



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 12:50 AM UTC

PDB ID : 6TLJ / pdb_00006tlj
EMDB ID : EMD-10516
Title : Cryo-EM structure of the Anaphase-promoting complex/Cyclosome, in complex with the Mitotic checkpoint complex (APC/C-MCC) at 3.8 angstrom resolution
Authors : Alfieri, C.; Barford, D.
Deposited on : 2019-12-02
Resolution : 3.80 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

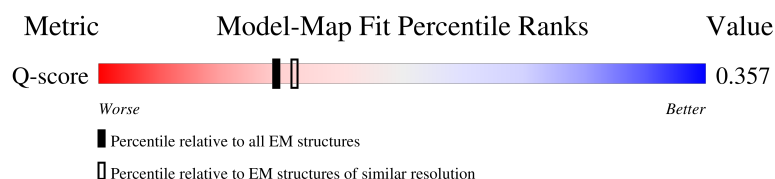
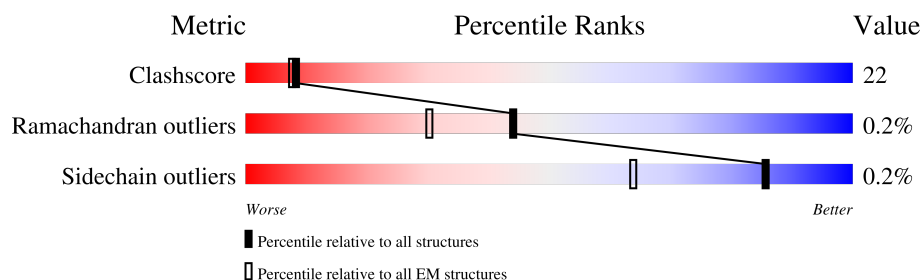
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10198 (3.30 - 4.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1944	
2	B	84	
3	C	597	
3	P	597	

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Mol	Chain	Length	Quality of chain
4	D	121	
5	E	110	
6	F	824	
6	H	824	
7	G	85	
7	W	85	
8	I	808	
9	J	620	
9	K	620	
10	L	185	
11	M	74	
12	N	822	
13	O	755	
14	Q	374	
15	R	499	
16	S	1050	
17	X	599	
17	Y	599	
18	Z	205	

2 Entry composition [i](#)

There are 18 unique types of molecules in this entry. The entry contains 72305 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 Anaphase-promoting complex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1441	Total	C	N	O	S	0	0
			10949	7039	1853	1983	74		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	356	PHE	PRO	conflict	UNP Q9H1A4

- Molecule 2 is a protein called Anaphase-promoting complex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	79	Total	C	N	O	S	0	0
			643	411	116	100	16		

- Molecule 3 is a protein called Cell division cycle protein 23 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	524	Total	C	N	O	S	0	0
			4306	2774	727	781	24		
3	P	491	Total	C	N	O	S	0	0
			4043	2611	679	729	24		

- Molecule 4 is a protein called Anaphase-promoting complex subunit 15.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	18	Total	C	N	O	0	0
			153	104	23	26		

- Molecule 5 is a protein called Anaphase-promoting complex subunit 16.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	56	Total	C	N	O	S	0	0
			450	290	74	85	1		

- Molecule 6 is a protein called Cell division cycle protein 27 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	483	Total	C	N	O	S	0	0
			3849	2470	649	704	26		
6	H	483	Total	C	N	O	S	0	0
			3853	2473	650	704	26		

- Molecule 7 is a protein called Anaphase-promoting complex subunit CDC26.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	25	Total	C	N	O	S	0	0
			213	133	40	39	1		
7	W	25	Total	C	N	O	S	0	0
			213	133	40	39	1		

- Molecule 8 is a protein called Anaphase-promoting complex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	733	Total	C	N	O	S	0	0
			5728	3675	953	1067	33		

- Molecule 9 is a protein called Cell division cycle protein 16 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	504	Total	C	N	O	S	0	0
			4047	2601	684	737	25		
9	K	493	Total	C	N	O	S	0	0
			3988	2563	672	729	24		

- Molecule 10 is a protein called Anaphase-promoting complex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	182	Total	C	N	O	S	0	0
			1435	898	263	268	6		

- Molecule 11 is a protein called Anaphase-promoting complex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	59	Total	C	N	O	S	0	0
			493	310	79	102	2		

- Molecule 12 is a protein called Anaphase-promoting complex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	N	703	Total	C	N	O	S	0	0
			5403	3436	971	971	25		

- Molecule 13 is a protein called Anaphase-promoting complex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	O	685	Total	C	N	O	S	0	0
			5402	3446	940	988	28		

- Molecule 14 is a protein called Cell division cycle protein 20 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Q	365	Total	C	N	O	S	0	0
			2739	1720	503	505	11		

- Molecule 15 is a protein called Cell division cycle protein 20 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	R	383	Total	C	N	O	S	0	0
			2953	1855	538	548	12		

- Molecule 16 is a protein called Mitotic checkpoint serine/threonine-protein kinase BUB1 beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	S	293	Total	C	N	O	S	0	0
			2227	1397	405	420	5		

- Molecule 17 is a protein called Anaphase-promoting complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	X	484	Total	C	N	O	S	0	0
			3773	2393	652	704	24		
17	Y	496	Total	C	N	O	S	0	0
			3868	2449	669	724	26		

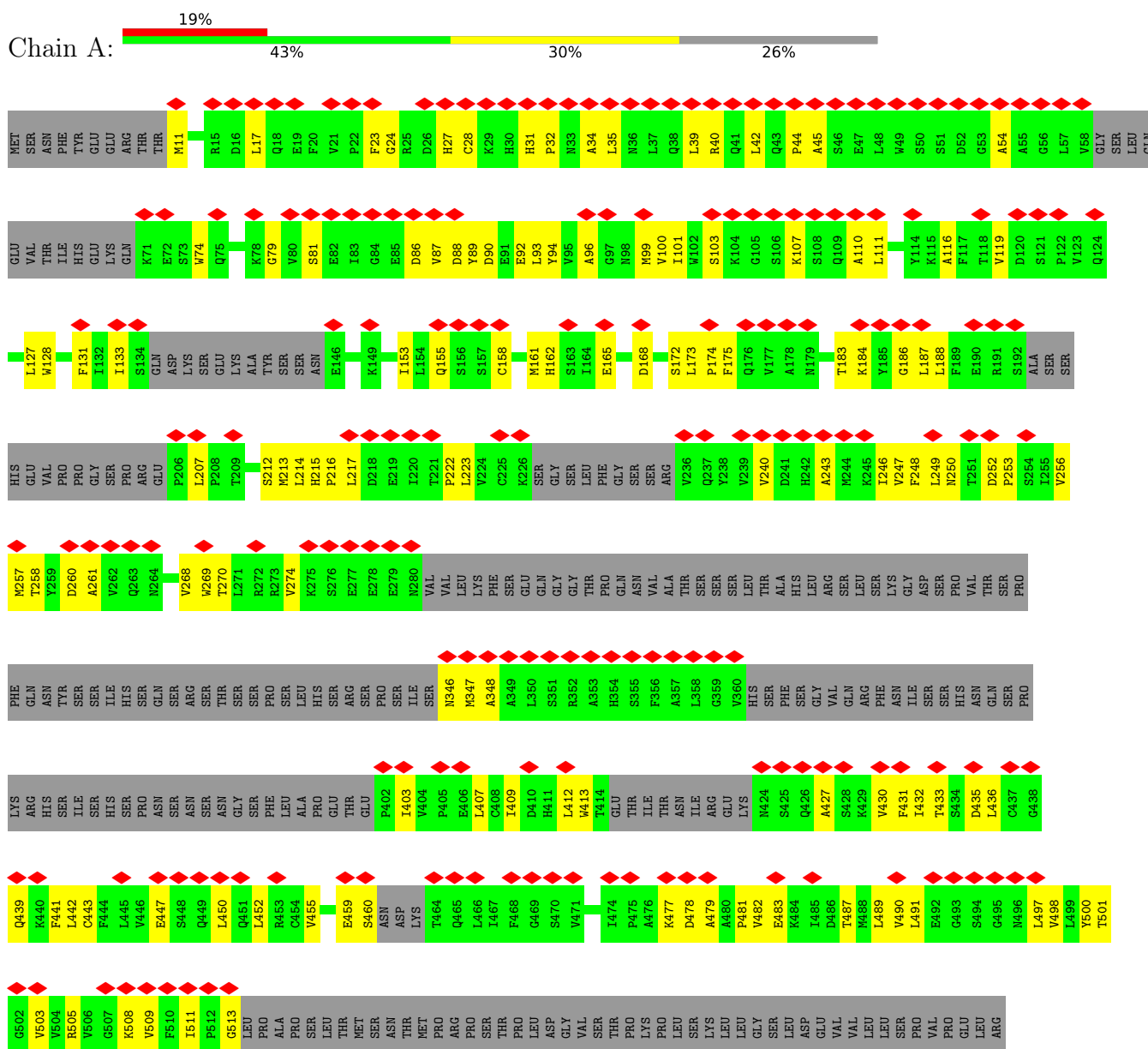
- Molecule 18 is a protein called Mitotic spindle assembly checkpoint protein MAD2A.

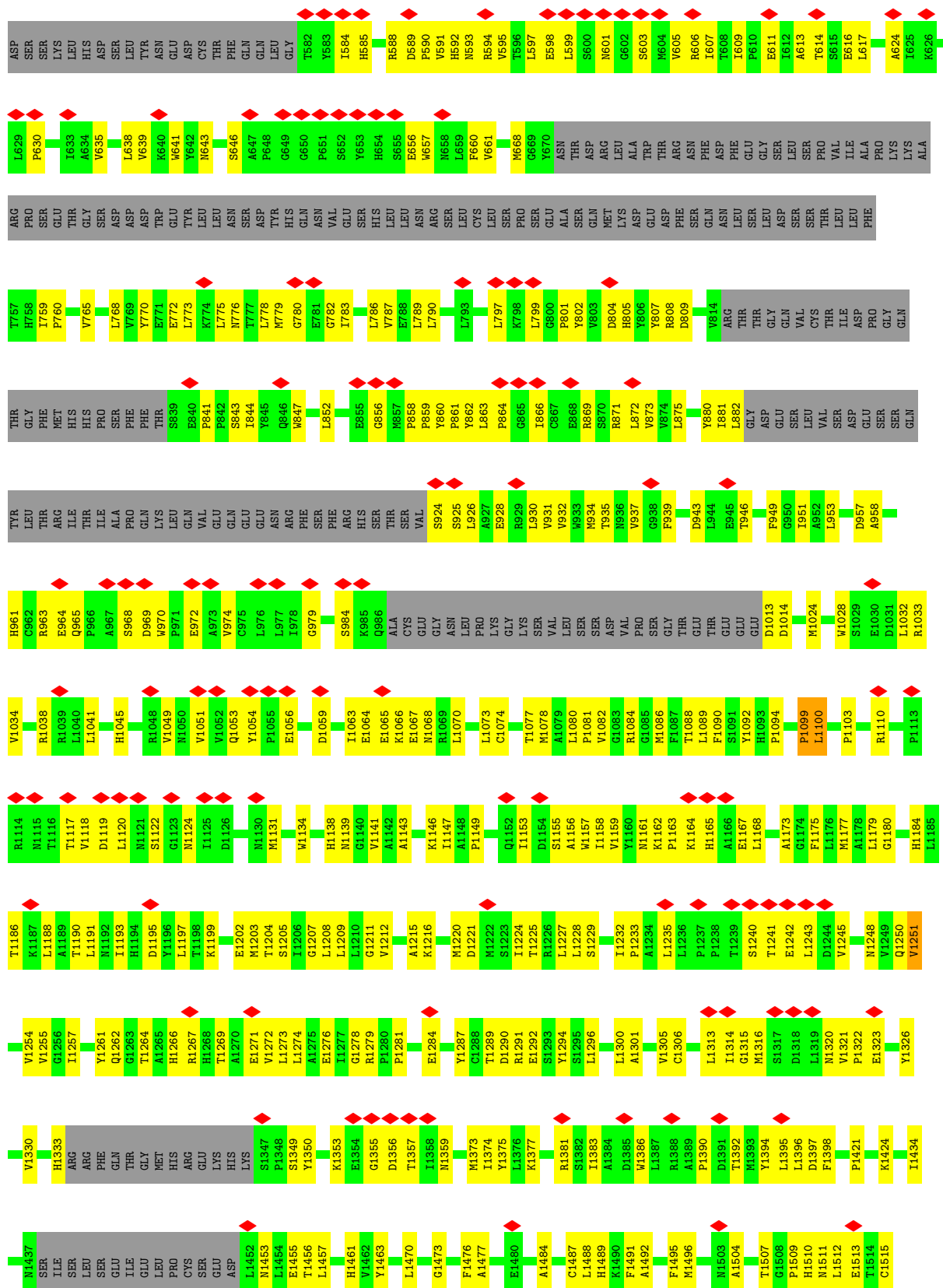
Mol	Chain	Residues	Atoms					AltConf	Trace
18	Z	195	Total	C	N	O	S	0	0
			1577	1012	256	305	4		

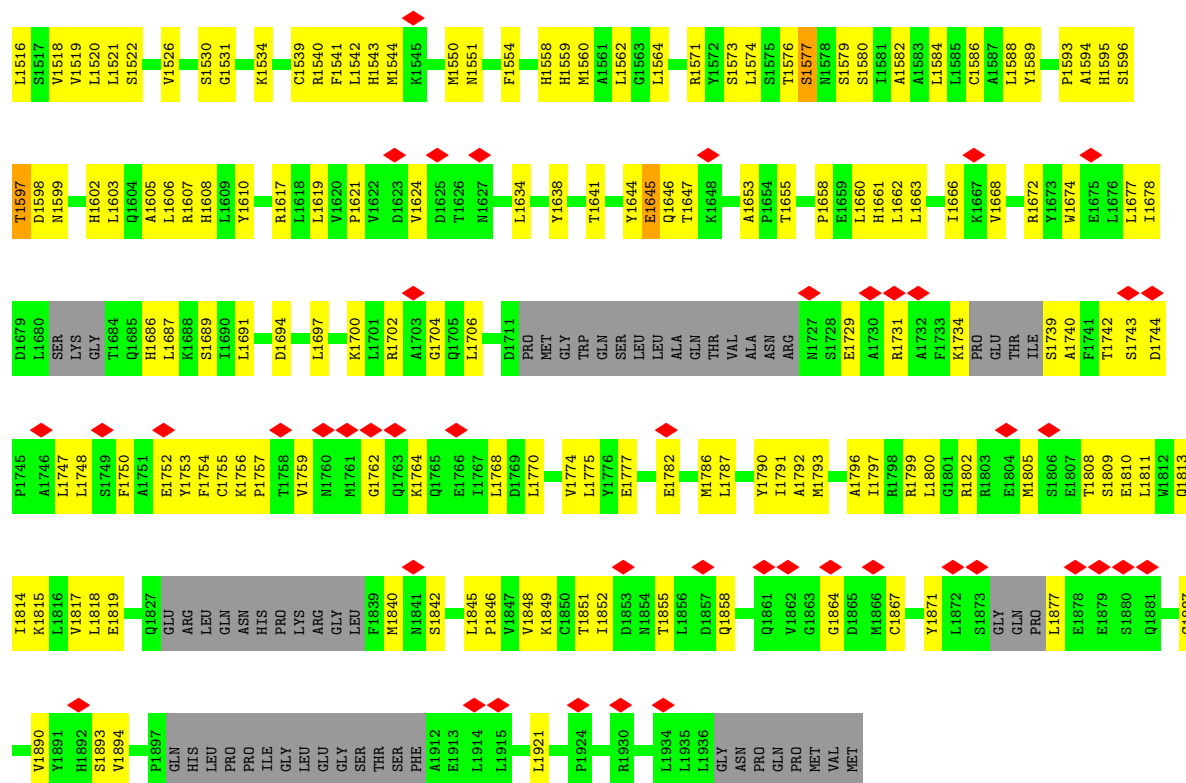
3 Residue-property plots [i](#)

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.

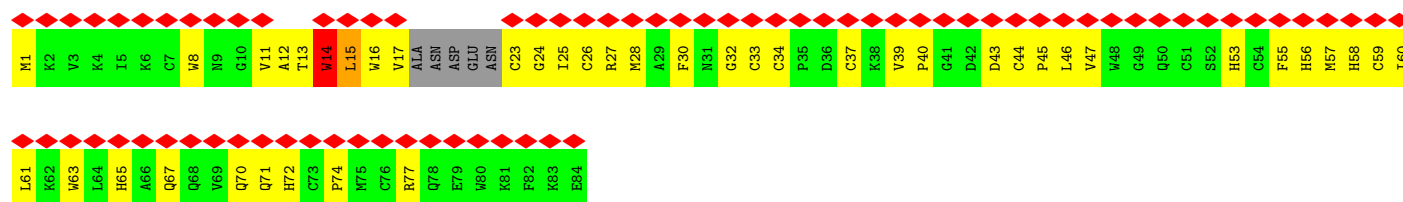
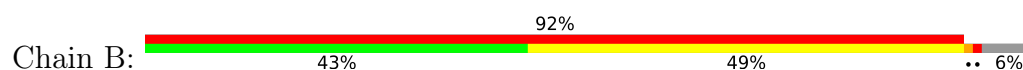
- Molecule 1: Anaphase-promoting complex subunit 1



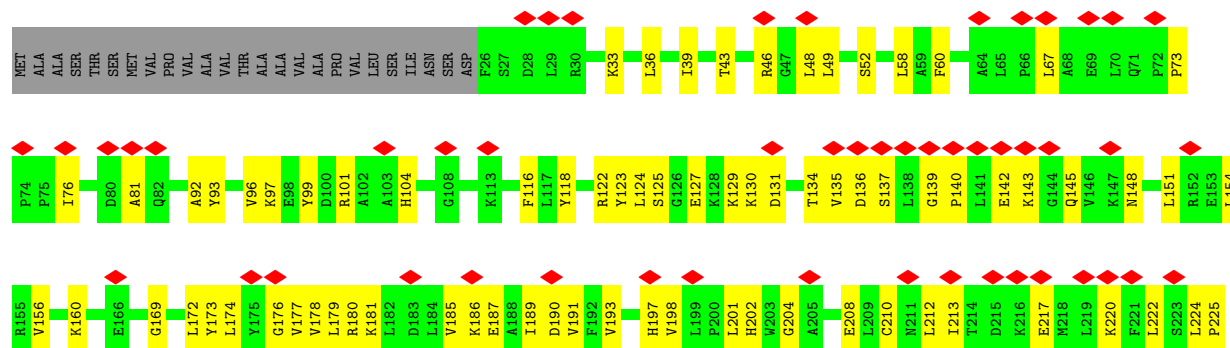


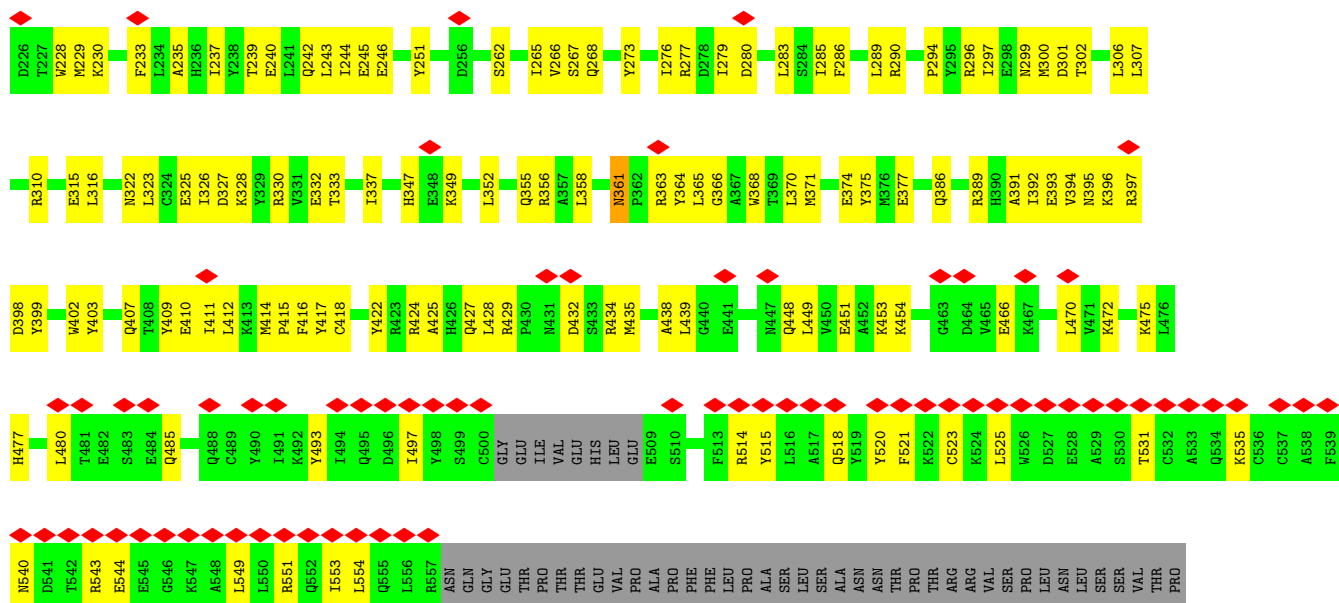


• Molecule 2: Anaphase-promoting complex subunit 11

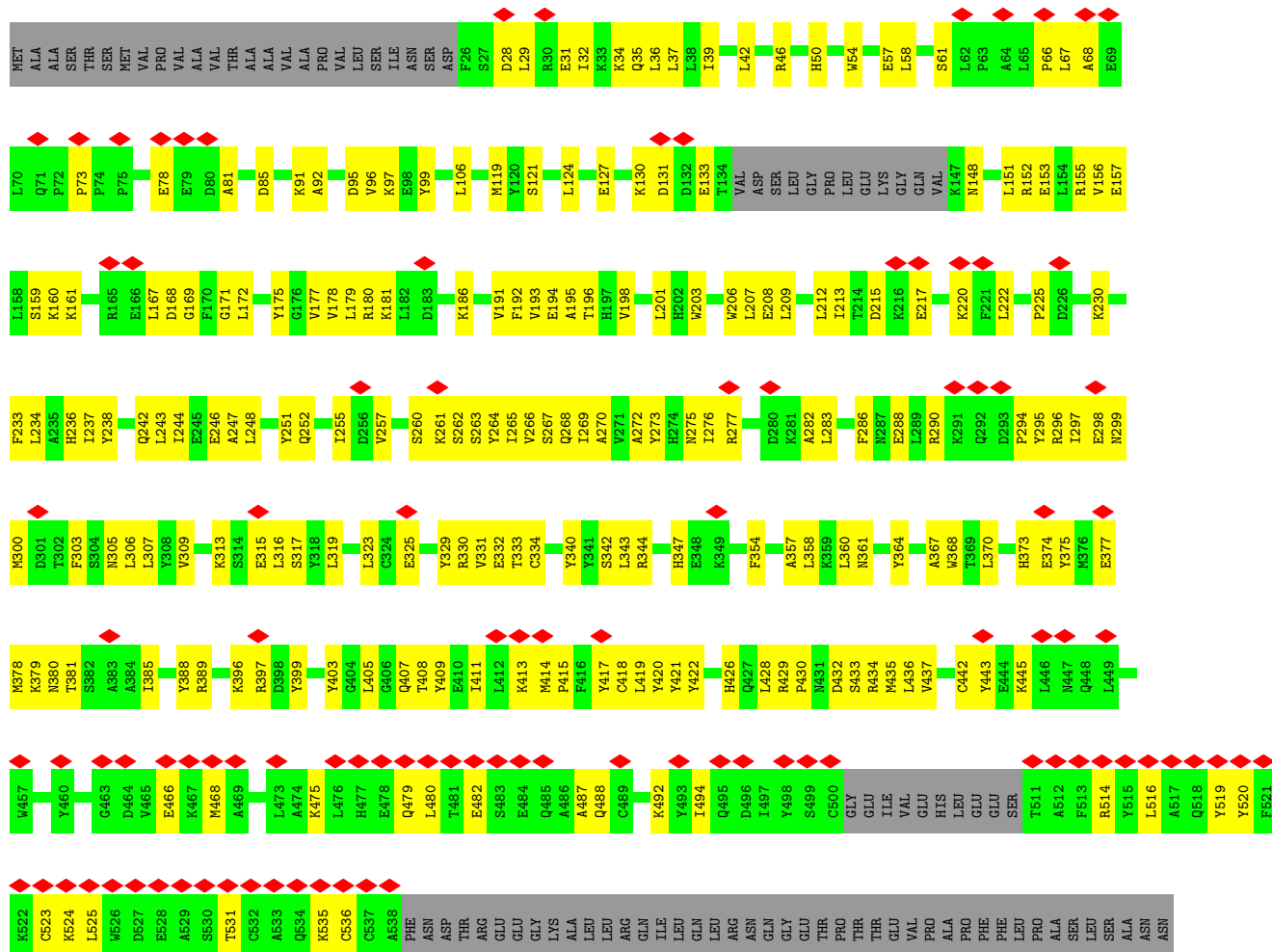


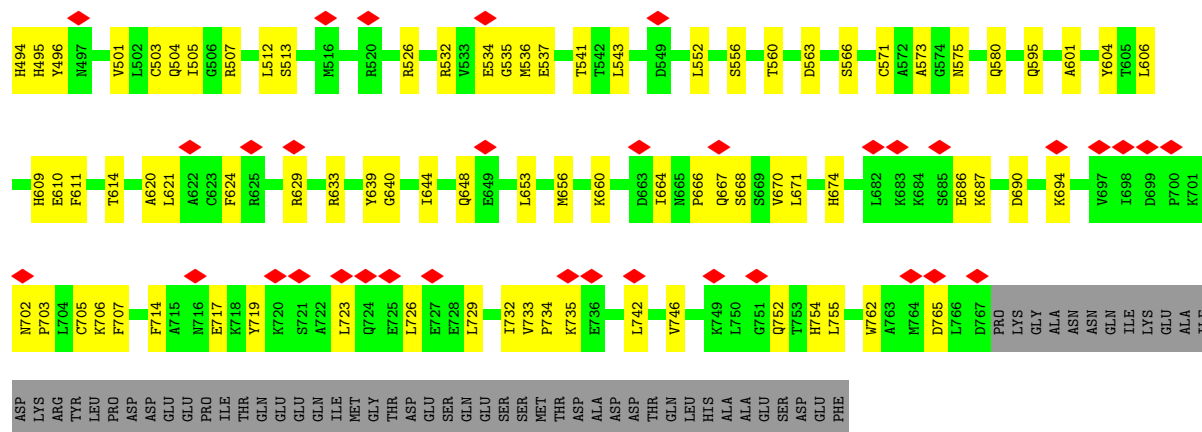
• Molecule 3: Cell division cycle protein 23 homolog





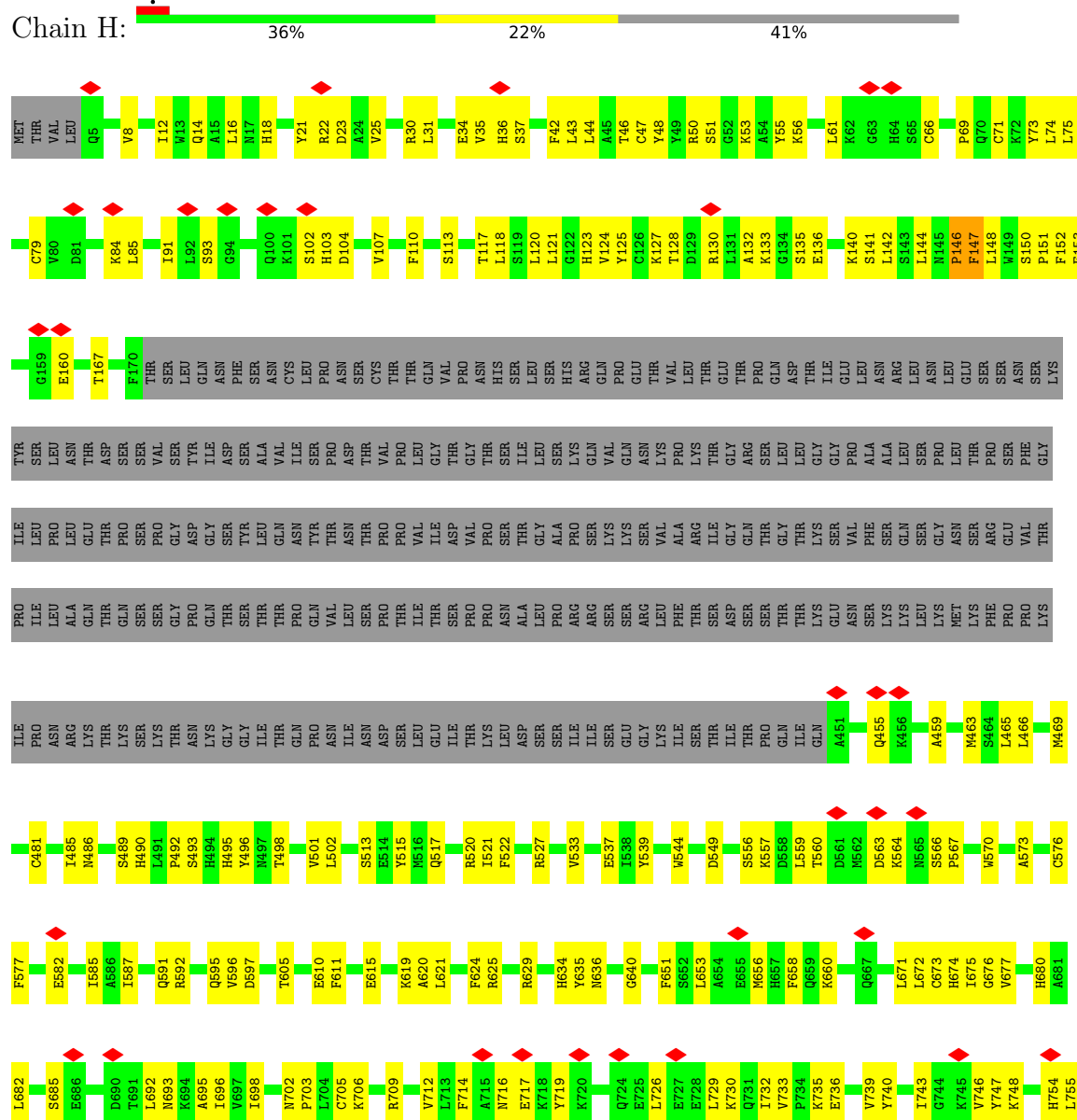
• Molecule 3: Cell division cycle protein 23 homolog

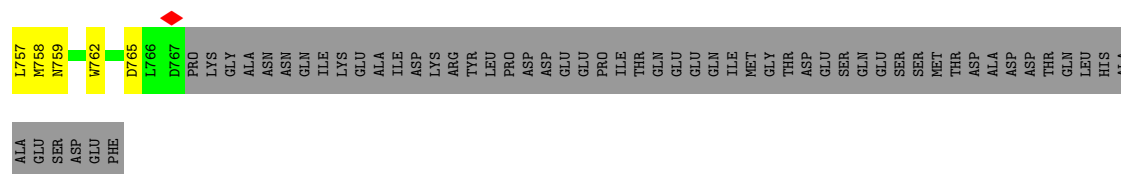




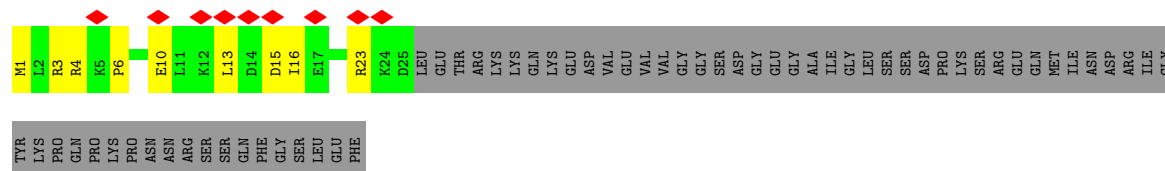
• Molecule 6: Cell division cycle protein 27 homolog

Chain H:

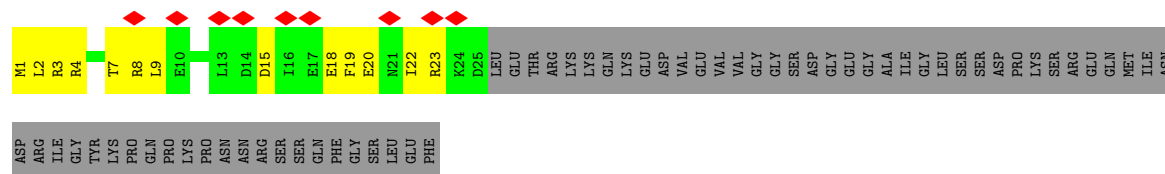




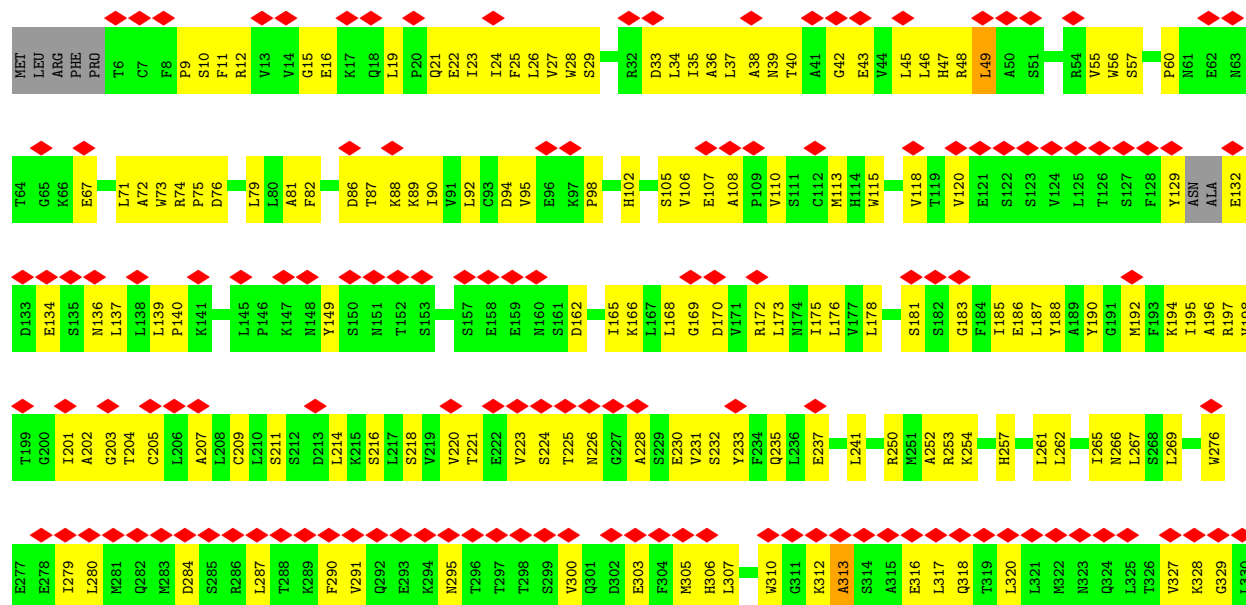
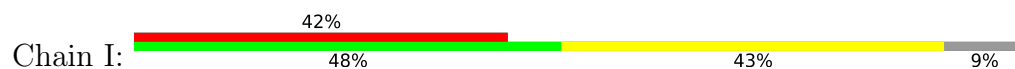
• Molecule 7: Anaphase-promoting complex subunit CDC26

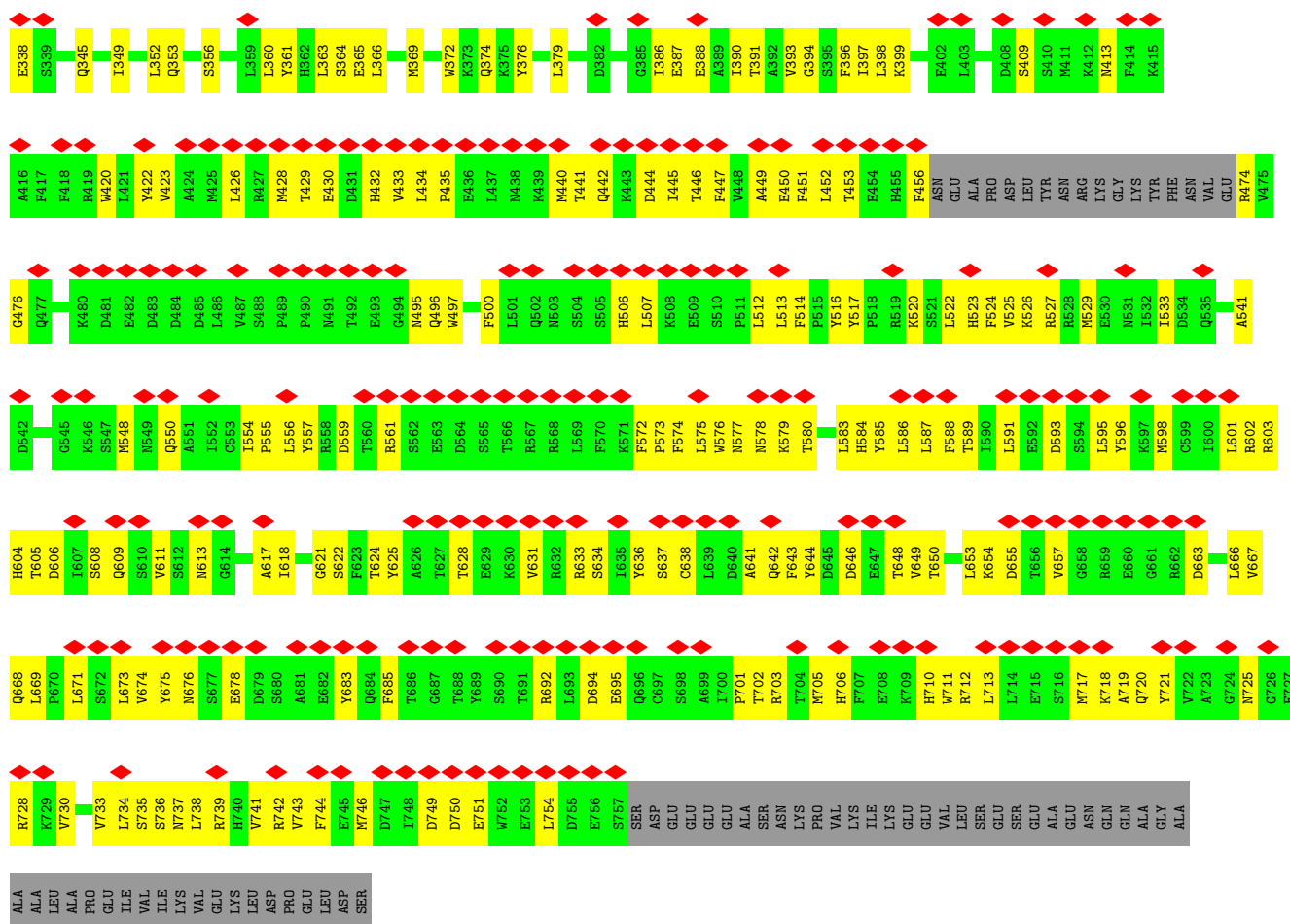


• Molecule 7: Anaphase-promoting complex subunit CDC26

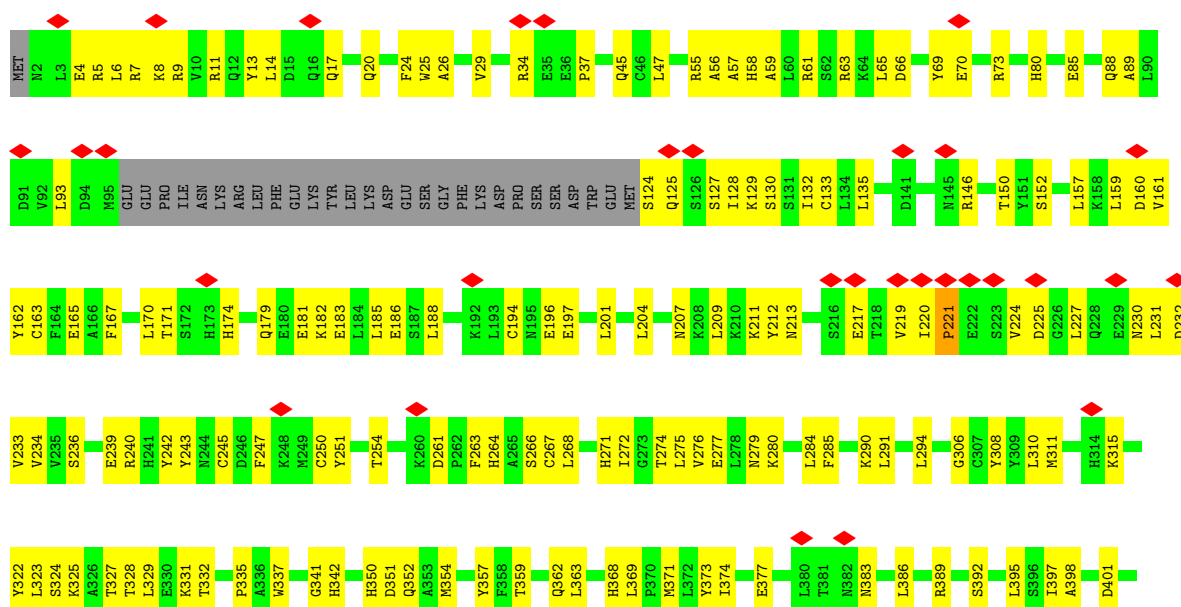


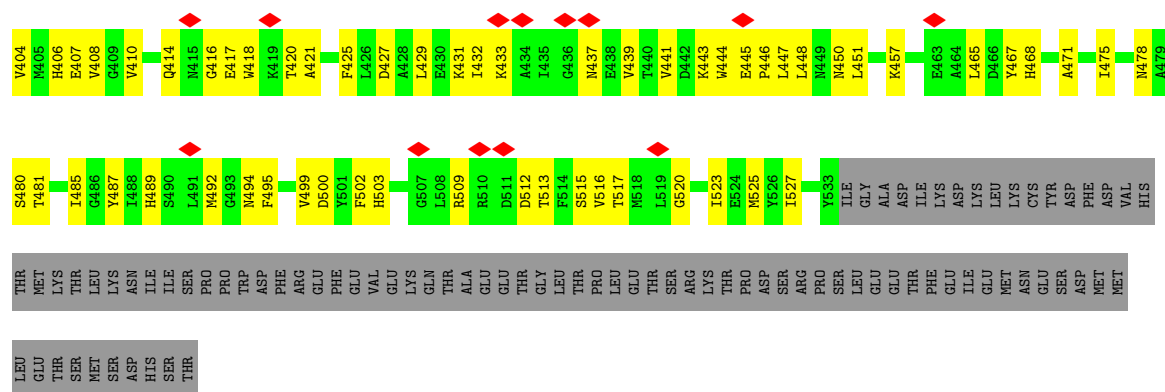
• Molecule 8: Anaphase-promoting complex subunit 4



