



Full wwPDB EM Validation Report ⓘ

Nov 6, 2022 – 02:30 PM EST

PDB ID : 6CNB
EMDB ID : EMD-7530
Title : Yeast RNA polymerase III initial transcribing complex
Authors : Han, Y.; He, Y.
Deposited on : 2018-03-08
Resolution : 4.10 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:

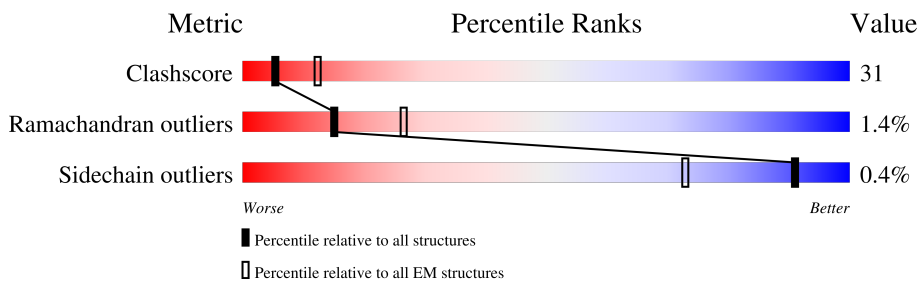
EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

1 Overall quality at a glance

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

The reported resolution of this entry is 4.10 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	1460	
2	B	1149	
3	C	335	
4	D	161	
5	E	215	
6	F	155	
7	G	212	
8	H	146	

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Mol	Chain	Length	Quality of chain
9	I	110	18% 16% 62%
10	J	70	60% 36%
11	K	142	45% 26% 29%
12	L	70	34% 30% 34%
13	M	282	24% 32% 42%
14	N	422	14% 12% 74%
15	O	654	6% 39% 41% 18%
16	P	317	20% 44% 43% 13%
17	Q	251	15% 6% 78%
18	R	736	7% 38% 33% 29%
19	S	594	8% 24% 12% 63%
20	X	71	8% 63% 28%
21	Y	71	6% 13% 72% 14%

2 Entry composition [i](#)

There are 22 unique types of molecules in this entry. The entry contains 47837 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called DNA-directed RNA polymerase III subunit RPC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1428	11159	7029	1972	2099	59	0	0

- Molecule 2 is a protein called DNA-directed RNA polymerase III subunit RPC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	1114	8788	5558	1516	1654	60	0	0

- Molecule 3 is a protein called DNA-directed RNA polymerases I and III subunit RPAC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	335	2655	1681	454	511	9	0	0

- Molecule 4 is a protein called DNA-directed RNA polymerase III subunit RPC9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	119	977	628	156	187	6	0	0

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	215	1759	1116	310	321	12	0	0

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	83	671	429	114	125	3	0	0

- Molecule 7 is a protein called DNA-directed RNA polymerase III subunit RPC8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	184	Total	C	N	O	S	0	0
			1484	972	239	267	6		

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	140	Total	C	N	O	S	0	0
			1120	703	188	224	5		

- Molecule 9 is a protein called DNA-directed RNA polymerase III subunit RPC10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	42	Total	C	N	O	S	0	0
			321	204	47	64	6		

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	67	Total	C	N	O	S	0	0
			549	350	95	98	6		

- Molecule 11 is a protein called DNA-directed RNA polymerases I and III subunit RPAC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	K	101	Total	C	N	O	S	0	0
			792	496	130	161	5		

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	L	46	Total	C	N	O	S	0	0
			363	224	72	63	4		

- Molecule 13 is a protein called DNA-directed RNA polymerase III subunit RPC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	M	164	Total	C	N	O	S	0	0
			1338	857	227	253	1		

- Molecule 14 is a protein called DNA-directed RNA polymerase III subunit RPC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	N	110	845	536	152	154	3	0	0

- Molecule 15 is a protein called DNA-directed RNA polymerase III subunit RPC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	O	539	4329	2756	741	813	19	0	0

- Molecule 16 is a protein called DNA-directed RNA polymerase III subunit RPC6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	P	277	2242	1438	368	425	11	0	0

- Molecule 17 is a protein called DNA-directed RNA polymerase III subunit RPC7,DNA-directed RNA polymerase III subunit RPC7,DNA-directed RNA polymerase III subunit RPC7,DNA-directed RNA polymerase III subunit RPC7,DNA-directed RNA polymerase III subunit RPC7.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
17	Q	54	368	238	64	66	0	0

- Molecule 18 is a protein called Transcription factor IIIB 70 kDa subunit,TATA-box-binding protein,Transcription factor IIIB 70 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	R	522	4131	2621	733	757	20	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	383	ALA	-	linker	UNP P29056
R	384	MET	-	linker	UNP P29056
R	385	PRO	-	linker	UNP P29056
R	386	TRP	-	linker	UNP P29056
R	567	GLY	-	linker	UNP P13393
R	568	SER	-	linker	UNP P13393
R	569	GLY	-	linker	UNP P13393
R	570	SER	-	linker	UNP P13393
R	571	GLY	-	linker	UNP P13393

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Chain	Residue	Modelled	Actual	Comment	Reference
R	572	SER	-	linker	UNP P13393
R	573	GLY	-	linker	UNP P13393
R	574	SER	-	linker	UNP P13393
R	575	GLY	-	linker	UNP P13393
R	576	SER	-	linker	UNP P13393
R	577	GLY	-	linker	UNP P13393
R	578	SER	CYS	engineered mutation	UNP P29056

- Molecule 19 is a protein called Transcription factor TFIIB component B",Transcription factor TFIIB component B",Transcription factor TFIIB component B",Transcription factor TFIIB component B",Transcription factor TFIIB component B".

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	S	217	1649	1035	286	321	7	0	0

- Molecule 20 is a DNA chain called DNA (71-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
20	X	51	1036	501	177	308	50	0	0

- Molecule 21 is a DNA chain called DNA (71-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
21	Y	61	1254	603	228	363	60	0	0

- Molecule 22 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
22	A	2	Total 2	Zn 2	0
22	B	1	Total 1	Zn 1	0
22	I	1	Total 1	Zn 1	0
22	J	1	Total 1	Zn 1	0
22	L	1	Total 1	Zn 1	0

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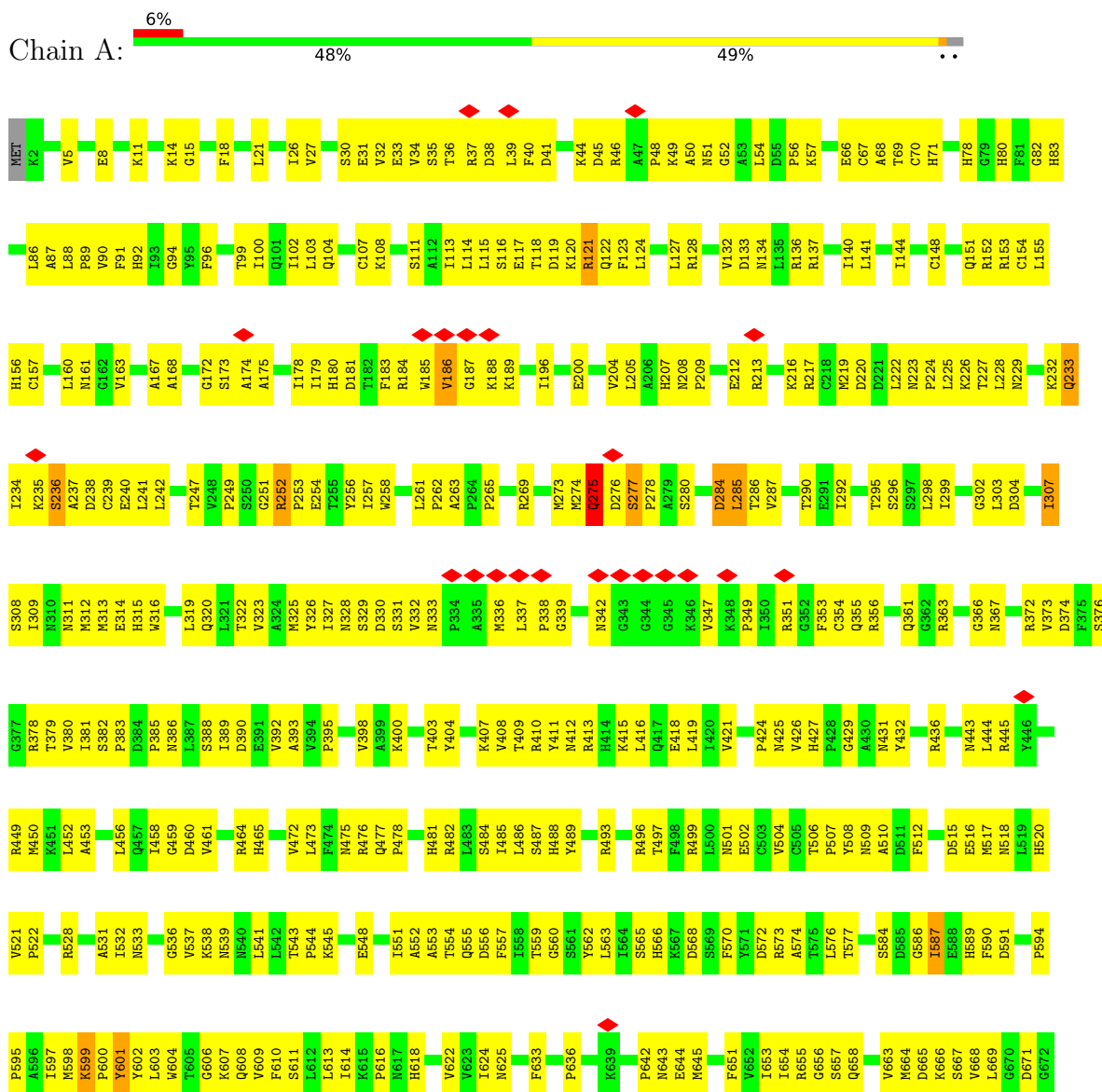
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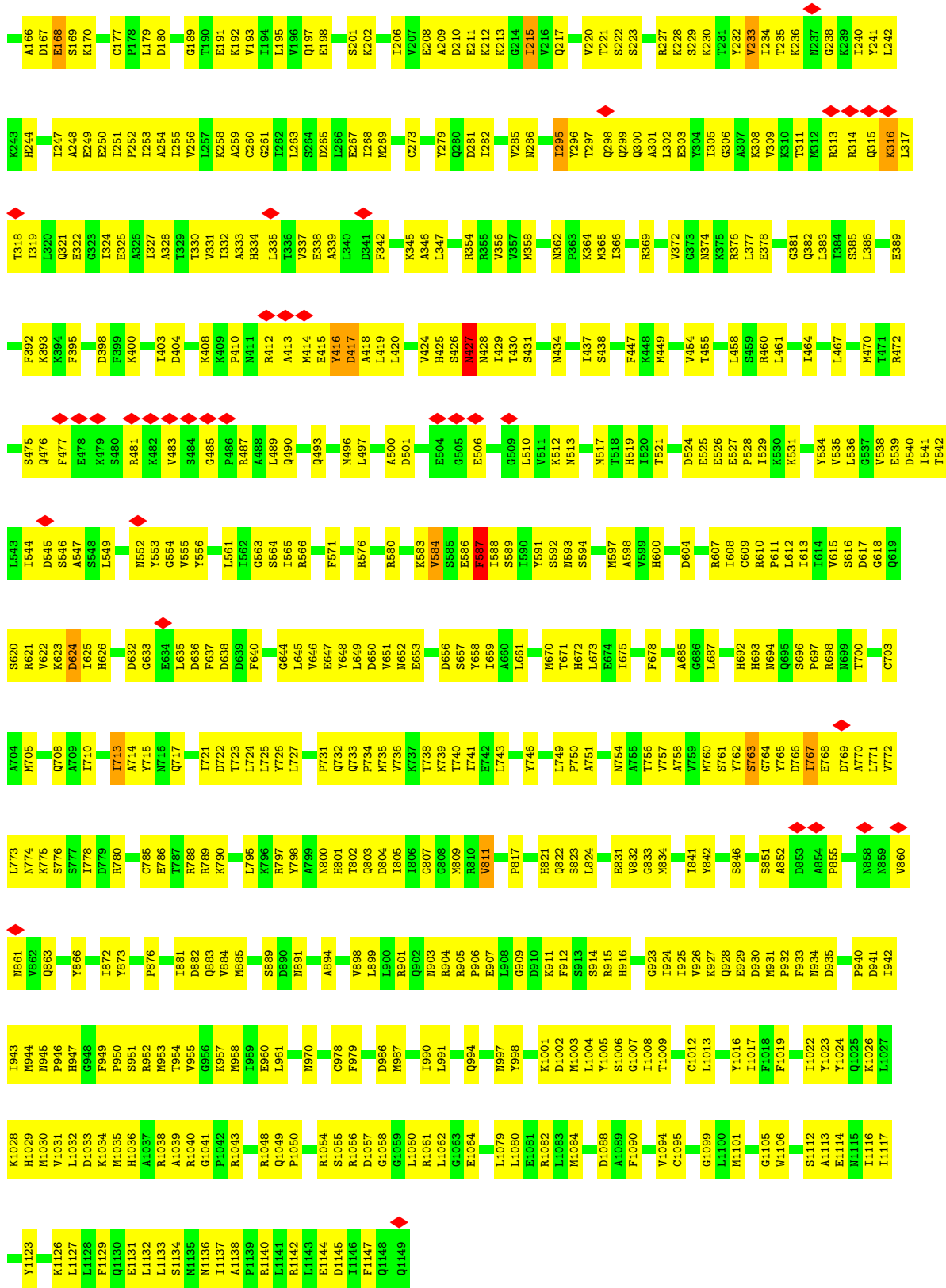
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
22	R	1	1	1	0

3 Residue-property plots

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

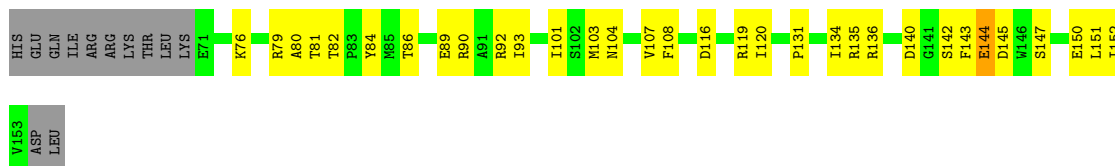
- Molecule 1: DNA-directed RNA polymerase III subunit RPC1



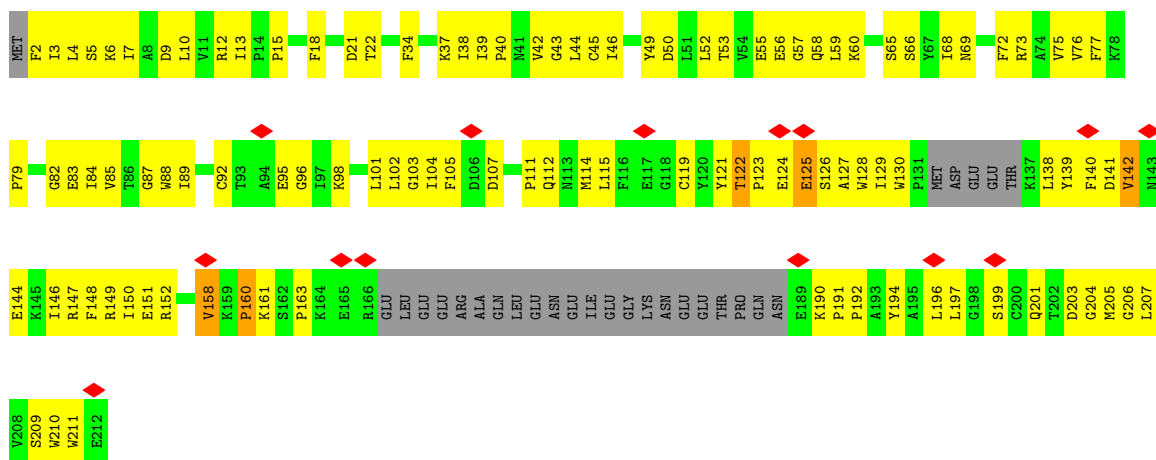


• Molecule 3: DNA-directed RNA polymerases I and III subunit RPAC1

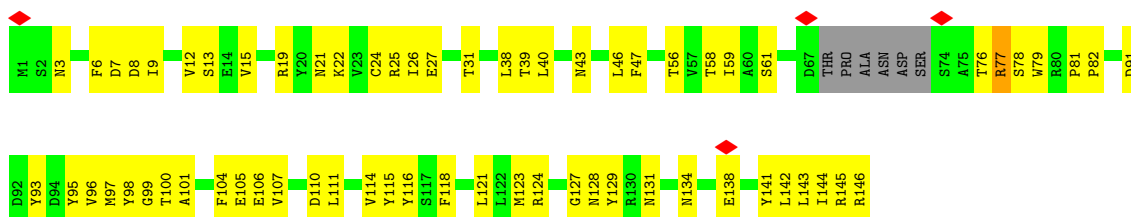




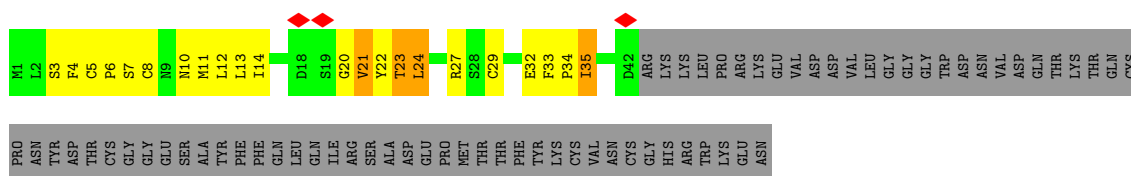
• Molecule 7: DNA-directed RNA polymerase III subunit RPC8



• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

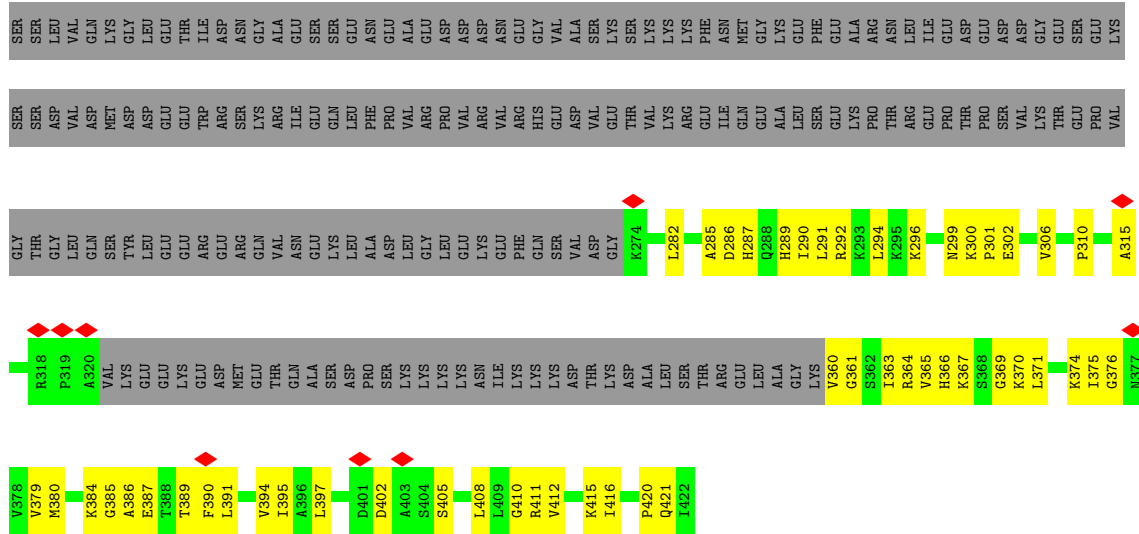


• Molecule 9: DNA-directed RNA polymerase III subunit RPC10

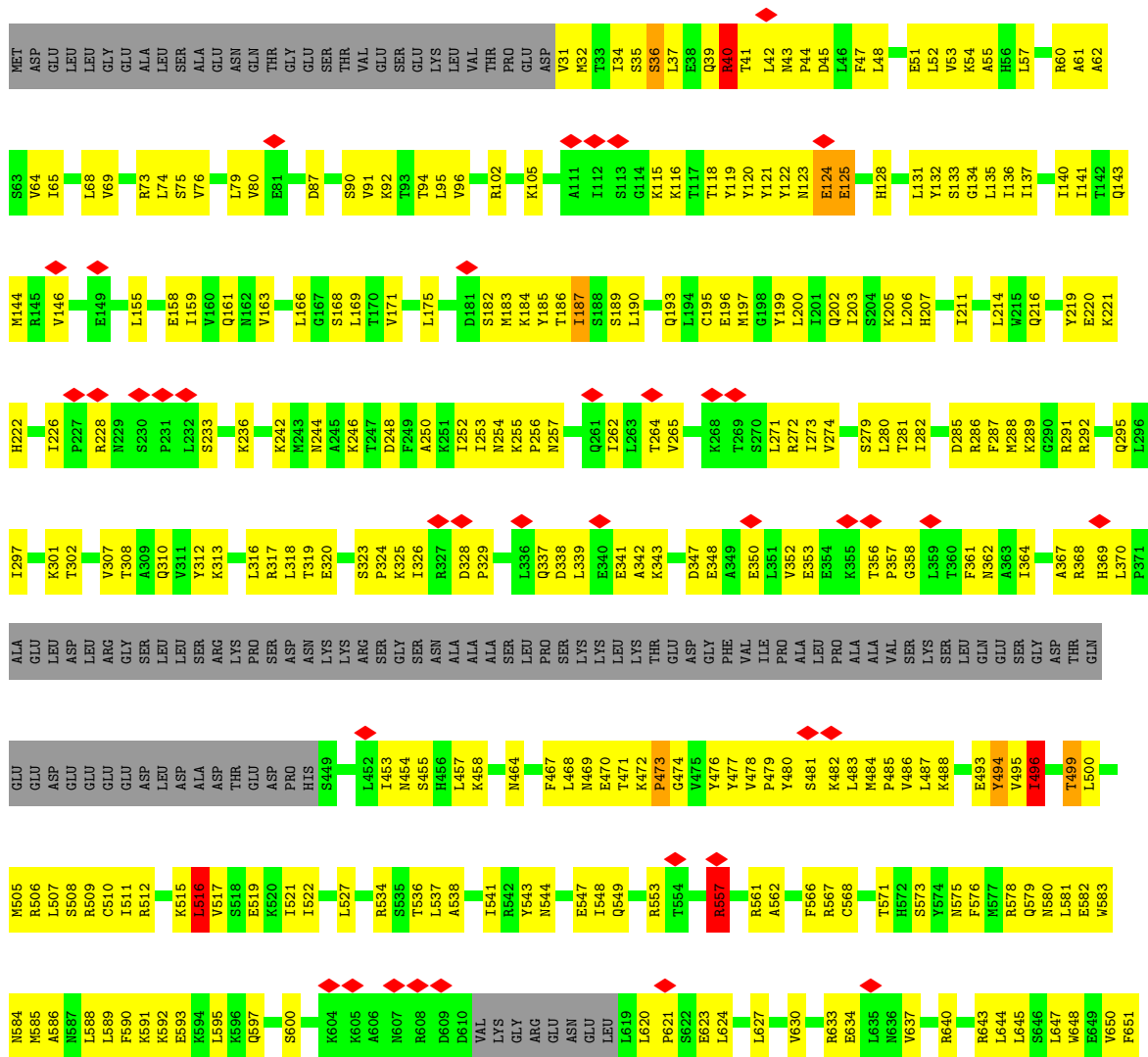


• Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5





• Molecule 15: DNA-directed RNA polymerase III subunit RPC3



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	103391	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY; CTF amplitude correction was performed following 3D auto refinement in relion.	Depositor
Microscope	JEOL 3200FS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	68.9	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.232	Depositor
Minimum map value	-0.136	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.0334	Depositor
Map size (\AA)	339.84, 339.84, 339.84	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.18, 1.18, 1.18	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.43	0/11358	0.62	0/15345
2	B	0.45	0/8943	0.63	0/12068
3	C	0.44	0/2711	0.59	0/3676
4	D	0.28	0/991	0.50	0/1328
5	E	0.37	0/1795	0.54	0/2416
6	F	0.45	0/683	0.64	0/923
7	G	0.32	0/1523	0.56	0/2066
8	H	0.42	0/1138	0.59	0/1540
9	I	0.37	0/328	0.64	0/445
10	J	0.51	0/558	0.62	0/750
11	K	0.44	0/803	0.61	0/1083
12	L	0.36	0/365	0.65	0/485
13	M	0.34	0/1369	0.60	0/1851
14	N	0.28	0/855	0.60	0/1149
15	O	0.35	0/4394	0.60	0/5928
16	P	0.31	0/2282	0.54	0/3075
17	Q	0.34	0/281	0.48	0/381
18	R	0.30	0/4200	0.50	0/5659
19	S	0.27	0/1464	0.49	0/1971
20	X	0.65	0/1158	1.04	0/1782
21	Y	0.64	0/1407	1.03	1/2169 (0.0%)
All	All	0.41	0/48606	0.63	1/66090 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	Y	65	DG	O4'-C1'-N9	5.67	111.97	108.00

There are no chirality outliers.

There are no planarity outliers.

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	11159	0	11285	789	0
2	B	8788	0	8901	631	0
3	C	2655	0	2628	165	0
4	D	977	0	983	85	0
5	E	1759	0	1788	105	0
6	F	671	0	692	32	0
7	G	1484	0	1485	125	0
8	H	1120	0	1089	65	0
9	I	321	0	303	40	0
10	J	549	0	559	36	0
11	K	792	0	790	37	0
12	L	363	0	386	33	0
13	M	1338	0	1307	142	0
14	N	845	0	891	67	0
15	O	4329	0	4497	349	0
16	P	2242	0	2265	144	0
17	Q	368	0	307	14	0
18	R	4131	0	4230	259	0
19	S	1649	0	1456	73	0
20	X	1036	0	584	75	0
21	Y	1254	0	695	92	0
22	A	2	0	0	0	0
22	B	1	0	0	0	0
22	I	1	0	0	0	0
22	J	1	0	0	0	0
22	L	1	0	0	0	0
22	R	1	0	0	0	0
All	All	47837	0	47121	2955	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 31.

