



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 02:13 PM UTC

PDB ID : 6CND / pdb_00006cnd
EMDB ID : EMD-7532
Title : Yeast RNA polymerase III natural open complex (nOC)
Authors : Han, Y.; He, Y.
Deposited on : 2018-03-08
Resolution : 4.80 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

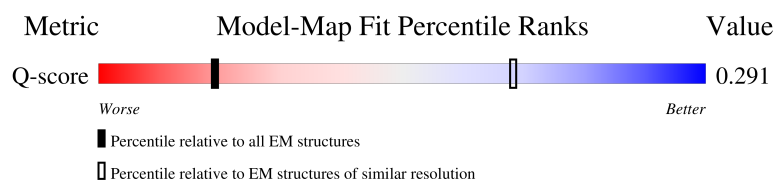
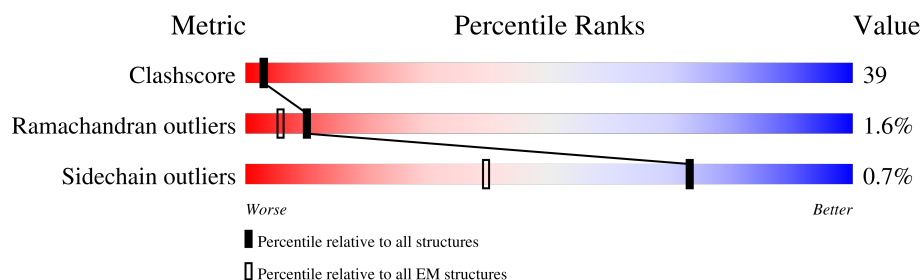
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 4.80 Å.

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



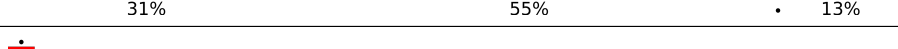
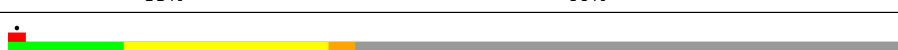
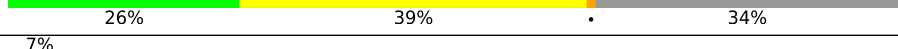
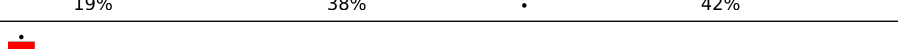
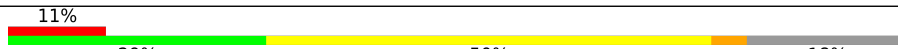
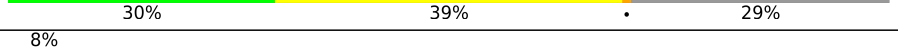
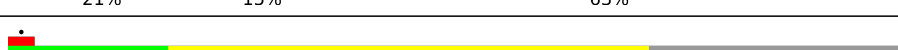
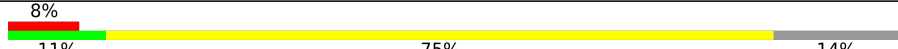
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	1575 (4.30 - 5.30)

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

Mol	Chain	Length	Quality of chain
1	A	1460	 9% 38% 57% ..
2	B	1149	 5% 38% 57% ..
3	C	335	 43% 54% .
4	D	161	 9% 39% 34% .. 26%

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Mol	Chain	Length	Quality of chain
5	E	215	
6	F	155	
7	G	212	
8	H	146	
9	I	110	
10	J	70	
11	K	142	
12	L	70	
13	M	282	
14	N	422	
15	O	654	
16	P	317	
17	Q	251	
18	R	736	
19	S	594	
20	X	71	
21	Y	71	

2 Entry composition

There are 22 unique types of molecules in this entry. The entry contains 47836 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
1	A	1428	Total	C	N	O	S	0	0
			11159	7029	1972	2099	59		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- 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
17	Q	54	Total	C	N	O	0	0
			368	238	64	66		

- 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
18	R	522	Total	C	N	O	S	0	0
			4131	2621	733	757	20		

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	conflict	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
19	S	217	Total	C	N	O	S	0	0
			1649	1035	286	321	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	X	51	Total	C	N	O	P	0	0
			1040	503	181	306	50		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Y	61	Total	C	N	O	P	0	0
			1249	602	223	364	60		

- Molecule 22 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

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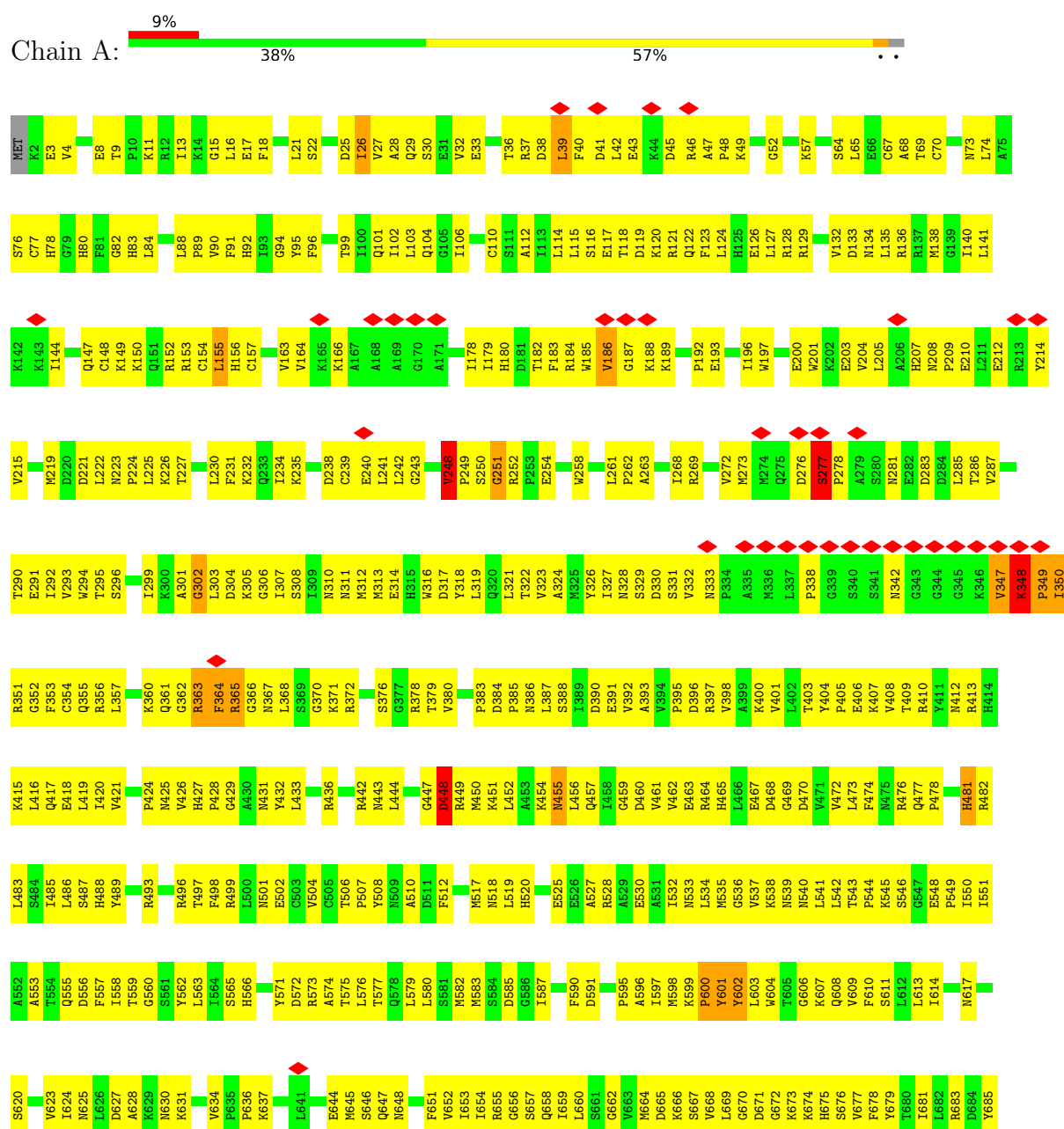
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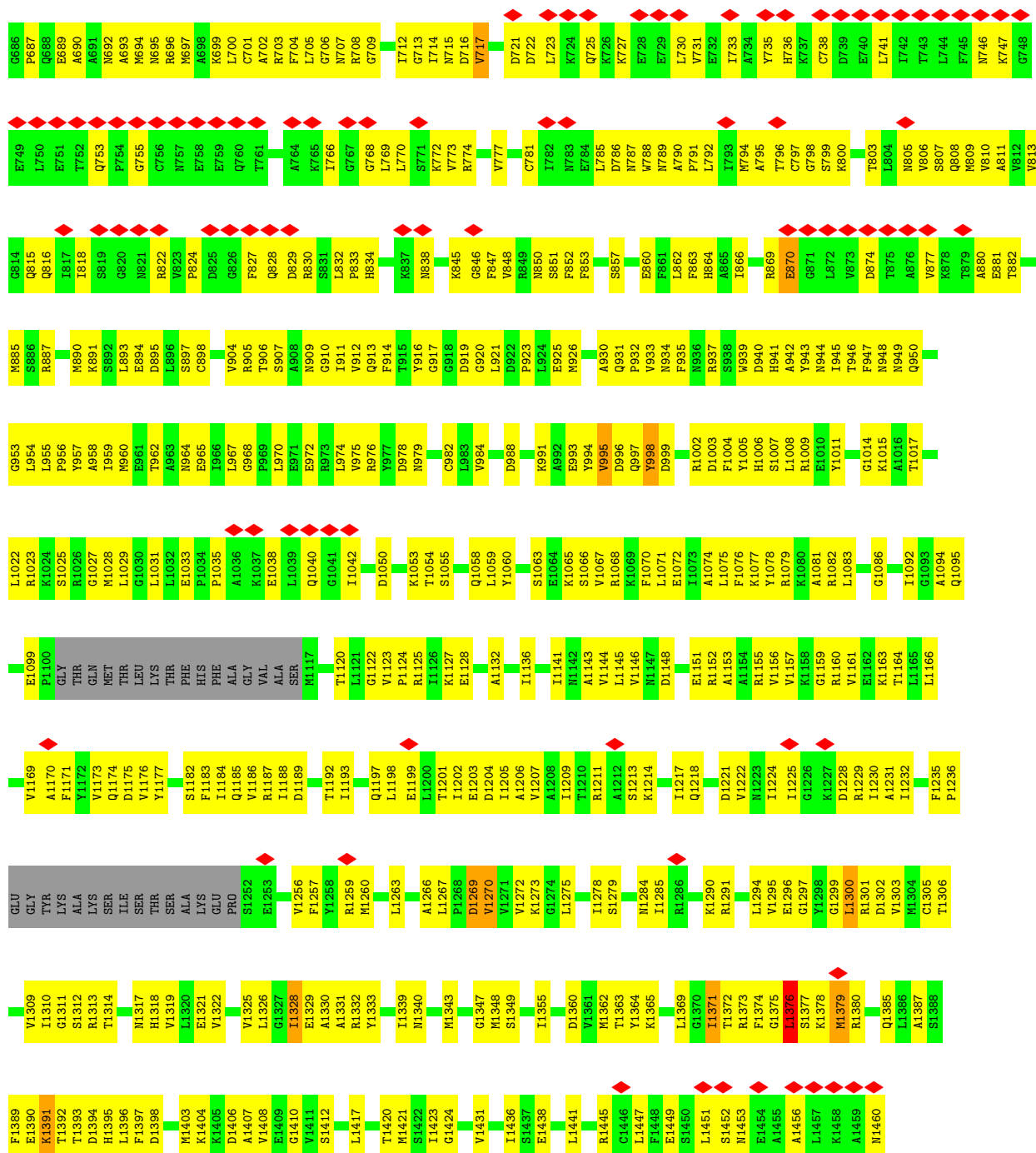
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
22	R	1	1	1	0

3 Residue-property plots

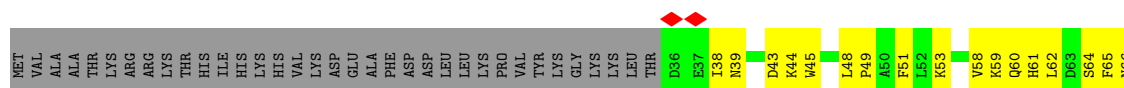
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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

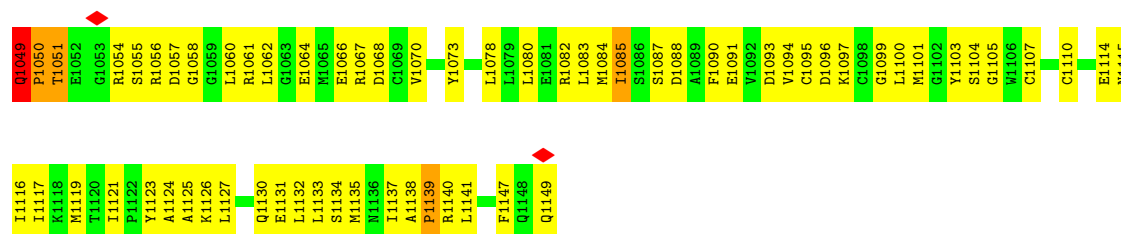




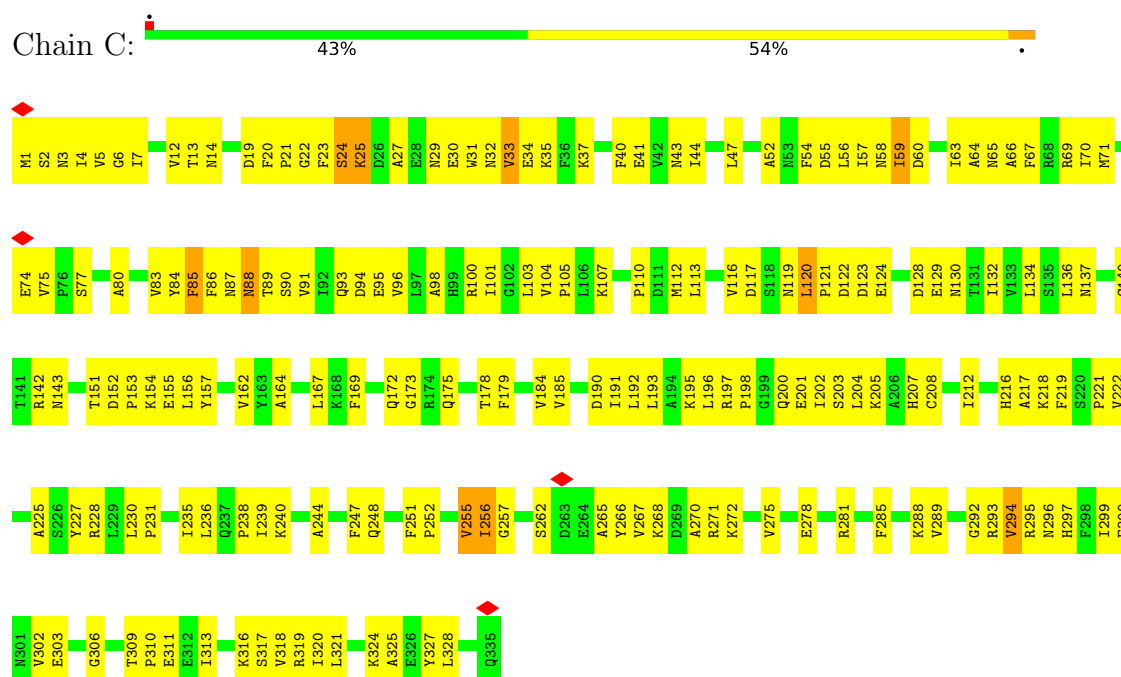
• Molecule 2: DNA-directed RNA polymerase III subunit RPC2



