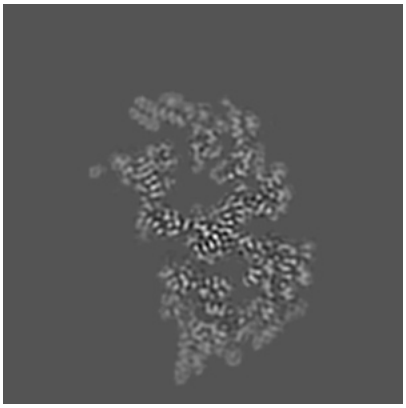
6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 149

Y Index: 101

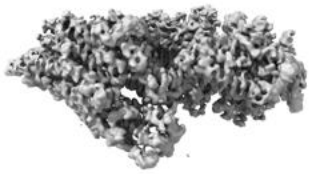


Z Index: 147

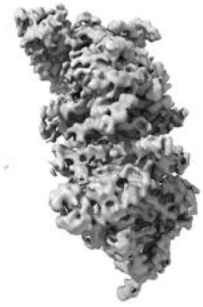
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

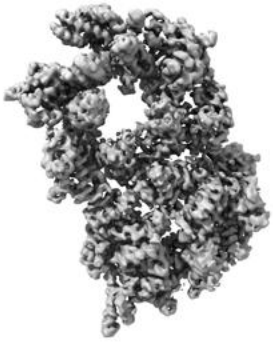
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

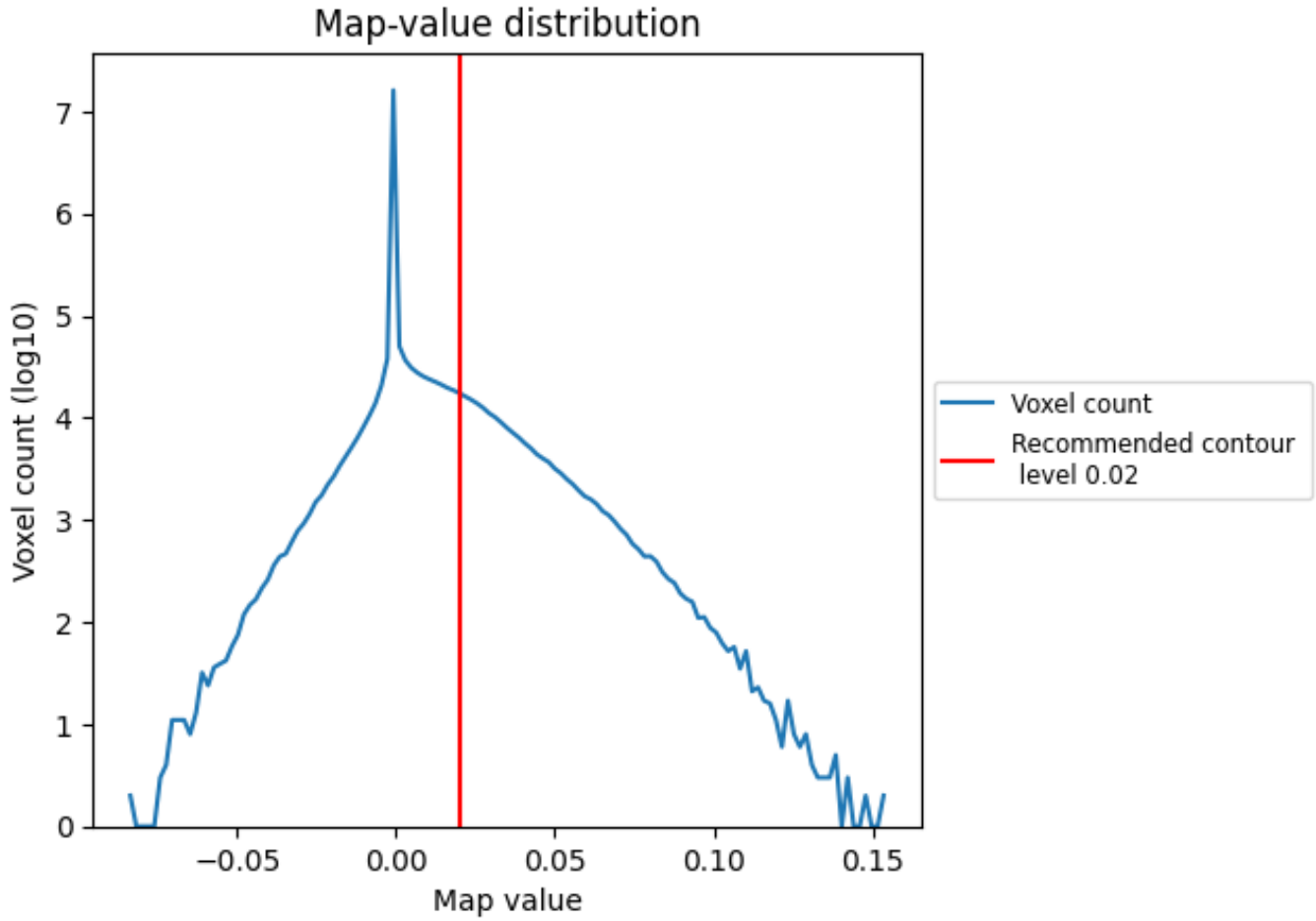
6.5 Mask visualisation (i)