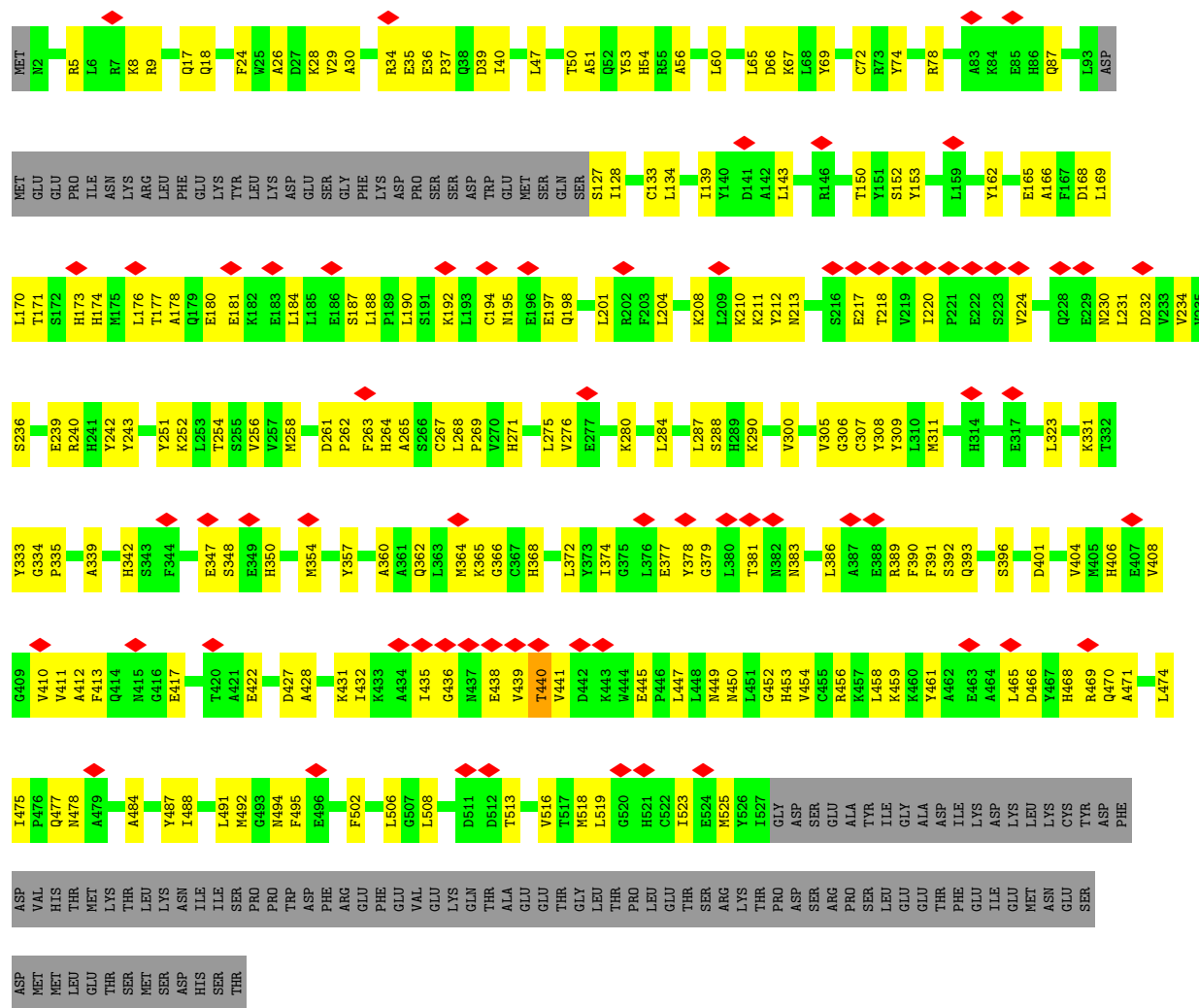


• Molecule 9: Cell division cycle protein 16 homolog



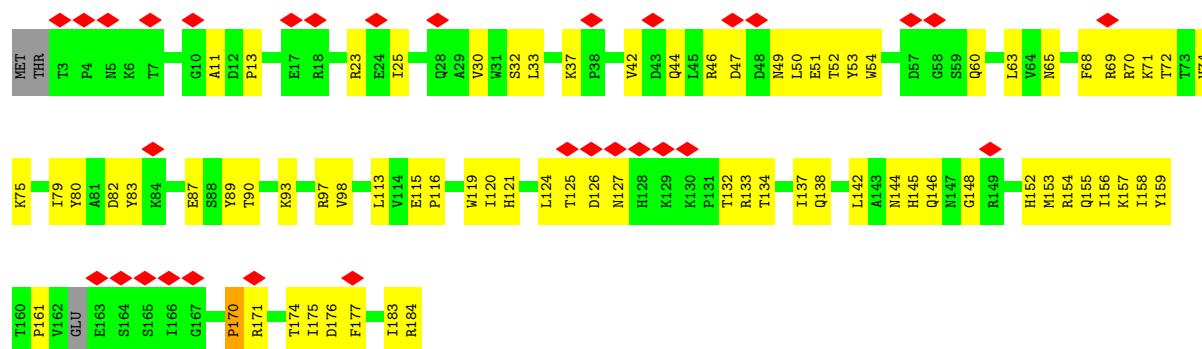


• Molecule 9: Cell division cycle protein 16 homolog



• Molecule 10: Anaphase-promoting complex subunit 10



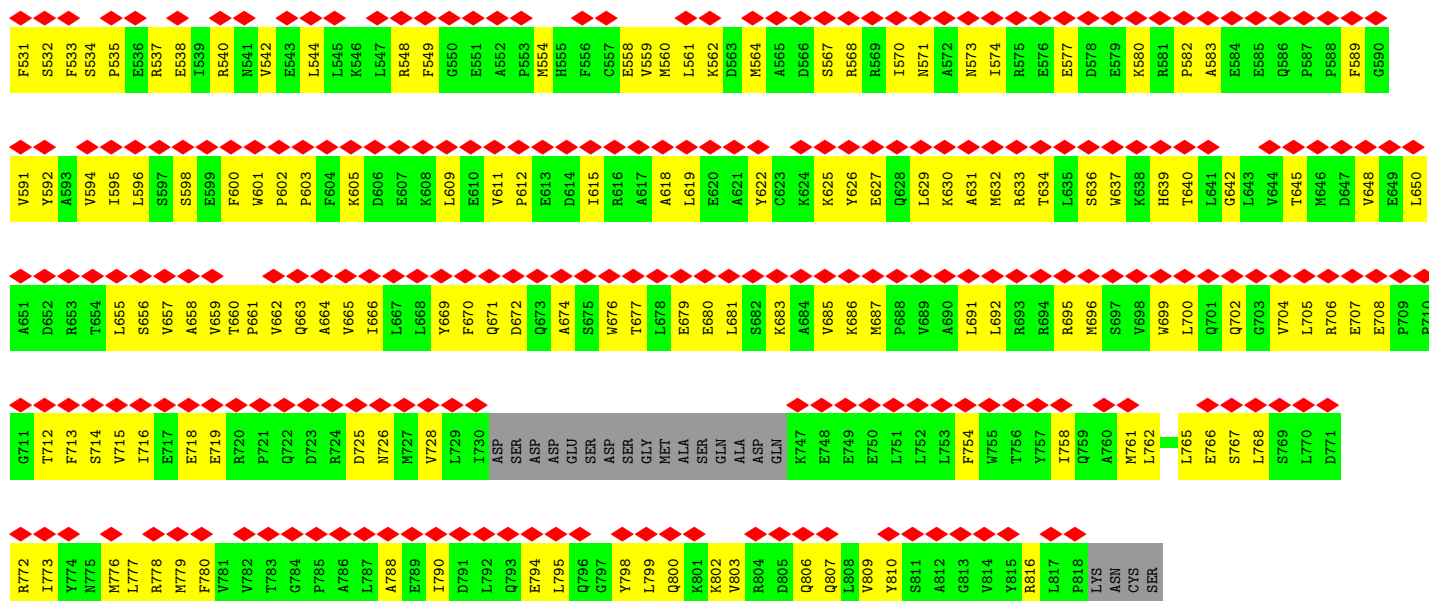


• Molecule 11: Anaphase-promoting complex subunit 13

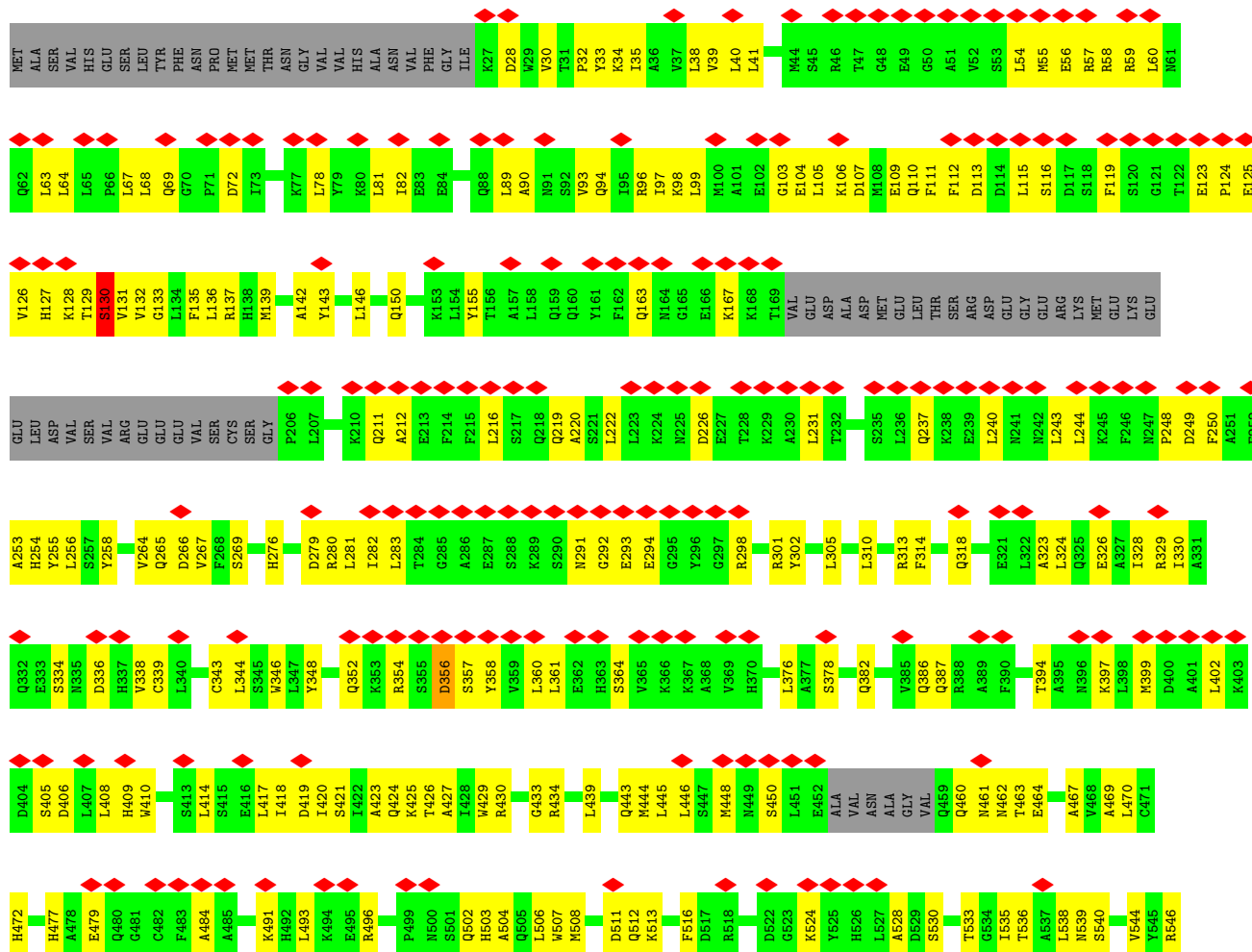


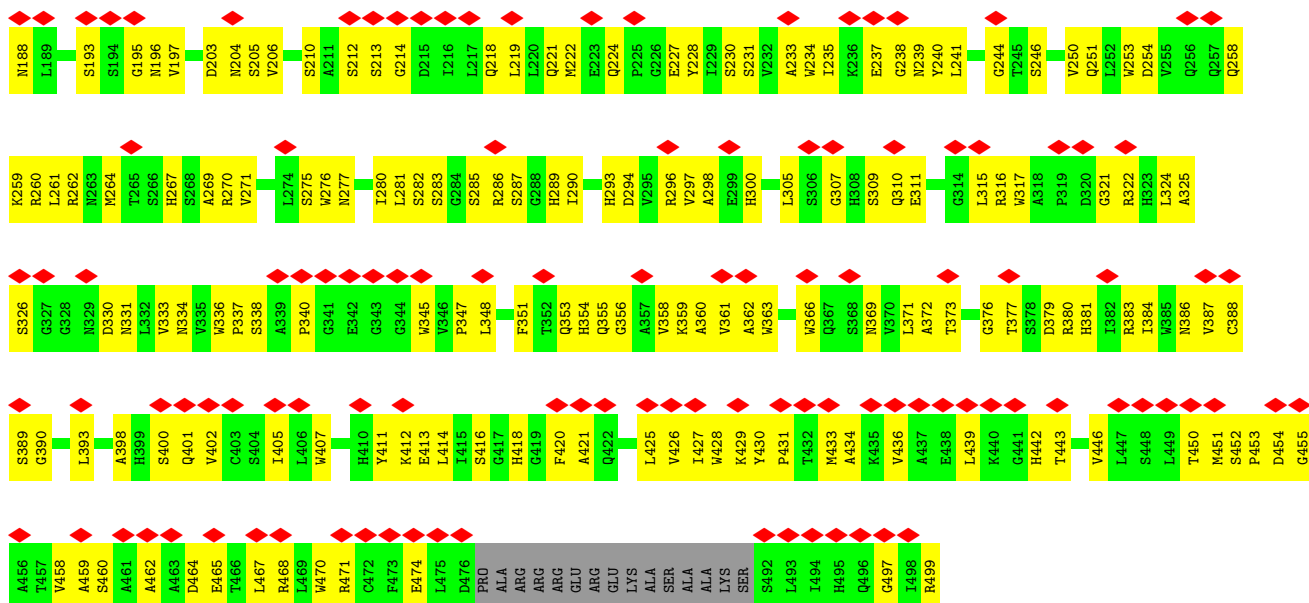
• Molecule 12: Anaphase-promoting complex subunit 2



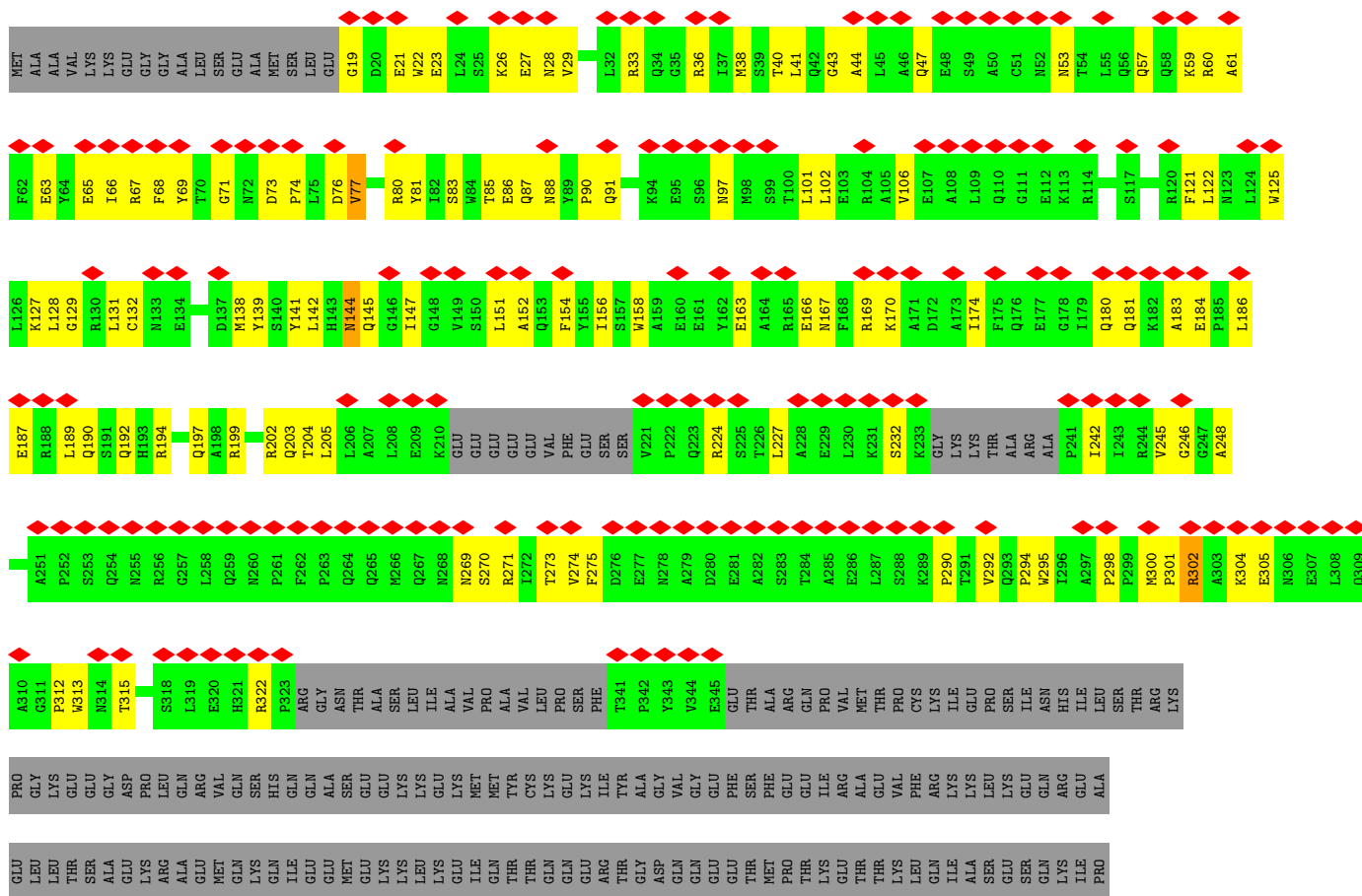


• Molecule 13: Anaphase-promoting complex subunit 5



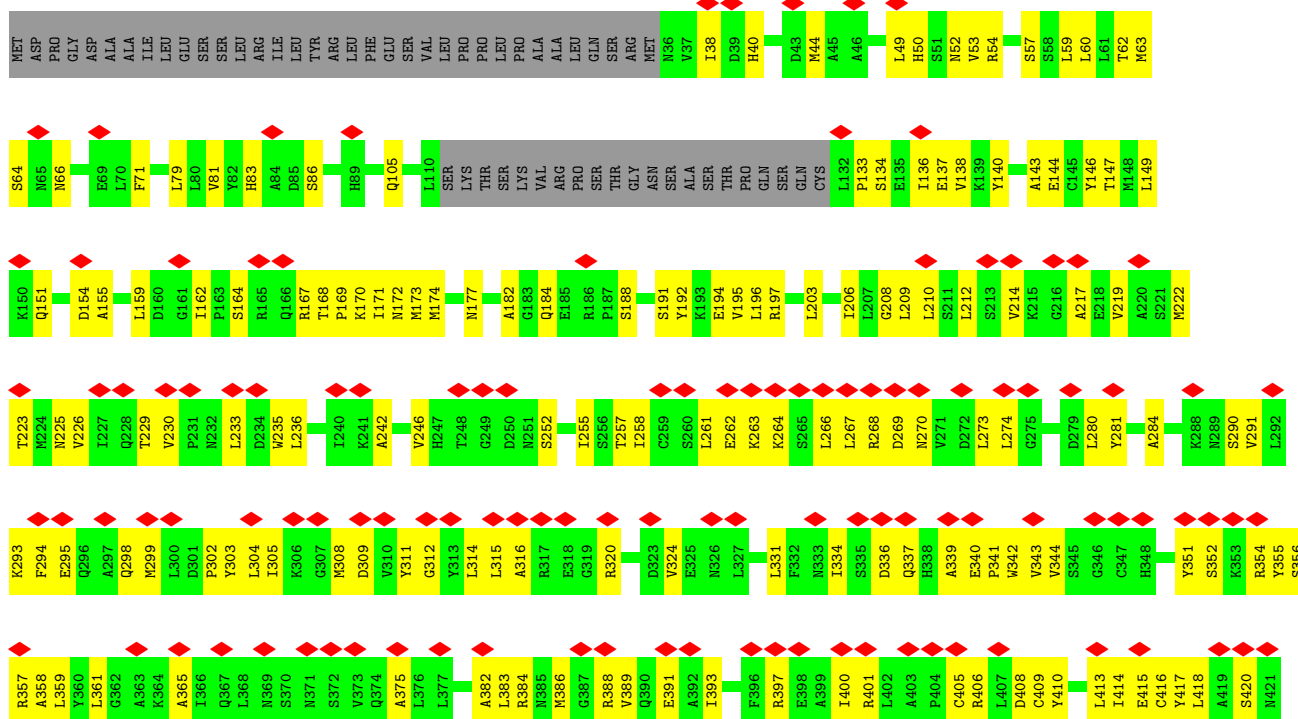


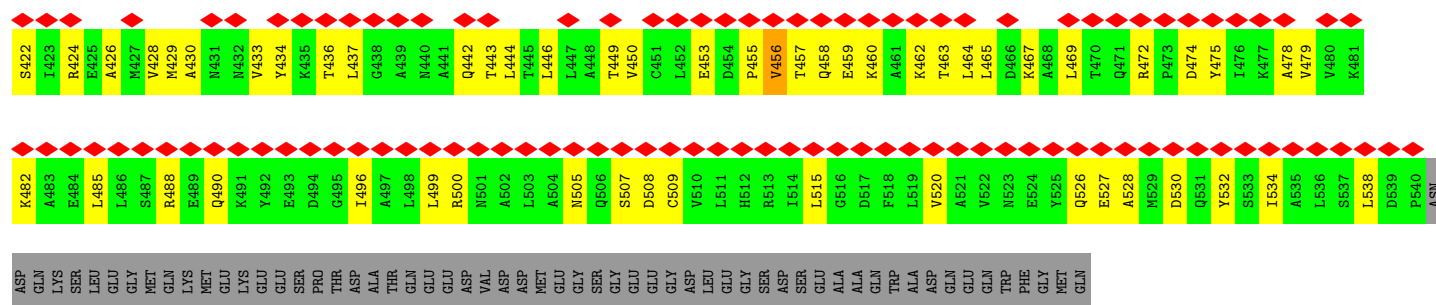
• Molecule 16: Mitotic checkpoint serine/threonine-protein kinase BUB1 beta



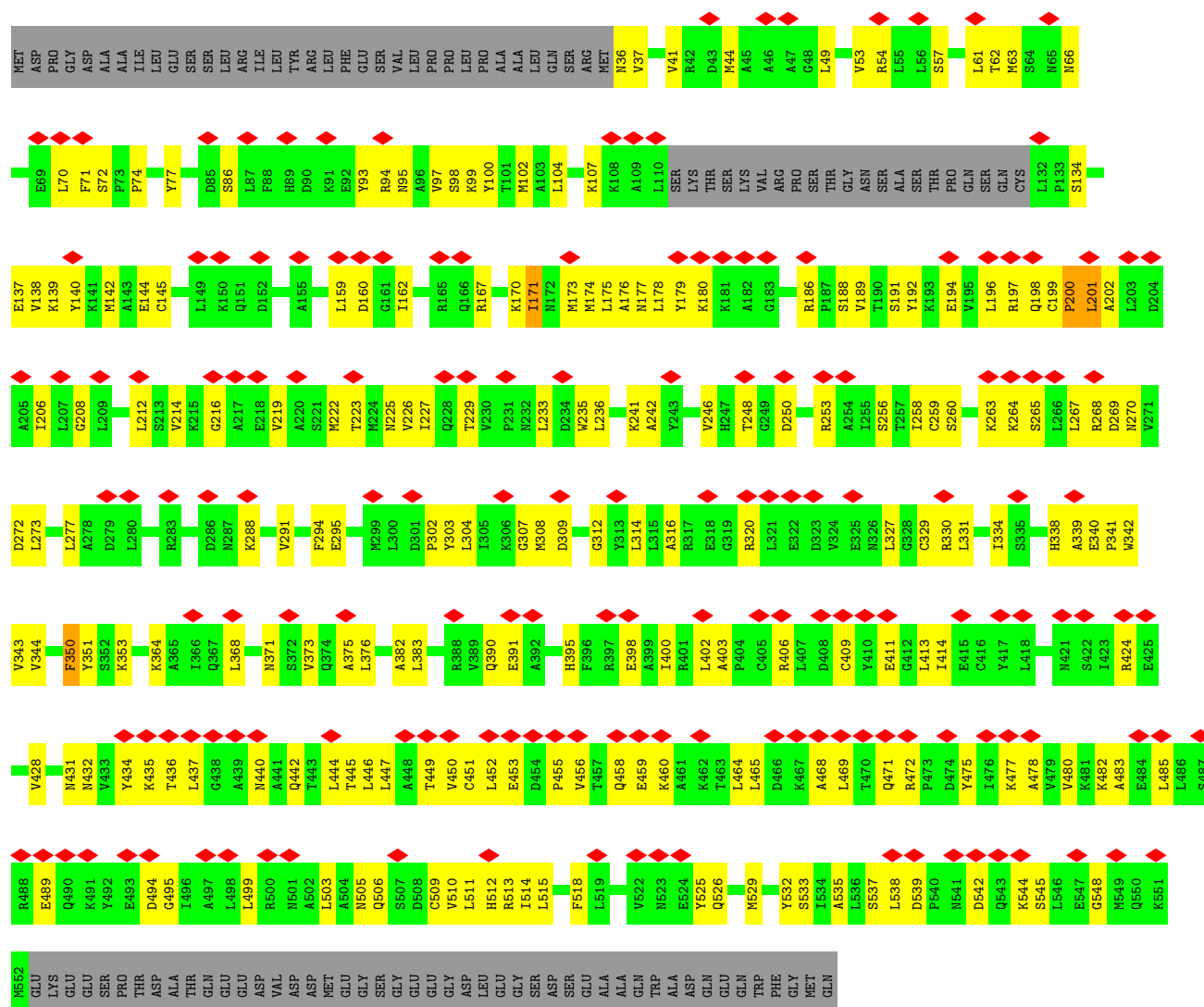
[illegible]

- Molecule 17: Anaphase-promoting complex subunit 7





• Molecule 17: Anaphase-promoting complex subunit 7



• Molecule 18: Mitotic spindle assembly checkpoint protein MAD2A





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	343551	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	27	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.206	Depositor
Minimum map value	-0.097	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	359.04, 359.04, 359.04	wwPDB
Map dimensions	264, 264, 264	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.36, 1.36, 1.36	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	A	0.30	1/11191 (0.0%)	0.55	2/15239 (0.0%)
2	B	0.22	0/665	0.56	0/896
3	C	0.29	0/4404	0.50	2/5945 (0.0%)
3	P	0.27	0/4138	0.48	0/5587
4	D	0.26	0/159	0.50	0/218
5	E	0.28	0/459	0.45	0/619
6	F	0.29	0/3939	0.46	1/5325 (0.0%)
6	H	0.32	0/3943	0.47	0/5329
7	G	0.26	0/214	0.55	0/284
7	W	0.27	0/214	0.55	0/284
8	I	0.22	0/5849	0.49	0/7932
9	J	0.31	0/4146	0.51	0/5616
9	K	0.29	0/4086	0.49	0/5534
10	L	0.31	0/1468	0.54	0/1993
11	M	0.31	0/502	0.61	0/680
12	N	0.24	0/5496	0.67	9/7444 (0.1%)
13	O	0.26	0/5501	0.51	2/7432 (0.0%)
14	Q	0.22	0/2807	0.51	0/3830
15	R	0.25	0/3029	0.51	0/4124
16	S	0.23	0/2272	0.55	1/3088 (0.0%)
17	X	0.22	0/3833	0.47	0/5187
17	Y	0.22	0/3928	0.48	0/5311
18	Z	0.17	0/1605	0.42	0/2176
All	All	0.27	1/73848 (0.0%)	0.52	17/100073 (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
1	A	0	4
2	B	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
8	I	0	2
9	J	0	2
9	K	0	3
12	N	0	9
13	O	0	1
14	Q	0	1
16	S	0	1
All	All	0	25

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1278	GLY	C-N	-5.98	1.25	1.33

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	N	125	TYR	CA-C-N	10.42	140.45	121.70
12	N	125	TYR	C-N-CA	10.42	140.45	121.70
12	N	63	ALA	N-CA-C	8.32	128.51	110.80
12	N	508	ILE	CA-C-N	-6.68	108.78	121.54
12	N	508	ILE	C-N-CA	-6.68	108.78	121.54
12	N	63	ALA	CA-C-N	6.62	133.62	121.70
12	N	63	ALA	C-N-CA	6.62	133.62	121.70
16	S	77	VAL	N-CA-C	-6.51	107.53	113.71
6	F	165	ASP	N-CA-C	-5.80	107.19	114.56
13	O	356	ASP	CA-C-N	5.54	131.68	121.70
13	O	356	ASP	C-N-CA	5.54	131.68	121.70
3	C	361	ASN	CA-C-N	5.47	140.13	127.00
3	C	361	ASN	C-N-CA	5.47	140.13	127.00
1	A	1278	GLY	CA-C-N	-5.40	110.85	122.67
1	A	1278	GLY	C-N-CA	-5.40	110.85	122.67
12	N	62	ARG	CA-C-N	5.17	131.42	121.54
12	N	62	ARG	C-N-CA	5.17	131.42	121.54

There are no chirality outliers.

All (25) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1356	ASP	Peptide
1	A	274	VAL	Peptide

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Mol	Chain	Res	Type	Group
1	A	856	GLY	Peptide
1	A	859	PRO	Peptide
2	B	14	TRP	Peptide
2	B	15	LEU	Peptide
8	I	313	ALA	Peptide
8	I	432	HIS	Peptide
9	J	220	ILE	Peptide
9	J	34	ARG	Peptide
9	K	34	ARG	Peptide
9	K	440	THR	Peptide
9	K	87	GLN	Peptide
12	N	281	TYR	Peptide
12	N	284	SER	Peptide
12	N	387	LEU	Peptide
12	N	394	CYS	Peptide
12	N	395	ASP	Peptide
12	N	411	ASP	Peptide
12	N	496	ARG	Peptide
12	N	509	TYR	Peptide
12	N	63	ALA	Peptide
13	O	130	SER	Peptide
14	Q	163	LYS	Peptide
16	S	298	PRO	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	A	10949	0	10691	486	0
2	B	643	0	617	59	0
3	C	4306	0	4275	189	0
3	P	4043	0	4000	175	0
4	D	153	0	148	6	0
5	E	450	0	435	19	0
6	F	3849	0	3783	124	0
6	H	3853	0	3794	161	0
7	G	213	0	220	14	0
7	W	213	0	220	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	I	5728	0	5615	295	0
9	J	4047	0	3949	186	0
9	K	3988	0	3908	164	0
10	L	1435	0	1382	67	0
11	M	493	0	469	33	0
12	N	5403	0	5104	261	0
13	O	5402	0	5436	258	0
14	Q	2739	0	2582	186	0
15	R	2953	0	2839	192	0
16	S	2227	0	2028	114	0
17	X	3773	0	3831	181	0
17	Y	3868	0	3926	188	0
18	Z	1577	0	1593	74	0
All	All	72305	0	70845	3110	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 22.