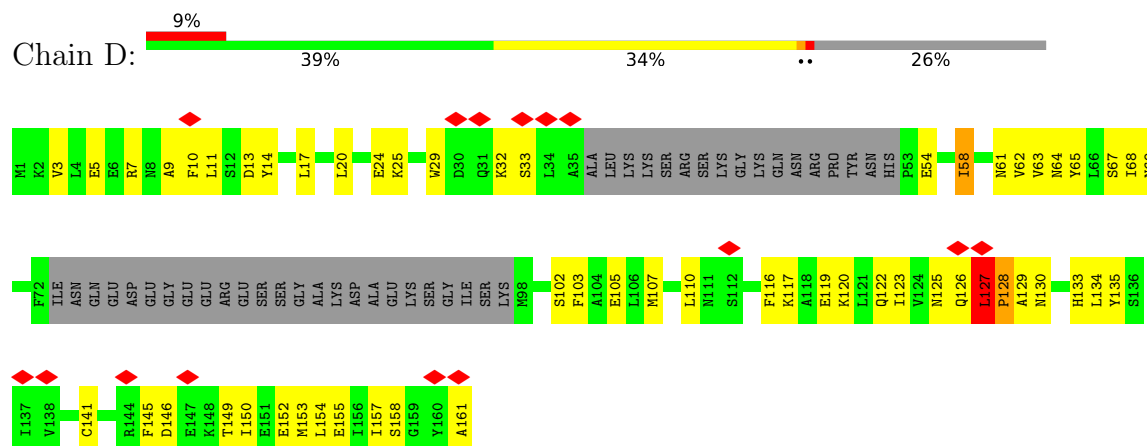




• Molecule 3: DNA-directed RNA polymerases I and III subunit RPAC1

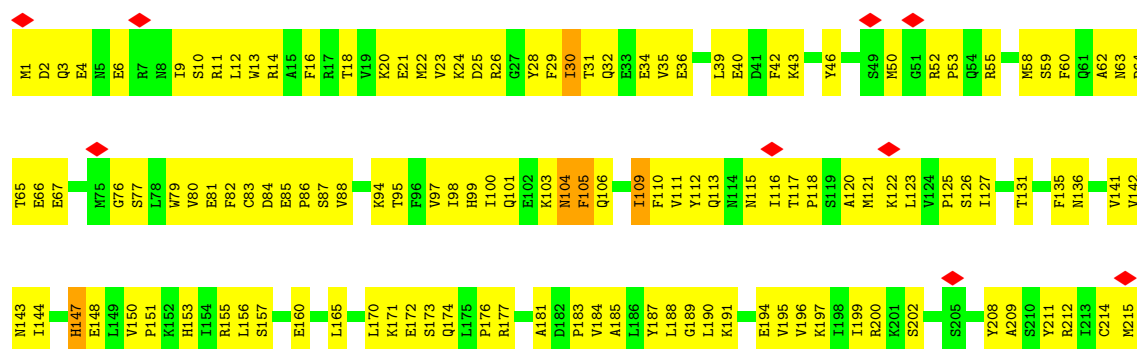


• Molecule 4: DNA-directed RNA polymerase III subunit RPC9

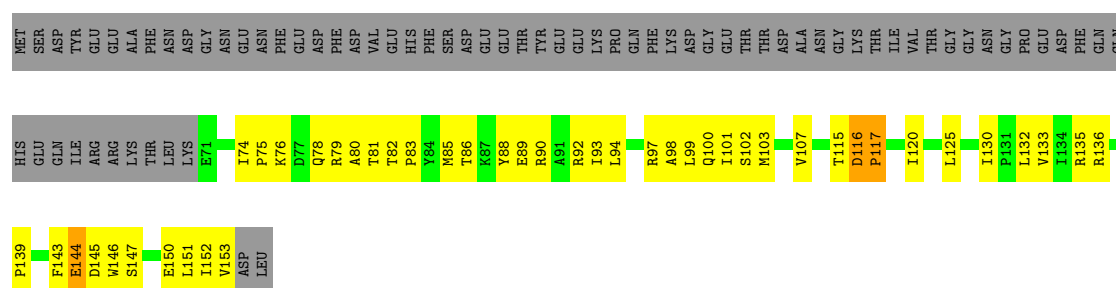
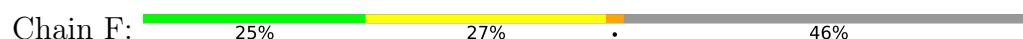


• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

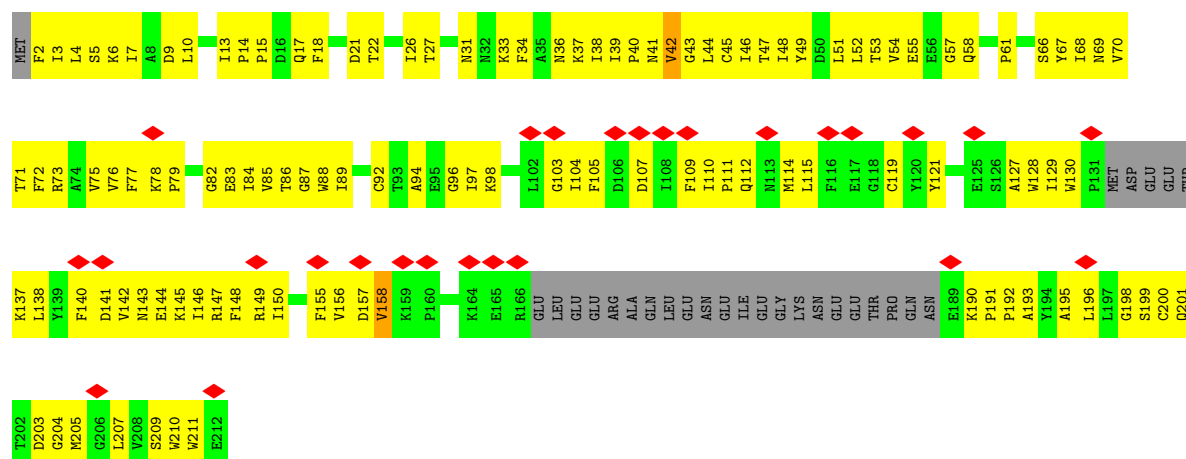




- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

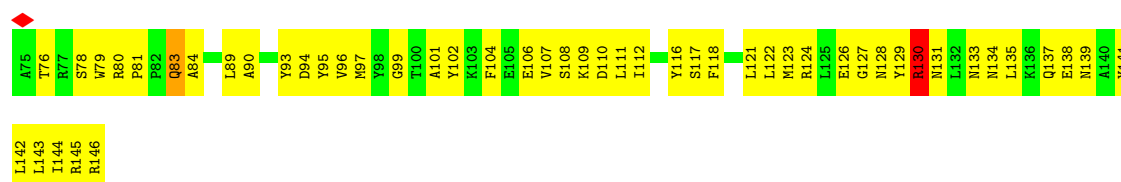


- Molecule 7: DNA-directed RNA polymerase III subunit RPC8

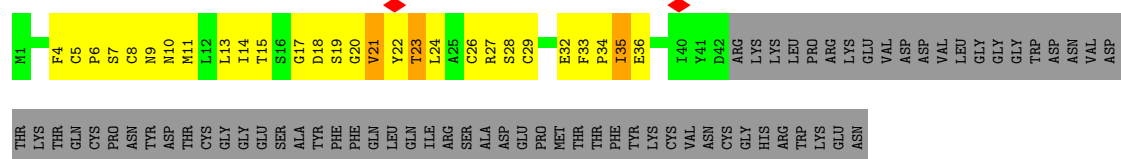


- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3





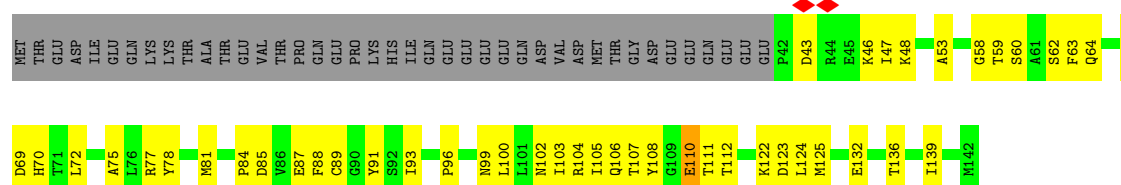
- Molecule 9: DNA-directed RNA polymerase III subunit RPC10



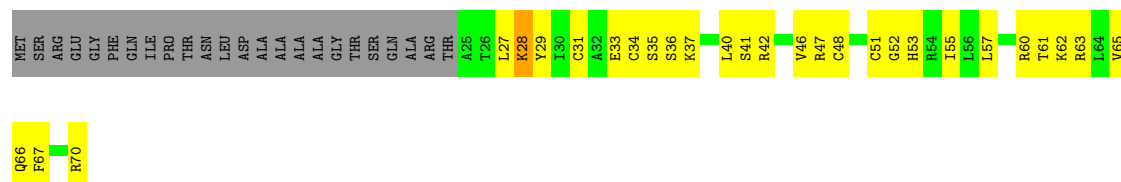
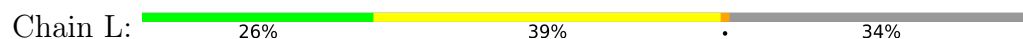
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5



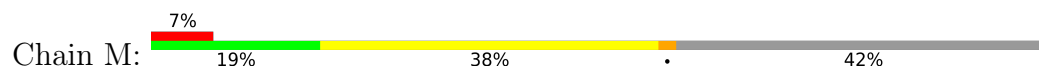
- Molecule 11: DNA-directed RNA polymerases I and III subunit RPAC2

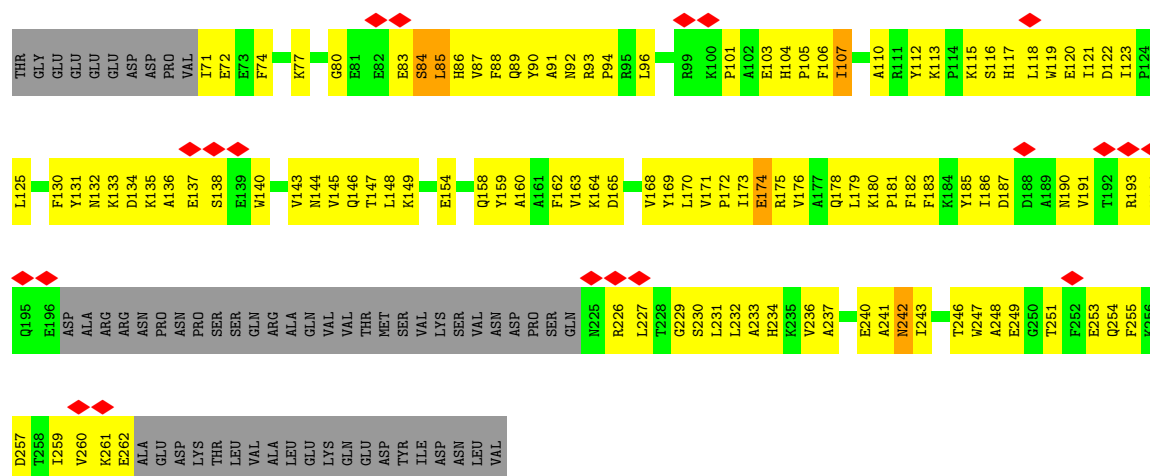


- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4



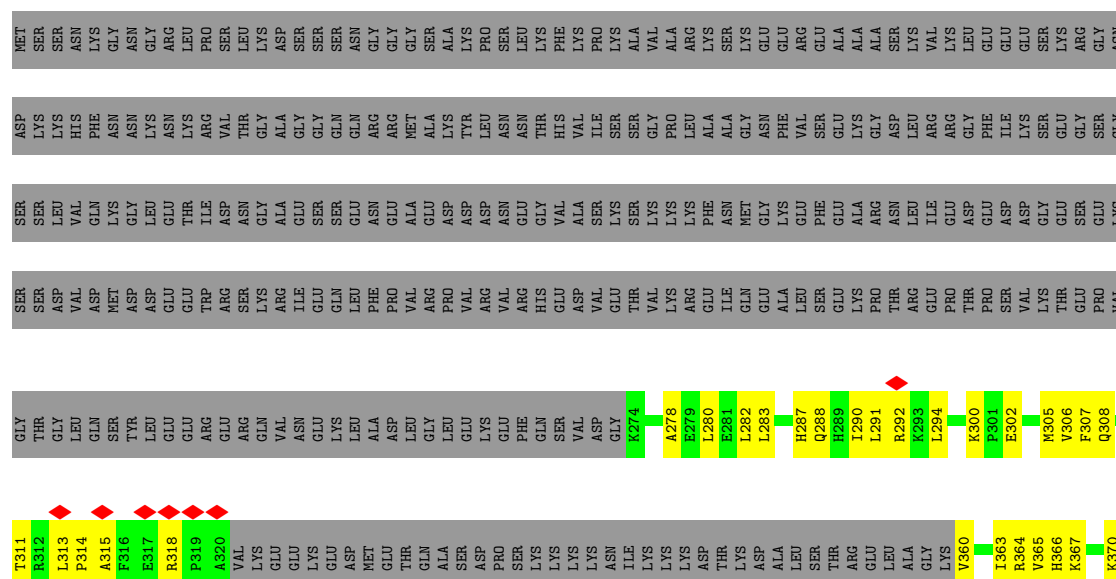
- Molecule 13: DNA-directed RNA polymerase III subunit RPC5





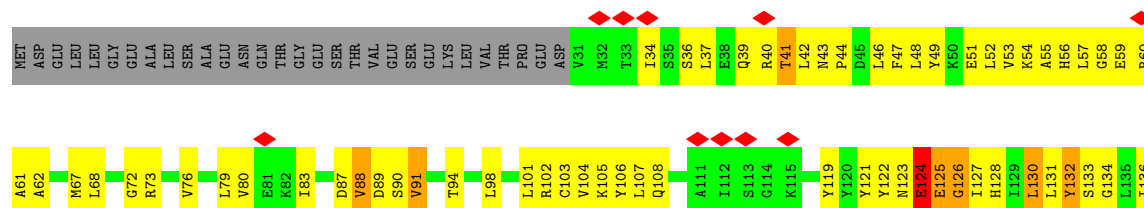
• Molecule 14: DNA-directed RNA polymerase III subunit RPC4

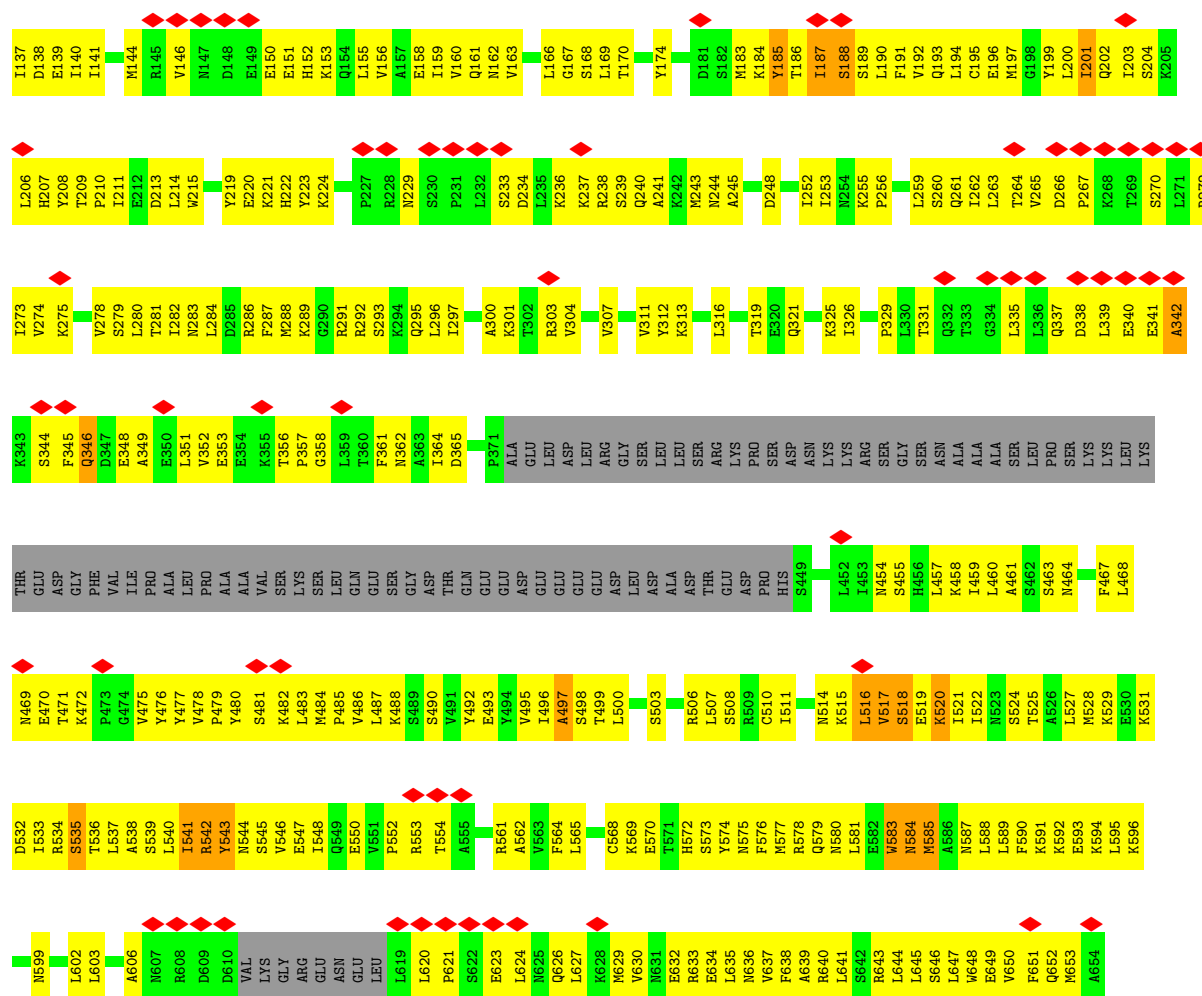
Chain N: 12% 14% 74%



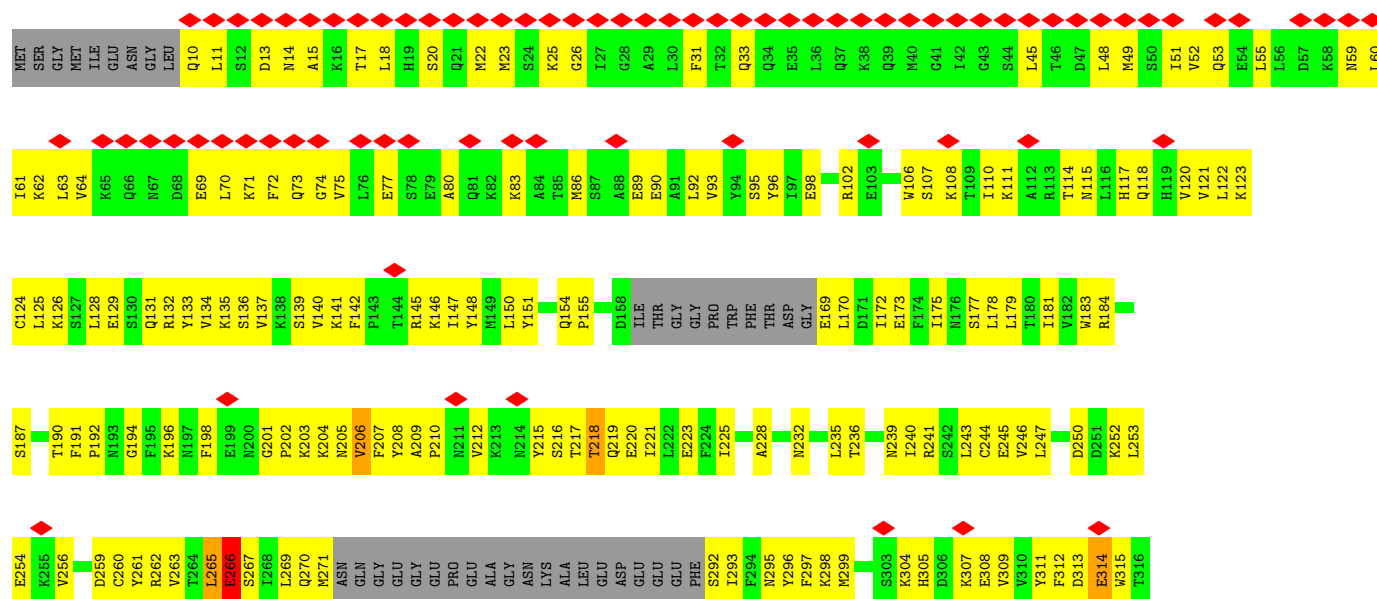
• Molecule 15: DNA-directed RNA polymerase III subunit RPC3