All (2955) 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)
20:X:4:DT:H2''	20:X:5:DC:C5'	1.26	1.57
2:B:587:PHE:CZ	2:B:607:ARG:HD3	1.32	1.56
20:X:4:DT:C2'	20:X:5:DC:H5'	1.35	1.54
1:A:200:GLU:HB3	15:O:516:LEU:CD2	1.48	1.43
1:A:235:LYS:HD3	15:O:44:PRO:CG	1.49	1.40
2:B:587:PHE:HZ	2:B:607:ARG:CD	1.35	1.38
1:A:154:CYS:HB3	1:A:157:CYS:SG	1.66	1.36
4:D:127:LEU:HD22	4:D:133:HIS:CD2	1.66	1.29
15:O:495:VAL:O	15:O:496:ILE:HG12	1.36	1.26
12:L:34:CYS:SG	12:L:51:CYS:HB3	1.75	1.25
7:G:82:GLY:HA2	7:G:150:ILE:O	1.32	1.25
1:A:235:LYS:NZ	15:O:44:PRO:CB	2.04	1.21
1:A:200:GLU:CB	15:O:516:LEU:HD21	1.72	1.19
1:A:598:MET:O	1:A:599:LYS:HG2	1.38	1.19
1:A:599:LYS:HB2	1:A:600:PRO:CD	1.73	1.19
1:A:232:LYS:O	1:A:235:LYS:HE3	1.42	1.16
1:A:235:LYS:HA	1:A:252:ARG:HD3	1.22	1.16
1:A:235:LYS:NZ	15:O:44:PRO:HB2	1.61	1.16
1:A:235:LYS:CD	15:O:44:PRO:HG2	1.77	1.15
21:Y:20:DT:C7	21:Y:21:DT:H73	1.75	1.15
1:A:599:LYS:HB2	1:A:600:PRO:HD2	1.15	1.14
1:A:235:LYS:HZ3	15:O:44:PRO:HB3	1.12	1.13
15:O:495:VAL:O	15:O:496:ILE:CG1	1.96	1.12
9:I:8:CYS:HB3	9:I:29:CYS:SG	1.87	1.12
1:A:235:LYS:CD	15:O:44:PRO:CG	2.28	1.11
1:A:102:ILE:HD12	1:A:242:LEU:HD13	1.79	1.10
18:R:219:ARG:HA	18:R:514:GLU:CG	1.81	1.10
8:H:58:THR:O	8:H:143:LEU:HB3	1.50	1.09
7:G:126:SER:CB	7:G:139:TYR:HB2	1.82	1.09
1:A:235:LYS:HD3	15:O:44:PRO:CB	1.83	1.08
20:X:3:DT:H2''	20:X:4:DT:C7	1.82	1.08
1:A:256:TYR:CE2	1:A:1401:PHE:CE1	2.42	1.08
1:A:102:ILE:HD12	1:A:242:LEU:HD13	1.14	1.07
3:C:93:GLN:HB3	3:C:95:GLU:HG2	1.34	1.07
4:D:127:LEU:CD2	4:D:133:HIS:HD2	1.66	1.07
1:A:252:ARG:HB3	1:A:253:PRO:HD2	1.31	1.06
7:G:87:GLY:O	7:G:146:ILE:HB	1.55	1.06
15:O:184:LYS:HA	15:O:187:ILE:HD11	1.35	1.06
15:O:584:ASN:O	15:O:588:LEU:HB3	1.56	1.05
20:X:3:DT:H2''	20:X:4:DT:H71	1.35	1.05
18:R:219:ARG:HA	18:R:514:GLU:HG3	1.36	1.05
1:A:598:MET:O	1:A:599:LYS:CG	2.05	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:111:THR:HG22	11:K:112:THR:H	1.18	1.04
1:A:102:ILE:CD1	1:A:242:LEU:HD13	1.88	1.04
1:A:1174:GLN:HB3	1:A:1185:GLN:O	1.54	1.04
19:S:470:GLU:O	19:S:474:ARG:HB3	1.56	1.04
1:A:235:LYS:CD	15:O:44:PRO:HB2	1.88	1.04
4:D:11:LEU:HD21	4:D:16:VAL:HG21	1.40	1.03
7:G:126:SER:HB3	7:G:139:TYR:CB	1.89	1.02
15:O:73:ARG:HG2	15:O:121:TYR:CE1	1.94	1.01
15:O:36:SER:O	15:O:40:ARG:HB2	1.60	1.01
2:B:521:THR:HG21	2:B:587:PHE:CD1	1.96	1.00
15:O:125:GLU:HB3	15:O:128:HIS:HB2	1.40	0.99
2:B:316:LYS:HZ2	13:M:226:ARG:HH21	0.99	0.99
1:A:235:LYS:CA	1:A:252:ARG:HD3	1.93	0.99
1:A:100:ILE:O	1:A:104:GLN:HB2	1.63	0.98
1:A:235:LYS:HA	1:A:252:ARG:CD	1.94	0.97
7:G:126:SER:HB3	7:G:139:TYR:HB2	1.00	0.97
1:A:102:ILE:CD1	1:A:242:LEU:CD1	2.41	0.97
20:X:4:DT:C2'	20:X:5:DC:C5'	2.12	0.97
18:R:558:PRO:O	18:R:562:GLU:HB2	1.65	0.97
8:H:105:GLU:HG2	8:H:106:GLU:H	1.28	0.97
1:A:599:LYS:CB	1:A:600:PRO:CD	2.41	0.97
2:B:135:TYR:CE1	2:B:419:LEU:HB3	1.99	0.97
4:D:14:TYR:CD1	4:D:15:GLU:N	2.32	0.97
3:C:172:GLN:H	3:C:175:GLN:HB3	1.29	0.96
13:M:85:LEU:O	14:N:397:LEU:O	1.84	0.96
19:S:483:GLU:O	19:S:487:GLU:HB2	1.63	0.95
1:A:235:LYS:CD	15:O:44:PRO:CB	2.43	0.95
2:B:419:LEU:HD12	2:B:420:LEU:N	1.81	0.95
1:A:252:ARG:HB3	1:A:253:PRO:CD	1.96	0.95
18:R:83:ALA:O	18:R:87:LEU:HG	1.67	0.94
19:S:418:ASP:HB3	19:S:449:ARG:HH12	1.32	0.94
2:B:772:VAL:HG13	2:B:943:ILE:HG23	1.47	0.94
18:R:219:ARG:HD3	18:R:514:GLU:HG3	1.50	0.94
9:I:24:LEU:HD23	9:I:33:PHE:CD1	2.04	0.93
2:B:521:THR:CG2	2:B:609:CYS:SG	2.56	0.93
1:A:235:LYS:HZ2	15:O:44:PRO:HB2	1.19	0.93
2:B:417:ASP:HB3	2:B:419:LEU:HG	1.50	0.93
1:A:235:LYS:HD3	15:O:44:PRO:HG2	0.93	0.92
13:M:182:PHE:O	13:M:183:PHE:HD1	1.51	0.92
14:N:371:LEU:HD22	14:N:384:LYS:HD3	1.52	0.92
1:A:228:LEU:HB3	1:A:257:ILE:HD11	1.52	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:TYR:CZ	1:A:1401:PHE:CD1	2.59	0.91
1:A:179:ILE:CD1	15:O:557:ARG:HH21	1.82	0.91
2:B:315:GLN:O	2:B:316:LYS:HB2	1.68	0.91
2:B:552:ASN:ND2	2:B:566:ARG:HA	1.86	0.91
12:L:48:CYS:SG	12:L:51:CYS:O	2.29	0.90
15:O:143:GLN:HE21	15:O:196:GLU:HG2	1.34	0.90
15:O:470:GLU:HB2	15:O:479:PRO:HG3	1.52	0.90
11:K:111:THR:CG2	11:K:112:THR:H	1.83	0.90
11:K:111:THR:HG22	11:K:112:THR:N	1.87	0.89
1:A:228:LEU:HD12	1:A:229:ASN:N	1.87	0.89
3:C:94:ASP:O	12:L:67:PHE:HE2	1.55	0.89
1:A:273:MET:HG3	1:A:275:GLN:HG2	1.51	0.89
2:B:143:MET:SD	19:S:399:GLU:HB2	2.12	0.89
2:B:587:PHE:CZ	2:B:607:ARG:CD	2.24	0.89
9:I:29:CYS:HB3	13:M:183:PHE:CE2	2.08	0.89
1:A:235:LYS:NZ	15:O:44:PRO:HB3	1.78	0.88
4:D:14:TYR:CD1	4:D:15:GLU:HG2	2.08	0.88
2:B:55:LYS:NZ	2:B:59:LYS:HE3	1.89	0.88
2:B:55:LYS:HZ3	2:B:59:LYS:HE3	1.37	0.88
15:O:44:PRO:HA	15:O:582:GLU:HG2	1.54	0.88
15:O:184:LYS:HA	15:O:187:ILE:CD1	2.03	0.88
1:A:235:LYS:CE	15:O:44:PRO:CB	2.51	0.88
2:B:552:ASN:HD21	2:B:566:ARG:HA	1.37	0.88
13:M:85:LEU:HD23	13:M:86:HIS:O	1.74	0.88
15:O:105:LYS:HG2	15:O:123:ASN:HA	1.56	0.88
1:A:256:TYR:CE2	1:A:1401:PHE:HE1	1.90	0.88
15:O:583:TRP:HH2	16:P:314:GLU:HG3	1.37	0.88
2:B:316:LYS:NZ	13:M:226:ARG:HH21	1.71	0.88
15:O:515:LYS:O	15:O:516:LEU:HG	1.73	0.87
1:A:235:LYS:CE	15:O:44:PRO:HB2	2.03	0.87
16:P:266:GLU:O	16:P:269:LEU:HG	1.74	0.87
1:A:89:PRO:HG3	1:A:228:LEU:HD21	1.54	0.87
1:A:178:ILE:HD11	1:A:222:LEU:HB2	1.54	0.86
18:R:83:ALA:O	18:R:87:LEU:CG	2.22	0.86
18:R:135:ARG:HH12	18:R:513:PRO:HG3	1.39	0.86
15:O:547:GLU:HG2	15:O:548:ILE:H	1.40	0.86
20:X:4:DT:H71	20:X:4:DT:OP2	1.75	0.86
1:A:1448:PHE:HZ	4:D:16:VAL:CG2	1.88	0.86
2:B:587:PHE:CE2	2:B:604:ASP:O	2.28	0.86
1:A:15:GLY:H	1:A:1408:VAL:HG12	1.41	0.86
4:D:127:LEU:HD22	4:D:133:HIS:HD2	0.76	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1026:LYS:NZ	2:B:1030:MET:SD	2.48	0.86
13:M:182:PHE:O	13:M:183:PHE:CD1	2.28	0.86
18:R:219:ARG:CA	18:R:514:GLU:HG3	2.05	0.85
21:Y:20:DT:H73	21:Y:21:DT:H73	1.55	0.85
15:O:200:LEU:HB3	15:O:280:LEU:HB3	1.57	0.85
15:O:125:GLU:CB	15:O:128:HIS:HB2	2.05	0.85
1:A:234:ILE:HD11	1:A:237:ALA:HB3	1.57	0.85
1:A:1366:GLY:HA3	5:E:179:GLN:HG3	1.59	0.85
2:B:521:THR:HG21	2:B:609:CYS:SG	2.17	0.84
14:N:306:VAL:HG23	14:N:415:LYS:HD3	1.56	0.84
15:O:467:PHE:HD2	15:O:468:LEU:HD13	1.42	0.84
1:A:235:LYS:HZ3	15:O:44:PRO:CB	1.73	0.84
2:B:717:GLN:HE21	2:B:727:LEU:HD22	1.43	0.84
15:O:583:TRP:CH2	16:P:314:GLU:HG3	2.11	0.84
13:M:241:ALA:O	13:M:242:ASN:HB3	1.78	0.84
1:A:232:LYS:O	1:A:235:LYS:CE	2.25	0.84
3:C:85:PHE:HE2	3:C:94:ASP:O	1.60	0.84
2:B:587:PHE:CZ	2:B:607:ARG:HB3	2.13	0.83
13:M:245:LEU:HD22	14:N:405:SER:OG	1.78	0.83
15:O:73:ARG:HG2	15:O:121:TYR:CZ	2.14	0.83
15:O:123:ASN:O	15:O:124:GLU:O	1.97	0.82
1:A:393:ALA:HB3	1:A:499:ARG:HB2	1.60	0.82
1:A:476:ARG:HG2	1:A:477:GLN:HG3	1.59	0.82
1:A:200:GLU:HB3	15:O:516:LEU:HD21	0.84	0.82
1:A:234:ILE:HD11	1:A:237:ALA:CB	2.09	0.82
1:A:598:MET:O	1:A:599:LYS:CB	2.26	0.82
2:B:587:PHE:HE2	2:B:604:ASP:O	1.60	0.82
4:D:110:LEU:HB3	4:D:120:LYS:HE3	1.62	0.82
1:A:723:LEU:O	1:A:727:LYS:HB2	1.78	0.82
1:A:200:GLU:CB	15:O:516:LEU:CD2	2.45	0.82
1:A:601:TYR:CD1	3:C:23:PHE:HE2	1.97	0.82
3:C:105:PRO:HG3	10:J:6:ARG:HH21	1.42	0.82
1:A:256:TYR:CZ	1:A:1401:PHE:CE1	2.68	0.81
2:B:536:LEU:HD22	2:B:571:PHE:HD1	1.45	0.81
15:O:43:ASN:HB3	15:O:47:PHE:HB2	1.63	0.81
2:B:230:LYS:HE2	2:B:334:HIS:HE1	1.43	0.81
2:B:316:LYS:HZ2	13:M:226:ARG:NH2	1.79	0.81
7:G:5:SER:O	7:G:73:ARG:HA	1.79	0.81
1:A:980:SER:HA	5:E:163:GLU:HG2	1.63	0.81
1:A:1378:LYS:HG3	1:A:1379:MET:H	1.46	0.81
16:P:33:GLN:NE2	16:P:49:MET:SD	2.54	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:741:ILE:HG23	2:B:746:TYR:HB3	1.64	0.80
3:C:231:PRO:HA	3:C:293:ARG:HG2	1.62	0.80
3:C:222:VAL:HG11	3:C:225:ALA:HB2	1.63	0.80
15:O:48:LEU:HD22	15:O:581:LEU:HD11	1.62	0.80
2:B:521:THR:HG23	2:B:609:CYS:SG	2.20	0.80
2:B:141:ILE:HG23	2:B:142:ILE:H	1.44	0.80
14:N:290:ILE:O	14:N:294:LEU:CB	2.30	0.80
7:G:126:SER:CB	7:G:139:TYR:CB	2.55	0.80
18:R:218:ARG:O	18:R:514:GLU:HG2	1.82	0.80
2:B:464:ILE:HD11	2:B:746:TYR:HE1	1.46	0.79
7:G:119:CYS:HB2	7:G:128:TRP:HB3	1.64	0.79
1:A:597:ILE:HD11	1:A:603:LEU:HD12	1.65	0.79
4:D:145:PHE:HB2	4:D:149:THR:HG21	1.64	0.79
13:M:89:GLN:HE21	13:M:178:GLN:HE22	1.29	0.79
20:X:4:DT:H2'	20:X:5:DC:C6	2.18	0.79
15:O:297:ILE:O	15:O:301:LYS:HB2	1.83	0.79
21:Y:20:DT:H71	21:Y:21:DT:H73	1.63	0.79
2:B:228:LYS:HD2	2:B:333:ALA:HA	1.64	0.79
4:D:14:TYR:HD1	4:D:15:GLU:HG2	1.44	0.79
14:N:290:ILE:O	14:N:294:LEU:HB2	1.83	0.79
14:N:287:HIS:O	14:N:291:LEU:HB2	1.82	0.78
15:O:509:ARG:O	15:O:512:ARG:HB3	1.83	0.78
1:A:235:LYS:CE	15:O:44:PRO:CG	2.61	0.78
1:A:235:LYS:O	1:A:236:SER:HB3	1.80	0.78
5:E:29:PHE:HB2	5:E:65:THR:HB	1.65	0.78
8:H:97:MET:HB2	8:H:142:LEU:HB3	1.65	0.78
1:A:1178:LYS:HB2	1:A:1181:LEU:HD12	1.65	0.78
1:A:1213:SER:HB2	1:A:1217:ILE:HB	1.63	0.78
17:Q:54:LEU:O	17:Q:58:TYR:HB2	1.83	0.78
21:Y:20:DT:C5	21:Y:21:DT:H73	2.17	0.78
2:B:587:PHE:HZ	2:B:607:ARG:CG	1.95	0.78
1:A:400:LYS:HA	1:A:465:HIS:HD2	1.49	0.78
2:B:403:ILE:HD11	2:B:418:ALA:HB1	1.65	0.78
1:A:1151:GLU:HG3	1:A:1152:ARG:HG3	1.66	0.77
16:P:33:GLN:NE2	19:S:372:MET:SD	2.58	0.77
2:B:1006:SER:HB2	2:B:1013:LEU:HD21	1.67	0.77
19:S:494:THR:HB	19:S:497:ASP:HB2	1.67	0.77
20:X:53:DT:H2''	20:X:54:DG:H8	1.49	0.77
1:A:121:ARG:HG3	15:O:73:ARG:CD	2.15	0.77
1:A:395:PRO:HB3	1:A:496:ARG:HA	1.66	0.76
2:B:122:ASP:HA	2:B:189:GLY:HA3	1.65	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:332:ILE:HG13	2:B:333:ALA:H	1.50	0.76
2:B:766:ASP:OD1	2:B:945:ASN:HB2	1.86	0.76
10:J:17:LYS:HB3	10:J:39:LEU:HD21	1.67	0.76
1:A:179:ILE:CD1	15:O:557:ARG:NH2	2.48	0.76
3:C:94:ASP:O	12:L:67:PHE:CE2	2.38	0.76
7:G:138:LEU:HD12	7:G:139:TYR:O	1.85	0.76
13:M:112:TYR:HD1	13:M:119:TRP:HE1	1.31	0.76
18:R:219:ARG:CA	18:R:514:GLU:CG	2.63	0.76
2:B:427:ASN:OD1	2:B:431:SER:HB3	1.85	0.76
21:Y:20:DT:C4	21:Y:21:DT:C4	2.73	0.76
1:A:1380:ARG:HH11	1:A:1385:GLN:HE22	1.32	0.76
18:R:219:ARG:HA	18:R:514:GLU:HG2	1.64	0.76
20:X:53:DT:H2'	20:X:54:DG:C8	2.21	0.76
16:P:176:ASN:HA	16:P:179:LEU:HB2	1.66	0.76
1:A:431:ASN:OD1	1:A:432:TYR:N	2.19	0.76
2:B:230:LYS:CE	2:B:334:HIS:HE1	1.98	0.76
2:B:1112:SER:HB2	2:B:1114:GLU:HG2	1.67	0.76
3:C:113:LEU:HD11	3:C:132:ILE:HD11	1.68	0.76
2:B:735:MET:HB2	2:B:754:ASN:HD21	1.51	0.76
1:A:642:PRO:HB2	1:A:644:GLU:OE1	1.86	0.75
2:B:137:ARG:HG2	2:B:141:ILE:HG12	1.66	0.75
15:O:105:LYS:HB2	15:O:121:TYR:HB2	1.66	0.75
4:D:127:LEU:HD21	7:G:147:ARG:HD2	1.68	0.75
1:A:308:SER:HA	15:O:534:ARG:HD2	1.68	0.75
2:B:135:TYR:OH	2:B:419:LEU:HB2	1.86	0.75
18:R:515:LEU:O	18:R:516:PHE:HB2	1.86	0.75
1:A:1448:PHE:HZ	4:D:16:VAL:HG23	1.52	0.75
2:B:68:PHE:CE1	2:B:385:SER:OG	2.40	0.75
1:A:117:GLU:HG2	1:A:119:ASP:H	1.52	0.74
1:A:330:ASP:OD1	1:A:331:SER:N	2.19	0.74
1:A:955:LEU:HB2	1:A:958:ALA:HB3	1.69	0.74
20:X:8:DC:O2	21:Y:62:DG:N2	2.13	0.74
1:A:153:ARG:NH2	15:O:337:GLN:O	2.20	0.74
3:C:256:ILE:HG22	3:C:267:VAL:HA	1.69	0.74
5:E:123:LEU:HD21	5:E:126:SER:HB2	1.68	0.74
3:C:33:VAL:O	3:C:34:GLU:HB2	1.85	0.74
8:H:105:GLU:HG2	8:H:106:GLU:N	2.01	0.74
12:L:61:THR:HG23	12:L:63:ARG:H	1.53	0.74
15:O:584:ASN:O	15:O:588:LEU:CB	2.33	0.74
15:O:584:ASN:HB3	15:O:588:LEU:HB2	1.69	0.74
2:B:364:LYS:HG3	2:B:365:MET:H	1.53	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:122:ASP:HB3	13:M:145:VAL:HG21	1.69	0.74
8:H:21:ASN:OD1	8:H:22:LYS:N	2.19	0.74
12:L:51:CYS:SG	12:L:53:HIS:HB3	2.28	0.74
15:O:620:LEU:HD12	15:O:621:PRO:HD2	1.68	0.74
2:B:135:TYR:CE1	2:B:419:LEU:CB	2.70	0.74
15:O:196:GLU:HG3	15:O:197:MET:H	1.53	0.74
1:A:946:THR:HG21	1:A:1066:SER:HA	1.70	0.74
3:C:256:ILE:HA	3:C:268:LYS:H	1.53	0.74
18:R:245:VAL:HA	18:R:248:SER:HB3	1.70	0.74
15:O:200:LEU:HA	15:O:281:THR:O	1.87	0.73
15:O:480:TYR:HA	15:O:483:LEU:HB3	1.69	0.73
18:R:202:ALA:O	18:R:205:LEU:HB3	1.87	0.73
10:J:9:SER:OG	10:J:45:CYS:SG	2.44	0.73
20:X:26:DT:H2'	20:X:27:DT:C6	2.23	0.73
1:A:378:ARG:NE	1:A:516:GLU:OE1	2.20	0.73
1:A:476:ARG:HD2	1:A:508:TYR:HB3	1.70	0.73
1:A:599:LYS:HG3	8:H:96:VAL:HG13	1.70	0.73
20:X:5:DC:O2	21:Y:65:DG:N2	2.17	0.73
2:B:416:TYR:CE1	18:R:151:GLN:HB2	2.23	0.73
7:G:92:CYS:SG	7:G:98:LYS:N	2.57	0.73
15:O:183:MET:O	15:O:187:ILE:HG13	1.89	0.73
1:A:276:ASP:O	1:A:277:SER:HB2	1.88	0.73
2:B:412:ARG:HG2	2:B:413:ALA:H	1.53	0.73
15:O:37:LEU:HD23	15:O:40:ARG:HD2	1.70	0.73
2:B:296:TYR:HB2	2:B:300:GLN:HE22	1.53	0.73
18:R:220:PRO:HD3	18:R:514:GLU:HG2	1.71	0.73
2:B:831:GLU:N	2:B:831:GLU:OE1	2.21	0.73
2:B:758:ALA:HA	2:B:1019:PHE:HB3	1.69	0.73
1:A:1184:ILE:HB	1:A:1232:ILE:HB	1.69	0.72
1:A:1395:HIS:O	1:A:1399:ALA:HB2	1.88	0.72
2:B:321:GLN:H	2:B:324:ILE:HB	1.54	0.72
2:B:754:ASN:O	10:J:48:ARG:NH1	2.22	0.72
18:R:468:ILE:HG13	18:R:610:LEU:HD11	1.71	0.72
1:A:212:GLU:CD	1:A:213:ARG:H	1.93	0.72
2:B:316:LYS:NZ	13:M:226:ARG:NH2	2.36	0.72
2:B:415:GLU:HG3	2:B:416:TYR:H	1.55	0.72
3:C:239:ILE:HG22	3:C:288:LYS:HD2	1.70	0.72
15:O:123:ASN:O	15:O:124:GLU:C	2.27	0.72
1:A:123:PHE:CG	1:A:144:ILE:HD13	2.25	0.72
1:A:777:VAL:HG12	1:A:811:ALA:HB1	1.71	0.72
14:N:384:LYS:HA	14:N:416:ILE:HD11	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:11:LEU:O	16:P:15:ALA:HB2	1.90	0.72
7:G:105:PHE:HD1	7:G:107:ASP:H	1.36	0.72
1:A:599:LYS:CB	1:A:600:PRO:HD2	2.02	0.72
14:N:380:MET:SD	14:N:421:GLN:NE2	2.62	0.72
15:O:515:LYS:C	15:O:516:LEU:HG	2.08	0.72
16:P:75:VAL:HG22	16:P:77:GLU:H	1.55	0.72
1:A:367:ASN:OD1	2:B:1049:GLN:NE2	2.23	0.72
2:B:797:ARG:HG2	2:B:803:GLN:HG2	1.68	0.72
2:B:822:GLN:O	2:B:824:LEU:N	2.22	0.72
13:M:112:TYR:O	13:M:243:ILE:CG2	2.37	0.72
1:A:598:MET:O	8:H:96:VAL:HG22	1.90	0.72
1:A:124:LEU:HB3	1:A:128:ARG:HH12	1.54	0.72
1:A:174:ALA:HB2	15:O:557:ARG:CB	2.19	0.72
1:A:1121:LEU:O	1:A:1346:HIS:NE2	2.22	0.72
3:C:93:GLN:HB3	3:C:95:GLU:CG	2.18	0.72
3:C:228:ARG:HH21	3:C:299:ILE:HD13	1.54	0.72
5:E:21:GLU:HB3	5:E:35:VAL:HG21	1.70	0.72
3:C:100:ARG:NH2	3:C:192:LEU:O	2.23	0.72
13:M:164:LYS:HG3	14:N:300:LYS:HD3	1.71	0.72
16:P:170:LEU:HD23	16:P:172:ILE:H	1.55	0.72
21:Y:20:DT:O4	21:Y:21:DT:O4	2.07	0.72
2:B:501:ASP:HB3	2:B:703:CYS:CB	2.20	0.71
9:I:24:LEU:HD23	9:I:33:PHE:CE1	2.25	0.71
2:B:295:ILE:O	2:B:300:GLN:NE2	2.23	0.71
2:B:554:GLY:HA2	2:B:564:SER:HA	1.71	0.71
4:D:17:LEU:HD11	4:D:63:VAL:HG23	1.72	0.71
15:O:495:VAL:O	15:O:496:ILE:HG13	1.91	0.71
1:A:328:ASN:OD1	1:A:329:SER:N	2.22	0.71
16:P:69:GLU:HG3	16:P:70:LEU:H	1.55	0.71
20:X:12:DT:H2'	20:X:13:DA:N7	2.05	0.71
20:X:4:DT:C2'	20:X:5:DC:O5'	2.36	0.71
2:B:428:ASN:OD1	2:B:429:ILE:N	2.23	0.71
2:B:694:ASN:HD21	2:B:916:HIS:CE1	2.08	0.71
15:O:183:MET:O	15:O:187:ILE:CG1	2.38	0.71
15:O:289:LYS:HE2	15:O:323:SER:HB3	1.72	0.71
19:S:470:GLU:O	19:S:474:ARG:CB	2.36	0.71
3:C:152:ASP:OD2	3:C:154:LYS:NZ	2.20	0.71
2:B:68:PHE:CD1	2:B:385:SER:OG	2.43	0.71
1:A:598:MET:C	1:A:599:LYS:HG2	2.11	0.71
4:D:11:LEU:HD21	4:D:16:VAL:CG2	2.20	0.71
21:Y:20:DT:C4	21:Y:21:DT:O4	2.44	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:LEU:HB3	1:A:257:ILE:CD1	2.20	0.71
1:A:432:TYR:OH	18:R:20:ASN:ND2	2.24	0.71
15:O:45:ASP:N	15:O:582:GLU:OE2	2.20	0.71
18:R:267:ALA:HA	18:R:270:LEU:HB3	1.73	0.71
21:Y:47:DG:H2'	21:Y:48:DT:H71	1.73	0.71
6:F:79:ARG:NH1	6:F:145:ASP:O	2.24	0.70
15:O:35:SER:HB2	15:O:40:ARG:HH21	1.56	0.70
2:B:261:GLY:O	13:M:180:LYS:NZ	2.23	0.70
19:S:483:GLU:O	19:S:487:GLU:CB	2.39	0.70
2:B:227:ARG:HD3	2:B:449:MET:HG3	1.73	0.70
2:B:566:ARG:HD3	14:N:386:ALA:O	1.92	0.70
2:B:785:CYS:SG	2:B:1026:LYS:NZ	2.57	0.70
5:E:86:PRO:HA	5:E:113:GLN:HB3	1.71	0.70
2:B:934:ASN:HB3	2:B:1004:LEU:HD23	1.72	0.70
9:I:32:GLU:HB2	13:M:130:PHE:HB3	1.73	0.70
2:B:137:ARG:H	2:B:141:ILE:HG21	1.56	0.70
2:B:315:GLN:O	2:B:316:LYS:CB	2.40	0.70
2:B:417:ASP:HB3	2:B:419:LEU:CG	2.20	0.70
1:A:92:HIS:CD2	1:A:94:GLY:H	2.09	0.70
15:O:493:GLU:O	15:O:494:TYR:O	2.09	0.70
2:B:265:ASP:O	2:B:268:ILE:N	2.22	0.70
16:P:310:VAL:HG11	17:Q:43:ILE:HD11	1.74	0.70
18:R:239:ARG:NH1	19:S:291:UNK:O	2.24	0.70
18:R:515:LEU:O	18:R:516:PHE:CB	2.40	0.70
1:A:999:ASP:OD1	1:A:1002:ARG:NH1	2.24	0.70
18:R:467:ARG:HG3	18:R:610:LEU:HD22	1.74	0.70
7:G:39:ILE:HD12	7:G:40:PRO:HD2	1.73	0.70
16:P:172:ILE:HG22	16:P:173:GLU:H	1.57	0.70
2:B:738:THR:HB	2:B:741:ILE:HD12	1.74	0.70
4:D:14:TYR:CG	4:D:15:GLU:N	2.56	0.70
1:A:338:PRO:HG2	1:A:342:ASN:HB2	1.74	0.69
1:A:1305:CYS:SG	5:E:11:ARG:NH1	2.65	0.69
2:B:221:THR:HG21	2:B:334:HIS:HA	1.72	0.69
18:R:463:ARG:NH1	18:R:601:ASN:O	2.25	0.69
18:R:528:ILE:HG12	18:R:543:ALA:HB2	1.73	0.69
1:A:429:GLY:C	1:A:465:HIS:HD1	1.95	0.69
1:A:1448:PHE:CE1	4:D:12:SER:O	2.45	0.69
2:B:259:ALA:HB1	2:B:302:LEU:HD23	1.74	0.69
15:O:591:LYS:O	15:O:633:ARG:NH2	2.25	0.69
18:R:219:ARG:HD3	18:R:514:GLU:CG	2.21	0.69
18:R:436:LYS:NZ	19:S:462:GLU:OE2	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:215:ASP:OD2	12:L:70:ARG:NH2	2.25	0.69
5:E:83:CYS:SG	5:E:84:ASP:N	2.66	0.69
18:R:218:ARG:HH12	18:R:258:ARG:HB2	1.57	0.69
15:O:516:LEU:HD12	15:O:516:LEU:O	1.92	0.69
1:A:601:TYR:CD1	3:C:23:PHE:CE2	2.81	0.69
2:B:758:ALA:HB3	2:B:943:ILE:HD13	1.73	0.69
1:A:228:LEU:O	1:A:232:LYS:HG3	1.92	0.69
1:A:1448:PHE:CZ	4:D:16:VAL:CG2	2.73	0.69
2:B:195:LEU:HD11	2:B:472:ARG:HB3	1.73	0.69
2:B:1036:HIS:NE2	2:B:1058:GLY:HA2	2.07	0.69
8:H:105:GLU:CG	8:H:106:GLU:H	2.03	0.69
13:M:149:LYS:HB3	13:M:182:PHE:HE1	1.56	0.69
1:A:486:LEU:HD23	1:A:537:VAL:HG22	1.74	0.69
2:B:698:ARG:HE	2:B:952:ARG:HB3	1.58	0.69
2:B:775:LYS:HG3	2:B:925:ILE:HG22	1.73	0.69
2:B:584:VAL:HB	2:B:588:ILE:HD12	1.75	0.69
3:C:132:ILE:O	3:C:208:CYS:HB3	1.93	0.69
2:B:760:MET:HB3	2:B:943:ILE:HD11	1.75	0.69
5:E:172:GLU:HG2	5:E:173:SER:H	1.57	0.69
16:P:191:PHE:HB2	16:P:192:PRO:HD2	1.75	0.69
2:B:197:GLN:NE2	2:B:476:GLN:OE1	2.25	0.68
3:C:33:VAL:HG12	3:C:34:GLU:H	1.58	0.68
1:A:89:PRO:HG3	1:A:228:LEU:CD2	2.23	0.68
1:A:543:THR:HG22	1:A:548:GLU:H	1.57	0.68
1:A:1447:LEU:HD23	1:A:1450:SER:HB3	1.74	0.68
2:B:253:ILE:HG22	2:B:286:ASN:HD21	1.58	0.68
14:N:364:ARG:NH1	14:N:365:VAL:O	2.26	0.68
15:O:292:ARG:HH12	15:O:650:VAL:HA	1.57	0.68
5:E:82:PHE:HD1	5:E:111:VAL:HB	1.58	0.68
15:O:75:SER:HB2	15:O:119:TYR:CE1	2.29	0.68
1:A:1448:PHE:CE1	4:D:14:TYR:CE2	2.82	0.68
16:P:266:GLU:HB3	16:P:269:LEU:CD2	2.24	0.68
1:A:400:LYS:HA	1:A:465:HIS:CD2	2.28	0.68
1:A:1177:TYR:HE2	9:I:14:ILE:HG13	1.59	0.68
2:B:412:ARG:NH1	2:B:415:GLU:OE2	2.27	0.68
18:R:213:TRP:HE1	18:R:495:PRO:HB3	1.58	0.68
2:B:335:LEU:HD12	2:B:335:LEU:O	1.94	0.68
2:B:882:ASP:OD1	2:B:883:GLN:N	2.27	0.68
8:H:24:CYS:SG	8:H:25:ARG:N	2.66	0.68
1:A:790:ALA:HB1	1:A:794:MET:HE2	1.76	0.68
10:J:52:THR:HG22	10:J:53:HIS:H	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:112:TYR:O	13:M:243:ILE:HG22	1.93	0.68
1:A:89:PRO:HG2	1:A:225:LEU:HA	1.74	0.68
4:D:11:LEU:CD2	4:D:16:VAL:HG21	2.22	0.68
4:D:14:TYR:CE1	4:D:15:GLU:HB2	2.28	0.68
15:O:73:ARG:CG	15:O:121:TYR:CE1	2.75	0.67
15:O:595:LEU:HD21	15:O:630:VAL:HG23	1.76	0.67
20:X:57:DT:O2	21:Y:14:DG:N2	2.27	0.67
1:A:1136:ILE:HG21	1:A:1318:HIS:HB3	1.76	0.67
6:F:80:ALA:O	6:F:81:THR:OG1	2.11	0.67
15:O:80:VAL:HG11	15:O:87:ASP:HB2	1.76	0.67
15:O:288:MET:SD	15:O:291:ARG:NH2	2.66	0.67
2:B:1101:MET:SD	2:B:1126:LYS:HG3	2.33	0.67
3:C:165:ARG:NH2	3:C:190:ASP:OD1	2.28	0.67
7:G:129:ILE:HG12	7:G:139:TYR:HB3	1.76	0.67
16:P:311:TYR:HA	17:Q:40:PRO:HA	1.77	0.67
1:A:179:ILE:HD11	15:O:557:ARG:HH21	1.58	0.67
1:A:716:ASP:OD2	1:A:790:ALA:N	2.27	0.67
2:B:501:ASP:HB3	2:B:703:CYS:HB2	1.77	0.67
3:C:283:GLU:O	3:C:286:ALA:N	2.27	0.67
14:N:395:ILE:HA	14:N:411:ARG:HA	1.76	0.67
20:X:2:DT:O4	21:Y:67:DA:N6	2.27	0.67
11:K:68:GLU:HG3	11:K:69:ASP:H	1.59	0.67
3:C:238:PRO:O	3:C:239:ILE:HG13	1.95	0.67
1:A:927:GLU:HG2	1:A:928:GLY:H	1.58	0.67
7:G:126:SER:O	7:G:128:TRP:N	2.26	0.67
2:B:241:TYR:HB3	2:B:250:GLU:HB2	1.76	0.67
1:A:121:ARG:HG3	15:O:73:ARG:HD2	1.76	0.67
13:M:103:GLU:OE1	13:M:103:GLU:O	2.13	0.67
15:O:353:GLU:H	15:O:481:SER:HB2	1.60	0.67
18:R:420:TYR:O	18:R:627:TRP:NE1	2.28	0.66
1:A:1425:THR:HG23	6:F:92:ARG:HB2	1.77	0.66
5:E:109:ILE:HG22	5:E:133:GLU:HB3	1.76	0.66
12:L:31:CYS:SG	12:L:48:CYS:HB2	2.35	0.66
13:M:160:ALA:HA	14:N:306:VAL:HG12	1.77	0.66
13:M:245:LEU:HD13	14:N:405:SER:OG	1.95	0.66
19:S:480:ASN:OD1	19:S:481:PHE:N	2.25	0.66
1:A:209:PRO:O	1:A:212:GLU:HB2	1.95	0.66
2:B:247:ILE:HG12	2:B:251:ILE:HD11	1.77	0.66
4:D:7:ARG:HE	4:D:10:PHE:HZ	1.41	0.66
16:P:11:LEU:O	16:P:15:ALA:CB	2.43	0.66
1:A:26:ILE:HD13	1:A:262:PRO:HG3	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:CYS:SG	1:A:80:HIS:HE1	2.18	0.66
2:B:461:LEU:HD21	2:B:1028:LYS:HD3	1.77	0.66
9:I:29:CYS:HB3	13:M:183:PHE:HE2	1.56	0.66
18:R:558:PRO:O	18:R:562:GLU:CB	2.43	0.66
1:A:303:LEU:HG	15:O:538:ALA:HB1	1.77	0.66
2:B:722:ASP:OD1	2:B:723:THR:N	2.27	0.66
7:G:13:ILE:HG13	7:G:66:SER:HB3	1.77	0.66
15:O:31:VAL:HG12	15:O:32:MET:HG3	1.78	0.66
18:R:213:TRP:CD1	18:R:287:PRO:HD3	2.30	0.66
1:A:120:LYS:HG3	1:A:241:LEU:HD11	1.78	0.66
1:A:1125:ARG:NH2	1:A:1338:GLU:OE2	2.27	0.66
1:A:1284:ASN:OD1	1:A:1285:ILE:N	2.25	0.66
5:E:117:THR:HG23	5:E:120:ALA:H	1.60	0.66
8:H:131:ASN:O	8:H:134:ASN:N	2.27	0.66
18:R:581:ASN:ND2	18:R:583:HIS:O	2.29	0.66
2:B:914:SER:O	2:B:915:ARG:HG2	1.96	0.66
4:D:122:GLN:HE22	7:G:83:GLU:HG3	1.61	0.66
16:P:269:LEU:HB3	16:P:297:PHE:CE1	2.30	0.66
18:R:123:GLN:HG2	18:R:150:LEU:HD21	1.78	0.66
1:A:572:ASP:OD1	1:A:573:ARG:N	2.28	0.66
2:B:416:TYR:CE1	18:R:151:GLN:CB	2.78	0.66
3:C:231:PRO:HB3	3:C:275:VAL:HG22	1.77	0.66
13:M:253:GLU:O	13:M:257:ASP:N	2.28	0.66
15:O:168:SER:HB3	15:O:279:SER:HB3	1.76	0.66
1:A:735:TYR:O	1:A:739:ASP:HB2	1.96	0.66
2:B:297:THR:HA	2:B:301:ALA:HB3	1.78	0.66
2:B:483:VAL:HG12	2:B:485:GLY:H	1.60	0.66
2:B:723:THR:HG23	2:B:724:LEU:H	1.61	0.66
2:B:1038:ARG:HE	2:B:1041:GLY:H	1.43	0.66
5:E:141:VAL:HG23	5:E:142:VAL:H	1.61	0.66
18:R:208:ARG:O	18:R:212:ASP:N	2.28	0.66
1:A:31:GLU:HG3	1:A:69:THR:HG21	1.77	0.66
1:A:183:PHE:CD2	1:A:184:ARG:HG3	2.31	0.66
2:B:762:TYR:O	2:B:764:GLY:N	2.29	0.66
5:E:101:GLN:O	5:E:104:ASN:ND2	2.29	0.66
16:P:190:THR:HA	16:P:215:TYR:CE1	2.31	0.66
10:J:8:PHE:CG	10:J:49:MET:HE1	2.31	0.65
18:R:639:GLU:HG3	18:R:642:ARG:HE	1.61	0.65
1:A:49:LYS:HG3	1:A:56:PRO:HD3	1.78	0.65
2:B:49:PRO:HG3	2:B:743:LEU:HD21	1.78	0.65
19:S:426:ILE:HA	19:S:429:TYR:HD2	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:LEU:HD12	1:A:228:LEU:C	2.17	0.65
1:A:274:MET:HA	1:A:280:SER:HB3	1.79	0.65
1:A:895:ASP:HB2	1:A:1411:VAL:HG12	1.79	0.65
1:A:1161:VAL:HG22	1:A:1275:LEU:HD13	1.77	0.65
1:A:1411:VAL:HG13	1:A:1412:SER:H	1.60	0.65
5:E:1:MET:HG3	5:E:3:GLN:H	1.60	0.65
18:R:209:MET:HA	18:R:212:ASP:HB2	1.78	0.65
19:S:432:LEU:O	19:S:476:LYS:NZ	2.29	0.65
2:B:542:THR:O	13:M:178:GLN:NE2	2.28	0.65
1:A:1256:VAL:O	1:A:1260:MET:HB2	1.96	0.65
2:B:763:SER:OG	2:B:764:GLY:N	2.30	0.65
5:E:18:THR:HG23	5:E:143:ASN:HB3	1.77	0.65
15:O:643:ARG:NH1	16:P:292:SER:OG	2.29	0.65
13:M:226:ARG:HG3	13:M:227:LEU:H	1.62	0.65
1:A:1026:ARG:NH2	8:H:129:TYR:OH	2.30	0.65
1:A:1038:GLU:HB3	1:A:1042:ILE:HD11	1.78	0.65
2:B:427:ASN:O	2:B:430:THR:N	2.29	0.65
18:R:12:PHE:HB3	18:R:23:LEU:HD11	1.78	0.65
1:A:541:LEU:HG	1:A:551:ILE:HD11	1.78	0.65
18:R:640:SER:OG	19:S:506:GLN:NE2	2.30	0.65
1:A:589:HIS:HA	11:K:104:ARG:HH21	1.62	0.65
15:O:338:ASP:HB3	15:O:341:GLU:HB3	1.79	0.65
2:B:242:LEU:HD12	2:B:256:VAL:HG21	1.78	0.65
2:B:901:ARG:HH11	3:C:93:GLN:NE2	1.94	0.65
7:G:104:ILE:HG23	7:G:105:PHE:H	1.61	0.65
15:O:316:LEU:O	15:O:320:GLU:N	2.29	0.65
7:G:104:ILE:HG12	7:G:105:PHE:CD2	2.31	0.64
15:O:91:VAL:O	15:O:95:LEU:HB3	1.95	0.64
1:A:234:ILE:O	1:A:234:ILE:HG23	1.96	0.64
1:A:425:ASN:OD1	1:A:426:VAL:N	2.29	0.64
2:B:49:PRO:O	2:B:53:LYS:N	2.30	0.64
2:B:552:ASN:ND2	2:B:565:ILE:O	2.29	0.64
2:B:587:PHE:CZ	2:B:607:ARG:CB	2.78	0.64
2:B:832:VAL:O	12:L:60:ARG:NH1	2.30	0.64
2:B:1028:LYS:HG2	2:B:1029:HIS:H	1.62	0.64
14:N:302:GLU:HB3	14:N:410:GLY:HA2	1.78	0.64
15:O:644:LEU:O	15:O:647:LEU:N	2.30	0.64
16:P:296:TYR:CD1	16:P:297:PHE:N	2.64	0.64
20:X:16:DA:H61	21:Y:55:DA:H61	1.44	0.64
1:A:153:ARG:HH11	15:O:339:LEU:HG	1.62	0.64
1:A:741:LEU:HD13	1:A:765:LYS:HD3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:77:ILE:HD13	2:B:98:ILE:HG12	1.79	0.64
2:B:426:SER:O	2:B:428:ASN:N	2.27	0.64
16:P:64:VAL:HB	16:P:71:LYS:HB2	1.78	0.64
1:A:599:LYS:NZ	8:H:91:ASP:HA	2.12	0.64
2:B:235:THR:HG22	2:B:236:LYS:HG3	1.78	0.64
4:D:1:MET:HG3	4:D:2:LYS:H	1.61	0.64
15:O:648:TRP:NE1	15:O:652:GLN:OE1	2.30	0.64
14:N:395:ILE:HD12	14:N:411:ARG:HA	1.80	0.64
1:A:746:ASN:OD1	1:A:747:LYS:N	2.31	0.64
2:B:723:THR:HA	2:B:790:LYS:HG2	1.80	0.64
15:O:128:HIS:HE1	15:O:652:GLN:HE22	1.44	0.64
18:R:131:TYR:OH	18:R:135:ARG:NH1	2.30	0.64
18:R:513:PRO:O	18:R:515:LEU:N	2.30	0.64
18:R:636:LEU:HD13	19:S:502:LEU:HD21	1.80	0.64
1:A:353:PHE:O	1:A:356:ARG:HG2	1.97	0.64
1:A:843:GLN:H	1:A:847:PHE:HB3	1.63	0.64
5:E:80:VAL:HG23	5:E:109:ILE:HD11	1.80	0.64
14:N:287:HIS:CD2	14:N:384:LYS:HE2	2.31	0.64
1:A:1451:LEU:O	4:D:111:ASN:ND2	2.30	0.64
2:B:131:VAL:HG23	2:B:133:ILE:HD11	1.78	0.64
2:B:416:TYR:O	2:B:418:ALA:N	2.30	0.64
2:B:613:ILE:HA	2:B:646:VAL:HG12	1.80	0.64
1:A:1384:LEU:HB2	1:A:1413:GLU:OE1	1.98	0.64
2:B:932:PRO:HG2	2:B:940:PRO:HG3	1.78	0.64
16:P:21:GLN:O	16:P:26:GLY:N	2.30	0.64
18:R:464:LYS:NZ	18:R:605:VAL:O	2.25	0.64
18:R:514:GLU:OE1	18:R:514:GLU:HA	1.97	0.64
19:S:413:ARG:NH1	20:X:12:DT:OP2	2.30	0.64
1:A:602:TYR:HB2	3:C:23:PHE:O	1.98	0.64
2:B:801:HIS:ND1	18:R:137:GLU:OE2	2.29	0.64
1:A:332:VAL:HG13	1:A:333:ASN:H	1.62	0.63
1:A:489:TYR:CE1	1:A:532:ILE:HG12	2.33	0.63
1:A:873:VAL:HG21	2:B:487:ARG:HG2	1.78	0.63
18:R:463:ARG:NH1	18:R:598:ASP:O	2.29	0.63
18:R:619:ALA:O	18:R:623:LYS:HB3	1.98	0.63
1:A:892:SER:O	1:A:1380:ARG:NH2	2.32	0.63
1:A:1395:HIS:O	1:A:1399:ALA:CB	2.46	0.63
2:B:55:LYS:HG2	2:B:59:LYS:HD3	1.80	0.63
2:B:202:LYS:HD3	2:B:222:SER:HB2	1.81	0.63
13:M:149:LYS:HB3	13:M:182:PHE:CE1	2.32	0.63
18:R:7:CYS:HB3	18:R:28:CYS:SG	2.39	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:485:ASN:OD1	18:R:486:ILE:N	2.31	0.63
1:A:33:GLU:HG3	1:A:83:HIS:NE2	2.13	0.63
1:A:100:ILE:O	1:A:104:GLN:CB	2.44	0.63
1:A:443:ASN:OD1	1:A:444:LEU:N	2.32	0.63
2:B:230:LYS:CE	2:B:334:HIS:CE1	2.81	0.63
13:M:95:ARG:HB3	13:M:101:PRO:HB3	1.81	0.63
1:A:373:VAL:HG12	1:A:374:ASP:H	1.62	0.63
1:A:476:ARG:CZ	1:A:510:ALA:HA	2.28	0.63
2:B:295:ILE:HG23	2:B:296:TYR:HD2	1.63	0.63
2:B:536:LEU:HD22	2:B:571:PHE:CD1	2.32	0.63
2:B:915:ARG:HD2	2:B:1023:TYR:HD2	1.61	0.63
2:B:1038:ARG:NH1	2:B:1050:PRO:HB3	2.13	0.63
3:C:86:PHE:HE1	12:L:64:LEU:HD12	1.64	0.63
7:G:45:CYS:SG	7:G:46:ILE:N	2.71	0.63
7:G:52:LEU:HD12	7:G:53:THR:HG22	1.79	0.63
1:A:493:ARG:HB2	1:A:499:ARG:HH21	1.62	0.63
1:A:276:ASP:O	1:A:277:SER:CB	2.47	0.63
7:G:83:GLU:H	7:G:150:ILE:H	1.47	0.63
13:M:112:TYR:HD1	13:M:119:TRP:NE1	1.96	0.63
15:O:326:ILE:HD12	15:O:653:MET:HB3	1.81	0.63
16:P:202:PRO:O	16:P:204:LYS:N	2.29	0.63
18:R:190:ASP:O	18:R:195:LYS:NZ	2.25	0.63
21:Y:20:DT:C7	21:Y:21:DT:C7	2.67	0.63
1:A:235:LYS:O	1:A:236:SER:CB	2.47	0.63
2:B:230:LYS:HE2	2:B:334:HIS:CE1	2.30	0.63
2:B:713:ILE:HG13	2:B:725:LEU:HD11	1.81	0.63
2:B:805:ILE:HG22	2:B:807:GLY:H	1.62	0.63
1:A:224:PRO:HD2	1:A:316:TRP:HH2	1.62	0.63
7:G:6:LYS:HA	7:G:72:PHE:O	1.99	0.63
7:G:112:GLN:HG2	7:G:115:LEU:HD13	1.81	0.63
16:P:45:LEU:HA	19:S:372:MET:HE2	1.79	0.63
16:P:106:TRP:CH2	16:P:108:LYS:HB3	2.32	0.63
18:R:419:GLU:O	18:R:428:VAL:HA	1.97	0.63
2:B:137:ARG:HG3	2:B:138:GLY:N	2.13	0.63
2:B:273:CYS:O	2:B:354:ARG:NH1	2.31	0.63
2:B:335:LEU:HD12	2:B:335:LEU:C	2.19	0.63
3:C:240:LYS:HB3	3:C:264:GLU:HB3	1.80	0.63
6:F:76:LYS:HD2	6:F:79:ARG:HH21	1.64	0.63
1:A:67:CYS:HB3	1:A:71:HIS:HA	1.80	0.62
1:A:153:ARG:HA	1:A:160:LEU:HA	1.81	0.62
1:A:261:LEU:HD12	1:A:262:PRO:HD2	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1225:ILE:H	1:A:1229:ARG:HE	1.46	0.62
2:B:930:ASP:O	2:B:931:MET:HG2	1.99	0.62
11:K:89:CYS:HA	11:K:104:ARG:O	1.99	0.62
15:O:102:ARG:NH2	15:O:282:ILE:O	2.31	0.62
1:A:86:LEU:HD21	1:A:319:LEU:HD21	1.81	0.62
2:B:201:SER:OG	2:B:376:ARG:NH1	2.32	0.62
18:R:195:LYS:O	18:R:199:VAL:N	2.26	0.62
2:B:626:HIS:HE1	2:B:640:PHE:CE1	2.18	0.62
2:B:1038:ARG:HB2	2:B:1058:GLY:HA3	1.81	0.62
5:E:185:ALA:O	5:E:189:GLY:N	2.32	0.62
1:A:1323:PHE:HA	1:A:1327:GLY:HA2	1.80	0.62
2:B:658:TYR:CE2	2:B:670:MET:HG2	2.35	0.62
3:C:95:GLU:HG3	3:C:96:VAL:H	1.64	0.62
15:O:285:ASP:OD1	15:O:286:ARG:N	2.32	0.62
15:O:519:GLU:HA	15:O:522:ILE:HB	1.81	0.62
7:G:96:GLY:HA3	7:G:111:PRO:HA	1.81	0.62
18:R:619:ALA:O	18:R:623:LYS:CB	2.47	0.62
1:A:41:ASP:OD2	1:A:50:ALA:N	2.31	0.62
1:A:128:ARG:NH2	1:A:240:GLU:OE2	2.32	0.62
1:A:1265:ARG:HH21	2:B:285:VAL:HG22	1.65	0.62
1:A:1448:PHE:CZ	4:D:14:TYR:CE2	2.88	0.62
2:B:279:TYR:HE1	2:B:358:MET:HA	1.65	0.62
2:B:299:GLN:HE22	13:M:190:ASN:HB2	1.63	0.62
2:B:698:ARG:HH21	2:B:952:ARG:HG2	1.65	0.62
5:E:32:GLN:HA	5:E:35:VAL:HG12	1.82	0.62
7:G:204:GLY:HA2	7:G:210:TRP:HB2	1.80	0.62
13:M:90:TYR:HB3	13:M:179:LEU:HB3	1.82	0.62
18:R:4:CYS:HB3	18:R:7:CYS:SG	2.40	0.62
1:A:921:LEU:HD23	1:A:932:PRO:HG3	1.82	0.62
1:A:1272:VAL:HG13	1:A:1273:LYS:H	1.64	0.62
1:A:1367:GLU:HG3	1:A:1369:LEU:HD23	1.81	0.62
2:B:612:LEU:HD13	2:B:672:HIS:HB3	1.81	0.62
18:R:455:GLU:HG2	18:R:588:THR:HG23	1.81	0.62
19:S:506:GLN:O	19:S:510:LYS:HB2	1.99	0.62
21:Y:20:DT:C5	21:Y:21:DT:C7	2.82	0.62
1:A:974:LEU:HD21	1:A:998:TYR:HB3	1.81	0.62
3:C:255:VAL:O	3:C:268:LYS:HB2	2.00	0.62
4:D:58:ILE:O	4:D:61:ASN:HB2	2.00	0.62
9:I:34:PRO:O	9:I:35:ILE:HG13	1.99	0.62
12:L:31:CYS:SG	12:L:34:CYS:HB2	2.39	0.62
2:B:415:GLU:O	2:B:416:TYR:O	2.18	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:767:ILE:HG22	2:B:768:GLU:N	2.15	0.62
15:O:455:SER:HA	15:O:458:LYS:HD3	1.81	0.62
16:P:128:LEU:HA	16:P:131:GLN:HB2	1.82	0.62
18:R:219:ARG:CD	18:R:514:GLU:HG3	2.26	0.62
2:B:901:ARG:HH11	3:C:93:GLN:HE22	1.46	0.61
1:A:520:HIS:HE1	2:B:1062:LEU:HD21	1.65	0.61
1:A:1163:LYS:HG3	1:A:1164:THR:H	1.64	0.61
1:A:1447:LEU:HD23	1:A:1450:SER:CB	2.28	0.61
2:B:137:ARG:HG2	2:B:141:ILE:HG21	1.81	0.61
2:B:566:ARG:HH22	14:N:282:LEU:HD23	1.63	0.61
2:B:1012:CYS:SG	3:C:293:ARG:NH2	2.69	0.61
15:O:495:VAL:O	15:O:495:VAL:HG23	2.00	0.61
16:P:62:LYS:HB2	16:P:73:GLN:O	2.00	0.61
1:A:378:ARG:HH11	1:A:518:ASN:HD21	1.48	0.61
1:A:395:PRO:HG2	1:A:398:VAL:HG22	1.81	0.61
1:A:577:THR:HG23	11:K:88:PHE:CD1	2.35	0.61
3:C:116:VAL:HB	3:C:209:ILE:HD11	1.82	0.61
18:R:116:PHE:CZ	18:R:120:ARG:NH1	2.68	0.61
18:R:419:GLU:HB2	18:R:429:ILE:HB	1.82	0.61
1:A:1048:VAL:HG11	1:A:1053:LYS:HG3	1.81	0.61
2:B:926:VAL:CG1	2:B:930:ASP:HB2	2.31	0.61
11:K:111:THR:CG2	11:K:112:THR:N	2.51	0.61
18:R:214:MET:O	18:R:258:ARG:NH1	2.29	0.61
21:Y:20:DT:H73	21:Y:21:DT:C7	2.29	0.61
1:A:225:LEU:O	1:A:228:LEU:HG	2.01	0.61
7:G:138:LEU:CD1	7:G:139:TYR:O	2.47	0.61
2:B:192:LYS:NZ	2:B:438:SER:O	2.27	0.61
2:B:1054:ARG:HG2	2:B:1055:SER:H	1.66	0.61
3:C:255:VAL:HG13	3:C:256:ILE:N	2.16	0.61
4:D:135:TYR:HA	4:D:141:CYS:SG	2.41	0.61
11:K:69:ASP:OD1	11:K:70:HIS:N	2.31	0.61
15:O:40:ARG:O	15:O:40:ARG:HG2	2.00	0.61
20:X:3:DT:C2'	20:X:4:DT:C7	2.70	0.61
1:A:11:LYS:HD3	2:B:1145:ASP:HA	1.83	0.61
1:A:429:GLY:O	1:A:465:HIS:ND1	2.30	0.61
2:B:126:SER:OG	2:B:151:ARG:HB3	2.01	0.61
2:B:137:ARG:NH2	2:B:419:LEU:CD2	2.64	0.61
2:B:524:ASP:OD2	2:B:588:ILE:HD11	2.00	0.61
2:B:786:GLU:OE2	3:C:93:GLN:HG3	2.01	0.61
2:B:1080:LEU:O	2:B:1084:MET:HB3	2.01	0.61
4:D:24:GLU:HG3	4:D:29:TRP:HA	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:115:TYR:HE1	8:H:124:ARG:HG3	1.65	0.61
14:N:287:HIS:HD2	14:N:384:LYS:HE2	1.64	0.61
1:A:141:LEU:HA	1:A:144:ILE:HG22	1.82	0.61
1:A:913:GLN:NE2	1:A:917:GLY:H	1.99	0.61
1:A:1202:ILE:HD13	1:A:1224:ILE:HB	1.82	0.61
15:O:171:VAL:O	15:O:175:LEU:HB3	2.00	0.61
18:R:219:ARG:N	21:Y:60:DA:OP1	2.30	0.61
21:Y:11:DG:H2'	21:Y:12:DG:C8	2.35	0.61
1:A:235:LYS:HE2	15:O:44:PRO:HG3	1.82	0.61
1:A:1384:LEU:O	1:A:1388:SER:N	2.34	0.61
11:K:95:HIS:HD2	11:K:96:PRO:HD2	1.66	0.61
18:R:289:SER:HB2	18:R:535:SER:HB2	1.81	0.61
5:E:9:ILE:HG22	5:E:53:PRO:HG3	1.82	0.60
19:S:387:ALA:O	19:S:391:ASN:N	2.30	0.60
1:A:373:VAL:HG12	1:A:374:ASP:N	2.16	0.60
18:R:467:ARG:HB3	18:R:610:LEU:HD13	1.82	0.60
20:X:54:DG:H2'	20:X:55:DA:C8	2.36	0.60
8:H:93:TYR:CD1	8:H:145:ARG:HD3	2.36	0.60
15:O:175:LEU:HD11	15:O:184:LYS:HB3	1.83	0.60
18:R:80:LEU:O	18:R:83:ALA:N	2.34	0.60
1:A:115:LEU:CD2	1:A:123:PHE:CE2	2.84	0.60
1:A:995:VAL:HG23	1:A:996:ASP:H	1.66	0.60
1:A:552:ALA:HB3	1:A:671:ASP:HB2	1.82	0.60
10:J:7:CYS:HA	10:J:49:MET:SD	2.41	0.60
15:O:91:VAL:O	15:O:95:LEU:CB	2.49	0.60
18:R:434:GLU:HA	18:R:436:LYS:H	1.66	0.60
2:B:129:ILE:HD11	2:B:152:MET:HB2	1.81	0.60
18:R:439:ALA:HA	18:R:450:THR:H	1.66	0.60
1:A:388:SER:OG	1:A:695:ASN:ND2	2.34	0.60
1:A:622:VAL:HA	1:A:685:TYR:CE2	2.37	0.60
13:M:121:ILE:N	13:M:148:LEU:O	2.34	0.60
14:N:366:HIS:HB3	14:N:370:LYS:HB2	1.84	0.60
18:R:516:PHE:CD1	18:R:517:PRO:HD2	2.37	0.60
1:A:1217:ILE:HG22	1:A:1218:GLN:H	1.67	0.60
2:B:210:ASP:OD1	2:B:211:GLU:N	2.34	0.60
4:D:1:MET:HG2	7:G:9:ASP:HA	1.84	0.60
4:D:125:ASN:OD1	4:D:126:GLN:N	2.30	0.60
9:I:8:CYS:SG	9:I:29:CYS:HB2	2.41	0.60
14:N:290:ILE:O	14:N:294:LEU:HB3	2.00	0.60
15:O:166:LEU:HB3	15:O:169:LEU:HD11	1.84	0.60
15:O:197:MET:HB2	15:O:286:ARG:HD2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:191:LEU:HD21	18:R:239:ARG:HE	1.67	0.60
1:A:376:SER:HB2	2:B:1060:LEU:HD12	1.83	0.60