All (3110) 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)
16:S:290:PRO:HB2	16:S:292:VAL:HG23	1.37	1.01
14:Q:141:PRO:HB2	16:S:202:ARG:HE	1.26	0.95
9:J:264:HIS:HE2	9:J:266:SER:HG	1.11	0.93
1:A:1134:TRP:HD1	1:A:1597:THR:HA	1.36	0.90
2:B:11:VAL:HG22	12:N:642:GLY:HA2	1.54	0.89
12:N:350:ASP:HB3	12:N:351:PHE:HA	1.52	0.89
17:X:434:TYR:HA	17:X:444:LEU:HD13	1.54	0.88
17:Y:437:LEU:HB3	17:Y:444:LEU:HD11	1.55	0.88
8:I:266:ASN:HA	8:I:526:LYS:HZ3	1.38	0.87
9:K:449:ASN:HD22	7:W:8:ARG:HE	1.20	0.87
17:X:354:ARG:HD2	17:X:357:ARG:HH11	1.37	0.87
2:B:14:TRP:HA	2:B:15:LEU:HG	1.57	0.86
3:C:554:LEU:HD13	9:K:386:LEU:HD11	1.58	0.86
16:S:38:MET:HG2	18:Z:181:VAL:HB	1.58	0.85
9:J:219:VAL:HG12	9:J:221:PRO:HD3	1.56	0.85
17:X:60:LEU:HB3	17:X:79:LEU:HD11	1.58	0.84
15:R:333:VAL:HB	15:R:351:PHE:HB2	1.57	0.83
12:N:570:ILE:HG12	12:N:626:TYR:HE1	1.44	0.82
3:P:475:LYS:HG3	3:P:479:GLN:HE22	1.44	0.82
17:Y:452:LEU:HD12	17:Y:455:PRO:HG2	1.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:X:393:ILE:HG12	17:X:416:CYS:HB3	1.60	0.82
14:Q:401:GLN:HE21	14:Q:420:PHE:H	1.24	0.82
8:I:676:ASN:H	8:I:703:ARG:HH12	1.23	0.81
1:A:1540:ARG:NH1	12:N:486:ASP:O	2.12	0.81
9:J:383:ASN:HB3	9:J:386:LEU:HD13	1.63	0.81
13:O:40:LEU:HD23	13:O:93:VAL:HG21	1.60	0.81
15:R:360:ALA:HB1	15:R:405:ILE:HG13	1.63	0.81
14:Q:129:LYS:HG3	18:Z:159:LYS:HD3	1.63	0.80
5:E:105:PHE:HZ	6:H:619:LYS:HG3	1.47	0.80
1:A:250:ASN:HD22	1:A:432:ILE:HD12	1.48	0.79
12:N:284:SER:HA	12:N:285:PHE:CD1	2.17	0.79
1:A:158:CYS:SG	3:C:427:GLN:NE2	2.55	0.79
12:N:199:LEU:O	12:N:283:ARG:NH1	2.15	0.79
13:O:41:LEU:HD21	13:O:132:VAL:HG13	1.64	0.78
8:I:666:LEU:HD21	8:I:746:MET:HE1	1.65	0.78
17:X:343:VAL:HG22	17:X:375:ALA:HB2	1.65	0.78
13:O:617:GLN:HE21	13:O:650:PRO:HB2	1.49	0.78
14:Q:290:ILE:HB	14:Q:305:LEU:HB2	1.66	0.78
9:K:276:VAL:HA	9:K:311:MET:HE2	1.63	0.78
17:X:263:LYS:O	17:X:268:ARG:NH2	2.17	0.78
8:I:624:THR:O	8:I:711:TRP:NE1	2.15	0.78
3:C:180:ARG:NH1	3:C:208:GLU:OE2	2.17	0.77
6:H:703:PRO:HB2	10:L:177:PHE:HE1	1.49	0.77
3:C:472:LYS:HA	3:C:475:LYS:HE3	1.66	0.77
8:I:113:MET:HB3	8:I:176:LEU:HD11	1.67	0.77
12:N:648:VAL:HB	12:N:655:LEU:HB3	1.65	0.77
1:A:661:VAL:HG13	1:A:789:LEU:HD12	1.66	0.77
14:Q:333:VAL:HB	14:Q:351:PHE:HB2	1.65	0.77
9:J:331:LYS:HD3	9:J:332:THR:HG23	1.66	0.76
8:I:209:CYS:HB2	8:I:575:LEU:HB3	1.67	0.76
13:O:657:ILE:HG13	13:O:704:VAL:HG22	1.67	0.76
6:H:610:GLU:OE2	10:L:184:ARG:NH2	2.19	0.76
13:O:226:ASP:OD1	13:O:462:ASN:ND2	2.18	0.76
6:H:527:ARG:NH1	17:Y:303:TYR:OH	2.19	0.76
3:C:267:SER:OG	3:C:299:ASN:OD1	2.04	0.76
18:Z:104:ILE:HG12	18:Z:193:VAL:HG22	1.68	0.76
8:I:719:ALA:HA	8:I:735:SER:HA	1.67	0.75
15:R:254:ASP:H	15:R:261:LEU:HD13	1.52	0.75
3:C:36:LEU:HD21	3:C:58:LEU:HB2	1.68	0.75
17:X:270:ASN:HA	17:Y:62:THR:HG21	1.68	0.75
8:I:48:ARG:HD2	8:I:55:VAL:HG22	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:R:261:LEU:HD23	16:S:274:VAL:HG11	1.67	0.75
1:A:1792:ALA:HB2	13:O:598:THR:HG21	1.68	0.75
17:X:397:ARG:O	17:X:401:ARG:NH1	2.19	0.75
12:N:577:GLU:HG2	12:N:583:ALA:HB2	1.69	0.75
13:O:552:GLN:NE2	13:O:589:GLU:OE1	2.15	0.74
15:R:411:TYR:O	15:R:429:LYS:NZ	2.20	0.74
9:J:475:ILE:HD11	9:J:478:ASN:HB2	1.70	0.74
1:A:88:ASP:O	1:A:594:ARG:NH2	2.20	0.74
6:F:34:GLU:HB2	6:H:495:HIS:HE1	1.52	0.74
6:F:610:GLU:OE2	15:R:499:ARG:NH1	2.21	0.74
9:K:208:LYS:O	9:K:211:LYS:NZ	2.21	0.74
15:R:204:ASN:HD21	15:R:221:GLN:HE21	1.33	0.74
2:B:23:CYS:SG	2:B:26:CYS:N	2.60	0.74
12:N:598:SER:OG	12:N:605:LYS:NZ	2.20	0.74
2:B:13:THR:HB	12:N:598:SER:HB2	1.70	0.74
14:Q:282:SER:OG	14:Q:317:TRP:NE1	2.20	0.74
15:R:269:ALA:HB1	15:R:286:ARG:HB3	1.68	0.74
1:A:188:LEU:HD11	1:A:223:LEU:HD11	1.69	0.73
8:I:9:PRO:HG2	8:I:750:ASP:HB3	1.67	0.73
12:N:622:TYR:O	12:N:626:TYR:HB2	1.88	0.73
14:Q:398:ALA:HB1	14:Q:418:HIS:HE1	1.50	0.73
1:A:964:GLU:HG3	1:A:965:GLN:HG2	1.70	0.73
12:N:573:ASN:OD1	12:N:625:LYS:NZ	2.20	0.73
14:Q:425:LEU:HB2	14:Q:439:LEU:HB2	1.70	0.73
9:K:242:TYR:O	7:W:3:ARG:NH2	2.21	0.73
13:O:382:GLN:NE2	13:O:424:GLN:OE1	2.21	0.73
6:F:32:TYR:OH	6:F:64:HIS:NE2	2.19	0.73
3:C:176:GLY:HA2	3:C:179:LEU:HD12	1.68	0.73
10:L:11:ALA:O	10:L:121:HIS:NE2	2.20	0.73
12:N:702:GLN:OE1	12:N:726:ASN:ND2	2.21	0.73
6:F:73:TYR:OH	6:H:18:HIS:O	2.06	0.73
1:A:1357:THR:O	10:L:69:ARG:NH2	2.22	0.73
6:F:580:GLN:HG3	11:M:62:LEU:HD21	1.70	0.73
13:O:675:ALA:HA	13:O:678:TYR:HB2	1.71	0.73
1:A:1815:LYS:NZ	1:A:1893:SER:OG	2.21	0.72
15:R:176:LEU:HB2	15:R:467:LEU:HB3	1.70	0.72
1:A:584:ILE:HA	1:A:599:LEU:HA	1.69	0.72
17:Y:343:VAL:HG22	17:Y:375:ALA:HB2	1.71	0.72
14:Q:149:LYS:NZ	14:Q:420:PHE:O	2.22	0.72
15:R:165:CYS:SG	15:R:166:ARG:N	2.60	0.72
17:Y:499:LEU:HB3	17:Y:515:LEU:HD12	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:VAL:O	1:A:155:GLN:NE2	2.22	0.72
12:N:704:VAL:HA	12:N:719:GLU:HG2	1.71	0.72
13:O:448:MET:O	13:O:460:GLN:NE2	2.22	0.72
1:A:1574:LEU:O	1:A:1617:ARG:NH2	2.21	0.72
8:I:169:GLY:O	8:I:253:ARG:NH2	2.21	0.72
17:X:449:THR:HG21	17:X:465:LEU:HD12	1.71	0.72
14:Q:324:LEU:HB3	14:Q:336:TRP:HB2	1.70	0.72
17:Y:304:LEU:O	17:Y:308:MET:HG2	1.90	0.72
16:S:199:ARG:O	16:S:202:ARG:HG2	1.89	0.72
2:B:45:PRO:HG3	12:N:630:LYS:HG3	1.71	0.72
7:G:15:ASP:O	9:J:487:TYR:OH	2.08	0.72
17:Y:186:ARG:HA	17:Y:189:VAL:HG12	1.72	0.72
8:I:129:TYR:O	8:I:132:GLU:N	2.23	0.71
12:N:425:ARG:HD3	12:N:507:SER:HB3	1.72	0.71
1:A:1551:ASN:HD22	1:A:1594:ALA:HA	1.55	0.71
17:X:134:SER:HB2	17:X:137:GLU:HG2	1.72	0.71
6:H:605:THR:HG21	6:H:636:ASN:HB3	1.71	0.71
12:N:290:HIS:HA	12:N:293:ILE:HB	1.72	0.71
12:N:333:TYR:OH	12:N:367:ARG:NH2	2.24	0.71
1:A:1092:TYR:HB3	1:A:1146:LYS:HG2	1.71	0.71
10:L:47:ASP:OD2	10:L:49:ASN:ND2	2.23	0.71
1:A:256:VAL:HB	1:A:269:TRP:HB2	1.70	0.71
1:A:1110:ARG:HG2	1:A:1117:THR:HG22	1.73	0.71
8:I:209:CYS:HB3	8:I:218:SER:HB2	1.72	0.71
9:J:327:THR:OG1	9:J:337:TRP:NE1	2.22	0.71
13:O:450:SER:HB2	13:O:461:ASN:HB2	1.71	0.71
18:Z:119:LYS:HD2	18:Z:189:THR:HG23	1.72	0.71
10:L:44:GLN:HB3	10:L:52:THR:HB	1.73	0.70
13:O:130:SER:HB2	13:O:133:GLY:H	1.55	0.70
14:Q:262:ARG:NH1	14:Q:297:VAL:O	2.23	0.70
14:Q:275:SER:HB2	14:Q:282:SER:HB2	1.71	0.70
14:Q:414:LEU:HB3	14:Q:428:TRP:HB2	1.71	0.70
3:C:127:GLU:OE2	3:C:130:LYS:NZ	2.23	0.70
8:I:673:LEU:O	8:I:703:ARG:NH1	2.25	0.70
1:A:1134:TRP:CD1	1:A:1597:THR:HA	2.25	0.70
8:I:429:THR:HG22	8:I:430:GLU:H	1.56	0.70
1:A:252:ASP:HB2	1:A:253:PRO:HD3	1.71	0.70
1:A:1753:TYR:O	13:O:631:GLN:NE2	2.24	0.70
12:N:455:THR:O	12:N:548:ARG:NH2	2.25	0.70
13:O:28:ASP:OD1	13:O:34:LYS:NZ	2.22	0.70
14:Q:377:THR:HG22	14:Q:401:GLN:HB3	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Y:308:MET:HG3	17:Y:331:LEU:HD21	1.74	0.70
8:I:586:LEU:HB3	8:I:601:LEU:HB3	1.73	0.70
4:D:10:PRO:O	13:O:313:ARG:NH2	2.24	0.70
9:K:362:GLN:O	9:K:365:LYS:NZ	2.24	0.69
3:P:217:GLU:HA	3:P:220:LYS:HD2	1.74	0.69
14:Q:166:ARG:HA	16:S:248:ALA:HA	1.74	0.69
1:A:74:TRP:O	1:A:588:ARG:NH2	2.22	0.69
9:K:502:PHE:HB3	9:K:519:LEU:HD12	1.74	0.69
8:I:496:GLN:HB2	13:O:496:ARG:HH21	1.57	0.69
15:R:218:GLN:HE21	15:R:221:GLN:HB2	1.58	0.69
3:C:429:ARG:HG2	3:C:432:ASP:HB2	1.74	0.69
8:I:409:SER:OG	8:I:474:ARG:NH2	2.25	0.69
17:Y:383:LEU:HD13	17:Y:391:GLU:HG2	1.74	0.69
1:A:1811:LEU:HD22	1:A:1887:CYS:HB2	1.74	0.69
2:B:26:CYS:SG	2:B:56:HIS:ND1	2.59	0.69
8:I:224:SER:HB3	8:I:230:GLU:H	1.57	0.69
10:L:60:GLN:NE2	10:L:148:GLY:O	2.26	0.69
13:O:648:ILE:HA	13:O:651:ILE:HD12	1.74	0.69
14:Q:128:ALA:HB3	18:Z:156:TYR:CZ	2.28	0.69
15:R:179:PRO:HB3	16:S:224:ARG:HG2	1.72	0.69
17:Y:308:MET:HB3	17:Y:327:LEU:HD21	1.74	0.69
12:N:92:TRP:O	12:N:93:ASN:N	2.26	0.69
1:A:1084:ARG:NH2	1:A:1139:ASN:OD1	2.25	0.69
8:I:576:TRP:NE1	8:I:646:ASP:OD1	2.22	0.69
16:S:145:GLN:NE2	16:S:295:TRP:O	2.26	0.69
17:Y:267:LEU:HG	17:Y:270:ASN:HD21	1.58	0.69
6:F:130:ARG:NH1	17:Y:505:ASN:O	2.25	0.68
17:X:81:VAL:HG11	17:X:133:PRO:HG2	1.75	0.68
1:A:81:SER:H	1:A:87:VAL:HG22	1.58	0.68
3:C:386:GLN:HE22	13:O:282:ILE:HG13	1.58	0.68
6:F:12:ILE:HG21	6:F:43:LEU:HD21	1.74	0.68
10:L:98:VAL:HG12	10:L:137:ILE:HG12	1.75	0.68
12:N:663:GLN:HE21	12:N:695:ARG:HD2	1.57	0.68
14:Q:197:VAL:HA	14:Q:210:SER:HA	1.75	0.68
7:G:3:ARG:HH12	9:J:243:TYR:HA	1.59	0.68
9:J:417:GLU:OE1	9:J:420:THR:OG1	2.08	0.68
12:N:612:PRO:HG2	12:N:615:ILE:HG12	1.76	0.68
3:P:127:GLU:OE1	3:P:181:LYS:NZ	2.24	0.68
14:Q:329:ASN:ND2	16:S:23:GLU:O	2.26	0.68
12:N:247:LEU:HA	12:N:251:SER:HB2	1.76	0.68
17:Y:371:ASN:HA	17:Y:402:LEU:HD21	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:357:TYR:HB3	9:K:374:ILE:HG13	1.76	0.68
1:A:1599:ASN:HB2	1:A:1603:LEU:HA	1.76	0.68
1:A:1658:PRO:HG2	1:A:1663:LEU:HD11	1.74	0.68
6:F:504:GLN:OE1	6:F:507:ARG:NH1	2.26	0.68
8:I:374:GLN:HE22	13:O:671:GLN:HE22	1.40	0.68
17:X:462:LYS:HG3	17:X:485:LEU:HD13	1.75	0.68
8:I:644:TYR:HB2	8:I:650:THR:HG23	1.76	0.68
15:R:321:GLY:O	15:R:338:SER:OG	2.07	0.68
3:C:151:LEU:HD22	3:C:178:VAL:HG13	1.76	0.68
1:A:852:LEU:HD11	1:A:1819:GLU:HB3	1.75	0.67
14:Q:398:ALA:HB1	14:Q:418:HIS:CE1	2.30	0.67
3:C:515:TYR:HA	3:C:518:GLN:HE21	1.60	0.67
12:N:274:GLU:OE2	12:N:278:ARG:NH2	2.27	0.67
13:O:687:LEU:HD23	13:O:724:LEU:HG	1.76	0.67
3:P:344:ARG:NH1	3:P:344:ARG:O	2.26	0.67
14:Q:160:SER:O	14:Q:163:LYS:NZ	2.26	0.67
12:N:706:ARG:HB3	12:N:714:SER:HB2	1.76	0.67
16:S:144:ASN:HD22	16:S:145:GLN:N	1.92	0.67
9:J:125:GLN:HA	9:J:128:ILE:HD12	1.76	0.67
9:J:194:CYS:O	9:J:197:GLU:N	2.28	0.67
15:R:262:ARG:NH1	15:R:297:VAL:O	2.27	0.67
3:P:361:ASN:HD22	3:P:364:TYR:HB2	1.60	0.67
15:R:81:PRO:HG3	15:R:131:LEU:HD21	1.77	0.67
1:A:963:ARG:NH2	1:A:1782:GLU:O	2.26	0.67
9:K:342:HIS:NE2	7:W:2:LEU:O	2.27	0.67
14:Q:179:PRO:HA	14:Q:465:GLU:HB3	1.77	0.67
17:X:331:LEU:HB3	17:X:341:PRO:HG3	1.74	0.67
9:J:133:CYS:O	9:J:152:SER:OG	2.11	0.67
17:X:57:SER:HB2	17:X:83:HIS:HB2	1.77	0.67
1:A:808:ARG:NH1	1:A:1871:TYR:OH	2.24	0.67
3:C:280:ASP:OD1	3:C:310:ARG:NH2	2.27	0.67
15:R:287:SER:HG	16:S:295:TRP:CD1	2.13	0.67
2:B:28:MET:SD	12:N:800:GLN:NE2	2.67	0.66
8:I:589:THR:HG22	8:I:598:MET:HA	1.77	0.66
15:R:186:TYR:OH	16:S:305:GLU:N	2.27	0.66
15:R:230:SER:N	15:R:244:GLY:O	2.25	0.66
1:A:1355:GLY:H	10:L:30:VAL:HG12	1.60	0.66
8:I:23:ILE:HA	8:I:39:ASN:HA	1.77	0.66
8:I:43:GLU:HB3	8:I:60:PRO:HD3	1.76	0.66
15:R:380:ARG:O	15:R:398:ALA:N	2.20	0.66
1:A:808:ARG:NH2	1:A:1894:VAL:O	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:125:TYR:HE2	6:H:133:LYS:HD2	1.59	0.66
9:J:401:ASP:HB3	9:J:404:VAL:HG12	1.76	0.66
10:L:174:THR:O	10:L:176:ASP:N	2.28	0.66
8:I:12:ARG:HH12	8:I:751:GLU:HB3	1.59	0.66
14:Q:129:LYS:N	18:Z:157:THR:O	2.25	0.66
17:X:336:ASP:OD1	17:X:337:GLN:N	2.28	0.66
1:A:74:TRP:NE1	1:A:589:ASP:OD2	2.27	0.66
1:A:161:MET:HE3	1:A:216:PRO:HB3	1.78	0.66
1:A:442:LEU:HB3	1:A:455:VAL:HG13	1.76	0.66
6:H:621:LEU:HB3	6:H:625:ARG:HH21	1.59	0.66
15:R:193:SER:OG	15:R:197:VAL:N	2.24	0.66
15:R:377:THR:O	15:R:380:ARG:NH1	2.29	0.66
13:O:356:ASP:HA	13:O:357:SER:OG	1.96	0.66
3:P:203:TRP:HA	3:P:206:TRP:HD1	1.61	0.66
6:F:153:GLU:OE1	6:H:22:ARG:NH2	2.29	0.65
9:K:243:TYR:HA	7:W:3:ARG:HH22	1.61	0.65
13:O:592:TRP:HH2	13:O:630:ALA:HA	1.61	0.65
17:Y:199:CYS:HB3	17:Y:201:LEU:HD12	1.78	0.65
1:A:100:VAL:HG21	1:A:153:ILE:HD12	1.78	0.65
9:K:168:ASP:HA	9:K:171:THR:HG22	1.78	0.65
7:W:20:GLU:OE2	7:W:23:ARG:NH1	2.29	0.65
17:X:136:ILE:HG22	17:X:162:ILE:HD13	1.77	0.65
17:X:266:LEU:HD13	17:Y:63:MET:HE3	1.78	0.65
17:Y:196:LEU:O	17:Y:200:PRO:HB3	1.95	0.65
8:I:303:GLU:HG2	8:I:317:LEU:HD21	1.77	0.65
17:X:173:MET:HE3	17:X:177:ASN:HD21	1.61	0.65
17:Y:376:LEU:HD21	17:Y:398:GLU:HG3	1.78	0.65
1:A:489:LEU:HD22	1:A:497:LEU:HD21	1.79	0.65
6:H:615:GLU:OE2	10:L:23:ARG:NH2	2.28	0.65
15:R:310:GLN:OE1	16:S:304:LYS:NZ	2.29	0.65
18:Z:47:GLN:OE1	18:Z:52:THR:OG1	2.15	0.65
3:C:33:LYS:NZ	3:P:85:ASP:OD2	2.29	0.65
1:A:1049:VAL:HG12	1:A:1073:LEU:HD12	1.78	0.65
1:A:1067:GLU:OE2	1:A:1122:SER:OG	2.13	0.65
2:B:12:ALA:H	12:N:594:VAL:HG22	1.60	0.65
3:P:161:LYS:HB3	3:P:167:LEU:HB2	1.77	0.65
18:Z:100:TRP:HH2	18:Z:138:THR:HG21	1.62	0.65
3:C:410:GLU:OE2	15:R:83:ARG:NH2	2.29	0.65
8:I:655:ASP:N	8:I:663:ASP:O	2.29	0.65
12:N:696:MET:SD	12:N:712:THR:OG1	2.55	0.65
3:P:180:ARG:NH1	3:P:208:GLU:OE1	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:ALA:O	3:C:180:ARG:NH2	2.29	0.65
1:A:641:TRP:HE1	1:A:660:PHE:HA	1.61	0.65
6:H:537:GLU:OE1	6:H:537:GLU:N	2.25	0.65
8:I:118:VAL:HG12	8:I:214:LEU:HD11	1.79	0.65
13:O:64:LEU:O	13:O:68:LEU:N	2.28	0.65
13:O:462:ASN:O	13:O:463:THR:OG1	2.14	0.65
14:Q:290:ILE:N	14:Q:305:LEU:O	2.30	0.65
8:I:49:LEU:HD13	8:I:730:VAL:HG21	1.77	0.65
13:O:146:LEU:HD22	13:O:150:GLN:HB3	1.78	0.65
3:P:243:LEU:HG	3:P:246:GLU:HB3	1.78	0.65
3:P:475:LYS:O	3:P:479:GLN:NE2	2.29	0.65
1:A:39:LEU:HD12	13:O:244:LEU:HB3	1.78	0.65
1:A:1033:ARG:NH1	1:A:1531:GLY:O	2.30	0.65
9:K:406:HIS:HD2	9:K:447:LEU:HD12	1.62	0.65
18:Z:43:PHE:HA	18:Z:56:THR:HA	1.78	0.65
12:N:517:ASN:OD1	12:N:520:ARG:NH2	2.30	0.64
3:P:29:LEU:HA	3:P:32:ILE:HD12	1.79	0.64
3:C:81:ALA:HB2	3:P:67:LEU:HD13	1.80	0.64
14:Q:184:ASP:OD1	16:S:28:ASN:ND2	2.24	0.64
6:F:101:LYS:HB3	6:F:105:ASP:HB2	1.78	0.64
6:H:66:CYS:HB2	6:H:71:CYS:HB3	1.80	0.64
3:P:432:ASP:HB3	3:P:435:MET:HG2	1.78	0.64
14:Q:188:ASN:OD1	14:Q:359:LYS:NZ	2.24	0.64
3:C:301:ASP:OD2	3:C:364:TYR:OH	2.16	0.64
7:G:3:ARG:NH2	9:J:245:CYS:SG	2.70	0.64
8:I:692:ARG:NH1	8:I:695:GLU:OE2	2.30	0.64
9:K:166:ALA:HA	9:K:169:LEU:HD12	1.80	0.64
16:S:22:TRP:HH2	16:S:38:MET:HA	1.62	0.64
17:Y:442:GLN:H	17:Y:442:GLN:CD	2.05	0.64
1:A:1193:ILE:HG23	1:A:1208:LEU:HD23	1.79	0.64
1:A:1240:SER:HB2	1:A:1242:GLU:HG2	1.78	0.64
6:F:30:ARG:HD2	6:H:469:MET:HE1	1.79	0.64
6:F:629:ARG:HD3	17:Y:537:SER:HB2	1.78	0.64
9:K:466:ASP:OD2	9:K:470:GLN:NE2	2.31	0.64
12:N:423:PRO:HA	12:N:426:ARG:HD3	1.79	0.64
13:O:631:GLN:HB3	13:O:636:ILE:HG13	1.80	0.64
14:Q:360:ALA:HB1	14:Q:405:ILE:HG13	1.79	0.64
17:Y:434:TYR:HA	17:Y:444:LEU:HD13	1.80	0.64
3:P:179:LEU:HD12	3:P:191:VAL:HG11	1.77	0.64
15:R:316:ARG:NH1	15:R:361:VAL:O	2.30	0.64
12:N:277:CYS:O	12:N:340:ARG:NH2	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Y:442:GLN:NE2	17:Y:471:GLN:OE1	2.31	0.64
14:Q:337:PRO:HD3	14:Q:348:LEU:HG	1.79	0.64
1:A:880:TYR:HA	1:A:926:LEU:HD21	1.80	0.64
1:A:1729:GLU:O	1:A:1731:ARG:NH1	2.31	0.64
2:B:15:LEU:HD12	12:N:626:TYR:HE2	1.63	0.64
9:J:368:HIS:NE2	9:J:401:ASP:OD2	2.30	0.64
3:P:297:ILE:HD13	3:P:330:ARG:HD3	1.80	0.64
17:X:463:THR:HG23	17:X:464:LEU:HD12	1.79	0.64
6:H:69:PRO:HB3	6:H:110:PHE:HA	1.81	0.63
9:K:502:PHE:HE2	9:K:518:MET:HG3	1.62	0.63
12:N:626:TYR:CD2	12:N:633:ARG:HB3	2.33	0.63
17:X:50:His:HA	17:X:53:VAL:HG22	1.80	0.63
17:X:309:ASP:HB2	17:X:340:GLU:HG3	1.80	0.63
1:A:187:LEU:N	1:A:213:MET:O	2.30	0.63
1:A:1641:THR:H	1:A:1645:GLU:HA	1.63	0.63
3:C:233:PHE:O	3:C:237:ILE:HG12	1.98	0.63
8:I:34:LEU:H	8:I:34:LEU:HD23	1.63	0.63
1:A:979:GLY:O	1:A:1700:LYS:NZ	2.32	0.63
9:J:468:HIS:HB3	9:J:485:ILE:HG22	1.81	0.63
12:N:280:GLU:O	12:N:354:SER:OG	2.15	0.63
1:A:924:SER:OG	1:A:925:SER:N	2.19	0.63
1:A:89:TYR:HD1	13:O:536:THR:HG23	1.64	0.63
1:A:1014:ASP:OD2	1:A:1038:ARG:NH2	2.30	0.63
18:Z:105:GLU:N	18:Z:192:LYS:O	2.30	0.63
1:A:624:ALA:HB1	1:A:765:VAL:HG22	1.81	0.63
8:I:23:ILE:HG21	8:I:26:LEU:HD23	1.79	0.63
9:K:162:TYR:OH	9:K:197:GLU:OE1	2.14	0.63
12:N:666:ILE:HG12	12:N:681:LEU:HD21	1.79	0.63
15:R:224:GLN:N	15:R:227:GLU:OE2	2.31	0.63
17:X:496:ILE:O	17:X:500:ARG:HG2	1.99	0.63
1:A:1186:THR:HG23	1:A:1215:ALA:HB1	1.79	0.63
1:A:1797:ILE:HD12	1:A:1851:THR:HG21	1.81	0.63
8:I:11:PHE:O	8:I:712:ARG:NH1	2.31	0.63
8:I:279:ILE:HD11	8:I:337:ILE:HG12	1.81	0.63
8:I:734:LEU:HD11	8:I:738:LEU:HA	1.81	0.63
9:K:450:ASN:OD1	7:W:9:LEU:N	2.24	0.63
13:O:386:GLN:HB3	13:O:424:GLN:NE2	2.14	0.63
1:A:1232:ILE:HD12	1:A:1233:PRO:HD2	1.80	0.63
8:I:185:ILE:HG13	8:I:201:ILE:HG13	1.81	0.63
9:J:59:ALA:O	9:J:63:ARG:NH1	2.32	0.63
9:J:502:PHE:HE1	9:J:515:SER:HA	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:407:GLN:HE22	15:R:81:PRO:HG2	1.63	0.63
15:R:173:ASP:OD1	15:R:471:ARG:N	2.28	0.63
17:Y:54:ARG:HB2	17:Y:86:SER:HB2	1.81	0.63
17:Y:225:ASN:O	17:Y:229:THR:OG1	2.11	0.63
3:C:189:ILE:O	3:C:193:VAL:HG23	1.99	0.62
6:H:42:PHE:O	6:H:46:THR:HG23	1.99	0.62
9:J:157:LEU:HD21	9:J:167:PHE:HD2	1.63	0.62
9:K:401:ASP:HB3	9:K:404:VAL:HG22	1.81	0.62
13:O:414:LEU:HD13	13:O:417:LEU:HB2	1.79	0.62
15:R:218:GLN:NE2	15:R:221:GLN:HB2	2.14	0.62
15:R:262:ARG:NH2	15:R:298:ALA:O	2.30	0.62
17:X:389:VAL:O	17:X:393:ILE:HG13	1.98	0.62
1:A:127:LEU:HD11	1:A:187:LEU:HD11	1.79	0.62
1:A:1571:ARG:NH1	1:A:1694:ASP:O	2.31	0.62
3:C:361:ASN:HD22	3:C:364:TYR:HB2	1.63	0.62
10:L:44:GLN:O	10:L:52:THR:OG1	2.17	0.62
12:N:187:SER:HA	12:N:190:LYS:HD2	1.81	0.62
17:X:455:PRO:O	17:X:457:THR:N	2.32	0.62
17:X:54:ARG:HG3	17:X:86:SER:HB2	1.79	0.62
5:E:99:ILE:O	5:E:102:LEU:N	2.32	0.62
9:J:179:GLN:O	9:J:183:GLU:HG2	1.99	0.62
12:N:164:SER:H	12:N:165:THR:HA	1.63	0.62
9:J:306:GLY:HA3	9:J:323:LEU:HD22	1.82	0.62
9:K:487:TYR:OH	7:W:15:ASP:O	2.14	0.62
3:P:91:LYS:NZ	3:P:95:ASP:OD2	2.33	0.62
17:Y:331:LEU:HB3	17:Y:341:PRO:HG3	1.81	0.62
6:H:130:ARG:HG2	9:K:469:ARG:HD3	1.81	0.62
8:I:621:GLY:N	8:I:705:MET:O	2.33	0.62
12:N:630:LYS:HB3	12:N:633:ARG:HD2	1.81	0.62
1:A:1797:ILE:HG22	1:A:1852:ILE:HD11	1.81	0.62
6:F:541:THR:HA	6:F:575:ASN:HD21	1.65	0.62
7:G:4:ARG:HB2	9:J:342:HIS:HE2	1.65	0.62
9:J:70:GLU:HA	9:J:73:ARG:HB3	1.81	0.62
9:K:178:ALA:HA	9:K:181:GLU:HB2	1.80	0.62
9:K:190:LEU:O	9:K:198:GLN:NE2	2.30	0.62
11:M:15:ILE:HG22	11:M:17:ASP:H	1.65	0.62
11:M:31:ILE:HG22	11:M:33:LEU:H	1.65	0.62
12:N:767:SER:OG	12:N:816:ARG:NH1	2.33	0.62
13:O:589:GLU:HA	13:O:592:TRP:HD1	1.65	0.62
1:A:1141:VAL:HG11	1:A:1608:HIS:CD2	2.35	0.62
13:O:378:SER:HB2	13:O:408:LEU:HD11	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:S:19:GLY:N	16:S:21:GLU:OE1	2.32	0.62
17:Y:223:THR:HA	17:Y:226:VAL:HG12	1.81	0.62
1:A:248:PHE:CZ	1:A:250:ASN:HB2	2.34	0.62
13:O:55:MET:SD	13:O:58:ARG:NH1	2.73	0.62
17:X:168:THR:HB	17:X:169:PRO:HD2	1.81	0.62
17:X:386:MET:HG3	17:X:388:ARG:HH21	1.65	0.62
1:A:1470:LEU:HA	1:A:1522:SER:OG	1.99	0.62
6:H:685:SER:HB2	6:H:716:ASN:HD21	1.64	0.62
17:X:526:GLN:HG2	17:X:527:GLU:H	1.65	0.62
1:A:611:GLU:OE1	1:A:613:ALA:N	2.29	0.61
1:A:1455:GLU:HG2	1:A:1456:THR:H	1.64	0.61
3:C:297:ILE:HD11	3:C:333:THR:HB	1.82	0.61
3:C:453:LYS:HZ2	3:C:480:LEU:HD22	1.65	0.61
6:F:633:ARG:HA	6:F:664:ILE:HD13	1.82	0.61
8:I:42:GLY:HA3	8:I:67:GLU:HA	1.80	0.61
11:M:4:GLU:OE2	3:P:50:HIS:ND1	2.32	0.61
12:N:331:PHE:CZ	12:N:335:ILE:HD11	2.35	0.61
6:F:14:GLN:O	6:F:18:HIS:ND1	2.28	0.61
12:N:780:PHE:HB2	16:S:205:LEU:HD12	1.82	0.61
3:P:244:ILE:HD13	3:P:276:ILE:HG13	1.82	0.61
14:Q:444:SER:HB3	14:Q:463:ALA:HB3	1.82	0.61
17:Y:291:VAL:HG22	17:Y:314:LEU:HB3	1.81	0.61
1:A:489:LEU:HD11	1:A:609:ILE:HD11	1.82	0.61
1:A:880:TYR:OH	1:A:957:ASP:OD2	2.14	0.61
8:I:721:TYR:HB2	8:I:734:LEU:HB3	1.82	0.61
9:K:449:ASN:ND2	7:W:8:ARG:HE	1.96	0.61
12:N:150:ARG:HE	12:N:153:VAL:HG21	1.64	0.61
12:N:185:MET:HE1	12:N:295:ARG:HD3	1.82	0.61
14:Q:179:PRO:HD3	16:S:315:THR:HG22	1.82	0.61
1:A:1065:GLU:HA	1:A:1068:ASN:HD22	1.64	0.61
8:I:88:LYS:NZ	8:I:107:GLU:O	2.31	0.61
8:I:636:TYR:HB3	8:I:653:LEU:HB3	1.81	0.61
9:J:276:VAL:HA	9:J:311:MET:SD	2.41	0.61
9:K:37:PRO:HA	9:K:65:LEU:HD21	1.82	0.61
9:K:465:LEU:HG	9:K:488:ILE:HG21	1.81	0.61
12:N:529:HIS:O	12:N:530:GLN:HG2	2.01	0.61
15:R:281:LEU:HB3	15:R:293:HIS:HB2	1.82	0.61
17:X:140:TYR:HD1	17:X:171:ILE:HG13	1.64	0.61
17:X:417:TYR:HB3	17:X:426:ALA:HB2	1.82	0.61
1:A:1551:ASN:ND2	1:A:1593:PRO:O	2.34	0.61
10:L:113:LEU:HB3	10:L:116:PRO:HG3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:467:ALA:HB1	13:O:506:LEU:HD11	1.83	0.61
14:Q:165:CYS:HA	16:S:224:ARG:HH21	1.65	0.61
1:A:1333:HIS:HB2	1:A:1357:THR:HA	1.82	0.61
9:J:433:LYS:NZ	9:J:437:ASN:O	2.24	0.61
14:Q:180:GLU:N	14:Q:465:GLU:OE1	2.31	0.61
1:A:441:PHE:HE2	1:A:503:VAL:HG23	1.64	0.61
1:A:1243:LEU:HD22	15:R:116:TRP:CD1	2.34	0.61
9:J:230:ASN:HB3	9:J:233:VAL:HG22	1.82	0.61
4:D:13:THR:HG22	13:O:255:TYR:HE2	1.66	0.61
14:Q:209:TRP:HD1	14:Q:216:ILE:HG13	1.64	0.61
1:A:597:LEU:HD11	1:A:607:ILE:HD13	1.83	0.61
13:O:328:ILE:HG22	13:O:343:CYS:HB3	1.82	0.61
13:O:700:TYR:O	13:O:704:VAL:HG23	2.00	0.61
3:C:262:SER:OG	3:C:265:ILE:HB	2.01	0.61
6:F:668:SER:OG	6:F:671:LEU:HB2	2.00	0.61
17:Y:465:LEU:HD21	17:Y:482:LYS:HB2	1.83	0.61
8:I:262:LEU:HD11	8:I:533:ILE:HG21	1.82	0.60
9:K:74:TYR:OH	9:K:78:ARG:NH1	2.33	0.60
14:Q:176:LEU:HD22	16:S:312:PRO:HD2	1.81	0.60
15:R:228:TYR:OH	15:R:270:ARG:NH2	2.34	0.60
15:R:251:GLN:OE1	15:R:253:TRP:NE1	2.29	0.60
15:R:414:LEU:O	15:R:428:TRP:N	2.24	0.60
17:X:38:ILE:HD11	17:X:79:LEU:HD12	1.81	0.60
3:C:101:ARG:HG3	3:P:295:TYR:HB2	1.81	0.60
8:I:162:ASP:HA	8:I:165:ILE:HD12	1.82	0.60
12:N:297:VAL:HG21	12:N:325:ARG:HG3	1.82	0.60
14:Q:183:ASN:HD21	16:S:91:GLN:HG3	1.66	0.60
15:R:333:VAL:HG22	15:R:358:VAL:HG11	1.82	0.60
17:X:488:ARG:O	17:X:490:GLN:NE2	2.33	0.60
17:Y:312:GLY:HA3	17:Y:344:VAL:HG12	1.82	0.60
1:A:54:ALA:HB3	3:C:395:ASN:HD21	1.66	0.60
1:A:601:ASN:ND2	1:A:603:SER:OG	2.34	0.60
1:A:1191:LEU:HD23	1:A:1191:LEU:H	1.66	0.60
9:J:85:GLU:OE2	9:J:88:GLN:NE2	2.34	0.60
9:K:342:HIS:CD2	7:W:4:ARG:HB3	2.36	0.60
12:N:803:VAL:O	12:N:806:GLN:NE2	2.33	0.60
14:Q:142:GLU:H	16:S:202:ARG:HD2	1.65	0.60
18:Z:183:LEU:HD11	18:Z:197:VAL:HB	1.83	0.60
1:A:487:THR:HG23	1:A:501:THR:HA	1.84	0.60
1:A:500:TYR:CZ	1:A:505:ARG:HB2	2.35	0.60
3:C:307:LEU:HD11	3:C:315:GLU:HG3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:74:ARG:NH2	8:I:76:ASP:OD2	2.34	0.60
8:I:231:VAL:HG23	8:I:556:LEU:HB2	1.82	0.60
9:J:5:ARG:O	9:J:9:ARG:HG2	2.01	0.60
12:N:284:SER:HA	12:N:285:PHE:CG	2.37	0.60
15:R:267:HIS:NE2	15:R:283:SER:OG	2.30	0.60
3:C:393:GLU:OE1	13:O:280:ARG:NH1	2.35	0.60
8:I:235:GLN:NE2	8:I:604:HIS:O	2.29	0.60
9:J:162:TYR:HE1	9:J:201:LEU:HD11	1.64	0.60
13:O:112:PHE:HA	13:O:115:LEU:HD12	1.83	0.60
14:Q:144:TYR:HE1	18:Z:146:GLU:HA	1.66	0.60
18:Z:117:ARG:NH1	18:Z:189:THR:O	2.35	0.60
9:J:272:ILE:O	9:J:276:VAL:HG23	2.02	0.60
9:J:410:VAL:O	9:J:414:GLN:HG2	2.02	0.60
9:K:393:GLN:O	9:K:396:SER:OG	2.17	0.60
17:Y:446:LEU:O	17:Y:450:VAL:HG23	2.01	0.60
17:Y:452:LEU:HD21	17:Y:460:LYS:HB3	1.82	0.60
9:J:503:HIS:HE1	3:P:421:TYR:OH	1.85	0.60
17:Y:390:GLN:OE1	17:Y:390:GLN:N	2.34	0.60
17:Y:424:ARG:O	17:Y:428:VAL:HG23	2.01	0.60
17:Y:495:GLY:HA3	17:Y:518:PHE:HE2	1.67	0.60
1:A:1134:TRP:CZ3	1:A:1605:ALA:HB2	2.35	0.60
8:I:387:GLU:HA	8:I:390:ILE:HD12	1.84	0.60
17:Y:160:ASP:OD1	17:Y:179:TYR:OH	2.19	0.60
17:Y:194:GLU:HA	17:Y:197:ARG:HG2	1.83	0.60
17:Y:265:SER:OG	17:Y:268:ARG:NH1	2.34	0.60
1:A:39:LEU:HD23	1:A:39:LEU:H	1.67	0.60
6:F:705:CYS:SG	6:F:706:LYS:N	2.74	0.60
6:F:707:PHE:HB2	6:F:729:LEU:HD21	1.84	0.60
6:H:636:ASN:ND2	10:L:184:ARG:O	2.34	0.60
6:H:696:ILE:HG23	6:H:706:LYS:HZ2	1.67	0.60
8:I:34:LEU:HD12	8:I:46:LEU:HD11	1.83	0.60
8:I:90:ILE:HD11	8:I:110:VAL:HG21	1.82	0.60
9:K:502:PHE:CE2	9:K:518:MET:HG3	2.36	0.60
10:L:75:LYS:HB2	10:L:161:PRO:HG3	1.83	0.60
12:N:204:ASP:HB2	12:N:282:GLU:HG3	1.82	0.60
13:O:669:LYS:NZ	13:O:755:LEU:O	2.35	0.60
3:P:297:ILE:HD11	3:P:333:THR:HB	1.84	0.60
1:A:11:MET:HB2	1:A:508:LYS:HG3	1.84	0.60
8:I:139:LEU:HB2	8:I:165:ILE:HG23	1.84	0.60
3:P:251:TYR:HB3	3:P:269:ILE:HD11	1.84	0.60
1:A:215:HIS:CD2	1:A:217:LEU:H	2.20	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:89:LYS:HA	8:I:105:SER:HA	1.83	0.59
15:R:206:VAL:HG13	15:R:219:LEU:HB3	1.84	0.59
1:A:23:PHE:HB2	1:A:111:LEU:HD13	1.84	0.59
1:A:1619:LEU:HD11	1:A:1697:LEU:HB2	1.83	0.59
2:B:34:CYS:HB3	2:B:56:HIS:CG	2.36	0.59
9:J:350:HIS:O	9:J:354:MET:HG2	2.01	0.59
9:J:371:MET:HA	9:J:374:ILE:HD12	1.84	0.59
12:N:802:LYS:HD2	12:N:807:GLN:HE21	1.66	0.59
3:P:389:ARG:NH2	3:P:409:TYR:OH	2.34	0.59
17:X:290:SER:HB3	17:X:314:LEU:HD11	1.84	0.59
1:A:1262:GLN:HE22	1:A:1579:SER:HB2	1.68	0.59
6:H:496:TYR:HA	6:H:501:VAL:HG11	1.84	0.59
8:I:188:TYR:CZ	8:I:194:LYS:HB2	2.38	0.59
10:L:32:SER:HB2	10:L:65:ASN:HB2	1.84	0.59
12:N:570:ILE:HG12	12:N:626:TYR:CE1	2.32	0.59
13:O:445:LEU:HD23	13:O:469:ALA:HB2	1.84	0.59
1:A:1162:LYS:HG3	1:A:1163:PRO:HD2	1.83	0.59
2:B:14:TRP:HA	2:B:15:LEU:CG	2.31	0.59
6:F:55:TYR:CE2	6:F:56:LYS:HG3	2.37	0.59
9:J:224:VAL:HG12	9:J:225:ASP:H	1.68	0.59
9:K:133:CYS:O	9:K:152:SER:OG	2.21	0.59
9:K:453:HIS:HA	9:K:456:ARG:NH1	2.16	0.59
15:R:355:GLN:H	15:R:379:ASP:CG	2.10	0.59
3:C:243:LEU:HG	3:C:246:GLU:HB2	1.84	0.59
6:H:128:THR:OG1	6:H:130:ARG:NH1	2.35	0.59
15:R:182:ARG:NH1	15:R:203:ASP:OD1	2.35	0.59
5:E:63:VAL:HG21	17:Y:364:LYS:HB2	1.84	0.59
12:N:609:LEU:HD13	12:N:639:HIS:HD2	1.67	0.59
14:Q:193:SER:HB3	14:Q:234:TRP:CE2	2.37	0.59
14:Q:322:ARG:NH2	14:Q:369:ASN:OD1	2.30	0.59
16:S:144:ASN:ND2	16:S:145:GLN:N	2.49	0.59
16:S:145:GLN:HA	16:S:294:PRO:HB3	1.84	0.59
17:Y:260:SER:O	17:Y:264:LYS:NZ	2.30	0.59
1:A:1313:LEU:HD12	1:A:1316:MET:HG3	1.83	0.59
2:B:70:GLN:HB3	2:B:72:HIS:HD2	1.67	0.59
12:N:559:VAL:HG13	12:N:560:MET:HE3	1.85	0.59
14:Q:270:ARG:HG2	14:Q:286:ARG:HB2	1.84	0.59
17:X:40:HIS:HD2	17:Y:201:LEU:HD11	1.66	0.59
1:A:1320:ASN:ND2	1:A:1323:GLU:OE1	2.34	0.59
9:K:491:LEU:HD21	7:W:19:PHE:HA	1.84	0.59
15:R:471:ARG:HD2	15:R:474:GLU:HB2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1074:CYS:O	1:A:1078:MET:HG2	2.02	0.59
2:B:17:VAL:HG21	12:N:634:THR:H	1.67	0.59
2:B:23:CYS:O	2:B:27:ARG:NH2	2.36	0.59
6:H:142:LEU:HD11	6:H:152:PHE:HB2	1.85	0.59
9:K:410:VAL:HG13	7:W:9:LEU:HD21	1.84	0.59
12:N:619:LEU:HD13	12:N:637:TRP:CE2	2.38	0.59
14:Q:377:THR:O	14:Q:380:ARG:NH1	2.35	0.59
16:S:73:ASP:HB2	16:S:74:PRO:HD3	1.85	0.59
1:A:24:GLY:HA3	1:A:94:TYR:CG	2.38	0.59
12:N:186:GLN:HA	12:N:189:ARG:HD2	1.85	0.59
12:N:630:LYS:HB3	12:N:633:ARG:CD	2.32	0.59
14:Q:262:ARG:NH2	14:Q:298:ALA:O	2.35	0.59
18:Z:107:ASP:OD2	18:Z:117:ARG:NH1	2.36	0.59
1:A:1225:THR:O	1:A:1229:SER:OG	2.18	0.58
1:A:1274:LEU:HD11	1:A:1321:VAL:HG12	1.85	0.58
3:C:140:PRO:HB3	13:O:248:PRO:HD2	1.85	0.58
5:E:78:ARG:NH2	17:Y:329:CYS:SG	2.75	0.58
5:E:93:GLU:OE2	6:H:595:GLN:NE2	2.34	0.58
17:Y:72:SER:OG	17:Y:74:PRO:HD2	2.02	0.58
2:B:34:CYS:SG	2:B:37:CYS:HB2	2.43	0.58
3:C:36:LEU:HD13	3:C:228:TRP:HH2	1.67	0.58
6:F:686:GLU:HG2	6:F:687:LYS:H	1.68	0.58
8:I:224:SER:OG	8:I:228:ALA:O	2.18	0.58
9:J:217:GLU:HG3	9:J:240:ARG:HD2	1.86	0.58
13:O:57:ARG:HA	13:O:60:LEU:HD12	1.85	0.58
3:P:399:TYR:HB3	3:P:428:LEU:HD22	1.86	0.58
3:P:442:CYS:HA	3:P:445:LYS:HE3	1.85	0.58
3:C:46:ARG:HB3	3:C:116:PHE:CE2	2.38	0.58
8:I:606:ASP:HB3	8:I:609:GLN:HB2	1.85	0.58
9:K:284:LEU:HD21	9:K:307:CYS:SG	2.43	0.58
10:L:74:VAL:HG11	10:L:137:ILE:HD11	1.85	0.58
10:L:126:ASP:HB2	10:L:132:THR:HG22	1.86	0.58
13:O:446:LEU:HD21	13:O:470:LEU:HD21	1.85	0.58
3:P:523:CYS:O	3:P:524:LYS:HG3	2.03	0.58
17:X:214:VAL:HG12	17:X:217:ALA:H	1.69	0.58
17:Y:411:GLU:O	17:Y:414:ILE:HG22	2.03	0.58
1:A:1156:ALA:HB2	13:O:329:ARG:HG3	1.86	0.58
1:A:1799:ARG:HH21	1:A:1805:MET:HG2	1.68	0.58
3:C:470:LEU:HD13	3:C:493:TYR:HA	1.84	0.58
14:Q:380:ARG:O	14:Q:398:ALA:N	2.32	0.58
17:Y:267:LEU:HG	17:Y:270:ASN:ND2	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:808:ARG:HH22	1:A:1871:TYR:HE2	1.51	0.58
1:A:1573:SER:C	1:A:1617:ARG:HH21	2.11	0.58
6:H:35:VAL:HG12	6:H:37:SER:H	1.69	0.58
9:K:217:GLU:HG2	9:K:218:THR:HG23	1.84	0.58
12:N:80:GLN:HG2	12:N:129:LEU:HD13	1.86	0.58
16:S:85:THR:HA	16:S:88:ASN:HD22	1.69	0.58
8:I:56:TRP:CE3	8:I:98:PRO:HB3	2.38	0.58
9:K:263:PHE:HZ	9:K:290:LYS:HB3	1.68	0.58
13:O:113:ASP:O	13:O:116:SER:OG	2.16	0.58
13:O:656:ALA:O	13:O:659:ASP:N	2.35	0.58
3:C:73:PRO:HG3	3:P:73:PRO:HG2	1.86	0.58
3:C:137:SER:O	3:C:143:LYS:NZ	2.35	0.58
3:C:322:ASN:O	3:C:325:GLU:HG3	2.02	0.58
6:H:85:LEU:HD22	6:H:124:VAL:HG13	1.84	0.58
8:I:94:ASP:OD1	8:I:95:VAL:N	2.36	0.58
1:A:961:HIS:HA	1:A:964:GLU:CD	2.29	0.58
10:L:49:ASN:HB2	10:L:52:THR:HG23	1.84	0.58
12:N:393:THR:OG1	12:N:431:ARG:HD3	2.04	0.58
15:R:264:MET:HG2	15:R:300:HIS:CG	2.39	0.58
17:Y:510:VAL:HG13	17:Y:513:ARG:HH21	1.69	0.58
1:A:17:LEU:HD11	1:A:605:VAL:HB	1.85	0.58
1:A:1205:SER:O	1:A:1209:LEU:HG	2.04	0.58
1:A:1813:GLN:O	1:A:1817:VAL:HG23	2.04	0.58
6:F:7:PRO:HG3	6:H:455:GLN:HG2	1.85	0.58
8:I:241:LEU:HD13	8:I:548:MET:HE1	1.86	0.58
8:I:583:LEU:HD21	8:I:611:VAL:HG21	1.86	0.58
12:N:629:LEU:HD23	12:N:630:LYS:HB2	1.85	0.58
13:O:219:GLN:HE22	13:O:231:LEU:H	1.52	0.58
3:P:233:PHE:CZ	3:P:237:ILE:HD11	2.39	0.58
15:R:205:SER:HB3	15:R:221:GLN:HG3	1.86	0.58
17:Y:432:ASN:OD1	17:Y:435:LYS:NZ	2.36	0.58
1:A:133:ILE:HA	3:C:454:LYS:HZ1	1.67	0.58
1:A:1292:GLU:OE1	1:A:1292:GLU:N	2.34	0.58
3:C:289:LEU:HD21	3:C:296:ARG:HG2	1.86	0.58
3:C:355:GLN:HB2	3:C:371:MET:HE3	1.85	0.58
6:H:693:ASN:OD1	6:H:709:ARG:NH1	2.37	0.58
6:H:714:PHE:HD2	6:H:746:VAL:HG22	1.68	0.58
9:J:17:GLN:O	9:K:78:ARG:NH2	2.35	0.58
12:N:681:LEU:O	12:N:685:VAL:HG22	2.04	0.58
14:Q:288:GLY:HA2	14:Q:312:VAL:HG23	1.86	0.58
17:X:303:TYR:HB2	17:Y:95:ASN:HD21	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:HIS:CD2	1:A:168:ASP:HB3	2.39	0.57
3:P:290:ARG:NH2	3:P:300:MET:SD	2.71	0.57
17:X:172:ASN:O	17:X:191:SER:OG	2.22	0.57
17:X:520:VAL:HG23	17:X:528:ALA:HB1	1.85	0.57
17:Y:316:ALA:HB1	17:Y:351:TYR:CE2	2.39	0.57
6:H:582:GLU:HB3	6:H:585:ILE:HD12	1.85	0.57
8:I:185:ILE:O	8:I:198:VAL:N	2.28	0.57
8:I:667:VAL:HG22	8:I:711:TRP:HB2	1.86	0.57
12:N:708:GLU:H	12:N:712:THR:HA	1.69	0.57
1:A:1301:ALA:O	1:A:1305:VAL:HG23	2.03	0.57
3:C:118:TYR:CZ	3:C:122:ARG:HD2	2.38	0.57
6:F:155:LEU:HA	6:F:158:ILE:HD12	1.85	0.57
13:O:663:ALA:O	13:O:667:VAL:HG23	2.03	0.57
14:Q:249:GLU:OE1	14:Q:263:ASN:ND2	2.35	0.57
6:F:526:ARG:HH11	6:F:536:MET:HE3	1.70	0.57
8:I:269:LEU:HD21	8:I:523:HIS:CE1	2.39	0.57
8:I:394:GLY:O	8:I:398:LEU:HG	2.04	0.57
9:J:429:LEU:HA	9:J:432:ILE:HG22	1.85	0.57
3:P:334:CYS:HB3	3:P:357:ALA:HB2	1.86	0.57
17:X:270:ASN:HD22	17:Y:62:THR:HG21	1.70	0.57
17:X:472:ARG:HB3	17:X:475:TYR:HB2	1.86	0.57
1:A:86:ASP:OD2	13:O:547:LYS:HG2	2.05	0.57
1:A:1289:THR:OG1	1:A:1290:ASP:OD2	2.18	0.57
2:B:55:PHE:HB2	2:B:60:ILE:HD13	1.87	0.57
5:E:105:PHE:CZ	6:H:619:LYS:HG3	2.35	0.57
13:O:464:GLU:HA	13:O:467:ALA:HB3	1.86	0.57
14:Q:373:THR:OG1	14:Q:385:TRP:NE1	2.38	0.57
1:A:42:LEU:HD11	3:C:394:VAL:HG13	1.86	0.57
8:I:734:LEU:HA	8:I:741:VAL:HG12	1.86	0.57
9:J:264:HIS:NE2	9:J:266:SER:OG	2.25	0.57
14:Q:353:GLN:NE2	18:Z:47:GLN:OE1	2.36	0.57
15:R:429:LYS:HB3	15:R:434:ALA:HB3	1.87	0.57
17:X:174:MET:HA	17:X:177:ASN:HD22	1.70	0.57
17:Y:174:MET:O	17:Y:178:LEU:HG	2.04	0.57
6:F:495:HIS:HE1	6:H:34:GLU:HB2	1.69	0.57
6:F:723:LEU:HG	6:F:746:VAL:HG11	1.87	0.57
8:I:287:LEU:O	8:I:291:VAL:HG23	2.04	0.57
10:L:144:ASN:ND2	10:L:148:GLY:O	2.36	0.57
12:N:609:LEU:HA	12:N:686:LYS:HB2	1.86	0.57
12:N:716:ILE:HG13	12:N:718:GLU:H	1.67	0.57
3:P:488:GLN:HG3	3:P:492:LYS:HD2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:49:LEU:O	3:C:52:SER:OG	2.22	0.57
8:I:28:TRP:CE3	8:I:35:ILE:HB	2.39	0.57
8:I:312:LYS:HG2	8:I:428:MET:HB3	1.86	0.57
12:N:516:ILE:HD11	12:N:549:PHE:HD2	1.69	0.57
13:O:348:TYR:CZ	13:O:352:GLN:HG3	2.39	0.57
3:P:480:LEU:HD23	3:P:482:GLU:HB2	1.87	0.57
17:Y:159:LEU:HD13	17:Y:171:ILE:HG23	1.87	0.57
1:A:776:ASN:ND2	1:A:779:MET:HE2	2.20	0.57
6:F:130:ARG:NH1	17:Y:506:GLN:HB3	2.18	0.57
6:F:150:SER:HB3	6:H:23:ASP:HB3	1.87	0.57
9:J:162:TYR:CE1	9:J:201:LEU:HD11	2.40	0.57
15:R:94:LEU:HD21	15:R:125:VAL:O	2.04	0.57
16:S:59:LYS:NZ	16:S:63:GLU:OE2	2.38	0.57
1:A:162:HIS:HD2	1:A:168:ASP:HB3	1.69	0.57
5:E:89:LEU:HD11	6:H:592:ARG:HB2	1.86	0.57
6:H:567:PRO:HG3	6:H:597:ASP:HB2	1.86	0.57
6:H:717:GLU:HA	6:H:719:TYR:CE1	2.40	0.57
14:Q:384:ILE:HG22	14:Q:393:LEU:HD12	1.86	0.57
18:Z:185:SER:OG	18:Z:193:VAL:O	2.22	0.57
1:A:968:SER:HG	1:A:970:TRP:CD1	2.23	0.56
9:J:445:GLU:OE1	9:J:475:ILE:HD13	2.05	0.56
12:N:754:PHE:HD1	12:N:777:LEU:HD22	1.69	0.56
3:C:134:THR:HG23	3:C:143:LYS:HG3	1.85	0.56
6:H:544:TRP:CZ3	10:L:184:ARG:HD2	2.40	0.56
12:N:612:PRO:HB3	12:N:665:VAL:HG23	1.85	0.56
1:A:776:ASN:HD22	1:A:779:MET:HE2	1.70	0.56
1:A:1063:ILE:HA	1:A:1066:LYS:HE2	1.87	0.56
1:A:1704:GLY:H	1:A:1742:THR:HG21	1.69	0.56
2:B:14:TRP:HD1	12:N:596:LEU:C	2.13	0.56
3:C:96:VAL:N	3:C:97:LYS:HA	2.21	0.56
6:H:624:PHE:CE1	6:H:640:GLY:HA3	2.40	0.56
8:I:676:ASN:HD21	8:I:678:GLU:HB2	1.70	0.56
9:K:127:SER:OG	9:K:128:ILE:N	2.37	0.56
13:O:565:GLN:O	13:O:569:VAL:HG23	2.06	0.56
3:P:397:ARG:HA	3:P:428:LEU:HD11	1.87	0.56
17:Y:442:GLN:O	17:Y:445:THR:OG1	2.23	0.56
1:A:1810:GLU:O	1:A:1813:GLN:HG2	2.05	0.56
9:K:35:GLU:HB3	9:K:40:ILE:HG12	1.87	0.56
11:M:3:SER:OG	3:P:180:ARG:NH2	2.38	0.56
12:N:674:ALA:HB1	12:N:715:VAL:HG21	1.87	0.56
3:P:303:PHE:CD2	3:P:319:LEU:HD22	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:X:146:TYR:HB2	17:X:155:ALA:HB2	1.87	0.56
17:X:316:ALA:HB1	17:X:351:TYR:HE1	1.70	0.56
1:A:1284:GLU:HB2	1:A:1350:TYR:CZ	2.41	0.56
3:C:370:LEU:HD22	15:R:78:ARG:NH2	2.21	0.56
6:H:625:ARG:CZ	9:K:506:LEU:HD22	2.35	0.56
8:I:29:SER:O	8:I:725:ASN:ND2	2.39	0.56
12:N:574:ILE:HG13	12:N:625:LYS:HD2	1.88	0.56
13:O:682:LYS:O	13:O:685:GLU:HG2	2.06	0.56
15:R:369:ASN:ND2	15:R:388:CYS:SG	2.79	0.56
1:A:127:LEU:HD23	1:A:127:LEU:H	1.71	0.56
1:A:491:LEU:HA	1:A:497:LEU:HA	1.87	0.56
3:C:327:ASP:O	3:C:333:THR:HG21	2.05	0.56
6:F:15:ALA:HB1	6:F:20:ALA:HB3	1.88	0.56
8:I:428:MET:SD	8:I:429:THR:OG1	2.62	0.56
8:I:669:LEU:HD11	8:I:674:VAL:HG23	1.87	0.56
9:J:395:LEU:HD11	9:J:408:VAL:HG21	1.86	0.56
9:K:450:ASN:HD21	7:W:8:ARG:HA	1.70	0.56
12:N:506:VAL:HA	12:N:510:GLY:O	2.06	0.56
14:Q:401:GLN:HG3	14:Q:419:GLY:HA3	1.87	0.56
15:R:219:LEU:HD12	15:R:258:GLN:HG3	1.87	0.56
17:X:170:LYS:HG3	17:X:171:ILE:HD12	1.88	0.56
18:Z:105:GLU:HB3	18:Z:192:LYS:HB3	1.87	0.56
6:F:53:LYS:HB3	6:F:56:LYS:HD3	1.86	0.56
9:J:171:THR:OG1	9:J:181:GLU:OE2	2.20	0.56
9:J:212:TYR:HB3	9:J:243:TYR:HB3	1.88	0.56
12:N:619:LEU:HD13	12:N:637:TRP:CZ2	2.41	0.56
13:O:682:LYS:HB3	13:O:685:GLU:CD	2.31	0.56
3:P:263:SER:OG	3:P:296:ARG:NH1	2.32	0.56
1:A:34:ALA:O	13:O:237:GLN:NE2	2.38	0.56
12:N:799:LEU:O	12:N:803:VAL:HG23	2.06	0.56
3:P:332:GLU:N	3:P:332:GLU:OE1	2.36	0.56
15:R:277:ASN:HB3	15:R:280:ILE:HB	1.88	0.56
15:R:322:ARG:HH22	15:R:369:ASN:HD21	1.54	0.56
17:X:465:LEU:HD22	17:X:482:LYS:HB2	1.87	0.56
17:Y:134:SER:HB3	17:Y:137:GLU:HG3	1.87	0.56
17:Y:339:ALA:O	17:Y:343:VAL:HG23	2.06	0.56
17:Y:475:TYR:HB3	17:Y:478:ALA:HB3	1.87	0.56
1:A:258:THR:OG1	1:A:269:TRP:NE1	2.38	0.56
7:G:1:MET:HG2	9:J:335:PRO:HG3	1.86	0.56
8:I:495:ASN:HA	13:O:460:GLN:HB2	1.88	0.56
9:J:55:ARG:NH1	9:K:265:ALA:H	2.02	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:N:778:ARG:HH22	12:N:779:MET:HG3	1.71	0.56
6:H:21:TYR:HB3	6:H:51:SER:OG	2.06	0.56
6:H:735:LYS:NZ	17:X:182:ALA:O	2.30	0.56
8:I:27:VAL:HG23	8:I:73:TRP:CD1	2.41	0.56
10:L:90:THR:HG21	10:L:116:PRO:HD2	1.86	0.56
13:O:292:GLY:HA3	13:O:336:ASP:HB3	1.87	0.56
17:Y:432:ASN:O	17:Y:436:THR:HG23	2.06	0.56
1:A:23:PHE:HB2	1:A:111:LEU:HD22	1.87	0.55
8:I:742:ARG:HD2	8:I:744:PHE:CZ	2.41	0.55
11:M:7:ARG:HB2	11:M:12:LEU:HD21	1.88	0.55
12:N:659:VAL:HG23	12:N:728:VAL:HG23	1.86	0.55
13:O:103:GLY:O	13:O:155:TYR:OH	2.18	0.55
14:Q:424:GLN:OE1	14:Q:424:GLN:N	2.39	0.55
1:A:1377:LYS:NZ	1:A:1577:SER:O	2.36	0.55
6:F:42:PHE:O	6:F:46:THR:HG23	2.07	0.55
6:F:72:LYS:HG2	6:F:91:ILE:HD11	1.89	0.55
8:I:310:TRP:HA	13:O:127:HIS:HB2	1.87	0.55
9:J:129:LYS:O	9:J:132:ILE:HG22	2.06	0.55
13:O:82:ILE:HG23	13:O:90:ALA:HB2	1.87	0.55
14:Q:457:THR:HA	14:Q:471:ARG:HA	1.88	0.55
18:Z:76:LEU:HD21	18:Z:104:ILE:HD13	1.88	0.55
3:C:46:ARG:HB3	3:C:116:PHE:HE2	1.71	0.55
8:I:46:LEU:HG	8:I:55:VAL:HG21	1.88	0.55
3:P:168:ASP:OD1	3:P:169:GLY:N	2.39	0.55
14:Q:204:ASN:HD21	14:Q:221:GLN:HE21	1.54	0.55
15:R:379:ASP:O	15:R:381:HIS:ND1	2.37	0.55
1:A:1810:GLU:OE1	1:A:1810:GLU:N	2.40	0.55
8:I:413:ASN:HD21	8:I:450:GLU:CD	2.14	0.55
9:K:372:LEU:HD22	9:K:404:VAL:HG12	1.87	0.55
3:P:230:LYS:HE2	3:P:234:LEU:HD11	1.88	0.55
14:Q:308:HIS:CE1	14:Q:332:LEU:HB2	2.41	0.55
17:X:464:LEU:HA	17:X:467:LYS:HD3	1.87	0.55
1:A:1596:SER:O	1:A:1597:THR:HG22	2.07	0.55
3:C:148:ASN:HB3	3:C:151:LEU:HG	1.88	0.55
4:D:16:LEU:HD13	13:O:302:TYR:CZ	2.41	0.55
6:F:22:ARG:NH2	6:H:153:GLU:OE1	2.30	0.55
9:J:160:ASP:O	9:J:163:CYS:N	2.33	0.55
9:K:176:LEU:HB3	9:K:180:GLU:HB2	1.87	0.55
10:L:145:HIS:O	10:L:146:GLN:HG2	2.06	0.55
12:N:670:PHE:HE2	12:N:715:VAL:HA	1.72	0.55
13:O:641:LEU:HD11	13:O:671:GLN:HG2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:S:132:CYS:HA	16:S:301:PRO:HB3	1.89	0.55
17:Y:242:ALA:O	17:Y:246:VAL:HG23	2.07	0.55
1:A:1086:MET:HG2	1:A:1610:TYR:CZ	2.41	0.55
1:A:1326:TYR:HB2	1:A:1386:TRP:CH2	2.41	0.55
8:I:434:LEU:HD22	8:I:435:PRO:HD2	1.89	0.55
12:N:185:MET:HE2	12:N:292:TRP:HD1	1.71	0.55
12:N:531:PHE:CE2	12:N:534:SER:HB3	2.42	0.55
13:O:419:ASP:OD1	13:O:448:MET:HE2	2.06	0.55
13:O:701:PHE:HB3	13:O:710:ILE:HG12	1.88	0.55
1:A:183:THR:OG1	1:A:184:LYS:O	2.23	0.55
8:I:441:THR:HB	8:I:444:ASP:HB2	1.89	0.55
8:I:637:SER:OG	8:I:654:LYS:HB3	2.07	0.55
9:J:410:VAL:HG22	9:J:414:GLN:HE21	1.72	0.55
9:K:194:CYS:O	9:K:197:GLU:N	2.38	0.55
3:P:296:ARG:NH2	3:P:298:GLU:OE1	2.40	0.55
16:S:61:ALA:O	16:S:65:GLU:HG2	2.07	0.55
16:S:86:GLU:OE2	16:S:127:LYS:NZ	2.31	0.55
17:X:203:LEU:HA	17:X:206:ILE:HD12	1.89	0.55
17:X:235:TRP:CD1	17:X:235:TRP:H	2.25	0.55
17:Y:194:GLU:O	17:Y:198:GLN:HG2	2.06	0.55
18:Z:134:GLN:HE22	18:Z:183:LEU:HA	1.72	0.55
1:A:1078:MET:HE3	1:A:1131:MET:HG2	1.89	0.55
3:C:187:GLU:O	3:C:191:VAL:HG23	2.07	0.55
6:F:481:CYS:O	6:F:485:ILE:HG12	2.06	0.55
8:I:573:PRO:HB2	8:I:586:LEU:HD11	1.89	0.55
8:I:671:LEU:HD13	8:I:675:TYR:HE2	1.71	0.55
12:N:663:GLN:HB3	12:N:699:TRP:CZ2	2.40	0.55
13:O:617:GLN:NE2	13:O:650:PRO:HB2	2.19	0.55
15:R:425:LEU:HB2	15:R:439:LEU:HB2	1.87	0.55
1:A:31:HIS:CG	1:A:32:PRO:HD2	2.42	0.55
1:A:87:VAL:HG12	1:A:89:TYR:H	1.71	0.55
2:B:13:THR:OG1	12:N:636:SER:OG	2.24	0.55
8:I:574:PHE:CD1	8:I:642:GLN:HG2	2.42	0.55
9:J:146:ARG:O	9:J:150:THR:HG23	2.07	0.55
10:L:51:GLU:OE1	10:L:51:GLU:N	2.34	0.55
15:R:294:ASP:OD2	15:R:296:ARG:NH1	2.33	0.55
1:A:1560:MET:HE1	1:A:1607:ARG:HB3	1.88	0.55
3:C:151:LEU:HA	3:C:154:LEU:HB2	1.89	0.55
6:H:104:ASP:N	6:H:104:ASP:OD1	2.40	0.55
8:I:266:ASN:HA	8:I:526:LYS:NZ	2.18	0.55
8:I:361:TYR:O	8:I:364:SER:OG	2.24	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:717:MET:HE2	8:I:733:VAL:HG13	1.88	0.55
11:M:1:MET:HB3	11:M:4:GLU:HB2	1.88	0.55
12:N:380:ALA:O	12:N:384:THR:HG23	2.07	0.55
13:O:409:HIS:HB3	13:O:418:ILE:HG12	1.89	0.55
3:P:99:TYR:O	3:P:121:SER:OG	2.24	0.55
17:X:173:MET:O	17:X:177:ASN:ND2	2.39	0.55
17:Y:456:VAL:O	17:Y:458:GLN:N	2.40	0.55
1:A:1250:GLN:O	1:A:1254:VAL:HG23	2.08	0.54
1:A:1777:GLU:OE2	1:A:1842:SER:OG	2.15	0.54
6:F:624:PHE:CE1	6:F:640:GLY:HA3	2.41	0.54
8:I:442:GLN:O	8:I:446:THR:HG23	2.05	0.54
9:J:251:TYR:HA	9:J:254:THR:HG22	1.89	0.54
12:N:609:LEU:HD11	12:N:640:THR:HG22	1.88	0.54
3:P:296:ARG:HH21	3:P:298:GLU:HB2	1.72	0.54
15:R:411:TYR:OH	15:R:474:GLU:O	2.25	0.54
16:S:76:ASP:OD2	16:S:80:ARG:NH2	2.40	0.54
3:C:277:ARG:HD3	15:R:77:ASP:HB3	1.88	0.54
3:C:422:TYR:CE2	3:C:438:ALA:HB1	2.42	0.54
6:H:696:ILE:HG12	6:H:706:LYS:HD2	1.88	0.54
13:O:434:ARG:HA	13:O:654:ASP:OD2	2.07	0.54
3:P:215:ASP:CG	3:P:217:GLU:HG2	2.33	0.54
3:P:433:SER:O	3:P:437:VAL:HG23	2.06	0.54
14:Q:249:GLU:HA	14:Q:265:THR:HG22	1.89	0.54
17:X:52:ASN:HD21	17:Y:173:MET:HE2	1.72	0.54
17:X:334:ILE:O	17:Y:94:ARG:NE	2.40	0.54
1:A:968:SER:OG	1:A:970:TRP:NE1	2.40	0.54
1:A:1686:HIS:O	1:A:1689:SER:OG	2.19	0.54
12:N:602:PRO:N	12:N:603:PRO:HD2	2.22	0.54
3:P:66:PRO:HG2	3:P:68:ALA:HB3	1.88	0.54
17:X:246:VAL:HG22	17:X:280:LEU:HD21	1.88	0.54
17:X:315:LEU:HD22	17:X:320:ARG:HH21	1.70	0.54
1:A:247:VAL:HG21	1:A:427:ALA:HB3	1.88	0.54
3:C:432:ASP:HB3	3:C:435:MET:HG2	1.89	0.54
8:I:25:PHE:O	8:I:38:ALA:N	2.31	0.54
14:Q:187:LEU:HB3	14:Q:189:LEU:HD21	1.89	0.54
15:R:386:ASN:HB2	15:R:393:LEU:HD11	1.89	0.54
16:S:38:MET:HE2	18:Z:179:GLU:HG3	1.90	0.54
1:A:1028:TRP:HZ2	1:A:1531:GLY:H	1.56	0.54
1:A:1470:LEU:HD12	1:A:1518:VAL:HG13	1.90	0.54
3:C:185:VAL:HG23	3:C:212:LEU:HD22	1.89	0.54
6:F:734:PRO:HG2	6:F:735:LYS:HD3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:6:LEU:HD12	9:J:9:ARG:HB2	1.89	0.54
9:J:207:ASN:HA	9:J:240:ARG:HH21	1.71	0.54
9:K:453:HIS:CD2	9:K:456:ARG:HH22	2.25	0.54
12:N:570:ILE:HA	12:N:573:ASN:ND2	2.23	0.54
13:O:358:TYR:HB3	13:O:387:GLN:HE22	1.73	0.54
13:O:548:ALA:HB2	13:O:563:LEU:HD22	1.88	0.54
1:A:478:ASP:HB3	1:A:491:LEU:HD21	1.90	0.54
3:C:409:TYR:OH	13:O:279:ASP:OD1	2.21	0.54
6:H:587:ILE:O	6:H:591:GLN:HG3	2.07	0.54
9:J:204:LEU:HD13	9:K:24:PHE:HZ	1.71	0.54
12:N:699:TRP:HB3	12:N:705:LEU:HB2	1.88	0.54
3:P:96:VAL:N	3:P:97:LYS:HA	2.21	0.54
15:R:275:SER:HB3	15:R:282:SER:HB2	1.89	0.54
18:Z:42:THR:O	18:Z:57:THR:N	2.40	0.54
18:Z:89:SER:O	18:Z:150:SER:N	2.23	0.54
1:A:79:GLY:C	1:A:87:VAL:HG11	2.32	0.54
1:A:260:ASP:OD1	1:A:261:ALA:N	2.41	0.54
1:A:1216:LYS:NZ	1:A:1221:ASP:OD1	2.41	0.54
6:H:25:VAL:HG13	6:H:48:TYR:HE1	1.72	0.54
8:I:196:ALA:HA	8:I:541:ALA:HA	1.89	0.54
8:I:305:MET:HE2	13:O:57:ARG:HD2	1.89	0.54
3:P:373:HIS:CD2	14:Q:497:GLY:H	2.25	0.54
14:Q:316:ARG:CZ	14:Q:363:TRP:H	2.21	0.54
17:X:208:GLY:O	17:X:212:LEU:HG	2.08	0.54
1:A:40:ARG:HG3	3:C:393:GLU:HB3	1.88	0.54
1:A:1179:LEU:HD12	1:A:1184:HIS:HB2	1.90	0.54
1:A:1577:SER:N	1:A:1580:SER:OG	2.41	0.54
1:A:1810:GLU:HA	1:A:1813:GLN:NE2	2.22	0.54
5:E:100:GLU:O	5:E:105:PHE:HB2	2.08	0.54
6:F:142:LEU:HA	6:F:146:PRO:HB3	1.89	0.54
6:H:680:HIS:CD2	6:H:712:VAL:HG23	2.43	0.54
8:I:602:ARG:HH21	8:I:613:ASN:HB2	1.72	0.54
12:N:425:ARG:CD	12:N:507:SER:HB3	2.38	0.54
17:X:225:ASN:O	17:X:229:THR:OG1	2.10	0.54
17:X:437:LEU:CB	17:X:444:LEU:HD11	2.38	0.54
1:A:92:GLU:N	1:A:103:SER:O	2.27	0.54
8:I:216:SER:HG	8:I:584:HIS:HE2	1.56	0.54
12:N:519:TYR:O	12:N:523:LEU:HG	2.08	0.54
13:O:129:THR:C	13:O:133:GLY:HA3	2.33	0.54
17:Y:432:ASN:HA	17:Y:435:LYS:HD2	1.89	0.54
18:Z:127:GLU:O	18:Z:131:VAL:HG23	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Z:130:SER:OG	18:Z:184:ARG:NE	2.40	0.54
1:A:186:GLY:HA3	1:A:214:LEU:HA	1.90	0.54
1:A:1086:MET:HE1	1:A:1560:MET:HG3	1.90	0.54
6:F:503:CYS:SG	6:F:535:GLY:HA3	2.48	0.54
9:J:58:HIS:CD2	9:K:262:PRO:HD3	2.42	0.54
9:J:527:ILE:HD11	3:P:420:TYR:HB2	1.90	0.54
12:N:296:VAL:O	12:N:299:TRP:HB3	2.07	0.54
3:P:316:LEU:HD21	3:P:340:TYR:HA	1.90	0.54
1:A:250:ASN:ND2	1:A:432:ILE:HD12	2.19	0.53
6:H:527:ARG:HB3	17:Y:302:PRO:HG3	1.90	0.53
8:I:81:ALA:HA	8:I:92:LEU:HA	1.91	0.53
9:K:360:ALA:O	9:K:364:MET:HB2	2.07	0.53
3:P:267:SER:HB2	3:P:299:ASN:ND2	2.23	0.53
3:P:466:GLU:HB2	3:P:468:MET:HE3	1.89	0.53
14:Q:175:ILE:HG12	14:Q:468:ARG:HG2	1.90	0.53
1:A:94:TYR:HE1	1:A:96:ALA:HB2	1.72	0.53
1:A:222:PRO:HD3	1:A:403:ILE:HD11	1.91	0.53
1:A:797:LEU:HB3	1:A:799:LEU:HD13	1.90	0.53
7:G:4:ARG:HB2	9:J:342:HIS:NE2	2.23	0.53
7:G:15:ASP:OD1	9:J:457:LYS:NZ	2.39	0.53
9:K:192:LYS:HD3	9:K:198:GLN:HG3	1.90	0.53
13:O:119:PHE:CZ	13:O:128:LYS:HA	2.43	0.53
14:Q:165:CYS:SG	16:S:224:ARG:NE	2.81	0.53
15:R:124:ASP:O	15:R:127:GLU:N	2.33	0.53
16:S:273:THR:OG1	16:S:274:VAL:N	2.41	0.53
1:A:1089:LEU:HD23	1:A:1090:PHE:HB2	1.90	0.53
1:A:1921:LEU:HA	12:N:78:VAL:HG21	1.90	0.53
2:B:1:MET:HB3	12:N:671:GLN:HG3	1.90	0.53
6:F:609:HIS:CD2	15:R:499:ARG:HB3	2.42	0.53
8:I:426:LEU:HG	8:I:434:LEU:HD21	1.90	0.53
10:L:83:TYR:CG	10:L:115:GLU:HG2	2.43	0.53
14:Q:464:ASP:OD2	14:Q:468:ARG:NH1	2.41	0.53
1:A:801:PRO:HB2	1:A:841:PRO:HG3	1.90	0.53
1:A:1153:ILE:HD11	1:A:1184:HIS:CD2	2.43	0.53
2:B:25:ILE:HG23	2:B:63:TRP:HE3	1.73	0.53
3:C:235:ALA:O	3:C:239:THR:HG23	2.07	0.53
3:C:448:GLN:HB3	3:C:451:GLU:OE2	2.08	0.53
8:I:295:ASN:H	8:I:316:GLU:HG3	1.72	0.53
8:I:318:GLN:HG3	8:I:428:MET:HE2	1.89	0.53
12:N:124:PRO:HA	12:N:127:ARG:CB	2.39	0.53
14:Q:144:TYR:CE1	18:Z:146:GLU:HA	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:Q:456:ALA:HA	14:Q:473:PHE:HB2	1.91	0.53
17:X:194:GLU:HA	17:X:197:ARG:HG2	1.90	0.53
17:Y:373:VAL:HG11	17:Y:403:ALA:HB2	1.89	0.53
17:Y:506:GLN:HE22	17:Y:512:HIS:HE2	1.55	0.53
18:Z:19:ILE:HD11	18:Z:121:GLN:HE22	1.73	0.53
1:A:1155:SER:HA	1:A:1158:ILE:HD12	1.89	0.53
6:H:42:PHE:HB2	6:H:71:CYS:SG	2.48	0.53
9:J:66:ASP:OD1	9:J:66:ASP:N	2.41	0.53
12:N:687:MET:HE1	12:N:695:ARG:HG3	1.91	0.53
14:Q:191:ASP:HA	14:Q:450:THR:HG21	1.89	0.53
16:S:142:LEU:HD22	16:S:147:ILE:HB	1.90	0.53
17:X:66:ASN:HD21	17:Y:268:ARG:HB3	1.73	0.53
17:Y:475:TYR:HE2	17:Y:477:LYS:HB2	1.74	0.53
3:C:129:LYS:NZ	3:P:325:GLU:OE1	2.37	0.53
8:I:500:PHE:HE2	8:I:507:LEU:HD12	1.73	0.53
12:N:677:THR:H	12:N:680:GLU:HB2	1.73	0.53
13:O:135:PHE:O	13:O:139:MET:HG2	2.08	0.53
3:P:234:LEU:HA	3:P:237:ILE:HD12	1.90	0.53
14:Q:186:TYR:CZ	16:S:27:GLU:HB2	2.44	0.53
15:R:446:VAL:HA	15:R:462:ALA:HA	1.90	0.53
17:X:442:GLN:CD	17:X:442:GLN:H	2.14	0.53
17:Y:177:ASN:HA	17:Y:180:LYS:HE2	1.90	0.53
1:A:799:LEU:C	1:A:801:PRO:HD2	2.34	0.53
8:I:643:PHE:HD1	8:I:649:VAL:HG13	1.74	0.53
13:O:106:LYS:O	13:O:110:GLN:HG3	2.09	0.53
13:O:354:ARG:NH2	13:O:572:GLN:O	2.42	0.53
1:A:93:LEU:HB2	1:A:128:TRP:CH2	2.44	0.53
1:A:269:TRP:HB3	1:A:409:ILE:HG22	1.90	0.53
1:A:772:GLU:OE1	1:A:869:ARG:HB2	2.09	0.53
2:B:44:CYS:H	12:N:630:LYS:HE3	1.73	0.53
3:C:407:GLN:O	3:C:411:ILE:HG12	2.09	0.53
9:J:500:ASP:OD1	3:P:396:LYS:NZ	2.37	0.53
9:K:306:GLY:HA3	9:K:323:LEU:HG	1.89	0.53
9:K:406:HIS:HE1	7:W:7:THR:O	1.92	0.53
12:N:247:LEU:HB3	12:N:253:LEU:HB3	1.91	0.53
12:N:434:THR:O	12:N:438:ILE:HG13	2.08	0.53
13:O:96:ARG:O	13:O:99:LEU:HG	2.09	0.53
14:Q:253:TRP:CE2	14:Q:260:ARG:HB2	2.44	0.53
8:I:24:ILE:N	8:I:38:ALA:O	2.41	0.53
9:J:20:GLN:HB2	9:K:165:GLU:CD	2.33	0.53
9:J:448:LEU:HB3	9:J:471:ALA:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:466:ASP:O	9:K:470:GLN:HG3	2.08	0.53
11:M:50:VAL:O	11:M:54:GLU:HG2	2.09	0.53
13:O:119:PHE:HE2	13:O:137:ARG:HG3	1.74	0.53
13:O:687:LEU:HG	13:O:720:LEU:HD11	1.91	0.53
3:P:167:LEU:HD11	3:P:171:GLY:HA3	1.91	0.53
3:P:373:HIS:HD2	14:Q:497:GLY:H	1.57	0.53
14:Q:185:TYR:CG	16:S:27:GLU:HB3	2.44	0.53
15:R:468:ARG:HD3	15:R:470:TRP:CZ2	2.44	0.53
1:A:1313:LEU:HG	1:A:1316:MET:HB2	1.91	0.53
1:A:1473:GLY:HA2	1:A:1526:VAL:HG23	1.89	0.53
6:F:464:SER:O	6:F:468:GLU:HG2	2.09	0.53
6:F:702:ASN:HB3	6:F:705:CYS:SG	2.49	0.53
12:N:387:LEU:HD21	12:N:424:ILE:HA	1.91	0.53
13:O:581:ILE:HG13	13:O:619:LEU:HD22	1.91	0.53
13:O:652:LEU:HA	13:O:660:LYS:HE3	1.90	0.53
3:P:307:LEU:HD21	3:P:315:GLU:HB2	1.90	0.53
15:R:287:SER:HB3	15:R:289:HIS:HD1	1.73	0.53
16:S:97:ASN:O	16:S:101:LEU:HG	2.09	0.53
16:S:194:ARG:HA	16:S:197:GLN:NE2	2.23	0.53
17:Y:406:ARG:HB3	17:Y:409:CYS:SG	2.48	0.53
1:A:1070:LEU:HD22	1:A:1118:VAL:HG23	1.91	0.52
1:A:1808:THR:HB	1:A:1890:VAL:HG21	1.90	0.52
3:C:434:ARG:HD3	15:R:80:ILE:HG21	1.92	0.52
6:H:747:TYR:CD2	6:H:755:LEU:HB3	2.44	0.52
8:I:136:ASN:O	8:I:253:ARG:NH1	2.42	0.52
8:I:202:ALA:O	8:I:221:THR:OG1	2.27	0.52
9:K:389:ARG:O	9:K:392:SER:OG	2.25	0.52
3:P:92:ALA:O	3:P:96:VAL:HG23	2.09	0.52
3:P:277:ARG:HH22	3:P:434:ARG:HD3	1.74	0.52
3:P:305:ASN:O	3:P:309:VAL:HG23	2.10	0.52
14:Q:166:ARG:NH1	14:Q:168:ILE:HD11	2.24	0.52
15:R:204:ASN:ND2	15:R:221:GLN:HE21	2.02	0.52
1:A:935:THR:HG21	1:A:974:VAL:HG23	1.91	0.52
1:A:1082:VAL:HG13	1:A:1608:HIS:CE1	2.44	0.52