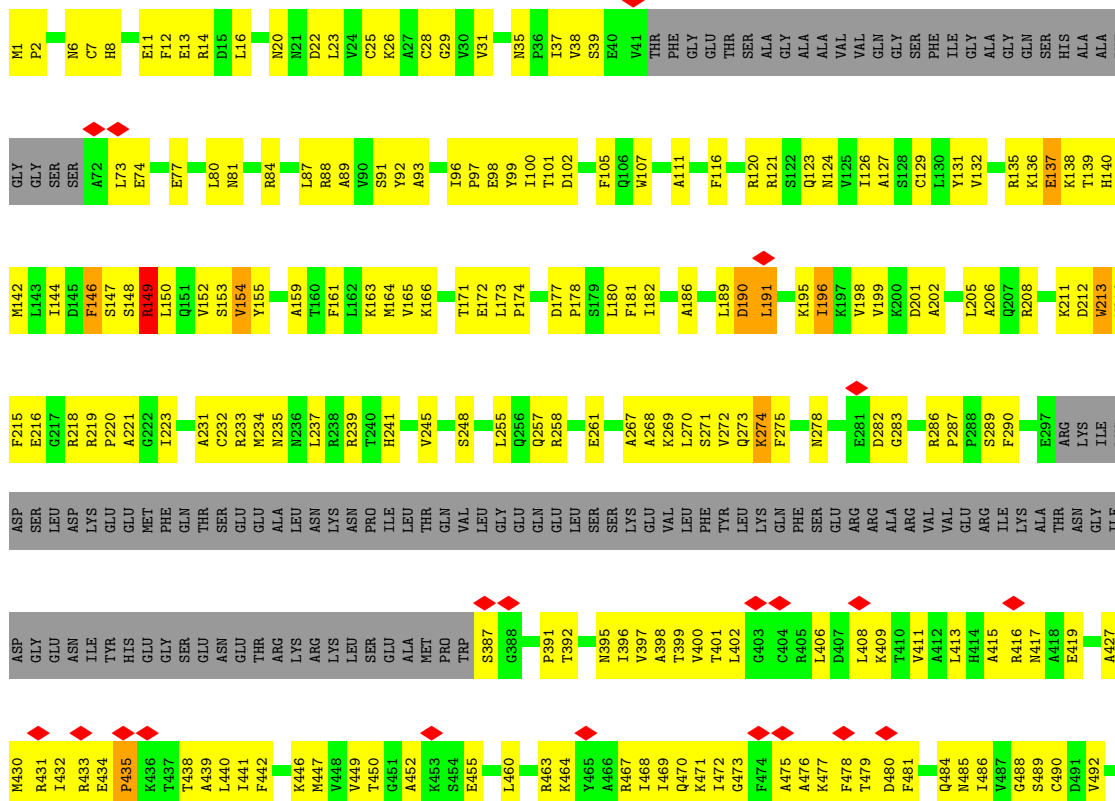
Chain O: 11% 29% 50% 18%

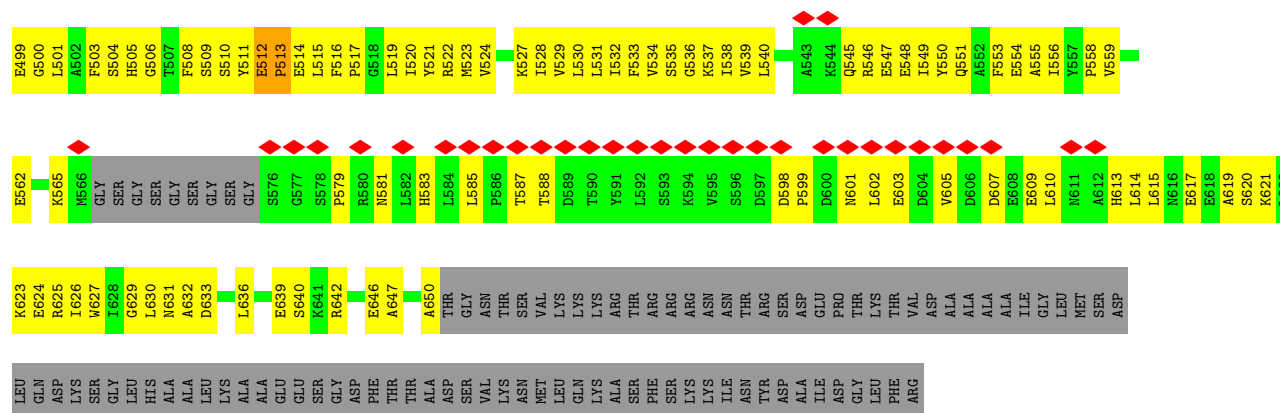




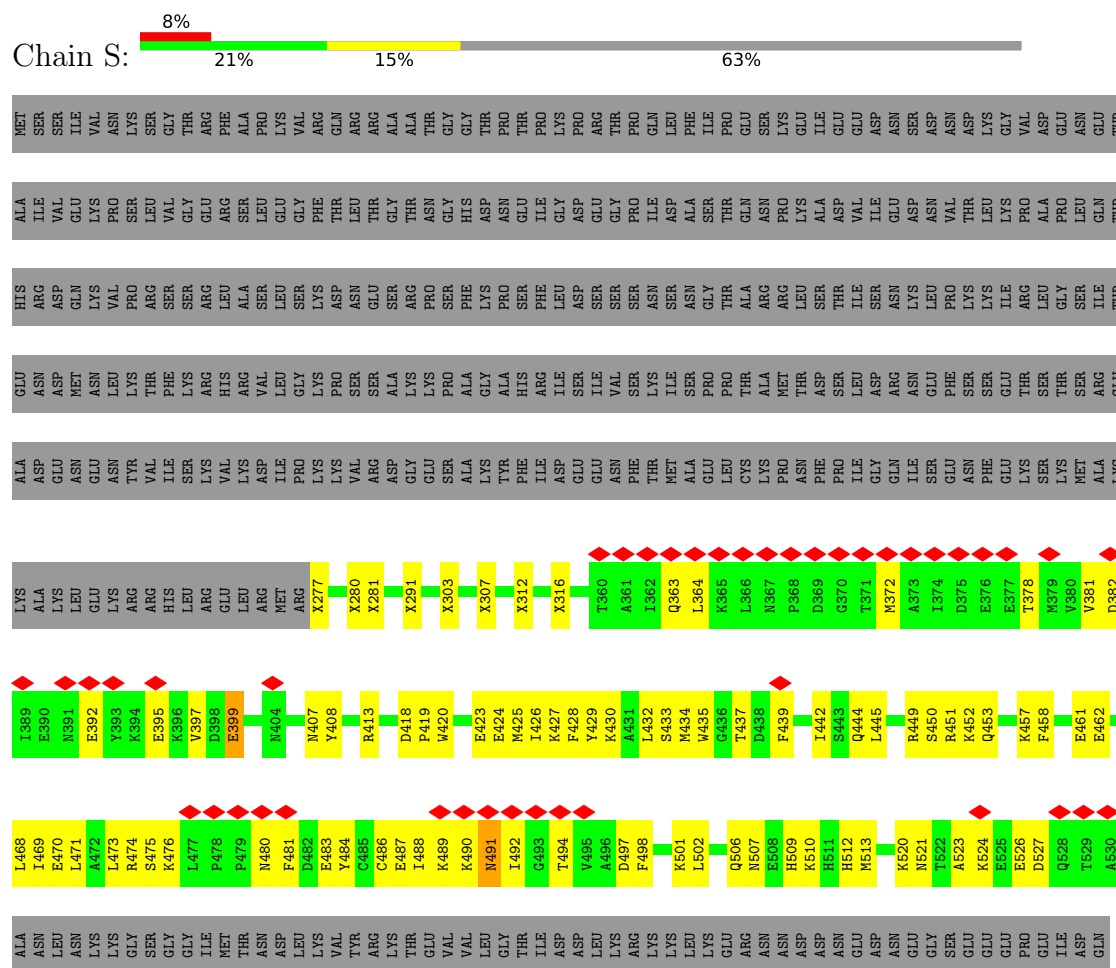
● Molecule 16: DNA-directed RNA polymerase III subunit RPC6



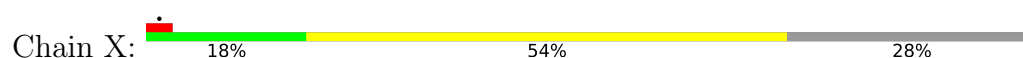




- Molecule 19: Transcription factor TFIIB component B",Transcription factor TFIIB component B",Transcription factor TFIIB component B",Transcription factor TFIIB component B"

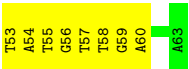
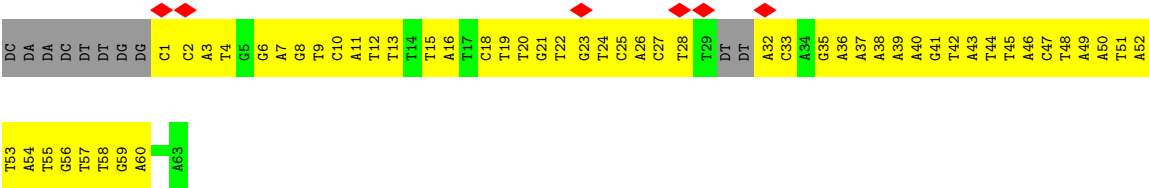


- Molecule 20: DNA (71-MER)





● Molecule 21: DNA (71-MER)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	96971	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	0.185	Depositor
Minimum map value	-0.101	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.035	Depositor
Map size (Å)	339.84, 339.84, 339.84	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.18, 1.18, 1.18	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.36	1/11358 (0.0%)	0.76	20/15345 (0.1%)
2	B	0.36	1/8943 (0.0%)	0.79	14/12068 (0.1%)
3	C	0.35	0/2711	0.75	5/3676 (0.1%)
4	D	0.22	0/991	0.64	0/1328
5	E	0.28	0/1795	0.69	4/2416 (0.2%)
6	F	0.36	0/683	0.77	1/923 (0.1%)
7	G	0.25	0/1523	0.64	0/2066
8	H	0.33	0/1138	0.77	3/1540 (0.2%)
9	I	0.32	0/328	0.80	0/445
10	J	0.39	0/558	0.74	0/750
11	K	0.37	0/803	0.76	1/1083 (0.1%)
12	L	0.31	0/365	0.79	1/485 (0.2%)
13	M	0.24	0/1369	0.68	4/1851 (0.2%)
14	N	0.25	0/855	0.64	0/1149
15	O	0.31	1/4394 (0.0%)	0.80	17/5928 (0.3%)
16	P	0.22	0/2282	0.64	1/3075 (0.0%)
17	Q	0.28	0/281	0.61	0/381
18	R	0.24	0/4200	0.70	10/5659 (0.2%)
19	S	0.19	0/1464	0.59	4/1971 (0.2%)
20	X	0.29	0/1164	0.51	0/1792
21	Y	0.28	0/1400	0.52	0/2157
All	All	0.32	3/48605 (0.0%)	0.73	85/66088 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	O	125	GLU	CA-C	8.75	1.64	1.52
2	B	517	MET	CA-CB	-5.45	1.46	1.52
1	A	348	LYS	CA-C	5.07	1.59	1.52

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	R	190	ASP	CB-CA-C	-11.34	103.50	116.54
18	R	512	GLU	CA-C-N	9.88	132.19	119.84
18	R	512	GLU	C-N-CA	9.88	132.19	119.84
18	R	190	ASP	N-CA-C	9.53	122.80	108.31
18	R	211	LYS	N-CA-C	9.36	121.48	111.28
1	A	347	VAL	N-CA-C	9.06	122.37	111.05
15	O	461	ALA	N-CA-C	8.61	121.74	111.33
15	O	524	SER	N-CA-C	8.39	121.55	111.82
18	R	146	PHE	N-CA-C	8.02	120.93	111.71
2	B	1043	ARG	N-CA-C	7.73	121.52	109.07
19	S	489	LYS	N-CA-C	-7.65	103.01	113.18
2	B	877	GLU	N-CA-C	7.55	114.79	108.07
3	C	151	THR	CA-C-N	-7.54	110.39	120.65
3	C	151	THR	C-N-CA	-7.54	110.39	120.65
15	O	585	MET	N-CA-C	7.39	120.03	111.02
15	O	522	ILE	N-CA-C	7.34	117.43	110.53
5	E	181	ALA	CA-C-N	-7.26	110.17	120.49
5	E	181	ALA	C-N-CA	-7.26	110.17	120.49
3	C	24	SER	N-CA-C	7.05	120.89	109.40
15	O	130	LEU	N-CA-C	7.01	119.52	111.11
1	A	248	VAL	CA-C-N	6.91	128.48	119.84
1	A	248	VAL	C-N-CA	6.91	128.48	119.84
15	O	463	SER	N-CA-C	-6.86	99.75	109.96
15	O	584	ASN	N-CA-C	6.82	120.82	112.23
15	O	525	THR	N-CA-C	6.80	118.77	111.36
1	A	1375	GLY	N-CA-C	6.79	121.11	112.83
5	E	104	ASN	CB-CA-C	-6.70	108.12	117.23
1	A	481	HIS	N-CA-C	6.69	117.07	108.24
1	A	1391	LYS	CB-CA-C	-6.52	102.28	111.80
1	A	600	PRO	CB-CA-C	-6.38	104.41	113.09
1	A	870	GLU	N-CA-C	6.35	118.73	111.11
11	K	110	GLU	N-CA-C	6.33	119.24	108.67
2	B	1047	THR	N-CA-C	-6.26	105.68	113.38
1	A	717	VAL	N-CA-C	6.24	118.85	111.05
8	H	130	ARG	N-CA-C	-6.22	97.55	110.80
2	B	863	GLN	N-CA-C	-6.18	105.39	113.17
15	O	132	TYR	N-CA-C	-6.15	103.19	112.04
2	B	976	GLY	N-CA-C	-6.14	106.45	115.72
15	O	125	GLU	CA-C-O	6.13	126.61	119.32
1	A	451	LYS	N-CA-C	6.13	119.59	111.75
8	H	108	SER	CB-CA-C	-5.98	109.66	116.54
19	S	399	GLU	CA-C-N	-5.96	109.32	121.48
19	S	399	GLU	C-N-CA	-5.96	109.32	121.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	R	213	TRP	N-CA-C	5.92	119.82	112.24
1	A	302	GLY	N-CA-C	-5.90	105.14	111.93
1	A	1376	LEU	N-CA-C	-5.90	104.76	111.07
13	M	174	GLU	CB-CA-C	-5.85	109.28	117.23
13	M	103	GLU	CA-C-N	-5.83	109.90	122.67
13	M	103	GLU	C-N-CA	-5.83	109.90	122.67
2	B	934	ASN	CB-CA-C	-5.82	108.19	116.34
2	B	877	GLU	CA-C-N	5.78	127.06	119.84
2	B	877	GLU	C-N-CA	5.78	127.06	119.84
18	R	139	THR	N-CA-C	-5.74	101.02	109.81
15	O	342	ALA	N-CA-C	-5.70	104.68	111.69
2	B	1141	LEU	N-CA-CB	-5.65	101.21	110.41
16	P	266	GLU	N-CA-C	-5.65	106.47	113.19
8	H	83	GLN	CB-CA-C	-5.60	108.50	116.34
18	R	137	GLU	N-CA-C	-5.56	106.16	113.17
3	C	85	PHE	N-CA-C	5.47	118.38	109.24
6	F	117	PRO	N-CA-CB	-5.47	98.27	103.41
15	O	125	GLU	CB-CA-C	-5.46	100.95	110.17
1	A	1379	MET	N-CA-C	-5.43	105.71	112.93
19	S	491	ASN	N-CA-C	5.41	122.32	110.80
15	O	124	GLU	CA-C-N	-5.34	114.22	122.49
15	O	124	GLU	C-N-CA	-5.34	114.22	122.49
2	B	588	ILE	N-CA-C	-5.33	98.26	109.34
1	A	448	ASP	N-CA-C	5.31	122.12	110.80
5	E	105	PHE	CB-CA-C	-5.25	108.96	115.89
18	R	196	ILE	N-CA-C	5.22	115.84	110.36
13	M	174	GLU	N-CA-C	5.21	117.38	108.67
15	O	346	GLN	N-CA-C	-5.21	106.08	112.90
2	B	384	ILE	N-CA-C	5.21	116.55	110.62
2	B	1135	MET	CA-C-N	-5.16	115.55	122.42
2	B	1135	MET	C-N-CA	-5.16	115.55	122.42
1	A	652	VAL	N-CA-C	-5.16	102.94	109.80
1	A	788	TRP	N-CA-C	-5.12	106.34	112.58
2	B	934	ASN	N-CA-C	5.11	115.56	108.00
15	O	525	THR	CB-CA-C	-5.11	102.17	110.85
1	A	1082	ARG	CA-C-N	-5.08	113.93	121.24
1	A	1082	ARG	C-N-CA	-5.08	113.93	121.24
1	A	602	TYR	N-CA-CB	5.07	117.66	110.46
1	A	348	LYS	CA-C-O	5.03	127.05	120.16
12	L	28	LYS	N-CA-C	5.03	116.57	111.14
3	C	306	GLY	N-CA-C	-5.02	108.19	115.27
15	O	520	LYS	N-CA-C	-5.01	105.82	111.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11159	0	11285	991	0
2	B	8788	0	8902	775	0
3	C	2655	0	2628	234	0
4	D	977	0	983	60	0
5	E	1759	0	1788	126	0
6	F	671	0	692	56	0
7	G	1484	0	1485	131	0
8	H	1120	0	1089	87	0
9	I	321	0	305	35	0
10	J	549	0	559	45	0
11	K	792	0	790	55	0
12	L	363	0	386	29	0
13	M	1338	0	1307	135	0
14	N	845	0	891	80	0
15	O	4329	0	4497	473	0
16	P	2242	0	2265	179	0
17	Q	368	0	308	23	0
18	R	4131	0	4230	324	0
19	S	1649	0	1456	92	0
20	X	1040	0	584	45	0
21	Y	1249	0	696	82	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	47836	0	47126	3646	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 39.