8:H:101:ALA:HB2	8:H:116:TYR:HE1	1.66	0.60
15:O:184:LYS:HA	15:O:187:ILE:CG1	2.32	0.60
18:R:186:ALA:HA	18:R:189:LEU:HD12	1.83	0.60
18:R:546:ARG:HA	18:R:549:ILE:HD12	1.83	0.60
1:A:49:LYS:HD2	1:A:54:LEU:HB3	1.82	0.60
1:A:91:PHE:HD1	1:A:224:PRO:HB3	1.65	0.60
1:A:476:ARG:NH2	1:A:515:ASP:OD2	2.35	0.60
2:B:801:HIS:O	2:B:863:GLN:NE2	2.34	0.60
3:C:30:GLU:HG3	11:K:84:PRO:HG3	1.84	0.60
4:D:127:LEU:CD2	7:G:147:ARG:HD2	2.32	0.60
19:S:507:ASN:HA	19:S:510:LYS:HB3	1.84	0.60
1:A:1347:GLY:O	1:A:1348:MET:HG2	2.01	0.59
17:Q:54:LEU:O	17:Q:58:TYR:CB	2.50	0.59
1:A:204:VAL:HG23	15:O:516:LEU:HD12	1.84	0.59
1:A:599:LYS:CB	1:A:600:PRO:HD3	2.29	0.59
2:B:658:TYR:O	2:B:671:THR:OG1	2.21	0.59
16:P:236:THR:HG23	16:P:239:ASN:H	1.66	0.59
1:A:1028:MET:SD	1:A:1048:VAL:HG22	2.43	0.59
1:A:1382:SER:HB2	1:A:1385:GLN:HG2	1.83	0.59
3:C:19:ASP:O	3:C:29:ASN:ND2	2.35	0.59
3:C:195:LYS:HD2	10:J:57:ILE:HG21	1.84	0.59
3:C:209:ILE:HG13	3:C:210:LEU:H	1.67	0.59
5:E:21:GLU:OE2	5:E:143:ASN:ND2	2.36	0.59
5:E:87:SER:HA	5:E:115:ASN:HB3	1.83	0.59
2:B:316:LYS:CE	13:M:226:ARG:HE	2.16	0.59
2:B:417:ASP:HB3	2:B:419:LEU:CD2	2.32	0.59
13:M:80:GLY:HA3	13:M:261:LYS:HE2	1.83	0.59
15:O:364:ILE:HA	15:O:476:TYR:CZ	2.37	0.59
1:A:921:LEU:HA	1:A:1082:ARG:HA	1.85	0.59
1:A:1145:LEU:H	1:A:1292:GLU:HG2	1.68	0.59
15:O:339:LEU:O	15:O:343:LYS:NZ	2.36	0.59
16:P:14:ASN:HB3	16:P:51:ILE:HD13	1.84	0.59
18:R:470:GLN:OE1	18:R:602:LEU:HD22	2.02	0.59
21:Y:2:DC:H2''	21:Y:3:DT:H71	1.85	0.59
1:A:235:LYS:HB3	1:A:252:ARG:NE	2.17	0.59
2:B:811:VAL:HA	2:B:817:PRO:HA	1.84	0.59
3:C:134:LEU:HD23	3:C:167:LEU:HD23	1.84	0.59
13:M:92:ASN:ND2	13:M:148:LEU:HD21	2.18	0.59
14:N:287:HIS:O	14:N:291:LEU:CB	2.50	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:52:LEU:HD11	15:O:131:LEU:HD12	1.84	0.59
20:X:3:DT:H2''	20:X:4:DT:C5	2.38	0.59
20:X:25:DT:H2'	20:X:26:DT:H71	1.84	0.59
1:A:957:TYR:CE2	1:A:1035:PRO:HD3	2.38	0.59
2:B:500:ALA:O	2:B:700:THR:HA	2.02	0.59
8:H:47:PHE:HZ	8:H:146:ARG:HG3	1.67	0.59
15:O:75:SER:HB2	15:O:119:TYR:CD1	2.38	0.59
15:O:128:HIS:O	15:O:132:TYR:HD1	1.86	0.59
1:A:786:ASP:OD1	1:A:787:ASN:N	2.36	0.59
1:A:974:LEU:HD11	1:A:998:TYR:CD1	2.38	0.59
1:A:1161:VAL:HG13	1:A:1275:LEU:HB2	1.84	0.59
13:M:72:GLU:H	14:N:364:ARG:HE	1.48	0.59
1:A:32:VAL:HG11	1:A:57:LYS:HD2	1.84	0.59
1:A:235:LYS:CE	15:O:44:PRO:HG3	2.32	0.59
2:B:1002:ASP:N	2:B:1017:ILE:O	2.30	0.59
7:G:207:LEU:HD22	7:G:210:TRP:CD1	2.38	0.59
11:K:85:ASP:OD1	11:K:86:VAL:N	2.35	0.59
13:M:94:PRO:HB3	14:N:391:LEU:HA	1.83	0.59
16:P:53:GLN:NE2	19:S:363:GLN:HA	2.18	0.59
16:P:153:LEU:HB3	16:P:155:PRO:HD3	1.83	0.59
1:A:37:ARG:HG2	1:A:38:ASP:H	1.67	0.59
1:A:653:ILE:HD11	1:A:655:ARG:NH2	2.18	0.59
2:B:817:PRO:HG2	2:B:822:GLN:OE1	2.03	0.59
13:M:112:TYR:O	13:M:243:ILE:HG21	2.03	0.59
15:O:597:GLN:HA	15:O:600:SER:HB2	1.84	0.59
1:A:123:PHE:CD2	1:A:144:ILE:HD13	2.38	0.58
2:B:832:VAL:HG12	12:L:60:ARG:HD2	1.83	0.58
3:C:103:LEU:HD21	10:J:6:ARG:HG3	1.83	0.58
7:G:115:LEU:HG	7:G:130:TRP:HZ2	1.68	0.58
8:H:8:ASP:OD1	8:H:9:ILE:N	2.35	0.58
15:O:233:SER:O	15:O:236:LYS:HG2	2.03	0.58
15:O:480:TYR:O	15:O:484:MET:N	2.35	0.58
21:Y:23:DT:H2''	21:Y:24:DC:H6	1.68	0.58
3:C:19:ASP:HB2	3:C:29:ASN:HD21	1.68	0.58
5:E:153:HIS:CD2	5:E:198:ILE:HG12	2.38	0.58
7:G:83:GLU:O	7:G:149:ARG:HA	2.03	0.58
13:M:83:GLU:O	13:M:84:SER:HB2	2.02	0.58
16:P:75:VAL:HG21	16:P:80:ALA:HB2	1.84	0.58
16:P:135:LYS:NZ	16:P:153:LEU:O	2.34	0.58
18:R:219:ARG:HD3	18:R:514:GLU:HB3	1.84	0.58
18:R:469:ILE:O	18:R:473:GLY:N	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:THR:HA	1:A:102:ILE:HG22	1.85	0.58
1:A:598:MET:O	1:A:599:LYS:HB2	2.04	0.58
1:A:703:ARG:NH2	11:K:93:ILE:O	2.36	0.58
2:B:538:VAL:HG12	2:B:565:ILE:HB	1.85	0.58
2:B:802:THR:OG1	2:B:863:GLN:NE2	2.25	0.58
2:B:1040:ARG:HD3	18:R:35:ASN:HD21	1.69	0.58
3:C:20:PHE:CZ	3:C:23:PHE:HB3	2.37	0.58
15:O:141:ILE:HA	15:O:144:MET:HB2	1.85	0.58
15:O:186:THR:O	15:O:187:ILE:C	2.42	0.58
1:A:666:LYS:HG2	1:A:667:SER:H	1.66	0.58
2:B:926:VAL:HG12	2:B:930:ASP:HB2	1.85	0.58
13:M:89:GLN:HB3	14:N:394:VAL:HG22	1.84	0.58
15:O:51:GLU:O	15:O:55:ALA:N	2.30	0.58
1:A:27:VAL:HG11	15:O:37:LEU:HD13	1.85	0.58
1:A:339:GLY:O	1:A:342:ASN:HB3	2.04	0.58
1:A:702:ALA:HB1	2:B:764:GLY:HA3	1.84	0.58
1:A:1125:ARG:NH2	1:A:1317:ASN:HB3	2.18	0.58
7:G:9:ASP:OD1	7:G:10:LEU:N	2.35	0.58
9:I:33:PHE:CD1	9:I:34:PRO:HD2	2.37	0.58
15:O:581:LEU:O	15:O:585:MET:HB2	2.03	0.58
18:R:467:ARG:O	18:R:471:LYS:CB	2.51	0.58
1:A:1026:ARG:HH12	8:H:110:ASP:HA	1.68	0.58
2:B:961:LEU:HD12	2:B:1022:ILE:HD11	1.86	0.58
16:P:54:GLU:O	16:P:58:LYS:N	2.34	0.58
17:Q:64:THR:O	17:Q:68:GLY:N	2.37	0.58
1:A:418:GLU:O	1:A:421:VAL:HG12	2.03	0.58
1:A:436:ARG:HH11	1:A:459:GLY:HA3	1.69	0.58
1:A:599:LYS:O	1:A:601:TYR:N	2.32	0.58
13:M:85:LEU:CD2	13:M:86:HIS:O	2.51	0.58
15:O:134:GLY:HA2	15:O:137:ILE:HD12	1.85	0.58
1:A:108:LYS:HG2	1:A:180:HIS:CD2	2.38	0.58
1:A:600:PRO:O	1:A:601:TYR:HB2	2.04	0.58
1:A:1127:LYS:O	1:A:1131:ASN:HB2	2.04	0.58
1:A:1152:ARG:O	1:A:1156:VAL:N	2.33	0.58
1:A:1431:VAL:HG13	7:G:57:GLY:O	2.03	0.58
2:B:137:ARG:HG3	2:B:138:GLY:H	1.69	0.58
2:B:626:HIS:CE1	2:B:635:LEU:HD21	2.38	0.58
3:C:137:ASN:HA	3:C:202:ILE:O	2.03	0.58
7:G:96:GLY:HA2	7:G:112:GLN:HG3	1.84	0.58
1:A:413:ARG:NH1	1:A:456:LEU:O	2.37	0.58
2:B:166:ALA:HB1	2:B:170:LYS:HB2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:223:SER:N	2:B:335:LEU:HD21	2.19	0.58
3:C:275:VAL:HG21	3:C:293:ARG:HD3	1.86	0.58
18:R:470:GLN:NE2	18:R:476:ALA:O	2.37	0.58
1:A:174:ALA:HB2	15:O:557:ARG:HB3	1.86	0.57
1:A:1202:ILE:O	1:A:1205:ILE:HG13	2.04	0.57
4:D:14:TYR:CE1	4:D:15:GLU:HG2	2.38	0.57
6:F:135:ARG:NH1	7:G:58:GLN:HE21	2.02	0.57
7:G:149:ARG:NH1	7:G:151:GLU:OE1	2.31	0.57
18:R:523:MET:O	18:R:527:LYS:HA	2.04	0.57
1:A:123:PHE:O	1:A:127:LEU:HD13	2.04	0.57
1:A:308:SER:N	1:A:311:ASN:OD1	2.37	0.57
1:A:890:MET:O	1:A:894:GLU:N	2.36	0.57
2:B:763:SER:OG	2:B:765:TYR:N	2.37	0.57
2:B:1057:ASP:OD1	2:B:1058:GLY:N	2.36	0.57
4:D:128:PRO:O	4:D:129:ALA:C	2.41	0.57
10:J:1:MET:O	10:J:53:HIS:NE2	2.37	0.57
13:M:106:PHE:CD2	13:M:107:ILE:HB	2.39	0.57
15:O:36:SER:O	15:O:40:ARG:CB	2.42	0.57
16:P:190:THR:HA	16:P:215:TYR:CZ	2.39	0.57
2:B:223:SER:H	2:B:335:LEU:HD21	1.68	0.57
2:B:269:MET:O	2:B:273:CYS:HB3	2.03	0.57
2:B:1048:ARG:HD2	2:B:1123:TYR:CZ	2.39	0.57
13:M:86:HIS:HD2	13:M:175:ARG:O	1.88	0.57
15:O:90:SER:O	15:O:94:THR:N	2.35	0.57
16:P:31:PHE:O	16:P:71:LYS:HA	2.05	0.57
1:A:556:ASP:OD1	2:B:947:HIS:NE2	2.37	0.57
1:A:584:SER:O	1:A:586:GLY:N	2.36	0.57
2:B:378:GLU:OE2	2:B:382:GLN:HB2	2.04	0.57
15:O:132:TYR:CE2	15:O:645:LEU:HD21	2.39	0.57
15:O:195:CYS:SG	15:O:196:GLU:N	2.78	0.57
16:P:296:TYR:CZ	16:P:297:PHE:HD1	2.23	0.57
18:R:94:LEU:HD23	18:R:149:ARG:HH21	1.69	0.57
19:S:434:MET:HE3	19:S:479:PRO:HB3	1.85	0.57
1:A:482:ARG:HD3	1:A:544:PRO:HB3	1.85	0.57
2:B:314:ARG:O	2:B:317:LEU:HD23	2.05	0.57
2:B:416:TYR:O	2:B:417:ASP:C	2.41	0.57
13:M:117:HIS:HB2	13:M:119:TRP:HE1	1.68	0.57
15:O:307:VAL:HG13	15:O:308:THR:H	1.69	0.57
15:O:624:LEU:HA	15:O:627:LEU:HD12	1.84	0.57
18:R:271:SER:HB2	18:R:277:GLU:HG3	1.87	0.57
18:R:420:TYR:HB2	18:R:428:VAL:HG22	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:587:THR:O	18:R:590:THR:OG1	2.21	0.57
1:A:475:ASN:OD1	1:A:476:ARG:N	2.38	0.57
1:A:599:LYS:HB2	1:A:600:PRO:HD3	1.76	0.57
1:A:1396:LEU:HD13	2:B:1132:LEU:HD21	1.86	0.57
3:C:59:ILE:HD13	3:C:63:ILE:HD11	1.86	0.57
15:O:102:ARG:O	15:O:123:ASN:ND2	2.38	0.57
21:Y:53:DC:H2'	21:Y:54:DT:C5	2.39	0.57
2:B:738:THR:HG22	2:B:740:THR:H	1.69	0.57
5:E:26:ARG:HH22	5:E:189:GLY:HA3	1.69	0.57
16:P:62:LYS:O	16:P:72:PHE:HA	2.04	0.57
20:X:6:DA:H4'	20:X:7:DA:H5'	1.86	0.57
21:Y:42:DA:H1'	21:Y:43:DA:H5'	1.85	0.57
2:B:97:ASP:OD1	2:B:98:ILE:N	2.38	0.57
2:B:475:SER:HB3	2:B:510:LEU:HB3	1.86	0.57
2:B:961:LEU:HD11	2:B:1019:PHE:HA	1.87	0.57
15:O:128:HIS:CE1	15:O:652:GLN:HE22	2.23	0.57
15:O:171:VAL:O	15:O:175:LEU:CB	2.53	0.57
15:O:353:GLU:N	15:O:481:SER:HB2	2.20	0.57
18:R:388:GLY:HA3	18:R:576:SER:HB2	1.86	0.57
1:A:389:ILE:HG22	1:A:390:ASP:H	1.70	0.57
1:A:978:ASP:HB2	1:A:984:VAL:HB	1.87	0.57
1:A:1305:CYS:HB2	5:E:141:VAL:HG21	1.86	0.57
2:B:687:LEU:HA	2:B:741:ILE:HD11	1.87	0.57
2:B:998:TYR:CD1	3:C:281:ARG:HD2	2.40	0.57
13:M:96:LEU:HB2	13:M:101:PRO:HA	1.86	0.57
15:O:496:ILE:O	15:O:496:ILE:HG22	2.05	0.57
18:R:623:LYS:HE2	19:S:435:TRP:HD1	1.69	0.57
1:A:890:MET:O	1:A:893:LEU:N	2.38	0.57
2:B:325:GLU:HG3	2:B:328:ALA:HB3	1.86	0.57
2:B:780:ARG:HE	3:C:217:ALA:HB1	1.70	0.57
2:B:1002:ASP:OD1	2:B:1003:MET:N	2.37	0.57
7:G:55:GLU:N	7:G:55:GLU:OE1	2.38	0.57
13:M:255:PHE:O	13:M:258:THR:OG1	2.22	0.57
16:P:118:GLN:HE22	21:Y:41:DG:H3'	1.70	0.57
18:R:218:ARG:NH1	18:R:258:ARG:HB2	2.19	0.57
1:A:113:ILE:HB	1:A:238:ASP:OD2	2.05	0.56
2:B:613:ILE:HG13	2:B:675:ILE:HG22	1.85	0.56
2:B:758:ALA:HA	2:B:1019:PHE:CB	2.34	0.56
2:B:800:ASN:ND2	2:B:851:SER:O	2.37	0.56
9:I:32:GLU:CG	13:M:132:ASN:HB2	2.34	0.56
13:M:255:PHE:O	13:M:259:ILE:HG12	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:Y:49:DA:H5'	21:Y:49:DA:C8	2.39	0.56
1:A:167:ALA:HB1	15:O:557:ARG:HD3	1.88	0.56
1:A:1448:PHE:CE1	4:D:14:TYR:CD2	2.93	0.56
3:C:96:VAL:O	3:C:99:HIS:N	2.38	0.56
7:G:151:GLU:N	7:G:197:LEU:O	2.28	0.56
9:I:3:SER:HB2	9:I:12:LEU:HD12	1.87	0.56
13:M:251:THR:OG1	14:N:302:GLU:OE2	2.24	0.56
1:A:735:TYR:O	1:A:739:ASP:CB	2.54	0.56
1:A:1399:ALA:HA	1:A:1404:LYS:HE2	1.88	0.56
2:B:38:ILE:HG13	2:B:43:ASP:HB3	1.86	0.56
2:B:177:CYS:SG	2:B:714:ALA:HB1	2.45	0.56
2:B:593:ASN:OD1	2:B:594:SER:N	2.38	0.56
5:E:85:GLU:HG3	5:E:87:SER:H	1.70	0.56
7:G:203:ASP:HB3	7:G:211:TRP:HE1	1.69	0.56
15:O:220:GLU:HG2	15:O:221:LYS:H	1.70	0.56
15:O:370:LEU:HD22	15:O:453:ILE:HD11	1.87	0.56
19:S:430:LYS:O	19:S:434:MET:HG2	2.05	0.56
21:Y:51:DT:H2'	21:Y:52:DA:H8	1.70	0.56
1:A:327:ILE:O	1:A:354:CYS:HB2	2.06	0.56
2:B:281:ASP:OD1	2:B:282:ILE:N	2.38	0.56
2:B:541:ILE:HA	2:B:544:ILE:HD12	1.86	0.56
3:C:85:PHE:CE2	3:C:94:ASP:O	2.49	0.56
10:J:53:HIS:ND1	10:J:53:HIS:O	2.38	0.56
15:O:471:THR:OG1	15:O:477:TYR:HB3	2.06	0.56
16:P:216:SER:HB2	16:P:261:TYR:H	1.70	0.56
19:S:460:ASN:ND2	20:X:9:DA:OP2	2.38	0.56
1:A:133:ASP:OD1	1:A:134:ASN:N	2.36	0.56
1:A:1177:TYR:CE2	9:I:14:ILE:HG13	2.41	0.56
2:B:640:PHE:HB3	2:B:645:LEU:HB2	1.88	0.56
15:O:362:ASN:HD21	15:O:478:VAL:HG23	1.70	0.56
18:R:138:LYS:NZ	18:R:173:LEU:O	2.29	0.56
18:R:172:GLU:OE1	18:R:172:GLU:N	2.34	0.56
1:A:722:ASP:O	1:A:725:GLN:N	2.38	0.56
1:A:733:ILE:HD12	1:A:736:HIS:NE2	2.21	0.56
2:B:316:LYS:HZ3	13:M:226:ARG:NE	2.04	0.56
5:E:31:THR:HG22	5:E:34:GLU:HG2	1.88	0.56
7:G:2:PHE:N	7:G:76:VAL:O	2.38	0.56
13:M:107:ILE:HG21	13:M:124:PRO:HD3	1.86	0.56
14:N:361:GLY:HA3	14:N:374:LYS:O	2.05	0.56
15:O:183:MET:O	15:O:187:ILE:HG12	2.06	0.56
15:O:316:LEU:HA	15:O:319:THR:HG22	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:THR:O	1:A:325:MET:N	2.39	0.56
9:I:22:TYR:O	9:I:23:THR:C	2.42	0.56
15:O:288:MET:O	15:O:291:ARG:HG2	2.06	0.56
1:A:26:ILE:CD1	1:A:262:PRO:HG3	2.36	0.56
1:A:978:ASP:N	1:A:982:CYS:O	2.35	0.56
3:C:33:VAL:HG12	3:C:34:GLU:N	2.21	0.56
5:E:127:ILE:HG22	5:E:130:ALA:H	1.69	0.56
6:F:116:ASP:OD2	6:F:119:ARG:NH1	2.39	0.56
9:I:5:CYS:HB3	9:I:10:ASN:H	1.71	0.56
18:R:418:ALA:HA	18:R:429:ILE:O	2.06	0.56
2:B:334:HIS:HB2	2:B:345:LYS:NZ	2.21	0.56
9:I:29:CYS:HB3	13:M:183:PHE:CZ	2.41	0.56
13:M:86:HIS:CD2	13:M:175:ARG:HB2	2.40	0.56
15:O:137:ILE:O	15:O:140:ILE:HG12	2.06	0.56
16:P:269:LEU:HD22	16:P:296:TYR:OH	2.05	0.56
18:R:13:GLU:CD	18:R:26:LYS:HG3	2.26	0.56
21:Y:26:DT:H1'	21:Y:27:DG:C5	2.41	0.56
4:D:119:GLU:HA	4:D:122:GLN:HB3	1.88	0.56
7:G:122:THR:O	7:G:124:GLU:N	2.39	0.56
9:I:24:LEU:C	9:I:24:LEU:HD12	2.27	0.56
10:J:10:CYS:SG	10:J:43:ARG:NE	2.68	0.56
15:O:361:PHE:HB2	15:O:477:TYR:HE1	1.71	0.56
18:R:195:LYS:HA	18:R:198:VAL:HB	1.88	0.56
18:R:395:ASN:H	18:R:487:VAL:HB	1.71	0.56
18:R:519:LEU:HB3	18:R:532:ILE:HB	1.88	0.56
21:Y:17:DA:H2''	21:Y:18:DT:C5	2.41	0.56
1:A:409:THR:O	1:A:411:TYR:N	2.33	0.55
1:A:476:ARG:CD	1:A:508:TYR:HB3	2.36	0.55
1:A:723:LEU:O	1:A:727:LYS:CB	2.52	0.55
2:B:58:VAL:HG12	2:B:58:VAL:O	2.06	0.55
2:B:1105:GLY:O	2:B:1116:ILE:HD12	2.05	0.55
5:E:121:MET:HA	5:E:124:VAL:HB	1.88	0.55
5:E:176:PRO:HB2	5:E:212:ARG:HG2	1.88	0.55
15:O:553:ARG:HB3	15:O:562:ALA:HA	1.87	0.55
20:X:67:DA:H2''	20:X:68:DG:C8	2.42	0.55
1:A:1186:VAL:H	1:A:1230:ILE:HG12	1.70	0.55
2:B:775:LYS:HB2	2:B:927:LYS:HA	1.88	0.55
5:E:153:HIS:CE1	5:E:184:VAL:HG11	2.41	0.55
12:L:26:THR:HA	12:L:62:LYS:HE3	1.87	0.55
12:L:31:CYS:SG	12:L:48:CYS:CB	2.93	0.55
16:P:10:GLN:HB3	16:P:13:ASP:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:95:SER:HA	16:P:98:GLU:HG2	1.88	0.55
16:P:314:GLU:HB3	17:Q:37:PRO:HB3	1.88	0.55
1:A:1079:ARG:HG2	6:F:84:TYR:HE2	1.71	0.55
2:B:517:MET:SD	2:B:675:ILE:HD11	2.46	0.55
2:B:1079:LEU:O	2:B:1082:ARG:N	2.39	0.55
2:B:1106:TRP:NE1	7:G:163:PRO:HD3	2.22	0.55
14:N:364:ARG:HH11	14:N:365:VAL:H	1.54	0.55
18:R:219:ARG:HG2	21:Y:60:DA:OP1	2.05	0.55
18:R:485:ASN:ND2	20:X:15:DT:O4'	2.39	0.55
1:A:302:GLY:C	1:A:304:ASP:H	2.09	0.55
1:A:363:ARG:NH1	2:B:1131:GLU:OE2	2.39	0.55
1:A:919:ASP:OD2	1:A:921:LEU:HB2	2.07	0.55
2:B:767:ILE:O	2:B:945:ASN:ND2	2.39	0.55
8:H:99:GLY:HA3	8:H:118:PHE:CD1	2.42	0.55
13:M:253:GLU:HB2	13:M:257:ASP:HB2	1.88	0.55
14:N:286:ASP:O	14:N:289:HIS:N	2.39	0.55
1:A:235:LYS:HZ2	15:O:44:PRO:CB	1.88	0.55
1:A:252:ARG:HH21	15:O:44:PRO:HD2	1.70	0.55
1:A:937:ARG:HG3	1:A:938:SER:N	2.19	0.55
1:A:1173:VAL:HA	1:A:1186:VAL:HG12	1.88	0.55
2:B:68:PHE:HE1	2:B:385:SER:OG	1.86	0.55
2:B:762:TYR:OH	2:B:930:ASP:HB3	2.05	0.55
3:C:197:ARG:HG3	10:J:61:LEU:HD13	1.89	0.55
4:D:14:TYR:CE1	4:D:15:GLU:CG	2.89	0.55
6:F:101:ILE:HG21	6:F:120:ILE:HD11	1.88	0.55
12:L:27:LEU:HD11	12:L:37:LYS:HB2	1.89	0.55
15:O:353:GLU:HA	15:O:357:PRO:HG2	1.89	0.55
18:R:470:GLN:HG3	18:R:476:ALA:HB3	1.89	0.55
19:S:310:UNK:O	19:S:314:UNK:N	2.40	0.55
1:A:389:ILE:HG22	1:A:390:ASP:N	2.21	0.55
2:B:427:ASN:C	2:B:429:ILE:N	2.60	0.55
2:B:536:LEU:HD23	2:B:536:LEU:O	2.07	0.55
2:B:1038:ARG:CZ	2:B:1050:PRO:HB3	2.36	0.55
2:B:1088:ASP:OD2	2:B:1123:TYR:N	2.40	0.55
4:D:127:LEU:CD2	7:G:147:ARG:CD	2.85	0.55
4:D:130:ASN:HA	4:D:154:LEU:HD11	1.88	0.55
15:O:168:SER:HG	15:O:281:THR:HG1	1.54	0.55
16:P:90:GLU:HA	16:P:93:VAL:HB	1.88	0.55
18:R:468:ILE:O	18:R:472:ILE:N	2.39	0.55
19:S:399:GLU:O	19:S:400:ASN:C	2.43	0.55
1:A:818:ILE:HD11	1:A:824:PRO:HD2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:64:SER:HB3	2:B:381:GLY:HA3	1.89	0.55
3:C:127:THR:H	3:C:130:ASN:HB3	1.71	0.55
3:C:259:ASP:HB2	3:C:266:TYR:CD1	2.42	0.55
5:E:1:MET:HB3	5:E:4:GLU:HG2	1.88	0.55
6:F:135:ARG:HH12	7:G:58:GLN:HE21	1.54	0.55
18:R:106:GLN:O	18:R:109:LYS:HB3	2.07	0.55
18:R:610:LEU:HA	18:R:613:HIS:HB2	1.88	0.55
19:S:429:TYR:HA	19:S:432:LEU:HD12	1.88	0.55
1:A:673:LYS:O	1:A:676:SER:OG	2.23	0.55
2:B:821:HIS:NE2	2:B:824:LEU:HD12	2.21	0.55
2:B:926:VAL:HG12	2:B:927:LYS:H	1.71	0.55
3:C:31:TRP:CZ2	11:K:123:ASP:HB3	2.42	0.55
4:D:14:TYR:CD1	4:D:15:GLU:CG	2.87	0.55
5:E:112:TYR:N	5:E:135:PHE:O	2.27	0.55
15:O:80:VAL:HG21	15:O:87:ASP:HA	1.89	0.55
1:A:1221:ASP:OD1	1:A:1222:VAL:N	2.39	0.55
6:F:101:ILE:HD12	6:F:107:VAL:HG12	1.88	0.55
13:M:163:VAL:HG22	13:M:168:VAL:HG22	1.88	0.55
15:O:35:SER:CB	15:O:40:ARG:HH21	2.20	0.55
15:O:516:LEU:HA	15:O:566:PHE:O	2.06	0.55
1:A:716:ASP:CG	1:A:791:PRO:HD2	2.27	0.54
2:B:128:PRO:HA	2:B:151:ARG:HG2	1.87	0.54
2:B:525:GLU:HG3	2:B:528:PRO:HD2	1.90	0.54
2:B:778:ILE:HG13	2:B:906:PRO:HG2	1.89	0.54
9:I:24:LEU:HG	9:I:24:LEU:O	2.06	0.54
1:A:66:GLU:HB3	1:A:71:HIS:HB2	1.89	0.54
1:A:102:ILE:CD1	1:A:242:LEU:HD12	2.31	0.54
1:A:643:ASN:HB2	1:A:651:PHE:CZ	2.42	0.54
1:A:1120:THR:H	1:A:1138:THR:HG21	1.71	0.54
1:A:1130:ILE:HG23	1:A:1371:ILE:HG13	1.90	0.54
1:A:1448:PHE:CZ	4:D:11:LEU:HG	2.42	0.54
2:B:317:LEU:O	2:B:319:ILE:N	2.41	0.54
2:B:362:ASN:ND2	2:B:365:MET:SD	2.72	0.54
15:O:47:PHE:CE2	15:O:586:ALA:HB1	2.41	0.54
15:O:105:LYS:N	15:O:121:TYR:O	2.35	0.54
15:O:292:ARG:NH2	15:O:653:MET:O	2.39	0.54
15:O:581:LEU:HB2	15:O:648:TRP:CH2	2.42	0.54
18:R:274:LYS:H	19:S:277:UNK:H	1.56	0.54
19:S:523:ALA:HA	19:S:526:GLU:HB3	1.90	0.54
2:B:208:GLU:O	2:B:215:ILE:HA	2.06	0.54
2:B:252:PRO:HD2	2:B:255:ILE:HD12	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:587:PHE:CD2	2:B:604:ASP:O	2.61	0.54
2:B:592:SER:N	2:B:656:ASP:OD2	2.38	0.54
5:E:117:THR:HG23	5:E:120:ALA:N	2.23	0.54
16:P:203:LYS:HD2	16:P:206:VAL:HG23	1.89	0.54
18:R:105:PHE:O	18:R:108:TYR:HB3	2.07	0.54
1:A:44:LYS:HG3	1:A:45:ASP:H	1.72	0.54
1:A:916:TYR:CE1	1:A:1089:ILE:HG21	2.43	0.54
2:B:83:ILE:HG13	2:B:93:LEU:HB3	1.88	0.54
3:C:66:ALA:O	3:C:70:ILE:HG22	2.07	0.54
15:O:168:SER:OG	15:O:281:THR:OG1	2.25	0.54
16:P:45:LEU:HD21	19:S:366:LEU:HB3	1.90	0.54
1:A:1174:GLN:CB	1:A:1185:GLN:O	2.43	0.54
1:A:1448:PHE:CE1	4:D:14:TYR:HE2	2.25	0.54
2:B:60:GLN:H	2:B:60:GLN:CD	2.10	0.54
2:B:914:SER:C	2:B:916:HIS:H	2.10	0.54
3:C:31:TRP:CG	3:C:32:ASN:N	2.72	0.54
4:D:127:LEU:HD21	7:G:147:ARG:CD	2.37	0.54
1:A:38:ASP:O	1:A:40:PHE:N	2.36	0.54
1:A:120:LYS:HG3	1:A:241:LEU:CD1	2.37	0.54
2:B:167:ASP:O	2:B:169:SER:N	2.41	0.54
2:B:1003:MET:SD	3:C:293:ARG:NH2	2.80	0.54
2:B:1038:ARG:NE	2:B:1041:GLY:H	2.05	0.54
11:K:136:THR:HA	11:K:139:ILE:HG22	1.90	0.54
18:R:213:TRP:HD1	18:R:287:PRO:HD3	1.73	0.54
18:R:395:ASN:ND2	21:Y:54:DT:O2	2.40	0.54
21:Y:23:DT:H2'	21:Y:24:DC:H5'	1.90	0.54
1:A:949:ASN:OD1	1:A:950:GLN:N	2.40	0.54
1:A:1059:LEU:HD11	8:H:106:GLU:HB3	1.90	0.54
1:A:1160:ARG:HA	1:A:1273:LYS:HE3	1.88	0.54
2:B:556:TYR:HD2	2:B:600:HIS:CE1	2.26	0.54
8:H:81:PRO:HD2	11:K:108:TYR:OH	2.08	0.54
15:O:578:ARG:HE	15:O:652:GLN:HA	1.73	0.54
19:S:439:PHE:HD1	19:S:454:VAL:HG12	1.71	0.54
1:A:233:GLN:HE21	15:O:575:ASN:ND2	2.06	0.54
1:A:277:SER:HB3	1:A:278:PRO:HD2	1.88	0.54
1:A:408:VAL:O	1:A:458:ILE:O	2.26	0.54
1:A:528:ARG:O	1:A:531:ALA:N	2.34	0.54
1:A:1153:ALA:HA	1:A:1156:VAL:HB	1.90	0.54
2:B:141:ILE:HG23	2:B:142:ILE:N	2.21	0.54
2:B:476:GLN:HG2	2:B:477:PHE:H	1.73	0.54
2:B:769:ASP:OD2	2:B:952:ARG:NH2	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:152:ARG:HB3	7:G:197:LEU:HD11	1.90	0.54
13:M:117:HIS:HB2	13:M:119:TRP:NE1	2.23	0.54
13:M:135:LYS:HE3	13:M:140:TRP:HE1	1.73	0.54
15:O:73:ARG:CG	15:O:121:TYR:HE1	2.19	0.54
16:P:217:THR:HA	16:P:220:GLU:HB3	1.90	0.54
18:R:83:ALA:O	18:R:87:LEU:CD1	2.55	0.54
18:R:406:LEU:HD13	18:R:411:VAL:HG21	1.89	0.54
1:A:45:ASP:OD1	1:A:46:ARG:N	2.41	0.54
1:A:476:ARG:HH11	1:A:517:MET:HE2	1.73	0.54
2:B:554:GLY:HA2	2:B:564:SER:CA	2.38	0.54
2:B:565:ILE:HG12	2:B:566:ARG:N	2.22	0.54
3:C:75:VAL:HG23	3:C:221:PRO:HG3	1.89	0.54
3:C:227:TYR:HB3	3:C:300:PHE:CD1	2.43	0.54
4:D:64:ASN:ND2	7:G:102:LEU:HD22	2.23	0.54
7:G:121:TYR:HD2	7:G:127:ALA:O	1.90	0.54
13:M:93:ARG:HH21	13:M:105:PRO:HB3	1.73	0.54
16:P:55:LEU:HD22	16:P:60:LEU:HD12	1.90	0.54
16:P:63:LEU:HD11	16:P:70:LEU:HD13	1.89	0.54
1:A:407:LYS:HG2	1:A:461:VAL:HG22	1.90	0.54
1:A:416:LEU:HD11	1:A:464:ARG:HH21	1.72	0.54
1:A:501:ASN:O	1:A:504:VAL:HG22	2.07	0.54
1:A:931:GLN:O	1:A:933:VAL:N	2.35	0.54
1:A:1166:LEU:O	1:A:1170:ALA:N	2.41	0.54
2:B:347:LEU:HD13	2:B:541:ILE:HD11	1.89	0.54
5:E:31:THR:HG23	5:E:34:GLU:H	1.74	0.54
8:H:7:ASP:OD1	8:H:7:ASP:O	2.26	0.54
13:M:113:LYS:HG3	13:M:116:SER:O	2.08	0.54
15:O:347:ASP:OD1	15:O:348:GLU:N	2.41	0.54
15:O:581:LEU:HB2	15:O:648:TRP:CZ3	2.43	0.54
18:R:219:ARG:CA	18:R:514:GLU:HG2	2.36	0.54
1:A:573:ARG:NH2	11:K:87:GLU:OE1	2.40	0.53
1:A:599:LYS:HG2	8:H:96:VAL:HG22	1.90	0.53
2:B:55:LYS:CG	2:B:59:LYS:HD3	2.38	0.53
2:B:916:HIS:CD2	2:B:957:LYS:HB2	2.43	0.53
3:C:85:PHE:HE1	3:C:204:LEU:HD22	1.72	0.53
1:A:232:LYS:HD3	16:P:315:TRP:CH2	2.44	0.53
1:A:599:LYS:HZ1	8:H:91:ASP:HA	1.72	0.53
2:B:306:GLY:O	2:B:309:VAL:HG12	2.08	0.53
2:B:427:ASN:C	2:B:430:THR:H	2.12	0.53
2:B:1054:ARG:O	2:B:1055:SER:OG	2.25	0.53
7:G:45:CYS:HA	7:G:76:VAL:HA	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:96:ILE:HG22	18:R:141:HIS:CE1	2.43	0.53
20:X:66:DA:N1	21:Y:4:DT:N3	2.56	0.53
21:Y:10:DT:H2''	21:Y:11:DG:C8	2.43	0.53
1:A:92:HIS:CD2	1:A:258:TRP:HE1	2.26	0.53
1:A:1300:LEU:HD22	1:A:1316:THR:HG21	1.90	0.53
2:B:330:THR:HA	2:B:345:LYS:HE3	1.90	0.53
2:B:337:VAL:HG23	2:B:338:GLU:H	1.72	0.53
2:B:846:SER:OG	2:B:866:TYR:HB3	2.08	0.53
3:C:211:GLY:HA3	3:C:219:PHE:CE2	2.43	0.53
3:C:285:PHE:HA	3:C:288:LYS:NZ	2.23	0.53
4:D:14:TYR:CE1	4:D:15:GLU:CB	2.91	0.53
8:H:38:LEU:HD21	8:H:40:LEU:HB2	1.89	0.53
9:I:29:CYS:CB	13:M:183:PHE:CE2	2.88	0.53
13:M:159:TYR:HD1	13:M:172:PRO:HA	1.71	0.53
18:R:2:PRO:HG2	18:R:12:PHE:HE2	1.73	0.53
18:R:478:PHE:HB3	18:R:599:PRO:HA	1.90	0.53
1:A:196:ILE:O	1:A:200:GLU:HG3	2.09	0.53
1:A:599:LYS:CG	8:H:96:VAL:HG13	2.38	0.53
2:B:143:MET:CG	19:S:399:GLU:HB2	2.38	0.53
2:B:944:MET:HE1	2:B:957:LYS:HE2	1.90	0.53
3:C:1:MET:HB3	3:C:14:ASN:HD21	1.74	0.53
3:C:260:GLU:O	3:C:264:GLU:N	2.42	0.53
11:K:63:PHE:HD2	11:K:117:LEU:HD13	1.74	0.53
15:O:537:LEU:HD11	15:O:566:PHE:CE2	2.43	0.53
18:R:18:ASN:HD21	18:R:20:ASN:ND2	2.07	0.53
1:A:816:GLN:HG2	1:A:864:HIS:HA	1.91	0.53
2:B:328:ALA:O	2:B:332:ILE:HG23	2.08	0.53
2:B:395:PHE:HA	2:B:428:ASN:HD21	1.73	0.53
7:G:88:TRP:HA	7:G:146:ILE:HD12	1.90	0.53
13:M:88:PHE:HB2	14:N:395:ILE:CG2	2.38	0.53
16:P:215:TYR:OH	16:P:262:ARG:NE	2.42	0.53
1:A:1222:VAL:HA	1:A:1231:ALA:O	2.09	0.53
2:B:263:LEU:HD12	2:B:297:THR:HG22	1.91	0.53
5:E:88:VAL:HG23	5:E:117:THR:HG22	1.90	0.53
7:G:49:TYR:HB2	7:G:75:VAL:HG23	1.89	0.53
11:K:80:ILE:HG22	11:K:86:VAL:HG11	1.90	0.53
13:M:113:LYS:HE2	13:M:118:LEU:HB2	1.90	0.53
13:M:134:ASP:O	13:M:138:SER:N	2.42	0.53
16:P:131:GLN:HB3	16:P:133:TYR:CD2	2.44	0.53
1:A:34:VAL:HG13	1:A:35:SER:H	1.72	0.53
1:A:574:ALA:HA	11:K:81:MET:HE3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:727:LEU:HD21	2:B:788:ARG:HE	1.74	0.53
2:B:1043:ARG:HH12	18:R:35:ASN:ND2	2.07	0.53
9:I:24:LEU:HD23	9:I:33:PHE:CG	2.44	0.53
18:R:215:PHE:HD1	18:R:223:ILE:HD13	1.72	0.53
18:R:219:ARG:HD3	18:R:514:GLU:CB	2.39	0.53
20:X:66:DA:H2'	20:X:67:DA:C8	2.44	0.53
1:A:557:PHE:HA	1:A:701:CYS:SG	2.48	0.53
1:A:600:PRO:O	1:A:601:TYR:CB	2.57	0.53
2:B:714:ALA:O	2:B:717:GLN:HB2	2.09	0.53
2:B:766:ASP:CG	2:B:945:ASN:HB2	2.28	0.53
8:H:76:THR:O	8:H:78:SER:N	2.42	0.53
13:M:251:THR:OG1	13:M:254:GLN:NE2	2.42	0.53
16:P:217:THR:HB	16:P:221:ILE:HB	1.91	0.53
1:A:252:ARG:CB	1:A:253:PRO:CD	2.70	0.53
1:A:986:ARG:H	1:A:989:LEU:HD11	1.73	0.53
1:A:1229:ARG:HH12	1:A:1231:ALA:HB2	1.74	0.53
2:B:657:SER:OG	2:B:658:TYR:N	2.42	0.53
3:C:197:ARG:HB3	3:C:198:PRO:HD2	1.90	0.53
18:R:136:LYS:HE2	18:R:173:LEU:HD13	1.91	0.53
21:Y:9:DA:H2'	21:Y:10:DT:H71	1.91	0.53
21:Y:44:DA:H1'	21:Y:45:DA:H5'	1.91	0.53
1:A:124:LEU:HB3	1:A:128:ARG:NH1	2.22	0.53
1:A:200:GLU:CA	15:O:516:LEU:HD21	2.35	0.53
1:A:957:TYR:HD1	1:A:1031:LEU:HG	1.74	0.53
1:A:1343:MET:HE1	1:A:1355:ILE:HD11	1.90	0.53
2:B:244:HIS:O	2:B:247:ILE:HG22	2.09	0.53
2:B:539:GLU:OE1	2:B:539:GLU:N	2.42	0.53
2:B:647:GLU:OE1	2:B:647:GLU:N	2.42	0.53
7:G:21:ASP:OD1	7:G:22:THR:N	2.42	0.53
15:O:254:ASN:HA	15:O:257:ASN:HB2	1.91	0.53
15:O:640:ARG:NH1	17:Q:44:ASN:OD1	2.41	0.53
21:Y:24:DC:H6	21:Y:24:DC:H5'	1.74	0.53
21:Y:25:DT:H2'	21:Y:26:DT:C4	2.43	0.53
1:A:926:MET:HA	1:A:932:PRO:HB3	1.90	0.52
2:B:135:TYR:CZ	2:B:419:LEU:CB	2.91	0.52
2:B:416:TYR:CZ	18:R:151:GLN:HB2	2.44	0.52
2:B:526:GLU:O	2:B:529:ILE:HG22	2.09	0.52
2:B:901:ARG:NH1	3:C:93:GLN:NE2	2.56	0.52
2:B:1147:PHE:HD2	7:G:10:LEU:HD11	1.73	0.52
4:D:130:ASN:OD1	4:D:133:HIS:ND1	2.42	0.52
15:O:457:LEU:HD21	15:O:476:TYR:CZ	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:504:VAL:O	1:A:507:PRO:HD2	2.09	0.52
1:A:516:GLU:OE2	2:B:1034:LYS:HD3	2.09	0.52
1:A:1022:LEU:HD22	1:A:1060:TYR:HE2	1.74	0.52
1:A:1408:VAL:HG23	1:A:1413:GLU:HG3	1.90	0.52
2:B:531:LYS:O	2:B:535:VAL:HG23	2.09	0.52
2:B:763:SER:HB2	2:B:765:TYR:HD1	1.75	0.52
2:B:832:VAL:CG1	12:L:60:ARG:HD2	2.37	0.52
12:L:29:TYR:HB3	12:L:58:LYS:HA	1.91	0.52
15:O:484:MET:HB2	15:O:485:PRO:HD3	1.91	0.52
16:P:90:GLU:O	16:P:94:TYR:N	2.42	0.52
18:R:213:TRP:CD1	18:R:285:ALA:HB1	2.44	0.52
18:R:218:ARG:HD3	21:Y:60:DA:OP1	2.09	0.52
18:R:397:VAL:HA	18:R:449:VAL:O	2.09	0.52
1:A:188:LYS:NZ	21:Y:7:DC:H3'	2.24	0.52
1:A:449:ARG:O	1:A:452:LEU:N	2.25	0.52
1:A:1448:PHE:CE2	4:D:11:LEU:HG	2.43	0.52
5:E:26:ARG:NH2	5:E:133:GLU:OE2	2.43	0.52
5:E:96:PHE:HZ	5:E:108:GLY:HA3	1.74	0.52
8:H:118:PHE:HB2	8:H:121:LEU:HB2	1.91	0.52
13:M:184:LYS:O	13:M:187:ASP:HB3	2.08	0.52
15:O:255:LYS:HB3	15:O:256:PRO:HD3	1.90	0.52
18:R:116:PHE:CE1	18:R:120:ARG:NH1	2.78	0.52
1:A:91:PHE:HE2	1:A:96:PHE:HD1	1.56	0.52
3:C:255:VAL:HG13	3:C:256:ILE:H	1.73	0.52
7:G:46:ILE:N	7:G:75:VAL:O	2.41	0.52
13:M:77:LYS:HA	14:N:360:VAL:HG22	1.90	0.52
16:P:106:TRP:HE1	16:P:145:ARG:HA	1.75	0.52
20:X:5:DC:N3	21:Y:65:DG:N1	2.40	0.52
5:E:23:VAL:HG22	5:E:28:TYR:HB2	1.90	0.52
10:J:21:TYR:OH	10:J:32:GLU:OE1	2.26	0.52
10:J:48:ARG:O	10:J:52:THR:N	2.22	0.52
13:M:135:LYS:HZ1	13:M:140:TRP:HZ2	1.55	0.52
15:O:73:ARG:HG2	15:O:121:TYR:OH	2.10	0.52
18:R:83:ALA:O	18:R:87:LEU:CB	2.56	0.52
1:A:517:MET:O	1:A:518:ASN:ND2	2.43	0.52
1:A:774:ARG:HH21	1:A:808:GLN:HE21	1.55	0.52
2:B:400:LYS:O	2:B:403:ILE:N	2.42	0.52
4:D:102:SER:HA	4:D:105:GLU:HB2	1.91	0.52
15:O:95:LEU:HD21	15:O:120:TYR:CZ	2.44	0.52
1:A:67:CYS:HB3	1:A:70:CYS:O	2.10	0.52
1:A:115:LEU:HD21	1:A:123:PHE:HE2	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:CYS:SG	1:A:155:LEU:N	2.83	0.52
1:A:235:LYS:CG	15:O:44:PRO:HG2	2.40	0.52
1:A:676:SER:HB2	1:A:679:TYR:HB3	1.91	0.52
1:A:830:ARG:NH2	1:A:833:PRO:O	2.43	0.52
2:B:658:TYR:CD2	2:B:670:MET:HG2	2.45	0.52
5:E:82:PHE:HE1	5:E:112:TYR:O	1.92	0.52
1:A:897:SER:HB2	1:A:1423:ILE:HG22	1.92	0.52
1:A:997:GLN:C	1:A:999:ASP:H	2.13	0.52
2:B:120:LEU:HD23	2:B:885:MET:SD	2.49	0.52
2:B:132:ASP:OD1	2:B:146:ASP:HA	2.10	0.52
2:B:588:ILE:O	2:B:588:ILE:HG22	2.10	0.52
3:C:255:VAL:HG22	3:C:256:ILE:H	1.75	0.52
14:N:395:ILE:HD11	14:N:408:LEU:HD21	1.91	0.52
15:O:544:ASN:HB3	15:O:576:PHE:CZ	2.44	0.52
16:P:221:ILE:O	16:P:225:ILE:HG12	2.09	0.52
1:A:1325:VAL:HG23	1:A:1326:LEU:H	1.74	0.52
5:E:77:SER:O	5:E:105:PHE:HB3	2.09	0.52
5:E:93:MET:SD	5:E:120:ALA:HA	2.50	0.52
7:G:87:GLY:HA3	7:G:148:PHE:HE1	1.74	0.52
15:O:634:GLU:O	15:O:637:VAL:HG12	2.10	0.52
16:P:55:LEU:HB3	16:P:60:LEU:HB2	1.91	0.52
18:R:140:HIS:ND1	18:R:140:HIS:O	2.43	0.52
18:R:191:LEU:HB2	18:R:195:LYS:HD3	1.91	0.52
20:X:4:DT:H2'	20:X:5:DC:C5'	2.32	0.52
20:X:24:DT:H2'	20:X:25:DT:C6	2.43	0.52
2:B:137:ARG:HH22	2:B:419:LEU:CD2	2.23	0.52
7:G:104:ILE:HG23	7:G:105:PHE:N	2.25	0.52
8:H:116:TYR:HB2	8:H:123:MET:HB3	1.91	0.52
15:O:507:LEU:O	15:O:511:ILE:HG12	2.09	0.52
16:P:184:ARG:O	16:P:187:SER:OG	2.21	0.52
20:X:61:DT:H2''	20:X:62:DG:C8	2.45	0.52
21:Y:12:DG:H2''	21:Y:13:DA:C8	2.45	0.52
1:A:716:ASP:CG	1:A:789:ASN:HB2	2.30	0.51
1:A:1171:PHE:HB3	1:A:1187:ARG:O	2.10	0.51
2:B:934:ASN:OD1	2:B:935:ASP:N	2.44	0.51
5:E:90:VAL:O	5:E:94:LYS:N	2.39	0.51
7:G:57:GLY:HA3	7:G:68:ILE:HG12	1.92	0.51
7:G:149:ARG:HD3	7:G:201:GLN:HE22	1.75	0.51
13:M:106:PHE:O	13:M:107:ILE:HG22	2.10	0.51
18:R:232:CYS:HB3	18:R:237:LEU:HD11	1.91	0.51
18:R:498:LEU:HD22	18:R:519:LEU:HD13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:X:17:DG:H1	21:Y:53:DC:H42	1.58	0.51
1:A:223:ASN:O	1:A:226:LYS:N	2.42	0.51
9:I:24:LEU:CD2	9:I:33:PHE:CD1	2.86	0.51
13:M:243:ILE:HG13	13:M:244:GLU:N	2.24	0.51
19:S:364:LEU:HA	19:S:375:ASP:HB3	1.92	0.51
19:S:421:THR:HG23	19:S:424:GLU:H	1.73	0.51
1:A:174:ALA:HB2	15:O:557:ARG:HB2	1.91	0.51
1:A:247:THR:HG23	1:A:249:PRO:HD3	1.91	0.51
2:B:400:LYS:O	2:B:403:ILE:HG22	2.10	0.51
2:B:587:PHE:CZ	2:B:607:ARG:CG	2.81	0.51
2:B:771:LEU:O	2:B:923:GLY:N	2.43	0.51
2:B:775:LYS:HA	2:B:778:ILE:HG22	1.92	0.51
3:C:278:GLU:N	3:C:278:GLU:OE1	2.43	0.51
13:M:151:VAL:HG12	13:M:152:GLY:H	1.74	0.51
20:X:17:DG:O6	21:Y:52:DA:N6	2.42	0.51
21:Y:24:DC:H5'	21:Y:24:DC:C6	2.45	0.51
1:A:385:PRO:HD2	2:B:765:TYR:CE2	2.46	0.51
1:A:477:GLN:NE2	1:A:515:ASP:OD2	2.43	0.51
1:A:1160:ARG:NH1	1:A:1307:ASP:OD2	2.44	0.51
1:A:1187:ARG:HA	1:A:1228:ASP:O	2.10	0.51
1:A:1316:THR:OG1	1:A:1317:ASN:N	2.41	0.51
1:A:1317:ASN:O	1:A:1318:HIS:ND1	2.44	0.51
1:A:1456:ALA:O	1:A:1460:ASN:ND2	2.43	0.51
2:B:81:GLN:N	2:B:81:GLN:OE1	2.43	0.51
2:B:295:ILE:HG12	2:B:296:TYR:H	1.75	0.51
2:B:316:LYS:NZ	13:M:226:ARG:HE	2.08	0.51
7:G:89:ILE:HG23	7:G:142:VAL:HG12	1.92	0.51
18:R:440:LEU:O	18:R:447:MET:HB2	2.10	0.51
1:A:179:ILE:HD12	15:O:557:ARG:NH2	2.26	0.51
1:A:1285:ILE:HA	1:A:1291:ARG:HG2	1.93	0.51
3:C:57:ILE:HD13	3:C:297:HIS:CD2	2.44	0.51
3:C:230:LEU:HD13	3:C:297:HIS:ND1	2.25	0.51
7:G:114:MET:HB2	7:G:199:SER:HB2	1.90	0.51
13:M:230:SER:O	13:M:234:HIS:N	2.44	0.51
15:O:242:LYS:O	15:O:246:LYS:N	2.32	0.51
15:O:356:THR:HB	15:O:357:PRO:HD3	1.92	0.51
18:R:485:ASN:HD21	18:R:542:GLY:H	1.57	0.51
1:A:204:VAL:CG2	15:O:516:LEU:HD12	2.40	0.51
1:A:247:THR:CG2	1:A:249:PRO:HD3	2.41	0.51
1:A:314:GLU:N	1:A:314:GLU:OE1	2.43	0.51
1:A:379:THR:HG21	1:A:497:THR:HA	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1318:HIS:CD2	1:A:1321:GLU:HB3	2.46	0.51
2:B:198:GLU:HA	2:B:377:LEU:HA	1.93	0.51
2:B:501:ASP:O	2:B:501:ASP:OD1	2.28	0.51
2:B:904:ARG:NH2	2:B:1033:ASP:OD1	2.44	0.51
2:B:929:GLU:OE1	3:C:69:ARG:NH2	2.44	0.51
2:B:1094:VAL:O	2:B:1116:ILE:HA	2.11	0.51
3:C:164:ALA:O	3:C:186:PRO:HG3	2.11	0.51
5:E:83:CYS:HG	5:E:92:THR:HG1	1.53	0.51
7:G:15:PRO:HA	7:G:18:PHE:CZ	2.45	0.51
8:H:98:TYR:HD1	8:H:141:TYR:CE2	2.29	0.51
14:N:290:ILE:HG21	14:N:384:LYS:HZ1	1.76	0.51
16:P:180:THR:O	16:P:184:ARG:HG2	2.10	0.51
16:P:187:SER:HA	16:P:263:VAL:HG21	1.91	0.51
19:S:425:MET:O	19:S:428:PHE:HB3	2.11	0.51
21:Y:59:DT:H2'	21:Y:60:DA:H8	1.75	0.51
1:A:595:PRO:HB3	1:A:604:TRP:CE2	2.46	0.51
1:A:788:TRP:HA	1:A:793:ILE:HD11	1.92	0.51
1:A:955:LEU:HD12	1:A:959:ILE:HG13	1.92	0.51
2:B:250:GLU:H	2:B:308:LYS:NZ	2.09	0.51
2:B:766:ASP:O	2:B:770:ALA:HB3	2.10	0.51
2:B:1105:GLY:O	2:B:1113:ALA:HA	2.11	0.51
3:C:55:ASP:OD2	3:C:297:HIS:NE2	2.42	0.51
5:E:136:ASN:HB3	5:E:139:ALA:HB2	1.93	0.51
15:O:159:ILE:O	15:O:163:VAL:HG23	2.10	0.51
15:O:312:TYR:HE1	15:O:468:LEU:HD11	1.74	0.51
16:P:117:HIS:HB2	16:P:120:VAL:HG22	1.93	0.51
16:P:235:LEU:HD21	16:P:239:ASN:HB3	1.93	0.51
18:R:467:ARG:O	18:R:471:LYS:HB2	2.11	0.51
1:A:116:SER:OG	1:A:117:GLU:OE1	2.23	0.51
1:A:273:MET:O	1:A:275:GLN:CG	2.59	0.51
1:A:559:THR:HG21	2:B:947:HIS:HE1	1.76	0.51
1:A:976:ARG:HD3	1:A:989:LEU:HD22	1.92	0.51
2:B:1106:TRP:NE1	7:G:161:LYS:O	2.44	0.51
4:D:17:LEU:HB2	4:D:66:LEU:HD23	1.92	0.51
4:D:133:HIS:CE1	7:G:211:TRP:HB3	2.46	0.51
5:E:112:TYR:CD1	5:E:116:ILE:HG12	2.45	0.51
6:F:135:ARG:NH2	7:G:56:GLU:OE1	2.44	0.51
15:O:47:PHE:CD2	15:O:586:ALA:HB1	2.46	0.51
15:O:222:HIS:CE1	15:O:244:ASN:HB3	2.45	0.51
16:P:31:PHE:HD2	16:P:72:PHE:HB2	1.76	0.51
18:R:147:SER:OG	18:R:154:VAL:HG22	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:427:LYS:HB2	19:S:446:TYR:OH	2.10	0.51
21:Y:3:DT:H1'	21:Y:4:DT:H5'	1.93	0.51
1:A:587:ILE:HA	11:K:53:ALA:HB2	1.93	0.51
1:A:633:PHE:CZ	1:A:643:ASN:HB3	2.46	0.51
1:A:653:ILE:HD11	1:A:655:ARG:HH21	1.75	0.51
1:A:1448:PHE:CZ	4:D:14:TYR:HE2	2.29	0.51
8:H:115:TYR:CE1	8:H:124:ARG:HG3	2.46	0.51
9:I:29:CYS:CB	13:M:183:PHE:HE2	2.23	0.51
1:A:625:ASN:HD21	1:A:941:HIS:HA	1.75	0.51
1:A:1454:GLU:HG2	1:A:1457:LEU:HD12	1.93	0.51
2:B:767:ILE:HG22	2:B:768:GLU:H	1.75	0.51
4:D:17:LEU:HD22	4:D:66:LEU:HB3	1.93	0.51
8:H:26:ILE:HG23	8:H:40:LEU:HB3	1.93	0.51
13:M:139:GLU:HB3	13:M:140:TRP:CE3	2.46	0.51
15:O:538:ALA:HA	15:O:541:ILE:HG22	1.92	0.51
1:A:502:GLU:CD	2:B:767:ILE:HG13	2.31	0.50
1:A:1299:GLY:C	1:A:1301:ARG:H	2.14	0.50
2:B:404:ASP:O	2:B:408:LYS:HG3	2.12	0.50
2:B:501:ASP:HB3	2:B:703:CYS:HB3	1.92	0.50
2:B:510:LEU:HD21	2:B:512:LYS:HE3	1.93	0.50
4:D:15:GLU:O	4:D:19:PHE:N	2.40	0.50
5:E:64:PRO:HD3	5:E:77:SER:HA	1.93	0.50
15:O:132:TYR:HD2	15:O:135:LEU:HD23	1.75	0.50
16:P:55:LEU:O	16:P:60:LEU:N	2.32	0.50
18:R:510:SER:O	18:R:520:ILE:HG13	2.10	0.50
1:A:185:TRP:O	1:A:186:VAL:HG22	2.10	0.50
1:A:408:VAL:O	1:A:408:VAL:HG13	2.11	0.50
1:A:624:ILE:HG22	1:A:625:ASN:N	2.26	0.50
1:A:911:ILE:HG23	5:E:176:PRO:HD3	1.93	0.50
1:A:1332:ARG:O	1:A:1335:ILE:HG22	2.11	0.50
2:B:94:LYS:HB3	2:B:134:GLU:HB3	1.93	0.50
2:B:997:ASN:OD1	2:B:998:TYR:N	2.44	0.50
15:O:133:SER:O	15:O:136:ILE:N	2.44	0.50
15:O:297:ILE:HD13	15:O:313:LYS:HG3	1.93	0.50
21:Y:50:DT:H2''	21:Y:51:DT:C6	2.46	0.50
1:A:103:LEU:HD11	1:A:222:LEU:HD22	1.93	0.50
1:A:111:SER:HB2	1:A:233:GLN:HG2	1.94	0.50
1:A:273:MET:O	1:A:275:GLN:HG2	2.12	0.50
1:A:913:GLN:HG2	1:A:915:THR:O	2.11	0.50
1:A:1449:GLU:O	4:D:117:LYS:NZ	2.45	0.50
2:B:137:ARG:NH2	2:B:419:LEU:HD23	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:611:PRO:HG3	2:B:648:TYR:HE1	1.77	0.50
2:B:756:THR:N	10:J:48:ARG:HH12	2.09	0.50
3:C:321:LEU:HD21	11:K:124:LEU:HD21	1.93	0.50
6:F:84:TYR:HD1	6:F:152:ILE:HG23	1.77	0.50
8:H:97:MET:HG3	8:H:142:LEU:HD23	1.93	0.50
11:K:99:ASN:O	11:K:100:LEU:HD12	2.11	0.50
13:M:93:ARG:NH2	13:M:105:PRO:HB3	2.26	0.50
14:N:387:GLU:OE2	14:N:415:LYS:NZ	2.34	0.50