9:J:9:ARG:NH2	9:J:13:TYR:OH	2.41	0.52
10:L:87:GLU:O	10:L:146:GLN:NE2	2.42	0.52
13:O:123:GLU:N	13:O:124:PRO:HA	2.24	0.52
3:P:180:ARG:HG3	3:P:212:LEU:HD21	1.92	0.52
15:R:363:TRP:CD2	15:R:371:LEU:HD13	2.44	0.52
15:R:451:MET:HG2	15:R:455:GLY:HA2	1.91	0.52
1:A:775:LEU:HD23	1:A:869:ARG:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:799:LEU:O	1:A:801:PRO:HD2	2.10	0.52
1:A:1674:TRP:HB3	1:A:1702:ARG:NH2	2.24	0.52
10:L:13:PRO:HB2	10:L:159:TYR:OH	2.10	0.52
12:N:754:PHE:HE2	12:N:788:ALA:HB3	1.73	0.52
14:Q:132:ARG:N	18:Z:168:GLU:O	2.42	0.52
14:Q:132:ARG:HB2	18:Z:170:SER:HB3	1.91	0.52
18:Z:58:ASP:HB3	18:Z:61:LEU:HB3	1.91	0.52
1:A:1871:TYR:HB2	1:A:1877:LEU:HD21	1.91	0.52
3:C:202:HIS:CD2	3:C:204:GLY:H	2.27	0.52
6:H:146:PRO:O	6:H:148:LEU:N	2.42	0.52
9:J:211:LYS:HE3	9:J:240:ARG:HE	1.74	0.52
9:K:242:TYR:OH	7:W:1:MET:O	2.25	0.52
12:N:372:GLN:O	12:N:376:VAL:HG23	2.09	0.52
13:O:593:ARG:HD2	13:O:753:ASN:HB3	1.91	0.52
17:X:339:ALA:O	17:X:343:VAL:HG23	2.09	0.52
18:Z:106:CYS:HA	18:Z:190:ILE:O	2.09	0.52
1:A:27:HIS:HE1	13:O:264:VAL:HG22	1.74	0.52
1:A:107:LYS:HB2	1:A:110:ALA:HB3	1.92	0.52
1:A:1063:ILE:HA	1:A:1066:LYS:HG2	1.91	0.52
2:B:43:ASP:C	2:B:45:PRO:HD3	2.34	0.52
3:C:521:PHE:CD1	3:C:553:ILE:HG22	2.45	0.52
8:I:225:THR:OG1	8:I:226:ASN:N	2.42	0.52
9:J:37:PRO:HB3	9:J:69:TYR:CE2	2.44	0.52
9:K:300:VAL:HG12	9:K:333:TYR:OH	2.10	0.52
13:O:581:ILE:HD11	13:O:619:LEU:HD13	1.91	0.52
3:P:487:ALA:HB1	3:P:519:TYR:CE1	2.45	0.52
17:X:443:THR:O	17:X:446:LEU:HG	2.10	0.52
17:Y:140:TYR:O	17:Y:144:GLU:HG3	2.10	0.52
1:A:1504:ALA:HA	1:A:1507:THR:HG22	1.92	0.52
2:B:26:CYS:HB3	2:B:59:CYS:SG	2.49	0.52
2:B:56:HIS:O	2:B:60:ILE:N	2.36	0.52
6:F:639:TYR:HB2	6:F:671:LEU:HD21	1.90	0.52
6:H:55:TYR:OH	6:H:56:LYS:NZ	2.43	0.52
8:I:345:GLN:NE2	13:O:410:TRP:HB3	2.25	0.52
8:I:557:TYR:HB3	8:I:694:ASP:HB3	1.92	0.52
8:I:625:TYR:HB2	8:I:628:THR:HG23	1.91	0.52
9:K:188:LEU:HD12	9:K:190:LEU:HB2	1.90	0.52
13:O:143:TYR:O	13:O:146:LEU:HB2	2.10	0.52
14:Q:187:LEU:HD13	14:Q:230:SER:HA	1.91	0.52
17:Y:57:SER:O	17:Y:61:LEU:HB2	2.10	0.52
1:A:435:ASP:OD1	1:A:439:GLN:HB3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:420:TRP:HA	8:I:423:VAL:HG12	1.92	0.52
12:N:670:PHE:HE1	12:N:713:PHE:HB3	1.75	0.52
3:P:31:GLU:O	3:P:34:LYS:HG2	2.10	0.52
15:R:400:SER:OG	15:R:401:GLN:N	2.43	0.52
18:Z:85:VAL:HB	18:Z:154:LEU:HB2	1.92	0.52
6:H:651:PHE:HB2	6:H:682:LEU:HD21	1.91	0.52
9:K:153:TYR:HB2	9:K:170:LEU:HD21	1.91	0.52
14:Q:411:TYR:OH	14:Q:474:GLU:O	2.26	0.52
16:S:102:LEU:O	16:S:106:VAL:HG23	2.09	0.52
1:A:42:LEU:HG	3:C:142:GLU:HG2	1.92	0.52
13:O:423:ALA:O	13:O:426:THR:HG22	2.10	0.52
14:Q:219:LEU:HD12	14:Q:258:GLN:HG3	1.90	0.52
15:R:231:SER:O	15:R:244:GLY:N	2.38	0.52
15:R:400:SER:HB3	15:R:418:HIS:HB3	1.91	0.52
17:X:312:GLY:HA3	17:X:344:VAL:HG23	1.92	0.52
17:X:342:TRP:HB2	17:X:365:ALA:HB2	1.91	0.52
18:Z:105:GLU:O	18:Z:192:LYS:N	2.41	0.52
1:A:1141:VAL:HG11	1:A:1608:HIS:CG	2.44	0.52
1:A:1276:GLU:HG3	1:A:1294:TYR:HE2	1.75	0.52
1:A:1306:CYS:HB2	1:A:1374:ILE:HG12	1.91	0.52
1:A:1373:MET:HE1	1:A:1582:ALA:HA	1.91	0.52
2:B:53:HIS:HB3	2:B:55:PHE:CE2	2.45	0.52
3:C:139:GLY:HA3	3:C:145:GLN:HE22	1.73	0.52
3:C:283:LEU:HD13	3:C:306:LEU:HD11	1.91	0.52
6:H:658:PHE:HB3	6:H:675:ILE:HG12	1.90	0.52
9:J:9:ARG:HA	9:J:9:ARG:HH11	1.74	0.52
9:J:47:LEU:HB3	9:J:56:ALA:HB2	1.92	0.52
9:J:389:ARG:O	9:J:392:SER:OG	2.23	0.52
9:K:252:LYS:O	9:K:256:VAL:HG23	2.09	0.52
12:N:432:GLU:OE1	12:N:509:TYR:OH	2.23	0.52
12:N:522:LEU:O	12:N:526:ARG:HG3	2.09	0.52
13:O:254:HIS:CD2	13:O:276:HIS:ND1	2.78	0.52
14:Q:220:LEU:HD11	14:Q:229:ILE:HD11	1.91	0.52
16:S:60:ARG:HA	16:S:63:GLU:CD	2.35	0.52
1:A:1232:ILE:HG23	1:A:1235:LEU:HB2	1.92	0.51
1:A:1540:ARG:HG2	1:A:1544:MET:HE2	1.91	0.51
2:B:14:TRP:HB3	12:N:595:ILE:HG23	1.91	0.51
3:C:156:VAL:O	3:C:160:LYS:HG2	2.11	0.51
6:F:644:ILE:O	6:F:648:GLN:HB2	2.10	0.51
6:H:520:ARG:NH2	17:X:154:ASP:OD1	2.43	0.51
9:J:324:SER:O	9:J:328:THR:HG23	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:Q:292:HIS:HD2	14:Q:303:ALA:HB3	1.75	0.51
15:R:85:ALA:HA	15:R:88:MET:HB2	1.93	0.51
16:S:141:TYR:CD1	16:S:295:TRP:HB2	2.45	0.51
1:A:81:SER:OG	1:A:87:VAL:HG22	2.10	0.51
1:A:585:HIS:N	1:A:598:GLU:O	2.33	0.51
3:C:352:LEU:HD21	3:C:356:ARG:CZ	2.40	0.51
8:I:71:LEU:HA	8:I:82:PHE:HB3	1.91	0.51
8:I:140:PRO:HB3	8:I:257:HIS:CE1	2.45	0.51
9:J:80:HIS:HB2	9:J:89:ALA:HB2	1.92	0.51
9:K:372:LEU:HD13	9:K:404:VAL:HG12	1.92	0.51
10:L:63:LEU:HD13	10:L:138:GLN:HE21	1.74	0.51
15:R:87:GLN:HG3	15:R:132:ARG:HG3	1.91	0.51
15:R:398:ALA:HB1	15:R:418:HIS:CE1	2.45	0.51
17:X:446:LEU:O	17:X:450:VAL:HG23	2.10	0.51
18:Z:103:ASP:O	18:Z:194:ASN:N	2.28	0.51
1:A:775:LEU:HD11	1:A:951:ILE:HG21	1.91	0.51
2:B:8:TRP:HE3	12:N:591:VAL:HA	1.75	0.51
3:C:449:LEU:HD13	3:C:480:LEU:HD11	1.92	0.51
8:I:15:GLY:O	8:I:743:VAL:N	2.40	0.51
8:I:393:VAL:O	8:I:397:ILE:HG13	2.11	0.51
10:L:50:LEU:O	10:L:154:ARG:HD2	2.10	0.51
13:O:35:ILE:HD12	13:O:38:LEU:HD12	1.91	0.51
13:O:504:ALA:HA	13:O:507:TRP:CD1	2.44	0.51
3:P:155:ARG:HH12	3:P:159:SER:HB3	1.75	0.51
14:Q:204:ASN:O	14:Q:222:MET:N	2.35	0.51
14:Q:406:LEU:HD13	14:Q:451:MET:HB2	1.93	0.51
1:A:498:VAL:HG12	1:A:508:LYS:HA	1.91	0.51
1:A:847:TRP:HD1	1:A:858:PRO:HG2	1.74	0.51
2:B:16:TRP:HD1	2:B:32:GLY:C	2.18	0.51
3:C:60:PHE:HD1	3:P:85:ASP:HB3	1.74	0.51
3:C:330:ARG:HG2	3:C:332:GLU:OE2	2.11	0.51
3:C:412:LEU:O	13:O:330:ILE:HD11	2.10	0.51
6:F:89:GLU:OE1	6:F:130:ARG:NH2	2.43	0.51
7:G:13:LEU:HA	7:G:16:ILE:HG13	1.93	0.51
6:H:136:GLU:O	6:H:140:LYS:HG2	2.11	0.51
9:J:268:LEU:HD22	9:J:291:LEU:HD11	1.92	0.51
9:K:192:LYS:NZ	9:K:195:ASN:OD1	2.40	0.51
3:P:277:ARG:HH12	3:P:434:ARG:HH11	1.57	0.51
14:Q:308:HIS:ND1	14:Q:332:LEU:HB2	2.25	0.51
15:R:324:LEU:HB3	15:R:336:TRP:HB2	1.92	0.51
17:Y:77:TYR:CE1	17:Y:107:LYS:HB2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1155:SER:OG	1:A:1188:LEU:HD12	2.10	0.51
8:I:211:SER:OG	8:I:216:SER:OG	2.08	0.51
12:N:533:PHE:HZ	12:N:568:ARG:HD2	1.74	0.51
12:N:685:VAL:HG23	12:N:687:MET:H	1.75	0.51
3:P:531:THR:O	3:P:535:LYS:HG2	2.09	0.51
17:Y:307:GLY:O	17:Y:309:ASP:N	2.44	0.51
18:Z:46:VAL:N	18:Z:53:LEU:O	2.38	0.51
18:Z:175:ILE:HB	18:Z:178:SER:HB2	1.93	0.51
1:A:1266:HIS:CD2	1:A:1269:THR:HG23	2.46	0.51
1:A:1757:PRO:C	1:A:1759:VAL:H	2.19	0.51
3:C:377:GLU:HA	15:R:130:ILE:HG22	1.93	0.51
6:F:34:GLU:HB2	6:H:495:HIS:CE1	2.40	0.51
8:I:388:GLU:O	8:I:391:THR:OG1	2.21	0.51
9:J:418:TRP:CE3	9:J:457:LYS:HB3	2.45	0.51
12:N:559:VAL:HA	12:N:562:LYS:HG2	1.92	0.51
13:O:119:PHE:HE1	13:O:126:VAL:HB	1.76	0.51
15:R:177:ASP:O	16:S:227:LEU:N	2.36	0.51
17:Y:391:GLU:O	17:Y:395:HIS:HD2	1.93	0.51
1:A:1375:TYR:CE2	1:A:1383:ILE:HD13	2.45	0.51
3:C:193:VAL:HG12	3:C:197:HIS:CE1	2.46	0.51
6:F:15:ALA:O	6:F:19:TYR:N	2.44	0.51
6:F:762:TRP:CE2	9:J:362:GLN:HB2	2.45	0.51
9:J:512:ASP:O	9:J:516:VAL:HG23	2.09	0.51
10:L:97:ARG:NH1	10:L:138:GLN:OE1	2.43	0.51
15:R:430:TYR:CG	15:R:431:PRO:HA	2.45	0.51
17:X:270:ASN:HB3	17:X:273:LEU:HB2	1.93	0.51
17:X:449:THR:O	17:X:453:GLU:HG2	2.11	0.51
17:Y:270:ASN:HB2	17:Y:273:LEU:HB2	1.92	0.51
17:Y:542:ASP:OD2	17:Y:545:SER:OG	2.29	0.51
1:A:1550:MET:HA	1:A:1554:PHE:HD2	1.76	0.51
8:I:49:LEU:HD13	8:I:730:VAL:CG2	2.39	0.51
9:K:263:PHE:CZ	9:K:290:LYS:HB3	2.45	0.51
12:N:180:PHE:CD2	12:N:299:TRP:HH2	2.28	0.51
13:O:324:LEU:O	13:O:328:ILE:HG23	2.11	0.51
14:Q:286:ARG:NH1	14:Q:311:GLU:OE2	2.41	0.51
14:Q:442:HIS:CE1	14:Q:468:ARG:HD2	2.45	0.51
17:Y:513:ARG:HD2	17:Y:544:LYS:HB2	1.93	0.51
18:Z:16:SER:O	18:Z:20:VAL:HG23	2.11	0.51
1:A:511:ILE:HG22	1:A:513:GLY:H	1.75	0.51
1:A:1134:TRP:CE2	1:A:1203:MET:HE1	2.46	0.51
3:C:266:VAL:HG12	3:C:289:LEU:HD12	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:409:TYR:HB3	3:C:418:CYS:HB3	1.93	0.51
6:H:489:SER:O	17:X:105:GLN:NE2	2.34	0.51
8:I:433:VAL:HG23	8:I:434:LEU:H	1.76	0.51
9:J:236:SER:HA	9:J:239:GLU:CD	2.36	0.51
9:K:230:ASN:OD1	9:K:232:ASP:N	2.39	0.51
13:O:104:GLU:N	13:O:107:ASP:OD2	2.44	0.51
13:O:265:GLN:HE21	13:O:502:GLN:HE21	1.58	0.51
18:Z:127:GLU:O	18:Z:130:SER:OG	2.21	0.51
1:A:90:ASP:HB3	1:A:591:VAL:HG11	1.92	0.51
1:A:1241:THR:HA	15:R:119:ASN:HD21	1.76	0.51
1:A:1251:VAL:HG12	1:A:1294:TYR:CD1	2.46	0.51
1:A:1394:TYR:OH	10:L:70:ARG:NH1	2.44	0.51
1:A:1542:LEU:HB3	1:A:1558:HIS:ND1	2.26	0.51
1:A:1595:HIS:NE2	1:A:1598:ASP:HB2	2.25	0.51
1:A:1621:PRO:HG3	1:A:1653:ALA:HB1	1.92	0.51
6:H:16:LEU:HD21	6:H:47:CYS:HA	1.92	0.51
8:I:497:TRP:NE1	8:I:516:TYR:OH	2.28	0.51
12:N:661:PRO:HA	12:N:664:ALA:HB3	1.92	0.51
12:N:772:ARG:HB3	12:N:776:MET:HE3	1.92	0.51
3:P:290:ARG:HH22	3:P:323:LEU:HD21	1.75	0.51
16:S:40:THR:HB	16:S:87:GLN:HB3	1.93	0.51
17:X:284:ALA:O	17:X:472:ARG:NH2	2.44	0.51
18:Z:188:THR:O	18:Z:189:THR:OG1	2.28	0.51
1:A:1661:HIS:CE1	1:A:1662:LEU:HB3	2.45	0.50
3:C:97:LYS:HD2	3:C:99:TYR:OH	2.11	0.50
6:H:104:ASP:HA	6:H:107:VAL:HG22	1.93	0.50
12:N:502:ILE:O	12:N:506:VAL:HG12	2.09	0.50
16:S:199:ARG:O	16:S:203:GLN:HG2	2.11	0.50
1:A:1267:ARG:NH1	1:A:1271:GLU:OE1	2.43	0.50
6:H:758:MET:HE1	17:X:429:MET:SD	2.51	0.50
9:J:509:ARG:HH11	9:J:512:ASP:HB2	1.76	0.50
9:K:66:ASP:OD1	9:K:67:LYS:N	2.44	0.50
12:N:180:PHE:CG	12:N:299:TRP:HH2	2.29	0.50
16:S:144:ASN:ND2	16:S:145:GLN:HG2	2.26	0.50
17:X:40:HIS:CD2	17:Y:201:LEU:HD11	2.46	0.50
17:X:242:ALA:HA	17:X:257:THR:HG21	1.92	0.50
17:X:298:GLN:HB3	17:X:299:MET:HE2	1.92	0.50
1:A:1729:GLU:HB3	1:A:1731:ARG:CZ	2.40	0.50
1:A:1787:LEU:O	1:A:1791:ILE:HG12	2.12	0.50
6:H:125:TYR:CE2	6:H:133:LYS:HD2	2.43	0.50
8:I:237:GLU:HB3	8:I:550:GLN:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:251:TYR:HA	9:K:254:THR:HG22	1.93	0.50
14:Q:209:TRP:NE1	14:Q:214:GLY:O	2.45	0.50
16:S:158:TRP:CG	16:S:174:ILE:HD13	2.47	0.50
17:X:304:LEU:H	17:X:308:MET:HE2	1.76	0.50
17:Y:248:THR:OG1	17:Y:250:ASP:OD1	2.28	0.50
18:Z:75:TRP:HB3	18:Z:81:VAL:HG23	1.93	0.50
1:A:23:PHE:CD1	1:A:111:LEU:HB3	2.47	0.50
1:A:436:LEU:H	1:A:501:THR:CG2	2.23	0.50
1:A:482:VAL:HG21	1:A:609:ILE:HD12	1.93	0.50
1:A:1147:ILE:HD11	1:A:1157:TRP:HH2	1.76	0.50
1:A:1261:TYR:O	1:A:1264:THR:HG22	2.11	0.50
6:F:27:LEU:HD11	6:H:147:PHE:O	2.10	0.50
6:F:42:PHE:HB2	6:F:71:CYS:SG	2.51	0.50
6:H:714:PHE:HE2	6:H:746:VAL:HA	1.75	0.50
12:N:533:PHE:CZ	12:N:568:ARG:HD2	2.47	0.50
3:P:286:PHE:HB3	3:P:303:PHE:CE1	2.46	0.50
15:R:366:TRP:CH2	15:R:407:TRP:HE3	2.29	0.50
17:X:331:LEU:HD23	17:X:334:ILE:HD11	1.93	0.50
17:X:430:ALA:HA	17:X:433:VAL:HG12	1.93	0.50
3:C:417:TYR:HB2	13:O:326:GLU:OE1	2.12	0.50
6:H:765:ASP:O	17:X:397:ARG:NH2	2.45	0.50
8:I:34:LEU:HD12	8:I:46:LEU:HD21	1.94	0.50
9:J:285:PHE:HB2	9:J:308:TYR:CE1	2.47	0.50
12:N:580:LYS:HB3	12:N:582:PRO:HD2	1.92	0.50
12:N:648:VAL:N	12:N:655:LEU:O	2.36	0.50
14:Q:168:ILE:HG21	14:Q:439:LEU:HD11	1.94	0.50
15:R:97:LYS:HE2	15:R:98:GLU:HB2	1.93	0.50
1:A:1059:ASP:OD1	1:A:1059:ASP:N	2.44	0.50
1:A:1359:ASN:HB3	10:L:30:VAL:HG11	1.93	0.50
1:A:1489:HIS:CE1	1:A:1534:LYS:HG3	2.46	0.50
3:C:93:TYR:CD1	3:C:101:ARG:HB3	2.45	0.50
6:F:501:VAL:O	6:F:505:ILE:HG13	2.12	0.50
8:I:376:TYR:HA	8:I:379:LEU:HD13	1.93	0.50
12:N:384:THR:OG1	12:N:385:ARG:HG3	2.12	0.50
12:N:790:ILE:HG13	12:N:794:GLU:CD	2.37	0.50
13:O:344:LEU:HD22	13:O:364:SER:HB2	1.93	0.50
3:P:354:PHE:CE2	3:P:370:LEU:HB3	2.47	0.50
1:A:770:TYR:HB2	1:A:786:LEU:HD22	1.94	0.50
3:C:371:MET:HE2	3:C:375:TYR:CE2	2.47	0.50
3:C:477:HIS:CE1	3:C:485:GLN:HB3	2.47	0.50
5:E:57:SER:HB2	17:X:361:LEU:HD21	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:195:ILE:HD13	8:I:252:ALA:HB2	1.94	0.50
8:I:517:TYR:HD2	8:I:525:VAL:HG22	1.77	0.50
8:I:578:ASN:N	8:I:583:LEU:O	2.45	0.50
12:N:778:ARG:NH2	12:N:779:MET:HG3	2.27	0.50
13:O:30:VAL:HG13	13:O:142:ALA:HB3	1.93	0.50
14:Q:363:TRP:CH2	14:Q:387:VAL:HG11	2.47	0.50
17:X:191:SER:O	17:X:195:VAL:HG13	2.12	0.50
17:X:437:LEU:HB2	17:X:444:LEU:HD11	1.92	0.50
17:Y:506:GLN:HE22	17:Y:512:HIS:CE1	2.30	0.50
1:A:1100:LEU:HD12	1:A:1175:PHE:CE1	2.47	0.50
8:I:447:PHE:HA	8:I:450:GLU:HB3	1.94	0.50
9:J:213:ASN:N	9:J:213:ASN:OD1	2.44	0.50
12:N:74:TRP:CG	12:N:76:VAL:HG12	2.47	0.50
13:O:301:ARG:NH2	13:O:334:SER:OG	2.45	0.50
14:Q:353:GLN:HG3	18:Z:52:THR:HG21	1.94	0.50
15:R:109:LYS:O	15:R:113:GLN:HG3	2.10	0.50
1:A:90:ASP:OD1	1:A:90:ASP:N	2.42	0.50
3:C:76:ILE:H	3:C:76:ILE:HD12	1.75	0.50
3:C:402:TRP:HB3	3:C:425:ALA:HB2	1.92	0.50
6:H:634:HIS:CE1	6:H:636:ASN:HB2	2.46	0.50
6:H:765:ASP:OD2	17:X:401:ARG:NH2	2.37	0.50
8:I:254:LYS:NZ	8:I:365:GLU:OE1	2.30	0.50
10:L:93:LYS:HG3	10:L:142:LEU:HD12	1.94	0.50
13:O:240:LEU:HD22	13:O:253:ALA:HB1	1.94	0.50
3:P:29:LEU:HD21	3:P:257:VAL:O	2.11	0.50
3:P:313:LYS:HE3	3:P:343:LEU:HG	1.92	0.50
3:P:364:TYR:HD2	3:P:367:ALA:H	1.59	0.50
15:R:167:TYR:CE2	15:R:169:PRO:HG3	2.47	0.50
15:R:195:GLY:HA3	15:R:238:GLY:HA3	1.94	0.50
16:S:67:ARG:HB2	16:S:77:VAL:HG11	1.93	0.50
17:X:393:ILE:O	17:X:397:ARG:HG3	2.12	0.50
17:Y:104:LEU:HD11	17:Y:139:LYS:HG2	1.94	0.50
17:Y:512:HIS:HB2	17:Y:535:ALA:HB2	1.94	0.50
17:Y:532:TYR:CE1	17:Y:548:GLY:HA3	2.47	0.50
1:A:27:HIS:CE1	13:O:264:VAL:HG22	2.47	0.49
1:A:871:ARG:HG3	1:A:875:LEU:HD12	1.93	0.49
1:A:1799:ARG:HE	1:A:1805:MET:HB3	1.76	0.49
5:E:78:ARG:HG2	6:H:557:LYS:HD3	1.94	0.49
9:J:432:ILE:HG12	9:J:444:TRP:CD1	2.47	0.49
9:K:478:ASN:ND2	7:W:8:ARG:HH22	2.10	0.49
12:N:347:ILE:HG21	12:N:358:ILE:HG23	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:N:663:GLN:HA	12:N:666:ILE:HD12	1.94	0.49
3:P:42:LEU:HD22	3:P:46:ARG:HH12	1.77	0.49
3:P:238:TYR:HB2	3:P:247:ALA:HB2	1.94	0.49
3:P:263:SER:HG	3:P:296:ARG:HH11	1.58	0.49
3:P:361:ASN:HD22	3:P:364:TYR:CB	2.25	0.49
3:P:373:HIS:O	3:P:377:GLU:HG2	2.12	0.49
3:P:388:TYR:HB3	3:P:405:LEU:HG	1.93	0.49
14:Q:323:HIS:HB3	14:Q:335:VAL:HG13	1.94	0.49
15:R:180:GLU:N	15:R:465:GLU:OE1	2.24	0.49
17:Y:70:LEU:HD22	17:Y:71:PHE:CE2	2.47	0.49
17:Y:200:PRO:O	17:Y:202:ALA:N	2.44	0.49
1:A:93:LEU:HD22	1:A:128:TRP:CE2	2.47	0.49
1:A:1053:GLN:N	1:A:1053:GLN:OE1	2.45	0.49
1:A:1103:PRO:HD2	1:A:1143:ALA:HB2	1.94	0.49
1:A:1455:GLU:HG2	1:A:1456:THR:N	2.27	0.49
8:I:250:ARG:NH2	13:O:649:GLU:OE2	2.45	0.49
9:J:527:ILE:HD12	3:P:419:LEU:HD22	1.94	0.49
12:N:245:GLN:HG2	12:N:249:ARG:HE	1.77	0.49
13:O:32:PRO:O	13:O:35:ILE:HG22	2.12	0.49
14:Q:166:ARG:HG3	14:Q:166:ARG:O	2.12	0.49
17:X:143:ALA:O	17:X:147:THR:HG23	2.12	0.49
3:C:407:GLN:NE2	15:R:81:PRO:HG2	2.27	0.49
4:D:13:THR:HG22	13:O:255:TYR:CE2	2.45	0.49
6:H:714:PHE:CD2	6:H:746:VAL:HG22	2.46	0.49
8:I:221:THR:O	8:I:232:SER:N	2.43	0.49
11:M:35:GLU:OE2	11:M:35:GLU:N	2.45	0.49
12:N:172:MET:O	12:N:176:LEU:HG	2.12	0.49
12:N:570:ILE:HA	12:N:573:ASN:HD21	1.76	0.49
15:R:267:HIS:CE1	15:R:285:SER:HB3	2.47	0.49
16:S:21:GLU:H	16:S:21:GLU:CD	2.20	0.49
1:A:40:ARG:CZ	13:O:248:PRO:HB2	2.43	0.49
1:A:1155:SER:O	1:A:1159:VAL:HG23	2.12	0.49
2:B:34:CYS:HB3	2:B:56:HIS:CD2	2.48	0.49
6:F:96:VAL:HG12	6:F:97:PHE:HD1	1.78	0.49
10:L:63:LEU:HD13	10:L:138:GLN:NE2	2.28	0.49
10:L:90:THR:O	10:L:145:HIS:ND1	2.35	0.49
12:N:669:TYR:HB3	12:N:676:TRP:CZ2	2.47	0.49
13:O:399:MET:HE3	13:O:429:TRP:CZ2	2.48	0.49
14:Q:429:LYS:HB3	14:Q:434:ALA:HB3	1.93	0.49
17:X:408:ASP:OD1	17:X:408:ASP:N	2.44	0.49
17:Y:340:GLU:OE1	17:Y:340:GLU:N	2.31	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1041:LEU:HA	1:A:1080:LEU:HD22	1.93	0.49
1:A:1255:VAL:HG11	1:A:1606:LEU:HD21	1.94	0.49
1:A:1491:PHE:O	1:A:1495:PHE:HD2	1.94	0.49
1:A:1638:TYR:HB3	1:A:1644:TYR:HE2	1.77	0.49
1:A:1810:GLU:H	1:A:1810:GLU:CD	2.19	0.49
3:C:210:CYS:HB3	3:C:240:GLU:OE2	2.12	0.49
9:J:230:ASN:OD1	9:J:232:ASP:N	2.35	0.49
13:O:56:GLU:HG3	13:O:59:ARG:HH21	1.76	0.49
13:O:64:LEU:HA	13:O:67:LEU:HB2	1.94	0.49
3:P:192:PHE:O	3:P:196:THR:HG23	2.12	0.49
3:P:286:PHE:HB3	3:P:303:PHE:CD1	2.47	0.49
15:R:234:TRP:CD2	15:R:241:LEU:HD13	2.47	0.49
15:R:353:GLN:O	15:R:383:ARG:NH1	2.46	0.49
15:R:386:ASN:O	15:R:390:GLY:N	2.34	0.49
16:S:53:ASN:O	16:S:57:GLN:HG3	2.13	0.49
1:A:1487:CYS:SG	1:A:1488:LEU:N	2.85	0.49
1:A:1799:ARG:NH2	1:A:1805:MET:HG2	2.27	0.49
2:B:14:TRP:CB	12:N:595:ILE:HG23	2.43	0.49
3:C:173:TYR:CG	3:C:202:HIS:HE1	2.30	0.49
3:C:415:PRO:HA	3:C:418:CYS:SG	2.53	0.49
6:H:465:LEU:HD22	6:H:495:HIS:CE1	2.47	0.49
6:H:726:LEU:HD22	6:H:739:VAL:HG23	1.95	0.49
9:K:47:LEU:HB3	9:K:56:ALA:HB2	1.94	0.49
12:N:790:ILE:HG12	12:N:795:LEU:HG	1.93	0.49
13:O:55:MET:HE3	13:O:59:ARG:HH12	1.76	0.49
13:O:127:HIS:C	13:O:129:THR:H	2.19	0.49
3:P:209:LEU:O	3:P:213:ILE:HG12	2.12	0.49
15:R:230:SER:OG	15:R:271:VAL:O	2.26	0.49
16:S:36:ARG:O	18:Z:199:TYR:OH	2.28	0.49
1:A:1232:ILE:HD13	1:A:1254:VAL:HG22	1.95	0.49
1:A:1463:TYR:HE2	1:A:1511:ASN:HB3	1.76	0.49
8:I:186:GLU:OE1	8:I:197:ARG:NE	2.41	0.49
8:I:513:LEU:HD21	13:O:477:HIS:HE1	1.78	0.49
8:I:523:HIS:HB3	8:I:527:ARG:HH12	1.78	0.49
8:I:622:SER:H	8:I:706:HIS:HA	1.77	0.49
9:J:306:GLY:HA3	9:J:323:LEU:CD2	2.43	0.49
9:J:406:HIS:CE1	9:J:450:ASN:HD22	2.30	0.49
9:J:439:VAL:HG21	9:J:444:TRP:HB2	1.95	0.49
9:K:309:TYR:OH	11:M:59:ASP:OD1	2.28	0.49
13:O:249:ASP:OD1	13:O:249:ASP:N	2.44	0.49
13:O:427:ALA:HA	13:O:472:HIS:HE1	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:272:ALA:O	3:P:275:ASN:N	2.45	0.49
17:X:384:ARG:NH2	17:X:415:GLU:OE1	2.26	0.49
17:Y:53:VAL:HG23	17:Y:86:SER:HB3	1.94	0.49
1:A:116:ALA:O	13:O:266:ASP:HA	2.13	0.49
1:A:860:TYR:CD1	1:A:861:PRO:HD2	2.47	0.49
1:A:1672:ARG:NE	1:A:1706:LEU:O	2.40	0.49
3:C:323:LEU:O	3:C:326:ILE:N	2.46	0.49
8:I:209:CYS:SG	8:I:584:HIS:ND1	2.79	0.49
8:I:329:GLY:O	8:I:332:LYS:HG3	2.13	0.49
8:I:451:PHE:CD2	8:I:452:LEU:HD22	2.46	0.49
8:I:586:LEU:N	8:I:601:LEU:O	2.36	0.49
9:K:354:MET:HE1	9:K:381:THR:HG21	1.94	0.49
14:Q:429:LYS:O	14:Q:433:MET:N	2.44	0.49
15:R:250:VAL:HG13	15:R:264:MET:HB2	1.93	0.49
15:R:442:HIS:CE1	15:R:468:ARG:HB2	2.48	0.49
1:A:435:ASP:OD1	1:A:435:ASP:N	2.35	0.49
1:A:1421:PRO:HG3	1:A:1476:PHE:CZ	2.48	0.49
1:A:1660:LEU:HD11	1:A:1687:LEU:HD23	1.94	0.49
3:C:251:TYR:OH	3:C:268:GLN:HG2	2.13	0.49
3:C:398:ASP:N	3:C:398:ASP:OD1	2.46	0.49
6:F:621:LEU:HG	6:F:644:ILE:HG21	1.95	0.49
6:H:611:PHE:CB	6:H:620:ALA:HB2	2.43	0.49
8:I:21:GLN:HG3	8:I:39:ASN:HD22	1.78	0.49
8:I:233:TYR:CE1	8:I:575:LEU:HD21	2.48	0.49
9:J:275:LEU:HD22	9:J:280:LYS:HB2	1.93	0.49
9:K:190:LEU:HD13	9:K:201:LEU:HD23	1.94	0.49
12:N:809:VAL:HG23	12:N:816:ARG:HB2	1.95	0.49
3:P:130:LYS:O	3:P:133:GLU:HG2	2.13	0.49
14:Q:204:ASN:ND2	14:Q:221:GLN:HE21	2.10	0.49
16:S:180:GLN:HG3	16:S:181:GLN:HE21	1.75	0.49
1:A:1512:LEU:HA	1:A:1515:CYS:SG	2.53	0.49
2:B:65:HIS:HB3	2:B:67:GLN:OE1	2.13	0.49
6:F:157:GLU:O	6:F:633:ARG:NH1	2.44	0.49
6:H:676:GLY:HA3	6:H:692:LEU:HD21	1.94	0.49
8:I:356:SER:HB2	8:I:397:ILE:HG12	1.95	0.49
8:I:663:ASP:OD1	8:I:663:ASP:N	2.46	0.49
9:J:351:ASP:OD1	9:J:352:GLN:N	2.42	0.49
10:L:46:ARG:NH1	10:L:156:ILE:O	2.46	0.49
13:O:493:LEU:HD13	13:O:507:TRP:HB2	1.94	0.49
3:P:466:GLU:HG2	3:P:468:MET:H	1.78	0.49
17:X:59:LEU:O	17:X:62:THR:OG1	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:X:66:ASN:ND2	17:Y:268:ARG:HB3	2.28	0.49
17:Y:268:ARG:HG2	17:Y:269:ASP:CG	2.38	0.49
1:A:1770:LEU:O	1:A:1774:VAL:HG23	2.13	0.48
3:C:135:VAL:HG11	11:M:13:ASP:HB3	1.95	0.48
3:C:240:GLU:O	3:C:242:GLN:NE2	2.45	0.48
6:H:93:SER:HB3	6:H:121:LEU:HD21	1.95	0.48
6:H:120:LEU:O	6:H:124:VAL:HG23	2.12	0.48
6:H:135:SER:OG	6:H:160:GLU:OE2	2.31	0.48
6:H:695:ALA:HA	6:H:698:ILE:HG12	1.95	0.48
8:I:46:LEU:HD12	8:I:47:HIS:H	1.77	0.48
8:I:48:ARG:NH1	12:N:392:ASN:OD1	2.46	0.48
9:J:24:PHE:HD2	9:J:25:TRP:CD1	2.31	0.48
9:J:63:ARG:HB2	9:J:65:LEU:HD13	1.95	0.48
12:N:408:ARG:O	12:N:413:SER:HA	2.13	0.48
13:O:733:CYS:HA	13:O:736:LEU:HD12	1.95	0.48
3:P:35:GLN:HG2	3:P:201:LEU:HD11	1.95	0.48
15:R:210:SER:OG	15:R:214:GLY:N	2.45	0.48
17:X:509:CYS:HB3	17:X:538:LEU:HB2	1.94	0.48
1:A:346:ASN:O	1:A:348:ALA:N	2.45	0.48
1:A:869:ARG:NH1	1:A:943:ASP:OD1	2.34	0.48
1:A:1266:HIS:HD2	1:A:1269:THR:HG23	1.78	0.48
1:A:1543:HIS:HB2	1:A:1559:HIS:HE1	1.77	0.48
1:A:1602:HIS:O	1:A:1606:LEU:HD12	2.13	0.48
1:A:1887:CYS:HA	1:A:1890:VAL:HG22	1.93	0.48
3:C:224:LEU:O	3:C:230:LYS:NZ	2.35	0.48
6:F:504:GLN:HE22	6:F:507:ARG:NH2	2.11	0.48
6:F:532:ARG:NH2	6:F:534:GLU:OE2	2.47	0.48
9:J:230:ASN:OD1	9:J:231:LEU:N	2.45	0.48
9:J:427:ASP:O	9:J:431:LYS:HG2	2.13	0.48
9:K:441:VAL:HG13	9:K:474:LEU:HD22	1.95	0.48
10:L:113:LEU:HD13	10:L:120:ILE:HD13	1.94	0.48
3:P:494:ILE:HD13	3:P:516:LEU:HD13	1.96	0.48
17:X:442:GLN:NE2	17:X:472:ARG:HG3	2.28	0.48
1:A:172:SER:OG	1:A:173:LEU:N	2.46	0.48
1:A:1321:VAL:HG23	1:A:1322:PRO:HD3	1.95	0.48
1:A:1492:ALA:O	1:A:1496:MET:HG2	2.12	0.48
1:A:1762:GLY:C	1:A:1764:LYS:H	2.21	0.48
6:H:736:GLU:HG2	10:L:177:PHE:CE2	2.48	0.48
8:I:48:ARG:CD	8:I:55:VAL:HG22	2.42	0.48
8:I:209:CYS:SG	8:I:577:ASN:HB2	2.53	0.48
9:K:150:THR:HA	9:K:153:TYR:HD2	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:445:GLU:HA	9:K:474:LEU:HD12	1.95	0.48
3:P:358:LEU:HD11	3:P:368:TRP:CE2	2.48	0.48
14:Q:189:LEU:HB3	14:Q:201:ALA:HB3	1.96	0.48
17:Y:509:CYS:HA	17:Y:512:HIS:HD2	1.79	0.48
1:A:1574:LEU:HD13	1:A:1584:LEU:HD11	1.96	0.48
1:A:1818:LEU:HD21	1:A:1849:LYS:HB2	1.94	0.48
3:C:186:LYS:NZ	3:C:190:ASP:OD2	2.46	0.48
8:I:705:MET:HE3	8:I:705:MET:HB2	1.77	0.48
8:I:718:LYS:HZ3	8:I:737:ASN:HB2	1.77	0.48
9:J:325:LYS:HE3	9:J:329:LEU:HB2	1.95	0.48
12:N:269:THR:HA	12:N:292:TRP:HH2	1.77	0.48
14:Q:248:ALA:HA	14:Q:271:VAL:HG23	1.95	0.48
16:S:85:THR:HG21	16:S:101:LEU:HD11	1.96	0.48
1:A:42:LEU:HD23	3:C:363:ARG:HG3	1.93	0.48
1:A:1024:MET:HG2	1:A:1034:VAL:HG11	1.96	0.48
1:A:1661:HIS:NE2	1:A:1662:LEU:HD23	2.29	0.48
1:A:1750:PHE:HD2	1:A:1775:LEU:HD12	1.77	0.48
1:A:1793:MET:O	1:A:1797:ILE:HG23	2.13	0.48
6:F:601:ALA:O	6:F:604:TYR:N	2.46	0.48
6:H:21:TYR:HE1	6:H:50:ARG:HB3	1.77	0.48
6:H:635:TYR:HE2	10:L:183:ILE:HD11	1.79	0.48
9:J:397:ILE:HG22	9:J:398:ALA:H	1.78	0.48
9:J:492:MET:HE3	9:J:494:ASN:ND2	2.28	0.48
13:O:219:GLN:NE2	13:O:231:LEU:H	2.11	0.48
14:Q:144:TYR:CD2	14:Q:148:LEU:HD13	2.48	0.48
14:Q:198:LEU:N	14:Q:209:TRP:O	2.30	0.48
15:R:402:VAL:HG22	15:R:418:HIS:ND1	2.29	0.48
16:S:22:TRP:CD1	16:S:22:TRP:H	2.30	0.48
17:X:66:ASN:ND2	17:Y:265:SER:O	2.46	0.48
17:X:305:ILE:HA	17:X:308:MET:HG2	1.95	0.48
17:X:456:VAL:O	17:X:458:GLN:N	2.44	0.48
17:X:507:SER:OG	17:X:508:ASP:N	2.46	0.48
3:C:67:LEU:HD22	3:P:78:GLU:HA	1.96	0.48
3:C:277:ARG:NH1	3:C:434:ARG:HH22	2.12	0.48
6:H:673:CYS:O	6:H:677:VAL:HG23	2.14	0.48
8:I:134:GLU:O	8:I:137:LEU:HB2	2.14	0.48
8:I:446:THR:HG22	13:O:69:GLN:HE22	1.79	0.48
8:I:666:LEU:N	8:I:712:ARG:O	2.30	0.48
9:J:124:SER:O	9:J:127:SER:OG	2.18	0.48
9:J:445:GLU:OE1	9:J:475:ILE:HG21	2.13	0.48
12:N:281:TYR:CE1	12:N:356:PRO:HB2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:N:657:VAL:O	12:N:728:VAL:HG22	2.13	0.48
13:O:38:LEU:HD11	13:O:139:MET:HB3	1.96	0.48
3:P:148:ASN:HD22	3:P:152:ARG:HE	1.60	0.48
17:Y:445:THR:O	17:Y:449:THR:HG23	2.14	0.48
1:A:268:VAL:HG12	1:A:412:LEU:HD21	1.96	0.48
1:A:668:MET:HG2	1:A:759:ILE:HD11	1.94	0.48
1:A:1013:ASP:OD2	1:A:1045:HIS:NE2	2.36	0.48
2:B:25:ILE:HG23	2:B:63:TRP:CE3	2.48	0.48
6:F:537:GLU:OE1	6:F:537:GLU:N	2.36	0.48
8:I:413:ASN:ND2	8:I:450:GLU:OE1	2.46	0.48
9:K:176:LEU:HB2	9:K:181:GLU:HG3	1.95	0.48
9:K:471:ALA:O	9:K:474:LEU:N	2.47	0.48
13:O:621:SER:HB2	13:O:651:ILE:CG1	2.44	0.48
14:Q:192:TRP:HE1	14:Q:196:ASN:HA	1.79	0.48
14:Q:414:LEU:O	14:Q:428:TRP:N	2.26	0.48
17:X:159:LEU:HD22	17:X:171:ILE:HG23	1.95	0.48
17:X:230:VAL:HG21	17:Y:36:ASN:HB3	1.95	0.48
17:X:320:ARG:O	17:X:324:VAL:HG23	2.14	0.48
17:Y:350:PHE:O	17:Y:353:LYS:N	2.44	0.48
17:Y:525:TYR:O	17:Y:529:MET:HG2	2.14	0.48
18:Z:18:GLU:HG2	18:Z:73:LYS:HD3	1.94	0.48
1:A:35:LEU:HD11	13:O:269:SER:HA	1.94	0.48
1:A:270:THR:HG23	1:A:412:LEU:HD22	1.95	0.48
3:C:92:ALA:O	3:C:96:VAL:HG23	2.13	0.48
3:C:123:TYR:OH	3:C:181:LYS:NZ	2.21	0.48
6:F:543:LEU:HB2	6:F:552:LEU:HD13	1.95	0.48
6:H:113:SER:O	6:H:117:THR:HG23	2.14	0.48
6:H:702:ASN:OD1	6:H:705:CYS:N	2.39	0.48
8:I:578:ASN:OD1	8:I:580:THR:OG1	2.29	0.48
9:K:35:GLU:HB3	9:K:40:ILE:CG1	2.44	0.48
9:K:287:LEU:HD23	9:K:287:LEU:HA	1.72	0.48
11:M:6:GLN:NE2	3:P:360:LEU:HB3	2.29	0.48
11:M:7:ARG:NH1	3:P:131:ASP:HB3	2.29	0.48
3:P:487:ALA:HB1	3:P:519:TYR:HE1	1.79	0.48
14:Q:262:ARG:NH2	14:Q:300:HIS:HD2	2.12	0.48
15:R:264:MET:HG2	15:R:300:HIS:CD2	2.48	0.48
15:R:337:PRO:HD3	15:R:347:PRO:HA	1.96	0.48
1:A:1284:GLU:HB2	1:A:1350:TYR:CE2	2.48	0.48
6:F:136:GLU:HB3	6:F:140:LYS:HZ3	1.79	0.48
6:F:653:LEU:HA	6:F:656:MET:HE3	1.95	0.48
8:I:37:LEU:HD21	8:I:45:LEU:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:173:LEU:HD12	8:I:190:TYR:CE1	2.49	0.48
9:K:243:TYR:HA	7:W:3:ARG:NH2	2.27	0.48
9:K:264:HIS:HD2	9:K:267:CYS:H	1.61	0.48
9:K:453:HIS:HD2	9:K:456:ARG:HH22	1.61	0.48
10:L:125:THR:HA	10:L:126:ASP:HB3	1.94	0.48
12:N:534:SER:OG	12:N:537:ARG:HG2	2.13	0.48
12:N:611:VAL:HG11	12:N:637:TRP:CZ2	2.49	0.48
13:O:707:LYS:NZ	13:O:740:LEU:O	2.37	0.48
3:P:283:LEU:HD13	3:P:306:LEU:HD11	1.95	0.48
3:P:385:ILE:HG12	3:P:408:THR:HG21	1.96	0.48
15:R:105:GLN:C	15:R:107:PRO:HD3	2.39	0.48
16:S:304:LYS:HG3	16:S:305:GLU:N	2.28	0.48
1:A:802:TYR:CZ	1:A:841:PRO:HA	2.49	0.48
1:A:1180:GLY:HA3	1:A:1211:GLY:CA	2.44	0.48
1:A:1530:SER:O	1:A:1530:SER:OG	2.32	0.48
2:B:45:PRO:HD2	2:B:57:MET:CB	2.44	0.48
8:I:397:ILE:HG22	13:O:444:MET:HE2	1.95	0.48
8:I:606:ASP:OD1	8:I:608:SER:N	2.44	0.48
12:N:350:ASP:CB	12:N:351:PHE:HA	2.33	0.48
12:N:395:ASP:OD1	12:N:398:THR:HB	2.14	0.48
13:O:402:LEU:HD13	13:O:425:LYS:HG2	1.95	0.48
3:P:426:HIS:CD2	3:P:430:PRO:HA	2.49	0.48
14:Q:264:MET:HB3	14:Q:300:HIS:CE1	2.48	0.48
14:Q:414:LEU:N	14:Q:428:TRP:O	2.33	0.48
16:S:151:LEU:C	16:S:183:ALA:HB1	2.38	0.48
17:X:424:ARG:O	17:X:428:VAL:HG23	2.13	0.48
1:A:131:PHE:CD2	1:A:216:PRO:HD3	2.49	0.47
1:A:212:SER:HB3	1:A:223:LEU:HD21	1.96	0.47
1:A:1644:TYR:O	1:A:1645:GLU:HG3	2.13	0.47
1:A:1702:ARG:HD3	1:A:1782:GLU:OE2	2.14	0.47
6:F:142:LEU:HD11	6:F:152:PHE:HA	1.95	0.47
6:F:575:ASN:OD1	15:R:499:ARG:NH2	2.46	0.47
6:F:656:MET:SD	17:Y:526:GLN:N	2.87	0.47
8:I:335:GLN:O	8:I:338:GLU:HG2	2.13	0.47
8:I:500:PHE:HE1	13:O:491:LYS:HE2	1.78	0.47
12:N:404:ILE:HG23	12:N:417:LEU:HD11	1.96	0.47
15:R:326:SER:OG	15:R:334:ASN:O	2.21	0.47
17:X:222:MET:O	17:X:226:VAL:HG23	2.14	0.47
8:I:106:VAL:HG12	8:I:107:GLU:H	1.78	0.47
9:J:441:VAL:HG23	9:J:443:LYS:H	1.78	0.47
9:K:153:TYR:HB3	9:K:166:ALA:HB1	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:N:530:GLN:HG3	12:N:532:SER:HB3	1.96	0.47
12:N:662:VAL:HB	12:N:687:MET:SD	2.54	0.47
13:O:55:MET:HB3	13:O:59:ARG:HH12	1.79	0.47
13:O:301:ARG:NH1	13:O:336:ASP:OD1	2.47	0.47
13:O:540:SER:O	13:O:544:VAL:HG22	2.13	0.47
3:P:54:TRP:O	3:P:57:GLU:HB2	2.14	0.47
3:P:203:TRP:NE1	3:P:207:LEU:HD13	2.29	0.47
3:P:238:TYR:CB	3:P:247:ALA:HB2	2.44	0.47
3:P:313:LYS:HD2	3:P:343:LEU:HD21	1.95	0.47
15:R:224:GLN:O	15:R:227:GLU:HG2	2.14	0.47
15:R:246:SER:HA	15:R:270:ARG:HB2	1.95	0.47
15:R:450:THR:O	15:R:459:ALA:N	2.40	0.47
15:R:454:ASP:OD1	15:R:454:ASP:N	2.40	0.47
17:X:302:PRO:HG2	17:X:303:TYR:CD2	2.49	0.47
17:Y:214:VAL:HG22	17:Y:216:GLY:H	1.79	0.47
1:A:1644:TYR:C	1:A:1645:GLU:HG3	2.40	0.47
6:H:142:LEU:O	6:H:144:LEU:N	2.47	0.47
6:H:522:PHE:CD1	6:H:539:TYR:HB2	2.50	0.47
6:H:696:ILE:HG13	6:H:705:CYS:SG	2.54	0.47
13:O:266:ASP:OD2	13:O:269:SER:N	2.47	0.47
14:Q:426:VAL:HG13	14:Q:438:GLU:OE2	2.14	0.47
15:R:233:ALA:O	15:R:276:TRP:NE1	2.35	0.47
16:S:139:TYR:HB3	16:S:158:TRP:CE2	2.49	0.47
17:X:44:MET:SD	17:Y:201:LEU:HB3	2.53	0.47
17:X:269:ASP:H	17:Y:66:ASN:HD21	1.61	0.47
17:Y:270:ASN:HD22	17:Y:273:LEU:HB2	1.78	0.47
17:Y:308:MET:HB2	17:Y:331:LEU:HD11	1.97	0.47
18:Z:86:VAL:HB	18:Z:100:TRP:HB2	1.96	0.47
1:A:1119:ASP:OD1	1:A:1120:LEU:N	2.48	0.47
1:A:1173:ALA:HB2	1:A:1204:THR:HG22	1.96	0.47
1:A:1543:HIS:HD2	1:A:1559:HIS:CE1	2.32	0.47
1:A:1621:PRO:HA	1:A:1697:LEU:O	2.15	0.47
3:C:131:ASP:O	3:C:134:THR:HB	2.14	0.47
8:I:261:LEU:O	8:I:265:ILE:HG23	2.14	0.47
8:I:676:ASN:ND2	8:I:678:GLU:HB2	2.28	0.47
13:O:72:ASP:HB2	13:O:211:GLN:NE2	2.29	0.47
13:O:622:GLU:O	13:O:625:LEU:HG	2.14	0.47
13:O:727:THR:O	13:O:730:ARG:HB3	2.15	0.47
3:P:61:SER:OG	3:P:262:SER:N	2.48	0.47
14:Q:150:VAL:HG12	16:S:33:ARG:HD2	1.97	0.47
17:X:436:THR:HG23	17:X:437:LEU:HD22	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:X:475:TYR:O	17:X:479:VAL:HG23	2.14	0.47
18:Z:84:LEU:O	18:Z:102:PHE:N	2.46	0.47
1:A:243:ALA:HB1	1:A:260:ASP:OD1	2.15	0.47
1:A:1074:CYS:HA	1:A:1077:THR:OG1	2.15	0.47
1:A:1314:ILE:HG13	1:A:1315:GLY:N	2.30	0.47
3:C:213:ILE:HD11	3:C:222:LEU:HD11	1.96	0.47
3:C:377:GLU:HA	15:R:130:ILE:CG2	2.45	0.47
6:H:79:CYS:SG	6:H:84:LYS:HB2	2.55	0.47
8:I:205:CYS:HA	8:I:220:VAL:O	2.15	0.47
8:I:276:TRP:CZ2	8:I:476:GLY:HA3	2.50	0.47
12:N:363:TYR:OH	12:N:367:ARG:NH2	2.47	0.47
3:P:225:PRO:O	3:P:230:LYS:HD2	2.14	0.47
14:Q:275:SER:O	14:Q:282:SER:N	2.42	0.47
15:R:317:TRP:CG	15:R:324:LEU:HD13	2.50	0.47
17:X:266:LEU:HD22	17:Y:63:MET:HB3	1.96	0.47
6:F:164:PRO:HG2	6:F:471:LYS:HG3	1.96	0.47
8:I:22:GLU:HB3	8:I:738:LEU:HD12	1.97	0.47
9:J:70:GLU:HB2	9:J:73:ARG:NH2	2.30	0.47
12:N:167:ARG:HA	12:N:170:GLN:CD	2.39	0.47
13:O:105:LEU:O	13:O:109:GLU:HG3	2.14	0.47
3:P:419:LEU:HD11	3:P:443:TYR:CE1	2.49	0.47
14:Q:165:CYS:O	14:Q:166:ARG:HG2	2.15	0.47
15:R:384:ILE:HG22	15:R:393:LEU:HB2	1.97	0.47
15:R:420:PHE:HA	15:R:421:ALA:HA	1.46	0.47
18:Z:75:TRP:CZ2	18:Z:161:LEU:HD21	2.50	0.47
1:A:968:SER:HG	1:A:970:TRP:NE1	2.12	0.47
1:A:1232:ILE:HG21	1:A:1235:LEU:HD12	1.97	0.47
1:A:1754:PHE:CE2	13:O:631:GLN:HG2	2.49	0.47
2:B:1:MET:N	12:N:650:LEU:HB3	2.30	0.47
2:B:15:LEU:HD13	12:N:634:THR:O	2.15	0.47
3:C:386:GLN:NE2	13:O:282:ILE:HG13	2.26	0.47
6:H:653:LEU:HG	9:K:523:ILE:HG21	1.97	0.47
8:I:300:VAL:HG11	8:I:456:PHE:HB3	1.96	0.47
8:I:717:MET:HG3	8:I:719:ALA:HB2	1.96	0.47
9:J:45:GLN:HE21	9:K:17:GLN:NE2	2.12	0.47
9:J:211:LYS:C	9:J:213:ASN:H	2.22	0.47
9:K:391:PHE:CG	9:K:408:VAL:HG22	2.50	0.47
12:N:239:GLN:HA	12:N:242:GLN:CD	2.39	0.47
13:O:512:GLN:HB3	13:O:535:ILE:HG13	1.96	0.47
3:P:193:VAL:HG21	3:P:222:LEU:HD22	1.95	0.47
3:P:317:SER:HB2	3:P:340:TYR:HE1	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:407:GLN:O	3:P:411:ILE:HG12	2.15	0.47
14:Q:209:TRP:CD1	14:Q:216:ILE:HG13	2.48	0.47
14:Q:292:HIS:HE1	14:Q:324:LEU:HD22	1.80	0.47
15:R:286:ARG:HA	15:R:311:GLU:HA	1.96	0.47
15:R:286:ARG:HA	15:R:311:GLU:HG3	1.95	0.47
15:R:316:ARG:HG2	15:R:363:TRP:CD1	2.48	0.47
16:S:129:GLY:HA3	16:S:138:MET:HE2	1.96	0.47
17:X:144:GLU:O	17:X:147:THR:OG1	2.26	0.47
17:Y:485:LEU:O	17:Y:489:GLU:HG2	2.15	0.47
1:A:32:PRO:HD2	13:O:264:VAL:HG21	1.97	0.47
1:A:932:VAL:O	1:A:935:THR:HG22	2.15	0.47
5:E:63:VAL:HG11	17:Y:364:LYS:HD3	1.97	0.47
6:H:493:SER:HA	6:H:496:TYR:HB3	1.96	0.47
8:I:391:THR:HA	8:I:514:PHE:CD1	2.49	0.47
12:N:411:ASP:CG	12:N:415:VAL:HB	2.39	0.47
14:Q:166:ARG:HH12	14:Q:168:ILE:HD11	1.80	0.47
15:R:83:ARG:HH21	15:R:88:MET:HG3	1.78	0.47
15:R:196:ASN:HB2	15:R:453:PRO:HG3	1.97	0.47
1:A:592:HIS:O	1:A:593:ASN:HB3	2.14	0.47
1:A:1296:LEU:HD22	1:A:1589:TYR:CZ	2.50	0.47
1:A:1326:TYR:O	1:A:1330:VAL:HG22	2.14	0.47
3:C:67:LEU:HD13	3:P:81:ALA:HB2	1.97	0.47
9:J:324:SER:HA	9:J:327:THR:HG22	1.96	0.47
9:K:422:GLU:OE1	9:K:458:LEU:HD22	2.15	0.47
9:K:475:ILE:HD13	9:K:478:ASN:HD22	1.80	0.47
12:N:669:TYR:HA	12:N:672:ASP:OD2	2.15	0.47
12:N:758:ILE:HD13	12:N:761:MET:HE3	1.97	0.47
3:P:358:LEU:HD21	3:P:368:TRP:CH2	2.50	0.47
14:Q:291:HIS:NE2	14:Q:304:THR:HG23	2.30	0.47
15:R:363:TRP:CZ3	15:R:387:VAL:HG11	2.48	0.47
17:Y:206:ILE:HG12	17:Y:222:MET:HE2	1.97	0.47
17:Y:241:LYS:HE2	17:Y:241:LYS:HB2	1.67	0.47
17:Y:295:GLU:OE2	17:Y:320:ARG:NH2	2.47	0.47
17:Y:350:PHE:HZ	17:Y:382:ALA:N	2.13	0.47
1:A:1398:PHE:CE2	10:L:70:ARG:HD3	2.50	0.47
1:A:1595:HIS:CD2	1:A:1598:ASP:HB2	2.50	0.47
1:A:1691:LEU:HD23	1:A:1691:LEU:HA	1.79	0.47
1:A:1864:GLY:HA2	1:A:1867:CYS:SG	2.55	0.47
3:C:531:THR:O	3:C:535:LYS:HG2	2.15	0.47
6:F:629:ARG:NE	17:Y:533:SER:OG	2.47	0.47
7:G:1:MET:SD	9:J:174:HIS:NE2	2.88	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:6:PRO:HD2	9:J:446:PRO:HG3	1.96	0.47
9:J:4:GLU:O	9:J:8:LYS:HG3	2.14	0.47
9:J:294:LEU:HD23	9:J:294:LEU:HA	1.74	0.47
9:K:36:GLU:HB3	9:K:39:ASP:OD2	2.15	0.47
12:N:285:PHE:HB3	12:N:289:PHE:HD1	1.80	0.47
12:N:571:ASN:ND2	12:N:592:TYR:HA	2.30	0.47
12:N:773:ILE:HG21	12:N:799:LEU:HD11	1.97	0.47
13:O:54:LEU:O	13:O:58:ARG:HG3	2.15	0.47
15:R:93:PHE:O	15:R:97:LYS:HB2	2.15	0.47
16:S:313:TRP:N	16:S:313:TRP:CD1	2.81	0.47
1:A:805:HIS:NE2	1:A:843:SER:HB2	2.29	0.46
1:A:949:PHE:CZ	1:A:1813:GLN:HG3	2.50	0.46
2:B:14:TRP:CG	12:N:595:ILE:HG23	2.50	0.46
3:C:39:ILE:O	3:C:43:THR:HG23	2.15	0.46
3:C:136:ASP:OD2	3:C:136:ASP:N	2.46	0.46
6:F:639:TYR:HE2	6:F:674:HIS:CD2	2.33	0.46
6:H:658:PHE:CE2	6:H:674:HIS:HB3	2.50	0.46
8:I:526:LYS:HA	8:I:529:MET:HE2	1.96	0.46
9:J:204:LEU:HD13	9:K:24:PHE:CZ	2.50	0.46
9:J:211:LYS:HB2	9:J:243:TYR:CD2	2.50	0.46
12:N:247:LEU:CB	12:N:253:LEU:HB3	2.44	0.46
13:O:240:LEU:HA	13:O:240:LEU:HD23	1.66	0.46
13:O:516:PHE:CE1	13:O:546:ARG:HD2	2.50	0.46
15:R:176:LEU:O	15:R:467:LEU:N	2.31	0.46
15:R:234:TRP:CZ2	15:R:241:LEU:HD22	2.50	0.46
15:R:235:ILE:HG23	15:R:237:GLU:H	1.79	0.46
17:Y:37:VAL:O	17:Y:41:VAL:HG23	2.15	0.46
17:Y:272:ASP:OD1	17:Y:273:LEU:N	2.49	0.46
17:Y:525:TYR:HD2	17:Y:529:MET:HE2	1.80	0.46
18:Z:80:SER:O	18:Z:157:THR:HA	2.15	0.46
1:A:643:ASN:O	1:A:646:SER:OG	2.23	0.46
1:A:1274:LEU:HD23	1:A:1274:LEU:HA	1.78	0.46
6:H:513:SER:HA	6:H:515:TYR:CE1	2.50	0.46
6:H:549:ASP:N	6:H:549:ASP:OD1	2.47	0.46
6:H:611:PHE:HB2	6:H:620:ALA:HB2	1.96	0.46
12:N:165:THR:CB	12:N:170:GLN:HE21	2.28	0.46
12:N:241:HIS:CE1	12:N:302:LYS:HE3	2.49	0.46
12:N:798:TYR:CE1	12:N:802:LYS:HE2	2.50	0.46
14:Q:240:TYR:HB3	14:Q:252:LEU:HD11	1.98	0.46
17:X:134:SER:O	17:X:138:VAL:HG23	2.14	0.46
17:X:450:VAL:HA	17:X:453:GLU:HG3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Y:93:TYR:HD1	17:Y:145:CYS:HB3	1.79	0.46
17:Y:176:ALA:HB1	17:Y:192:TYR:CE2	2.50	0.46
1:A:246:ILE:HD11	1:A:249:LEU:HD21	1.97	0.46
1:A:483:GLU:OE2	1:A:592:HIS:N	2.47	0.46
1:A:1666:ILE:HG13	1:A:1666:ILE:O	2.15	0.46
2:B:47:VAL:HG11	2:B:60:ILE:HG21	1.96	0.46
8:I:27:VAL:O	8:I:35:ILE:HG13	2.15	0.46
8:I:497:TRP:CD1	13:O:446:LEU:HB3	2.49	0.46
8:I:596:TYR:H	8:I:637:SER:HB2	1.81	0.46
9:J:231:LEU:HB3	9:J:264:HIS:CE1	2.50	0.46
12:N:185:MET:HE2	12:N:292:TRP:CD1	2.49	0.46
12:N:245:GLN:O	12:N:249:ARG:HG3	2.15	0.46
15:R:429:LYS:O	15:R:433:MET:N	2.48	0.46
16:S:122:LEU:HD11	16:S:154:PHE:HB2	1.97	0.46
16:S:163:GLU:C	16:S:166:GLU:H	2.22	0.46
17:X:356:SER:HA	17:X:386:MET:HE1	1.96	0.46
17:X:462:LYS:HG2	17:X:482:LYS:HZ3	1.80	0.46
17:Y:134:SER:HB3	17:Y:137:GLU:CG	2.46	0.46
17:Y:338:HIS:O	17:Y:341:PRO:HD2	2.15	0.46
18:Z:145:LEU:HB3	18:Z:149:CYS:SG	2.56	0.46
1:A:1520:LEU:HD22	1:A:1542:LEU:HD12	1.98	0.46
3:C:104:HIS:CE1	3:P:294:PRO:HG3	2.51	0.46
6:F:136:GLU:HB3	6:F:140:LYS:NZ	2.31	0.46
6:F:472:GLY:HA3	6:F:488:LEU:HD21	1.98	0.46
8:I:250:ARG:HE	8:I:369:MET:HE2	1.81	0.46
8:I:512:LEU:HG	13:O:439:LEU:HD13	1.97	0.46
9:J:14:LEU:HD23	9:J:14:LEU:HA	1.79	0.46
12:N:63:ALA:HB3	12:N:64:ALA:HB3	1.97	0.46
12:N:91:PHE:O	12:N:93:ASN:N	2.48	0.46
12:N:197:PRO:HA	12:N:198:GLU:HA	1.59	0.46
13:O:55:MET:HB3	13:O:59:ARG:NH1	2.30	0.46
14:Q:411:TYR:HD1	14:Q:473:PHE:HD1	1.64	0.46
17:Y:444:LEU:HA	17:Y:447:LEU:HD12	1.97	0.46
18:Z:64:TYR:HD2	18:Z:65:LEU:HD23	1.79	0.46
18:Z:83:LYS:H	18:Z:156:TYR:HB3	1.80	0.46
1:A:431:PHE:HB2	1:A:481:PRO:HG3	1.98	0.46
1:A:1177:MET:HB2	1:A:1207:GLY:HA2	1.97	0.46
1:A:1848:VAL:O	1:A:1852:ILE:HG12	2.16	0.46
3:C:389:ARG:O	3:C:392:ILE:HG22	2.16	0.46
3:C:403:TYR:HD2	3:C:435:MET:SD	2.38	0.46
3:C:470:LEU:HB3	3:C:493:TYR:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:765:ASP:OD2	9:J:359:THR:OG1	2.34	0.46
6:H:592:ARG:HD3	6:H:596:VAL:HG23	1.96	0.46
9:J:93:LEU:HD23	9:J:93:LEU:HA	1.70	0.46
9:J:185:LEU:HD13	9:J:188:LEU:HD12	1.97	0.46
9:J:264:HIS:HD2	9:J:267:CYS:H	1.63	0.46
11:M:60:LEU:HB3	11:M:62:LEU:HD13	1.97	0.46
12:N:512:LYS:O	12:N:516:ILE:HG12	2.16	0.46
12:N:560:MET:HE3	12:N:600:PHE:HB2	1.98	0.46
12:N:670:PHE:CE2	12:N:715:VAL:HA	2.50	0.46
13:O:516:PHE:CE2	13:O:528:ALA:HB1	2.50	0.46
3:P:520:TYR:HA	3:P:523:CYS:SG	2.55	0.46
14:Q:167:TYR:CZ	15:R:464:ASP:HA	2.50	0.46
14:Q:301:HIS:NE2	14:Q:304:THR:OG1	2.42	0.46
15:R:97:LYS:HA	15:R:98:GLU:HA	1.66	0.46
16:S:131:LEU:HD12	16:S:131:LEU:O	2.15	0.46
17:Y:44:MET:HB3	17:Y:53:VAL:HG12	1.96	0.46
1:A:28:CYS:HA	1:A:31:HIS:HB2	1.98	0.46
1:A:165:GLU:OE1	13:O:318:GLN:HB2	2.16	0.46
1:A:436:LEU:H	1:A:501:THR:HG23	1.80	0.46
1:A:872:LEU:HD13	1:A:937:VAL:HG11	1.98	0.46
2:B:57:MET:HE3	2:B:61:LEU:HD21	1.98	0.46
6:H:103:HIS:O	6:H:107:VAL:HG13	2.16	0.46
6:H:730:LYS:HG2	6:H:740:TYR:HE1	1.80	0.46
8:I:86:ASP:OD1	8:I:87:THR:N	2.44	0.46
8:I:120:VAL:HG22	8:I:172:ARG:NH2	2.30	0.46
8:I:178:LEU:HD12	8:I:188:TYR:CD1	2.50	0.46
8:I:203:GLY:HA3	8:I:223:VAL:HG22	1.98	0.46
8:I:360:LEU:HD11	8:I:390:ILE:HG23	1.96	0.46
9:J:165:GLU:OE1	9:K:18:GLN:NE2	2.48	0.46
9:K:5:ARG:O	9:K:9:ARG:HG2	2.16	0.46
9:K:231:LEU:HA	9:K:234:VAL:HG22	1.98	0.46
9:K:506:LEU:HD11	9:K:516:VAL:HG22	1.98	0.46
13:O:508:MET:HA	13:O:511:ASP:OD1	2.16	0.46
3:P:426:HIS:CD2	3:P:436:LEU:HD21	2.50	0.46
14:Q:228:TYR:CE1	14:Q:246:SER:HB3	2.51	0.46
17:X:384:ARG:NH2	17:X:415:GLU:HB3	2.30	0.46
17:X:400:ILE:HG13	17:X:401:ARG:N	2.31	0.46
1:A:248:PHE:HD1	1:A:257:MET:HB2	1.81	0.46
1:A:1390:PRO:HG2	1:A:1396:LEU:HG	1.98	0.46
3:C:93:TYR:HD1	3:C:101:ARG:HB3	1.80	0.46
6:F:96:VAL:O	6:F:97:PHE:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:123:HIS:CE1	6:H:127:LYS:HE3	2.50	0.46
9:J:242:TYR:HB2	9:J:250:CYS:SG	2.56	0.46
9:J:279:ASN:HA	9:J:311:MET:HE3	1.97	0.46
9:J:406:HIS:CE1	9:J:447:LEU:HA	2.50	0.46
9:K:378:TYR:HE2	9:K:390:PHE:CE2	2.33	0.46
11:M:2:ASP:OD2	3:P:177:VAL:HG22	2.16	0.46
12:N:660:THR:HG21	12:N:695:ARG:HH22	1.81	0.46
13:O:63:LEU:HD21	13:O:81:LEU:HG	1.97	0.46
3:P:374:GLU:O	3:P:378:MET:HG2	2.15	0.46
14:Q:340:PRO:HD3	14:Q:345:TRP:CZ2	2.51	0.46
15:R:166:ARG:HH22	15:R:413:GLU:CD	2.24	0.46
16:S:125:TRP:CG	16:S:142:LEU:HD21	2.51	0.46
17:X:316:ALA:HB1	17:X:351:TYR:CE1	2.48	0.46
1:A:770:TYR:OH	1:A:809:ASP:OD2	2.30	0.46
1:A:847:TRP:CD1	1:A:858:PRO:HG2	2.51	0.46
8:I:209:CYS:O	8:I:218:SER:N	2.42	0.46
8:I:595:LEU:HB2	8:I:637:SER:HB3	1.98	0.46
9:J:194:CYS:SG	9:J:196:GLU:HB2	2.56	0.46
9:J:291:LEU:HD23	9:J:291:LEU:HA	1.76	0.46
12:N:400:TYR:OH	12:N:425:ARG:NE	2.49	0.46
12:N:691:LEU:O	12:N:695:ARG:HG2	2.16	0.46
3:P:248:LEU:O	3:P:252:GLN:HG2	2.16	0.46
3:P:405:LEU:HD23	3:P:405:LEU:HA	1.80	0.46
14:Q:361:VAL:HA	14:Q:372:ALA:O	2.16	0.46
15:R:309:SER:N	15:R:330:ASP:OD2	2.33	0.46
16:S:190:GLN:O	16:S:194:ARG:HG3	2.16	0.46
17:Y:180:LYS:HD3	17:Y:192:TYR:HE2	1.81	0.46
18:Z:135:ILE:O	18:Z:138:THR:HG22	2.15	0.46
1:A:436:LEU:HD13	1:A:638:LEU:HD23	1.98	0.46
1:A:1014:ASP:HB2	1:A:1045:HIS:CE1	2.51	0.46
1:A:1064:GLU:O	1:A:1068:ASN:ND2	2.49	0.46
1:A:1434:ILE:HA	1:A:1457:LEU:HD11	1.98	0.46
3:C:124:LEU:HD23	3:C:124:LEU:HA	1.78	0.46
6:F:532:ARG:HG2	6:F:534:GLU:H	1.81	0.46
8:I:175:ILE:HG21	8:I:187:LEU:HD23	1.97	0.46
8:I:394:GLY:HA3	8:I:514:PHE:CD2	2.50	0.46
8:I:603:ARG:HA	8:I:603:ARG:HD2	1.73	0.46
10:L:170:PRO:HA	10:L:171:ARG:HA	1.77	0.46
11:M:6:GLN:HE22	3:P:331:VAL:HG23	1.80	0.46
12:N:535:PRO:HA	12:N:538:GLU:HB3	1.98	0.46
3:P:379:LYS:HD3	3:P:379:LYS:HA	1.58	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:Q:406:LEU:HB2	14:Q:415:ILE:HG23	1.97	0.46
15:R:175:ILE:HA	15:R:468:ARG:HA	1.98	0.46
17:X:62:THR:HG21	17:Y:270:ASN:HA	1.98	0.46
17:Y:61:LEU:HD23	17:Y:61:LEU:HA	1.83	0.46
17:Y:233:LEU:HD13	17:Y:236:LEU:HD22	1.98	0.46
17:Y:442:GLN:HG2	17:Y:472:ARG:HB2	1.97	0.46
18:Z:26:PHE:CE2	18:Z:48:LYS:HG2	2.50	0.46
1:A:1149:PRO:HA	1:A:1184:HIS:CE1	2.50	0.46
1:A:1220:MET:HG2	1:A:1264:THR:HG21	1.98	0.46
1:A:1593:PRO:HB3	1:A:1598:ASP:O	2.16	0.46
1:A:1677:LEU:HD12	1:A:1678:ILE:H	1.81	0.46
6:F:116:PHE:HE2	6:H:14:GLN:HG2	1.81	0.46
9:J:341:GLY:HA3	9:J:357:TYR:CE1	2.51	0.46
9:K:139:ILE:O	9:K:143:LEU:HB2	2.16	0.46
9:K:217:GLU:O	9:K:218:THR:OG1	2.29	0.46
13:O:34:LYS:HD3	13:O:139:MET:SD	2.56	0.46
13:O:357:SER:HA	13:O:360:LEU:HD13	1.98	0.46
13:O:382:GLN:HE22	13:O:421:SER:HA	1.80	0.46
3:P:415:PRO:HA	3:P:418:CYS:SG	2.56	0.46
3:P:466:GLU:OE1	3:P:466:GLU:N	2.42	0.46
16:S:83:SER:OG	16:S:87:GLN:NE2	2.48	0.46
17:X:219:VAL:O	17:X:223:THR:HG23	2.16	0.46
17:X:469:LEU:HG	17:X:478:ALA:HB1	1.98	0.46
17:Y:199:CYS:HB2	17:Y:200:PRO:O	2.16	0.46
1:A:215:HIS:CG	1:A:216:PRO:HD2	2.50	0.45
1:A:500:TYR:CE1	1:A:505:ARG:HB2	2.51	0.45
3:C:366:GLY:O	3:C:370:LEU:HG	2.16	0.45
6:F:18:HIS:O	6:H:73:TYR:OH	2.18	0.45
8:I:34:LEU:HD22	12:N:390:GLY:HA3	1.99	0.45
8:I:497:TRP:CE2	13:O:446:LEU:HD13	2.51	0.45
8:I:555:PRO:HB2	8:I:692:ARG:HG3	1.99	0.45
12:N:612:PRO:HG3	12:N:665:VAL:HB	1.98	0.45
13:O:382:GLN:NE2	13:O:421:SER:HA	2.31	0.45
14:Q:353:GLN:NE2	18:Z:52:THR:OG1	2.49	0.45
16:S:66:ILE:HA	16:S:69:TYR:CD2	2.51	0.45
17:X:196:LEU:HD23	17:X:196:LEU:HA	1.67	0.45
17:X:354:ARG:HD2	17:X:357:ARG:HD2	1.98	0.45
1:A:614:THR:HB	1:A:656:GLU:OE1	2.16	0.45
1:A:768:LEU:HD23	1:A:768:LEU:HA	1.79	0.45
1:A:1748:LEU:O	1:A:1752:GLU:HG3	2.16	0.45
3:C:242:GLN:HA	3:C:244:ILE:HG23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:290:ARG:NH2	3:C:294:PRO:O	2.50	0.45
6:F:492:PRO:C	6:F:494:HIS:H	2.23	0.45
7:G:4:ARG:NH2	9:J:377:GLU:OE2	2.36	0.45
8:I:72:ALA:N	8:I:81:ALA:O	2.49	0.45
8:I:92:LEU:O	8:I:92:LEU:HD12	2.16	0.45
8:I:496:GLN:HB2	13:O:496:ARG:NH2	2.30	0.45
9:K:453:HIS:CD2	9:K:456:ARG:HH12	2.34	0.45
3:P:525:LEU:HD23	3:P:525:LEU:HA	1.84	0.45
14:Q:183:ASN:ND2	16:S:91:GLN:O	2.49	0.45
14:Q:309:SER:N	14:Q:330:ASP:OD2	2.49	0.45
14:Q:323:HIS:HE1	14:Q:348:LEU:HD12	1.80	0.45
14:Q:419:GLY:HA2	14:Q:445:ARG:HB2	1.99	0.45
17:X:192:TYR:O	17:X:195:VAL:HG22	2.15	0.45
17:X:311:TYR:CZ	17:X:315:LEU:HD21	2.51	0.45
17:Y:188:SER:O	17:Y:191:SER:OG	2.34	0.45
2:B:27:ARG:HB3	12:N:810:TYR:CZ	2.52	0.45
3:C:358:LEU:HD13	3:C:358:LEU:HA	1.80	0.45
8:I:27:VAL:HG23	8:I:73:TRP:HD1	1.81	0.45
9:K:379:GLY:HA3	9:K:411:VAL:HG22	1.98	0.45
13:O:55:MET:HE3	13:O:59:ARG:NH1	2.32	0.45
13:O:641:LEU:HG	13:O:670:CYS:SG	2.56	0.45
3:P:119:MET:HE1	3:P:157:GLU:CD	2.42	0.45
3:P:156:VAL:O	3:P:160:LYS:HG2	2.15	0.45
3:P:265:ILE:HG13	3:P:266:VAL:N	2.30	0.45
3:P:396:LYS:HA	3:P:396:LYS:HD3	1.83	0.45
3:P:494:ILE:HG21	3:P:516:LEU:HD13	1.97	0.45
14:Q:199:ALA:HB2	14:Q:234:TRP:CZ2	2.52	0.45
14:Q:458:VAL:HG12	14:Q:470:TRP:HB2	1.98	0.45
17:X:63:MET:SD	17:Y:235:TRP:NE1	2.89	0.45
1:A:248:PHE:HB3	1:A:257:MET:HB3	1.98	0.45
1:A:768:LEU:HD11	1:A:861:PRO:HB2	1.98	0.45
1:A:1251:VAL:CG2	1:A:1603:LEU:HD13	2.47	0.45
1:A:1397:ASP:HB3	10:L:71:LYS:HB3	1.99	0.45
2:B:23:CYS:HB2	2:B:55:PHE:HD1	1.79	0.45
6:F:512:LEU:O	6:F:513:SER:OG	2.30	0.45
6:H:142:LEU:O	6:H:146:PRO:HB3	2.16	0.45
6:H:703:PRO:HB2	10:L:177:PHE:CE1	2.39	0.45
8:I:74:ARG:HG2	8:I:75:PRO:HD2	1.98	0.45
8:I:269:LEU:HD13	8:I:526:LYS:HZ1	1.82	0.45
9:J:254:THR:HG23	9:J:271:HIS:HD2	1.81	0.45
9:J:275:LEU:HA	9:J:275:LEU:HD23	1.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:116:PRO:HB3	10:L:120:ILE:HD11	1.99	0.45
13:O:38:LEU:HD21	13:O:139:MET:HG3	1.97	0.45
13:O:126:VAL:HG11	13:O:132:VAL:HG12	1.98	0.45
3:P:130:LYS:HE3	3:P:130:LYS:HB3	1.69	0.45
3:P:255:ILE:HG13	3:P:260:SER:HA	1.98	0.45
14:Q:420:PHE:HA	14:Q:421:ALA:HA	1.46	0.45
16:S:156:ILE:HD13	16:S:192:GLN:HG3	1.99	0.45
17:Y:469:LEU:HD23	17:Y:469:LEU:HA	1.83	0.45
17:Y:495:GLY:HA3	17:Y:518:PHE:CE2	2.49	0.45
1:A:1595:HIS:HD2	1:A:1596:SER:O	1.99	0.45
3:C:422:TYR:CD2	3:C:438:ALA:HB1	2.51	0.45
6:H:121:LEU:O	6:H:125:TYR:HD1	1.99	0.45
8:I:33:ASP:N	8:I:728:ARG:HG3	2.31	0.45
8:I:593:ASP:OD1	8:I:593:ASP:N	2.41	0.45
8:I:602:ARG:NH2	8:I:613:ASN:HB2	2.31	0.45
8:I:618:ILE:HD12	8:I:705:MET:HE1	1.98	0.45
9:J:322:TYR:CE1	11:M:36:LEU:HD11	2.51	0.45
9:K:134:LEU:HD12	9:K:166:ALA:HB2	1.97	0.45
10:L:33:LEU:HD22	10:L:54:TRP:CE2	2.51	0.45
12:N:344:LEU:O	12:N:348:VAL:HG23	2.17	0.45
12:N:350:ASP:HB3	12:N:351:PHE:CA	2.36	0.45
13:O:291:ASN:OD1	13:O:298:ARG:NH2	2.49	0.45
13:O:701:PHE:CZ	13:O:709:ARG:HD2	2.52	0.45
3:P:97:LYS:HD2	3:P:99:TYR:OH	2.17	0.45
3:P:180:ARG:HG3	3:P:212:LEU:HD11	1.98	0.45
3:P:264:TYR:O	3:P:267:SER:OG	2.30	0.45
14:Q:222:MET:HE1	14:Q:251:GLN:NE2	2.31	0.45
15:R:290:ILE:HB	15:R:305:LEU:HB2	1.97	0.45
16:S:274:VAL:HG22	16:S:275:PHE:O	2.17	0.45
17:X:184:GLN:O	17:X:188:SER:OG	2.29	0.45
17:X:311:TYR:O	17:X:315:LEU:HG	2.16	0.45
1:A:497:LEU:HD22	1:A:509:VAL:HG11	1.99	0.45
1:A:635:VAL:O	1:A:639:VAL:HG22	2.16	0.45
1:A:804:ASP:HA	1:A:807:TYR:HB3	1.97	0.45
3:C:290:ARG:HG2	3:C:300:MET:HE1	1.98	0.45
3:C:551:ARG:HH11	9:K:383:ASN:HA	1.81	0.45
8:I:106:VAL:HG12	8:I:107:GLU:N	2.31	0.45
8:I:279:ILE:HD11	8:I:337:ILE:HA	1.98	0.45
8:I:513:LEU:HD22	13:O:443:GLN:CD	2.41	0.45
9:J:26:ALA:HA	9:J:29:VAL:HG12	1.97	0.45
9:J:475:ILE:HD11	9:J:478:ASN:HD22	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:502:PHE:CE1	9:J:515:SER:HA	2.50	0.45
12:N:561:LEU:O	12:N:564:MET:HB2	2.17	0.45
12:N:681:LEU:HB3	12:N:692:LEU:HD21	1.98	0.45
14:Q:149:LYS:NZ	14:Q:400:SER:HA	2.32	0.45
14:Q:289:HIS:CE1	14:Q:306:SER:HB2	2.52	0.45
16:S:129:GLY:HA2	16:S:132:CYS:SG	2.57	0.45
17:Y:223:THR:O	17:Y:227:ILE:HG12	2.17	0.45
1:A:937:VAL:C	1:A:939:PHE:H	2.25	0.45
1:A:1220:MET:SD	1:A:1264:THR:OG1	2.67	0.45
1:A:1424:LYS:HA	1:A:1424:LYS:HD2	1.83	0.45
6:F:754:HIS:CG	6:F:755:LEU:N	2.85	0.45
6:H:118:LEU:HB2	6:H:141:SER:HB3	1.97	0.45
6:H:160:GLU:H	6:H:160:GLU:CD	2.22	0.45
8:I:523:HIS:HB3	8:I:527:ARG:NH1	2.32	0.45
8:I:559:ASP:OD2	8:I:561:ARG:NE	2.50	0.45
9:J:520:GLY:O	9:J:523:ILE:HG22	2.17	0.45
9:K:459:LYS:HD2	9:K:461:TYR:HE2	1.82	0.45
10:L:68:PHE:CD2	10:L:72:THR:HB	2.51	0.45
12:N:80:GLN:HE22	12:N:84:GLN:NE2	2.15	0.45
12:N:211:ARG:O	12:N:215:LEU:HG	2.16	0.45
12:N:589:PHE:CE2	12:N:618:ALA:HB2	2.52	0.45
13:O:33:TYR:HE2	13:O:78:LEU:HD21	1.81	0.45
14:Q:172:PRO:HG3	14:Q:470:TRP:CZ2	2.51	0.45
14:Q:266:SER:OG	14:Q:291:HIS:ND1	2.43	0.45
15:R:99:ASN:N	15:R:100:GLN:HA	2.31	0.45
15:R:193:SER:OG	15:R:196:ASN:N	2.50	0.45
15:R:333:VAL:HG11	15:R:373:THR:HG21	1.97	0.45
17:Y:330:ARG:O	17:Y:334:ILE:HG23	2.17	0.45
18:Z:65:LEU:O	18:Z:69:VAL:HG23	2.16	0.45
1:A:1100:LEU:HD12	1:A:1175:PHE:HE1	1.80	0.45
2:B:57:MET:O	2:B:60:ILE:HG22	2.16	0.45
3:C:414:MET:HE2	13:O:330:ILE:HG13	1.99	0.45
6:H:656:MET:HE2	6:H:660:LYS:NZ	2.32	0.45
8:I:394:GLY:HA3	8:I:514:PHE:CE2	2.52	0.45
8:I:617:ALA:HB3	8:I:702:THR:OG1	2.17	0.45
9:K:347:GLU:O	9:K:348:SER:HB3	2.17	0.45
9:K:431:LYS:O	9:K:435:ILE:HG22	2.17	0.45
9:K:487:TYR:CE1	9:K:518:MET:HG2	2.52	0.45
11:M:2:ASP:OD1	11:M:3:SER:N	2.43	0.45
13:O:627:LEU:O	13:O:631:GLN:HG3	2.17	0.45
14:Q:336:TRP:CH2	14:Q:347:PRO:HG3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:R:187:LEU:O	15:R:359:LYS:NZ	2.38	0.45
15:R:366:TRP:CH2	15:R:412:LYS:HA	2.52	0.45
16:S:170:LYS:O	16:S:174:ILE:HG13	2.17	0.45
17:X:261:LEU:HD22	17:X:267:LEU:HD23	1.98	0.45
1:A:477:LYS:N	1:A:491:LEU:O	2.48	0.45
1:A:1077:THR:HA	1:A:1080:LEU:HD12	1.99	0.45
1:A:1138:HIS:HD2	1:A:1608:HIS:NE2	2.15	0.45
1:A:1190:THR:HA	1:A:1193:ILE:HD12	1.98	0.45