All (3646) 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)
1:A:364:PHE:CD2	1:A:365:ARG:HD3	1.42	1.49
1:A:248:VAL:CG2	1:A:249:PRO:HD2	1.41	1.46
1:A:248:VAL:HG23	1:A:249:PRO:CD	1.48	1.42
3:C:83:VAL:CG1	3:C:85:PHE:CE2	2.06	1.36
2:B:1049:GLN:HB2	2:B:1050:PRO:CD	1.49	1.31
15:O:200:LEU:O	15:O:201:ILE:HG13	1.32	1.29
18:R:22:ASP:CG	18:R:31:VAL:HG11	1.59	1.27
18:R:149:ARG:O	18:R:150:LEU:HD12	1.35	1.27
2:B:524:ASP:HB2	2:B:587:PHE:CZ	1.71	1.26
1:A:248:VAL:CG2	1:A:249:PRO:CD	2.10	1.25
15:O:124:GLU:CG	15:O:125:GLU:H	1.50	1.24
18:R:98:GLU:O	18:R:101:THR:HG22	1.32	1.24
3:C:83:VAL:HG12	3:C:85:PHE:CE2	1.67	1.23
2:B:695:GLN:CG	2:B:697:PRO:HD2	1.67	1.22
1:A:18:PHE:CE1	2:B:1139:PRO:HB3	1.74	1.21
1:A:154:CYS:HB3	1:A:157:CYS:SG	1.82	1.20
2:B:521:THR:HG22	2:B:586:GLU:OE2	1.40	1.20
3:C:83:VAL:HG11	3:C:85:PHE:CZ	1.76	1.20
3:C:83:VAL:HG11	3:C:85:PHE:CE2	1.75	1.17
1:A:364:PHE:CE2	1:A:365:ARG:HD3	1.80	1.17
2:B:776:SER:HA	2:B:779:ASP:HB3	1.22	1.16
2:B:695:GLN:HG3	2:B:697:PRO:CD	1.75	1.15
11:K:110:GLU:CD	11:K:111:THR:H	1.52	1.15
1:A:364:PHE:CD2	1:A:365:ARG:CD	2.31	1.14
15:O:190:LEU:HD23	15:O:194:LEU:HD23	1.29	1.14
18:R:429:ILE:HG21	18:R:431:ARG:NH1	1.61	1.14
1:A:319:LEU:O	1:A:322:THR:HG22	1.45	1.14
18:R:22:ASP:OD2	18:R:31:VAL:HG11	1.44	1.13
1:A:525:GLU:OE2	6:F:102:SER:HB2	1.47	1.13
1:A:363:ARG:NH2	2:B:1046:LEU:HD21	1.64	1.13
2:B:170:LYS:O	2:B:174:LEU:HB2	1.47	1.13
2:B:552:ASN:HD21	2:B:566:ARG:HD2	1.08	1.12
1:A:357:LEU:HD12	1:A:363:ARG:HB3	1.13	1.11
2:B:1049:GLN:HB2	2:B:1050:PRO:HD3	1.23	1.11
13:M:85:LEU:HG	14:N:398:SER:HB3	1.13	1.11
18:R:7:CYS:SG	18:R:28:CYS:HB3	1.89	1.11
1:A:248:VAL:HB	1:A:249:PRO:HD3	1.33	1.11
1:A:378:ARG:HD2	2:B:1060:LEU:CD2	1.78	1.11
1:A:110:CYS:SG	1:A:156:HIS:CE1	2.43	1.11
1:A:248:VAL:CB	1:A:249:PRO:CD	2.27	1.10
2:B:767:ILE:HG23	2:B:768:GLU:H	1.09	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:517:VAL:HG23	15:O:518:SER:H	1.07	1.10
1:A:18:PHE:HE1	2:B:1139:PRO:HB3	0.99	1.10
1:A:1376:LEU:O	1:A:1378:LYS:HG2	1.52	1.09
1:A:1176:VAL:O	1:A:1183:PHE:HB2	1.52	1.09
6:F:116:ASP:OD1	6:F:117:PRO:HD2	1.50	1.09
6:F:116:ASP:CG	6:F:117:PRO:HD2	1.76	1.08
1:A:525:GLU:OE1	6:F:99:LEU:HA	1.52	1.08
1:A:276:ASP:O	1:A:277:SER:HB2	1.52	1.07
15:O:200:LEU:HD22	15:O:281:THR:HA	1.29	1.07
1:A:444:LEU:HD22	1:A:449:ARG:HD3	1.33	1.07
1:A:347:VAL:C	1:A:349:PRO:HD3	1.81	1.06
1:A:18:PHE:HE1	2:B:1139:PRO:CB	1.67	1.06
13:M:112:TYR:H	13:M:243:ILE:HG21	1.11	1.06
15:O:297:ILE:O	15:O:301:LYS:HB2	1.55	1.06
19:S:470:GLU:O	19:S:474:ARG:HB3	1.54	1.05
15:O:200:LEU:HD23	15:O:282:ILE:N	1.72	1.05
2:B:776:SER:HB2	3:C:217:ALA:HB2	1.37	1.04
15:O:636:ASN:O	15:O:640:ARG:HB2	1.55	1.04
15:O:199:TYR:CZ	15:O:200:LEU:HD12	1.93	1.04
1:A:364:PHE:CE2	1:A:365:ARG:CD	2.41	1.03
3:C:83:VAL:CG1	3:C:85:PHE:CZ	2.36	1.03
15:O:124:GLU:HG2	15:O:125:GLU:N	1.30	1.03
2:B:1049:GLN:HB2	2:B:1050:PRO:HD2	1.38	1.02
1:A:357:LEU:CD1	1:A:363:ARG:HB3	1.89	1.01
1:A:444:LEU:CD2	1:A:449:ARG:HD3	1.90	1.01
15:O:200:LEU:HD22	15:O:281:THR:CA	1.90	1.01
15:O:215:TRP:O	15:O:219:TYR:HB2	1.61	1.01
1:A:1256:VAL:O	1:A:1260:MET:HB2	1.58	1.00
2:B:1049:GLN:CB	2:B:1050:PRO:CD	2.40	1.00
4:D:126:GLN:O	4:D:127:LEU:HG	1.58	0.99
16:P:137:VAL:HB	16:P:147:ILE:O	1.62	0.99
2:B:552:ASN:ND2	2:B:566:ARG:HD2	1.78	0.99
3:C:119:ASN:O	3:C:120:LEU:HG	1.63	0.99
15:O:195:CYS:SG	15:O:274:VAL:CG1	2.51	0.98
15:O:105:LYS:HE3	15:O:124:GLU:H	1.26	0.98
1:A:602:TYR:OH	3:C:25:LYS:HA	1.63	0.98
15:O:543:TYR:CD2	16:P:312:PHE:HZ	1.81	0.98
7:G:83:GLU:O	7:G:149:ARG:HA	1.64	0.97
6:F:116:ASP:OD1	6:F:117:PRO:CD	2.11	0.97
3:C:105:PRO:HG3	10:J:6:ARG:HH21	1.26	0.97
2:B:584:VAL:HB	2:B:588:ILE:HD12	1.47	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:772:VAL:HG13	2:B:943:ILE:HG23	1.47	0.97
15:O:190:LEU:CD2	15:O:194:LEU:HD23	1.95	0.96
15:O:288:MET:SD	15:O:291:ARG:NH2	2.39	0.96
3:C:117:ASP:CB	3:C:120:LEU:HD21	1.95	0.96
1:A:364:PHE:HZ	1:A:1389:PHE:O	1.48	0.95
15:O:37:LEU:O	15:O:41:THR:HB	1.64	0.95
1:A:347:VAL:HG12	1:A:349:PRO:CD	1.96	0.95
1:A:1166:LEU:HD13	1:A:1270:VAL:HG23	1.49	0.95
16:P:311:TYR:HA	17:Q:40:PRO:HA	1.44	0.95
1:A:362:GLY:O	1:A:367:ASN:HB3	1.66	0.95
1:A:248:VAL:CB	1:A:249:PRO:HD3	1.93	0.95
1:A:378:ARG:HD2	2:B:1060:LEU:HD21	1.45	0.95
1:A:378:ARG:HD2	2:B:1060:LEU:HD22	1.46	0.95
7:G:40:PRO:O	7:G:42:VAL:HG12	1.67	0.95
1:A:790:ALA:N	1:A:791:PRO:HD2	1.82	0.94
15:O:199:TYR:CE2	15:O:200:LEU:HB2	2.03	0.94
18:R:558:PRO:O	18:R:562:GLU:HB2	1.68	0.94
19:S:483:GLU:O	19:S:487:GLU:HB2	1.66	0.94
15:O:133:SER:HB3	17:Q:58:TYR:CE2	2.03	0.94
2:B:524:ASP:HB2	2:B:587:PHE:CE1	2.03	0.94
18:R:400:VAL:HA	18:R:480:ASP:O	1.68	0.94
14:N:290:ILE:O	14:N:294:LEU:HB2	1.69	0.93
16:P:33:GLN:NE2	16:P:49:MET:SD	2.40	0.93
18:R:22:ASP:OD1	18:R:31:VAL:HG11	1.69	0.93
1:A:364:PHE:HD2	1:A:365:ARG:CD	1.77	0.93
1:A:363:ARG:HH22	2:B:1046:LEU:HD21	1.30	0.93
15:O:200:LEU:CD2	15:O:282:ILE:N	2.32	0.92
1:A:250:SER:O	1:A:252:ARG:N	2.02	0.92
2:B:1022:ILE:HG22	2:B:1023:TYR:H	1.32	0.92
1:A:248:VAL:HB	1:A:249:PRO:CD	1.93	0.92
1:A:364:PHE:HZ	1:A:1389:PHE:C	1.77	0.92
18:R:190:ASP:CG	18:R:191:LEU:H	1.73	0.92
18:R:632:ALA:O	18:R:636:LEU:HB2	1.70	0.92
11:K:110:GLU:CD	11:K:111:THR:N	2.27	0.92
19:S:458:PHE:O	19:S:462:GLU:HB2	1.70	0.91
3:C:84:TYR:HB2	3:C:205:LYS:O	1.71	0.91
15:O:200:LEU:HB3	15:O:281:THR:N	1.86	0.91
1:A:200:GLU:C	15:O:516:LEU:HD21	1.95	0.90
1:A:1285:ILE:HA	1:A:1291:ARG:HG2	1.53	0.90
15:O:107:LEU:HB3	15:O:119:TYR:O	1.70	0.90
8:H:118:PHE:HB2	8:H:121:LEU:HB2	1.49	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:58:THR:O	8:H:143:LEU:HB3	1.69	0.90
1:A:1378:LYS:HG3	1:A:1379:MET:H	1.35	0.90
15:O:200:LEU:O	15:O:201:ILE:CG1	2.19	0.90
1:A:252:ARG:HH21	15:O:44:PRO:HD2	1.37	0.90
2:B:524:ASP:HB2	2:B:587:PHE:HZ	1.19	0.90
1:A:362:GLY:O	1:A:367:ASN:CB	2.21	0.89
7:G:87:GLY:O	7:G:146:ILE:HB	1.72	0.89
3:C:231:PRO:HA	3:C:293:ARG:HG2	1.55	0.89
8:H:97:MET:HB2	8:H:142:LEU:HB3	1.53	0.89
15:O:37:LEU:O	15:O:41:THR:CB	2.21	0.88
15:O:543:TYR:CD2	16:P:312:PHE:CZ	2.60	0.88
18:R:431:ARG:HH21	19:S:437:THR:HB	1.38	0.88
3:C:227:TYR:HB3	3:C:300:PHE:HD1	1.39	0.88
18:R:521:TYR:HB3	18:R:530:LEU:HB2	1.53	0.88
3:C:132:ILE:O	3:C:208:CYS:HB3	1.74	0.88
5:E:99:HIS:O	5:E:103:LYS:HB2	1.74	0.88
1:A:1067:VAL:O	1:A:1070:PHE:HB3	1.73	0.87
1:A:715:ASN:OD1	1:A:716:ASP:N	2.07	0.87
2:B:1043:ARG:HG2	2:B:1049:GLN:O	1.75	0.87
2:B:552:ASN:HD22	2:B:566:ARG:HA	1.40	0.87
3:C:117:ASP:HB3	3:C:120:LEU:HD21	1.54	0.87
13:M:241:ALA:O	13:M:242:ASN:HB3	1.71	0.87
1:A:18:PHE:HD1	2:B:1139:PRO:HA	1.40	0.87
1:A:357:LEU:HD12	1:A:363:ARG:CB	2.03	0.87
13:M:112:TYR:HD1	13:M:119:TRP:HE1	1.20	0.87
2:B:969:LEU:HD13	2:B:994:GLN:OE1	1.74	0.86
3:C:255:VAL:HG22	3:C:256:ILE:H	1.38	0.86
19:S:469:ILE:O	19:S:473:LEU:HB3	1.75	0.86
15:O:40:ARG:NH2	16:P:314:GLU:O	2.07	0.86
1:A:136:ARG:O	1:A:140:ILE:HB	1.75	0.86
2:B:915:ARG:HD2	2:B:1023:TYR:HD2	1.40	0.86
2:B:944:MET:HG2	2:B:945:ASN:H	1.41	0.86
19:S:491:ASN:OD1	19:S:492:ILE:N	2.08	0.86
1:A:277:SER:HB3	1:A:278:PRO:CD	2.04	0.86
3:C:228:ARG:O	3:C:299:ILE:HB	1.76	0.86
2:B:767:ILE:HG23	2:B:768:GLU:N	1.83	0.86
18:R:116:PHE:CE1	18:R:120:ARG:NH2	2.43	0.85
6:F:86:THR:HB	6:F:89:GLU:H	1.40	0.85
1:A:248:VAL:CG2	1:A:249:PRO:HD3	2.03	0.85
1:A:347:VAL:C	1:A:349:PRO:CD	2.50	0.85
15:O:341:GLU:O	15:O:345:PHE:HB3	1.76	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:93:ALA:HB1	18:R:149:ARG:HH21	1.41	0.85
1:A:277:SER:HB3	1:A:278:PRO:HD2	1.56	0.85
1:A:347:VAL:O	1:A:348:LYS:HB2	1.75	0.85
16:P:11:LEU:O	16:P:15:ALA:HB2	1.77	0.85
18:R:519:LEU:HB3	18:R:532:ILE:HB	1.58	0.85
1:A:482:ARG:HD3	1:A:544:PRO:HG3	1.57	0.85
1:A:988:ASP:HA	1:A:991:LYS:HB3	1.57	0.85
1:A:598:MET:HB2	8:H:96:VAL:HG21	1.55	0.85
1:A:364:PHE:HD2	1:A:365:ARG:HD3	1.04	0.84
1:A:601:TYR:CD1	3:C:23:PHE:CE2	2.65	0.84
1:A:926:MET:HG3	1:A:932:PRO:HG3	1.58	0.84
18:R:22:ASP:OD1	18:R:31:VAL:CG1	2.24	0.84
14:N:287:HIS:O	14:N:291:LEU:HB2	1.78	0.84
18:R:98:GLU:O	18:R:101:THR:CG2	2.22	0.84
18:R:417:ASN:OD1	19:S:437:THR:HG23	1.77	0.84
2:B:695:GLN:HG3	2:B:697:PRO:HD2	0.86	0.84
13:M:183:PHE:HB2	13:M:186:ILE:HG12	1.60	0.84
2:B:1049:GLN:CB	2:B:1050:PRO:HD3	2.06	0.84
18:R:619:ALA:O	18:R:623:LYS:HB3	1.78	0.84
1:A:476:ARG:HG2	1:A:478:PRO:HD2	1.60	0.83
1:A:272:VAL:HB	1:A:281:ASN:HB3	1.57	0.83
1:A:110:CYS:HB2	1:A:156:HIS:HE1	1.41	0.83
18:R:22:ASP:CG	18:R:31:VAL:CG1	2.50	0.83
18:R:101:THR:HG23	18:R:102:ASP:N	1.93	0.83
1:A:200:GLU:HB3	15:O:516:LEU:CD2	2.08	0.83
1:A:378:ARG:CD	2:B:1060:LEU:HD21	2.08	0.83
8:H:116:TYR:HB2	8:H:123:MET:HB3	1.61	0.83
2:B:776:SER:CA	2:B:779:ASP:HB3	2.06	0.83
10:J:36:LEU:HA	10:J:39:LEU:HB3	1.61	0.83
1:A:1141:ILE:HB	1:A:1295:VAL:HB	1.61	0.82
2:B:934:ASN:HB3	2:B:1004:LEU:HD23	1.59	0.82
1:A:364:PHE:CZ	1:A:1389:PHE:O	2.32	0.82
2:B:1043:ARG:HB3	2:B:1048:ARG:HA	1.61	0.82
7:G:129:ILE:HG23	7:G:138:LEU:HA	1.60	0.82
1:A:1174:GLN:O	1:A:1185:GLN:HB3	1.79	0.82
4:D:126:GLN:C	4:D:127:LEU:HG	2.02	0.82
7:G:5:SER:O	7:G:73:ARG:HA	1.80	0.82
7:G:119:CYS:HB2	7:G:128:TRP:HB3	1.61	0.82
15:O:517:VAL:HG23	15:O:518:SER:N	1.89	0.82
1:A:347:VAL:O	1:A:348:LYS:CB	2.26	0.82
14:N:302:GLU:HB3	14:N:410:GLY:HA2	1.62	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:199:TYR:O	15:O:282:ILE:HA	1.79	0.82