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

7 Map analysis

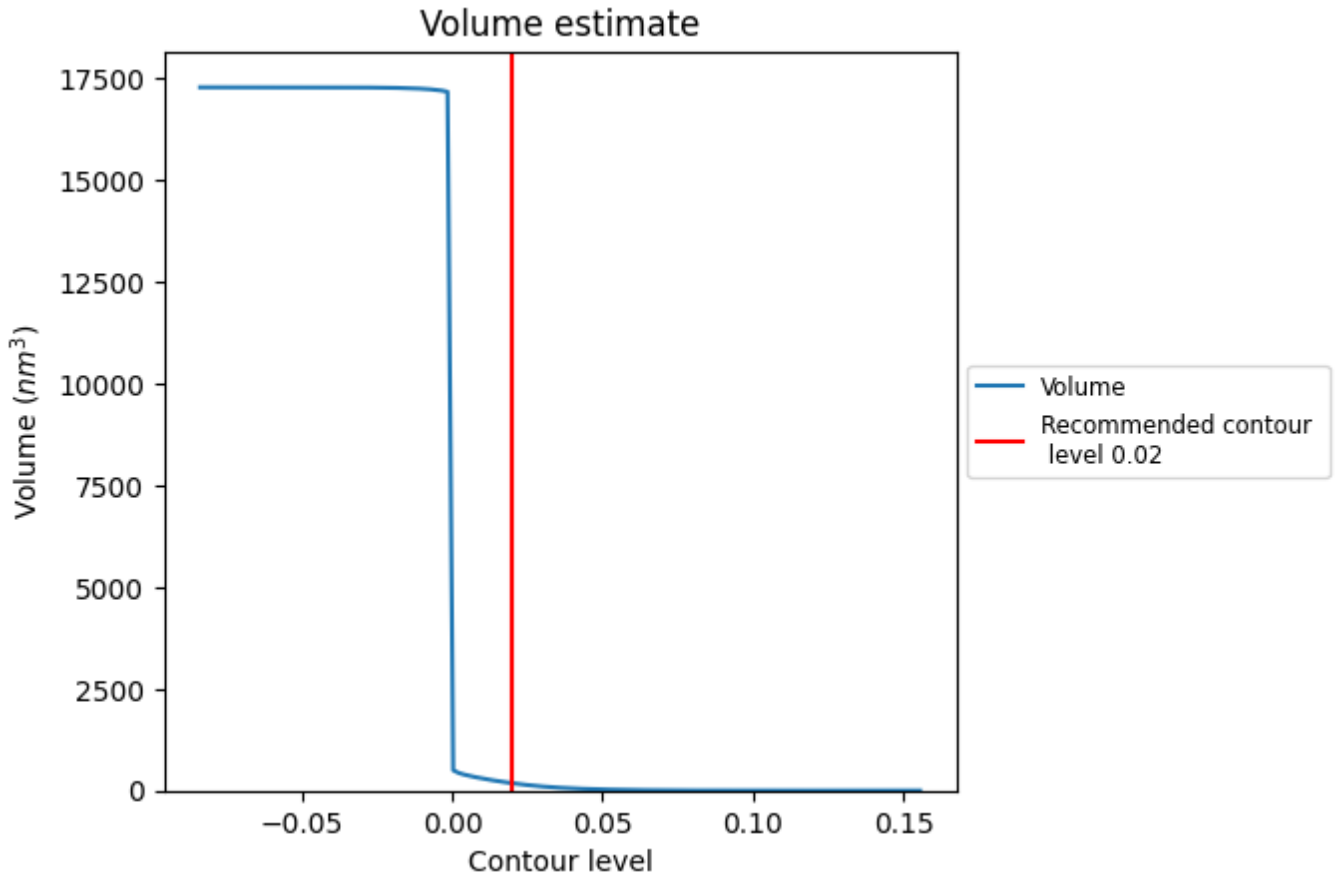
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