15:O:74:LEU:HG	15:O:79:LEU:HD12	1.93	0.50
15:O:589:LEU:O	15:O:592:LYS:HB3	2.11	0.50
18:R:11:GLU:N	18:R:11:GLU:OE1	2.43	0.50
18:R:431:ARG:HA	18:R:438:THR:HA	1.94	0.50
18:R:467:ARG:HA	18:R:602:LEU:HD21	1.93	0.50
19:S:432:LEU:HB3	19:S:472:ALA:HB1	1.94	0.50
20:X:57:DT:H2 ⁺	20:X:58:DC:C6	2.47	0.50
7:G:141:ASP:OD1	7:G:142:VAL:N	2.43	0.50
13:M:148:LEU:HD23	13:M:179:LEU:HG	1.93	0.50
16:P:209:ALA:C	16:P:211:ASN:H	2.15	0.50
1:A:431:ASN:O	1:A:444:LEU:HD13	2.11	0.50
1:A:809:MET:O	1:A:851:SER:HB3	2.11	0.50
2:B:56:GLY:O	2:B:59:LYS:HG2	2.12	0.50
2:B:68:PHE:HD1	2:B:385:SER:OG	1.93	0.50
2:B:540:ASP:OD1	2:B:541:ILE:N	2.44	0.50
2:B:772:VAL:HG23	2:B:924:ILE:O	2.12	0.50
2:B:906:PRO:HB3	2:B:1026:LYS:HE3	1.93	0.50
5:E:20:LYS:O	5:E:23:VAL:HG12	2.12	0.50
6:F:104:ASN:OD1	6:F:104:ASN:O	2.30	0.50
15:O:163:VAL:HG22	15:O:169:LEU:HD22	1.93	0.50
15:O:634:GLU:HA	15:O:637:VAL:HG12	1.94	0.50
19:S:422:VAL:O	19:S:426:ILE:N	2.44	0.50
1:A:186:VAL:HG23	1:A:188:LYS:HG2	1.94	0.50
1:A:265:PRO:O	1:A:269:ARG:HG2	2.12	0.50
1:A:392:VAL:HG23	1:A:488:HIS:CG	2.47	0.50
1:A:1145:LEU:HB2	1:A:1292:GLU:CG	2.42	0.50
2:B:135:TYR:CZ	2:B:419:LEU:HB2	2.45	0.50
2:B:372:VAL:HG11	2:B:608:ILE:HD12	1.93	0.50
6:F:143:PHE:O	6:F:144:GLU:HB2	2.11	0.50
12:L:29:TYR:CB	12:L:58:LYS:HA	2.40	0.50
15:O:53:VAL:HG21	15:O:65:ILE:HD12	1.93	0.50
15:O:506:ARG:HB3	16:P:250:ASP:OD1	2.11	0.50
17:Q:1079:UNK:O	17:Q:1083:UNK:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:512:GLU:OE1	18:R:512:GLU:N	2.42	0.50
20:X:3:DT:O4	21:Y:66:DA:N6	2.45	0.50
1:A:33:GLU:HB3	1:A:35:SER:OG	2.11	0.50
1:A:445:ARG:HG2	18:R:24:VAL:HG11	1.93	0.50
1:A:1431:VAL:HG21	6:F:135:ARG:CZ	2.42	0.50
2:B:736:VAL:HG21	2:B:960:GLU:HG3	1.93	0.50
2:B:1009:THR:O	3:C:65:ASN:ND2	2.44	0.50
4:D:13:ASP:OD1	4:D:17:LEU:N	2.44	0.50
8:H:106:GLU:N	8:H:106:GLU:OE1	2.45	0.50
15:O:248:ASP:O	15:O:252:ILE:HG12	2.11	0.50
16:P:27:ILE:HB	16:P:31:PHE:HB2	1.94	0.50
16:P:172:ILE:O	16:P:175:ILE:HD11	2.12	0.50
18:R:428:VAL:O	18:R:441:ILE:HG22	2.12	0.50
21:Y:46:DA:C6	21:Y:47:DG:C6	3.00	0.50
1:A:835:PHE:CE2	1:A:844:SER:HA	2.47	0.50
1:A:1207:VAL:O	1:A:1211:ARG:HG2	2.12	0.50
2:B:732:GLN:HB3	10:J:52:THR:CG2	2.42	0.50
2:B:957:LYS:HZ2	2:B:1022:ILE:HD13	1.76	0.50
3:C:34:GLU:C	3:C:36:PHE:N	2.65	0.50
3:C:284:GLU:O	3:C:288:LYS:NZ	2.45	0.50
7:G:95:GLU:HG3	7:G:96:GLY:H	1.77	0.50
1:A:716:ASP:OD2	1:A:791:PRO:HD2	2.12	0.50
1:A:1123:VAL:N	1:A:1124:PRO:HD2	2.26	0.50
1:A:1305:CYS:SG	5:E:141:VAL:HG11	2.52	0.50
2:B:780:ARG:NH1	10:J:9:SER:O	2.44	0.50
13:M:87:VAL:HG23	14:N:395:ILE:O	2.12	0.50
16:P:106:TRP:HB2	16:P:147:ILE:HG22	1.94	0.50
16:P:241:ARG:O	16:P:245:GLU:HG2	2.12	0.50
18:R:621:LYS:O	18:R:625:ARG:N	2.43	0.50
1:A:120:LYS:CG	1:A:241:LEU:HD11	2.41	0.49
1:A:485:ILE:O	1:A:486:LEU:HD12	2.12	0.49
1:A:1064:GLU:O	1:A:1067:VAL:N	2.45	0.49
1:A:1186:VAL:HG22	1:A:1230:ILE:HG12	1.94	0.49
3:C:103:LEU:HD22	10:J:5:VAL:HG23	1.92	0.49
7:G:59:LEU:C	7:G:59:LEU:HD12	2.33	0.49
13:M:113:LYS:HG2	13:M:117:HIS:O	2.12	0.49
13:M:183:PHE:HB3	13:M:185:TYR:HB2	1.94	0.49
15:O:202:GLN:N	15:O:280:LEU:HG	2.26	0.49
18:R:144:ILE:HD12	18:R:154:VAL:HG21	1.94	0.49
1:A:424:PRO:HB3	1:A:431:ASN:HB3	1.94	0.49
1:A:518:ASN:ND2	2:B:1060:LEU:HD13	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:316:LYS:HE2	13:M:226:ARG:HE	1.76	0.49
2:B:949:PHE:HB2	2:B:950:PRO:HD3	1.94	0.49
4:D:122:GLN:NE2	7:G:83:GLU:HG3	2.27	0.49
13:M:88:PHE:HZ	13:M:119:TRP:HE3	1.59	0.49
13:M:104:HIS:CG	13:M:105:PRO:HD2	2.47	0.49
14:N:287:HIS:ND1	14:N:369:GLY:O	2.35	0.49
15:O:182:SER:OG	15:O:187:ILE:HG21	2.12	0.49
18:R:287:PRO:O	18:R:289:SER:N	2.43	0.49
18:R:417:ASN:HA	19:S:437:THR:HG22	1.94	0.49
18:R:467:ARG:HG2	18:R:606:ASP:OD1	2.12	0.49
1:A:533:ASN:HD21	6:F:90:ARG:HG2	1.76	0.49
1:A:1458:LYS:NZ	4:D:112:SER:HA	2.27	0.49
2:B:649:LEU:HD22	2:B:653:GLU:OE1	2.12	0.49
3:C:69:ARG:HE	11:K:71:THR:HG22	1.78	0.49
7:G:119:CYS:HB3	7:G:130:TRP:HD1	1.77	0.49
8:H:15:VAL:HG13	8:H:24:CYS:SG	2.52	0.49
15:O:37:LEU:HD23	15:O:40:ARG:CD	2.41	0.49
18:R:468:ILE:HG23	18:R:472:ILE:HD12	1.93	0.49
21:Y:41:DG:H1'	21:Y:42:DA:H5'	1.95	0.49
1:A:309:ILE:HG12	15:O:566:PHE:CE1	2.47	0.49
2:B:876:PRO:HG2	2:B:1032:LEU:HD21	1.94	0.49
3:C:211:GLY:HA3	3:C:219:PHE:CD2	2.46	0.49
16:P:36:LEU:O	16:P:40:MET:N	2.46	0.49
16:P:154:GLN:HG2	19:S:520:LYS:HE2	1.95	0.49
16:P:296:TYR:CG	16:P:297:PHE:N	2.81	0.49
18:R:396:ILE:N	18:R:452:ALA:O	2.41	0.49
18:R:626:ILE:HD11	19:S:487:GLU:HG3	1.93	0.49
21:Y:55:DA:H1'	21:Y:56:DA:C4	2.46	0.49
1:A:69:THR:OG1	1:A:80:HIS:NE2	2.46	0.49
1:A:115:LEU:HD21	1:A:123:PHE:CE2	2.47	0.49
1:A:235:LYS:CA	1:A:252:ARG:CD	2.72	0.49
1:A:373:VAL:HG11	2:B:1082:ARG:HD2	1.93	0.49
1:A:538:LYS:HB3	1:A:687:PRO:HB2	1.94	0.49
1:A:541:LEU:HG	1:A:551:ILE:CD1	2.43	0.49
2:B:545:ASP:OD2	2:B:547:ALA:HB3	2.12	0.49
2:B:798:TYR:CG	2:B:851:SER:HB2	2.48	0.49
2:B:957:LYS:NZ	2:B:1022:ILE:HG21	2.28	0.49
7:G:50:ASP:OD1	7:G:73:ARG:N	2.40	0.49
21:Y:28:DT:H2''	21:Y:29:DG:H8	1.78	0.49
1:A:273:MET:HB3	18:R:39:SER:OG	2.12	0.49
1:A:1165:LEU:HD22	1:A:1198:LEU:HD21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1408:VAL:HG23	1:A:1413:GLU:CG	2.42	0.49
2:B:296:TYR:HE1	13:M:182:PHE:HA	1.78	0.49
4:D:1:MET:HG3	4:D:2:LYS:N	2.27	0.49
8:H:76:THR:C	8:H:78:SER:H	2.16	0.49
12:L:40:LEU:HD11	12:L:44:ASP:HB3	1.95	0.49
13:M:159:TYR:CD1	13:M:172:PRO:HA	2.47	0.49
15:O:39:GLN:O	15:O:40:ARG:HB2	2.12	0.49
15:O:92:LYS:O	15:O:96:VAL:HG22	2.13	0.49
16:P:31:PHE:CD2	16:P:72:PHE:HB2	2.48	0.49
20:X:2:DT:H1'	20:X:3:DT:H5'	1.95	0.49
21:Y:65:DG:H4'	21:Y:66:DA:H5'	1.94	0.49
1:A:90:VAL:HG13	1:A:258:TRP:HB2	1.93	0.49
2:B:55:LYS:HZ2	2:B:59:LYS:HE3	1.75	0.49
2:B:316:LYS:HE2	13:M:226:ARG:HB2	1.94	0.49
18:R:144:ILE:O	18:R:147:SER:OG	2.27	0.49
18:R:220:PRO:HD3	18:R:514:GLU:CG	2.41	0.49
1:A:181:ASP:HB2	1:A:219:MET:HG3	1.94	0.49
1:A:226:LYS:HD3	15:O:547:GLU:HG3	1.95	0.49
1:A:610:PHE:O	1:A:613:LEU:HB3	2.12	0.49
1:A:1217:ILE:H	1:A:1217:ILE:HD12	1.78	0.49
2:B:232:TYR:HD1	2:B:242:LEU:HD23	1.76	0.49
2:B:944:MET:SD	2:B:1024:TYR:OH	2.71	0.49
4:D:126:GLN:HE21	7:G:85:VAL:HA	1.77	0.49
13:M:247:TRP:CH2	13:M:249:GLU:HB2	2.48	0.49
16:P:221:ILE:O	16:P:225:ILE:N	2.40	0.49
18:R:83:ALA:O	18:R:87:LEU:HD12	2.13	0.49
18:R:140:HIS:ND1	18:R:184:HIS:HB2	2.28	0.49
20:X:3:DT:H2''	20:X:4:DT:H73	1.86	0.49
1:A:381:ILE:HG22	1:A:382:SER:H	1.78	0.49
1:A:611:SER:OG	1:A:658:GLN:HA	2.13	0.49
1:A:1127:LYS:O	1:A:1131:ASN:CB	2.60	0.49
2:B:81:GLN:HG2	2:B:82:LEU:HG	1.94	0.49
2:B:265:ASP:O	2:B:267:GLU:N	2.46	0.49
2:B:464:ILE:HD11	2:B:746:TYR:CE1	2.37	0.49
2:B:762:TYR:O	2:B:763:SER:OG	2.31	0.49
2:B:1112:SER:OG	2:B:1113:ALA:N	2.46	0.49
5:E:26:ARG:HH12	5:E:189:GLY:HA3	1.78	0.49
5:E:79:TRP:NE1	5:E:81:GLU:HB2	2.28	0.49
10:J:16:ASP:CG	10:J:17:LYS:HG3	2.33	0.49
12:L:41:SER:HB3	12:L:44:ASP:HB2	1.93	0.49
13:M:122:ASP:HB3	13:M:145:VAL:CG2	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:158:GLU:OE1	15:O:161:GLN:NE2	2.46	0.49
15:O:467:PHE:CD2	15:O:468:LEU:HD13	2.34	0.49
15:O:468:LEU:HD12	15:O:483:LEU:HD21	1.95	0.49
15:O:567:ARG:HG2	15:O:568:CYS:H	1.78	0.49
16:P:308:GLU:OE1	16:P:308:GLU:N	2.46	0.49
18:R:212:ASP:O	18:R:214:MET:HE2	2.13	0.49
1:A:36:THR:HG21	1:A:51:ASN:ND2	2.28	0.49
1:A:601:TYR:CE1	3:C:23:PHE:HE2	2.31	0.49
1:A:1152:ARG:O	1:A:1155:ARG:N	2.46	0.49
3:C:103:LEU:HD21	10:J:6:ARG:CD	2.43	0.49
4:D:61:ASN:HB3	7:G:103:GLY:O	2.13	0.49
7:G:147:ARG:NH2	7:G:204:GLY:O	2.45	0.49
11:K:85:ASP:OD1	11:K:86:VAL:HG23	2.12	0.49
15:O:73:ARG:HG2	15:O:121:TYR:HE1	1.64	0.49
15:O:302:THR:O	16:P:265:LEU:HD11	2.12	0.49
16:P:142:PHE:CZ	20:X:30:DT:H4'	2.47	0.49
16:P:263:VAL:HG12	16:P:265:LEU:H	1.77	0.49
18:R:583:HIS:NE2	18:R:585:LEU:O	2.46	0.49
1:A:238:ASP:OD1	1:A:238:ASP:N	2.45	0.48
1:A:482:ARG:HB3	1:A:544:PRO:HG3	1.96	0.48
1:A:753:GLN:O	1:A:755:GLY:N	2.36	0.48
1:A:818:ILE:HG22	1:A:867:SER:HA	1.94	0.48
1:A:912:VAL:HG12	1:A:1364:TYR:CD1	2.48	0.48
1:A:1099:GLU:OE1	1:A:1099:GLU:N	2.38	0.48
1:A:1205:ILE:O	1:A:1209:ILE:HG12	2.13	0.48
1:A:1448:PHE:CZ	4:D:16:VAL:HG23	2.39	0.48
2:B:539:GLU:O	2:B:563:GLY:HA2	2.13	0.48
2:B:1147:PHE:HB2	7:G:10:LEU:HD11	1.95	0.48
5:E:46:TYR:CZ	5:E:58:MET:HA	2.48	0.48
13:M:154:GLU:N	13:M:154:GLU:OE1	2.45	0.48
13:M:241:ALA:O	13:M:242:ASN:CB	2.51	0.48
18:R:198:VAL:O	18:R:201:ASP:HB2	2.13	0.48
1:A:172:GLY:HA3	1:A:331:SER:HB2	1.95	0.48
1:A:330:ASP:CG	1:A:331:SER:H	2.12	0.48
1:A:472:VAL:HG22	1:A:521:VAL:HG12	1.94	0.48
1:A:577:THR:HG21	11:K:89:CYS:H	1.78	0.48
1:A:919:ASP:OD1	1:A:921:LEU:HD13	2.13	0.48
2:B:112:LEU:HD23	2:B:113:THR:N	2.28	0.48
2:B:296:TYR:HB2	2:B:300:GLN:NE2	2.24	0.48
2:B:416:TYR:CZ	18:R:151:GLN:CB	2.96	0.48
2:B:693:HIS:HB3	2:B:955:VAL:HG23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:855:PRO:HD2	18:R:106:GLN:CD	2.34	0.48
8:H:39:THR:HB	8:H:124:ARG:HB3	1.95	0.48
10:J:16:ASP:OD1	10:J:17:LYS:N	2.46	0.48
15:O:369:HIS:CG	15:O:370:LEU:H	2.30	0.48
15:O:472:LYS:HG2	15:O:473:PRO:HD2	1.94	0.48
18:R:213:TRP:CG	18:R:285:ALA:HB1	2.48	0.48
18:R:214:MET:SD	18:R:288:PRO:HD3	2.53	0.48
1:A:5:VAL:HG22	7:G:37:LYS:HB3	1.96	0.48
1:A:269:ARG:O	1:A:269:ARG:HG3	2.12	0.48
1:A:493:ARG:HB2	1:A:499:ARG:NH2	2.28	0.48
1:A:520:HIS:CE1	2:B:1062:LEU:HD21	2.45	0.48
2:B:481:ARG:NH2	21:Y:21:DT:H2'	2.28	0.48
2:B:616:SER:HB2	2:B:621:ARG:HH21	1.78	0.48
2:B:809:MET:HA	2:B:821:HIS:CD2	2.47	0.48
2:B:986:ASP:OD1	2:B:987:MET:N	2.46	0.48
3:C:70:ILE:HG13	3:C:74:GLU:HB2	1.95	0.48
8:H:3:ASN:HB2	8:H:61:SER:O	2.14	0.48
16:P:292:SER:OG	16:P:293:ILE:N	2.46	0.48
1:A:654:ILE:HG23	1:A:658:GLN:O	2.14	0.48
1:A:997:GLN:O	1:A:999:ASP:N	2.46	0.48
1:A:1128:GLU:OE1	1:A:1136:ILE:HG13	2.14	0.48
2:B:493:GLN:HG3	2:B:497:LEU:HB2	1.96	0.48
2:B:587:PHE:CD1	2:B:609:CYS:SG	3.06	0.48
2:B:623:LYS:O	2:B:625:ILE:N	2.41	0.48
2:B:926:VAL:HG12	2:B:927:LYS:N	2.28	0.48
10:J:55:ASP:OD1	10:J:57:ILE:HG22	2.13	0.48
13:M:76:LEU:HD23	14:N:363:ILE:HG13	1.95	0.48
13:M:92:ASN:HD21	13:M:148:LEU:HD21	1.76	0.48
14:N:365:VAL:HG13	14:N:370:LYS:O	2.13	0.48
1:A:173:SER:OG	15:O:557:ARG:O	2.31	0.48
1:A:233:GLN:NE2	15:O:575:ASN:ND2	2.62	0.48
1:A:607:LYS:O	1:A:611:SER:HB2	2.13	0.48
2:B:434:ASN:HA	2:B:437:ILE:HG22	1.94	0.48
3:C:70:ILE:HD11	3:C:320:ILE:CG2	2.44	0.48
3:C:122:ASP:OD1	3:C:123:ASP:N	2.46	0.48
10:J:57:ILE:O	10:J:61:LEU:HG	2.12	0.48
13:M:72:GLU:OE1	14:N:364:ARG:NE	2.38	0.48
15:O:578:ARG:O	15:O:581:LEU:HB3	2.13	0.48
16:P:177:SER:O	16:P:180:THR:HG22	2.14	0.48
16:P:254:GLU:HB3	16:P:262:ARG:HB2	1.94	0.48
1:A:308:SER:HA	15:O:534:ARG:CD	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:416:TYR:C	2:B:418:ALA:N	2.65	0.48
2:B:731:PRO:HB2	2:B:750:PRO:HG2	1.95	0.48
8:H:107:VAL:O	8:H:111:LEU:HB2	2.14	0.48
18:R:121:ARG:HB2	18:R:124:ASN:HD22	1.78	0.48
18:R:467:ARG:O	18:R:471:LYS:HB3	2.12	0.48
19:S:409:GLY:N	21:Y:61:DT:H5''	2.28	0.48
1:A:1411:VAL:HG13	1:A:1412:SER:N	2.26	0.48
2:B:77:ILE:HG21	2:B:98:ILE:HD11	1.95	0.48
2:B:177:CYS:SG	2:B:179:LEU:N	2.87	0.48
2:B:327:ILE:HD13	13:M:231:LEU:HD13	1.95	0.48
2:B:733:GLN:HG3	10:J:54:VAL:HG13	1.95	0.48
5:E:112:TYR:CE1	5:E:116:ILE:HG12	2.49	0.48
6:F:89:GLU:OE1	6:F:90:ARG:N	2.47	0.48
6:F:147:SER:HB3	6:F:150:GLU:HG3	1.96	0.48
8:H:128:ASN:CG	8:H:129:TYR:H	2.16	0.48
18:R:79:THR:HG21	20:X:26:DT:H5''	1.96	0.48
19:S:462:GLU:HA	19:S:469:ILE:HG13	1.95	0.48
21:Y:26:DT:C2	21:Y:27:DG:C6	3.00	0.48
1:A:1378:LYS:HG3	1:A:1379:MET:N	2.22	0.48
2:B:103:LYS:HB3	2:B:130:TYR:CE2	2.49	0.48
2:B:721:ILE:HG12	2:B:899:LEU:HD23	1.94	0.48
2:B:1126:LYS:O	2:B:1129:PHE:N	2.46	0.48
3:C:31:TRP:HH2	11:K:127:LEU:HG	1.79	0.48
3:C:283:GLU:O	3:C:285:PHE:N	2.47	0.48
4:D:65:TYR:CE1	7:G:101:LEU:HD11	2.48	0.48
13:M:122:ASP:HA	13:M:146:GLN:O	2.14	0.48
14:N:376:GLY:H	14:N:379:VAL:HG12	1.78	0.48
16:P:175:ILE:O	16:P:178:LEU:HG	2.13	0.48
18:R:7:CYS:SG	18:R:27:ALA:HB3	2.54	0.48
18:R:104:ALA:O	18:R:107:TRP:HB2	2.13	0.48
21:Y:65:DG:H1'	21:Y:66:DA:C8	2.49	0.48
1:A:742:ILE:HG12	1:A:840:LYS:HB2	1.95	0.48
1:A:903:THR:HA	1:A:914:PHE:O	2.14	0.48
1:A:1050:ASP:O	1:A:1053:LYS:N	2.45	0.48
1:A:1193:ILE:HG12	1:A:1200:LEU:HD11	1.96	0.48
1:A:1300:LEU:HB3	1:A:1321:GLU:OE2	2.14	0.48
1:A:1386:LEU:HB3	1:A:1395:HIS:CD2	2.49	0.48
1:A:1449:GLU:OE2	4:D:10:PHE:N	2.47	0.48
2:B:419:LEU:HD12	2:B:419:LEU:C	2.33	0.48
2:B:496:MET:CG	2:B:610:ARG:HD2	2.44	0.48
2:B:776:SER:HB3	3:C:217:ALA:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:276:SER:OG	3:C:278:GLU:OE2	2.22	0.48
6:F:81:THR:HG21	6:F:136:ARG:HH11	1.78	0.48
11:K:88:PHE:HB3	11:K:106:GLN:HB3	1.95	0.48
16:P:266:GLU:HA	16:P:268:ILE:HG13	1.96	0.48
18:R:499:GLU:OE1	18:R:499:GLU:N	2.42	0.48
1:A:287:VAL:O	1:A:290:THR:HG22	2.14	0.48
1:A:962:THR:O	1:A:965:GLU:HB3	2.14	0.48
2:B:1057:ASP:OD1	18:R:19:ALA:HB1	2.13	0.48
3:C:100:ARG:HH22	10:J:2:ILE:HG21	1.79	0.48
5:E:81:GLU:HB3	5:E:110:PHE:HB3	1.95	0.48
8:H:101:ALA:HB2	8:H:116:TYR:CE1	2.47	0.48
13:M:159:TYR:CG	13:M:170:LEU:HD21	2.49	0.48
13:M:182:PHE:C	13:M:183:PHE:CD1	2.86	0.48
16:P:269:LEU:C	16:P:269:LEU:HD12	2.34	0.48
18:R:213:TRP:CH2	18:R:497:ARG:HB3	2.49	0.48
19:S:424:GLU:OE2	19:S:449:ARG:NE	2.37	0.48
20:X:13:DA:P	20:X:13:DA:H8	2.37	0.48
1:A:186:VAL:HG22	1:A:189:LYS:HG2	1.96	0.47
1:A:316:TRP:O	1:A:319:LEU:HB3	2.14	0.47
1:A:675:HIS:HA	1:A:937:ARG:HH22	1.78	0.47
1:A:1125:ARG:HH22	1:A:1317:ASN:HB3	1.79	0.47
3:C:258:ILE:HD13	3:C:265:ALA:HB2	1.97	0.47
7:G:203:ASP:O	7:G:205:MET:HG2	2.14	0.47
11:K:63:PHE:CD2	11:K:117:LEU:HD13	2.48	0.47
15:O:39:GLN:HG3	15:O:47:PHE:CZ	2.49	0.47
15:O:262:ILE:O	15:O:274:VAL:HA	2.14	0.47
15:O:472:LYS:CG	15:O:473:PRO:HD2	2.44	0.47
1:A:385:PRO:HD2	2:B:765:TYR:CD2	2.48	0.47
1:A:386:ASN:ND2	1:A:703:ARG:HH21	2.12	0.47
1:A:502:GLU:H	1:A:502:GLU:HG3	1.49	0.47
1:A:568:ASP:OD1	8:H:22:LYS:HG2	2.14	0.47
1:A:1203:GLU:HA	1:A:1206:ALA:HB3	1.96	0.47
2:B:640:PHE:O	2:B:644:GLY:N	2.47	0.47
2:B:678:PHE:HB3	2:B:978:CYS:O	2.13	0.47
2:B:705:MET:O	2:B:708:GLN:N	2.25	0.47
2:B:884:VAL:HB	2:B:898:VAL:HG12	1.96	0.47
3:C:32:ASN:CG	3:C:33:VAL:H	2.17	0.47
5:E:26:ARG:HH22	5:E:189:GLY:CA	2.26	0.47
9:I:22:TYR:O	9:I:23:THR:CG2	2.62	0.47
13:M:247:TRP:HE1	14:N:408:LEU:HB2	1.79	0.47
15:O:326:ILE:HG21	15:O:653:MET:SD	2.54	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:MET:O	1:A:316:TRP:N	2.47	0.47
1:A:363:ARG:NH1	2:B:1127:LEU:HG	2.28	0.47
1:A:372:ARG:HD2	2:B:1050:PRO:O	2.14	0.47
1:A:427:HIS:O	1:A:429:GLY:N	2.48	0.47
2:B:632:ASP:OD1	2:B:633:GLY:N	2.48	0.47
2:B:834:MET:CE	12:L:63:ARG:HD2	2.44	0.47
3:C:59:ILE:HD12	3:C:60:ASP:O	2.14	0.47
15:O:51:GLU:HB2	15:O:590:PHE:CZ	2.49	0.47
18:R:122:SER:N	20:X:25:DT:OP1	2.44	0.47
18:R:414:HIS:HB2	18:R:472:ILE:HD13	1.95	0.47
19:S:425:MET:HG2	19:S:429:TYR:CE2	2.48	0.47
1:A:857:SER:N	1:A:860:GLU:OE2	2.36	0.47
1:A:1164:THR:HB	1:A:1271:VAL:HA	1.97	0.47
2:B:248:ALA:HB3	2:B:308:LYS:HG2	1.96	0.47
2:B:389:GLU:O	2:B:393:LYS:HB2	2.14	0.47
6:F:136:ARG:O	6:F:144:GLU:HB3	2.13	0.47
15:O:483:LEU:O	15:O:487:LEU:N	2.47	0.47
18:R:501:LEU:HA	18:R:563:PHE:CE2	2.48	0.47
1:A:185:TRP:C	1:A:187:GLY:H	2.17	0.47
1:A:224:PRO:HA	1:A:227:THR:HG22	1.95	0.47
1:A:323:VAL:O	1:A:326:TYR:HB3	2.14	0.47
1:A:633:PHE:HZ	1:A:643:ASN:HB3	1.79	0.47
1:A:675:HIS:HA	1:A:937:ARG:NH2	2.30	0.47
1:A:711:SER:OG	2:B:1016:TYR:O	2.30	0.47
1:A:856:LEU:HD13	2:B:692:HIS:O	2.15	0.47
1:A:998:TYR:HB2	1:A:1002:ARG:HH12	1.79	0.47
3:C:33:VAL:C	3:C:35:LYS:H	2.18	0.47
9:I:4:PHE:O	9:I:6:PRO:HD3	2.15	0.47
15:O:140:ILE:O	15:O:144:MET:N	2.47	0.47
15:O:203:ILE:HB	15:O:207:HIS:CD2	2.48	0.47
16:P:78:SER:O	16:P:82:LYS:HB2	2.15	0.47
18:R:273:GLN:HB2	19:S:277:UNK:N	2.30	0.47
18:R:397:VAL:HG21	20:X:16:DA:H2	1.80	0.47
1:A:188:LYS:HZ3	21:Y:7:DC:H3'	1.78	0.47
1:A:1302:ASP:N	1:A:1302:ASP:OD1	2.45	0.47
5:E:151:PRO:HB2	5:E:199:ILE:O	2.14	0.47
15:O:124:GLU:CG	15:O:125:GLU:H	2.27	0.47
15:O:292:ARG:NH1	15:O:650:VAL:HA	2.27	0.47
16:P:203:LYS:HB2	16:P:206:VAL:H	1.80	0.47
18:R:223:ILE:HD12	18:R:258:ARG:HH21	1.79	0.47
1:A:18:PHE:CE2	1:A:1383:VAL:HG21	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:ARG:CZ	1:A:278:PRO:HA	2.44	0.47
1:A:96:PHE:O	1:A:99:THR:N	2.47	0.47
1:A:436:ARG:N	1:A:460:ASP:OD1	2.35	0.47
1:A:624:ILE:HG22	1:A:625:ASN:H	1.78	0.47
1:A:858:PRO:HD2	2:B:661:LEU:HD13	1.96	0.47
2:B:217:GLN:CG	2:B:232:TYR:HB3	2.44	0.47
2:B:220:VAL:HG12	2:B:229:SER:HA	1.96	0.47
2:B:316:LYS:HZ3	13:M:226:ARG:CZ	2.28	0.47
2:B:615:VAL:HG12	2:B:620:SER:HA	1.97	0.47
2:B:622:VAL:HG12	2:B:624:ASP:H	1.80	0.47
2:B:724:LEU:HD12	2:B:789:ARG:NH1	2.30	0.47
2:B:774:ASN:O	2:B:778:ILE:HG22	2.15	0.47
4:D:126:GLN:HG3	4:D:127:LEU:HG	1.95	0.47
5:E:82:PHE:CD1	5:E:111:VAL:HB	2.45	0.47
7:G:152:ARG:O	7:G:197:LEU:HG	2.15	0.47
11:K:132:GLU:O	11:K:136:THR:HG22	2.15	0.47
13:M:72:GLU:OE1	13:M:72:GLU:N	2.48	0.47
13:M:184:LYS:HD2	13:M:184:LYS:HA	1.44	0.47
15:O:472:LYS:O	15:O:474:GLY:N	2.48	0.47
16:P:151:TYR:OH	18:R:647:ALA:O	2.31	0.47
18:R:140:HIS:CE1	18:R:184:HIS:HB2	2.50	0.47
18:R:491:ASP:HB2	18:R:537:LYS:HD3	1.96	0.47
18:R:500:GLY:HA2	18:R:503:PHE:HB3	1.96	0.47
1:A:168:ALA:HB3	1:A:174:ALA:HB3	1.97	0.47
1:A:1163:LYS:HG3	1:A:1164:THR:N	2.30	0.47
2:B:556:TYR:HD1	2:B:561:LEU:HA	1.80	0.47
2:B:957:LYS:NZ	2:B:1022:ILE:HD13	2.30	0.47
3:C:96:VAL:O	3:C:99:HIS:HB3	2.15	0.47
5:E:188:LEU:HD23	5:E:190:LEU:HD11	1.96	0.47
7:G:119:CYS:CB	7:G:128:TRP:HB3	2.41	0.47
8:H:105:GLU:CG	8:H:106:GLU:N	2.69	0.47
13:M:151:VAL:HG12	13:M:152:GLY:N	2.29	0.47
16:P:51:ILE:O	16:P:55:LEU:HG	2.14	0.47
16:P:110:ILE:O	16:P:114:THR:HG22	2.15	0.47
16:P:304:LYS:HG3	16:P:305:HIS:CD2	2.50	0.47
18:R:610:LEU:HA	18:R:613:HIS:CD2	2.49	0.47
1:A:38:ASP:OD1	1:A:38:ASP:N	2.41	0.47
1:A:46:ARG:HD3	1:A:278:PRO:HA	1.97	0.47
1:A:223:ASN:ND2	1:A:225:LEU:HB3	2.30	0.47
1:A:450:MET:O	1:A:453:ALA:N	2.48	0.47
1:A:818:ILE:HG21	1:A:866:ILE:HG22	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1278:ILE:HG23	1:A:1296:GLU:O	2.14	0.47
1:A:1451:LEU:HD23	4:D:107:MET:HB3	1.96	0.47
2:B:244:HIS:HE1	2:B:332:ILE:O	1.97	0.47
2:B:415:GLU:HG3	2:B:416:TYR:N	2.28	0.47
2:B:889:SER:OG	2:B:891:ASN:OD1	2.32	0.47
10:J:16:ASP:OD1	10:J:17:LYS:HG3	2.14	0.47
18:R:229:LEU:HB2	18:R:244:ILE:HD13	1.96	0.47
19:S:424:GLU:O	19:S:446:TYR:OH	2.25	0.47
21:Y:18:DT:C6	21:Y:18:DT:H5'	2.50	0.47
1:A:573:ARG:O	1:A:577:THR:OG1	2.22	0.47
1:A:903:THR:O	1:A:905:ARG:HG3	2.14	0.47
2:B:657:SER:OG	2:B:671:THR:OG1	2.33	0.47
2:B:961:LEU:HD21	2:B:1019:PHE:C	2.35	0.47
3:C:227:TYR:HB3	3:C:300:PHE:HD1	1.80	0.47
7:G:149:ARG:HB3	7:G:199:SER:O	2.15	0.47
15:O:197:MET:HG3	15:O:286:ARG:HB3	1.96	0.47
15:O:216:GLN:O	15:O:219:TYR:HB3	2.15	0.47
16:P:127:SER:O	16:P:131:GLN:N	2.37	0.47
16:P:269:LEU:CB	16:P:297:PHE:CE1	2.97	0.47
18:R:191:LEU:CD2	18:R:239:ARG:HE	2.28	0.47
1:A:329:SER:OG	1:A:330:ASP:N	2.48	0.46
1:A:800:LYS:HB3	2:B:951:SER:OG	2.16	0.46
1:A:1202:ILE:HG21	1:A:1224:ILE:HG21	1.97	0.46
2:B:45:TRP:CD1	2:B:739:LYS:HD3	2.50	0.46
2:B:206:ILE:HD13	2:B:374:ASN:HD21	1.81	0.46
2:B:398:ASP:C	2:B:425:HIS:HE1	2.19	0.46
2:B:500:ALA:HB3	2:B:685:ALA:HB2	1.97	0.46
2:B:901:ARG:HH22	3:C:94:ASP:HB2	1.79	0.46
7:G:95:GLU:HG3	7:G:96:GLY:N	2.30	0.46
8:H:95:TYR:O	8:H:144:ILE:HB	2.15	0.46
15:O:64:VAL:HG13	15:O:65:ILE:H	1.80	0.46
18:R:623:LYS:HE2	19:S:435:TRP:CD1	2.49	0.46
20:X:16:DA:N6	21:Y:55:DA:H61	2.09	0.46
1:A:608:GLN:O	1:A:611:SER:N	2.49	0.46
2:B:298:GLN:HG3	13:M:182:PHE:CD2	2.50	0.46
2:B:490:GLN:H	2:B:490:GLN:CD	2.19	0.46
2:B:1040:ARG:HD3	18:R:35:ASN:ND2	2.30	0.46
3:C:1:MET:HB3	3:C:14:ASN:ND2	2.30	0.46
3:C:32:ASN:OD1	3:C:33:VAL:N	2.45	0.46
4:D:127:LEU:HD21	7:G:147:ARG:NH1	2.30	0.46
5:E:96:PHE:CZ	5:E:108:GLY:HA3	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:125:GLU:O	7:G:140:PHE:O	2.34	0.46
12:L:25:ALA:HB2	12:L:37:LYS:NZ	2.30	0.46
13:M:77:LYS:HZ3	13:M:262:GLU:HB2	1.80	0.46
18:R:506:GLY:HA2	18:R:509:SER:O	2.15	0.46
1:A:891:LYS:NZ	2:B:1064:GLU:OE2	2.47	0.46
1:A:1145:LEU:HB2	1:A:1292:GLU:HG3	1.97	0.46
2:B:424:VAL:HG23	18:R:89:ALA:O	2.16	0.46
3:C:251:PHE:CD2	3:C:255:VAL:HG21	2.50	0.46
4:D:8:ASN:HB3	7:G:4:LEU:O	2.15	0.46
4:D:58:ILE:O	4:D:62:VAL:N	2.31	0.46
5:E:200:ARG:HD2	5:E:208:TYR:OH	2.14	0.46
8:H:99:GLY:HA3	8:H:118:PHE:HD1	1.80	0.46
12:L:29:TYR:CE1	12:L:56:LEU:HD13	2.50	0.46
13:M:89:GLN:NE2	13:M:178:GLN:HE22	2.06	0.46
15:O:264:THR:HA	15:O:272:ARG:HE	1.79	0.46
15:O:285:ASP:O	15:O:288:MET:HB3	2.14	0.46
15:O:482:LYS:O	15:O:486:VAL:HG22	2.16	0.46
21:Y:40:DA:H1'	21:Y:41:DG:H5'	1.97	0.46
1:A:378:ARG:HG3	1:A:517:MET:O	2.16	0.46
2:B:141:ILE:CG2	2:B:142:ILE:H	2.23	0.46
2:B:167:ASP:OD1	2:B:168:GLU:HG2	2.15	0.46
2:B:212:LYS:HG3	2:B:213:LYS:H	1.80	0.46
2:B:233:VAL:HG22	2:B:234:ILE:N	2.30	0.46
2:B:447:PHE:O	2:B:449:MET:HG2	2.15	0.46
2:B:817:PRO:CG	2:B:822:GLN:OE1	2.64	0.46
3:C:6:GLY:HA3	3:C:13:THR:HB	1.97	0.46
7:G:38:ILE:HB	7:G:44:LEU:HB3	1.97	0.46
7:G:121:TYR:CD2	7:G:127:ALA:O	2.68	0.46
7:G:190:LYS:C	7:G:192:PRO:HD3	2.35	0.46
15:O:41:THR:HG22	15:O:42:LEU:N	2.31	0.46
15:O:118:THR:O	15:O:119:TYR:CD2	2.68	0.46
15:O:468:LEU:HG	15:O:478:VAL:HG11	1.97	0.46
16:P:201:GLY:N	16:P:202:PRO:CD	2.78	0.46
19:S:413:ARG:NH1	20:X:11:DA:H3'	2.30	0.46
1:A:235:LYS:HB3	1:A:252:ARG:CZ	2.46	0.46
1:A:251:GLY:O	1:A:252:ARG:HB2	2.15	0.46
1:A:522:PRO:HA	2:B:1082:ARG:NH2	2.30	0.46
2:B:217:GLN:HG3	2:B:232:TYR:HB3	1.98	0.46
2:B:242:LEU:O	2:B:250:GLU:HA	2.16	0.46
15:O:364:ILE:HA	15:O:476:TYR:OH	2.15	0.46
19:S:428:PHE:O	19:S:432:LEU:HG	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:VAL:HG23	1:A:83:HIS:NE2	2.31	0.46
1:A:882:THR:O	1:A:885:MET:HB3	2.16	0.46
1:A:896:LEU:HD11	1:A:912:VAL:HG21	1.98	0.46
1:A:953:GLY:HA2	1:A:1063:SER:HB2	1.97	0.46
2:B:295:ILE:HG12	2:B:296:TYR:N	2.30	0.46
2:B:609:CYS:HB3	2:B:648:TYR:HB3	1.98	0.46
3:C:103:LEU:HD21	10:J:6:ARG:CG	2.45	0.46
4:D:146:ASP:O	4:D:150:ILE:HG12	2.16	0.46
5:E:143:ASN:OD1	5:E:143:ASN:N	2.49	0.46
7:G:4:LEU:HG	7:G:73:ARG:HB3	1.98	0.46
7:G:34:PHE:O	7:G:37:LYS:HB2	2.16	0.46
7:G:146:ILE:HG23	7:G:206:GLY:HA2	1.97	0.46
9:I:22:TYR:O	9:I:23:THR:O	2.34	0.46
16:P:218:THR:O	16:P:221:ILE:HG22	2.16	0.46
16:P:266:GLU:HB3	16:P:269:LEU:HD23	1.98	0.46
18:R:414:HIS:HD2	18:R:615:LEU:O	1.98	0.46
1:A:88:LEU:HB3	1:A:316:TRP:HE1	1.81	0.46
1:A:373:VAL:CG1	1:A:374:ASP:H	2.26	0.46
1:A:573:ARG:O	1:A:577:THR:CB	2.63	0.46
2:B:949:PHE:O	2:B:953:MET:N	2.48	0.46
2:B:1147:PHE:CZ	7:G:60:LYS:HB3	2.50	0.46
3:C:5:VAL:HG22	3:C:293:ARG:H	1.80	0.46
3:C:110:PRO:O	3:C:111:ASP:HB2	2.16	0.46
7:G:119:CYS:HB3	7:G:130:TRP:CD1	2.50	0.46
8:H:93:TYR:HB2	8:H:143:LEU:HD11	1.98	0.46
13:M:154:GLU:OE1	13:M:175:ARG:HG2	2.16	0.46
14:N:315:ALA:HB1	14:N:376:GLY:HA3	1.97	0.46
15:O:265:VAL:O	15:O:273:ILE:N	2.25	0.46
18:R:107:TRP:O	18:R:111:ALA:N	2.37	0.46
18:R:416:ARG:HG2	18:R:613:HIS:O	2.16	0.46
21:Y:23:DT:H2 ⁺	21:Y:24:DC:C6	2.49	0.46
1:A:124:LEU:HG	1:A:241:LEU:HD21	1.97	0.46
1:A:553:ALA:HB3	1:A:669:LEU:HD13	1.98	0.46
1:A:563:LEU:HD13	1:A:708:ARG:NH1	2.31	0.46
1:A:565:SER:OG	1:A:663:VAL:HA	2.16	0.46
1:A:572:ASP:O	1:A:576:LEU:N	2.35	0.46
1:A:893:LEU:HD13	1:A:1361:VAL:HG21	1.97	0.46
2:B:45:TRP:NE1	2:B:739:LYS:HD3	2.31	0.46
2:B:328:ALA:HA	2:B:331:VAL:O	2.15	0.46
2:B:583:LYS:HG2	2:B:584:VAL:HG13	1.98	0.46
5:E:190:LEU:HD23	5:E:214:CYS:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:7:SER:OG	9:I:8:CYS:N	2.45	0.46
9:I:32:GLU:HG2	13:M:132:ASN:HB2	1.98	0.46
15:O:250:ALA:O	15:O:253:ILE:HG13	2.15	0.46
15:O:295:GLN:HE22	15:O:650:VAL:HB	1.79	0.46
15:O:353:GLU:HB2	15:O:481:SER:HB2	1.98	0.46
15:O:499:THR:HG22	15:O:500:LEU:HD12	1.98	0.46
15:O:592:LYS:NZ	15:O:593:GLU:OE2	2.39	0.46
19:S:461:GLU:OE1	19:S:465:ARG:NH2	2.38	0.46
20:X:7:DA:H4'	20:X:8:DC:OP1	2.16	0.46
21:Y:55:DA:H1'	21:Y:56:DA:C5	2.50	0.46
1:A:38:ASP:C	1:A:40:PHE:H	2.20	0.46
1:A:307:ILE:HB	1:A:311:ASN:OD1	2.15	0.46
1:A:667:SER:OG	1:A:668:VAL:N	2.48	0.46
1:A:668:VAL:O	1:A:677:VAL:N	2.37	0.46
1:A:1286:ARG:N	1:A:1290:LYS:O	2.41	0.46
1:A:1330:ALA:HB2	5:E:150:VAL:HG22	1.98	0.46
2:B:416:TYR:CE1	18:R:151:GLN:HB3	2.51	0.46
2:B:541:ILE:HA	2:B:544:ILE:CD1	2.46	0.46
2:B:713:ILE:O	2:B:749:LEU:HD13	2.15	0.46
2:B:723:THR:HG23	2:B:724:LEU:N	2.29	0.46
2:B:778:ILE:CD1	2:B:906:PRO:HG2	2.45	0.46
2:B:1145:ASP:OD1	2:B:1145:ASP:N	2.49	0.46
5:E:95:THR:O	5:E:99:HIS:ND1	2.38	0.46
13:M:149:LYS:HE3	13:M:182:PHE:CZ	2.51	0.46
15:O:515:LYS:O	15:O:516:LEU:C	2.53	0.46
18:R:402:LEU:HA	18:R:477:LYS:O	2.16	0.46
18:R:478:PHE:O	18:R:599:PRO:HB3	2.16	0.46
1:A:412:ASN:HB3	1:A:416:LEU:HD13	1.97	0.46
1:A:682:LEU:HD13	1:A:687:PRO:HA	1.98	0.46
1:A:822:ARG:NH2	1:A:845:LYS:HB2	2.31	0.46
1:A:829:ASP:OD1	1:A:838:ASN:ND2	2.49	0.46
2:B:297:THR:CA	2:B:301:ALA:HB3	2.44	0.46
3:C:242:GLU:O	3:C:245:ARG:N	2.43	0.46
5:E:66:GLU:HG3	5:E:67:GLU:H	1.81	0.46
6:F:136:ARG:HB2	6:F:144:GLU:HB3	1.96	0.46
10:J:36:LEU:H	10:J:36:LEU:HD12	1.81	0.46
13:M:86:HIS:O	13:M:87:VAL:HB	2.16	0.46
13:M:230:SER:C	13:M:234:HIS:HD1	2.18	0.46
15:O:128:HIS:CE1	15:O:132:TYR:CE1	3.04	0.46
15:O:307:VAL:HG13	15:O:308:THR:N	2.31	0.46
15:O:324:PRO:HD3	15:O:353:GLU:CD	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:494:TYR:CD2	16:P:294:PHE:HE2	2.34	0.46
15:O:573:SER:HA	15:O:576:PHE:HE1	1.80	0.46
15:O:633:ARG:CZ	16:P:308:GLU:HG2	2.46	0.46
16:P:118:GLN:O	16:P:122:LEU:HG	2.16	0.46
16:P:194:GLY:O	16:P:196:LYS:NZ	2.47	0.46
18:R:155:TYR:O	18:R:159:ALA:N	2.37	0.46
18:R:218:ARG:C	18:R:514:GLU:HG2	2.36	0.46
18:R:402:LEU:HB3	18:R:476:ALA:HA	1.98	0.46
18:R:467:ARG:HB2	18:R:602:LEU:HD11	1.98	0.46
18:R:609:GLU:O	18:R:613:HIS:N	2.47	0.46
1:A:134:ASN:HD21	1:A:1404:LYS:NZ	2.14	0.45
2:B:143:MET:HG2	19:S:399:GLU:HB2	1.97	0.45
2:B:565:ILE:CG1	2:B:566:ARG:N	2.78	0.45
2:B:586:GLU:HG3	2:B:648:TYR:HD2	1.80	0.45
2:B:933:PHE:CE2	2:B:1005:TYR:HD2	2.34	0.45
4:D:27:HIS:NE2	4:D:53:PRO:HG3	2.31	0.45
15:O:623:GLU:O	15:O:627:LEU:HG	2.15	0.45
16:P:49:MET:HE1	19:S:364:LEU:HD21	1.97	0.45
18:R:617:GLU:HG2	18:R:621:LYS:HE2	1.98	0.45
1:A:559:THR:HG21	2:B:947:HIS:CE1	2.50	0.45
1:A:560:GLY:HA3	1:A:701:CYS:SG	2.56	0.45
2:B:325:GLU:O	2:B:328:ALA:N	2.49	0.45
2:B:589:SER:OG	2:B:653:GLU:HB2	2.15	0.45
2:B:1106:TRP:HE1	7:G:163:PRO:HD3	1.81	0.45
5:E:82:PHE:HZ	5:E:113:GLN:HB2	1.82	0.45
7:G:10:LEU:HA	7:G:69:ASN:HA	1.98	0.45
10:J:2:ILE:H	10:J:2:ILE:HD12	1.81	0.45
11:K:107:THR:HG23	11:K:108:TYR:O	2.17	0.45
13:M:89:GLN:CB	14:N:394:VAL:HG22	2.45	0.45
13:M:148:LEU:HB3	13:M:179:LEU:HD11	1.97	0.45
14:N:389:THR:HG23	14:N:390:PHE:H	1.81	0.45
15:O:190:LEU:HD11	15:O:199:TYR:CE1	2.51	0.45
20:X:7:DA:C5	20:X:8:DC:C4	3.04	0.45
1:A:46:ARG:HH21	2:B:852:ALA:CB	2.29	0.45
1:A:351:ARG:HD2	1:A:355:GLN:CD	2.37	0.45
1:A:539:ASN:OD1	1:A:687:PRO:HG3	2.16	0.45
1:A:570:PHE:CG	1:A:603:LEU:HD13	2.51	0.45
2:B:300:GLN:O	2:B:303:GLU:N	2.50	0.45
2:B:970:ASN:OD1	2:B:990:ILE:HD13	2.16	0.45
2:B:1005:TYR:HE1	2:B:1012:CYS:HG	1.64	0.45
5:E:124:VAL:HG22	5:E:132:ILE:HG12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:2:PHE:N	7:G:77:PHE:HA	2.32	0.45
8:H:13:SER:HB3	8:H:27:GLU:O	2.17	0.45
15:O:468:LEU:HG	15:O:478:VAL:CG1	2.46	0.45
18:R:290:PHE:CE2	18:R:495:PRO:HG3	2.52	0.45
20:X:3:DT:C2	20:X:4:DT:N3	2.84	0.45
1:A:508:TYR:O	1:A:509:ASN:OD1	2.34	0.45
1:A:955:LEU:O	1:A:959:ILE:HG13	2.17	0.45
1:A:1225:ILE:N	1:A:1229:ARG:HE	2.13	0.45
1:A:1332:ARG:O	1:A:1335:ILE:N	2.50	0.45
2:B:137:ARG:HG2	2:B:141:ILE:CG1	2.42	0.45
2:B:587:PHE:CE1	2:B:609:CYS:SG	3.09	0.45
2:B:1031:VAL:O	2:B:1034:LYS:N	2.47	0.45
5:E:55:ARG:HD2	5:E:82:PHE:CE2	2.51	0.45
7:G:158:VAL:C	7:G:160:PRO:HD3	2.37	0.45
11:K:60:SER:HA	11:K:106:GLN:HA	1.98	0.45
15:O:163:VAL:HG12	15:O:282:ILE:HD11	1.97	0.45
20:X:6:DA:C2	21:Y:65:DG:C2	3.04	0.45
1:A:99:THR:HA	1:A:102:ILE:CG2	2.47	0.45
1:A:415:LYS:O	1:A:419:LEU:N	2.49	0.45
1:A:880:ALA:O	21:Y:22:DA:H5'	2.17	0.45
1:A:884:TYR:CZ	1:A:888:ARG:HD3	2.51	0.45
2:B:193:VAL:HG21	2:B:458:LEU:HD12	1.98	0.45
2:B:724:LEU:HD21	2:B:726:TYR:CE2	2.51	0.45
2:B:842:TYR:HB2	2:B:881:ILE:HD11	1.98	0.45
2:B:932:PRO:HB2	2:B:1004:LEU:HD22	1.97	0.45
5:E:132:ILE:HD13	5:E:134:THR:HG23	1.98	0.45
14:N:286:ASP:CG	14:N:385:GLY:H	2.20	0.45
15:O:211:ILE:O	15:O:214:LEU:HG	2.16	0.45
15:O:484:MET:O	15:O:488:LYS:HG2	2.16	0.45
16:P:195:PHE:HB3	16:P:201:GLY:HA3	1.97	0.45
18:R:268:ALA:O	18:R:272:VAL:HB	2.17	0.45
20:X:28:DT:H2''	20:X:29:DC:C6	2.51	0.45
1:A:11:LYS:HG3	2:B:1117:ILE:HD13	1.97	0.45
1:A:89:PRO:CG	1:A:225:LEU:HA	2.46	0.45
1:A:114:LEU:HD22	1:A:161:ASN:HD21	1.82	0.45
1:A:205:LEU:HG	1:A:212:GLU:HA	1.97	0.45
2:B:832:VAL:HG13	2:B:882:ASP:O	2.17	0.45
2:B:841:ILE:HD13	2:B:872:ILE:HA	1.99	0.45
2:B:1147:PHE:CD2	7:G:10:LEU:HD11	2.52	0.45
5:E:90:VAL:O	5:E:94:LYS:HG2	2.17	0.45
13:M:85:LEU:HD23	13:M:86:HIS:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:155:ASN:OD1	13:M:155:ASN:N	2.49	0.45
14:N:361:GLY:HA3	14:N:375:ILE:HA	1.98	0.45
1:A:894:GLU:OE2	1:A:1412:SER:HB3	2.17	0.45
1:A:1202:ILE:O	1:A:1205:ILE:N	2.50	0.45
2:B:392:PHE:O	2:B:395:PHE:HB3	2.17	0.45
7:G:194:TYR:CZ	7:G:196:LEU:HD11	2.51	0.45
18:R:607:ASP:C	18:R:609:GLU:H	2.18	0.45
1:A:88:LEU:HD11	1:A:303:LEU:HD13	1.98	0.45
1:A:228:LEU:C	1:A:228:LEU:CD1	2.85	0.45
1:A:678:PHE:CE2	1:A:694:MET:HG2	2.52	0.45
1:A:856:LEU:HD23	1:A:861:PHE:HA	1.98	0.45
1:A:988:ASP:OD1	1:A:992:ALA:N	2.50	0.45
1:A:1125:ARG:HH12	1:A:1136:ILE:HD11	1.82	0.45
1:A:1217:ILE:HG22	1:A:1218:GLN:N	2.30	0.45
2:B:591:TYR:CD1	2:B:652:ASN:HB3	2.52	0.45
3:C:110:PRO:C	3:C:112:MET:H	2.20	0.45
3:C:157:TYR:HE2	3:C:197:ARG:NH1	2.15	0.45
5:E:100:ILE:HG21	5:E:127:ILE:HG13	1.99	0.45
9:I:13:LEU:HD21	9:I:27:ARG:HB2	1.99	0.45
9:I:22:TYR:C	9:I:23:THR:HG22	2.37	0.45
14:N:395:ILE:HD12	14:N:411:ARG:CA	2.45	0.45
15:O:185:TYR:O	15:O:189:SER:HA	2.17	0.45
16:P:175:ILE:HG22	16:P:179:LEU:HD13	1.98	0.45
1:A:89:PRO:CB	1:A:228:LEU:HD23	2.46	0.45
1:A:90:VAL:HG23	1:A:320:GLN:HB3	1.98	0.45
1:A:1023:ARG:HG2	1:A:1028:MET:HB2	1.97	0.45
3:C:25:LYS:HE2	8:H:82:PRO:HG2	1.98	0.45
3:C:88:ASN:OD1	3:C:89:THR:N	2.49	0.45
8:H:111:LEU:HA	8:H:127:GLY:O	2.17	0.45
9:I:20:GLY:C	9:I:22:TYR:H	2.21	0.45
12:L:56:LEU:HD12	12:L:56:LEU:O	2.17	0.45
13:M:84:SER:HB3	13:M:85:LEU:H	1.60	0.45
14:N:385:GLY:O	14:N:416:ILE:HG13	2.17	0.45
15:O:37:LEU:HA	15:O:40:ARG:HB3	1.99	0.45
15:O:579:GLN:HG3	15:O:580:ASN:N	2.32	0.45
15:O:583:TRP:CZ3	16:P:315:TRP:HB2	2.51	0.45
16:P:82:LYS:O	16:P:86:MET:HG2	2.17	0.45
16:P:107:SER:O	16:P:110:ILE:HG22	2.17	0.45
16:P:269:LEU:HA	16:P:297:PHE:CE2	2.52	0.45
1:A:545:LYS:HA	1:A:1354:HIS:HE1	1.81	0.45
1:A:591:ASP:HB2	8:H:77:ARG:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:801:GLY:N	2:B:951:SER:OG	2.49	0.45
1:A:858:PRO:HA	2:B:979:PHE:CZ	2.52	0.45
1:A:862:LEU:O	1:A:866:ILE:HG12	2.17	0.45
1:A:873:VAL:CG2	2:B:487:ARG:HG2	2.46	0.45
1:A:884:TYR:CE2	1:A:888:ARG:HD3	2.52	0.45
1:A:957:TYR:OH	1:A:1040:GLN:NE2	2.50	0.45
1:A:1235:PHE:HB2	1:A:1236:PRO:HD2	1.98	0.45
2:B:256:VAL:O	2:B:260:CYS:N	2.43	0.45
2:B:316:LYS:NZ	13:M:226:ARG:NE	2.65	0.45
2:B:612:LEU:HD21	2:B:649:LEU:HD12	2.00	0.45
3:C:133:VAL:HG11	3:C:172:GLN:HE22	1.82	0.45
3:C:245:ARG:O	3:C:248:GLN:HG2	2.17	0.45
5:E:43:LYS:O	5:E:47:CYS:HB2	2.16	0.45
6:F:103:MET:O	6:F:104:ASN:HB3	2.17	0.45
13:M:112:TYR:H	13:M:243:ILE:CG2	2.30	0.45
15:O:317:ARG:HA	15:O:320:GLU:CD	2.36	0.45
15:O:318:LEU:HD21	15:O:368:ARG:CZ	2.47	0.45
15:O:353:GLU:H	15:O:481:SER:CB	2.29	0.45
15:O:495:VAL:CG1	15:O:647:LEU:HD11	2.47	0.45
18:R:397:VAL:HG21	20:X:16:DA:C2	2.52	0.45
20:X:18:DT:H71	20:X:19:DA:H62	1.82	0.45
1:A:114:LEU:HD11	1:A:148:CYS:HB2	1.99	0.44
1:A:1165:LEU:O	1:A:1169:VAL:N	2.48	0.44
1:A:1224:ILE:HG12	1:A:1226:GLY:N	2.32	0.44
1:A:1365:LYS:HE3	1:A:1379:MET:HB2	1.98	0.44
2:B:55:LYS:HD2	2:B:519:HIS:CD2	2.52	0.44
2:B:100:VAL:HG12	2:B:129:ILE:HD13	1.98	0.44
2:B:378:GLU:OE1	2:B:383:LEU:HD13	2.17	0.44
2:B:715:TYR:HA	10:J:60:PHE:HE1	1.82	0.44
5:E:72:PHE:HE1	5:E:157:SER:HA	1.82	0.44
14:N:299:ASN:CG	14:N:301:PRO:HD3	2.37	0.44
15:O:352:VAL:N	15:O:481:SER:OG	2.50	0.44
16:P:222:LEU:HA	16:P:225:ILE:HB	2.00	0.44
17:Q:55:ALA:O	17:Q:58:TYR:HB3	2.17	0.44
18:R:401:THR:O	18:R:479:THR:OG1	2.31	0.44
21:Y:25:DT:H2'	21:Y:26:DT:C5	2.51	0.44
1:A:49:LYS:CD	1:A:54:LEU:HB3	2.47	0.44
1:A:155:LEU:HD12	1:A:156:HIS:N	2.31	0.44
1:A:204:VAL:O	1:A:208:ASN:N	2.27	0.44
2:B:311:THR:HG23	2:B:313:ARG:H	1.82	0.44
2:B:1007:GLY:HA2	3:C:68:ARG:NH2	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:11:LEU:H	7:G:3:ILE:HG22	1.82	0.44
4:D:24:GLU:HG2	4:D:30:ASP:CG	2.38	0.44
5:E:115:ASN:OD1	5:E:116:ILE:N	2.50	0.44
6:F:108:PHE:HE2	6:F:131:PRO:HG3	1.82	0.44
7:G:207:LEU:HB3	7:G:210:TRP:CE2	2.52	0.44
15:O:95:LEU:HD21	15:O:120:TYR:CE1	2.52	0.44
15:O:507:LEU:HD21	15:O:536:THR:HG23	1.99	0.44
15:O:650:VAL:HG13	15:O:651:PHE:H	1.82	0.44
16:P:102:ARG:O	16:P:155:PRO:HG2	2.17	0.44
16:P:106:TRP:O	16:P:109:THR:HG22	2.17	0.44
18:R:2:PRO:HG2	18:R:12:PHE:CE2	2.52	0.44
18:R:211:LYS:HE2	18:R:282:ASP:HB3	1.99	0.44
18:R:391:PRO:HA	18:R:490:CYS:HB3	1.99	0.44
21:Y:23:DT:C2	21:Y:24:DC:H5	2.35	0.44
1:A:14:LYS:HD3	2:B:1144:GLU:CD	2.37	0.44