1:A:1674:TRP:CZ3	1:A:1702:ARG:HA	2.52	0.45
2:B:24:GLY:HA2	2:B:27:ARG:HH12	1.82	0.45
3:C:328:LYS:NZ	11:M:22:ASP:O	2.50	0.45
6:F:486:ASN:O	6:F:489:SER:OG	2.33	0.45
8:I:254:LYS:HG3	8:I:369:MET:HE1	1.99	0.45
8:I:666:LEU:O	8:I:712:ARG:N	2.30	0.45
8:I:668:GLN:HB2	8:I:710:HIS:HB3	1.99	0.45
9:K:173:HIS:O	9:K:364:MET:HG2	2.17	0.45
9:K:406:HIS:O	9:K:410:VAL:HG23	2.17	0.45
12:N:554:MET:O	12:N:558:GLU:HG3	2.17	0.45
13:O:39:VAL:HG11	13:O:97:ILE:HD13	1.99	0.45
13:O:684:ALA:O	13:O:688:GLU:HG2	2.16	0.45
3:P:267:SER:HB2	3:P:299:ASN:HD22	1.81	0.45
3:P:381:THR:O	3:P:385:ILE:HG13	2.16	0.45
15:R:362:ALA:O	15:R:371:LEU:HD12	2.17	0.45
16:S:33:ARG:HA	18:Z:144:LEU:HG	1.98	0.45
17:Y:294:PHE:HZ	17:Y:307:GLY:C	2.25	0.45
1:A:248:PHE:HZ	1:A:250:ASN:HB2	1.78	0.45
1:A:1086:MET:SD	1:A:1564:LEU:HG	2.56	0.45
1:A:1810:GLU:O	1:A:1814:ILE:HG13	2.16	0.45
3:C:139:GLY:HA3	3:C:145:GLN:NE2	2.32	0.45
6:F:726:LEU:HD11	6:F:742:LEU:HD23	1.98	0.45
6:H:121:LEU:HG	6:H:125:TYR:CE1	2.52	0.45
8:I:19:LEU:N	8:I:739:ARG:O	2.33	0.45
13:O:55:MET:HA	13:O:58:ARG:NE	2.32	0.45
14:Q:276:TRP:CE2	14:Q:281:LEU:HD13	2.52	0.45
16:S:158:TRP:CD2	16:S:174:ILE:HD13	2.52	0.45
17:X:262:GLU:O	17:X:268:ARG:HA	2.17	0.45
17:X:417:TYR:O	17:X:420:SER:OG	2.23	0.45
17:Y:291:VAL:CG2	17:Y:314:LEU:HB3	2.46	0.45
1:A:479:ALA:HA	1:A:490:VAL:HA	1.98	0.44
3:C:185:VAL:O	3:C:189:ILE:HG13	2.17	0.44
3:C:402:TRP:CD1	3:C:428:LEU:HD22	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:514:ARG:O	3:C:518:GLN:HG3	2.17	0.44
8:I:233:TYR:CD1	8:I:586:LEU:HD22	2.52	0.44
9:J:512:ASP:OD1	9:J:515:SER:N	2.37	0.44
9:K:220:ILE:O	9:K:224:VAL:HG23	2.17	0.44
9:K:439:VAL:O	9:K:440:THR:C	2.60	0.44
10:L:25:ILE:HG22	10:L:158:ILE:HG23	2.00	0.44
12:N:554:MET:HE2	12:N:554:MET:HA	1.98	0.44
14:Q:168:ILE:HD13	14:Q:168:ILE:HA	1.85	0.44
14:Q:317:TRP:CE2	14:Q:324:LEU:HD13	2.52	0.44
16:S:106:VAL:HG21	16:S:128:LEU:HD22	1.99	0.44
1:A:797:LEU:HB3	1:A:799:LEU:CD1	2.47	0.44
1:A:1634:LEU:HD23	1:A:1668:VAL:HA	1.99	0.44
6:F:717:GLU:OE1	6:F:719:TYR:OH	2.31	0.44
8:I:216:SER:HB2	8:I:235:GLN:HG2	1.99	0.44
8:I:604:HIS:CD2	8:I:611:VAL:HB	2.52	0.44
9:J:204:LEU:HA	9:J:204:LEU:HD23	1.69	0.44
12:N:208:ALA:HB1	12:N:212:TYR:CZ	2.52	0.44
12:N:627:GLU:HA	12:N:630:LYS:O	2.18	0.44
12:N:637:TRP:HB3	12:N:639:HIS:HB2	1.99	0.44
13:O:524:LYS:HD3	13:O:524:LYS:HA	1.60	0.44
14:Q:428:TRP:HA	14:Q:434:ALA:O	2.18	0.44
15:R:307:GLY:O	15:R:334:ASN:ND2	2.50	0.44
15:R:430:TYR:CD1	15:R:431:PRO:HA	2.52	0.44
1:A:1473:GLY:HA2	1:A:1526:VAL:CG2	2.48	0.44
3:C:122:ARG:O	3:C:125:SER:OG	2.19	0.44
4:D:10:PRO:HG2	13:O:346:TRP:CE2	2.52	0.44
8:I:45:LEU:HG	8:I:57:SER:HA	1.99	0.44
8:I:207:ALA:C	8:I:575:LEU:HD12	2.43	0.44
8:I:420:TRP:HB2	8:I:440:MET:HE1	1.98	0.44
8:I:520:LYS:HD3	8:I:524:PHE:CE1	2.53	0.44
8:I:655:ASP:OD1	8:I:657:VAL:HG22	2.18	0.44
8:I:713:LEU:HD21	8:I:754:LEU:HD11	2.00	0.44
10:L:80:TYR:HB2	10:L:119:TRP:CD2	2.52	0.44
10:L:87:GLU:OE1	10:L:146:GLN:NE2	2.51	0.44
14:Q:323:HIS:HB2	14:Q:363:TRP:CH2	2.53	0.44
14:Q:424:GLN:HB2	14:Q:440:LYS:HG2	1.98	0.44
14:Q:451:MET:HG2	14:Q:455:GLY:HA2	1.99	0.44
16:S:187:GLU:HA	16:S:190:GLN:OE1	2.17	0.44
17:X:226:VAL:HG22	17:X:236:LEU:HD23	1.99	0.44
1:A:223:LEU:HD22	1:A:407:LEU:O	2.18	0.44
3:C:279:ILE:HD11	15:R:76:GLY:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:207:ALA:HB3	8:I:220:VAL:HB	1.99	0.44
8:I:497:TRP:HE1	8:I:516:TYR:HH	1.57	0.44
8:I:575:LEU:HD23	8:I:575:LEU:HA	1.80	0.44
12:N:260:ALA:O	12:N:264:THR:HG23	2.17	0.44
13:O:111:PHE:O	13:O:115:LEU:HG	2.17	0.44
13:O:163:GLN:HB3	13:O:167:LYS:HE3	1.99	0.44
14:Q:438:GLU:O	14:Q:440:LYS:HG3	2.17	0.44
14:Q:445:ARG:NH1	16:S:27:GLU:O	2.34	0.44
17:X:406:ARG:HB2	17:X:409:CYS:SG	2.58	0.44
17:Y:208:GLY:O	17:Y:212:LEU:HG	2.18	0.44
17:Y:258:ILE:HG22	17:Y:277:LEU:HD22	1.98	0.44
1:A:119:VAL:HB	1:A:155:GLN:NE2	2.33	0.44
1:A:1092:TYR:CZ	1:A:1094:PRO:HA	2.53	0.44
1:A:1638:TYR:OH	1:A:1658:PRO:HG3	2.17	0.44
2:B:70:GLN:OE1	2:B:71:GLN:HG2	2.17	0.44
6:H:75:LEU:HG	6:H:91:ILE:HD13	1.99	0.44
6:H:754:HIS:CE1	6:H:755:LEU:HG	2.52	0.44
8:I:29:SER:HB2	8:I:73:TRP:CE2	2.53	0.44
8:I:276:TRP:CZ2	8:I:280:LEU:HD22	2.52	0.44
8:I:598:MET:N	8:I:638:CYS:SG	2.90	0.44
9:J:513:THR:O	9:J:517:THR:HG22	2.17	0.44
10:L:37:LYS:HE2	10:L:37:LYS:HB3	1.69	0.44
12:N:395:ASP:N	12:N:395:ASP:OD2	2.47	0.44
12:N:571:ASN:HA	12:N:574:ILE:HG22	2.00	0.44
12:N:663:GLN:NE2	12:N:695:ARG:HD2	2.30	0.44
14:Q:275:SER:OG	14:Q:315:LEU:O	2.35	0.44
17:Y:49:LEU:O	17:Y:53:VAL:HG13	2.18	0.44
17:Y:364:LYS:HE3	17:Y:368:LEU:HD11	1.98	0.44
17:Y:475:TYR:HD2	17:Y:478:ALA:H	1.65	0.44
18:Z:160:ASP:OD1	18:Z:160:ASP:N	2.48	0.44
1:A:1235:LEU:CD2	1:A:1272:VAL:HG11	2.48	0.44
3:C:434:ARG:HB3	3:C:466:GLU:OE2	2.16	0.44
8:I:188:TYR:CE1	8:I:194:LYS:HB2	2.53	0.44
8:I:718:LYS:NZ	8:I:737:ASN:HB2	2.33	0.44
12:N:574:ILE:CG1	12:N:625:LYS:HD2	2.46	0.44
13:O:67:LEU:HD21	13:O:81:LEU:HD23	2.00	0.44
13:O:293:GLU:HG2	13:O:294:GLU:N	2.32	0.44
16:S:81:TYR:CE2	16:S:101:LEU:HD22	2.52	0.44
17:X:474:ASP:OD2	17:X:505:ASN:HB2	2.18	0.44
17:Y:100:TYR:HB3	17:Y:142:MET:HG2	1.98	0.44
18:Z:85:VAL:HG22	18:Z:101:GLN:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:LEU:HD13	13:O:244:LEU:HD13	2.00	0.44
1:A:783:ILE:O	1:A:787:VAL:HG23	2.17	0.44
1:A:1603:LEU:HD23	1:A:1603:LEU:O	2.17	0.44
1:A:1744:ASP:HB2	1:A:1747:LEU:HD13	2.00	0.44
3:C:101:ARG:NH2	3:P:296:ARG:HA	2.33	0.44
3:C:224:LEU:HB2	3:C:230:LYS:HE3	1.99	0.44
3:C:414:MET:CE	13:O:330:ILE:HG13	2.48	0.44
6:F:124:VAL:O	6:F:128:THR:HG22	2.17	0.44
6:F:150:SER:H	6:H:23:ASP:HB3	1.83	0.44
8:I:10:SER:C	8:I:749:ASP:HA	2.43	0.44
8:I:16:GLU:HA	8:I:741:VAL:O	2.18	0.44
8:I:287:LEU:HD13	8:I:456:PHE:CD2	2.53	0.44
9:K:236:SER:HA	9:K:239:GLU:CD	2.43	0.44
9:K:484:ALA:O	9:K:488:ILE:HG12	2.17	0.44
10:L:33:LEU:HD22	10:L:54:TRP:CZ2	2.53	0.44
12:N:165:THR:N	12:N:166:PRO:HA	2.32	0.44
12:N:234:ARG:HA	12:N:237:LEU:HB2	1.99	0.44
12:N:395:ASP:O	12:N:398:THR:HG22	2.18	0.44
12:N:493:SER:HA	12:N:494:SER:HA	1.62	0.44
13:O:427:ALA:HA	13:O:472:HIS:CE1	2.53	0.44
14:Q:208:LEU:O	14:Q:217:LEU:N	2.51	0.44
16:S:152:ALA:HB1	16:S:189:LEU:HB2	1.99	0.44
17:X:340:GLU:OE1	17:X:340:GLU:N	2.51	0.44
17:X:359:LEU:CD1	17:X:383:LEU:HG	2.47	0.44
17:Y:414:ILE:HD11	17:Y:451:CYS:SG	2.58	0.44
1:A:1147:ILE:HD11	1:A:1157:TRP:CH2	2.52	0.44
1:A:1220:MET:HE1	3:C:544:GLU:HB2	2.00	0.44
1:A:1320:ASN:HB3	1:A:1323:GLU:HB3	1.98	0.44
6:F:72:LYS:HE2	6:F:91:ILE:HD11	1.98	0.44
6:F:127:LYS:HD3	6:F:127:LYS:HA	1.80	0.44
6:F:668:SER:HG	6:F:671:LEU:HB2	1.83	0.44
6:H:121:LEU:HG	6:H:125:TYR:HE1	1.83	0.44
8:I:183:GLY:C	8:I:201:ILE:HB	2.43	0.44
8:I:349:ILE:HA	8:I:353:GLN:HG3	1.99	0.44
9:J:159:LEU:HD23	9:J:159:LEU:HA	1.86	0.44
9:J:247:PHE:CE2	9:J:277:GLU:HG3	2.52	0.44
9:K:284:LEU:HD23	9:K:308:TYR:HA	2.00	0.44
10:L:79:ILE:HD11	10:L:153:MET:SD	2.58	0.44
13:O:105:LEU:H	13:O:105:LEU:HD12	1.82	0.44
13:O:249:ASP:HA	13:O:280:ARG:HH22	1.83	0.44
13:O:539:ASN:O	13:O:540:SER:OG	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:576:ASN:OD1	13:O:576:ASN:N	2.50	0.44
3:P:233:PHE:CE1	3:P:237:ILE:HD11	2.53	0.44
14:Q:235:ILE:HG22	14:Q:240:TYR:H	1.83	0.44
15:R:123:PHE:HB2	15:R:125:VAL:HG12	1.99	0.44
15:R:253:TRP:CZ2	15:R:260:ARG:HB2	2.53	0.44
15:R:317:TRP:CH2	15:R:324:LEU:HB2	2.53	0.44
15:R:340:PRO:HD3	15:R:345:TRP:CZ2	2.53	0.44
15:R:376:GLY:HA2	15:R:401:GLN:HG3	1.99	0.44
17:Y:98:SER:O	17:Y:102:MET:HG3	2.17	0.44
17:Y:180:LYS:HD3	17:Y:192:TYR:CE2	2.53	0.44
1:A:40:ARG:NH1	13:O:248:PRO:HB2	2.33	0.44
1:A:94:TYR:CE1	1:A:96:ALA:HB2	2.52	0.44
1:A:1212:VAL:HG22	1:A:1224:ILE:HD12	1.99	0.44
1:A:1245:VAL:HG23	1:A:1250:GLN:NE2	2.32	0.44
6:F:131:LEU:HD12	6:F:131:LEU:HA	1.84	0.44
6:F:703:PRO:HB3	6:F:733:VAL:HG21	1.99	0.44
6:F:726:LEU:HD23	6:F:726:LEU:HA	1.89	0.44
6:H:102:SER:C	6:H:104:ASP:H	2.26	0.44
8:I:186:GLU:HG2	8:I:197:ARG:HG3	2.00	0.44
8:I:300:VAL:HA	8:I:303:GLU:OE1	2.18	0.44
9:J:207:ASN:HA	9:J:240:ARG:NH2	2.33	0.44
9:J:418:TRP:HA	9:J:421:ALA:HB3	2.00	0.44
9:K:331:LYS:H	9:K:331:LYS:HG2	1.65	0.44
11:M:8:ASP:HB3	11:M:11:ILE:HG12	2.00	0.44
11:M:16:ASP:C	11:M:16:ASP:OD1	2.61	0.44
12:N:403:ALA:O	12:N:407:LEU:HG	2.17	0.44
12:N:540:ARG:O	12:N:544:LEU:HD13	2.18	0.44
12:N:656:SER:HB2	12:N:725:ASP:HA	2.00	0.44
12:N:779:MET:HE2	12:N:780:PHE:CZ	2.53	0.44
13:O:547:LYS:O	13:O:551:LEU:HB2	2.18	0.44
13:O:556:GLN:HG2	13:O:559:GLU:HB2	2.00	0.44
14:Q:229:ILE:HG23	14:Q:243:VAL:HG13	1.99	0.44
14:Q:316:ARG:NE	14:Q:363:TRP:H	2.15	0.44
14:Q:323:HIS:CE1	14:Q:348:LEU:HD12	2.53	0.44
16:S:312:PRO:HB3	16:S:322:ARG:O	2.18	0.44
17:X:196:LEU:HD12	17:X:209:LEU:HD12	1.99	0.44
17:X:291:VAL:HG13	17:X:311:TYR:HE1	1.83	0.44
17:X:472:ARG:HD3	17:X:475:TYR:CD1	2.52	0.44
18:Z:25:SER:O	18:Z:28:ILE:HG12	2.18	0.44
18:Z:185:SER:OG	18:Z:194:ASN:OD1	2.26	0.44
1:A:34:ALA:HB3	13:O:237:GLN:OE1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1797:ILE:HG21	1:A:1848:VAL:HG13	2.00	0.43
1:A:1809:SER:OG	1:A:1810:GLU:OE1	2.31	0.43
3:C:169:GLY:O	3:C:173:TYR:N	2.32	0.43
3:C:174:LEU:O	3:C:178:VAL:HG23	2.18	0.43
3:C:396:LYS:HG2	3:C:397:ARG:HD2	1.99	0.43
3:C:525:LEU:HD23	3:C:525:LEU:HA	1.81	0.43
8:I:318:GLN:OE1	14:Q:367:GLN:NE2	2.51	0.43
8:I:496:GLN:HE22	13:O:460:GLN:H	1.66	0.43
9:K:427:ASP:O	9:K:431:LYS:HG2	2.18	0.43
10:L:134:THR:HG21	10:L:137:ILE:HG13	2.00	0.43
12:N:754:PHE:CD1	12:N:777:LEU:HD22	2.50	0.43
13:O:577:THR:O	13:O:581:ILE:HG23	2.17	0.43
3:P:409:TYR:CD2	3:P:421:TYR:HE2	2.36	0.43
14:Q:184:ASP:OD2	14:Q:270:ARG:NH1	2.50	0.43
15:R:73:LYS:N	15:R:74:PRO:HD2	2.33	0.43
15:R:451:MET:HA	15:R:458:VAL:HA	1.99	0.43
1:A:1051:VAL:HG23	1:A:1051:VAL:O	2.18	0.43
1:A:1251:VAL:HG22	1:A:1603:LEU:HD13	1.99	0.43
1:A:1434:ILE:HG22	1:A:1461:HIS:HB2	1.99	0.43
1:A:1739:SER:N	1:A:1740:ALA:HB3	2.33	0.43
3:C:286:PHE:HZ	3:C:302:THR:HG23	1.83	0.43
3:C:397:ARG:O	3:C:399:TYR:N	2.50	0.43
3:C:402:TRP:CZ2	3:C:424:ARG:HG2	2.54	0.43
6:F:660:LYS:O	6:F:664:ILE:HG13	2.18	0.43
6:H:43:LEU:HD12	6:H:43:LEU:HA	1.73	0.43
9:J:495:PHE:CZ	9:J:525:MET:HG2	2.53	0.43
12:N:428:LEU:HD23	12:N:428:LEU:HA	1.85	0.43
13:O:538:LEU:HD23	13:O:538:LEU:HA	1.83	0.43
13:O:706:CYS:SG	13:O:708:GLU:HG3	2.58	0.43
3:P:151:LEU:HD22	3:P:178:VAL:HG23	2.00	0.43
15:R:94:LEU:HA	15:R:94:LEU:HD23	1.60	0.43
17:X:270:ASN:O	17:X:274:LEU:HG	2.18	0.43
17:Y:99:LYS:HD3	17:Y:102:MET:HE2	1.99	0.43
1:A:268:VAL:HB	1:A:413:TRP:HB3	2.00	0.43
1:A:972:GLU:OE2	1:A:984:SER:HB3	2.19	0.43
1:A:1084:ARG:O	1:A:1088:THR:HG22	2.19	0.43
6:F:729:LEU:HA	6:F:732:ILE:HG22	2.01	0.43
6:H:730:LYS:HE2	6:H:730:LYS:HB3	1.86	0.43
8:I:327:VAL:HG23	8:I:422:TYR:HE1	1.83	0.43
8:I:352:LEU:HD21	8:I:396:PHE:CE2	2.53	0.43
9:J:271:HIS:O	9:J:274:THR:HG22	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:26:ALA:HA	9:K:29:VAL:HG12	2.00	0.43
12:N:663:GLN:HB3	12:N:699:TRP:HZ2	1.82	0.43
3:P:233:PHE:CE2	3:P:237:ILE:HD11	2.53	0.43
14:Q:369:ASN:ND2	14:Q:388:CYS:SG	2.91	0.43
15:R:259:LYS:HG3	15:R:261:LEU:HD12	2.00	0.43
15:R:317:TRP:CD2	15:R:324:LEU:HD13	2.53	0.43
16:S:300:MET:O	16:S:302:ARG:N	2.51	0.43
17:X:281:TYR:HE2	17:X:293:LYS:HG3	1.82	0.43
17:Y:253:ARG:O	17:Y:256:SER:OG	2.28	0.43
17:Y:304:LEU:HD23	17:Y:304:LEU:HA	1.82	0.43
17:Y:509:CYS:SG	17:Y:510:VAL:N	2.91	0.43
18:Z:75:TRP:CE2	18:Z:161:LEU:HD21	2.53	0.43
1:A:459:GLU:HG2	1:A:460:SER:H	1.82	0.43
1:A:862:TYR:O	1:A:863:LEU:HD12	2.18	0.43
2:B:27:ARG:HB3	12:N:810:TYR:CE2	2.54	0.43
6:F:74:LEU:HA	6:F:74:LEU:HD23	1.71	0.43
8:I:276:TRP:HA	8:I:279:ILE:HG22	1.99	0.43
8:I:685:PHE:HA	8:I:701:PRO:HD3	2.01	0.43
9:J:209:LEU:O	9:J:211:LYS:HD2	2.18	0.43
9:J:231:LEU:HA	9:J:234:VAL:HG22	2.00	0.43
9:J:337:TRP:CD1	9:J:363:LEU:HD13	2.54	0.43
9:J:444:TRP:C	9:J:446:PRO:HD2	2.44	0.43
9:K:30:ALA:HB1	9:K:35:GLU:HG2	1.99	0.43
9:K:268:LEU:N	9:K:269:PRO:HD2	2.33	0.43
10:L:46:ARG:NH1	10:L:157:LYS:HA	2.32	0.43
12:N:154:HIS:O	12:N:158:ARG:HG3	2.17	0.43
12:N:279:GLY:O	12:N:280:GLU:HG2	2.19	0.43
13:O:376:LEU:HD12	13:O:376:LEU:HA	1.88	0.43
13:O:551:LEU:HG	13:O:556:GLN:HB3	2.00	0.43
3:P:186:LYS:H	3:P:186:LYS:HG2	1.60	0.43
3:P:466:GLU:CG	3:P:468:MET:HG2	2.48	0.43
14:Q:196:ASN:O	14:Q:211:ALA:N	2.50	0.43
14:Q:222:MET:HE1	14:Q:251:GLN:HE22	1.83	0.43
14:Q:292:HIS:CD2	14:Q:303:ALA:HB3	2.53	0.43
14:Q:369:ASN:O	14:Q:386:ASN:HA	2.18	0.43
14:Q:464:ASP:O	14:Q:466:THR:HG23	2.19	0.43
16:S:144:ASN:ND2	16:S:145:GLN:H	2.15	0.43
17:Y:308:MET:SD	17:Y:327:LEU:HD11	2.58	0.43
17:Y:477:LYS:HA	17:Y:480:VAL:HG12	2.00	0.43
18:Z:100:TRP:CH2	18:Z:138:THR:HG21	2.48	0.43
1:A:94:TYR:HB3	1:A:101:ILE:HB	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:930:LEU:HD23	1:A:958:ALA:CB	2.48	0.43
1:A:1099:PRO:O	1:A:1161:ASN:ND2	2.52	0.43
3:C:225:PRO:O	3:C:230:LYS:HD2	2.18	0.43
3:C:285:ILE:HD12	3:C:285:ILE:HA	1.90	0.43
7:G:10:GLU:OE1	9:J:480:SER:OG	2.20	0.43
6:H:44:LEU:HD11	6:H:48:TYR:CZ	2.53	0.43
6:H:556:SER:O	6:H:560:THR:OG1	2.35	0.43
9:J:162:TYR:HD2	9:K:9:ARG:CZ	2.32	0.43
13:O:256:LEU:HA	13:O:256:LEU:HD23	1.63	0.43
13:O:608:LEU:HD13	13:O:627:LEU:HD12	1.99	0.43
3:P:172:LEU:HB3	3:P:195:ALA:HB2	2.00	0.43
3:P:242:GLN:HE22	3:P:429:ARG:HH12	1.65	0.43
15:R:240:TYR:OH	16:S:273:THR:HB	2.18	0.43
18:Z:35:ARG:HA	18:Z:35:ARG:HD2	1.74	0.43
1:A:1300:LEU:HD21	1:A:1586:CYS:HA	2.00	0.43
3:C:493:TYR:O	3:C:497:ILE:HG12	2.18	0.43
3:C:520:TYR:HA	3:C:523:CYS:SG	2.59	0.43
6:H:146:PRO:HG3	6:H:167:THR:HA	2.00	0.43
8:I:139:LEU:HD21	8:I:192:MET:HE1	1.99	0.43
8:I:233:TYR:HD2	8:I:554:ILE:HD12	1.84	0.43
8:I:300:VAL:HG11	8:I:456:PHE:CB	2.48	0.43
9:J:167:PHE:O	9:J:170:LEU:HD23	2.18	0.43
9:J:182:LYS:O	9:J:186:GLU:HG3	2.18	0.43
9:J:465:LEU:HD11	9:J:489:HIS:CE1	2.52	0.43
9:K:204:LEU:HD23	9:K:204:LEU:HA	1.79	0.43
9:K:251:TYR:CZ	9:K:280:LYS:HE2	2.53	0.43
12:N:65:VAL:H	12:N:71:LEU:CB	2.31	0.43
12:N:125:TYR:HB2	12:N:126:LEU:CB	2.49	0.43
12:N:596:LEU:HD13	12:N:601:TRP:CE2	2.54	0.43
13:O:433:GLY:HA2	13:O:618:TYR:HD1	1.83	0.43
3:P:277:ARG:NH2	3:P:432:ASP:OD1	2.50	0.43
14:Q:132:ARG:O	18:Z:168:GLU:N	2.47	0.43
15:R:354:HIS:HD1	15:R:379:ASP:CG	2.27	0.43
15:R:362:ALA:O	15:R:372:ALA:N	2.48	0.43
16:S:63:GLU:O	16:S:67:ARG:HG3	2.18	0.43
17:X:52:ASN:OD1	17:Y:202:ALA:HB1	2.19	0.43
17:X:261:LEU:HA	17:X:264:LYS:HG2	1.99	0.43
17:X:400:ILE:HG21	17:X:413:LEU:HD13	2.00	0.43
17:X:526:GLN:HG2	17:X:527:GLU:N	2.30	0.43
17:Y:494:ASP:OD1	17:Y:494:ASP:N	2.49	0.43
1:A:1167:GLU:CD	1:A:1168:LEU:H	2.27	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1539:CYS:SG	1:A:1562:LEU:HB2	2.59	0.43
2:B:15:LEU:HD21	12:N:636:SER:H	1.84	0.43
5:E:67:LEU:HD22	17:Y:342:TRP:CH2	2.53	0.43
6:F:98:ASN:O	6:F:99:LYS:HG2	2.19	0.43
6:F:163:ASP:N	6:F:163:ASP:OD1	2.51	0.43
6:H:132:ALA:O	6:H:136:GLU:HG3	2.19	0.43
8:I:587:LEU:HD13	8:I:641:ALA:HB1	1.99	0.43
8:I:644:TYR:HB3	8:I:648:THR:OG1	2.19	0.43
9:J:332:THR:HA	9:J:363:LEU:HG	2.00	0.43
9:K:8:LYS:HA	9:K:8:LYS:HD2	1.74	0.43
9:K:212:TYR:HE1	9:K:368:HIS:CE1	2.36	0.43
12:N:435:VAL:HA	12:N:438:ILE:HD12	2.01	0.43
12:N:508:ILE:HG13	12:N:509:TYR:CE2	2.53	0.43
12:N:768:LEU:HD23	12:N:773:ILE:HG13	2.01	0.43
13:O:386:GLN:HB3	13:O:424:GLN:HE21	1.81	0.43
13:O:599:ILE:O	13:O:602:PRO:HD2	2.19	0.43
15:R:74:PRO:CB	15:R:75:GLY:HA2	2.48	0.43
16:S:59:LYS:HE3	16:S:59:LYS:HB3	1.89	0.43
17:Y:142:MET:HE2	17:Y:142:MET:HB3	1.78	0.43
18:Z:195:SER:OG	18:Z:196:MET:N	2.52	0.43
1:A:780:GLY:C	1:A:782:GLY:H	2.27	0.43
1:A:864:PRO:HA	1:A:871:ARG:HH12	1.84	0.43
1:A:1477:ALA:HB1	1:A:1574:LEU:HD11	2.00	0.43
1:A:1653:ALA:O	1:A:1655:THR:N	2.43	0.43
1:A:1694:ASP:OD1	1:A:1694:ASP:C	2.62	0.43
3:C:337:ILE:HD12	11:M:24:LEU:HD21	2.01	0.43
6:F:102:SER:C	6:F:104:ASP:H	2.27	0.43
8:I:79:LEU:HD23	8:I:79:LEU:HA	1.76	0.43
9:K:212:TYR:OH	9:K:368:HIS:ND1	2.38	0.43
10:L:93:LYS:HD2	10:L:93:LYS:HA	1.72	0.43
11:M:63:GLN:C	11:M:65:LEU:H	2.27	0.43
12:N:182:ARG:HH21	12:N:232:TRP:HZ2	1.65	0.43
12:N:410:LEU:O	12:N:411:ASP:C	2.61	0.43
13:O:394:THR:HA	13:O:615:ARG:NH1	2.34	0.43
13:O:479:GLU:OE1	13:O:618:TYR:OH	2.28	0.43
13:O:569:VAL:O	13:O:573:LYS:HG2	2.19	0.43
3:P:28:ASP:OD1	3:P:28:ASP:N	2.43	0.43
15:R:224:GLN:HB2	15:R:227:GLU:CD	2.44	0.43
16:S:40:THR:CB	16:S:87:GLN:HB3	2.48	0.43
17:X:255:ILE:HA	17:X:258:ILE:HG22	2.00	0.43
17:X:400:ILE:HG22	17:X:409:CYS:SG	2.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Z:106:CYS:HB3	18:Z:191:HIS:CD2	2.54	0.43
1:A:44:PRO:HG2	3:C:181:LYS:HA	2.00	0.43
1:A:1090:PHE:HA	1:A:1147:ILE:O	2.19	0.43
3:C:347:HIS:CE1	3:C:377:GLU:HB3	2.53	0.43
6:F:7:PRO:HG2	6:H:459:ALA:HB2	2.00	0.43
8:I:430:GLU:HG3	14:Q:429:LYS:HE2	2.00	0.43
9:J:315:LYS:HA	9:J:315:LYS:HD3	1.84	0.43
12:N:202:GLU:C	12:N:204:ASP:H	2.25	0.43
13:O:69:GLN:HE21	13:O:69:GLN:HB2	1.58	0.43
14:Q:249:GLU:HB3	14:Q:263:ASN:OD1	2.19	0.43
15:R:184:ASP:OD2	15:R:186:TYR:N	2.52	0.43
15:R:235:ILE:HG13	15:R:276:TRP:CE3	2.53	0.43
15:R:287:SER:O	15:R:287:SER:OG	2.37	0.43
15:R:290:ILE:N	15:R:305:LEU:O	2.42	0.43
17:X:382:ALA:O	17:X:386:MET:HG2	2.19	0.43
1:A:174:PRO:HG2	1:A:175:PHE:CD2	2.54	0.43
1:A:657:TRP:O	1:A:661:VAL:HG23	2.18	0.43
1:A:1216:LYS:HG3	1:A:1224:ILE:HG13	2.00	0.43
1:A:1281:PRO:HB2	1:A:1349:SER:HB2	2.01	0.43
1:A:1509:PRO:O	1:A:1513:GLU:HG2	2.18	0.43
2:B:30:PHE:HA	2:B:56:HIS:CE1	2.54	0.43
3:C:365:LEU:HD23	3:C:365:LEU:HA	1.85	0.43
6:F:489:SER:HA	6:F:496:TYR:CE2	2.54	0.43
6:F:686:GLU:HG2	6:F:687:LYS:N	2.32	0.43
6:H:621:LEU:HB3	6:H:625:ARG:NH2	2.30	0.43
8:I:267:LEU:HD12	8:I:267:LEU:HA	1.84	0.43
8:I:587:LEU:HD22	8:I:598:MET:HE3	2.01	0.43
9:K:495:PHE:CE1	9:K:525:MET:HG2	2.54	0.43
12:N:542:VAL:HG21	12:N:561:LEU:HD21	2.01	0.43
13:O:665:PHE:CZ	13:O:669:LYS:HD2	2.54	0.43
15:R:322:ARG:NH2	15:R:369:ASN:HD21	2.15	0.43
17:X:352:SER:OG	17:X:354:ARG:HG2	2.19	0.43
17:Y:162:ILE:O	17:Y:167:ARG:NE	2.52	0.43
1:A:1383:ILE:HG23	1:A:1386:TRP:CZ2	2.54	0.42
1:A:1521:LEU:HD13	1:A:1588:LEU:HD12	2.01	0.42
3:C:140:PRO:HD2	3:C:145:GLN:NE2	2.33	0.42
3:C:193:VAL:HG12	3:C:197:HIS:HE1	1.83	0.42
3:C:233:PHE:CE1	3:C:237:ILE:HD11	2.54	0.42
5:E:98:PRO:HG2	5:E:101:GLN:CB	2.49	0.42
8:I:186:GLU:HA	8:I:197:ARG:HA	2.01	0.42
9:J:437:ASN:N	9:J:437:ASN:OD1	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:212:TYR:HE1	9:K:368:HIS:HE1	1.66	0.42
11:M:2:ASP:OD1	11:M:2:ASP:N	2.52	0.42
12:N:345:PHE:CE2	12:N:386:LEU:HD23	2.53	0.42
12:N:484:PRO:HA	12:N:485:VAL:HA	1.82	0.42
12:N:532:SER:HA	12:N:533:PHE:HA	1.58	0.42
12:N:645:THR:HA	12:N:658:ALA:HA	2.01	0.42
13:O:258:TYR:HE1	13:O:310:LEU:HD13	1.84	0.42
13:O:645:HIS:C	13:O:646:MET:HE2	2.44	0.42
14:Q:165:CYS:CB	16:S:224:ARG:HE	2.32	0.42
14:Q:206:VAL:HG12	14:Q:220:LEU:HG	2.01	0.42
14:Q:262:ARG:HD3	14:Q:295:VAL:HG13	2.02	0.42
15:R:239:ASN:HD21	16:S:271:ARG:HH21	1.66	0.42
15:R:315:LEU:HD12	15:R:325:ALA:O	2.19	0.42
15:R:373:THR:OG1	15:R:383:ARG:HB2	2.19	0.42
15:R:427:ILE:HB	15:R:436:VAL:HB	2.01	0.42
15:R:468:ARG:HD3	15:R:470:TRP:HZ2	1.83	0.42
7:W:19:PHE:CE2	7:W:23:ARG:HD2	2.54	0.42
17:X:295:GLU:O	17:X:299:MET:HG2	2.19	0.42
17:Y:175:LEU:HD12	17:Y:175:LEU:HA	1.90	0.42
1:A:594:ARG:HB3	1:A:606:ARG:HH21	1.84	0.42
1:A:1276:GLU:OE2	1:A:1294:TYR:OH	2.24	0.42
2:B:46:LEU:HB2	12:N:632:MET:HG3	2.01	0.42
2:B:77:ARG:O	2:B:77:ARG:HD3	2.19	0.42
3:C:48:LEU:HD23	3:C:48:LEU:HA	1.79	0.42
6:F:556:SER:OG	6:F:573:ALA:HA	2.19	0.42
6:F:670:VAL:HG21	15:R:497:GLY:HA2	2.01	0.42
6:H:492:PRO:O	6:H:493:SER:OG	2.36	0.42
6:H:743:ILE:HG22	6:H:759:ASN:ND2	2.34	0.42
6:H:748:LYS:HE2	6:H:748:LYS:HB3	1.78	0.42
8:I:572:PHE:CZ	8:I:588:PHE:HA	2.54	0.42
8:I:742:ARG:HD2	8:I:744:PHE:HZ	1.81	0.42
9:J:263:PHE:CZ	9:J:290:LYS:HD3	2.54	0.42
9:J:263:PHE:CZ	9:J:294:LEU:HD12	2.53	0.42
9:J:481:THR:O	9:J:485:ILE:HG23	2.19	0.42
9:K:438:GLU:C	9:K:440:THR:H	2.26	0.42
12:N:702:GLN:NE2	12:N:728:VAL:HG12	2.34	0.42
12:N:707:GLU:HA	12:N:712:THR:HB	2.00	0.42
12:N:761:MET:HG2	16:S:204:THR:OG1	2.19	0.42
13:O:530:SER:O	13:O:533:THR:HG22	2.19	0.42
3:P:36:LEU:HA	3:P:39:ILE:HG22	2.00	0.42
3:P:399:TYR:HE2	14:Q:498:ILE:HG21	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:403:TYR:CG	3:P:422:TYR:HE1	2.38	0.42
14:Q:447:LEU:HG	14:Q:462:ALA:HA	2.01	0.42
15:R:239:ASN:HD21	16:S:271:ARG:NH2	2.17	0.42
15:R:354:HIS:ND1	15:R:379:ASP:OD2	2.47	0.42
17:X:252:SER:HA	17:X:255:ILE:HG22	2.01	0.42
17:X:417:TYR:HD1	17:X:422:SER:OG	2.03	0.42
17:Y:134:SER:O	17:Y:138:VAL:HG23	2.19	0.42
17:Y:219:VAL:O	17:Y:223:THR:HG23	2.19	0.42
17:Y:503:LEU:HD21	17:Y:511:LEU:HB3	2.00	0.42
18:Z:128:ILE:O	18:Z:132:ILE:HG13	2.19	0.42
1:A:1267:ARG:HA	1:A:1316:MET:SD	2.60	0.42
1:A:1375:TYR:CZ	1:A:1383:ILE:HD13	2.55	0.42
1:A:1453:ASN:HD21	10:L:133:ARG:CZ	2.32	0.42
1:A:1750:PHE:HB2	13:O:605:LEU:HD13	2.01	0.42
3:C:173:TYR:O	3:C:177:VAL:HG23	2.19	0.42
3:C:244:ILE:HD12	3:C:276:ILE:HB	2.01	0.42
6:H:757:LEU:HB2	17:X:428:VAL:HG11	2.00	0.42
6:H:762:TRP:CD1	17:X:401:ARG:HH21	2.37	0.42
8:I:444:ASP:HA	8:I:447:PHE:CE1	2.54	0.42
9:K:431:LYS:HA	9:K:431:LYS:HD3	1.83	0.42
10:L:70:ARG:O	10:L:72:THR:N	2.52	0.42
12:N:501:ILE:HD13	12:N:548:ARG:NH1	2.34	0.42
13:O:281:LEU:HD21	13:O:283:LEU:HD22	2.00	0.42
13:O:394:THR:HG23	13:O:397:LYS:H	1.84	0.42
13:O:691:ILE:HG12	13:O:721:TYR:CE1	2.54	0.42
3:P:375:TYR:O	3:P:380:ASN:N	2.43	0.42
15:R:222:MET:SD	15:R:227:GLU:HG3	2.58	0.42
7:W:18:GLU:O	7:W:22:ILE:HG12	2.19	0.42
17:X:233:LEU:HD21	17:Y:37:VAL:HG21	2.01	0.42
17:Y:538:LEU:HD23	17:Y:538:LEU:HA	1.77	0.42
1:A:99:MET:HE3	1:A:99:MET:HB2	1.88	0.42
1:A:969:ASP:OD1	1:A:969:ASP:N	2.52	0.42
1:A:1066:LYS:HE3	1:A:1118:VAL:HG11	2.01	0.42
1:A:1267:ARG:NH2	9:K:348:SER:OG	2.53	0.42
1:A:1755:CYS:O	1:A:1768:LEU:HD21	2.19	0.42
6:H:35:VAL:HG12	6:H:37:SER:N	2.34	0.42
8:I:276:TRP:O	8:I:279:ILE:HG22	2.20	0.42
8:I:506:HIS:HD2	13:O:484:ALA:HB1	1.85	0.42
9:J:135:LEU:HD12	9:J:135:LEU:HA	1.81	0.42
9:J:294:LEU:HD13	9:K:54:HIS:CD2	2.55	0.42
9:J:407:GLU:HA	9:J:410:VAL:HG12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:412:ALA:HB1	9:K:417:GLU:HG3	2.01	0.42
12:N:220:LEU:CB	12:N:232:TRP:HB3	2.50	0.42
12:N:432:GLU:HG3	12:N:433:ASP:H	1.84	0.42
12:N:798:TYR:CZ	12:N:802:LYS:HE2	2.54	0.42
13:O:216:LEU:HD12	13:O:250:PHE:HE2	1.84	0.42
14:Q:410:HIS:ND1	14:Q:473:PHE:HB3	2.33	0.42
15:R:337:PRO:HB3	15:R:348:LEU:HD21	2.01	0.42
16:S:144:ASN:HD22	16:S:144:ASN:C	2.27	0.42
17:Y:170:LYS:HG3	17:Y:171:ILE:HD12	2.00	0.42
17:Y:265:SER:HA	17:Y:268:ARG:HB2	2.01	0.42
1:A:215:HIS:HD2	1:A:217:LEU:H	1.65	0.42
1:A:443:CYS:HB3	1:A:452:LEU:HD12	2.02	0.42
1:A:511:ILE:HD12	1:A:607:ILE:HG21	2.00	0.42
1:A:1074:CYS:SG	1:A:1078:MET:HE2	2.59	0.42
1:A:1163:PRO:O	1:A:1164:LYS:HG2	2.19	0.42
1:A:1646:GLN:O	1:A:1647:THR:OG1	2.31	0.42
3:C:137:SER:C	3:C:143:LYS:HZ2	2.26	0.42
3:C:276:ILE:O	3:C:277:ARG:HG2	2.20	0.42
3:C:392:ILE:HD11	3:C:402:TRP:NE1	2.34	0.42
6:F:611:PHE:HA	6:F:614:THR:HG22	2.01	0.42
6:H:12:ILE:HG21	6:H:43:LEU:HG	2.02	0.42
6:H:481:CYS:O	6:H:485:ILE:HG12	2.19	0.42
6:H:706:LYS:HB3	6:H:729:LEU:HG	2.01	0.42
8:I:115:TRP:CD1	8:I:176:LEU:HB2	2.54	0.42
8:I:233:TYR:HE1	8:I:575:LEU:HD21	1.83	0.42
9:J:127:SER:O	9:J:130:SER:OG	2.28	0.42
9:K:60:LEU:HA	9:K:60:LEU:HD23	1.85	0.42
12:N:365:LEU:HD11	12:N:374:LEU:HD13	2.02	0.42
12:N:762:LEU:HD23	12:N:762:LEU:HA	1.82	0.42
13:O:222:LEU:HD23	13:O:222:LEU:HA	1.80	0.42
13:O:627:LEU:HD23	13:O:627:LEU:HA	1.78	0.42
3:P:411:ILE:O	3:P:413:LYS:NZ	2.50	0.42
15:R:188:ASN:OD1	15:R:359:LYS:NZ	2.33	0.42
17:Y:350:PHE:HD1	17:Y:350:PHE:HA	1.68	0.42
17:Y:440:ASN:O	17:Y:442:GLN:NE2	2.53	0.42
18:Z:44:THR:N	18:Z:55:VAL:O	2.51	0.42
1:A:773:LEU:HD22	1:A:779:MET:HG3	2.00	0.42
1:A:930:LEU:HG	1:A:934:MET:HE2	2.01	0.42
1:A:1496:MET:HE1	1:A:1541:PHE:CE2	2.55	0.42
1:A:1731:ARG:HD3	12:N:163:PHE:HE1	1.84	0.42
2:B:17:VAL:O	12:N:632:MET:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:389:ARG:HD2	3:C:392:ILE:HG21	2.01	0.42
3:C:453:LYS:NZ	3:C:477:HIS:HD2	2.18	0.42
5:E:89:LEU:HA	5:E:89:LEU:HD12	1.72	0.42
6:F:150:SER:N	6:F:151:PRO:HD2	2.34	0.42
6:F:717:GLU:HA	6:F:719:TYR:CE1	2.54	0.42
8:I:23:ILE:H	8:I:738:LEU:HB3	1.85	0.42
8:I:118:VAL:HG13	8:I:173:LEU:O	2.20	0.42
9:J:55:ARG:NH2	9:K:261:ASP:OD2	2.53	0.42
9:J:369:LEU:HD23	9:J:369:LEU:HA	1.88	0.42
9:K:230:ASN:O	9:K:234:VAL:HG13	2.20	0.42
9:K:288:SER:HB3	9:K:305:VAL:HG22	2.01	0.42
9:K:513:THR:HA	9:K:516:VAL:HB	2.01	0.42
12:N:662:VAL:O	12:N:665:VAL:HG12	2.19	0.42
13:O:382:GLN:O	13:O:424:GLN:NE2	2.33	0.42
13:O:591:TYR:HA	13:O:594:SER:OG	2.19	0.42
13:O:593:ARG:HA	13:O:753:ASN:CG	2.44	0.42
3:P:61:SER:HA	3:P:261:LYS:HB2	2.02	0.42
16:S:121:PHE:HE2	16:S:147:ILE:HD13	1.85	0.42
17:X:206:ILE:O	17:X:210:LEU:HD23	2.20	0.42
17:X:520:VAL:HG23	17:X:532:TYR:HE2	1.85	0.42
17:Y:199:CYS:HB2	17:Y:200:PRO:C	2.45	0.42
18:Z:85:VAL:O	18:Z:154:LEU:N	2.31	0.42
1:A:759:ILE:N	1:A:760:PRO:HD2	2.34	0.42
1:A:1392:THR:OG1	1:A:1395:LEU:N	2.36	0.42
1:A:1619:LEU:HD21	1:A:1697:LEU:HD22	2.00	0.42
2:B:16:TRP:CD1	2:B:33:CYS:HA	2.54	0.42
3:C:251:TYR:CZ	3:C:268:GLN:HG2	2.55	0.42
3:C:323:LEU:HD23	3:C:323:LEU:HA	1.72	0.42
3:C:389:ARG:HG3	13:O:279:ASP:HB3	2.01	0.42
5:E:87:GLU:HA	5:E:90:GLU:OE1	2.19	0.42
6:F:552:LEU:HA	6:F:552:LEU:HD12	1.74	0.42
6:H:463:MET:HE3	6:H:466:LEU:HB3	2.01	0.42
6:H:513:SER:HA	6:H:515:TYR:HE1	1.83	0.42
6:H:629:ARG:HD2	9:K:477:GLN:HE22	1.83	0.42
6:H:732:ILE:HG22	6:H:733:VAL:HG13	2.01	0.42
8:I:178:LEU:HD12	8:I:188:TYR:CE1	2.54	0.42
9:J:7:ARG:O	9:J:11:ARG:HG3	2.19	0.42
9:K:210:LYS:HD2	9:K:240:ARG:NH2	2.34	0.42
12:N:398:THR:HG23	12:N:399:LEU:N	2.34	0.42
13:O:78:LEU:O	13:O:82:ILE:HG22	2.20	0.42
13:O:305:LEU:HD13	13:O:343:CYS:SG	2.60	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:273:TYR:HB3	3:P:282:ALA:HB2	2.01	0.42
14:Q:193:SER:HB3	14:Q:234:TRP:CD2	2.54	0.42
17:X:164:SER:HA	17:X:167:ARG:HE	1.84	0.42
17:X:459:GLU:HG2	17:X:460:LYS:N	2.35	0.42
1:A:1273:LEU:HD23	1:A:1273:LEU:HA	1.77	0.42
1:A:1274:LEU:HD11	1:A:1321:VAL:HA	2.02	0.42
1:A:1421:PRO:HB3	1:A:1484:ALA:HB2	2.00	0.42
3:C:229:MET:HE3	3:C:229:MET:HB3	1.89	0.42
3:C:472:LYS:HG2	3:C:475:LYS:HE3	2.01	0.42
5:E:101:GLN:HG2	5:E:106:THR:O	2.19	0.42
6:F:140:LYS:O	6:F:143:SER:OG	2.25	0.42
6:H:150:SER:N	6:H:151:PRO:HD2	2.35	0.42
8:I:46:LEU:HD23	8:I:56:TRP:NE1	2.34	0.42
8:I:276:TRP:CH2	8:I:476:GLY:HA3	2.54	0.42
8:I:441:THR:O	8:I:445:ILE:HG12	2.19	0.42
8:I:634:SER:HB2	8:I:636:TYR:CZ	2.54	0.42
9:J:523:ILE:O	9:J:527:ILE:HG12	2.19	0.42
9:K:258:MET:HG3	9:K:271:HIS:CD2	2.54	0.42
9:K:271:HIS:HE1	9:K:275:LEU:HD11	1.85	0.42
10:L:53:TYR:HE2	10:L:152:HIS:CE1	2.38	0.42
11:M:2:ASP:CG	11:M:3:SER:H	2.27	0.42
12:N:273:MET:SD	12:N:339:LEU:HD12	2.59	0.42
12:N:330:ARG:O	12:N:334:ARG:HG2	2.19	0.42
13:O:405:SER:OG	13:O:406:ASP:N	2.53	0.42
13:O:464:GLU:HB2	13:O:503:HIS:ND1	2.35	0.42
13:O:630:ALA:O	13:O:634:LEU:HG	2.20	0.42
3:P:31:GLU:HA	3:P:34:LYS:HG2	2.02	0.42
3:P:106:LEU:HD23	3:P:106:LEU:HA	1.84	0.42
3:P:153:GLU:N	3:P:153:GLU:OE1	2.53	0.42
14:Q:128:ALA:O	18:Z:159:LYS:HE2	2.19	0.42
14:Q:411:TYR:O	14:Q:413:GLU:HG2	2.20	0.42
15:R:171:LEU:HD11	16:S:242:ILE:HA	2.01	0.42
15:R:224:GLN:HG2	16:S:167:ASN:CG	2.44	0.42
16:S:304:LYS:HG3	16:S:305:GLU:H	1.85	0.42
17:X:140:TYR:CD1	17:X:171:ILE:HG13	2.50	0.42
17:X:433:VAL:HA	17:X:436:THR:HG22	2.02	0.42
17:Y:70:LEU:HD22	17:Y:71:PHE:CZ	2.55	0.42
17:Y:100:TYR:HB3	17:Y:142:MET:SD	2.60	0.42
18:Z:101:GLN:HB3	18:Z:196:MET:SD	2.59	0.42
1:A:953:LEU:HD21	1:A:1786:MET:HE1	2.01	0.42
1:A:1078:MET:O	1:A:1081:PRO:HD2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1251:VAL:HG12	1:A:1294:TYR:HD1	1.84	0.42
1:A:1855:THR:O	1:A:1858:GLN:HG3	2.20	0.42
2:B:15:LEU:HD12	12:N:626:TYR:CE2	2.50	0.42
6:F:469:MET:HE2	6:F:491:LEU:HD21	2.01	0.42
6:F:563:ASP:OD2	6:F:566:SER:HB3	2.20	0.42
9:J:57:ALA:HB1	9:J:80:HIS:CE1	2.54	0.42
9:J:523:ILE:HD11	3:P:420:TYR:HB3	2.01	0.42
10:L:74:VAL:HG21	10:L:158:ILE:HD11	2.02	0.42
12:N:181:LEU:HD13	12:N:299:TRP:CD2	2.54	0.42
12:N:250:LEU:O	12:N:252:LEU:HG	2.20	0.42
12:N:508:ILE:HD12	12:N:508:ILE:HA	1.91	0.42
12:N:699:TRP:CH2	12:N:728:VAL:HG21	2.55	0.42
13:O:624:VAL:HG13	13:O:643:LEU:HD11	2.01	0.42
3:P:342:SER:HA	3:P:347:HIS:HD2	1.85	0.42
14:Q:186:TYR:CE2	16:S:27:GLU:HB2	2.54	0.42
15:R:324:LEU:O	15:R:336:TRP:N	2.27	0.42
15:R:386:ASN:O	15:R:389:SER:N	2.53	0.42
17:X:499:LEU:HB3	17:X:515:LEU:HG	2.00	0.42
17:Y:93:TYR:O	17:Y:97:VAL:HG23	2.20	0.42
1:A:433:THR:HG23	1:A:441:PHE:HB2	2.01	0.42
1:A:863:LEU:HD22	1:A:866:ILE:HD11	2.01	0.42
2:B:44:CYS:HB2	2:B:58:HIS:CE1	2.55	0.42
2:B:45:PRO:HB2	12:N:631:ALA:HB3	2.01	0.42
6:F:611:PHE:HB3	6:F:620:ALA:HB2	2.02	0.42
6:H:30:ARG:HA	6:H:30:ARG:HD3	1.79	0.42
8:I:181:SER:HA	8:I:204:THR:HA	2.01	0.42
8:I:254:LYS:HA	8:I:254:LYS:HD3	1.70	0.42
8:I:363:LEU:HD23	8:I:363:LEU:HA	1.91	0.42
8:I:366:LEU:HG	8:I:386:ILE:HD13	2.02	0.42
9:J:58:HIS:CG	9:K:262:PRO:HG3	2.55	0.42
9:J:451:LEU:HD11	9:J:467:TYR:CD1	2.55	0.42
9:K:50:THR:HG22	9:K:50:THR:O	2.20	0.42
9:K:174:HIS:HB3	9:K:366:GLY:C	2.44	0.42
9:K:428:ALA:O	9:K:432:ILE:HG22	2.20	0.42
9:K:459:LYS:HD2	9:K:461:TYR:CE2	2.55	0.42
9:K:465:LEU:O	9:K:469:ARG:HG3	2.20	0.42
9:K:491:LEU:HA	9:K:491:LEU:HD23	1.78	0.42
12:N:387:LEU:HD22	12:N:427:TYR:HB3	2.00	0.42
13:O:608:LEU:HD23	13:O:612:LYS:HE2	2.01	0.42
16:S:269:ASN:O	16:S:270:SER:OG	2.30	0.42
17:Y:431:ASN:O	17:Y:434:TYR:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Z:87:VAL:HG21	18:Z:173:GLN:NE2	2.35	0.42
1:A:594:ARG:HB3	1:A:606:ARG:NH2	2.35	0.41
1:A:928:GLU:HA	1:A:931:VAL:HG12	2.02	0.41
1:A:1032:LEU:H	1:A:1032:LEU:HD23	1.83	0.41
1:A:1197:LEU:CD1	1:A:1227:LEU:HD11	2.49	0.41
1:A:1743:SER:HA	1:A:1748:LEU:HD21	2.01	0.41
3:C:368:TRP:HB3	3:C:391:ALA:HB2	2.02	0.41
8:I:280:LEU:O	8:I:284:ASP:N	2.35	0.41
8:I:399:LYS:HG3	8:I:522:LEU:HD23	2.02	0.41
8:I:718:LYS:HE3	8:I:718:LYS:HB3	1.86	0.41
9:J:61:ARG:HD2	9:J:80:HIS:HE1	1.84	0.41
9:J:475:ILE:O	9:J:475:ILE:HG13	2.17	0.41
9:K:177:THR:O	9:K:177:THR:HG22	2.20	0.41
9:K:413:PHE:HD1	9:K:454:VAL:HG22	1.85	0.41
13:O:33:TYR:CD1	13:O:72:ASP:HA	2.55	0.41
14:Q:427:ILE:HD12	14:Q:437:ALA:HB3	2.02	0.41
15:R:262:ARG:NH2	15:R:300:HIS:HD2	2.18	0.41
16:S:44:ALA:HA	16:S:47:GLN:CD	2.45	0.41
17:X:291:VAL:HG13	17:X:311:TYR:CE1	2.55	0.41
17:X:405:CYS:HA	17:X:410:TYR:HE2	1.85	0.41
17:Y:138:VAL:O	17:Y:142:MET:HG3	2.20	0.41
17:Y:475:TYR:CE2	17:Y:477:LYS:HB2	2.55	0.41
18:Z:78:LYS:HB2	18:Z:78:LYS:HE3	1.74	0.41
1:A:1067:GLU:OE1	1:A:1124:ASN:HB3	2.20	0.41
1:A:1261:TYR:HD1	1:A:1264:THR:HG21	1.84	0.41
3:C:549:LEU:O	3:C:553:ILE:HG23	2.20	0.41
6:F:30:ARG:HH22	6:H:498:THR:HG21	1.84	0.41
6:F:666:PRO:O	6:F:667:GLN:HG2	2.20	0.41
8:I:149:TYR:O	8:I:267:LEU:HD11	2.20	0.41
9:J:227:LEU:HD11	9:K:28:LYS:HD2	2.01	0.41
9:J:261:ASP:HB3	9:J:264:HIS:HB2	2.02	0.41
9:J:509:ARG:NH1	9:J:512:ASP:HB2	2.35	0.41
9:K:339:ALA:HB2	7:W:2:LEU:HD22	2.02	0.41
9:K:519:LEU:O	9:K:523:ILE:HG12	2.21	0.41
11:M:10:ARG:HD3	11:M:14:LEU:HD22	2.01	0.41
12:N:277:CYS:HA	12:N:285:PHE:HE2	1.85	0.41
12:N:765:LEU:HD23	12:N:768:LEU:HD13	2.02	0.41
14:Q:130:ILE:HG12	18:Z:156:TYR:HD1	1.85	0.41
15:R:287:SER:C	15:R:289:HIS:H	2.28	0.41
17:X:414:ILE:O	17:X:418:LEU:HG	2.19	0.41
17:Y:140:TYR:HB2	17:Y:171:ILE:HD11	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Y:400:ILE:HD13	17:Y:413:LEU:HD22	2.02	0.41
17:Y:445:THR:OG1	17:Y:468:ALA:HB2	2.21	0.41
18:Z:90:ASN:ND2	18:Z:147:VAL:HG21	2.35	0.41
1:A:1086:MET:HG2	1:A:1610:TYR:CE1	2.55	0.41
1:A:1617:ARG:HA	1:A:1691:LEU:HD13	2.03	0.41
3:C:307:LEU:HD22	3:C:316:LEU:HB2	2.01	0.41
3:C:370:LEU:O	3:C:374:GLU:HG2	2.20	0.41
3:C:416:PHE:CE2	13:O:323:ALA:HB2	2.55	0.41
3:C:448:GLN:HB3	3:C:451:GLU:CD	2.45	0.41
6:H:8:VAL:HG11	6:H:31:LEU:HD13	2.02	0.41
6:H:61:LEU:HD11	6:H:74:LEU:HD22	2.02	0.41
6:H:726:LEU:HA	6:H:726:LEU:HD23	1.79	0.41
8:I:22:GLU:O	8:I:40:THR:N	2.50	0.41
8:I:166:LYS:HA	8:I:170:ASP:OD1	2.20	0.41
8:I:186:GLU:OE2	8:I:194:LYS:HD3	2.20	0.41
8:I:372:TRP:HH2	13:O:667:VAL:HG11	1.85	0.41
12:N:363:TYR:HA	12:N:366:GLU:CD	2.45	0.41
12:N:392:ASN:HB3	12:N:394:CYS:SG	2.59	0.41
12:N:766:GLU:HG3	16:S:169:ARG:HG3	2.02	0.41
13:O:132:VAL:HG12	13:O:136:LEU:HD23	2.03	0.41
3:P:39:ILE:HG12	3:P:201:LEU:O	2.21	0.41
3:P:194:GLU:O	3:P:198:VAL:HG12	2.20	0.41
15:R:239:ASN:OD1	15:R:239:ASN:N	2.52	0.41
15:R:354:HIS:CE1	15:R:383:ARG:HE	2.38	0.41
17:X:233:LEU:HD22	17:X:235:TRP:HZ2	1.85	0.41
17:Y:259:CYS:O	17:Y:263:LYS:HG2	2.20	0.41
1:A:770:TYR:HB2	1:A:790:LEU:HD11	2.01	0.41
1:A:872:LEU:HD21	1:A:939:PHE:CD2	2.56	0.41
1:A:1175:PHE:CD2	1:A:1175:PHE:C	2.98	0.41
1:A:1202:GLU:HG2	1:A:1203:MET:N	2.35	0.41
1:A:1248:ASN:OD1	1:A:1603:LEU:HD12	2.21	0.41
1:A:1774:VAL:HG13	1:A:1790:TYR:HD2	1.85	0.41
1:A:1800:LEU:HD23	1:A:1800:LEU:HA	1.89	0.41
2:B:14:TRP:CD1	12:N:596:LEU:C	2.97	0.41
3:C:39:ILE:HG12	3:C:201:LEU:HB2	2.03	0.41
3:C:540:ASN:HB3	3:C:543:ARG:HG2	2.02	0.41
6:F:30:ARG:NH2	6:H:498:THR:HG21	2.35	0.41
6:H:672:LEU:HB3	6:H:695:ALA:HB2	2.01	0.41
8:I:624:THR:HB	8:I:631:VAL:HG22	2.02	0.41
9:J:397:ILE:O	9:J:398:ALA:C	2.63	0.41
9:K:51:ALA:HA	9:K:53:TYR:CE1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:435:ILE:HG23	9:K:436:GLY:H	1.85	0.41
10:L:155:GLN:HG3	10:L:156:ILE:N	2.36	0.41
12:N:253:LEU:O	12:N:255:ARG:N	2.53	0.41
12:N:323:ARG:HD3	12:N:323:ARG:HA	1.91	0.41
13:O:94:GLN:HE22	13:O:98:LYS:HD3	1.85	0.41
13:O:212:ALA:HB1	13:O:243:LEU:HD21	2.02	0.41
13:O:533:THR:HA	13:O:536:THR:HG22	2.02	0.41
13:O:732:ARG:O	13:O:735:MET:HG3	2.20	0.41
3:P:475:LYS:HG3	3:P:479:GLN:NE2	2.24	0.41
14:Q:133:LEU:HD12	14:Q:134:SER:H	1.84	0.41
15:R:300:HIS:CD2	15:R:300:HIS:H	2.36	0.41
17:X:334:ILE:HA	17:Y:94:ARG:HE	1.84	0.41
17:X:383:LEU:HD13	17:X:391:GLU:C	2.45	0.41
17:X:406:ARG:HB3	17:X:408:ASP:OD1	2.20	0.41
17:X:465:LEU:HD21	17:X:478:ALA:O	2.20	0.41
17:Y:44:MET:HE2	17:Y:53:VAL:HG12	2.02	0.41
17:Y:459:GLU:CD	17:Y:459:GLU:H	2.28	0.41
1:A:248:PHE:O	1:A:249:LEU:HD22	2.21	0.41
1:A:447:GLU:O	1:A:450:LEU:HG	2.20	0.41
1:A:1512:LEU:HA	1:A:1512:LEU:HD23	1.71	0.41
6:F:571:CYS:SG	6:F:606:LEU:HD12	2.60	0.41
7:G:23:ARG:NH2	9:J:525:MET:HE2	2.36	0.41
8:I:307:LEU:HD13	8:I:313:ALA:HB2	2.01	0.41
8:I:683:TYR:HD2	8:I:703:ARG:HH21	1.68	0.41
9:J:310:LEU:HA	9:J:310:LEU:HD23	1.83	0.41
9:K:350:HIS:ND1	9:K:377:GLU:OE1	2.53	0.41
9:K:492:MET:HE2	9:K:494:ASN:HD21	1.84	0.41
10:L:127:ASN:OD1	10:L:127:ASN:N	2.53	0.41
12:N:758:ILE:HG12	12:N:777:LEU:HD21	2.03	0.41
13:O:82:ILE:HD11	13:O:89:LEU:HD23	2.02	0.41
13:O:125:GLU:O	13:O:126:VAL:C	2.63	0.41
13:O:254:HIS:NE2	13:O:276:HIS:CE1	2.89	0.41
13:O:551:LEU:HD23	13:O:560:ALA:HA	2.01	0.41
14:Q:178:ALA:HB1	14:Q:202:LEU:HD21	2.03	0.41
14:Q:251:GLN:HA	14:Q:262:ARG:O	2.21	0.41
14:Q:366:TRP:CD1	14:Q:367:GLN:HG2	2.55	0.41
14:Q:445:ARG:HH22	16:S:28:ASN:HA	1.86	0.41
15:R:331:ASN:HA	15:R:356:GLY:O	2.21	0.41
16:S:29:VAL:HG13	16:S:36:ARG:HH11	1.85	0.41
1:A:81:SER:H	1:A:87:VAL:CG2	2.28	0.41
1:A:1195:ASP:O	1:A:1199:LYS:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1281:PRO:O	1:A:1287:TYR:HB3	2.20	0.41
3:C:244:ILE:H	3:C:244:ILE:HG12	1.63	0.41
3:C:349:LYS:HB3	3:C:349:LYS:HE2	1.65	0.41
6:F:690:ASP:O	6:F:694:LYS:HG2	2.21	0.41
6:F:762:TRP:CZ3	9:J:362:GLN:HG3	2.56	0.41
6:H:502:LEU:HA	6:H:502:LEU:HD12	1.76	0.41
6:H:729:LEU:HD23	6:H:729:LEU:HA	1.81	0.41
6:H:762:TRP:CD1	17:X:401:ARG:NH2	2.88	0.41
6:H:765:ASP:OD1	17:X:397:ARG:NE	2.52	0.41
9:J:425:PHE:CE2	9:J:450:ASN:HB3	2.55	0.41
12:N:269:THR:HG23	12:N:292:TRP:CZ3	2.55	0.41
12:N:478:GLU:H	12:N:479:ASP:HA	1.85	0.41
12:N:505:LEU:O	12:N:508:ILE:HG22	2.21	0.41
12:N:529:HIS:C	12:N:531:PHE:H	2.29	0.41
3:P:270:ALA:HB1	3:P:286:PHE:CE2	2.56	0.41
14:Q:208:LEU:HD22	14:Q:219:LEU:HD13	2.02	0.41
14:Q:329:ASN:OD1	16:S:26:LYS:HE2	2.20	0.41
14:Q:357:ALA:O	14:Q:376:GLY:N	2.53	0.41
15:R:210:SER:HB2	15:R:213:SER:H	1.86	0.41
17:X:49:LEU:HD12	17:X:52:ASN:ND2	2.35	0.41
17:X:294:PHE:CE2	17:X:311:TYR:HB2	2.56	0.41
17:Y:95:ASN:O	17:Y:99:LYS:HG2	2.20	0.41
1:A:489:LEU:HD12	1:A:595:VAL:HG21	2.02	0.41
1:A:1434:ILE:HG23	1:A:1457:LEU:HG	2.03	0.41
1:A:1796:ALA:O	1:A:1799:ARG:HG2	2.21	0.41
3:C:389:ARG:HH11	3:C:392:ILE:HG21	1.85	0.41
6:F:493:SER:HA	6:F:496:TYR:HB3	2.01	0.41
6:F:629:ARG:HD3	17:Y:537:SER:CB	2.49	0.41
6:H:53:LYS:HB3	6:H:56:LYS:HB2	2.03	0.41
6:H:533:VAL:HG23	6:H:559:LEU:HD22	2.03	0.41
6:H:671:LEU:HA	6:H:671:LEU:HD23	1.77	0.41
8:I:591:LEU:HB3	8:I:596:TYR:CE1	2.54	0.41
9:J:429:LEU:HD13	9:J:451:LEU:HD21	2.02	0.41
9:K:184:LEU:HA	9:K:187:SER:HB3	2.01	0.41
10:L:124:LEU:HD23	10:L:124:LEU:HA	1.87	0.41
13:O:283:LEU:O	13:O:283:LEU:HG	2.20	0.41
13:O:679:ASP:HA	13:O:683:LYS:HE3	2.03	0.41
14:Q:262:ARG:HH22	14:Q:298:ALA:C	2.29	0.41
14:Q:414:LEU:HA	14:Q:414:LEU:HD12	1.78	0.41
16:S:36:ARG:NH1	16:S:90:PRO:O	2.50	0.41
16:S:68:PHE:C	16:S:71:GLY:H	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:X:149:LEU:HB3	17:X:151:GLN:HE21	1.85	0.41
17:X:235:TRP:CE3	17:X:236:LEU:HA	2.56	0.41
17:X:355:TYR:O	17:X:358:ALA:HB3	2.21	0.41
17:Y:509:CYS:SG	17:Y:539:ASP:HB2	2.61	0.41
3:C:392:ILE:HD12	3:C:392:ILE:HA	1.78	0.41
3:C:493:TYR:CE1	3:C:497:ILE:HD11	2.56	0.41
6:F:543:LEU:HD23	6:F:543:LEU:HA	1.81	0.41
8:I:92:LEU:HG	8:I:102:HIS:O	2.21	0.41
8:I:328:LYS:HA	8:I:331:LYS:HD2	2.03	0.41
8:I:667:VAL:HA	8:I:711:TRP:HA	2.02	0.41
9:J:161:VAL:HG12	9:J:188:LEU:HD22	2.02	0.41
9:K:69:TYR:HB2	9:K:72:CYS:SG	2.61	0.41
9:K:177:THR:HA	9:K:366:GLY:HA2	2.02	0.41
9:K:435:ILE:HG23	9:K:436:GLY:N	2.35	0.41
13:O:216:LEU:HD22	13:O:256:LEU:HD12	2.02	0.41
13:O:220:ALA:HB2	13:O:256:LEU:HD21	2.01	0.41
13:O:267:VAL:HG22	13:O:314:PHE:CE2	2.56	0.41
13:O:348:TYR:CZ	13:O:361:LEU:HD11	2.56	0.41
3:P:516:LEU:HG	3:P:520:TYR:CE2	2.55	0.41
16:S:184:GLU:HA	16:S:186:LEU:N	2.35	0.41
1:A:1353:LYS:HB2	10:L:42:VAL:HG11	2.02	0.41
1:A:1477:ALA:HB3	1:A:1576:THR:CG2	2.51	0.41
1:A:1551:ASN:ND2	1:A:1594:ALA:HA	2.31	0.41
1:A:1624:VAL:HG12	1:A:1700:LYS:HA	2.01	0.41
1:A:1704:GLY:H	1:A:1742:THR:CG2	2.33	0.41
1:A:1790:TYR:OH	1:A:1840:MET:HE3	2.21	0.41
1:A:1802:ARG:HB3	1:A:1802:ARG:NH1	2.36	0.41
1:A:1845:LEU:N	1:A:1846:PRO:HD2	2.35	0.41
2:B:39:VAL:N	2:B:40:PRO:HD2	2.36	0.41
3:C:356:ARG:HB3	11:M:19:TRP:CH2	2.56	0.41
3:C:389:ARG:HH21	13:O:276:HIS:CB	2.34	0.41
6:F:483:GLU:O	6:F:487:ILE:HG12	2.21	0.41
6:F:560:THR:HG21	11:M:65:LEU:HD11	2.03	0.41
6:F:714:PHE:CD1	6:F:746:VAL:HG22	2.56	0.41
6:F:752:GLN:HA	9:J:389:ARG:NH1	2.36	0.41
6:H:563:ASP:OD2	6:H:566:SER:OG	2.37	0.41
6:H:564:LYS:HB3	6:H:570:TRP:HE1	1.85	0.41
6:H:577:PHE:HD1	6:H:582:GLU:HB2	1.86	0.41
8:I:168:LEU:HD23	8:I:168:LEU:HA	1.90	0.41
8:I:372:TRP:HD1	8:I:376:TYR:CD2	2.39	0.41
8:I:374:GLN:NE2	13:O:689:ALA:HB1	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:718:LYS:O	8:I:718:LYS:HD2	2.21	0.41
8:I:733:VAL:HG12	8:I:744:PHE:HE1	1.86	0.41
9:J:264:HIS:CD2	9:J:266:SER:HG	2.36	0.41
9:K:508:LEU:HD23	9:K:508:LEU:HA	1.88	0.41
10:L:89:TYR:HB3	10:L:152:HIS:N	2.36	0.41
11:M:9:GLY:HA3	3:P:329:TYR:CG	2.55	0.41
11:M:31:ILE:HD13	11:M:31:ILE:HA	1.82	0.41
12:N:162:PHE:HB3	12:N:255:ARG:HH21	1.86	0.41
12:N:180:PHE:HB2	12:N:240:PHE:CZ	2.55	0.41
12:N:203:LEU:O	12:N:206:ARG:HB3	2.20	0.41
13:O:54:LEU:HB3	13:O:58:ARG:HH21	1.86	0.41
13:O:119:PHE:CZ	13:O:136:LEU:HD11	2.56	0.41
13:O:119:PHE:CE2	13:O:128:LYS:HA	2.56	0.41
13:O:291:ASN:HA	13:O:338:VAL:HG22	2.02	0.41
14:Q:141:PRO:HB2	16:S:202:ARG:NE	2.11	0.41
14:Q:209:TRP:CE2	14:Q:214:GLY:HA2	2.56	0.41
14:Q:252:LEU:HD22	14:Q:295:VAL:HG11	2.03	0.41
14:Q:280:ILE:HG23	14:Q:292:HIS:HB3	2.01	0.41
15:R:85:ALA:O	15:R:89:GLU:HG2	2.21	0.41
15:R:93:PHE:CE1	15:R:97:LYS:HG3	2.55	0.41
15:R:353:GLN:H	15:R:353:GLN:CD	2.29	0.41
15:R:401:GLN:NE2	16:S:305:GLU:HB3	2.36	0.41
17:X:261:LEU:HA	17:X:261:LEU:HD23	1.96	0.41
17:Y:442:GLN:HE21	17:Y:471:GLN:HB3	1.85	0.41
18:Z:88:ILE:HB	18:Z:98:GLU:HB3	2.03	0.41
1:A:590:PRO:HB3	1:A:595:VAL:HG22	2.02	0.41
1:A:616:GLU:OE1	1:A:779:MET:HE1	2.21	0.41
1:A:617:LEU:HD11	1:A:782:GLY:HA2	2.03	0.41
1:A:1510:HIS:CD2	1:A:1554:PHE:HZ	2.39	0.41
2:B:25:ILE:HG21	2:B:59:CYS:O	2.20	0.41
2:B:25:ILE:HG13	2:B:74:PRO:HB3	2.03	0.41
5:E:89:LEU:HD11	6:H:592:ARG:CB	2.50	0.41
7:G:3:ARG:HH22	9:J:243:TYR:C	2.29	0.41
6:H:559:LEU:HD23	6:H:559:LEU:HA	1.90	0.41
6:H:573:ALA:O	6:H:576:CYS:HB2	2.21	0.41
8:I:36:ALA:HA	8:I:46:LEU:HA	2.02	0.41
9:J:284:LEU:HD12	9:J:284:LEU:HA	1.89	0.41
9:J:369:LEU:HD22	9:J:373:TYR:HE2	1.86	0.41
9:J:416:GLY:HA2	9:J:418:TRP:HE1	1.86	0.41
9:K:36:GLU:HG3	9:K:37:PRO:HD2	2.03	0.41
9:K:37:PRO:HA	9:K:40:ILE:HD12	2.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:302:TYR:HE1	13:O:339:CYS:HB2	1.86	0.41
3:P:236:HIS:CE1	3:P:268:GLN:HE22	2.39	0.41
14:Q:333:VAL:N	14:Q:351:PHE:O	2.54	0.41
15:R:114:LYS:O	15:R:118:LEU:HD13	2.20	0.41
15:R:282:SER:HB3	15:R:315:LEU:HD21	2.03	0.41
16:S:180:GLN:HG3	16:S:181:GLN:NE2	2.35	0.41
17:X:49:LEU:HD23	17:X:49:LEU:H	1.86	0.41
1:A:1163:PRO:C	1:A:1165:HIS:H	2.28	0.40
1:A:1279:ARG:O	1:A:1291:ARG:NH2	2.54	0.40
1:A:1516:LEU:O	1:A:1519:VAL:HG12	2.21	0.40
1:A:1734:LYS:HB3	1:A:1756:LYS:NZ	2.37	0.40
3:C:439:LEU:HD23	3:C:439:LEU:HA	1.90	0.40
6:F:146:PRO:C	6:F:148:LEU:N	2.78	0.40
6:H:35:VAL:O	6:H:36:HIS:HB2	2.20	0.40
6:H:658:PHE:HB3	6:H:675:ILE:CG1	2.51	0.40
6:H:709:ARG:O	6:H:712:VAL:HG12	2.21	0.40
6:H:747:TYR:CE2	6:H:755:LEU:HB3	2.55	0.40
8:I:9:PRO:HG3	8:I:754:LEU:HD13	2.03	0.40
8:I:290:PHE:HA	8:I:320:LEU:HD11	2.03	0.40
8:I:622:SER:HB3	8:I:633:ARG:HE	1.87	0.40
9:J:225:ASP:OD2	9:J:225:ASP:N	2.53	0.40
9:J:418:TRP:CD1	9:J:418:TRP:N	2.89	0.40
11:M:51:LYS:HB3	11:M:51:LYS:HE2	1.70	0.40
12:N:275:ASP:OD1	12:N:276:ARG:N	2.54	0.40
12:N:700:LEU:HD22	12:N:707:GLU:CD	2.46	0.40
13:O:631:GLN:HB2	13:O:640:ALA:HB2	2.03	0.40
3:P:36:LEU:HD21	3:P:58:LEU:HB2	2.03	0.40
3:P:124:LEU:HA	3:P:124:LEU:HD23	1.87	0.40
15:R:193:SER:HB3	15:R:234:TRP:CE2	2.56	0.40
15:R:411:TYR:HB2	15:R:413:GLU:OE2	2.20	0.40
15:R:416:SER:O	15:R:426:VAL:N	2.54	0.40
15:R:452:SER:HB3	15:R:453:PRO:HD2	2.02	0.40
17:X:304:LEU:HD12	17:X:304:LEU:HA	1.84	0.40
17:Y:260:SER:O	17:Y:264:LYS:HG2	2.21	0.40
1:A:778:LEU:HD23	1:A:778:LEU:HA	1.91	0.40
1:A:972:GLU:N	1:A:972:GLU:OE1	2.54	0.40
1:A:1228:LEU:HB2	1:A:1257:ILE:HD11	2.03	0.40
1:A:1279:ARG:HD3	1:A:1287:TYR:CE1	2.56	0.40
1:A:1542:LEU:HA	1:A:1542:LEU:HD23	1.87	0.40
2:B:72:HIS:HB2	2:B:77:ARG:HG2	2.04	0.40
3:C:273:TYR:HA	3:C:276:ILE:HG22	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:389:ARG:HG3	13:O:279:ASP:CB	2.51	0.40
5:E:99:ILE:C	5:E:101:GLN:N	2.78	0.40
6:H:486:ASN:OD1	6:H:490:HIS:NE2	2.54	0.40
8:I:449:ALA:O	8:I:453:THR:OG1	2.36	0.40
8:I:584:HIS:HD2	8:I:605:THR:HA	1.86	0.40
9:J:211:LYS:HG2	9:J:240:ARG:HD3	2.03	0.40
9:J:439:VAL:HG11	9:J:448:LEU:HD21	2.03	0.40
9:K:334:GLY:N	9:K:335:PRO:HD2	2.36	0.40
10:L:82:ASP:HA	10:L:116:PRO:O	2.21	0.40
11:M:17:ASP:HA	11:M:20:ARG:HG2	2.03	0.40
12:N:567:SER:HA	12:N:595:ILE:HB	2.02	0.40
13:O:430:ARG:HD3	13:O:472:HIS:CD2	2.56	0.40
3:P:265:ILE:O	3:P:269:ILE:HG12	2.21	0.40
14:Q:242:ALA:HB2	14:Q:276:TRP:CZ2	2.56	0.40
14:Q:413:GLU:OE2	14:Q:429:LYS:HD3	2.21	0.40
15:R:237:GLU:HG2	16:S:271:ARG:HE	1.86	0.40
16:S:43:GLY:O	16:S:47:GLN:HG3	2.20	0.40
16:S:232:SER:H	16:S:245:VAL:HG22	1.86	0.40
17:X:308:MET:HG3	17:X:331:LEU:HD21	2.02	0.40
17:X:455:PRO:C	17:X:457:THR:H	2.30	0.40
17:X:460:LYS:HA	17:X:463:THR:HG22	2.03	0.40
17:Y:100:TYR:HD1	17:Y:138:VAL:HG13	1.86	0.40
1:A:207:LEU:O	1:A:240:VAL:HG23	2.21	0.40
1:A:844:ILE:HD11	1:A:873:VAL:HG11	2.03	0.40
1:A:862:TYR:C	1:A:863:LEU:HD12	2.46	0.40
1:A:881:ILE:HB	1:A:882:LEU:HD12	2.02	0.40
1:A:1274:LEU:CD1	1:A:1321:VAL:HG12	2.51	0.40
1:A:1666:ILE:HG13	1:A:1677:LEU:HB3	2.03	0.40
3:C:172:LEU:HD12	3:C:198:VAL:HG11	2.03	0.40
3:C:244:ILE:HD11	3:C:276:ILE:HD13	2.04	0.40
3:C:432:ASP:OD1	3:C:434:ARG:NH1	2.55	0.40
4:D:14:GLU:HB2	4:D:17:TRP:CZ3	2.56	0.40
6:H:53:LYS:HZ2	6:H:53:LYS:HG2	1.75	0.40
8:I:374:GLN:HE21	13:O:689:ALA:HB1	1.86	0.40
8:I:720:GLN:HB2	8:I:736:SER:HB2	2.04	0.40
9:K:452:GLY:HA3	9:K:468:HIS:CE1	2.55	0.40
10:L:53:TYR:HB3	10:L:154:ARG:HD3	2.02	0.40
12:N:269:THR:HG23	12:N:292:TRP:HZ3	1.86	0.40
12:N:679:GLU:O	12:N:683:LYS:HG2	2.20	0.40
13:O:513:LYS:HA	13:O:535:ILE:HD11	2.02	0.40
3:P:296:ARG:HD2	3:P:298:GLU:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:414:MET:HB3	3:P:417:TYR:CD2	2.56	0.40
3:P:514:ARG:HB2	3:P:536:CYS:SG	2.61	0.40
14:Q:224:GLN:O	14:Q:227:GLU:HG2	2.20	0.40
14:Q:373:THR:HG1	14:Q:385:TRP:HE1	1.63	0.40
15:R:166:ARG:NH2	15:R:413:GLU:OE2	2.53	0.40
15:R:287:SER:HB3	15:R:289:HIS:ND1	2.36	0.40
15:R:468:ARG:HH22	16:S:245:VAL:H	1.70	0.40
17:Y:104:LEU:HD23	17:Y:104:LEU:HA	1.94	0.40
17:Y:449:THR:O	17:Y:453:GLU:HG2	2.21	0.40
17:Y:483:ALA:HB1	17:Y:514:ILE:HG21	2.04	0.40
1:A:778:LEU:HG	1:A:946:THR:HG21	2.03	0.40
1:A:1229:SER:HA	1:A:1232:ILE:CG2	2.51	0.40
1:A:1381:ARG:HD3	1:A:1381:ARG:HA	1.89	0.40
3:C:217:GLU:HA	3:C:220:LYS:HD2	2.03	0.40
3:C:245:GLU:OE1	3:C:245:GLU:N	2.44	0.40
6:F:42:PHE:CE1	6:F:74:LEU:HD12	2.57	0.40
6:H:762:TRP:HA	6:H:765:ASP:HB3	2.03	0.40
9:K:213:ASN:O	9:K:240:ARG:HD3	2.21	0.40
13:O:38:LEU:HD11	13:O:139:MET:HG3	2.03	0.40
13:O:131:VAL:HG23	13:O:132:VAL:HG23	2.03	0.40
13:O:502:GLN:HG2	13:O:503:HIS:H	1.85	0.40
3:P:175:TYR:CE1	3:P:179:LEU:HD11	2.57	0.40
3:P:405:LEU:O	3:P:408:THR:HG22	2.21	0.40
14:Q:375:GLY:HA3	14:Q:379:ASP:OD2	2.22	0.40
15:R:443:THR:HG21	16:S:246:GLY:HA3	2.02	0.40
16:S:41:LEU:HD23	16:S:41:LEU:HA	1.87	0.40
17:X:530:ASP:O	17:X:534:ILE:HG12	2.22	0.40
17:Y:445:THR:HA	17:Y:464:LEU:HD12	2.03	0.40
1:A:1054:TYR:O	1:A:1056:GLU:N	2.47	0.40
2:B:16:TRP:HD1	2:B:32:GLY:O	2.04	0.40
3:C:409:TYR:CB	3:C:418:CYS:HB3	2.52	0.40
5:E:94:TRP:HE1	6:F:595:GLN:NE2	2.19	0.40
6:F:43:LEU:O	6:F:46:THR:OG1	2.30	0.40
6:F:59:ARG:NH1	6:F:59:ARG:HB2	2.36	0.40
6:F:671:LEU:HD23	6:F:671:LEU:HA	1.91	0.40
6:H:517:GLN:O	6:H:521:ILE:HG13	2.21	0.40
8:I:88:LYS:HD2	8:I:108:ALA:C	2.46	0.40
8:I:178:LEU:HD23	8:I:178:LEU:HA	1.90	0.40
8:I:306:HIS:CD2	8:I:313:ALA:HA	2.56	0.40
8:I:312:LYS:HE3	14:Q:412:LYS:HE3	2.02	0.40
8:I:429:THR:HG22	8:I:430:GLU:N	2.31	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:576:TRP:O	8:I:585:TYR:N	2.44	0.40
8:I:579:LYS:H	8:I:579:LYS:HG3	1.48	0.40
9:J:495:PHE:O	9:J:499:VAL:HG12	2.21	0.40
11:M:6:GLN:OE1	3:P:361:ASN:HA	2.21	0.40
12:N:273:MET:HE3	12:N:332:PHE:CE1	2.56	0.40
13:O:97:ILE:HD12	13:O:97:ILE:HA	1.97	0.40
13:O:556:GLN:NE2	13:O:559:GLU:OE1	2.54	0.40
3:P:37:LEU:HD23	3:P:37:LEU:HA	1.94	0.40
3:P:203:TRP:CE2	3:P:207:LEU:HD13	2.55	0.40
15:R:212:SER:OG	15:R:213:SER:N	2.55	0.40
15:R:442:HIS:NE2	15:R:468:ARG:HB2	2.36	0.40
15:R:460:SER:OG	15:R:470:TRP:NE1	2.52	0.40
17:X:64:SER:HB3	17:X:71:PHE:HD2	1.87	0.40
17:X:393:ILE:HG22	17:X:397:ARG:HD3	2.03	0.40
17:Y:288:LYS:HA	17:Y:288:LYS:HD2	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1399/1944 (72%)	1246 (89%)	147 (10%)	6 (0%)	30	62
2	B	75/84 (89%)	64 (85%)	11 (15%)	0	100	100
3	C	520/597 (87%)	490 (94%)	30 (6%)	0	100	100
3	P	485/597 (81%)	455 (94%)	30 (6%)	0	100	100
4	D	16/121 (13%)	13 (81%)	3 (19%)	0	100	100
5	E	54/110 (49%)	52 (96%)	2 (4%)	0	100	100
6	F	479/824 (58%)	448 (94%)	31 (6%)	0	100	100
6	H	479/824 (58%)	443 (92%)	34 (7%)	2 (0%)	30	62