1:A:666:LYS:HA	1:A:670:GLY:HA3	1.62	0.82
1:A:1141:ILE:O	1:A:1294:LEU:HA	1.80	0.82
4:D:24:GLU:HG3	4:D:29:TRP:HA	1.62	0.82
2:B:579:ARG:HH12	2:B:647:GLU:HG3	1.42	0.82
1:A:378:ARG:HG3	2:B:1060:LEU:HD11	1.62	0.81
13:M:174:GLU:HG2	13:M:175:ARG:HG3	1.60	0.81
14:N:290:ILE:O	14:N:294:LEU:CB	2.28	0.81
19:S:483:GLU:O	19:S:487:GLU:CB	2.27	0.81
1:A:18:PHE:CD1	2:B:1139:PRO:HA	2.15	0.81
1:A:1373:ARG:HA	1:A:1376:LEU:HD11	1.61	0.81
3:C:86:PHE:HB2	3:C:203:SER:CB	2.11	0.81
4:D:3:VAL:HG13	7:G:7:ILE:HG22	1.60	0.81
13:M:85:LEU:HG	14:N:398:SER:CB	2.06	0.81
13:M:174:GLU:HG2	13:M:175:ARG:N	1.94	0.81
1:A:342:ASN:HD21	21:Y:32:DA:H1'	1.45	0.81
1:A:424:PRO:HD3	1:A:444:LEU:HD23	1.62	0.81
1:A:1184:ILE:HB	1:A:1232:ILE:HB	1.61	0.81
5:E:21:GLU:HB3	5:E:35:VAL:HG21	1.62	0.81
2:B:376:ARG:HH21	2:B:607:ARG:HH12	1.29	0.81
1:A:18:PHE:CE1	2:B:1139:PRO:CB	2.49	0.81
15:O:206:LEU:HB2	15:O:214:LEU:HD22	1.63	0.81
15:O:467:PHE:HD2	15:O:468:LEU:HD13	1.45	0.80
10:J:12:LYS:HE2	10:J:43:ARG:HH22	1.46	0.80
1:A:520:HIS:HE1	2:B:1062:LEU:HD21	1.46	0.80
5:E:86:PRO:HA	5:E:113:GLN:HB3	1.64	0.80
3:C:117:ASP:OD2	3:C:120:LEU:HD23	1.80	0.80
18:R:531:LEU:HB2	18:R:539:VAL:O	1.80	0.80
1:A:178:ILE:HD11	1:A:222:LEU:HB2	1.62	0.80
1:A:378:ARG:HH22	21:Y:25:DC:H4'	1.45	0.80
2:B:267:GLU:HA	2:B:270:GLN:HB3	1.62	0.80
19:S:445:LEU:HD22	19:S:486:CYS:HB3	1.63	0.80
3:C:172:GLN:H	3:C:175:GLN:HB3	1.45	0.80
16:P:266:GLU:O	16:P:269:LEU:HB3	1.82	0.80
1:A:378:ARG:HG2	1:A:518:ASN:OD1	1.83	0.79
2:B:356:VAL:O	2:B:360:MET:HB2	1.82	0.79
18:R:232:CYS:HB3	18:R:237:LEU:HD11	1.64	0.79
1:A:322:THR:HG23	1:A:323:VAL:N	1.96	0.79
1:A:364:PHE:HE2	1:A:365:ARG:HD2	1.46	0.79
1:A:794:MET:HE1	2:B:950:PRO:HG2	1.65	0.79
18:R:237:LEU:HD13	18:R:239:ARG:HG2	1.62	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:110:LEU:HB3	4:D:120:LYS:HE3	1.64	0.79
1:A:1267:LEU:O	1:A:1270:VAL:HG22	1.83	0.79
15:O:195:CYS:SG	15:O:274:VAL:HG13	2.22	0.79
16:P:64:VAL:HB	16:P:71:LYS:HB2	1.63	0.79
18:R:198:VAL:O	18:R:201:ASP:HB2	1.83	0.79
16:P:145:ARG:HB3	16:P:147:ILE:HG23	1.64	0.79
5:E:172:GLU:HG2	5:E:173:SER:H	1.48	0.79
13:M:112:TYR:H	13:M:243:ILE:CG2	1.94	0.78
1:A:789:ASN:HB3	1:A:791:PRO:HD2	1.65	0.78
15:O:541:ILE:C	15:O:543:TYR:H	1.89	0.78
2:B:1040:ARG:HB3	18:R:35:ASN:HD21	1.47	0.78
3:C:80:ALA:HA	3:C:208:CYS:HA	1.63	0.78
10:J:10:CYS:SG	10:J:43:ARG:NE	2.55	0.78
1:A:1380:ARG:HH11	1:A:1385:GLN:HE22	1.28	0.78
3:C:117:ASP:OD2	3:C:120:LEU:CD2	2.32	0.78
6:F:116:ASP:CG	6:F:117:PRO:CD	2.52	0.78
2:B:141:ILE:HG23	2:B:142:ILE:H	1.47	0.78
2:B:213:LYS:HD3	2:B:216:VAL:HG23	1.65	0.78
1:A:328:ASN:OD1	1:A:329:SER:N	2.16	0.78
2:B:817:PRO:HB2	2:B:822:GLN:HA	1.63	0.78
3:C:119:ASN:C	3:C:120:LEU:HG	2.09	0.78
3:C:240:LYS:HD2	3:C:262:SER:HA	1.64	0.78
11:K:110:GLU:OE1	11:K:111:THR:N	2.15	0.78
20:X:13:DA:N6	21:Y:51:DT:O4	2.16	0.78
1:A:946:THR:HG21	1:A:1066:SER:HA	1.65	0.77
2:B:613:ILE:HA	2:B:646:VAL:HG12	1.66	0.77
5:E:100:ILE:HG21	5:E:127:ILE:HG13	1.66	0.77
2:B:1094:VAL:O	2:B:1116:ILE:HA	1.84	0.77
9:I:17:GLY:H	9:I:22:TYR:HA	1.48	0.77
13:M:246:THR:H	14:N:404:SER:HA	1.48	0.77
15:O:168:SER:HB3	15:O:279:SER:HB3	1.67	0.77
1:A:431:ASN:OD1	1:A:432:TYR:N	2.17	0.77
4:D:145:PHE:HB2	4:D:149:THR:HG21	1.65	0.77
15:O:199:TYR:CD2	15:O:200:LEU:N	2.51	0.77
1:A:1392:THR:O	1:A:1392:THR:HG22	1.83	0.77
2:B:586:GLU:HG3	2:B:648:TYR:HD2	1.48	0.77
18:R:245:VAL:HA	18:R:248:SER:HB3	1.65	0.77
3:C:83:VAL:CG1	3:C:85:PHE:HE2	1.90	0.77
11:K:58:GLY:HA2	11:K:112:THR:HG23	1.66	0.77
16:P:266:GLU:HG3	16:P:269:LEU:HD13	1.67	0.77
1:A:379:THR:HG22	1:A:380:VAL:H	1.48	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1390:GLU:HG3	21:Y:20:DT:H5'	1.66	0.77
14:N:395:ILE:HD12	14:N:411:ARG:HA	1.64	0.77
16:P:92:LEU:O	16:P:96:TYR:CB	2.33	0.76
1:A:1163:LYS:HG3	1:A:1164:THR:H	1.49	0.76
2:B:464:ILE:HD11	2:B:746:TYR:HE1	1.48	0.76
2:B:364:LYS:HG3	2:B:365:MET:H	1.50	0.76
2:B:1149:GLN:H	7:G:58:GLN:HE22	1.34	0.76
5:E:88:VAL:HG23	5:E:117:THR:HG22	1.65	0.76
7:G:39:ILE:CG2	7:G:43:GLY:O	2.33	0.76
2:B:279:TYR:HE1	2:B:358:MET:HA	1.49	0.76
1:A:348:LYS:N	1:A:349:PRO:CD	2.49	0.76
1:A:276:ASP:O	1:A:277:SER:CB	2.31	0.76
2:B:695:GLN:NE2	2:B:698:ARG:CZ	2.49	0.76
15:O:52:LEU:HB3	15:O:127:ILE:HG21	1.67	0.76
19:S:494:THR:HB	19:S:497:ASP:HB2	1.66	0.76
3:C:70:ILE:HG13	3:C:74:GLU:HB2	1.67	0.76
1:A:1438:GLU:O	1:A:1441:LEU:HB2	1.86	0.76
6:F:98:ALA:HB1	6:F:117:PRO:O	1.86	0.75
15:O:133:SER:HB3	17:Q:58:TYR:HE2	1.49	0.75
15:O:517:VAL:CG2	15:O:518:SER:H	1.91	0.75
19:S:458:PHE:O	19:S:462:GLU:CB	2.34	0.75
15:O:52:LEU:O	15:O:56:HIS:HB2	1.86	0.75
16:P:236:THR:HG23	16:P:239:ASN:H	1.51	0.75
2:B:723:THR:HA	2:B:790:LYS:HG2	1.67	0.75
2:B:739:LYS:HD2	2:B:977:THR:HG21	1.68	0.75
1:A:777:VAL:HG12	1:A:811:ALA:HB1	1.67	0.75
12:L:31:CYS:SG	12:L:34:CYS:HB2	2.26	0.75
15:O:188:SER:C	15:O:190:LEU:H	1.92	0.75
2:B:122:ASP:HA	2:B:189:GLY:HA3	1.69	0.75
1:A:40:PHE:HB3	1:A:47:ALA:HA	1.67	0.75
1:A:347:VAL:HG12	1:A:349:PRO:CG	2.17	0.75
10:J:6:ARG:HB3	10:J:11:GLY:HA2	1.67	0.75
15:O:592:LYS:HB2	15:O:637:VAL:HG21	1.67	0.75
1:A:449:ARG:O	1:A:450:MET:C	2.30	0.75
2:B:207:VAL:HG22	2:B:217:GLN:HB2	1.69	0.75
2:B:583:LYS:HG2	2:B:584:VAL:HG13	1.67	0.75
14:N:400:ALA:H	14:N:405:SER:HB2	1.51	0.75
15:O:297:ILE:O	15:O:301:LYS:CB	2.33	0.75
15:O:365:ASP:N	15:O:476:TYR:OH	2.20	0.75
1:A:601:TYR:CE1	3:C:23:PHE:HE2	2.04	0.75
2:B:949:PHE:O	2:B:953:MET:N	2.20	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:VAL:HG12	1:A:349:PRO:HD3	1.67	0.74
16:P:256:VAL:O	16:P:260:CYS:HB3	1.87	0.74
1:A:1144:VAL:HG23	1:A:1310:ILE:HG23	1.69	0.74
1:A:1199:GLU:H	1:A:1273:LYS:HE2	1.52	0.74
5:E:28:TYR:HA	5:E:64:PRO:HA	1.67	0.74
15:O:124:GLU:HG2	15:O:125:GLU:H	0.72	0.74
7:G:39:ILE:HG23	7:G:43:GLY:O	1.86	0.74
8:H:58:THR:HB	8:H:143:LEU:HD23	1.68	0.74
16:P:90:GLU:HA	16:P:93:VAL:HB	1.69	0.74
18:R:190:ASP:CG	18:R:191:LEU:N	2.35	0.74
9:I:32:GLU:HB2	13:M:130:PHE:HB3	1.70	0.74
16:P:170:LEU:HD23	16:P:172:ILE:H	1.52	0.74
2:B:521:THR:HG22	2:B:586:GLU:CD	2.13	0.74
18:R:152:VAL:HG22	18:R:154:VAL:H	1.52	0.74
1:A:238:ASP:HA	1:A:241:LEU:HD12	1.68	0.74
2:B:541:ILE:HA	2:B:544:ILE:HD12	1.69	0.74
2:B:667:VAL:HG12	2:B:669:SER:H	1.52	0.74
2:B:197:GLN:HE22	2:B:451:ARG:HD2	1.52	0.74
2:B:607:ARG:NH2	2:B:650:ASP:OD2	2.20	0.74
2:B:794:VAL:HG23	2:B:895:LEU:HD21	1.68	0.74
1:A:645:MET:HG2	8:H:122:LEU:HD23	1.69	0.74
5:E:29:PHE:HB2	5:E:65:THR:HB	1.70	0.74
14:N:364:ARG:HB3	14:N:372:SER:HB3	1.70	0.74
18:R:258:ARG:NH2	21:Y:54:DA:OP2	2.21	0.74
13:M:174:GLU:HG2	13:M:175:ARG:H	1.51	0.73
16:P:92:LEU:O	16:P:96:TYR:HB3	1.87	0.73
2:B:129:ILE:HD11	2:B:152:MET:HB2	1.70	0.73
3:C:86:PHE:HB2	3:C:203:SER:HB3	1.70	0.73
1:A:347:VAL:O	1:A:349:PRO:HD3	1.87	0.73
2:B:741:ILE:HG23	2:B:746:TYR:HB3	1.71	0.73
15:O:201:ILE:O	15:O:281:THR:HG22	1.88	0.73
19:S:432:LEU:O	19:S:476:LYS:NZ	2.20	0.73
1:A:601:TYR:CD1	3:C:23:PHE:HE2	2.04	0.73
1:A:1394:ASP:O	1:A:1398:ASP:HB2	1.89	0.73
2:B:615:VAL:HG12	2:B:673:LEU:HD23	1.70	0.73
2:B:728:MET:SD	2:B:753:GLN:NE2	2.60	0.73
15:O:573:SER:HA	15:O:576:PHE:CE2	2.23	0.73
2:B:776:SER:HB2	3:C:217:ALA:CB	2.18	0.73
1:A:379:THR:HG21	1:A:497:THR:HA	1.71	0.73
1:A:536:GLY:O	1:A:540:ASN:ND2	2.21	0.73
1:A:1225:ILE:H	1:A:1229:ARG:HE	1.35	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:141:VAL:HG23	5:E:142:VAL:H	1.54	0.73
1:A:1161:VAL:HG22	1:A:1275:LEU:HD13	1.71	0.73
2:B:415:GLU:HG3	2:B:416:TYR:H	1.54	0.73
2:B:800:ASN:ND2	2:B:851:SER:O	2.22	0.73
15:O:125:GLU:HB2	15:O:128:HIS:HB2	1.71	0.73
16:P:131:GLN:HB3	16:P:133:TYR:HD2	1.53	0.73
1:A:1161:VAL:HG13	1:A:1275:LEU:HB2	1.70	0.72
15:O:141:ILE:HA	15:O:144:MET:HB2	1.71	0.72
1:A:790:ALA:N	1:A:791:PRO:CD	2.51	0.72
2:B:780:ARG:NH1	10:J:9:SER:O	2.22	0.72
15:O:543:TYR:CE2	16:P:312:PHE:CZ	2.77	0.72
1:A:486:LEU:HD23	1:A:537:VAL:HG22	1.70	0.72
1:A:601:TYR:CE1	3:C:23:PHE:CE2	2.77	0.72
15:O:510:CYS:SG	15:O:514:ASN:ND2	2.62	0.72
1:A:103:LEU:HD11	1:A:222:LEU:HD22	1.71	0.72
1:A:1387:ALA:CB	1:A:1392:THR:HG23	2.20	0.72
2:B:521:THR:HB	2:B:587:PHE:CD2	2.23	0.72
2:B:735:MET:HB2	2:B:754:ASN:HD21	1.53	0.72
8:H:6:PHE:HB3	8:H:130:ARG:HH21	1.53	0.72
15:O:578:ARG:HA	15:O:648:TRP:HZ3	1.53	0.72
18:R:620:SER:O	18:R:624:GLU:HB3	1.88	0.72
19:S:418:ASP:O	19:S:449:ARG:NH1	2.22	0.72
2:B:410:PRO:HA	2:B:414:MET:HE2	1.71	0.72
7:G:150:ILE:HG21	7:G:196:LEU:HD23	1.72	0.72
14:N:365:VAL:HG13	14:N:370:LYS:H	1.54	0.72
3:C:231:PRO:HB3	3:C:275:VAL:HG22	1.71	0.72
6:F:80:ALA:O	6:F:81:THR:OG1	2.07	0.72
15:O:634:GLU:HA	15:O:637:VAL:HG12	1.72	0.72
16:P:172:ILE:HG22	16:P:173:GLU:H	1.54	0.72
16:P:313:ASP:O	16:P:315:TRP:N	2.21	0.72
1:A:364:PHE:CE2	1:A:365:ARG:HD2	2.21	0.72
2:B:297:THR:OG1	2:B:301:ALA:HB3	1.89	0.72
2:B:377:LEU:HD11	2:B:520:ILE:HD13	1.71	0.72
13:M:112:TYR:N	13:M:243:ILE:HG21	1.96	0.72
13:M:160:ALA:HA	14:N:306:VAL:HA	1.71	0.72
18:R:554:GLU:HG2	18:R:579:PRO:HB3	1.72	0.72
1:A:1438:GLU:HA	1:A:1441:LEU:HD13	1.72	0.72
2:B:616:SER:N	2:B:619:GLN:O	2.23	0.72
3:C:164:ALA:HA	3:C:167:LEU:HD13	1.72	0.72
2:B:877:GLU:HG3	2:B:878:PRO:HD2	1.72	0.72
12:L:31:CYS:SG	12:L:36:SER:OG	2.47	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:200:LEU:CD2	15:O:281:THR:C	2.62	0.72
15:O:104:VAL:HA	15:O:123:ASN:H	1.53	0.72