1:A:66:GLU:HB3	1:A:71:HIS:CB	2.48	0.44
1:A:92:HIS:CD2	1:A:258:TRP:NE1	2.85	0.44
1:A:234:ILE:O	1:A:234:ILE:CG2	2.64	0.44
1:A:342:ASN:ND2	21:Y:38:DA:H2''	2.33	0.44
1:A:481:HIS:HA	1:A:1095:GLN:OE1	2.17	0.44
1:A:1199:GLU:HG2	5:E:3:GLN:HE22	1.81	0.44
2:B:467:LEU:HA	2:B:470:MET:HB3	1.98	0.44
2:B:884:VAL:HG22	12:L:58:LYS:HB3	1.99	0.44
2:B:991:LEU:O	2:B:994:GLN:N	2.50	0.44
3:C:77:SER:OG	3:C:221:PRO:HB3	2.17	0.44
21:Y:49:DA:H5''	21:Y:49:DA:H8	1.79	0.44
1:A:753:GLN:OE1	1:A:761:THR:HG23	2.17	0.44
1:A:1446:CYS:HB2	4:D:14:TYR:OH	2.17	0.44
2:B:410:PRO:HA	2:B:414:MET:SD	2.57	0.44
2:B:586:GLU:O	2:B:587:PHE:O	2.34	0.44
2:B:1138:ALA:O	2:B:1140:ARG:N	2.50	0.44
3:C:40:PHE:CD1	3:C:59:ILE:HG23	2.52	0.44
3:C:108:VAL:HB	3:C:184:VAL:HG12	1.99	0.44
5:E:42:PHE:CE1	5:E:46:TYR:HD2	2.36	0.44
5:E:200:ARG:HD2	5:E:208:TYR:CZ	2.52	0.44
8:H:6:PHE:HB3	8:H:59:ILE:HG13	1.99	0.44
15:O:273:ILE:HG23	15:O:274:VAL:O	2.17	0.44
15:O:506:ARG:NH2	15:O:527:LEU:O	2.50	0.44
15:O:507:LEU:HD12	15:O:508:SER:N	2.32	0.44
15:O:517:VAL:HG23	15:O:521:ILE:HD11	1.98	0.44
18:R:486:ILE:N	18:R:543:ALA:O	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:VAL:HG13	1:A:35:SER:N	2.32	0.44
1:A:363:ARG:O	1:A:367:ASN:HB3	2.16	0.44
1:A:624:ILE:N	1:A:657:SER:OG	2.48	0.44
2:B:123:MET:O	2:B:189:GLY:N	2.50	0.44
2:B:247:ILE:HG13	2:B:248:ALA:H	1.83	0.44
2:B:338:GLU:CD	2:B:339:ALA:H	2.20	0.44
2:B:369:ARG:HG3	2:B:369:ARG:O	2.17	0.44
2:B:493:GLN:CG	2:B:497:LEU:HB2	2.48	0.44
2:B:773:LEU:HD21	2:B:912:PHE:HE2	1.81	0.44
2:B:833:GLY:HA3	12:L:60:ARG:CZ	2.47	0.44
2:B:842:TYR:HD2	2:B:873:TYR:HB2	1.81	0.44
2:B:911:LYS:HD3	2:B:1029:HIS:HB2	1.99	0.44
5:E:94:LYS:O	5:E:98:ILE:HG12	2.17	0.44
9:I:24:LEU:O	9:I:33:PHE:HB2	2.18	0.44
11:K:127:LEU:O	11:K:130:VAL:N	2.50	0.44
13:M:132:ASN:OD1	13:M:134:ASP:HB2	2.17	0.44
14:N:286:ASP:OD2	14:N:384:LYS:HB3	2.16	0.44
15:O:32:MET:O	15:O:34:ILE:N	2.51	0.44
15:O:118:THR:O	15:O:119:TYR:CG	2.70	0.44
15:O:292:ARG:HG2	15:O:325:LYS:HD2	1.98	0.44
15:O:578:ARG:HH21	15:O:652:GLN:HA	1.81	0.44
15:O:620:LEU:HD23	15:O:623:GLU:HB2	2.00	0.44
15:O:650:VAL:HG13	15:O:651:PHE:N	2.32	0.44
18:R:251:ALA:HB3	18:R:254:THR:OG1	2.18	0.44
20:X:9:DA:C5	20:X:10:DT:C4	3.05	0.44
20:X:14:DT:H2'	20:X:15:DT:H5'	1.99	0.44
1:A:614:ILE:O	1:A:622:VAL:HG21	2.18	0.44
1:A:940:ASP:O	1:A:943:TYR:N	2.50	0.44
1:A:943:TYR:O	1:A:947:PHE:N	2.50	0.44
1:A:1026:ARG:NH2	1:A:1055:SER:OG	2.51	0.44
2:B:553:TYR:HD1	2:B:597:MET:HB3	1.83	0.44
2:B:658:TYR:HE2	2:B:670:MET:HG2	1.78	0.44
2:B:860:VAL:HG13	2:B:861:ASN:N	2.33	0.44
2:B:1055:SER:OG	2:B:1056:ARG:N	2.51	0.44
3:C:94:ASP:C	12:L:67:PHE:HE2	2.20	0.44
3:C:256:ILE:HD13	3:C:265:ALA:HB1	1.99	0.44
8:H:104:PHE:HE1	8:H:114:VAL:HG13	1.82	0.44
13:M:245:LEU:CD2	14:N:405:SER:OG	2.59	0.44
18:R:198:VAL:HA	18:R:201:ASP:HB2	1.99	0.44
18:R:213:TRP:NE1	18:R:495:PRO:HB3	2.30	0.44
18:R:220:PRO:HD3	18:R:514:GLU:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:511:TYR:HB2	18:R:519:LEU:CD1	2.48	0.44
18:R:604:ASP:OD1	18:R:605:VAL:N	2.51	0.44
1:A:153:ARG:CZ	15:O:338:ASP:HA	2.47	0.44
1:A:476:ARG:HE	1:A:477:GLN:CD	2.21	0.44
1:A:555:GLN:HG2	1:A:800:LYS:HD3	2.00	0.44
1:A:683:ARG:HH12	1:A:925:GLU:HB2	1.82	0.44
1:A:813:VAL:O	1:A:848:VAL:HG13	2.18	0.44
1:A:1083:LEU:HA	1:A:1083:LEU:HD23	1.63	0.44
1:A:1299:GLY:O	1:A:1301:ARG:N	2.50	0.44
1:A:1328:ILE:O	1:A:1331:ALA:N	2.51	0.44
2:B:305:ILE:CG2	2:B:325:GLU:HG2	2.47	0.44
2:B:738:THR:O	2:B:741:ILE:N	2.51	0.44
3:C:81:GLU:OE2	12:L:70:ARG:NH1	2.49	0.44
3:C:89:THR:CG2	3:C:201:GLU:H	2.31	0.44
3:C:113:LEU:HD21	3:C:132:ILE:HD12	1.99	0.44
4:D:11:LEU:HB3	7:G:3:ILE:HA	1.99	0.44
7:G:203:ASP:OD1	7:G:204:GLY:N	2.40	0.44
15:O:64:VAL:HG13	15:O:65:ILE:N	2.33	0.44
18:R:130:LEU:HD23	18:R:146:PHE:HE1	1.82	0.44
18:R:198:VAL:O	18:R:202:ALA:N	2.33	0.44
18:R:424:ARG:HH21	21:Y:51:DT:H5''	1.83	0.44
19:S:420:TRP:CD1	19:S:457:LYS:HD2	2.52	0.44
21:Y:18:DT:H6	21:Y:18:DT:H2''	1.58	0.44
1:A:226:LYS:NZ	15:O:547:GLU:OE2	2.40	0.44
1:A:234:ILE:CD1	1:A:237:ALA:HB3	2.40	0.44
1:A:361:GLN:N	1:A:361:GLN:OE1	2.51	0.44
1:A:1078:TYR:O	1:A:1081:ALA:N	2.51	0.44
1:A:1332:ARG:NH2	5:E:200:ARG:NE	2.66	0.44
2:B:804:ASP:OD1	2:B:804:ASP:N	2.51	0.44
15:O:454:ASN:O	15:O:457:LEU:HB3	2.18	0.44
18:R:398:ALA:HB3	18:R:449:VAL:HB	2.00	0.44
19:S:502:LEU:HD12	19:S:505:LEU:HD23	1.99	0.44
19:S:509:HIS:HA	19:S:512:HIS:HB3	1.99	0.44
21:Y:44:DA:C6	21:Y:45:DA:C6	3.05	0.44
1:A:449:ARG:O	1:A:450:MET:C	2.56	0.44
1:A:590:PHE:O	11:K:106:GLN:NE2	2.51	0.44
1:A:665:ASP:OD2	1:A:797:CYS:HB3	2.18	0.44
1:A:774:ARG:NH2	1:A:808:GLN:HE21	2.15	0.44
1:A:988:ASP:CG	1:A:993:GLU:H	2.22	0.44
2:B:260:CYS:O	2:B:342:PHE:HB3	2.18	0.44
2:B:553:TYR:HA	2:B:597:MET:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:732:GLN:HB3	10:J:52:THR:HG22	1.99	0.44
2:B:824:LEU:O	2:B:831:GLU:HB3	2.18	0.44
3:C:95:GLU:HA	12:L:67:PHE:CE2	2.53	0.44
5:E:24:LYS:HB2	5:E:30:ILE:HD11	2.00	0.44
5:E:191:LYS:N	5:E:194:GLU:OE1	2.38	0.44
6:F:108:PHE:CE2	6:F:131:PRO:HG3	2.53	0.44
6:F:151:LEU:HD23	6:F:152:ILE:N	2.32	0.44
7:G:101:LEU:HB3	7:G:104:ILE:CG2	2.48	0.44
16:P:296:TYR:CZ	16:P:297:PHE:CD1	3.04	0.44
18:R:116:PHE:CE2	18:R:164:MET:HB3	2.53	0.44
19:S:414:GLY:HA3	20:X:11:DA:OP1	2.18	0.44
1:A:107:CYS:N	1:A:114:LEU:HD23	2.33	0.43
1:A:378:ARG:NH1	1:A:518:ASN:HD21	2.12	0.43
2:B:209:ALA:HA	2:B:215:ILE:HA	1.99	0.43
15:O:464:ASN:HA	15:O:469:ASN:CG	2.38	0.43
15:O:470:GLU:HB2	15:O:479:PRO:CG	2.36	0.43
15:O:495:VAL:HG11	15:O:647:LEU:HD11	2.00	0.43
15:O:583:TRP:CE3	15:O:583:TRP:HA	2.53	0.43
16:P:185:PHE:HE2	16:P:217:THR:HG22	1.83	0.43
18:R:191:LEU:HD21	18:R:237:LEU:HD13	2.00	0.43
18:R:417:ASN:O	18:R:430:MET:HG2	2.18	0.43
20:X:19:DA:H1'	20:X:20:DA:O4'	2.17	0.43
1:A:151:GLN:O	1:A:152:ARG:NH1	2.51	0.43
1:A:675:HIS:O	1:A:676:SER:OG	2.36	0.43
1:A:715:ASN:OD1	1:A:716:ASP:N	2.52	0.43
1:A:781:CYS:O	1:A:785:LEU:HB2	2.18	0.43
1:A:794:MET:HE3	2:B:950:PRO:HG2	2.01	0.43
1:A:890:MET:HE3	1:A:890:MET:HB2	1.78	0.43
2:B:954:THR:HG23	2:B:954:THR:O	2.18	0.43
3:C:95:GLU:HG3	3:C:96:VAL:N	2.33	0.43
7:G:38:ILE:HD11	7:G:43:GLY:HA2	2.00	0.43
13:M:74:PHE:HE2	14:N:364:ARG:HD2	1.83	0.43
15:O:362:ASN:O	15:O:477:TYR:HD1	2.00	0.43
15:O:505:MET:O	15:O:509:ARG:N	2.41	0.43
15:O:515:LYS:O	15:O:516:LEU:O	2.36	0.43
1:A:30:SER:OG	1:A:83:HIS:ND1	2.50	0.43
1:A:256:TYR:CD2	1:A:1401:PHE:HE1	2.34	0.43
1:A:506:THR:OG1	1:A:507:PRO:HD3	2.18	0.43
1:A:606:GLY:HA2	1:A:609:VAL:HG12	1.99	0.43
1:A:1165:LEU:HB3	1:A:1169:VAL:HG23	1.99	0.43
2:B:96:VAL:HG13	2:B:97:ASP:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:534:TYR:HA	2:B:538:VAL:HG22	1.99	0.43
2:B:544:ILE:HG22	2:B:546:SER:H	1.84	0.43
2:B:710:ILE:HG12	2:B:1026:LYS:O	2.16	0.43
2:B:795:LEU:HB2	2:B:894:ALA:HB3	2.00	0.43
3:C:15:THR:O	3:C:295:ARG:HD3	2.19	0.43
3:C:35:LYS:HD2	3:C:35:LYS:HA	1.43	0.43
3:C:157:TYR:HE2	3:C:197:ARG:HH11	1.66	0.43
3:C:209:ILE:HG13	3:C:210:LEU:N	2.33	0.43
4:D:61:ASN:O	4:D:64:ASN:HB3	2.18	0.43
5:E:171:LYS:H	5:E:174:GLN:NE2	2.15	0.43
6:F:86:THR:HG1	6:F:89:GLU:H	1.59	0.43
15:O:264:THR:HA	15:O:272:ARG:NE	2.32	0.43
15:O:287:PHE:HE2	15:O:291:ARG:HH11	1.65	0.43
15:O:547:GLU:HG2	15:O:548:ILE:N	2.20	0.43
18:R:97:PRO:HD2	18:R:100:ILE:HD12	1.99	0.43
18:R:622:LEU:HD22	19:S:483:GLU:OE2	2.18	0.43
20:X:13:DA:H2 ⁷	20:X:14:DT:H71	2.00	0.43
1:A:51:ASN:OD1	1:A:52:GLY:N	2.51	0.43
1:A:167:ALA:HB1	15:O:557:ARG:CD	2.48	0.43
1:A:616:PRO:HG3	1:A:696:ARG:NH1	2.34	0.43
2:B:306:GLY:CA	2:B:325:GLU:HB2	2.49	0.43
2:B:427:ASN:O	2:B:431:SER:N	2.51	0.43
3:C:89:THR:HG21	3:C:200:GLN:HA	2.00	0.43
5:E:178:ILE:HG13	5:E:212:ARG:HD3	2.00	0.43
6:F:104:ASN:OD1	6:F:104:ASN:C	2.55	0.43
9:I:6:PRO:C	9:I:7:SER:HG	2.18	0.43
15:O:105:LYS:HE3	15:O:123:ASN:OD1	2.18	0.43
15:O:310:GLN:NE2	15:O:313:LYS:HD3	2.33	0.43
15:O:573:SER:HA	15:O:576:PHE:CE1	2.54	0.43
15:O:623:GLU:OE1	15:O:624:LEU:HD12	2.19	0.43
16:P:296:TYR:CE1	16:P:297:PHE:HB3	2.53	0.43
18:R:516:PHE:CG	18:R:517:PRO:HD2	2.53	0.43
1:A:298:LEU:HD21	1:A:315:HIS:CE1	2.54	0.43
1:A:347:VAL:HG12	1:A:349:PRO:HD2	2.00	0.43
1:A:351:ARG:HD2	1:A:355:GLN:HG2	2.00	0.43
1:A:476:ARG:HA	1:A:517:MET:SD	2.58	0.43
1:A:562:TYR:HE1	1:A:663:VAL:HG21	1.84	0.43
2:B:698:ARG:NH2	2:B:952:ARG:HG2	2.30	0.43
2:B:765:TYR:CD2	2:B:924:ILE:HG12	2.53	0.43
2:B:834:MET:HE2	12:L:63:ARG:HD2	2.00	0.43
3:C:231:PRO:HB3	3:C:275:VAL:CG2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:144:ASN:CG	13:M:145:VAL:H	2.21	0.43
15:O:271:LEU:HD23	15:O:272:ARG:H	1.84	0.43
15:O:538:ALA:O	15:O:541:ILE:HG22	2.19	0.43
16:P:183:TRP:O	16:P:187:SER:HB3	2.18	0.43
20:X:4:DT:H2'	20:X:5:DC:O5'	2.15	0.43
20:X:31:DG:H8	20:X:31:DG:O5'	2.01	0.43
21:Y:39:DC:H6	21:Y:39:DC:H2'	1.69	0.43
1:A:207:HIS:O	1:A:209:PRO:HD3	2.18	0.43
1:A:473:LEU:HA	1:A:487:SER:HA	2.00	0.43
1:A:730:LEU:O	1:A:733:ILE:HG22	2.18	0.43
2:B:112:LEU:HD23	2:B:113:THR:H	1.83	0.43
2:B:612:LEU:HA	2:B:675:ILE:HG23	2.01	0.43
2:B:696:SER:OG	2:B:697:PRO:HD3	2.19	0.43
2:B:763:SER:CB	2:B:765:TYR:H	2.31	0.43
13:M:121:ILE:HG21	13:M:179:LEU:HD21	2.01	0.43
13:M:126:ASP:HB2	13:M:129:ALA:HB2	1.99	0.43
15:O:585:MET:HE2	15:O:644:LEU:HB3	2.00	0.43
16:P:175:ILE:HG22	16:P:179:LEU:CD1	2.49	0.43
18:R:171:THR:HG23	18:R:172:GLU:N	2.32	0.43
18:R:192:ALA:O	18:R:195:LYS:NZ	2.48	0.43
20:X:30:DT:H2''	20:X:31:DG:N7	2.33	0.43
1:A:541:LEU:HD11	1:A:694:MET:CE	2.49	0.43
1:A:753:GLN:HE22	1:A:765:LYS:HE2	1.83	0.43
2:B:324:ILE:HG23	2:B:325:GLU:N	2.33	0.43
2:B:496:MET:HG2	2:B:610:ARG:HD2	2.00	0.43
3:C:152:ASP:HB3	3:C:155:GLU:OE1	2.18	0.43
3:C:244:ALA:O	3:C:247:PHE:HB3	2.19	0.43
5:E:157:SER:HB2	5:E:160:GLU:HG3	1.99	0.43
7:G:12:ARG:NH2	7:G:65:SER:OG	2.51	0.43
12:L:31:CYS:CB	12:L:34:CYS:HB2	2.49	0.43
15:O:347:ASP:HA	15:O:350:GLU:HG2	1.99	0.43
15:O:358:GLY:HA2	15:O:361:PHE:CD2	2.53	0.43
15:O:367:ALA:HB2	15:O:453:ILE:HD13	2.01	0.43
16:P:60:LEU:HD23	16:P:60:LEU:HA	1.88	0.43
16:P:149:MET:SD	16:P:155:PRO:HD2	2.59	0.43
16:P:191:PHE:HZ	16:P:196:LYS:HZ1	1.66	0.43
18:R:195:LYS:O	18:R:198:VAL:HB	2.18	0.43
18:R:470:GLN:HG2	18:R:475:ALA:O	2.18	0.43
18:R:619:ALA:O	18:R:623:LYS:HB2	2.18	0.43
19:S:517:GLU:O	19:S:520:LYS:HB3	2.18	0.43
20:X:30:DT:H3	21:Y:40:DA:N6	2.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:Y:59:DT:C2	21:Y:60:DA:C8	3.06	0.43
1:A:21:LEU:HD11	2:B:1133:LEU:HD11	2.00	0.43
1:A:228:LEU:HD12	1:A:229:ASN:CA	2.48	0.43
1:A:665:ASP:CG	1:A:797:CYS:HB3	2.39	0.43
1:A:848:VAL:HG23	1:A:860:GLU:OE1	2.19	0.43
2:B:734:PRO:HB3	2:B:1023:TYR:CD2	2.53	0.43
2:B:774:ASN:HB2	2:B:941:ASP:O	2.19	0.43
2:B:803:GLN:O	2:B:805:ILE:HG12	2.18	0.43
5:E:80:VAL:HA	5:E:109:ILE:HG13	2.00	0.43
5:E:85:GLU:CD	5:E:86:PRO:HD2	2.38	0.43
5:E:153:HIS:HB3	5:E:196:VAL:HG21	2.00	0.43
8:H:95:TYR:CZ	8:H:97:MET:SD	3.12	0.43
9:I:29:CYS:HA	13:M:183:PHE:HE2	1.84	0.43
15:O:175:LEU:HD21	15:O:184:LYS:HD3	2.00	0.43
15:O:289:LYS:NZ	15:O:320:GLU:HA	2.34	0.43
16:P:98:GLU:HB2	16:P:150:LEU:HD11	2.01	0.43
16:P:145:ARG:HB3	16:P:147:ILE:HG23	2.01	0.43
18:R:601:ASN:HB3	18:R:604:ASP:OD2	2.18	0.43
1:A:496:ARG:O	1:A:497:THR:HB	2.18	0.43
1:A:594:PRO:HB3	8:H:79:TRP:CD1	2.54	0.43
1:A:645:MET:SD	8:H:124:ARG:HB2	2.59	0.43
1:A:911:ILE:HG22	5:E:174:GLN:O	2.18	0.43
1:A:1272:VAL:HG13	1:A:1273:LYS:N	2.32	0.43
1:A:1441:LEU:HD23	7:G:53:THR:H	1.84	0.43
2:B:694:ASN:OD1	2:B:916:HIS:NE2	2.51	0.43
2:B:786:GLU:HA	2:B:903:ASN:HA	2.00	0.43
5:E:9:ILE:HD13	5:E:43:LYS:HD3	2.00	0.43
8:H:56:THR:HB	8:H:145:ARG:HG3	2.01	0.43
13:M:117:HIS:CG	13:M:118:LEU:N	2.87	0.43
15:O:282:ILE:H	15:O:282:ILE:HD12	1.84	0.43
15:O:483:LEU:HA	15:O:486:VAL:HG22	2.01	0.43
18:R:627:TRP:O	18:R:631:ASN:ND2	2.36	0.43
19:S:479:PRO:HB3	19:S:483:GLU:HB2	2.00	0.43
20:X:16:DA:H2 ⁺	20:X:17:DG:N9	2.34	0.43
1:A:8:GLU:OE1	1:A:8:GLU:N	2.51	0.43
1:A:429:GLY:C	1:A:465:HIS:ND1	2.69	0.43
1:A:842:PRO:C	1:A:844:SER:H	2.22	0.43
1:A:857:SER:O	1:A:860:GLU:HG2	2.19	0.43
1:A:1224:ILE:HG13	1:A:1229:ARG:H	1.83	0.43
2:B:403:ILE:HD12	2:B:403:ILE:HA	1.77	0.43
7:G:15:PRO:HA	7:G:18:PHE:CE2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:69:VAL:HG22	15:O:122:TYR:CD1	2.54	0.43
15:O:470:GLU:O	15:O:479:PRO:HD3	2.17	0.43
18:R:267:ALA:O	18:R:271:SER:OG	2.33	0.43
21:Y:20:DT:C5	21:Y:21:DT:C5	3.07	0.43
21:Y:45:DA:C6	21:Y:46:DA:C6	3.06	0.43
1:A:295:THR:O	1:A:298:LEU:HB3	2.19	0.42
1:A:792:LEU:HD11	8:H:19:ARG:NH2	2.33	0.42
1:A:816:GLN:N	1:A:846:GLY:O	2.52	0.42
1:A:822:ARG:NE	1:A:845:LYS:HB2	2.34	0.42
2:B:77:ILE:HG13	2:B:78:LYS:N	2.34	0.42
2:B:86:ASP:O	16:P:117:HIS:CD2	2.72	0.42
2:B:1095:CYS:O	2:B:1099:GLY:HA2	2.19	0.42
3:C:19:ASP:HB2	3:C:29:ASN:ND2	2.34	0.42
3:C:77:SER:O	3:C:210:LEU:HD12	2.19	0.42
3:C:152:ASP:O	3:C:154:LYS:N	2.49	0.42
3:C:209:ILE:HD12	3:C:209:ILE:HA	1.92	0.42
4:D:24:GLU:OE2	4:D:30:ASP:N	2.25	0.42
8:H:100:THR:OG1	8:H:138:GLU:HA	2.19	0.42
13:M:72:GLU:OE1	14:N:364:ARG:NH2	2.51	0.42
13:M:115:LYS:O	13:M:175:ARG:NH2	2.52	0.42
18:R:434:GLU:HA	18:R:436:LYS:N	2.33	0.42
1:A:336:MET:HG3	1:A:337:LEU:O	2.20	0.42
1:A:432:TYR:HD1	1:A:443:ASN:HA	1.84	0.42
1:A:1164:THR:CB	1:A:1271:VAL:HA	2.48	0.42
2:B:234:ILE:HG13	2:B:240:ILE:HG22	1.99	0.42
2:B:254:ALA:O	2:B:258:LYS:HG2	2.19	0.42
2:B:1057:ASP:CG	2:B:1058:GLY:H	2.21	0.42
4:D:129:ALA:HB3	4:D:157:ILE:HG21	2.01	0.42
5:E:81:GLU:O	5:E:110:PHE:HA	2.20	0.42
15:O:500:LEU:HD11	15:O:543:TYR:CD2	2.54	0.42
15:O:547:GLU:O	15:O:548:ILE:HG13	2.19	0.42
15:O:591:LYS:HD3	16:P:308:GLU:HG3	2.01	0.42
18:R:590:THR:O	18:R:594:LYS:HG3	2.19	0.42
1:A:302:GLY:O	1:A:304:ASP:N	2.52	0.42
1:A:496:ARG:HB2	2:B:1035:MET:SD	2.59	0.42
1:A:811:ALA:O	1:A:851:SER:OG	2.37	0.42
1:A:1024:LYS:HG3	1:A:1025:SER:N	2.35	0.42
2:B:553:TYR:HB3	2:B:598:ALA:N	2.34	0.42
3:C:229:LEU:HB3	3:C:293:ARG:NH1	2.34	0.42
6:F:81:THR:HG22	6:F:82:THR:N	2.34	0.42
7:G:203:ASP:HB3	7:G:211:TRP:NE1	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:207:LEU:HB3	7:G:210:TRP:CD2	2.54	0.42
8:H:95:TYR:OH	8:H:97:MET:SD	2.69	0.42
14:N:282:LEU:HA	14:N:285:ALA:HB3	2.01	0.42
14:N:310:PRO:HG2	14:N:420:PRO:HD3	2.00	0.42
15:O:133:SER:HB2	17:Q:58:TYR:CE1	2.54	0.42
15:O:271:LEU:HD23	15:O:272:ARG:N	2.34	0.42
15:O:496:ILE:HA	15:O:499:THR:HB	2.01	0.42
18:R:511:TYR:HB2	18:R:519:LEU:HD12	2.01	0.42
20:X:3:DT:H2''	20:X:4:DT:OP2	2.19	0.42
1:A:366:GLY:O	2:B:1061:ARG:NH1	2.45	0.42
1:A:388:SER:OG	1:A:389:ILE:N	2.52	0.42
1:A:1189:ASP:OD2	1:A:1192:THR:N	2.53	0.42
2:B:555:VAL:CG1	2:B:563:GLY:H	2.31	0.42
2:B:710:ILE:O	2:B:751:ALA:HB1	2.20	0.42
2:B:776:SER:HB2	2:B:928:GLN:HB2	2.02	0.42
2:B:932:PRO:HB2	2:B:1004:LEU:HB3	2.01	0.42
3:C:122:ASP:CG	3:C:123:ASP:H	2.23	0.42
4:D:11:LEU:HD23	4:D:12:SER:O	2.20	0.42
10:J:48:ARG:HG3	10:J:49:MET:HG3	2.01	0.42
13:M:85:LEU:HD23	13:M:85:LEU:C	2.39	0.42
13:M:106:PHE:O	13:M:123:ILE:HG12	2.19	0.42
13:M:123:ILE:N	13:M:145:VAL:HG22	2.34	0.42
13:M:159:TYR:HB3	13:M:170:LEU:HG	2.02	0.42
15:O:54:LYS:HA	15:O:62:ALA:HB2	2.01	0.42
15:O:553:ARG:HB3	15:O:561:ARG:O	2.19	0.42
17:Q:1074:UNK:O	17:Q:1076:UNK:N	2.52	0.42
19:S:407:ASN:O	19:S:410:SER:N	2.49	0.42
1:A:91:PHE:CE2	1:A:96:PHE:HD1	2.35	0.42
1:A:114:LEU:CD1	1:A:148:CYS:HB2	2.49	0.42
1:A:380:VAL:O	1:A:497:THR:OG1	2.25	0.42
1:A:413:ARG:O	1:A:416:LEU:N	2.52	0.42
2:B:234:ILE:CB	2:B:240:ILE:HG22	2.50	0.42
2:B:426:SER:C	2:B:428:ASN:H	2.17	0.42
2:B:727:LEU:HD11	2:B:786:GLU:OE1	2.20	0.42
2:B:780:ARG:HH12	10:J:10:CYS:C	2.23	0.42
2:B:809:MET:HG2	2:B:811:VAL:HG23	2.01	0.42
3:C:33:VAL:C	3:C:35:LYS:N	2.72	0.42
3:C:309:THR:OG1	3:C:311:GLU:HG2	2.20	0.42
5:E:148:GLU:OE1	5:E:149:LEU:N	2.53	0.42
8:H:43:ASN:ND2	8:H:46:LEU:HD13	2.35	0.42
15:O:128:HIS:CE1	15:O:291:ARG:HH22	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:134:GLY:O	15:O:137:ILE:HB	2.19	0.42
16:P:69:GLU:HG3	16:P:70:LEU:N	2.29	0.42
16:P:209:ALA:O	16:P:212:VAL:HG12	2.19	0.42
16:P:256:VAL:HG22	16:P:257:THR:HG23	2.01	0.42
18:R:402:LEU:HD22	18:R:476:ALA:HB1	2.00	0.42
20:X:8:DC:N4	20:X:9:DA:H62	2.17	0.42
20:X:19:DA:H4'	20:X:20:DA:OP1	2.17	0.42
1:A:45:ASP:O	1:A:48:PRO:HD3	2.19	0.42
1:A:172:GLY:HA2	1:A:175:ALA:HB3	2.00	0.42
1:A:566:HIS:CD2	1:A:568:ASP:HB3	2.54	0.42
1:A:1065:LYS:HA	1:A:1068:ARG:HB2	2.00	0.42
2:B:191:GLU:OE1	2:B:458:LEU:HB3	2.20	0.42
2:B:809:MET:HG2	2:B:811:VAL:CG2	2.50	0.42
2:B:909:GLY:O	2:B:1031:VAL:HB	2.19	0.42
2:B:931:MET:HB2	2:B:932:PRO:HD2	2.01	0.42
3:C:216:HIS:CD2	12:L:70:ARG:HB2	2.54	0.42
5:E:41:ASP:O	5:E:45:LYS:N	2.52	0.42
7:G:207:LEU:HD23	7:G:209:SER:H	1.85	0.42
20:X:8:DC:H6	20:X:8:DC:H2'	1.69	0.42
21:Y:48:DT:C2	21:Y:49:DA:N7	2.87	0.42
21:Y:60:DA:H2'	21:Y:61:DT:H71	2.02	0.42
1:A:123:PHE:O	1:A:127:LEU:CD1	2.67	0.42
1:A:136:ARG:O	1:A:140:ILE:HG12	2.20	0.42
1:A:155:LEU:HD11	1:A:156:HIS:HD2	1.84	0.42
1:A:167:ALA:HB1	15:O:557:ARG:NE	2.35	0.42
1:A:636:PRO:HG2	1:A:643:ASN:HA	2.01	0.42
1:A:997:GLN:C	1:A:999:ASP:N	2.73	0.42
2:B:316:LYS:NZ	13:M:226:ARG:CZ	2.83	0.42
2:B:398:ASP:HB3	2:B:425:HIS:CE1	2.55	0.42
2:B:529:ILE:HD12	2:B:529:ILE:HA	1.95	0.42
2:B:932:PRO:HA	2:B:1005:TYR:O	2.19	0.42
2:B:943:ILE:HD12	2:B:944:MET:H	1.84	0.42
4:D:126:GLN:O	4:D:127:LEU:O	2.37	0.42
5:E:22:MET:CE	5:E:26:ARG:HH21	2.33	0.42
7:G:39:ILE:HG23	7:G:42:VAL:HG13	2.01	0.42
9:I:24:LEU:HG	9:I:33:PHE:HB2	2.02	0.42
15:O:183:MET:HB2	15:O:186:THR:HB	2.00	0.42
18:R:394:GLN:HB2	18:R:487:VAL:HG12	2.01	0.42
19:S:442:ILE:HA	19:S:445:LEU:HD12	2.01	0.42
1:A:284:ASP:O	1:A:286:THR:N	2.53	0.42
1:A:379:THR:HG22	1:A:380:VAL:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:786:ASP:OD2	3:C:9:TYR:HE2	2.02	0.42
1:A:968:GLY:O	1:A:972:GLU:HG2	2.19	0.42
1:A:1380:ARG:HH11	1:A:1385:GLN:NE2	2.07	0.42
2:B:260:CYS:O	2:B:346:ALA:HB2	2.19	0.42
2:B:762:TYR:CG	2:B:763:SER:N	2.87	0.42
2:B:833:GLY:N	2:B:881:ILE:O	2.28	0.42
3:C:173:GLY:C	3:C:175:GLN:H	2.23	0.42
3:C:239:ILE:O	3:C:244:ALA:HB2	2.20	0.42
14:N:286:ASP:O	14:N:290:ILE:HG22	2.20	0.42
16:P:49:MET:HE2	19:S:364:LEU:HD11	2.02	0.42
18:R:484:GLN:HA	18:R:544:LYS:HE2	2.02	0.42
18:R:540:LEU:HD13	18:R:549:ILE:HG23	2.02	0.42
1:A:118:THR:O	1:A:122:GLN:N	2.49	0.42
1:A:262:PRO:HB2	2:B:1134:SER:O	2.19	0.42
1:A:373:VAL:CG1	1:A:374:ASP:N	2.82	0.42
1:A:383:PRO:HG3	1:A:512:PHE:CZ	2.55	0.42
1:A:408:VAL:O	1:A:409:THR:CG2	2.68	0.42
2:B:96:VAL:HG13	2:B:97:ASP:N	2.35	0.42
2:B:489:LEU:HG	2:B:493:GLN:OE1	2.20	0.42
2:B:732:GLN:HE22	10:J:49:MET:HG2	1.85	0.42
2:B:1039:ALA:HB3	18:R:20:ASN:OD1	2.19	0.42
3:C:326:GLU:HB2	11:K:125:MET:SD	2.60	0.42
13:M:85:LEU:HD12	13:M:171:VAL:HG11	2.02	0.42
13:M:88:PHE:CZ	13:M:119:TRP:HE3	2.36	0.42
13:M:251:THR:HG23	13:M:254:GLN:CG	2.50	0.42
15:O:190:LEU:HG	15:O:193:GLN:HB3	2.01	0.42
15:O:478:VAL:HG12	15:O:479:PRO:O	2.20	0.42
16:P:221:ILE:HG21	16:P:240:ILE:HG21	2.01	0.42
18:R:171:THR:OG1	18:R:506:GLY:O	2.34	0.42
19:S:299:UNK:CB	19:S:400:ASN:HD21	2.33	0.42
19:S:479:PRO:HB2	19:S:483:GLU:OE1	2.19	0.42
21:Y:14:DG:C2	21:Y:15:DT:C2	3.08	0.42
1:A:78:HIS:ND1	2:B:1090:PHE:HZ	2.18	0.42
1:A:91:PHE:HE2	1:A:96:PHE:CD1	2.37	0.42
1:A:381:ILE:HG22	1:A:382:SER:N	2.35	0.42
1:A:565:SER:HB2	1:A:664:MET:HE2	2.02	0.42
1:A:733:ILE:HG13	1:A:737:LYS:HE2	2.01	0.42
2:B:135:TYR:HE1	2:B:419:LEU:HB3	1.74	0.42
2:B:143:MET:HG2	2:B:144:HIS:H	1.85	0.42
2:B:180:ASP:OD2	2:B:460:ARG:NH2	2.38	0.42
2:B:364:LYS:O	2:B:366:ILE:HG23	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:591:TYR:HB3	2:B:653:GLU:HA	2.01	0.42
3:C:163:TYR:HA	3:C:191:ILE:O	2.18	0.42
3:C:195:LYS:HD2	10:J:57:ILE:CG2	2.49	0.42
3:C:229:LEU:HD23	3:C:293:ARG:NH1	2.35	0.42
5:E:63:ASN:HA	5:E:77:SER:HA	2.01	0.42
7:G:141:ASP:OD1	7:G:142:VAL:HG22	2.20	0.42
9:I:33:PHE:CE2	9:I:35:ILE:HA	2.55	0.42
13:M:117:HIS:CG	13:M:118:LEU:H	2.38	0.42
14:N:402:ASP:O	14:N:405:SER:HB3	2.20	0.42
15:O:125:GLU:HB2	15:O:128:HIS:HB2	1.97	0.42
16:P:106:TRP:NE1	16:P:145:ARG:HA	2.35	0.42
16:P:202:PRO:C	16:P:203:LYS:HG2	2.41	0.42
16:P:253:LEU:HB2	16:P:262:ARG:O	2.20	0.42
19:S:367:ASN:HB3	19:S:370:GLY:O	2.20	0.42
21:Y:41:DG:C6	21:Y:42:DA:C6	3.08	0.42
1:A:14:LYS:HE3	2:B:1142:ARG:CZ	2.50	0.41
1:A:721:ASP:H	1:A:724:LYS:NZ	2.17	0.41
1:A:912:VAL:HG11	1:A:1361:VAL:HG12	2.02	0.41
2:B:250:GLU:H	2:B:308:LYS:HZ3	1.68	0.41
2:B:535:VAL:HG13	14:N:310:PRO:HB3	2.02	0.41
2:B:636:ASP:OD1	2:B:637:PHE:N	2.53	0.41
2:B:957:LYS:O	2:B:960:GLU:N	2.52	0.41
5:E:152:LYS:HE2	5:E:154:ILE:HD11	2.02	0.41
6:F:140:ASP:OD1	6:F:142:SER:N	2.52	0.41
7:G:147:ARG:NH2	7:G:211:TRP:HB2	2.35	0.41
15:O:190:LEU:HD11	15:O:199:TYR:HE1	1.85	0.41
16:P:206:VAL:HB	16:P:210:PRO:HA	2.02	0.41
18:R:128:SER:O	18:R:132:VAL:HG22	2.20	0.41
18:R:401:THR:HG23	18:R:446:LYS:HG2	2.01	0.41
18:R:485:ASN:ND2	18:R:542:GLY:H	2.17	0.41
1:A:134:ASN:O	1:A:137:ARG:HB2	2.20	0.41
1:A:1323:PHE:HD1	1:A:1328:ILE:H	1.68	0.41
1:A:1454:GLU:HA	1:A:1457:LEU:HD12	2.01	0.41
2:B:65:PHE:O	2:B:68:PHE:HB3	2.19	0.41
2:B:234:ILE:CG1	2:B:240:ILE:HG22	2.50	0.41
2:B:317:LEU:C	2:B:319:ILE:N	2.71	0.41
2:B:556:TYR:CD1	2:B:561:LEU:HA	2.55	0.41
2:B:576:ARG:O	2:B:580:ARG:HG2	2.21	0.41
3:C:93:GLN:HB2	3:C:96:VAL:HB	2.02	0.41
7:G:2:PHE:HE2	7:G:79:PRO:HB3	1.86	0.41
9:I:12:LEU:HD22	9:I:24:LEU:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:154:GLU:HB3	13:M:175:ARG:HA	2.02	0.41
15:O:506:ARG:O	15:O:510:CYS:N	2.46	0.41
15:O:634:GLU:O	15:O:637:VAL:N	2.52	0.41
18:R:83:ALA:O	18:R:87:LEU:HB2	2.19	0.41
19:S:416:TYR:OH	21:Y:64:DT:H5"	2.20	0.41
19:S:423:GLU:HA	19:S:426:ILE:HG12	2.02	0.41
19:S:427:LYS:HA	19:S:430:LYS:HD2	2.03	0.41
21:Y:10:DT:C2	21:Y:11:DG:C5	3.07	0.41
1:A:678:PHE:CD2	1:A:694:MET:HG2	2.55	0.41
2:B:855:PRO:HD2	18:R:106:GLN:NE2	2.34	0.41
3:C:270:ALA:O	3:C:271:ARG:HG2	2.20	0.41
4:D:127:LEU:HD23	7:G:147:ARG:CD	2.51	0.41
4:D:134:LEU:HD22	4:D:153:MET:SD	2.61	0.41
5:E:66:GLU:O	5:E:69:ILE:HG22	2.20	0.41
5:E:118:PRO:O	5:E:122:LYS:N	2.53	0.41
5:E:169:ARG:HD3	6:F:140:ASP:OD2	2.21	0.41
15:O:226:ILE:O	15:O:228:ARG:N	2.46	0.41
15:O:369:HIS:CG	15:O:370:LEU:N	2.89	0.41
16:P:25:LYS:HG3	16:P:26:GLY:N	2.35	0.41
18:R:515:LEU:HD23	18:R:515:LEU:HA	1.82	0.41
21:Y:28:DT:H2"	21:Y:29:DG:C8	2.55	0.41
1:A:238:ASP:CG	1:A:239:CYS:H	2.24	0.41
1:A:332:VAL:HG13	1:A:333:ASN:N	2.30	0.41
1:A:712:ILE:O	2:B:1001:LYS:NZ	2.49	0.41
1:A:958:ALA:O	1:A:961:GLU:HB2	2.20	0.41
2:B:249:GLU:H	2:B:308:LYS:HE2	1.85	0.41
2:B:553:TYR:HB3	2:B:598:ALA:CA	2.50	0.41
5:E:96:PHE:O	5:E:100:ILE:HG12	2.19	0.41
7:G:96:GLY:CA	7:G:112:GLN:HG3	2.49	0.41
8:H:110:ASP:O	8:H:128:ASN:HA	2.20	0.41
15:O:369:HIS:ND1	15:O:370:LEU:N	2.68	0.41
18:R:131:TYR:HA	18:R:134:CYS:SG	2.59	0.41
19:S:506:GLN:O	19:S:510:LYS:CB	2.67	0.41
1:A:404:TYR:CE1	1:A:528:ARG:HD2	2.55	0.41
1:A:668:VAL:HG23	1:A:669:LEU:N	2.35	0.41
1:A:717:VAL:O	1:A:810:VAL:HG22	2.20	0.41
1:A:1152:ARG:C	1:A:1156:VAL:HG23	2.41	0.41
2:B:193:VAL:HG23	2:B:458:LEU:HB2	2.03	0.41
2:B:611:PRO:HG3	2:B:648:TYR:CE1	2.56	0.41
2:B:914:SER:C	2:B:916:HIS:N	2.74	0.41
3:C:319:ARG:HB2	11:K:132:GLU:OE2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:292:ARG:O	14:N:296:LYS:HG2	2.19	0.41
16:P:256:VAL:O	16:P:260:CYS:HB3	2.19	0.41
18:R:484:GLN:NE2	20:X:16:DA:N3	2.68	0.41
18:R:537:LYS:O	18:R:538:ILE:HD13	2.21	0.41
1:A:91:PHE:CD1	1:A:224:PRO:HB3	2.52	0.41
1:A:953:GLY:HA3	1:A:1061:ARG:CG	2.50	0.41
1:A:1281:ALA:HB1	1:A:1295:VAL:HG22	2.03	0.41
2:B:68:PHE:HD1	2:B:385:SER:HG	1.55	0.41
2:B:234:ILE:HD11	2:B:238:GLY:H	1.86	0.41
2:B:354:ARG:NH1	2:B:549:LEU:HD13	2.35	0.41
2:B:1147:PHE:HZ	7:G:60:LYS:HB3	1.85	0.41
3:C:91:VAL:HG23	3:C:200:GLN:HE22	1.85	0.41
5:E:180:ARG:HH12	5:E:191:LYS:HA	1.86	0.41
9:I:21:VAL:C	9:I:23:THR:H	2.24	0.41
13:M:245:LEU:HD13	14:N:405:SER:HG	1.85	0.41
16:P:59:ASN:OD1	16:P:80:ALA:HB1	2.20	0.41
16:P:209:ALA:O	16:P:211:ASN:N	2.42	0.41
1:A:308:SER:O	1:A:312:MET:N	2.53	0.41
1:A:487:SER:OG	1:A:536:GLY:HA2	2.21	0.41
1:A:687:PRO:O	1:A:690:ALA:N	2.54	0.41
2:B:65:PHE:O	2:B:68:PHE:N	2.53	0.41
2:B:615:VAL:HA	2:B:620:SER:HA	2.02	0.41
2:B:723:THR:O	2:B:789:ARG:HA	2.21	0.41
2:B:947:HIS:O	2:B:950:PRO:HD2	2.21	0.41
3:C:44:ILE:HA	3:C:54:PHE:HB2	2.03	0.41
3:C:239:ILE:O	3:C:239:ILE:HD12	2.21	0.41
3:C:278:GLU:O	3:C:281:ARG:HG2	2.20	0.41
7:G:84:ILE:HG23	7:G:147:ARG:HB3	2.02	0.41
8:H:9:ILE:O	8:H:31:THR:HG22	2.20	0.41
14:N:286:ASP:OD2	14:N:384:LYS:HE3	2.20	0.41
15:O:155:LEU:O	15:O:159:ILE:HG12	2.21	0.41
15:O:328:ASP:OD1	15:O:329:PRO:HD3	2.20	0.41
15:O:571:THR:O	15:O:575:ASN:HB2	2.19	0.41
16:P:206:VAL:HB	16:P:210:PRO:HB3	2.01	0.41
20:X:15:DT:H2'	20:X:16:DA:C8	2.56	0.41
20:X:51:DA:C6	20:X:52:DA:C6	3.08	0.41
1:A:57:LYS:HA	1:A:68:ALA:HB3	2.03	0.41
1:A:132:VAL:HG13	1:A:136:ARG:HB2	2.01	0.41
1:A:220:ASP:HB3	15:O:549:GLN:HE22	1.86	0.41
1:A:389:ILE:O	1:A:390:ASP:OD1	2.37	0.41
1:A:822:ARG:CZ	1:A:845:LYS:HB2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:217:GLN:HB3	2:B:356:VAL:CG1	2.50	0.41
2:B:501:ASP:OD2	2:B:513:ASN:ND2	2.54	0.41
2:B:519:HIS:ND1	2:B:586:GLU:OE2	2.54	0.41
3:C:123:ASP:OD1	3:C:124:GLU:N	2.53	0.41
4:D:14:TYR:CD1	4:D:15:GLU:CB	3.03	0.41
8:H:7:ASP:HB3	8:H:58:THR:HG23	2.03	0.41
11:K:55:SER:O	11:K:56:GLU:HG3	2.20	0.41
13:M:133:LYS:O	13:M:137:GLU:N	2.47	0.41
15:O:68:LEU:HD21	15:O:121:TYR:C	2.41	0.41
16:P:309:VAL:HG21	16:P:311:TYR:CZ	2.56	0.41
17:Q:69:PRO:HG2	17:Q:70:PHE:CE2	2.55	0.41
18:R:195:LYS:HE2	18:R:195:LYS:HB2	1.86	0.41
18:R:196:ILE:O	18:R:199:VAL:HB	2.20	0.41
19:S:416:TYR:OH	19:S:419:PRO:HD3	2.21	0.41
21:Y:20:DT:C2'	21:Y:21:DT:H5'	2.51	0.41
21:Y:64:DT:H4'	21:Y:65:DG:H5'	2.02	0.41
1:A:11:LYS:HD3	2:B:1145:ASP:CA	2.49	0.41
1:A:163:VAL:HG13	1:A:184:ARG:HH12	1.86	0.41
1:A:258:TRP:CZ3	2:B:1136:ASN:HB2	2.56	0.41
1:A:484:SER:O	1:A:508:TYR:HE1	2.04	0.41
1:A:832:LEU:HD21	1:A:862:LEU:HD23	2.02	0.41
1:A:921:LEU:HG	1:A:1081:ALA:O	2.20	0.41
2:B:72:ASP:O	2:B:76:ILE:HG12	2.20	0.41
2:B:258:LYS:HE2	2:B:265:ASP:HA	2.03	0.41
2:B:454:VAL:HG13	2:B:455:THR:HG23	2.02	0.41
2:B:726:TYR:O	2:B:727:LEU:HB3	2.21	0.41
2:B:757:VAL:HA	2:B:942:ILE:O	2.21	0.41
2:B:905:ARG:O	2:B:907:GLU:N	2.53	0.41
2:B:932:PRO:CB	2:B:1004:LEU:HB3	2.51	0.41
2:B:1106:TRP:CD1	7:G:163:PRO:HD3	2.55	0.41
3:C:45:SER:HB2	3:C:53:ASN:O	2.21	0.41
3:C:67:PHE:O	3:C:71:MET:HB2	2.21	0.41
3:C:260:GLU:N	3:C:263:ASP:HB2	2.36	0.41
4:D:3:VAL:HG13	7:G:7:ILE:HG22	2.03	0.41
4:D:130:ASN:O	4:D:133:HIS:HB2	2.20	0.41
7:G:126:SER:HB2	7:G:139:TYR:CB	2.45	0.41
9:I:3:SER:CB	9:I:12:LEU:HD12	2.51	0.41
12:L:60:ARG:NH1	12:L:61:THR:HG22	2.36	0.41
13:M:237:ALA:O	13:M:241:ALA:HB2	2.20	0.41
14:N:290:ILE:HG21	14:N:384:LYS:NZ	2.35	0.41
14:N:366:HIS:CG	14:N:367:LYS:H	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:394:VAL:HB	14:N:412:VAL:HB	2.01	0.41
15:O:115:LYS:HB3	15:O:116:LYS:H	1.54	0.41
15:O:203:ILE:HG13	15:O:203:ILE:O	2.21	0.41
15:O:480:TYR:O	15:O:483:LEU:N	2.54	0.41
15:O:584:ASN:OD1	16:P:310:VAL:HG22	2.21	0.41
18:R:142:MET:HB2	18:R:181:PHE:HE1	1.86	0.41
18:R:227:CYS:HA	18:R:230:LEU:HD12	2.02	0.41
18:R:413:LEU:O	18:R:615:LEU:HD11	2.21	0.41
18:R:442:PHE:HD2	18:R:446:LYS:HB2	1.86	0.41
18:R:467:ARG:NH2	18:R:471:LYS:HZ3	2.19	0.41
18:R:492:VAL:HB	18:R:494:PHE:CE2	2.56	0.41
20:X:59:DC:H2 ⁷	20:X:60:DA:OP2	2.20	0.41
21:Y:40:DA:C6	21:Y:41:DG:C6	3.09	0.41
21:Y:42:DA:C6	21:Y:43:DA:C6	3.09	0.41
1:A:87:ALA:O	1:A:88:LEU:HB2	2.21	0.41
1:A:296:SER:O	1:A:299:ILE:N	2.54	0.41
1:A:618:HIS:CD2	8:H:77:ARG:HH11	2.39	0.41
1:A:859:PRO:HD3	2:B:661:LEU:HD11	2.03	0.41
1:A:1124:PRO:O	1:A:1127:LYS:HB2	2.20	0.41
1:A:1202:ILE:HG23	1:A:1203:GLU:N	2.36	0.41
2:B:916:HIS:CG	2:B:957:LYS:HB2	2.56	0.41
3:C:59:ILE:HD13	3:C:63:ILE:CD1	2.50	0.41
15:O:60:ARG:HG3	15:O:61:ALA:N	2.36	0.41
15:O:337:GLN:HB3	15:O:342:ALA:HB2	2.02	0.41
15:O:644:LEU:HD12	17:Q:43:ILE:HD12	2.03	0.41
16:P:98:GLU:HB3	16:P:150:LEU:HD21	2.03	0.41
18:R:13:GLU:OE2	18:R:26:LYS:HE2	2.20	0.41
18:R:229:LEU:HD13	18:R:244:ILE:HD11	2.03	0.41
18:R:492:VAL:HG11	18:R:560:LEU:HD13	2.03	0.41
18:R:510:SER:HB3	18:R:520:ILE:HD11	2.03	0.41
20:X:22:DA:C2	20:X:23:DC:C2	3.08	0.41
1:A:32:VAL:HG11	1:A:57:LYS:CD	2.49	0.40
1:A:89:PRO:CG	1:A:228:LEU:CD2	2.96	0.40
1:A:179:ILE:HD13	15:O:557:ARG:HH21	1.78	0.40
1:A:261:LEU:HA	1:A:262:PRO:HD3	1.84	0.40
1:A:302:GLY:C	1:A:304:ASP:N	2.74	0.40
1:A:666:LYS:O	1:A:667:SER:OG	2.39	0.40
1:A:716:ASP:OD1	1:A:789:ASN:HB2	2.21	0.40
1:A:1184:ILE:HD11	1:A:1260:MET:SD	2.61	0.40
1:A:1396:LEU:HD23	1:A:1396:LEU:HA	1.79	0.40
2:B:527:GLU:HB3	2:B:528:PRO:HD3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:673:LEU:O	2:B:673:LEU:HD12	2.21	0.40
2:B:751:ALA:C	2:B:1023:TYR:HH	2.23	0.40
2:B:915:ARG:HD2	2:B:1023:TYR:CD2	2.50	0.40
2:B:1088:ASP:OD1	2:B:1088:ASP:N	2.54	0.40
3:C:255:VAL:HG22	3:C:256:ILE:N	2.36	0.40
5:E:83:CYS:SG	5:E:92:THR:OG1	2.68	0.40
5:E:136:ASN:ND2	5:E:138:ALA:HB3	2.37	0.40
6:F:93:ILE:HD11	6:F:134:ILE:HG12	2.03	0.40
8:H:12:VAL:HG22	8:H:26:ILE:HD11	2.01	0.40
9:I:11:MET:HG3	9:I:12:LEU:N	2.35	0.40
15:O:73:ARG:NE	15:O:121:TYR:OH	2.53	0.40
15:O:579:GLN:O	15:O:583:TRP:N	2.54	0.40
16:P:20:SER:HA	16:P:23:MET:HG2	2.02	0.40
18:R:14:ARG:HA	18:R:22:ASP:O	2.21	0.40
18:R:133:ALA:O	18:R:136:LYS:N	2.53	0.40
18:R:598:ASP:HB3	18:R:601:ASN:OD1	2.21	0.40
21:Y:56:DA:N6	21:Y:57:DT:O4	2.54	0.40
1:A:82:GLY:O	1:A:263:ALA:N	2.41	0.40
1:A:103:LEU:HD11	1:A:222:LEU:CD2	2.50	0.40
1:A:183:PHE:CG	1:A:184:ARG:N	2.89	0.40
1:A:292:ILE:HA	1:A:295:THR:HG22	2.03	0.40
1:A:559:THR:HG23	1:A:560:GLY:N	2.36	0.40
2:B:58:VAL:HG11	2:B:470:MET:CE	2.51	0.40
2:B:386:LEU:HD23	2:B:386:LEU:HA	1.90	0.40
6:F:136:ARG:O	6:F:144:GLU:CB	2.69	0.40
9:I:34:PRO:C	9:I:35:ILE:HG13	2.41	0.40
14:N:389:THR:HG23	14:N:390:PHE:N	2.35	0.40
15:O:128:HIS:CE1	15:O:132:TYR:HE1	2.39	0.40
15:O:253:ILE:O	15:O:256:PRO:HD2	2.22	0.40
16:P:202:PRO:C	16:P:204:LYS:H	2.22	0.40
20:X:16:DA:H61	21:Y:55:DA:N6	2.14	0.40
21:Y:8:DC:C2	21:Y:9:DA:C5	3.10	0.40
1:A:403:THR:HG21	1:A:431:ASN:HD21	1.85	0.40
1:A:714:ILE:CD1	2:B:958:MET:HG2	2.51	0.40
1:A:891:LYS:HG3	1:A:1389:PHE:HD1	1.85	0.40
2:B:305:ILE:HG22	2:B:325:GLU:HG2	2.03	0.40
2:B:637:PHE:CG	2:B:638:ASP:N	2.90	0.40
2:B:1060:LEU:HA	2:B:1060:LEU:HD23	1.82	0.40
3:C:5:VAL:HG22	3:C:293:ARG:O	2.21	0.40
4:D:98:MET:HA	4:D:160:TYR:CZ	2.57	0.40
15:O:196:GLU:HG3	15:O:197:MET:N	2.28	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:48:LEU:O	16:P:52:VAL:HG23	2.22	0.40
18:R:213:TRP:HH2	18:R:497:ARG:HB3	1.84	0.40
18:R:218:ARG:HD3	21:Y:60:DA:P	2.62	0.40
20:X:3:DT:C2	20:X:4:DT:C4	3.10	0.40
1:A:478:PRO:HG3	21:Y:23:DT:O2	2.21	0.40
1:A:506:THR:HG21	1:A:554:THR:HG21	2.04	0.40
1:A:584:SER:C	1:A:586:GLY:H	2.25	0.40
1:A:706:GLY:HA2	2:B:761:SER:O	2.21	0.40
1:A:976:ARG:HG2	1:A:1002:ARG:NH2	2.36	0.40
1:A:1447:LEU:HB3	1:A:1450:SER:HB3	2.04	0.40
2:B:86:ASP:O	2:B:87:VAL:HB	2.21	0.40
2:B:303:GLU:OE1	2:B:322:GLU:HA	2.21	0.40
2:B:945:ASN:OD1	2:B:946:PRO:HD2	2.21	0.40
5:E:153:HIS:ND1	5:E:184:VAL:HG11	2.37	0.40
13:M:230:SER:O	13:M:234:HIS:ND1	2.50	0.40
15:O:457:LEU:HD21	15:O:476:TYR:OH	2.22	0.40
1:A:216:LYS:HG3	1:A:217:ARG:N	2.37	0.40
1:A:329:SER:HB3	1:A:351:ARG:HB3	2.03	0.40
1:A:562:TYR:CE2	1:A:793:ILE:HG23	2.57	0.40
1:A:656:GLY:H	1:A:944:ASN:ND2	2.19	0.40
1:A:827:PHE:HE2	1:A:833:PRO:HD3	1.87	0.40
1:A:834:HIS:HA	2:B:659:ILE:O	2.21	0.40
1:A:935:PHE:HE1	1:A:1008:LEU:HD13	1.86	0.40
1:A:1332:ARG:NH2	5:E:200:ARG:HE	2.20	0.40
2:B:230:LYS:HB2	2:B:333:ALA:CB	2.51	0.40
2:B:617:ASP:CG	2:B:618:GLY:H	2.25	0.40
2:B:650:ASP:OD1	2:B:651:VAL:N	2.55	0.40
2:B:924:ILE:HD13	2:B:924:ILE:HA	1.93	0.40
3:C:274:THR:HG22	3:C:274:THR:O	2.22	0.40
4:D:126:GLN:HG2	7:G:84:ILE:O	2.20	0.40
7:G:126:SER:CB	7:G:139:TYR:HB3	2.49	0.40
7:G:141:ASP:O	7:G:144:GLU:HB2	2.22	0.40
14:N:364:ARG:O	14:N:371:LEU:HD12	2.21	0.40
15:O:45:ASP:H	15:O:582:GLU:CD	2.17	0.40
15:O:53:VAL:HG23	15:O:57:LEU:HD12	2.04	0.40
15:O:205:LYS:HG3	15:O:206:LEU:N	2.36	0.40
15:O:583:TRP:HH2	16:P:314:GLU:CG	2.19	0.40
17:Q:39:ILE:O	17:Q:39:ILE:HG23	2.22	0.40
18:R:195:LYS:O	18:R:199:VAL:HG23	2.21	0.40
18:R:488:GLY:N	18:R:540:LEU:O	2.46	0.40
19:S:364:LEU:HB2	19:S:373:ALA:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:X:60:DA:H2''	20:X:61:DT:OP2	2.21	0.40
20:X:64:DC:H2''	20:X:65:DC:C6	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1422/1460 (97%)	1142 (80%)	260 (18%)	20 (1%)	11	45
2	B	1112/1149 (97%)	907 (82%)	185 (17%)	20 (2%)	8	40
3	C	333/335 (99%)	272 (82%)	58 (17%)	3 (1%)	17	54
4	D	113/161 (70%)	85 (75%)	26 (23%)	2 (2%)	8	40
5	E	213/215 (99%)	177 (83%)	35 (16%)	1 (0%)	29	67
6	F	81/155 (52%)	71 (88%)	9 (11%)	1 (1%)	13	48
7	G	178/212 (84%)	146 (82%)	27 (15%)	5 (3%)	5	32
8	H	136/146 (93%)	114 (84%)	21 (15%)	1 (1%)	22	60
9	I	40/110 (36%)	29 (72%)	8 (20%)	3 (8%)	1	15
10	J	65/70 (93%)	51 (78%)	14 (22%)	0	100	100
11	K	99/142 (70%)	79 (80%)	20 (20%)	0	100	100
12	L	44/70 (63%)	36 (82%)	8 (18%)	0	100	100
13	M	160/282 (57%)	128 (80%)	27 (17%)	5 (3%)	4	31
14	N	106/422 (25%)	80 (76%)	26 (24%)	0	100	100
15	O	533/654 (82%)	405 (76%)	116 (22%)	12 (2%)	6	36
16	P	271/317 (86%)	223 (82%)	45 (17%)	3 (1%)	14	50
17	Q	33/251 (13%)	27 (82%)	6 (18%)	0	100	100
18	R	514/736 (70%)	436 (85%)	75 (15%)	3 (1%)	25	63