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	G	23/85 (27%)	23 (100%)	0	0	100	100
7	W	23/85 (27%)	23 (100%)	0	0	100	100
8	I	727/808 (90%)	674 (93%)	53 (7%)	0	100	100
9	J	500/620 (81%)	454 (91%)	45 (9%)	1 (0%)	43	73
9	K	489/620 (79%)	445 (91%)	44 (9%)	0	100	100
10	L	180/185 (97%)	159 (88%)	19 (11%)	2 (1%)	11	41
11	M	55/74 (74%)	43 (78%)	12 (22%)	0	100	100
12	N	681/822 (83%)	575 (84%)	104 (15%)	2 (0%)	36	67
13	O	677/755 (90%)	639 (94%)	37 (6%)	1 (0%)	48	79
14	Q	361/374 (96%)	327 (91%)	32 (9%)	2 (1%)	21	54
15	R	377/499 (76%)	338 (90%)	39 (10%)	0	100	100
16	S	285/1050 (27%)	240 (84%)	45 (16%)	0	100	100
17	X	480/599 (80%)	456 (95%)	23 (5%)	1 (0%)	43	73
17	Y	492/599 (82%)	464 (94%)	26 (5%)	2 (0%)	30	62
18	Z	193/205 (94%)	187 (97%)	6 (3%)	0	100	100
All	All	9050/12481 (72%)	8258 (91%)	773 (8%)	19 (0%)	44	73