3:C:21:PRO:HG3	3:C:30:GLU:HB2	1.72	0.71
7:G:204:GLY:HA2	7:G:210:TRP:HB2	1.72	0.71
16:P:49:MET:HE3	19:S:364:LEU:HD13	1.72	0.71
19:S:470:GLU:O	19:S:474:ARG:CB	2.36	0.71
2:B:97:ASP:OD2	2:B:99:ARG:NH1	2.22	0.71
2:B:1028:LYS:HG2	2:B:1029:HIS:H	1.53	0.71
3:C:83:VAL:HG12	3:C:85:PHE:CD2	2.24	0.71
1:A:110:CYS:CB	1:A:156:HIS:HE1	2.02	0.71
18:R:429:ILE:CG2	18:R:431:ARG:NH1	2.49	0.71
15:O:201:ILE:H	15:O:280:LEU:HB3	1.56	0.71
2:B:109:LYS:NZ	2:B:111:TYR:O	2.21	0.71
15:O:590:PHE:O	15:O:594:LYS:N	2.20	0.71
1:A:388:SER:OG	1:A:695:ASN:ND2	2.23	0.71
20:X:8:DC:N3	20:X:9:DA:N6	2.38	0.71
1:A:372:ARG:HG2	2:B:1050:PRO:HG2	1.72	0.71
1:A:1372:THR:O	1:A:1376:LEU:HG	1.89	0.71
2:B:1003:MET:SD	3:C:293:ARG:NH2	2.63	0.71
16:P:75:VAL:HG22	16:P:77:GLU:H	1.52	0.71
5:E:22:MET:HE3	5:E:187:TYR:HA	1.72	0.71
18:R:87:LEU:CD2	18:R:101:THR:OG1	2.39	0.71
2:B:901:ARG:NH2	3:C:94:ASP:OD1	2.24	0.71
18:R:116:PHE:CZ	18:R:164:MET:HB3	2.26	0.71
18:R:131:TYR:OH	18:R:135:ARG:NH1	2.23	0.71
1:A:205:LEU:HD12	1:A:212:GLU:HG2	1.73	0.70
5:E:80:VAL:HG23	5:E:109:ILE:HD11	1.72	0.70
15:O:293:SER:HB3	15:O:316:LEU:HD23	1.73	0.70
18:R:101:THR:CG2	18:R:102:ASP:N	2.54	0.70
18:R:429:ILE:HG21	18:R:431:ARG:HH12	1.54	0.70
8:H:21:ASN:OD1	8:H:22:LYS:N	2.21	0.70
8:H:39:THR:HB	8:H:124:ARG:HB3	1.72	0.70
13:M:85:LEU:CG	14:N:398:SER:HB3	2.08	0.70
3:C:52:ALA:HB2	3:C:310:PRO:HG2	1.74	0.70
13:M:117:HIS:HD1	13:M:119:TRP:CD1	2.09	0.70
1:A:452:LEU:HA	1:A:455:ASN:ND2	2.06	0.70
2:B:1054:ARG:HG2	2:B:1055:SER:H	1.56	0.70
5:E:24:LYS:HB2	5:E:30:ILE:HD11	1.73	0.70
8:H:130:ARG:O	8:H:134:ASN:ND2	2.24	0.70
1:A:830:ARG:NH1	2:B:657:SER:O	2.24	0.70
1:A:1445:ARG:HG3	1:A:1447:LEU:HD12	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:201:SER:OG	2:B:376:ARG:NH1	2.22	0.70
15:O:353:GLU:HB2	15:O:481:SER:HB3	1.73	0.70
1:A:600:PRO:O	1:A:601:TYR:HB2	1.91	0.70
2:B:555:VAL:HG12	2:B:564:SER:H	1.56	0.70
2:B:1026:LYS:NZ	2:B:1030:MET:SD	2.65	0.70
15:O:620:LEU:HD12	15:O:621:PRO:HD2	1.72	0.70
14:N:383:GLY:HA3	14:N:418:VAL:HA	1.72	0.70
15:O:52:LEU:O	15:O:56:HIS:CB	2.40	0.70
18:R:467:ARG:HG3	18:R:610:LEU:HD22	1.74	0.70
1:A:204:VAL:HG21	15:O:517:VAL:HA	1.74	0.69
15:O:197:MET:HB2	15:O:286:ARG:HE	1.56	0.69
15:O:295:GLN:NE2	15:O:646:SER:O	2.24	0.69
16:P:102:ARG:HD2	16:P:155:PRO:HB2	1.74	0.69
18:R:12:PHE:HB3	18:R:23:LEU:HD11	1.73	0.69
19:S:480:ASN:OD1	19:S:481:PHE:N	2.25	0.69
15:O:470:GLU:H	15:O:479:PRO:HD3	1.56	0.69
15:O:575:ASN:OD1	15:O:578:ARG:NH1	2.25	0.69
15:O:592:LYS:NZ	15:O:593:GLU:OE2	2.25	0.69
18:R:432:ILE:HG13	18:R:434:GLU:H	1.55	0.69
2:B:524:ASP:CB	2:B:587:PHE:CZ	2.64	0.69
15:O:90:SER:O	15:O:94:THR:N	2.25	0.69
16:P:194:GLY:O	16:P:196:LYS:NZ	2.25	0.69
1:A:1128:GLU:O	1:A:1132:ALA:N	2.23	0.69
3:C:251:PHE:HB2	3:C:255:VAL:HG23	1.73	0.69
5:E:117:THR:HG23	5:E:120:ALA:H	1.56	0.69
18:R:429:ILE:HG21	18:R:431:ARG:HH11	1.54	0.69
2:B:776:SER:HA	2:B:779:ASP:CB	2.14	0.69
3:C:12:VAL:HG12	3:C:13:THR:N	2.07	0.69
9:I:26:CYS:HB3	9:I:29:CYS:SG	2.32	0.69
1:A:535:MET:HE1	2:B:1070:VAL:HG12	1.75	0.69
10:J:52:THR:HG22	10:J:53:HIS:H	1.57	0.69
15:O:200:LEU:HD22	15:O:281:THR:C	2.17	0.69
21:Y:25:DC:N3	21:Y:26:DA:N6	2.39	0.69
1:A:277:SER:CB	1:A:278:PRO:CD	2.70	0.69
1:A:877:VAL:HG21	2:B:487:ARG:HH12	1.56	0.69
2:B:43:ASP:OD1	2:B:44:LYS:N	2.25	0.69
3:C:134:LEU:O	3:C:205:LYS:HA	1.93	0.69
7:G:104:ILE:HG23	7:G:105:PHE:H	1.56	0.69
15:O:190:LEU:HD23	15:O:194:LEU:CD2	2.17	0.69
15:O:291:ARG:NH2	15:O:653:MET:SD	2.66	0.69
18:R:149:ARG:C	18:R:150:LEU:HD12	2.16	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:7:ARG:HE	4:D:10:PHE:HZ	1.40	0.69
2:B:202:LYS:HD3	2:B:222:SER:HB2	1.75	0.69
3:C:132:ILE:O	3:C:208:CYS:CB	2.41	0.69
7:G:112:GLN:HE22	7:G:128:TRP:CD1	2.11	0.69
16:P:11:LEU:O	16:P:15:ALA:CB	2.41	0.69
1:A:493:ARG:HB2	1:A:499:ARG:HH21	1.58	0.69
2:B:822:GLN:HG2	2:B:823:SER:H	1.58	0.69
5:E:31:THR:HG22	5:E:34:GLU:HG2	1.75	0.69
7:G:39:ILE:HD12	7:G:40:PRO:HD2	1.75	0.68
8:H:128:ASN:CG	8:H:129:TYR:H	2.01	0.68
15:O:541:ILE:O	15:O:543:TYR:N	2.26	0.68
15:O:577:MET:O	15:O:580:ASN:HB3	1.93	0.68
1:A:372:ARG:O	2:B:1050:PRO:HG3	1.92	0.68
2:B:192:LYS:NZ	2:B:438:SER:O	2.26	0.68
2:B:267:GLU:O	2:B:271:LEU:N	2.20	0.68
4:D:129:ALA:HB1	4:D:153:MET:HB3	1.73	0.68
18:R:551:GLN:O	18:R:555:ALA:HB2	1.93	0.68
20:X:26:DT:H2'	20:X:27:DT:C6	2.28	0.68
21:Y:47:DC:H2'	21:Y:48:DT:C4	2.28	0.68
2:B:287:LEU:HD21	9:I:11:MET:HG2	1.75	0.68
2:B:766:ASP:O	2:B:767:ILE:HG22	1.92	0.68
4:D:13:ASP:OD1	4:D:17:LEU:N	2.22	0.68
15:O:131:LEU:C	15:O:131:LEU:HD12	2.18	0.68
1:A:38:ASP:O	1:A:40:PHE:N	2.25	0.68
1:A:408:VAL:HA	1:A:412:ASN:HD22	1.58	0.68
1:A:1387:ALA:HB1	1:A:1392:THR:HG23	1.74	0.68
2:B:137:ARG:H	2:B:141:ILE:HG21	1.58	0.68
2:B:239:LYS:HG2	2:B:241:TYR:CE2	2.28	0.68
2:B:915:ARG:HD2	2:B:1023:TYR:CD2	2.26	0.68
3:C:84:TYR:CD2	3:C:207:HIS:HE1	2.12	0.68
3:C:100:ARG:HE	10:J:5:VAL:HG13	1.58	0.68
5:E:64:PRO:HD3	5:E:77:SER:HA	1.75	0.68
15:O:80:VAL:HG21	15:O:87:ASP:HA	1.75	0.68
18:R:219:ARG:NE	19:S:408:TYR:OH	2.27	0.68
18:R:464:LYS:NZ	18:R:605:VAL:O	2.27	0.68
1:A:251:GLY:HA3	15:O:42:LEU:HD13	1.75	0.68
1:A:766:ILE:HA	1:A:769:LEU:HB2	1.76	0.68
1:A:1305:CYS:SG	5:E:11:ARG:NH1	2.67	0.68
2:B:524:ASP:CB	2:B:587:PHE:CE1	2.76	0.68
15:O:162:ASN:HD22	15:O:174:TYR:HE1	1.41	0.68
1:A:974:LEU:HD21	1:A:998:TYR:HB3	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:467:LEU:HA	2:B:470:MET:HE3	1.75	0.68
1:A:114:LEU:HD11	1:A:148:CYS:HA	1.73	0.68
1:A:548:GLU:OE2	1:A:673:LYS:N	2.27	0.68
2:B:651:VAL:HG23	2:B:652:ASN:H	1.59	0.68
8:H:43:ASN:HD21	8:H:46:LEU:HD13	1.58	0.68
18:R:463:ARG:NH1	18:R:598:ASP:O	2.27	0.68
1:A:322:THR:HG23	1:A:323:VAL:H	1.59	0.68
1:A:38:ASP:C	1:A:40:PHE:H	2.01	0.68
1:A:363:ARG:HH21	2:B:1046:LEU:HD21	1.56	0.68
1:A:477:GLN:HE21	1:A:518:ASN:ND2	1.91	0.68
1:A:668:VAL:HB	1:A:677:VAL:HG23	1.74	0.68
3:C:85:PHE:CD1	3:C:204:LEU:HB3	2.29	0.68
5:E:95:THR:O	5:E:99:HIS:ND1	2.26	0.68
14:N:307:PHE:CD1	14:N:416:ILE:HG22	2.28	0.68
15:O:52:LEU:HD13	15:O:127:ILE:CG2	2.24	0.68
1:A:238:ASP:OD1	1:A:239:CYS:N	2.26	0.68
1:A:1285:ILE:HG12	1:A:1291:ARG:HE	1.59	0.68
16:P:254:GLU:HB3	16:P:262:ARG:O	1.93	0.68
18:R:455:GLU:OE1	18:R:546:ARG:NH2	2.27	0.68
1:A:303:LEU:HD12	1:A:312:MET:HE2	1.75	0.67
1:A:572:ASP:H	1:A:575:THR:HB	1.58	0.67
3:C:5:VAL:HG22	3:C:293:ARG:H	1.58	0.67
4:D:65:TYR:HA	4:D:68:ILE:HG22	1.76	0.67
11:K:89:CYS:HA	11:K:104:ARG:O	1.94	0.67
13:M:104:HIS:ND1	13:M:105:PRO:O	2.25	0.67
17:Q:41:LEU:O	17:Q:44:ASN:ND2	2.26	0.67
18:R:397:VAL:HB	18:R:485:ASN:H	1.57	0.67
1:A:610:PHE:HZ	1:A:697:MET:HE1	1.59	0.67
2:B:558:ASN:HD21	2:B:603:THR:HG22	1.57	0.67
2:B:797:ARG:HG2	2:B:803:GLN:HG2	1.76	0.67
18:R:101:THR:HG23	18:R:102:ASP:H	1.59	0.67
18:R:147:SER:O	18:R:152:VAL:HG11	1.93	0.67
1:A:597:ILE:HD11	1:A:603:LEU:HD12	1.75	0.67
1:A:1157:VAL:HG12	1:A:1160:ARG:HD2	1.77	0.67
7:G:2:PHE:HB2	7:G:78:LYS:H	1.59	0.67
15:O:46:LEU:HA	15:O:49:TYR:HD1	1.58	0.67
1:A:232:LYS:HD3	16:P:315:TRP:HH2	1.59	0.67
2:B:552:ASN:ND2	2:B:566:ARG:HA	2.10	0.67
2:B:1080:LEU:O	2:B:1084:MET:HB3	1.94	0.67
16:P:235:LEU:HD21	16:P:239:ASN:HB3	1.76	0.67
18:R:417:ASN:OD1	19:S:437:THR:CG2	2.42	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:506:GLN:O	19:S:510:LYS:HB2	1.94	0.67
1:A:916:TYR:HB3	1:A:920:GLY:HA2	1.76	0.67
2:B:1002:ASP:OD1	2:B:1003:MET:N	2.27	0.67
1:A:269:ARG:NH2	1:A:283:ASP:OD1	2.27	0.67
1:A:714:ILE:HD11	2:B:958:MET:HG2	1.77	0.67
2:B:327:ILE:HD11	13:M:231:LEU:HB2	1.76	0.67
15:O:199:TYR:CD2	15:O:200:LEU:HB2	2.30	0.67
18:R:101:THR:CG2	18:R:102:ASP:H	2.06	0.67
1:A:319:LEU:O	1:A:322:THR:CG2	2.35	0.67
15:O:166:LEU:HB3	15:O:169:LEU:HD11	1.76	0.67
15:O:554:THR:HG23	15:O:561:ARG:HB3	1.77	0.67
18:R:213:TRP:O	18:R:214:MET:HE2	1.94	0.67
16:P:120:VAL:HA	16:P:123:LYS:HE3	1.76	0.67
18:R:191:LEU:CD1	18:R:239:ARG:HH21	2.08	0.67
21:Y:32:DA:H5'	21:Y:33:DC:H5''	1.75	0.67
21:Y:59:DG:H4'	21:Y:60:DA:H5'	1.76	0.67
1:A:92:HIS:CD2	1:A:258:TRP:HE1	2.13	0.67
1:A:464:ARG:NH1	1:A:467:GLU:OE1	2.28	0.67
1:A:955:LEU:HB2	1:A:958:ALA:HB3	1.76	0.67
6:F:98:ALA:CB	6:F:117:PRO:O	2.43	0.67
15:O:538:ALA:O	15:O:542:ARG:HG3	1.95	0.67
1:A:1166:LEU:CD1	1:A:1270:VAL:HG23	2.23	0.67
1:A:182:THR:O	1:A:185:TRP:NE1	2.28	0.66
1:A:703:ARG:NH2	11:K:93:ILE:O	2.28	0.66
1:A:934:ASN:ND2	1:A:937:ARG:HE	1.93	0.66
2:B:167:ASP:O	2:B:169:SER:N	2.27	0.66
3:C:117:ASP:HB3	3:C:120:LEU:CD2	2.25	0.66
3:C:256:ILE:HD13	3:C:265:ALA:HB1	1.78	0.66
3:C:257:GLY:N	3:C:266:TYR:O	2.25	0.66
7:G:53:THR:HG21	7:G:71:THR:HG22	1.77	0.66
15:O:516:LEU:HB2	15:O:565:LEU:HD23	1.76	0.66
1:A:525:GLU:OE2	6:F:102:SER:CB	2.35	0.66
1:A:599:LYS:H	8:H:96:VAL:CG2	2.08	0.66
14:N:397:LEU:HG	14:N:408:LEU:HA	1.76	0.66
15:O:234:ASP:O	15:O:238:ARG:N	2.27	0.66
15:O:455:SER:HA	15:O:458:LYS:HD3	1.77	0.66
18:R:202:ALA:O	18:R:206:ALA:N	2.20	0.66
1:A:1002:ARG:O	1:A:1006:HIS:HB2	1.93	0.66
1:A:1202:ILE:O	1:A:1206:ALA:N	2.23	0.66
1:A:1387:ALA:HB1	1:A:1392:THR:CG2	2.24	0.66
16:P:217:THR:C	16:P:219:GLN:H	2.03	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:ARG:CG	2:B:1050:PRO:HG2	2.26	0.66
1:A:573:ARG:NH2	11:K:87:GLU:OE1	2.28	0.66
7:G:114:MET:HB3	7:G:201:GLN:HB3	1.78	0.66
9:I:32:GLU:HG3	13:M:132:ASN:HB2	1.77	0.66
15:O:48:LEU:HD22	15:O:581:LEU:HD21	1.76	0.66