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	S	172/594 (29%)	157 (91%)	15 (9%)	0	100	100
All	All	5625/7481 (75%)	4565 (81%)	981 (17%)	79 (1%)	15	45

All (79) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	186	VAL
1	A	236	SER
1	A	587	ILE
1	A	599	LYS
1	A	601	TYR
1	A	1371	ILE
2	B	416	TYR
2	B	417	ASP
2	B	427	ASN
2	B	587	PHE
2	B	823	SER
9	I	21	VAL
13	M	107	ILE
15	O	124	GLU
15	O	494	TYR
15	O	496	ILE
18	R	514	GLU
18	R	516	PHE
1	A	284	ASP
1	A	285	LEU
1	A	307	ILE
1	A	975	VAL
2	B	87	VAL
2	B	318	THR
4	D	129	ALA
9	I	23	THR
13	M	87	VAL
13	M	242	ASN
15	O	40	ARG
15	O	125	GLU
1	A	275	GLN
1	A	410	ARG
1	A	995	VAL
1	A	998	TYR
3	C	87	ASN
3	C	255	VAL

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Mol	Chain	Res	Type
6	F	144	GLU
7	G	123	PRO
7	G	191	PRO
9	I	35	ILE
15	O	36	SER
16	P	203	LYS
1	A	39	LEU
1	A	233	GLN
1	A	277	SER
1	A	1300	LEU
1	A	1328	ILE
2	B	506	GLU
2	B	713	ILE
2	B	763	SER
3	C	88	ASN
5	E	147	HIS
15	O	146	VAL
15	O	516	LEU
2	B	767	ILE
4	D	127	LEU
7	G	160	PRO
8	H	77	ARG
13	M	84	SER
13	M	85	LEU
15	O	557	ARG
1	A	252	ARG
2	B	168	GLU
2	B	295	ILE
2	B	624	ASP
15	O	499	THR
2	B	1008	ILE
2	B	584	VAL
15	O	473	PRO
2	B	215	ILE
2	B	811	VAL
2	B	233	VAL
7	G	142	VAL
15	O	76	VAL
16	P	192	PRO
16	P	206	VAL
2	B	1137	ILE
7	G	158	VAL