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1099	PRO
6	H	147	PHE
10	L	175	ILE
13	O	130	SER
17	X	456	VAL
1	A	630	PRO
1	A	1577	SER
12	N	64	ALA
1	A	347	MET
12	N	282	GLU
14	Q	476	ASP
1	A	1645	GLU
14	Q	477	PRO
17	Y	201	LEU
9	J	221	PRO
1	A	1100	LEU
10	L	170	PRO

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Mol	Chain	Res	Type
6	H	146	PRO
17	Y	200	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1151/1720 (67%)	1148 (100%)	3 (0%)	86	84
2	B	71/75 (95%)	70 (99%)	1 (1%)	59	70
3	C	452/520 (87%)	452 (100%)	0	100	100
3	P	422/520 (81%)	421 (100%)	1 (0%)	87	87
4	D	18/115 (16%)	18 (100%)	0	100	100
5	E	47/89 (53%)	47 (100%)	0	100	100
6	F	407/727 (56%)	407 (100%)	0	100	100
6	H	408/727 (56%)	408 (100%)	0	100	100
7	G	23/77 (30%)	23 (100%)	0	100	100
7	W	23/77 (30%)	23 (100%)	0	100	100
8	I	621/730 (85%)	620 (100%)	1 (0%)	87	87
9	J	424/548 (77%)	424 (100%)	0	100	100
9	K	423/548 (77%)	423 (100%)	0	100	100
10	L	155/170 (91%)	155 (100%)	0	100	100
11	M	55/67 (82%)	54 (98%)	1 (2%)	51	67
12	N	518/724 (72%)	516 (100%)	2 (0%)	84	83
13	O	577/650 (89%)	576 (100%)	1 (0%)	87	87
14	Q	275/310 (89%)	275 (100%)	0	100	100
15	R	311/411 (76%)	311 (100%)	0	100	100
16	S	208/938 (22%)	206 (99%)	2 (1%)	68	74
17	X	407/513 (79%)	407 (100%)	0	100	100
17	Y	418/513 (82%)	416 (100%)	2 (0%)	81	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	Z	181/190 (95%)	181 (100%)	0	100	100
All	All	7595/10959 (69%)	7581 (100%)	14 (0%)	85	87