15:O:188:SER:O	15:O:190:LEU:N	2.28	0.66
18:R:620:SER:O	18:R:624:GLU:CB	2.44	0.66
1:A:250:SER:O	1:A:251:GLY:C	2.37	0.66
1:A:870:GLU:O	1:A:874:ASP:HB2	1.95	0.66
2:B:265:ASP:H	2:B:268:ILE:HD12	1.61	0.66
6:F:116:ASP:OD1	6:F:117:PRO:HD3	1.95	0.66
7:G:2:PHE:N	7:G:76:VAL:O	2.28	0.66
7:G:89:ILE:HG13	7:G:92:CYS:SG	2.36	0.66
1:A:583:MET:HG3	1:A:700:LEU:HB2	1.78	0.66
4:D:17:LEU:HD21	4:D:63:VAL:HG23	1.75	0.66
7:G:112:GLN:HG2	7:G:115:LEU:HD13	1.77	0.66
18:R:558:PRO:O	18:R:562:GLU:CB	2.42	0.66
1:A:250:SER:CB	1:A:1403:MET:HE1	2.25	0.66
5:E:18:THR:HG23	5:E:143:ASN:HB3	1.78	0.66
5:E:190:LEU:HD23	5:E:214:CYS:HB2	1.78	0.66
8:H:9:ILE:HA	8:H:55:LEU:O	1.96	0.66
1:A:706:GLY:HA3	2:B:762:TYR:HA	1.77	0.66
2:B:204:ARG:NH2	2:B:604:ASP:OD2	2.22	0.66
2:B:459:SER:N	2:B:469:MET:SD	2.68	0.66
13:M:96:LEU:H	13:M:101:PRO:HA	1.61	0.66
16:P:69:GLU:HG3	16:P:70:LEU:H	1.60	0.66
16:P:263:VAL:HG12	16:P:265:LEU:H	1.61	0.66
2:B:613:ILE:O	2:B:673:LEU:N	2.27	0.66
2:B:760:MET:HE3	2:B:762:TYR:HB2	1.76	0.66
1:A:364:PHE:CZ	1:A:1389:PHE:C	2.68	0.66
15:O:338:ASP:OD2	15:O:340:GLU:HB2	1.95	0.66
18:R:191:LEU:HD12	18:R:239:ARG:HH21	1.59	0.66
1:A:127:LEU:HD21	1:A:141:LEU:HD21	1.78	0.65
1:A:421:VAL:O	1:A:449:ARG:NH1	2.29	0.65
1:A:1038:GLU:HB3	1:A:1042:ILE:HD11	1.77	0.65
1:A:15:GLY:HA2	1:A:1407:ALA:HA	1.79	0.65
1:A:365:ARG:HG2	1:A:365:ARG:O	1.97	0.65
1:A:366:GLY:O	2:B:1061:ARG:NH1	2.29	0.65
2:B:81:GLN:HG2	2:B:82:LEU:HG	1.78	0.65
3:C:47:LEU:HD21	11:K:139:ILE:HD11	1.78	0.65
15:O:506:ARG:NH2	15:O:528:MET:HG2	2.11	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:ALA:O	1:A:49:LYS:NZ	2.27	0.65
1:A:413:ARG:NH1	1:A:456:LEU:O	2.28	0.65
16:P:191:PHE:HB2	16:P:192:PRO:HD2	1.77	0.65
19:S:419:PRO:O	19:S:449:ARG:NH2	2.30	0.65
20:X:30:DT:O2	21:Y:35:DG:N2	2.29	0.65
1:A:420:ILE:HD11	1:A:462:VAL:HG21	1.77	0.65
2:B:612:LEU:HB2	2:B:674:GLU:HA	1.79	0.65
2:B:695:GLN:HE22	2:B:698:ARG:NH2	1.94	0.65
15:O:199:TYR:OH	15:O:200:LEU:HD12	1.97	0.65
18:R:116:PHE:CZ	18:R:120:ARG:NH2	2.65	0.65
1:A:354:CYS:SG	1:A:1393:THR:OG1	2.51	0.65
1:A:654:ILE:HG12	1:A:659:ILE:HA	1.79	0.65
1:A:1256:VAL:O	1:A:1260:MET:CB	2.39	0.65
2:B:731:PRO:HB2	2:B:750:PRO:HG2	1.79	0.65
2:B:997:ASN:OD1	2:B:998:TYR:N	2.30	0.65
15:O:134:GLY:H	17:Q:58:TYR:HD2	1.45	0.65
15:O:506:ARG:HH21	15:O:528:MET:HG2	1.62	0.65
16:P:154:GLN:HG2	19:S:520:LYS:HE3	1.78	0.65
18:R:136:LYS:HE2	18:R:173:LEU:HD13	1.79	0.65
18:R:235:ASN:HD22	18:R:237:LEU:HD23	1.61	0.65
1:A:1390:GLU:HG2	1:A:1391:LYS:HG2	1.78	0.65
18:R:619:ALA:O	18:R:623:LYS:CB	2.44	0.65
1:A:595:PRO:HA	1:A:604:TRP:NE1	2.12	0.65
2:B:524:ASP:CB	2:B:587:PHE:HZ	2.04	0.65
2:B:675:ILE:HG13	2:B:676:GLU:N	2.11	0.65
2:B:930:ASP:O	2:B:931:MET:HG2	1.96	0.65
15:O:195:CYS:SG	15:O:274:VAL:HG12	2.36	0.65
18:R:609:GLU:O	18:R:613:HIS:N	2.30	0.65
2:B:305:ILE:HB	2:B:325:GLU:HG2	1.79	0.65
6:F:76:LYS:HD3	6:F:79:ARG:HH21	1.60	0.65
8:H:131:ASN:HA	8:H:134:ASN:HD22	1.61	0.65
15:O:43:ASN:HB3	15:O:47:PHE:HB2	1.77	0.65
1:A:407:LYS:HG2	1:A:461:VAL:HG22	1.78	0.65
1:A:599:LYS:H	8:H:96:VAL:HG22	1.60	0.65
9:I:8:CYS:HB2	9:I:29:CYS:SG	2.37	0.65
13:M:83:GLU:O	13:M:84:SER:O	2.15	0.65
16:P:33:GLN:NE2	19:S:372:MET:SD	2.70	0.65
19:S:424:GLU:OE2	19:S:449:ARG:NE	2.29	0.65
1:A:1284:ASN:OD1	1:A:1285:ILE:N	2.29	0.64
1:A:1376:LEU:HD21	1:A:1389:PHE:CE2	2.32	0.64
2:B:94:LYS:HB3	2:B:134:GLU:O	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:210:ASP:HB3	2:B:213:LYS:HD2	1.78	0.64
2:B:687:LEU:O	2:B:915:ARG:NH2	2.29	0.64
3:C:121:PRO:O	3:C:122:ASP:OD1	2.13	0.64
2:B:303:GLU:O	2:B:307:ALA:HB2	1.96	0.64
2:B:473:ILE:O	2:B:511:VAL:HA	1.98	0.64
2:B:1004:LEU:HB2	2:B:1013:LEU:HD12	1.78	0.64
2:B:1005:TYR:OH	3:C:293:ARG:NH1	2.30	0.64
3:C:134:LEU:HD23	3:C:167:LEU:HD23	1.78	0.64
8:H:93:TYR:HD2	8:H:143:LEU:HD21	1.61	0.64
14:N:364:ARG:NH1	14:N:365:VAL:O	2.31	0.64
15:O:105:LYS:N	15:O:121:TYR:O	2.30	0.64
15:O:341:GLU:O	15:O:345:PHE:CB	2.45	0.64
18:R:81:ASN:OD1	18:R:84:ARG:NH2	2.30	0.64
1:A:400:LYS:HA	1:A:465:HIS:HD2	1.62	0.64
2:B:905:ARG:O	2:B:907:GLU:N	2.28	0.64
2:B:914:SER:C	2:B:916:HIS:H	2.05	0.64
3:C:248:GLN:HB3	3:C:256:ILE:HD11	1.80	0.64
4:D:133:HIS:CE1	7:G:211:TRP:HB3	2.33	0.64
18:R:87:LEU:HD21	18:R:101:THR:OG1	1.96	0.64
19:S:382:ASP:HB3	19:S:385:LYS:HG2	1.79	0.64
11:K:69:ASP:CG	11:K:70:HIS:H	2.04	0.64
15:O:215:TRP:O	15:O:219:TYR:CB	2.42	0.64
18:R:640:SER:OG	19:S:506:GLN:NE2	2.30	0.64
1:A:425:ASN:OD1	1:A:426:VAL:N	2.30	0.64
1:A:598:MET:HB2	8:H:96:VAL:CG2	2.27	0.64
2:B:417:ASP:HB2	2:B:419:LEU:HD13	1.80	0.64
2:B:464:ILE:HG12	2:B:687:LEU:HD11	1.79	0.64
3:C:197:ARG:HE	10:J:61:LEU:HB3	1.60	0.64
1:A:116:SER:HA	1:A:120:LYS:HE3	1.80	0.64
1:A:183:PHE:CD2	1:A:184:ARG:HG3	2.33	0.64
1:A:372:ARG:HD2	2:B:1050:PRO:O	1.97	0.64
1:A:787:ASN:ND2	8:H:19:ARG:O	2.31	0.64
1:A:1153:ALA:HA	1:A:1156:VAL:HB	1.78	0.64
2:B:609:CYS:HB3	2:B:648:TYR:HB3	1.78	0.64
2:B:630:LEU:HA	2:B:635:LEU:HB2	1.80	0.64
7:G:87:GLY:HA3	7:G:148:PHE:HE2	1.62	0.64
15:O:577:MET:O	15:O:580:ASN:CB	2.45	0.64
1:A:92:HIS:CD2	1:A:94:GLY:H	2.15	0.64
1:A:269:ARG:NH1	1:A:356:ARG:HH12	1.96	0.64
1:A:597:ILE:O	1:A:602:TYR:HA	1.97	0.64
15:O:54:LYS:HA	15:O:58:GLY:HA2	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:400:LYS:HA	1:A:465:HIS:CD2	2.32	0.64
3:C:107:LYS:HB3	3:C:185:VAL:HG23	1.80	0.64
15:O:221:LYS:H	15:O:224:LYS:HB3	1.61	0.64
16:P:267:SER:O	16:P:271:MET:N	2.30	0.64
2:B:553:TYR:HB3	2:B:598:ALA:N	2.13	0.64
3:C:33:VAL:HG12	3:C:34:GLU:H	1.63	0.64
16:P:253:LEU:HA	16:P:263:VAL:HA	1.80	0.64
18:R:241:HIS:HD2	18:R:255:LEU:HD23	1.63	0.64
1:A:625:ASN:HB2	1:A:655:ARG:HD3	1.80	0.64
1:A:887:ARG:NE	2:B:1064:GLU:OE1	2.31	0.64
1:A:1436:ILE:HG12	7:G:54:VAL:HG11	1.80	0.64
5:E:55:ARG:HG3	5:E:84:ASP:HA	1.79	0.64
12:L:27:LEU:HD11	12:L:37:LYS:HB2	1.79	0.64
14:N:288:GLN:HE21	14:N:292:ARG:HG3	1.63	0.64
16:P:75:VAL:HG21	16:P:80:ALA:HB2	1.80	0.64
1:A:572:ASP:OD1	1:A:573:ARG:N	2.30	0.63
1:A:628:ALA:O	1:A:651:PHE:HA	1.98	0.63
2:B:87:VAL:O	19:S:383:ARG:NH1	2.31	0.63
2:B:779:ASP:OD1	3:C:216:HIS:ND1	2.32	0.63
5:E:111:VAL:HG22	5:E:135:PHE:HB2	1.79	0.63
15:O:200:LEU:HD23	15:O:282:ILE:CA	2.28	0.63
2:B:735:MET:HE2	2:B:754:ASN:HD21	1.63	0.63
2:B:819:TRP:O	2:B:840:GLN:NE2	2.30	0.63
3:C:239:ILE:HG21	3:C:288:LYS:HD3	1.80	0.63
5:E:112:TYR:N	5:E:135:PHE:O	2.23	0.63
15:O:636:ASN:O	15:O:640:ARG:CB	2.40	0.63
18:R:511:TYR:CZ	18:R:513:PRO:HA	2.34	0.63
1:A:931:GLN:O	1:A:933:VAL:N	2.31	0.63
12:L:48:CYS:SG	12:L:51:CYS:N	2.64	0.63
14:N:384:LYS:HA	14:N:416:ILE:HD11	1.81	0.63
8:H:56:THR:O	8:H:144:ILE:HA	1.98	0.63
14:N:287:HIS:CD2	14:N:384:LYS:HE2	2.33	0.63
15:O:289:LYS:HD2	15:O:325:LYS:HZ2	1.62	0.63
18:R:213:TRP:C	18:R:214:MET:HE2	2.24	0.63
2:B:68:PHE:CD1	2:B:385:SER:OG	2.52	0.63
14:N:389:THR:HG23	14:N:390:PHE:H	1.62	0.63
1:A:118:THR:O	1:A:122:GLN:N	2.29	0.63
1:A:1257:PHE:HB2	9:I:14:ILE:HB	1.81	0.63
2:B:232:TYR:HD1	2:B:242:LEU:HD23	1.62	0.63
2:B:614:ILE:HG12	2:B:672:HIS:CD2	2.33	0.63
19:S:488:ILE:HG23	19:S:491:ASN:HB2	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:607:LYS:HZ1	1:A:662:GLY:H	1.47	0.63
2:B:659:ILE:HG12	2:B:672:HIS:HB2	1.79	0.63
2:B:903:ASN:ND2	3:C:95:GLU:HG2	2.14	0.63
3:C:239:ILE:HD13	3:C:288:LYS:HE3	1.81	0.63
15:O:199:TYR:CG	15:O:200:LEU:N	2.63	0.63
19:S:303:UNK:O	19:S:307:UNK:CB	2.47	0.63
1:A:45:ASP:OD1	1:A:46:ARG:N	2.32	0.63
1:A:322:THR:CG2	1:A:323:VAL:N	2.62	0.63
1:A:828:GLN:NE2	2:B:593:ASN:OD1	2.31	0.63
1:A:1050:ASP:HA	1:A:1053:LYS:HE2	1.81	0.63
2:B:521:THR:HG23	2:B:609:CYS:SG	2.38	0.63
1:A:452:LEU:HA	1:A:455:ASN:HD22	1.63	0.62
1:A:1014:GLY:O	1:A:1017:THR:HG22	1.99	0.62
2:B:332:ILE:HG13	2:B:333:ALA:H	1.62	0.62
3:C:32:ASN:OD1	3:C:33:VAL:N	2.32	0.62
4:D:14:TYR:CE2	4:D:103:PHE:HB2	2.34	0.62
6:F:147:SER:HB3	6:F:150:GLU:HG3	1.81	0.62
18:R:138:LYS:HG3	18:R:138:LYS:O	1.99	0.62
18:R:275:PHE:HD1	18:R:278:ASN:H	1.47	0.62
18:R:581:ASN:ND2	18:R:583:HIS:O	2.31	0.62
18:R:632:ALA:O	18:R:636:LEU:CB	2.44	0.62
1:A:391:GLU:HG3	1:A:489:TYR:HB2	1.80	0.62
1:A:432:TYR:OH	18:R:20:ASN:ND2	2.31	0.62
2:B:257:LEU:HD23	2:B:268:ILE:HG23	1.80	0.62
3:C:88:ASN:HB3	12:L:60:ARG:NH1	2.14	0.62
15:O:287:PHE:O	15:O:291:ARG:HG2	1.99	0.62
16:P:135:LYS:HD3	16:P:151:TYR:CD1	2.34	0.62
1:A:485:ILE:O	1:A:486:LEU:HD12	1.99	0.62
2:B:756:THR:HG23	2:B:941:ASP:H	1.63	0.62
15:O:541:ILE:C	15:O:543:TYR:N	2.56	0.62
18:R:549:ILE:O	18:R:553:PHE:HB3	1.98	0.62
1:A:372:ARG:C	2:B:1050:PRO:HG3	2.25	0.62
2:B:297:THR:CB	2:B:301:ALA:HB3	2.28	0.62
2:B:760:MET:HB3	2:B:943:ILE:HD11	1.81	0.62
18:R:446:LYS:NZ	20:X:18:DT:OP1	2.32	0.62
20:X:25:DT:H2'	20:X:26:DT:C6	2.33	0.62
1:A:91:PHE:HE2	1:A:96:PHE:HD1	1.47	0.62
2:B:536:LEU:HA	14:N:419:THR:HG21	1.82	0.62
5:E:55:ARG:NE	5:E:113:GLN:OE1	2.30	0.62
15:O:158:GLU:OE1	15:O:161:GLN:NE2	2.33	0.62
15:O:645:LEU:HA	15:O:648:TRP:HB3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:467:ARG:O	18:R:471:LYS:CB	2.48	0.62
2:B:933:PHE:HB2	2:B:937:GLY:HA2	1.81	0.62
6:F:75:PRO:HD2	6:F:78:GLN:HE21	1.65	0.62
15:O:53:VAL:O	15:O:57:LEU:N	2.32	0.62
15:O:183:MET:HB2	15:O:186:THR:HB	1.82	0.62
16:P:141:LYS:HG2	16:P:142:PHE:H	1.63	0.62
18:R:549:ILE:O	18:R:553:PHE:CB	2.48	0.62
1:A:286:THR:O	1:A:290:THR:HB	1.99	0.62
2:B:517:MET:HE2	2:B:611:PRO:HG2	1.82	0.62