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Mol	Chain	Res	Type
18	R	154	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1232/1257 (98%)	1227 (100%)	5 (0%)	91	94
2	B	975/1006 (97%)	971 (100%)	4 (0%)	91	94
3	C	296/296 (100%)	294 (99%)	2 (1%)	84	90
4	D	110/145 (76%)	110 (100%)	0	100	100
5	E	197/197 (100%)	197 (100%)	0	100	100
6	F	73/137 (53%)	73 (100%)	0	100	100
7	G	164/190 (86%)	162 (99%)	2 (1%)	71	83
8	H	123/128 (96%)	123 (100%)	0	100	100
9	I	38/98 (39%)	37 (97%)	1 (3%)	46	67
10	J	62/65 (95%)	62 (100%)	0	100	100
11	K	91/130 (70%)	91 (100%)	0	100	100
12	L	40/57 (70%)	39 (98%)	1 (2%)	47	68
13	M	142/249 (57%)	142 (100%)	0	100	100
14	N	92/360 (26%)	92 (100%)	0	100	100
15	O	495/593 (84%)	490 (99%)	5 (1%)	76	85
16	P	255/285 (90%)	255 (100%)	0	100	100
17	Q	31/195 (16%)	31 (100%)	0	100	100
18	R	450/623 (72%)	448 (100%)	2 (0%)	91	94
19	S	157/494 (32%)	157 (100%)	0	100	100
All	All	5023/6505 (77%)	5001 (100%)	22 (0%)	91	94