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	430	VAL
1	A	1251	VAL
1	A	1597	THR
2	B	14	TRP
8	I	49	LEU
11	M	62	LEU
12	N	285	PHE
12	N	368	THR
13	O	420	ILE
3	P	288	GLU
16	S	144	ASN
16	S	302	ARG
17	Y	171	ILE
17	Y	350	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (198) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	HIS
1	A	155	GLN
1	A	242	HIS
1	A	266	HIS
1	A	601	ASN
1	A	645	HIS
1	A	654	HIS
1	A	666	ASN
1	A	846	GLN
1	A	1068	ASN
1	A	1093	HIS
1	A	1138	HIS
1	A	1182	ASN
1	A	1184	HIS
1	A	1201	HIS
1	A	1262	GLN
1	A	1266	HIS

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Mol	Chain	Res	Type
1	A	1429	ASN
1	A	1453	ASN
1	A	1461	HIS
1	A	1489	HIS
1	A	1537	GLN
1	A	1555	HIS
1	A	1559	HIS
1	A	1591	HIS
1	A	1595	HIS
2	B	65	HIS
2	B	72	HIS
3	C	82	GLN
3	C	202	HIS
3	C	242	GLN
3	C	249	GLN
3	C	274	HIS
3	C	287	ASN
3	C	322	ASN
3	C	347	HIS
3	C	361	ASN
3	C	386	GLN
3	C	395	ASN
3	C	427	GLN
3	C	518	GLN
3	C	540	ASN
3	C	552	GLN
5	E	72	HIS
6	F	36	HIS
6	F	103	HIS
6	F	145	ASN
6	F	495	HIS
6	F	517	GLN
6	F	545	HIS
6	F	609	HIS
6	F	659	GLN
6	F	674	HIS
6	H	123	HIS
6	H	495	HIS
6	H	545	HIS
6	H	580	GLN
6	H	609	HIS
6	H	636	ASN

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Mol	Chain	Res	Type
6	H	648	GLN
6	H	674	HIS
6	H	680	HIS
6	H	708	HIS
6	H	716	ASN
8	I	257	HIS
8	I	266	ASN
8	I	306	HIS
8	I	318	GLN
8	I	323	ASN
8	I	353	GLN
8	I	413	ASN
8	I	455	HIS
8	I	496	GLN
8	I	506	HIS
8	I	523	HIS
8	I	642	GLN
8	I	740	HIS
9	J	17	GLN
9	J	38	GLN
9	J	54	HIS
9	J	58	HIS
9	J	80	HIS
9	J	271	HIS
9	J	289	HIS
9	J	406	HIS
9	J	414	GLN
9	J	503	HIS
9	K	16	GLN
9	K	17	GLN
9	K	58	HIS
9	K	80	HIS
9	K	88	GLN
9	K	244	ASN
9	K	271	HIS
9	K	289	HIS
9	K	362	GLN
9	K	449	ASN
9	K	453	HIS
9	K	477	GLN
9	K	494	ASN
10	L	49	ASN

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Mol	Chain	Res	Type
10	L	101	ASN
10	L	152	HIS
11	M	6	GLN
11	M	63	GLN
12	N	80	GLN
12	N	186	GLN
12	N	239	GLN
12	N	241	HIS
12	N	242	GLN
12	N	266	HIS
12	N	290	HIS
12	N	639	HIS
12	N	663	GLN
12	N	702	GLN
12	N	726	ASN
12	N	806	GLN
12	N	807	GLN
13	O	61	ASN
13	O	69	GLN
13	O	219	GLN
13	O	254	HIS
13	O	261	ASN
13	O	265	GLN
13	O	342	HIS
13	O	382	GLN
13	O	387	GLN
13	O	412	HIS
13	O	472	HIS
13	O	477	HIS
13	O	500	ASN
13	O	617	GLN
13	O	645	HIS
13	O	671	GLN
13	O	722	HIS
13	O	731	ASN
13	O	741	HIS
3	P	148	ASN
3	P	162	HIS
3	P	202	HIS
3	P	242	GLN
3	P	268	GLN
3	P	274	HIS

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Mol	Chain	Res	Type
3	P	287	ASN
3	P	299	ASN
3	P	305	ASN
3	P	321	HIS
3	P	361	ASN
3	P	426	HIS
3	P	427	GLN
3	P	477	HIS
3	P	485	GLN
3	P	495	GLN
14	Q	183	ASN
14	Q	204	ASN
14	Q	292	HIS
14	Q	353	GLN
14	Q	367	GLN
15	R	204	ASN
15	R	300	HIS
15	R	369	ASN
15	R	422	GLN
16	S	57	GLN
16	S	87	GLN
16	S	88	ASN
16	S	91	GLN
16	S	144	ASN
16	S	181	GLN
16	S	192	GLN
16	S	197	GLN
16	S	293	GLN
17	X	66	ASN
17	X	78	GLN
17	X	106	GLN
17	X	177	ASN
17	X	198	GLN
17	X	287	ASN
17	X	385	ASN
17	X	471	GLN
17	Y	78	GLN
17	Y	89	HIS
17	Y	95	ASN
17	Y	151	GLN
17	Y	270	ASN
17	Y	298	GLN

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Mol	Chain	Res	Type
17	Y	326	ASN
17	Y	385	ASN
17	Y	442	GLN
17	Y	471	GLN
17	Y	506	GLN
17	Y	523	ASN
17	Y	531	GLN
18	Z	29	ASN
18	Z	71	GLN
18	Z	101	GLN
18	Z	121	GLN
18	Z	125	GLN
18	Z	173	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
12	N	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	N	92:TRP	C	93:ASN	N	2.97

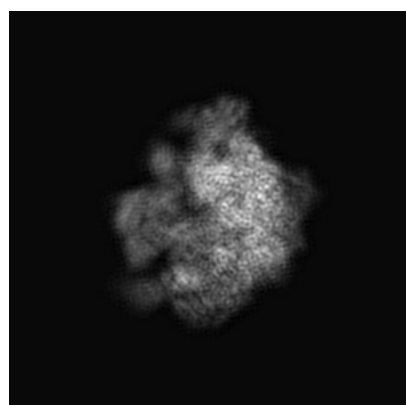
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10516. These allow visual inspection of the internal detail of the map and identification of artifacts.

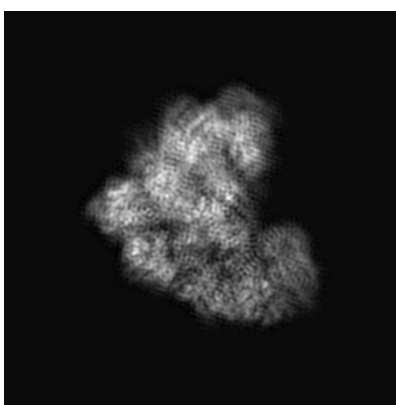
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

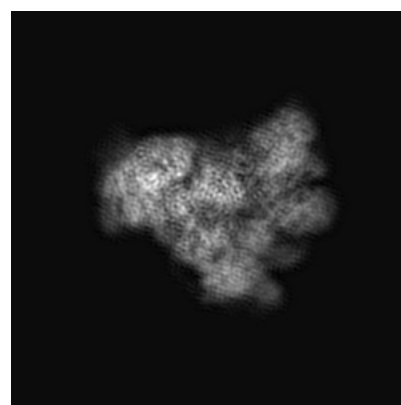
6.1.1 Primary map



X



Y

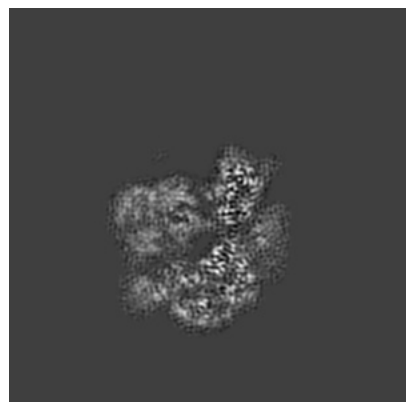


Z

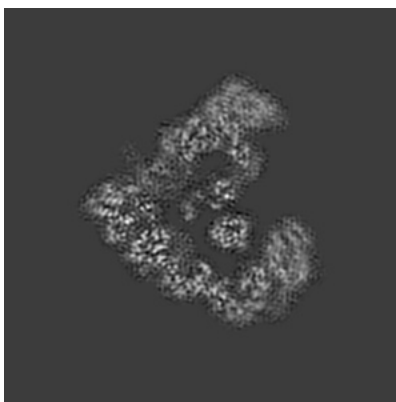
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

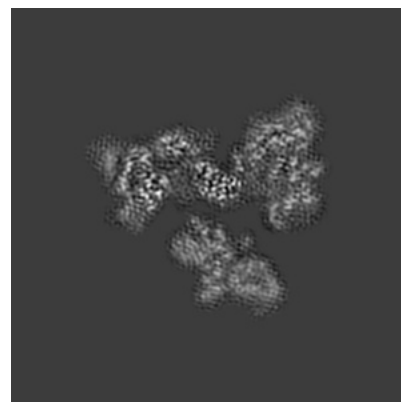
6.2.1 Primary map



X Index: 132



Y Index: 132

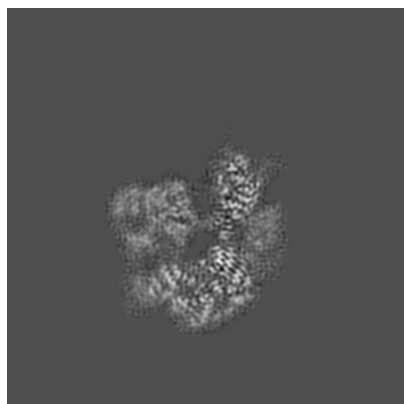


Z Index: 132

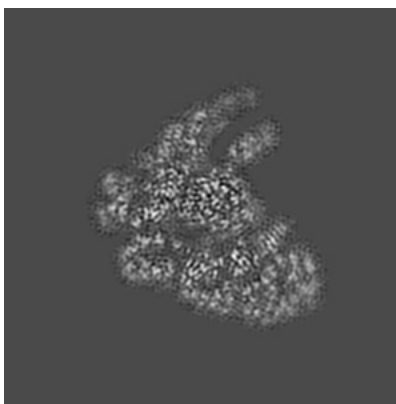
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

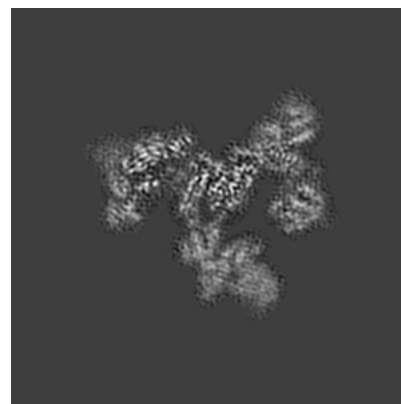
6.3.1 Primary map



X Index: 129



Y Index: 147

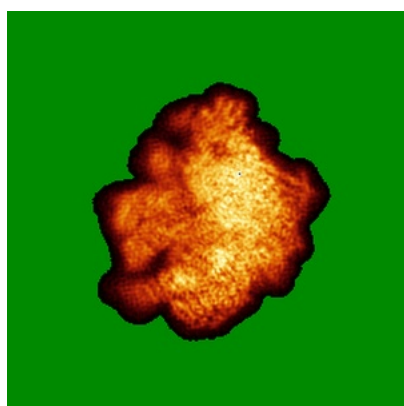


Z Index: 139

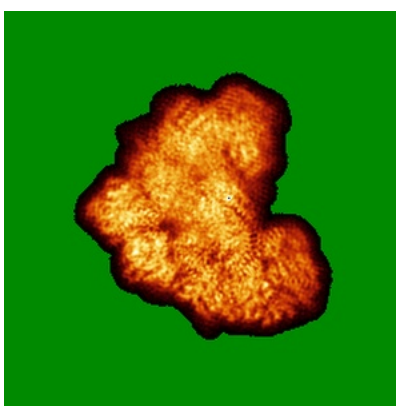
The images above show the largest variance slices of the map in three orthogonal directions.

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

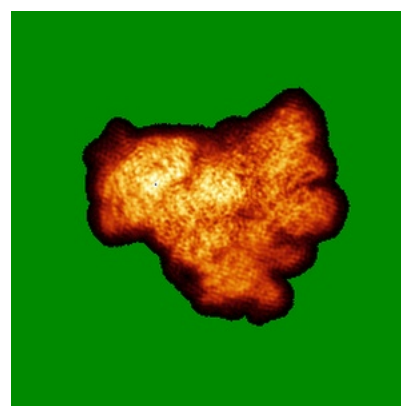
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.06. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

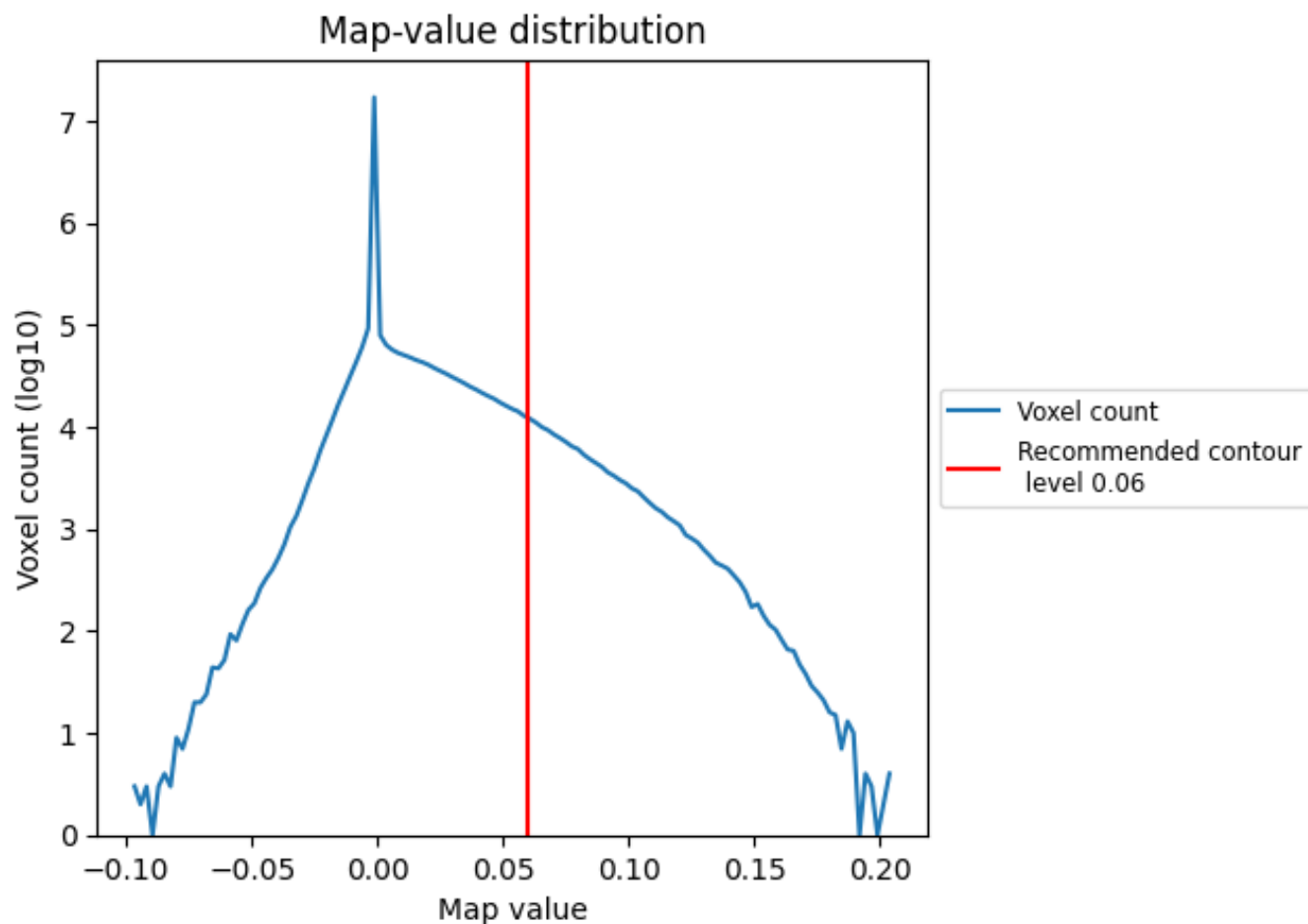
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

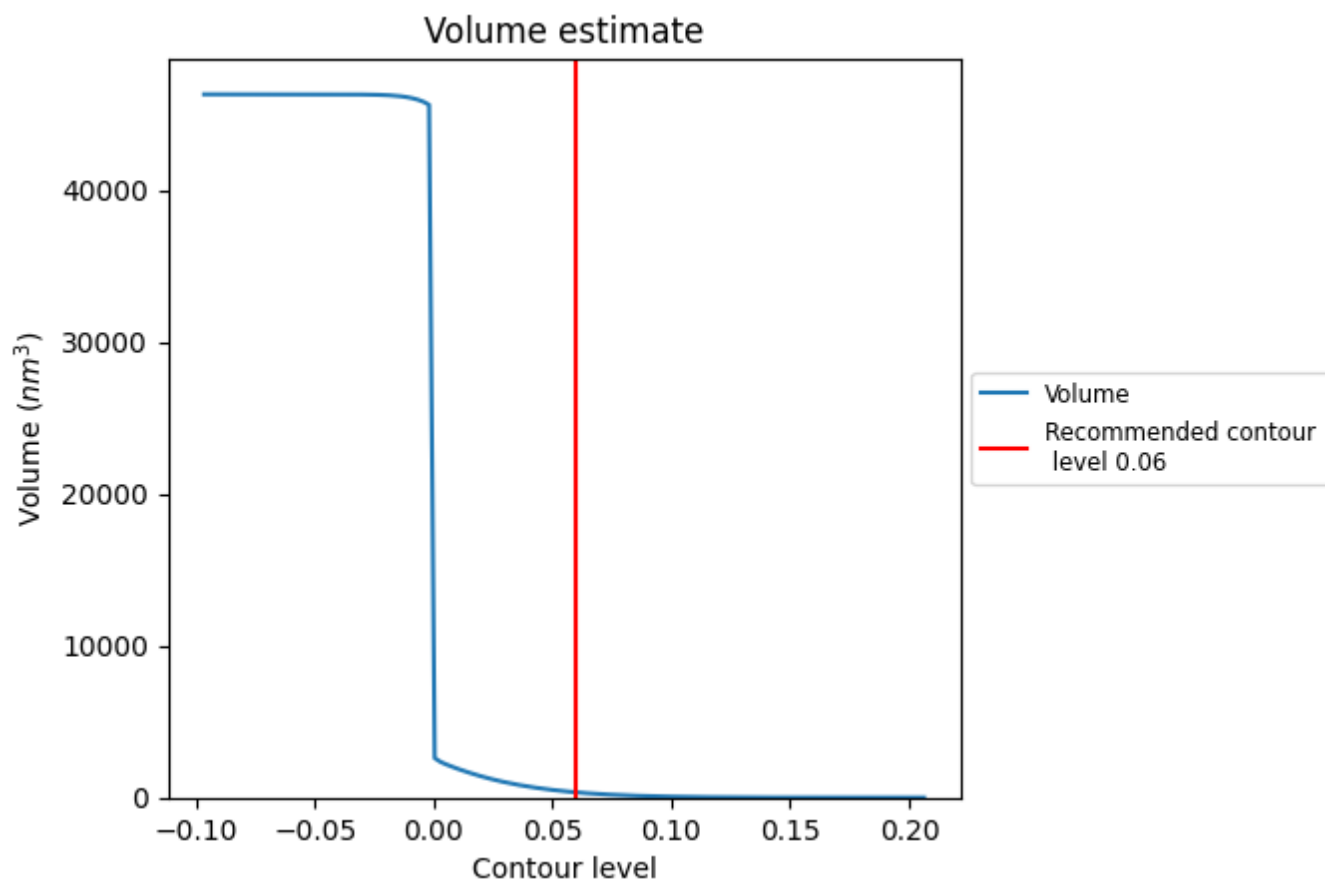
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

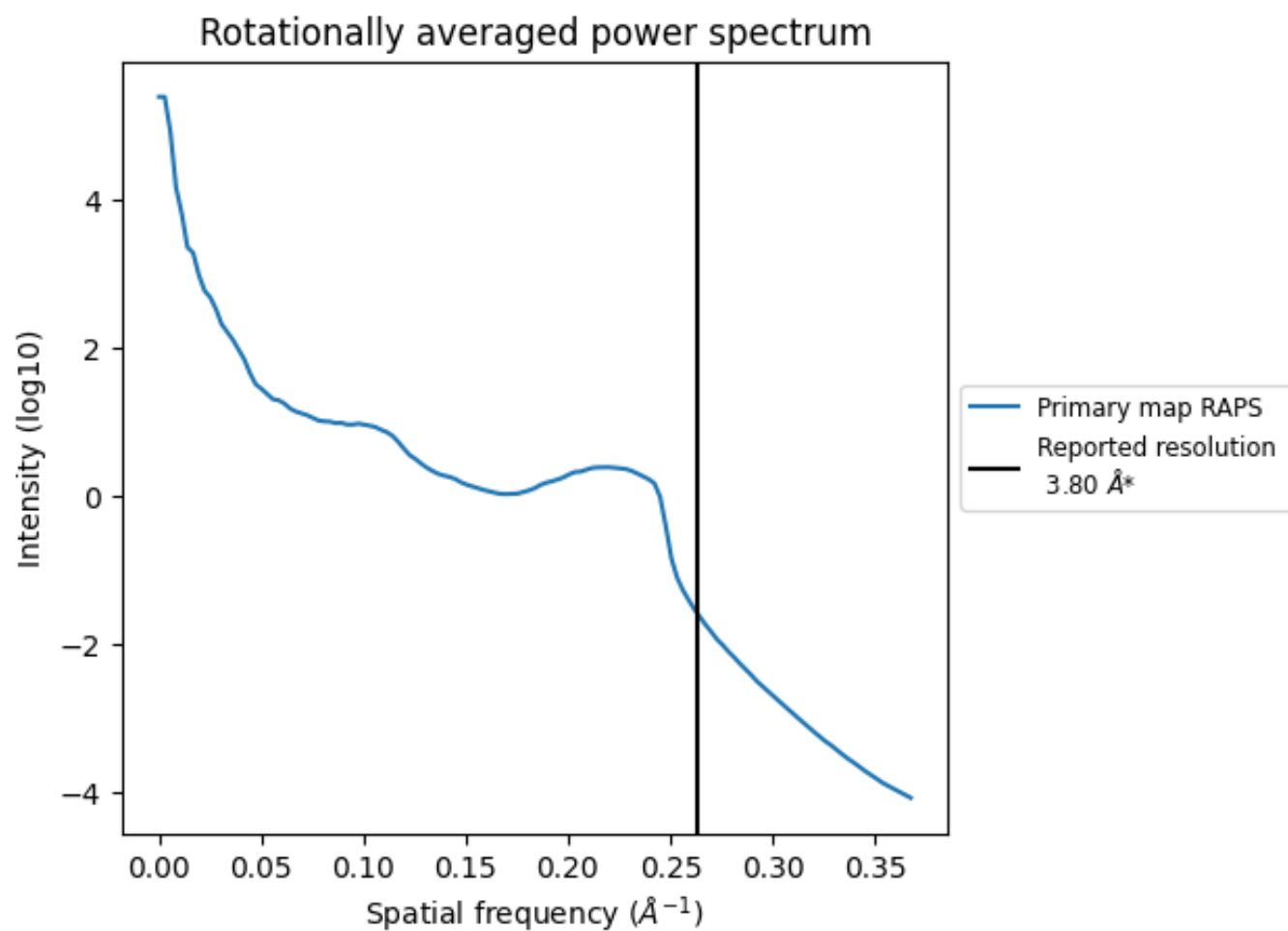
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 343 nm³; this corresponds to an approximate mass of 310 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

8 Fourier-Shell correlation

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

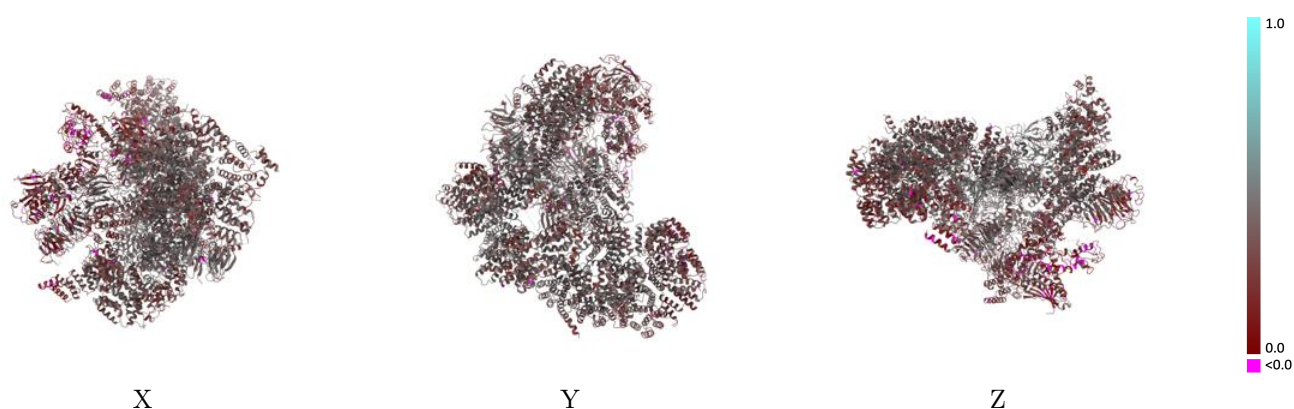
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-10516 and PDB model 6TLJ. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)

This section was not generated.

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

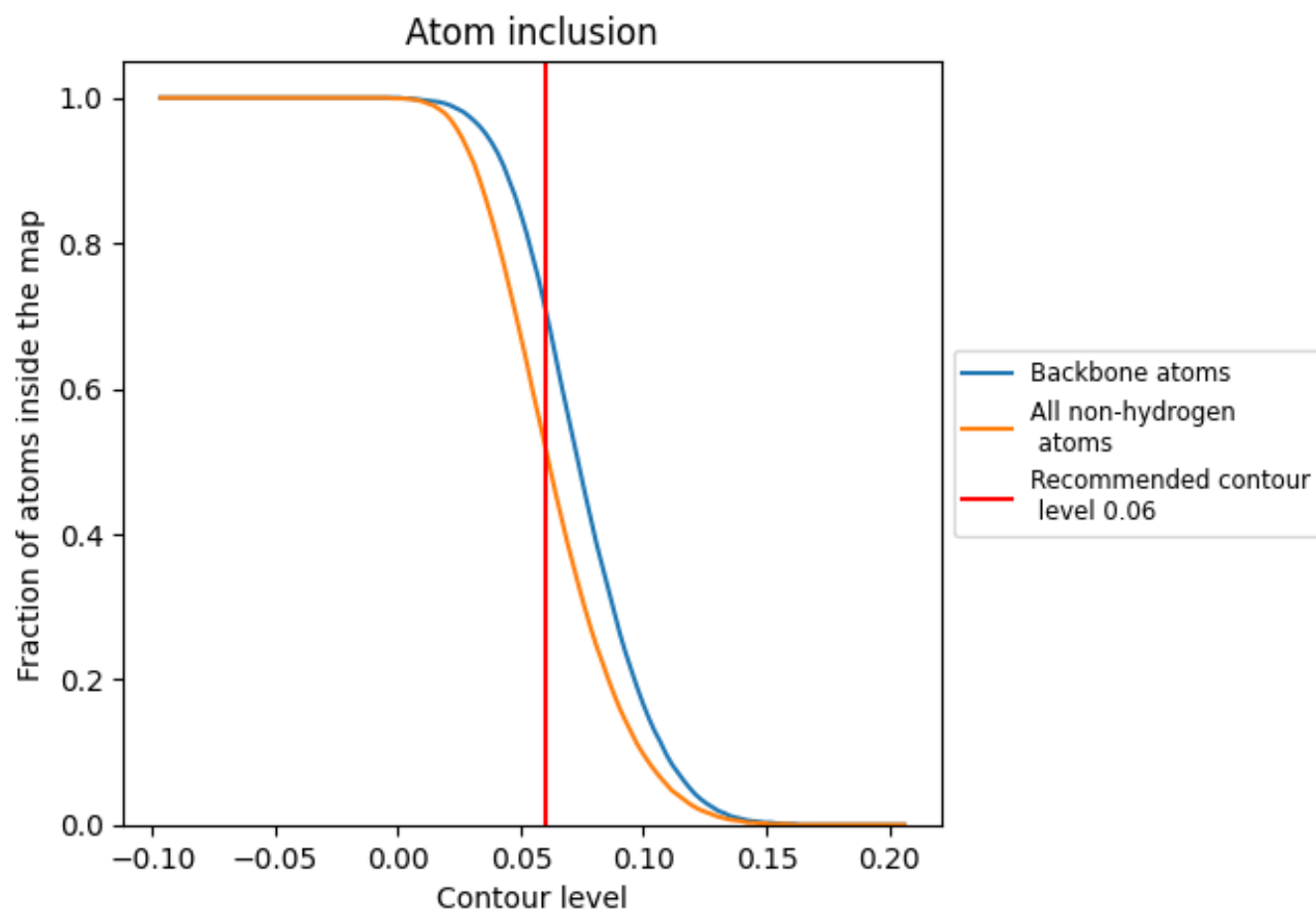


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 71% of all backbone atoms, 52% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5200	 0.3570
A	 0.5550	 0.4080
B	 0.0250	 0.1810
C	 0.5580	 0.3750
D	 0.4600	 0.4830
E	 0.6330	 0.4370
F	 0.6350	 0.4030
G	 0.5270	 0.4060
H	 0.6880	 0.4100
I	 0.4270	 0.3240
J	 0.6720	 0.4070
K	 0.6300	 0.3790
L	 0.6040	 0.4320
M	 0.5030	 0.4120
N	 0.3890	 0.2730
O	 0.4950	 0.3820
P	 0.5830	 0.3540
Q	 0.4320	 0.2950
R	 0.4840	 0.3450
S	 0.3730	 0.2790
W	 0.5410	 0.4030
X	 0.4380	 0.3000
Y	 0.4940	 0.3270
Z	 0.2870	 0.2380