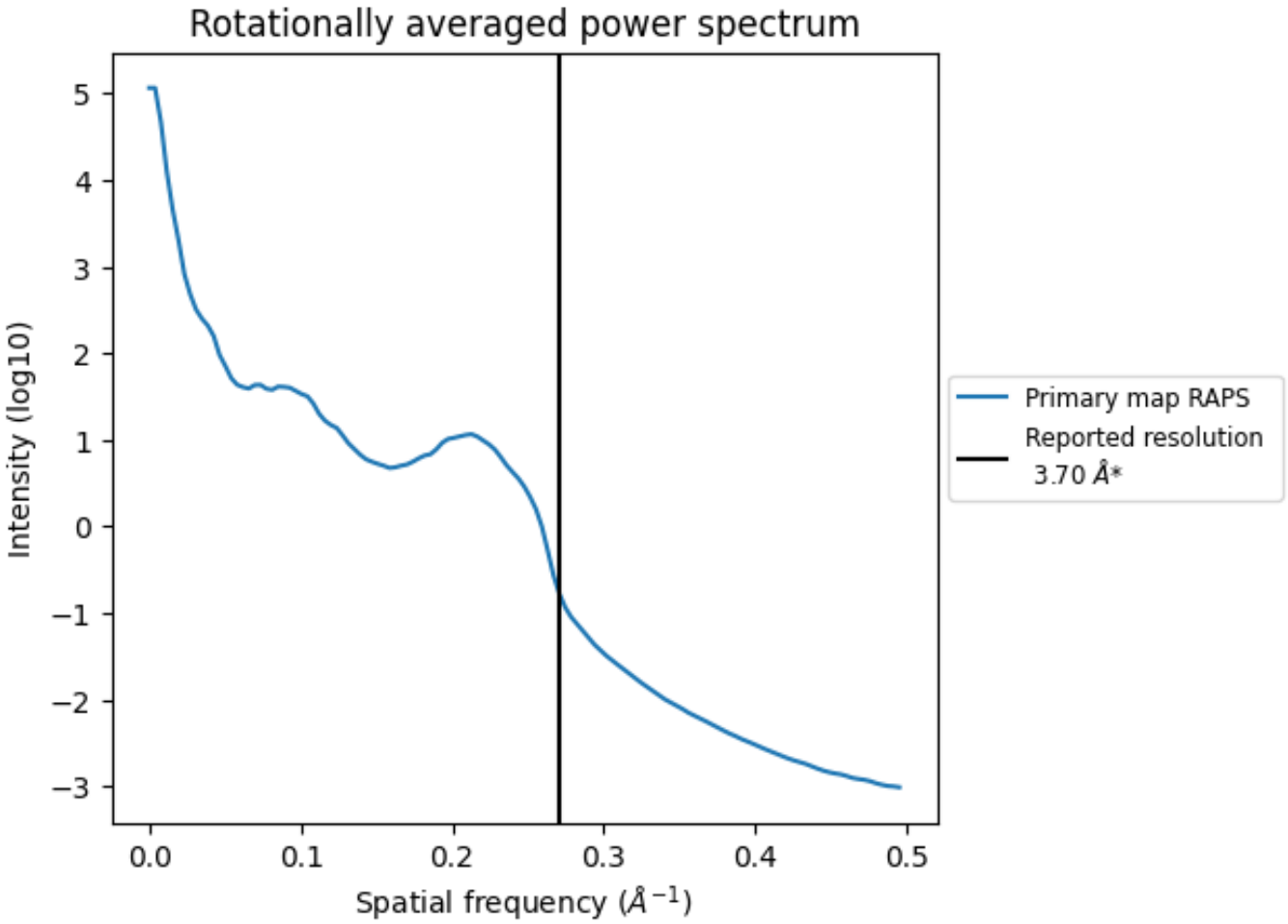
7.2 Volume estimate



The volume at the recommended contour level is 181 nm^3; 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 (i)



*Reported resolution corresponds to spatial frequency of 0.270 Å^{-1}

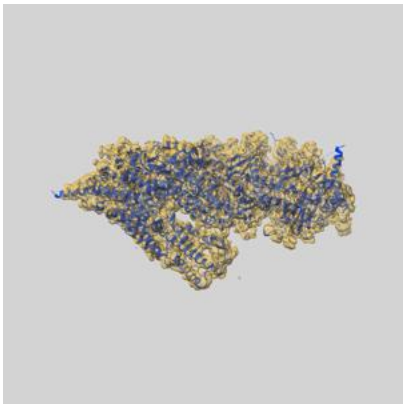
8 Fourier-Shell correlation (i)