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	121	ARG
1	A	254	GLU
1	A	275	GLN
1	A	285	LEU
1	A	1145	LEU
2	B	59	LYS
2	B	316	LYS
2	B	427	ASN
2	B	587	PHE
3	C	35	LYS
3	C	120	LEU
7	G	122	THR
7	G	125	GLU
9	I	24	LEU
12	L	61	THR
15	O	40	ARG
15	O	187	ILE
15	O	496	ILE
15	O	516	LEU
15	O	557	ARG
18	R	514	GLU
18	R	515	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (83) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	HIS
1	A	156	HIS
1	A	233	GLN
1	A	315	HIS
1	A	386	ASN
1	A	518	ASN
1	A	520	HIS
1	A	523	GLN
1	A	533	ASN
1	A	566	HIS
1	A	589	HIS
1	A	618	HIS
1	A	619	ASN
1	A	643	ASN
1	A	808	GLN
1	A	838	ASN
1	A	913	GLN

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Mol	Chain	Res	Type
1	A	1058	GLN
1	A	1385	GLN
2	B	116	HIS
2	B	140	ASN
2	B	197	GLN
2	B	244	HIS
2	B	275	ASN
2	B	286	ASN
2	B	299	GLN
2	B	334	HIS
2	B	374	ASN
2	B	396	ASN
2	B	411	ASN
2	B	425	HIS
2	B	550	HIS
2	B	600	HIS
2	B	626	HIS
2	B	693	HIS
2	B	717	GLN
2	B	754	ASN
2	B	803	GLN
2	B	865	GLN
2	B	902	GLN
2	B	918	GLN
2	B	1148	GLN
3	C	14	ASN
3	C	29	ASN
3	C	93	GLN
3	C	99	HIS
3	C	175	GLN
4	D	64	ASN
4	D	122	GLN
5	E	3	GLN
5	E	54	GLN
5	E	104	ASN
5	E	153	HIS
5	E	174	GLN
7	G	28	HIS
13	M	86	HIS
13	M	89	GLN
13	M	190	ASN
13	M	254	GLN

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Mol	Chain	Res	Type
14	N	288	GLN
15	O	43	ASN
15	O	128	HIS
15	O	222	HIS
15	O	295	GLN
15	O	310	GLN
15	O	332	GLN
15	O	337	GLN
15	O	456	HIS
16	P	33	GLN
16	P	118	GLN
16	P	119	HIS
16	P	131	GLN
16	P	239	ASN
16	P	305	HIS
18	R	20	ASN
18	R	35	ASN
18	R	235	ASN
18	R	278	ASN
18	R	394	GLN
18	R	414	HIS
19	S	444	GLN
19	S	499	ASN
19	S	506	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 7 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
19	S	1
17	Q	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	S	319:UNK	C	360:THR	N	37.31
1	Q	70:PHE	C	1070:UNK	N	13.25

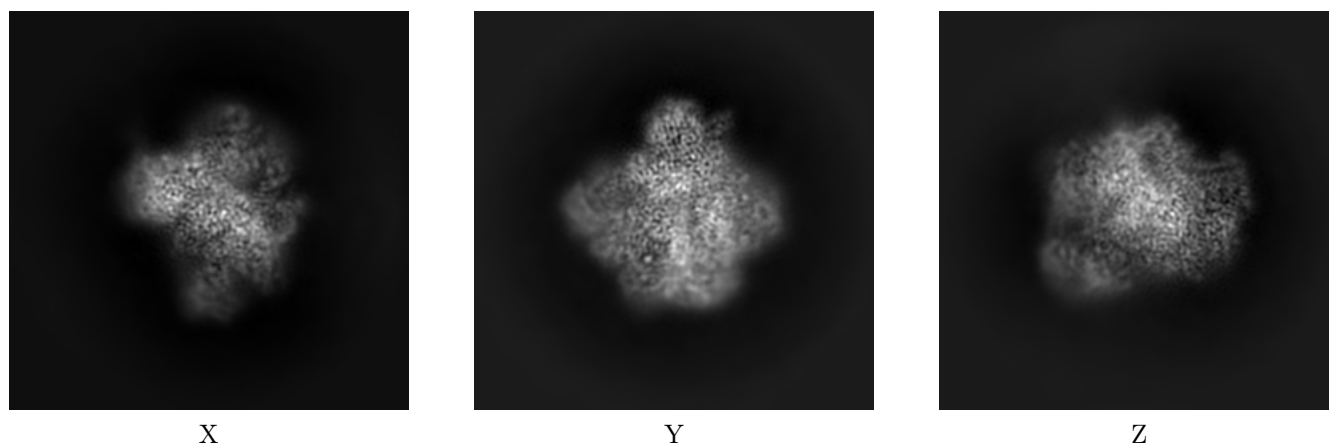
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7530. 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](#)

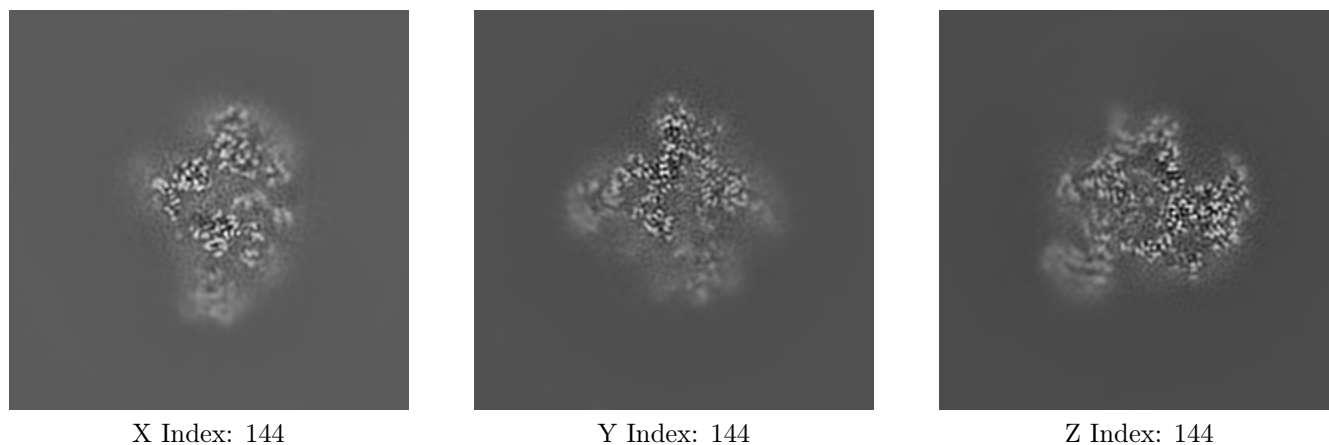
6.1.1 Primary map



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

6.2 Central slices [i](#)

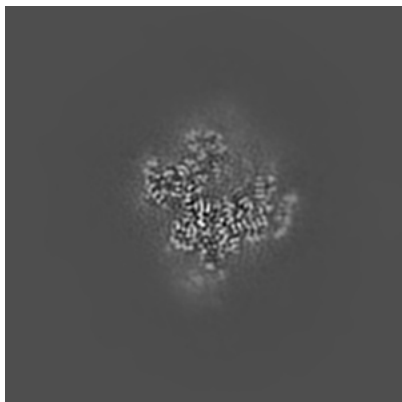
6.2.1 Primary map



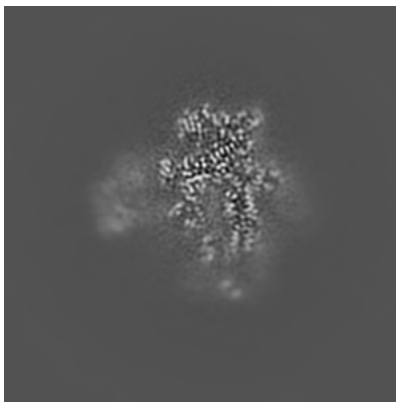
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

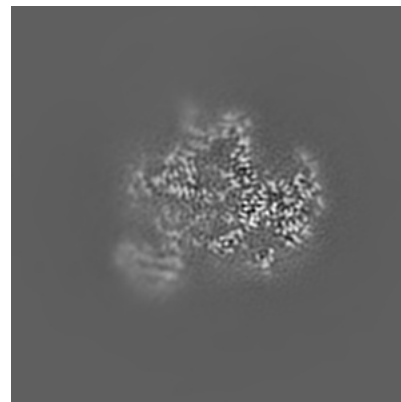
6.3.1 Primary map



X Index: 168



Y Index: 134



Z Index: 143

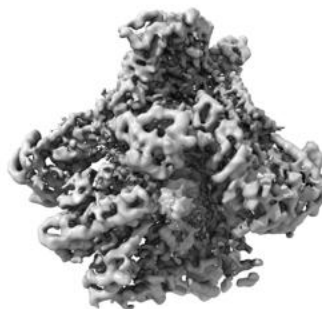
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0334. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

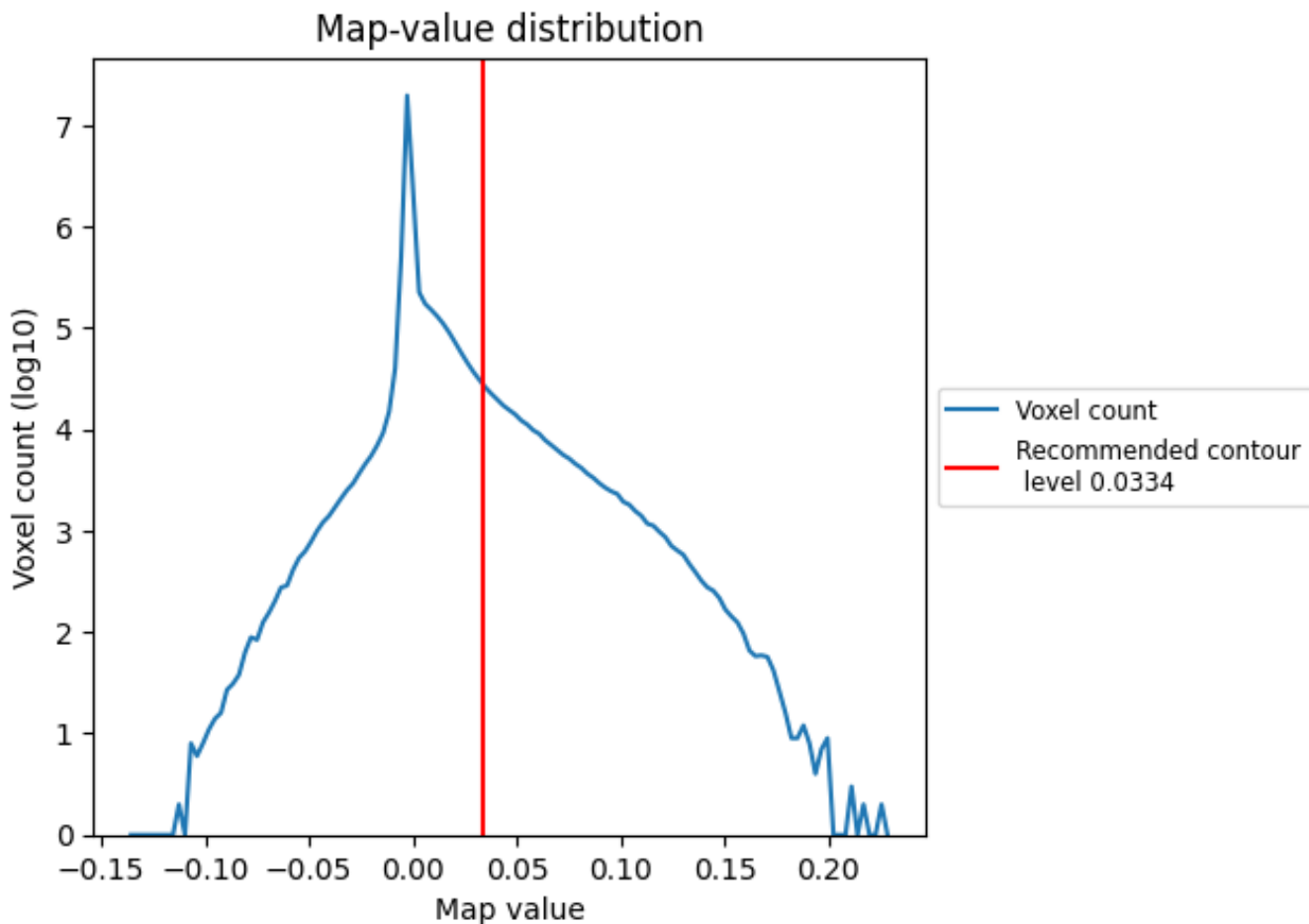
6.5 Mask visualisation

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

7 Map analysis [i](#)

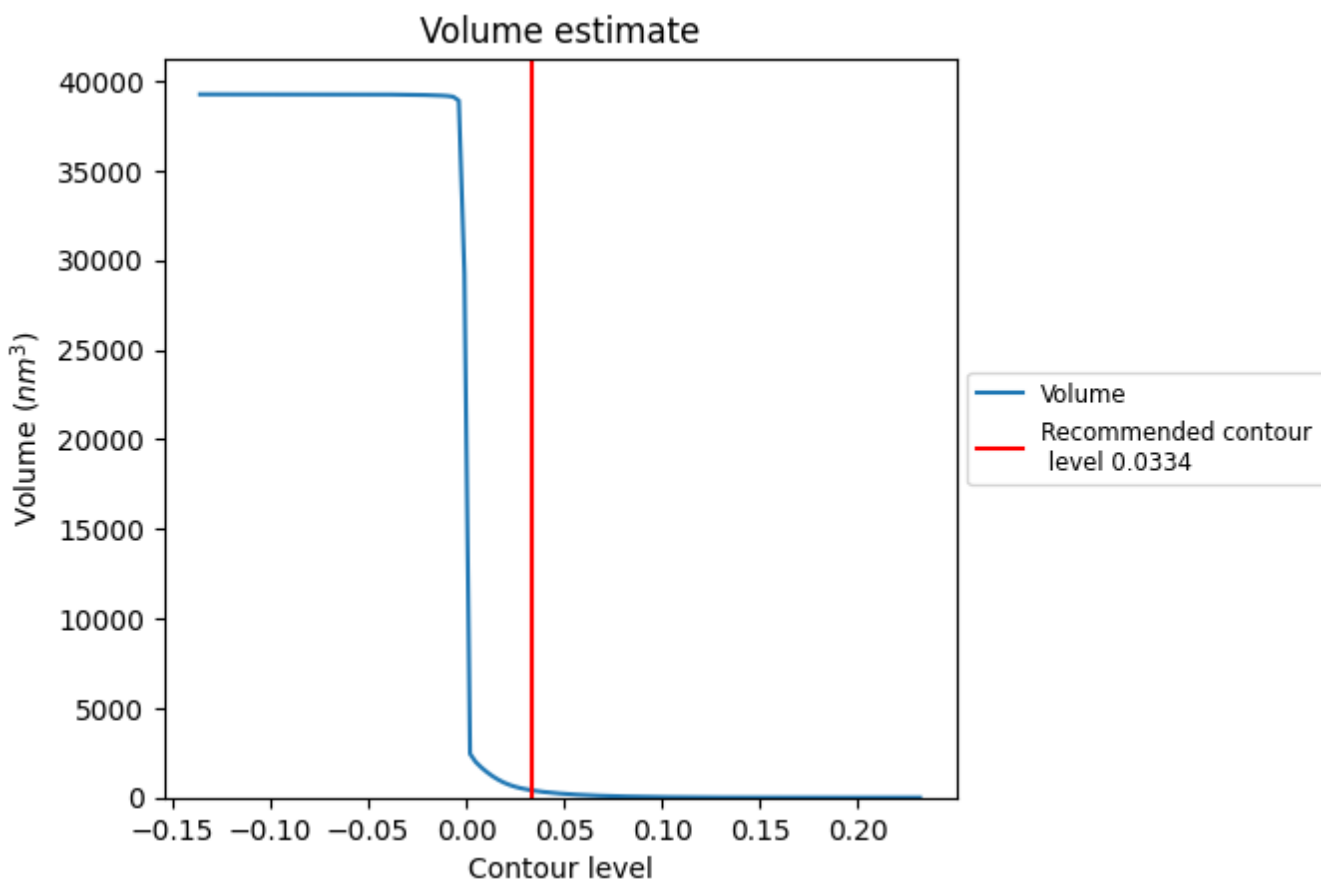
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

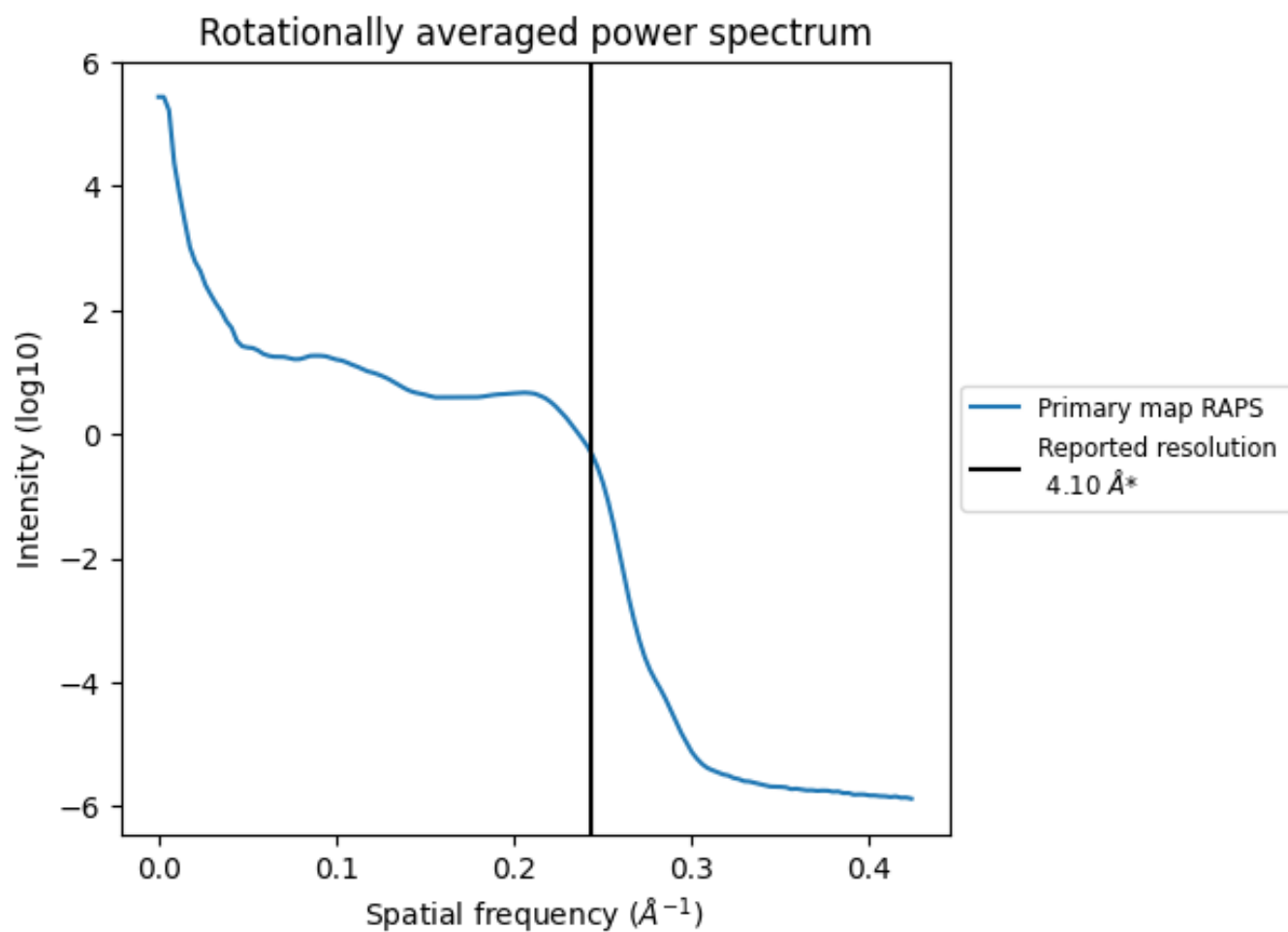
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 406 nm³; this corresponds to an approximate mass of 366 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

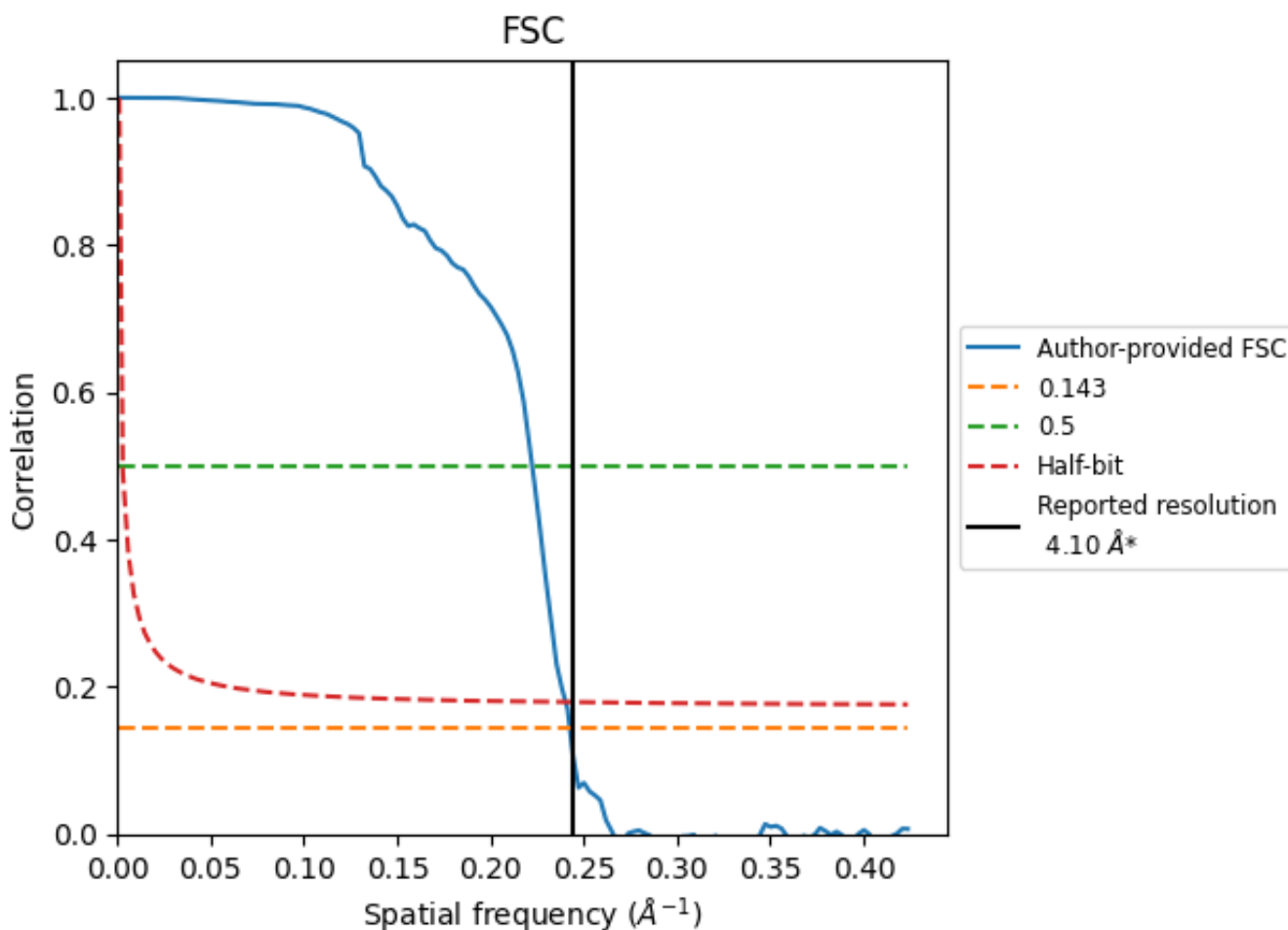


*Reported resolution corresponds to spatial frequency of 0.244\AA^{-1}

8 Fourier-Shell correlation [\(i\)](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [\(i\)](#)



*Reported resolution corresponds to spatial frequency of 0.244 Å⁻¹

8.2 Resolution estimates [i](#)

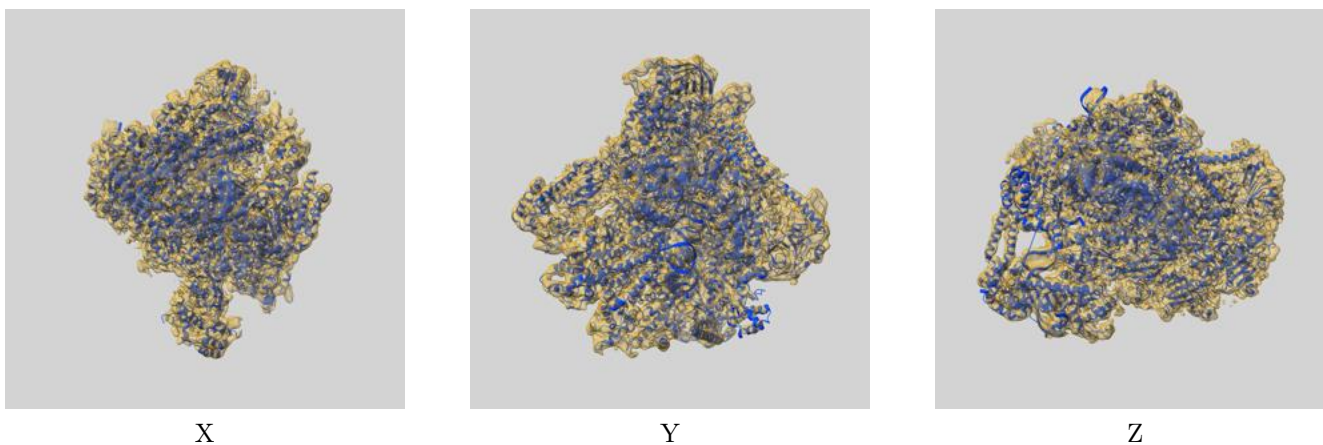
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.10	-	-
Author-provided FSC curve	4.12	4.50	4.16
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

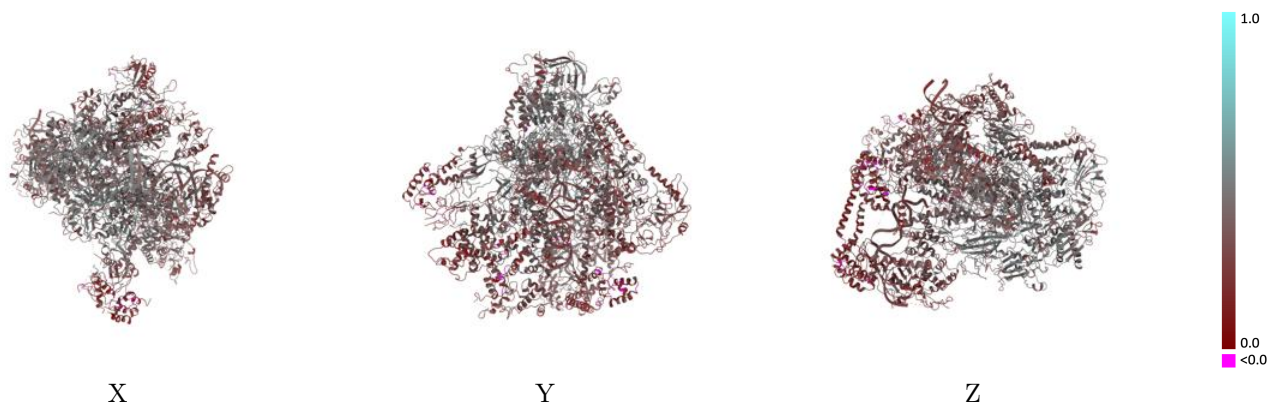
This section contains information regarding the fit between EMDB map EMD-7530 and PDB model 6CNB. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)



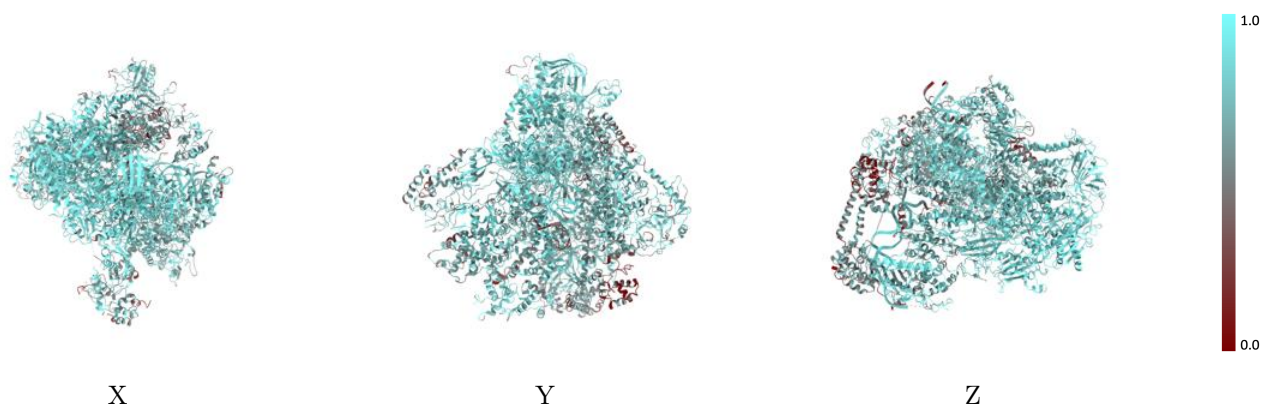
The images above show the 3D surface view of the map at the recommended contour level 0.0334 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



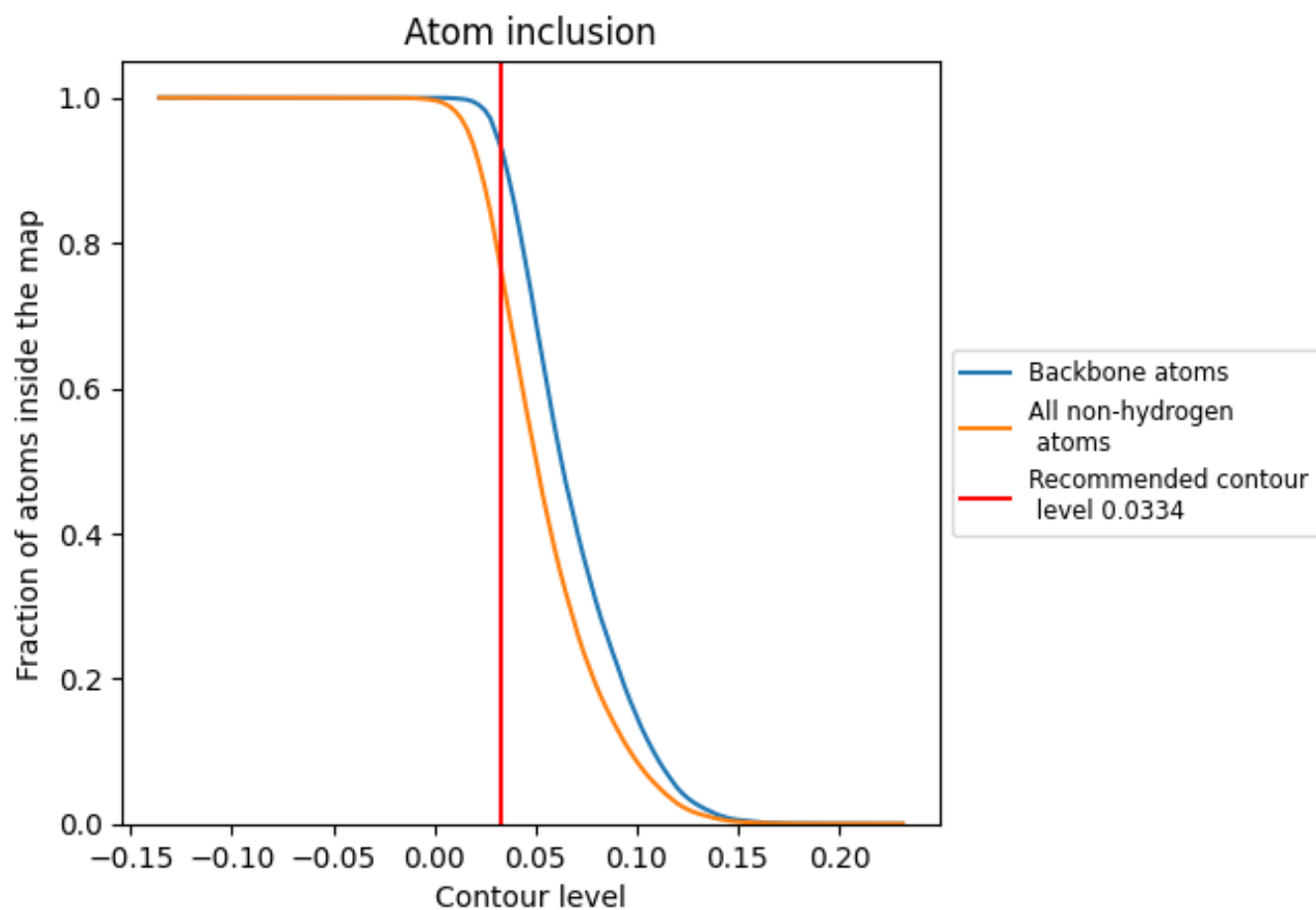
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0334).













































9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 76% 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 (0.0334) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7583	 0.3550
A	 0.7802	 0.3950
B	 0.7981	 0.4100
C	 0.8808	 0.4270
D	 0.6118	 0.2080
E	 0.7902	 0.3510
F	 0.8790	 0.4450
G	 0.7437	 0.2830
H	 0.8352	 0.4160
I	 0.7350	 0.3120
J	 0.8951	 0.4390
K	 0.8608	 0.4380
L	 0.8205	 0.4270
M	 0.6700	 0.2820
N	 0.6999	 0.2880
O	 0.7072	 0.3040
P	 0.6070	 0.2680
Q	 0.8658	 0.3680
R	 0.6677	 0.2830
S	 0.5591	 0.2440
X	 0.8890	 0.3240
Y	 0.8461	 0.3270