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

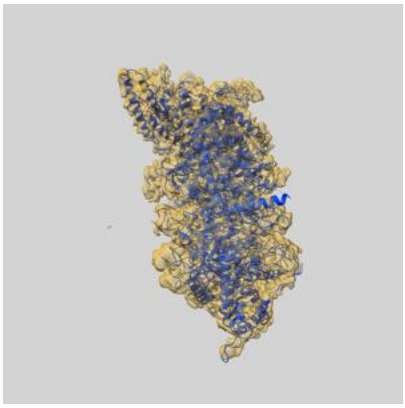
9 Map-model fit

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.

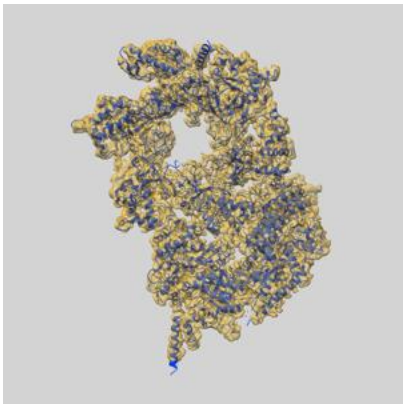
9.1 Map-model overlay



X



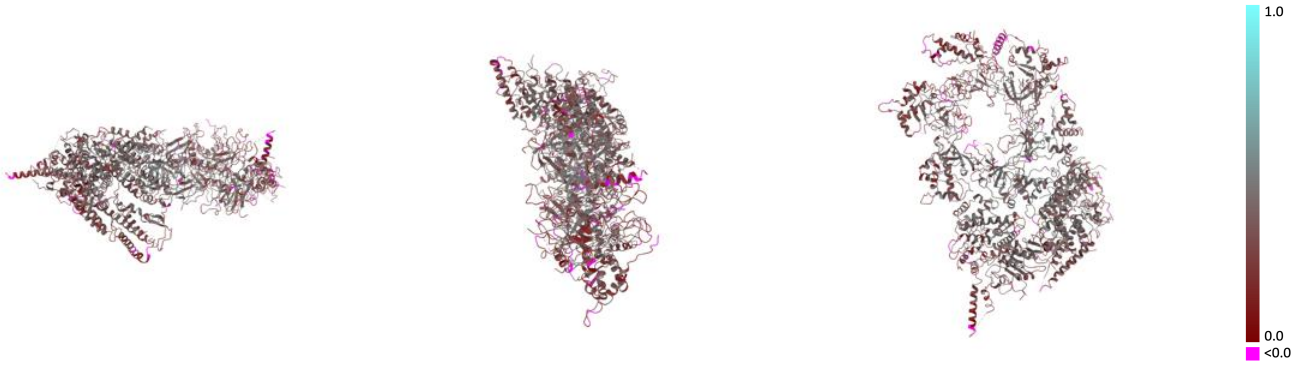
Y



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.

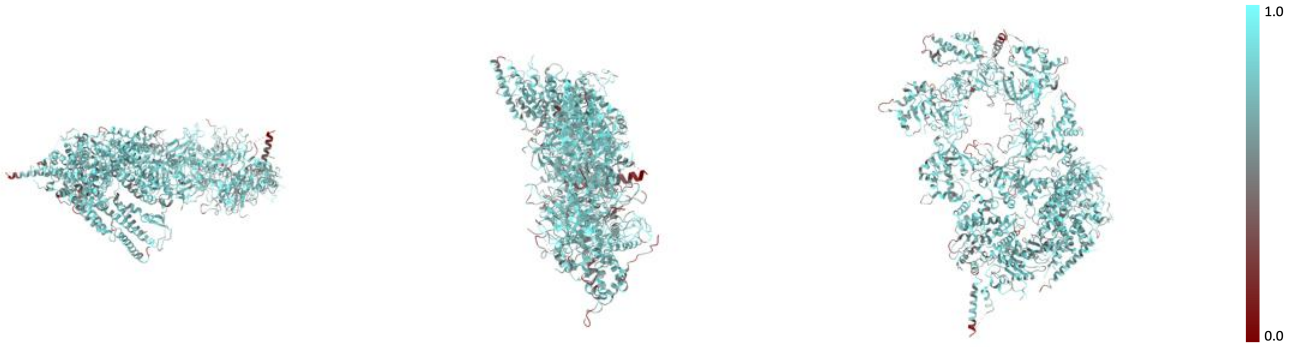
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

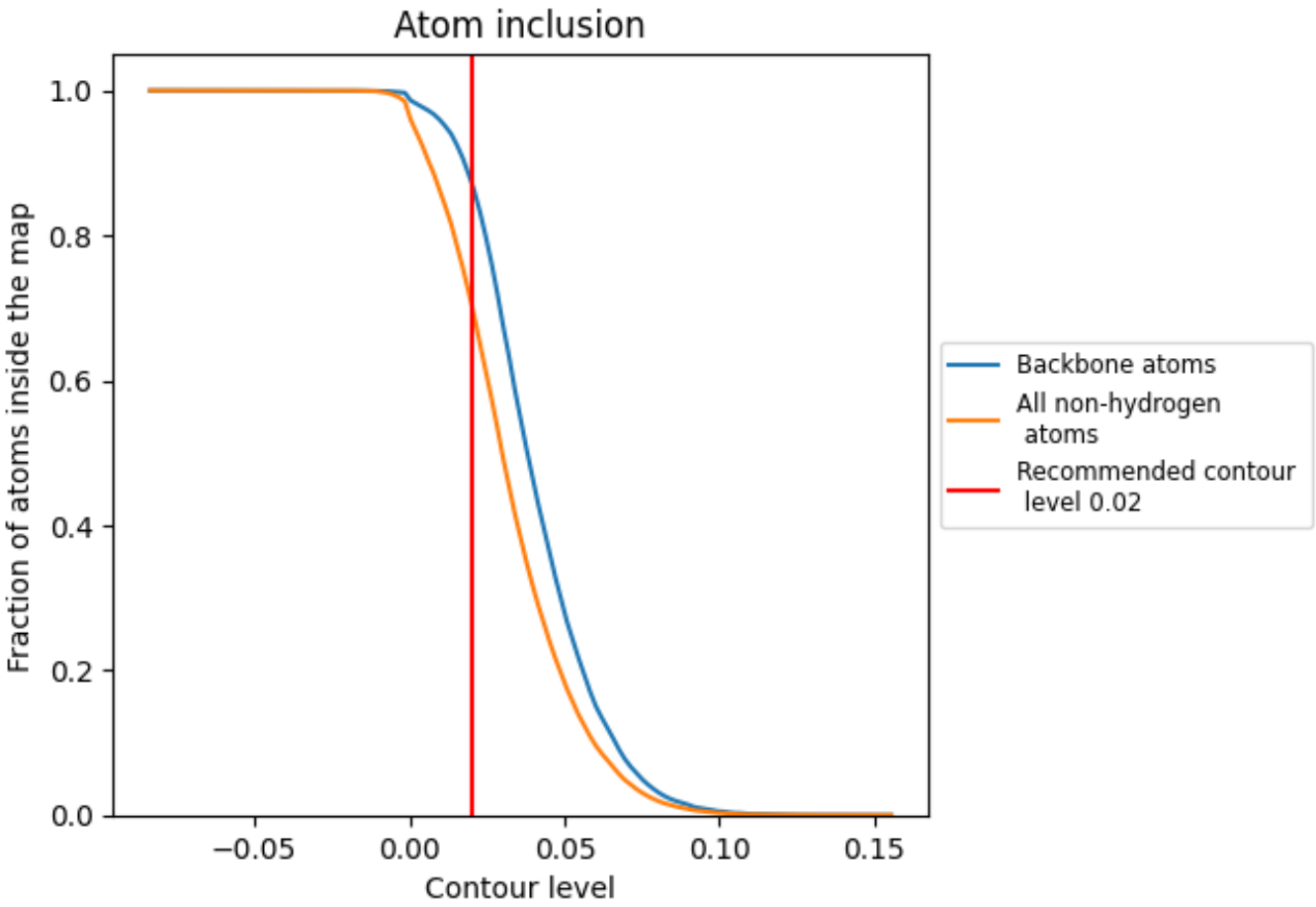
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (i)



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	0.7055	0.3290
2	0.7000	0.3380
3	0.7451	0.3680
4	0.6763	0.2630
5	0.7681	0.4160
6	0.6793	0.2950
7	0.6517	0.2910
A	0.6494	0.2820
B	0.7470	0.3740
C	0.7679	0.3830
D	0.7241	0.3260
E	0.6999	0.3270