13:M:71:ILE:HG12	14:N:367:LYS:HZ3	1.64	0.62
21:Y:25:DC:H2''	21:Y:26:DA:C8	2.35	0.62
1:A:116:SER:OG	1:A:117:GLU:OE1	2.15	0.62
1:A:231:PHE:HD1	1:A:234:ILE:HD12	1.65	0.62
1:A:909:ASN:OD1	6:F:139:PRO:HB3	2.00	0.62
2:B:102:LYS:HG2	2:B:104:SER:H	1.65	0.62
4:D:122:GLN:NE2	7:G:83:GLU:OE2	2.32	0.62
4:D:125:ASN:OD1	4:D:126:GLN:N	2.32	0.62
11:K:63:PHE:O	11:K:102:ASN:HA	1.99	0.62
13:M:253:GLU:HB2	13:M:257:ASP:HB2	1.81	0.62
15:O:262:ILE:HG22	15:O:274:VAL:HB	1.82	0.62
1:A:1186:VAL:HG22	1:A:1230:ILE:HG12	1.81	0.62
5:E:80:VAL:HA	5:E:109:ILE:HG13	1.81	0.62
8:H:1:MET:HG3	8:H:3:ASN:H	1.65	0.62
8:H:8:ASP:OD1	8:H:9:ILE:N	2.32	0.62
10:J:10:CYS:HB3	10:J:43:ARG:HH21	1.65	0.62
18:R:255:LEU:O	18:R:258:ARG:N	2.31	0.62
2:B:914:SER:O	2:B:915:ARG:HG2	2.00	0.62
7:G:92:CYS:SG	7:G:98:LYS:N	2.59	0.62
2:B:586:GLU:HG3	2:B:648:TYR:CD2	2.34	0.61
11:K:99:ASN:O	11:K:100:LEU:HD12	2.00	0.61
1:A:133:ASP:HB3	1:A:136:ARG:HG2	1.83	0.61
1:A:313:MET:O	1:A:317:ASP:N	2.27	0.61
1:A:403:THR:HA	1:A:464:ARG:O	2.00	0.61
1:A:1456:ALA:O	1:A:1460:ASN:ND2	2.32	0.61
2:B:658:TYR:CE2	2:B:670:MET:HG2	2.35	0.61
3:C:14:ASN:O	3:C:295:ARG:NH1	2.32	0.61
13:M:85:LEU:HD23	14:N:397:LEU:O	2.00	0.61
15:O:517:VAL:O	15:O:518:SER:HB3	2.00	0.61
15:O:585:MET:HG2	15:O:644:LEU:HD23	1.81	0.61
18:R:190:ASP:OD2	18:R:191:LEU:N	2.24	0.61
5:E:23:VAL:HG22	5:E:28:TYR:HB2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:265:VAL:O	15:O:273:ILE:N	2.26	0.61
15:O:507:LEU:O	15:O:511:ILE:HG12	2.00	0.61
15:O:585:MET:HE2	15:O:644:LEU:HB3	1.82	0.61
2:B:209:ALA:HB2	2:B:366:ILE:HG21	1.81	0.61
2:B:252:PRO:HB2	2:B:255:ILE:HD12	1.82	0.61
4:D:119:GLU:HG3	4:D:123:ILE:HG23	1.82	0.61
5:E:32:GLN:HA	5:E:35:VAL:HG12	1.81	0.61
5:E:77:SER:O	5:E:105:PHE:HB3	2.00	0.61
6:F:130:ILE:HG22	6:F:132:LEU:H	1.65	0.61
13:M:123:ILE:O	13:M:146:GLN:N	2.31	0.61
13:M:163:VAL:HG22	13:M:168:VAL:HG22	1.82	0.61
2:B:44:LYS:HZ2	2:B:663:GLU:HB2	1.65	0.61
2:B:420:LEU:HD13	18:R:149:ARG:HD3	1.83	0.61
2:B:755:ALA:N	2:B:1022:ILE:O	2.31	0.61
3:C:3:ASN:O	3:C:294:VAL:HA	2.00	0.61
3:C:288:LYS:HG3	3:C:289:VAL:HG23	1.83	0.61
16:P:190:THR:HA	16:P:215:TYR:CE1	2.35	0.61
1:A:781:CYS:O	1:A:785:LEU:HB2	2.00	0.61
1:A:978:ASP:N	1:A:982:CYS:O	2.27	0.61
18:R:469:ILE:O	18:R:473:GLY:N	2.34	0.61
20:X:60:DA:H2'	20:X:61:DT:C6	2.35	0.61
1:A:141:LEU:HA	1:A:144:ILE:HG22	1.83	0.61
8:H:97:MET:HG3	8:H:142:LEU:HD23	1.83	0.61
13:M:74:PHE:N	14:N:363:ILE:O	2.32	0.61
14:N:278:ALA:O	14:N:282:LEU:N	2.22	0.61
15:O:128:HIS:NE2	15:O:132:TYR:HE2	1.99	0.61
1:A:1391:LYS:HD3	21:Y:19:DT:H4'	1.83	0.61
2:B:49:PRO:O	2:B:53:LYS:N	2.34	0.61
2:B:454:VAL:HG13	2:B:455:THR:HG23	1.82	0.61
7:G:88:TRP:CD1	7:G:143:ASN:H	2.18	0.61
16:P:135:LYS:HB2	16:P:151:TYR:HD1	1.64	0.61
18:R:583:HIS:NE2	18:R:585:LEU:O	2.33	0.61
1:A:235:LYS:HE3	15:O:44:PRO:HB2	1.83	0.61
2:B:556:TYR:CZ	2:B:561:LEU:HD12	2.35	0.61
2:B:763:SER:O	2:B:765:TYR:N	2.33	0.61
2:B:834:MET:HE1	12:L:63:ARG:HH11	1.66	0.61
4:D:152:GLU:HA	4:D:155:GLU:HG2	1.83	0.61
9:I:29:CYS:HA	13:M:183:PHE:HZ	1.66	0.61
1:A:29:GLN:NE2	2:B:1100:LEU:HD13	2.16	0.61
15:O:202:GLN:HA	15:O:280:LEU:HA	1.81	0.61
15:O:573:SER:C	15:O:575:ASN:H	2.09	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:116:PHE:CD1	18:R:120:ARG:NH2	2.67	0.61
18:R:149:ARG:O	18:R:150:LEU:CD1	2.30	0.61
18:R:215:PHE:HD1	18:R:223:ILE:HD13	1.65	0.61
1:A:624:ILE:HD11	1:A:681:ILE:HG12	1.83	0.60
1:A:911:ILE:HG23	5:E:176:PRO:HD3	1.82	0.60
2:B:833:GLY:N	2:B:881:ILE:O	2.28	0.60
3:C:221:PRO:HG2	3:C:222:VAL:HG23	1.83	0.60
15:O:263:LEU:HA	15:O:274:VAL:HA	1.83	0.60
15:O:265:VAL:HG12	15:O:267:PRO:HD3	1.83	0.60
15:O:580:ASN:O	15:O:583:TRP:CB	2.49	0.60
18:R:166:LYS:HG2	18:R:522:ARG:HH22	1.63	0.60
1:A:385:PRO:HD2	2:B:765:TYR:CD1	2.36	0.60
2:B:739:LYS:HG3	2:B:977:THR:HB	1.82	0.60
6:F:135:ARG:HH12	7:G:58:GLN:HE21	1.48	0.60
15:O:106:TYR:HB3	15:O:208:TYR:HE2	1.64	0.60
15:O:580:ASN:O	15:O:583:TRP:HB2	2.00	0.60
1:A:954:LEU:O	1:A:956:PRO:HD3	2.01	0.60
1:A:1217:ILE:HG22	1:A:1218:GLN:H	1.65	0.60
2:B:695:GLN:CG	2:B:697:PRO:CD	2.55	0.60
3:C:86:PHE:HB2	3:C:203:SER:OG	2.02	0.60
5:E:177:ARG:HD3	5:E:215:MET:HG2	1.84	0.60
15:O:578:ARG:HA	15:O:648:TRP:CZ3	2.34	0.60
1:A:200:GLU:HA	15:O:515:LYS:HD2	1.82	0.60
1:A:250:SER:HB3	1:A:1403:MET:HE1	1.83	0.60
3:C:32:ASN:CG	3:C:33:VAL:H	2.08	0.60
15:O:52:LEU:HD13	15:O:127:ILE:HG21	1.83	0.60
16:P:86:MET:HE1	16:P:131:GLN:HG3	1.83	0.60
16:P:221:ILE:O	16:P:225:ILE:HG12	2.01	0.60
18:R:402:LEU:HD22	18:R:476:ALA:HB1	1.82	0.60
1:A:154:CYS:CB	1:A:157:CYS:SG	2.61	0.60
1:A:208:ASN:O	1:A:210:GLU:N	2.34	0.60
1:A:347:VAL:O	1:A:348:LYS:CG	2.49	0.60
1:A:448:ASP:HB3	1:A:452:LEU:HD12	1.83	0.60
3:C:140:CYS:HB2	3:C:196:LEU:HD13	1.83	0.60
7:G:141:ASP:OD1	7:G:142:VAL:N	2.34	0.60
13:M:247:TRP:CH2	13:M:249:GLU:HB2	2.36	0.60
15:O:484:MET:O	15:O:488:LYS:HG2	2.01	0.60
1:A:128:ARG:NH2	1:A:240:GLU:OE2	2.34	0.60
1:A:384:ASP:HA	2:B:765:TYR:CE1	2.36	0.60
1:A:1221:ASP:OD1	1:A:1222:VAL:N	2.34	0.60
2:B:239:LYS:HG2	2:B:241:TYR:HE2	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:325:GLU:O	2:B:329:THR:N	2.32	0.60
2:B:405:LYS:HG2	2:B:408:LYS:HE2	1.82	0.60
2:B:650:ASP:OD1	2:B:651:VAL:N	2.35	0.60
5:E:100:ILE:O	5:E:104:ASN:ND2	2.35	0.60
16:P:14:ASN:O	16:P:18:LEU:CB	2.50	0.60
1:A:357:LEU:HD12	1:A:363:ARG:C	2.27	0.60
1:A:444:LEU:HD21	1:A:449:ARG:HD3	1.81	0.60
1:A:791:PRO:HB3	1:A:806:VAL:HG21	1.83	0.60
1:A:1198:LEU:HD23	1:A:1273:LYS:HD3	1.84	0.60
2:B:134:GLU:HB2	2:B:144:HIS:HB3	1.82	0.60
2:B:611:PRO:HG3	2:B:648:TYR:CE1	2.36	0.60
2:B:934:ASN:OD1	2:B:935:ASP:N	2.35	0.60
15:O:460:LEU:HD23	15:O:476:TYR:HB2	1.83	0.60
18:R:202:ALA:O	18:R:205:LEU:HB3	2.02	0.60
1:A:110:CYS:CB	1:A:156:HIS:CE1	2.81	0.60
2:B:782:PHE:O	2:B:784:ARG:N	2.34	0.60
5:E:79:TRP:HE1	5:E:81:GLU:HB3	1.65	0.60
5:E:183:PRO:O	5:E:187:TYR:N	2.34	0.60
8:H:101:ALA:HB2	8:H:116:TYR:CE2	2.36	0.60
15:O:191:PHE:CE1	15:O:273:ILE:HD12	2.37	0.60
18:R:28:CYS:SG	18:R:29:GLY:N	2.74	0.60
18:R:87:LEU:HB2	18:R:126:ILE:HD11	1.83	0.60
1:A:457:GLN:N	1:A:460:ASP:OD2	2.35	0.60
6:F:136:ARG:HB2	6:F:144:GLU:HB3	1.82	0.60
7:G:21:ASP:OD1	7:G:22:THR:N	2.34	0.60
13:M:71:ILE:HB	14:N:366:HIS:CD2	2.37	0.60
13:M:159:TYR:HD1	13:M:172:PRO:HA	1.66	0.60
13:M:251:THR:OG1	13:M:254:GLN:NE2	2.34	0.60
1:A:21:LEU:HD11	2:B:1133:LEU:HD12	1.84	0.60
1:A:448:ASP:CB	1:A:452:LEU:HD12	2.31	0.60
2:B:539:GLU:OE1	2:B:539:GLU:N	2.35	0.60
2:B:695:GLN:HE22	2:B:698:ARG:CZ	2.15	0.60
2:B:739:LYS:HG2	2:B:975:TYR:CE1	2.36	0.60
15:O:49:TYR:HA	15:O:52:LEU:HD12	1.83	0.60
15:O:292:ARG:HH22	15:O:649:GLU:C	2.10	0.60
18:R:467:ARG:O	18:R:471:LYS:HB3	2.02	0.60
1:A:249:PRO:C	1:A:251:GLY:H	2.09	0.59
1:A:330:ASP:OD1	1:A:331:SER:N	2.34	0.59
1:A:805:ASN:ND2	2:B:951:SER:O	2.36	0.59
2:B:256:VAL:O	2:B:260:CYS:N	2.33	0.59
2:B:417:ASP:OD1	2:B:419:LEU:N	2.23	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:528:PRO:O	2:B:532:LEU:HB2	2.02	0.59
3:C:236:LEU:N	3:C:288:LYS:O	2.35	0.59
4:D:9:ALA:HB3	7:G:4:LEU:HB3	1.83	0.59
13:M:113:LYS:HD3	13:M:241:ALA:HA	1.85	0.59
15:O:206:LEU:HA	15:O:209:THR:HB	1.84	0.59
15:O:602:LEU:HD22	15:O:626:GLN:HE21	1.66	0.59
1:A:133:ASP:OD1	1:A:134:ASN:N	2.35	0.59
2:B:247:ILE:HD12	2:B:309:VAL:HG23	1.84	0.59
2:B:279:TYR:HA	2:B:282:ILE:HD12	1.83	0.59
3:C:228:ARG:HH21	3:C:299:ILE:HD13	1.67	0.59
5:E:155:ARG:HB2	5:E:188:LEU:HD21	1.83	0.59
11:K:136:THR:HA	11:K:139:ILE:HG22	1.83	0.59
15:O:200:LEU:HA	15:O:281:THR:O	2.02	0.59
20:X:59:DC:C2	20:X:60:DA:N7	2.70	0.59
1:A:224:PRO:HA	1:A:227:THR:HG22	1.82	0.59
1:A:322:THR:CG2	1:A:323:VAL:H	2.16	0.59
1:A:925:GLU:CD	1:A:1081:ALA:HA	2.28	0.59
1:A:955:LEU:O	1:A:959:ILE:HG13	2.02	0.59
2:B:59:LYS:HA	2:B:62:LEU:HB2	1.83	0.59
2:B:301:ALA:O	2:B:304:TYR:HB3	2.02	0.59
8:H:5:LEU:HG	8:H:133:ASN:HB3	1.84	0.59
11:K:88:PHE:HB3	11:K:106:GLN:HB3	1.83	0.59
13:M:110:ALA:HA	13:M:120:GLU:O	2.03	0.59
15:O:76:VAL:HA	15:O:79:LEU:HD13	1.84	0.59
15:O:202:GLN:N	15:O:280:LEU:HG	2.17	0.59
16:P:92:LEU:O	16:P:96:TYR:HB2	2.01	0.59
1:A:545:LYS:HG3	1:A:546:SER:H	1.68	0.59
1:A:1055:SER:O	1:A:1059:LEU:HB2	2.03	0.59
1:A:1145:LEU:HD11	1:A:1157:VAL:HG21	1.85	0.59
7:G:54:VAL:HA	7:G:70:VAL:HG12	1.83	0.59
13:M:112:TYR:HD1	13:M:119:TRP:NE1	1.97	0.59
1:A:361:GLN:O	1:A:361:GLN:HG2	2.02	0.59
1:A:501:ASN:OD1	1:A:502:GLU:N	2.36	0.59
1:A:811:ALA:O	1:A:851:SER:OG	2.20	0.59
2:B:44:LYS:NZ	2:B:663:GLU:HB2	2.18	0.59
2:B:191:GLU:OE2	2:B:460:ARG:NH2	2.35	0.59
2:B:297:THR:HA	2:B:301:ALA:HB3	1.83	0.59
2:B:805:ILE:HG22	2:B:807:GLY:H	1.67	0.59
4:D:128:PRO:O	4:D:157:ILE:HG21	2.03	0.59
5:E:20:LYS:O	5:E:23:VAL:HG12	2.03	0.59
14:N:388:THR:HG23	14:N:390:PHE:CD2	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:467:PHE:CD2	15:O:468:LEU:HD13	2.33	0.59
16:P:313:ASP:C	16:P:315:TRP:H	2.10	0.59
1:A:67:CYS:HB3	1:A:70:CYS:O	2.01	0.59
1:A:630:ASN:HA	1:A:667:SER:OG	2.01	0.59
1:A:957:TYR:OH	1:A:1040:GLN:NE2	2.35	0.59
1:A:1002:ARG:O	1:A:1006:HIS:CB	2.50	0.59
2:B:267:GLU:HG3	2:B:546:SER:HB3	1.84	0.59
2:B:320:LEU:HA	2:B:324:ILE:HD12	1.83	0.59
2:B:767:ILE:CG2	2:B:768:GLU:N	2.58	0.59
3:C:86:PHE:CB	3:C:203:SER:HB3	2.32	0.59
6:F:81:THR:HG22	6:F:82:THR:H	1.68	0.59
15:O:57:LEU:HD22	17:Q:70:PHE:HB2	1.84	0.59
15:O:140:ILE:O	15:O:144:MET:N	2.36	0.59
20:X:25:DT:C6	20:X:26:DT:H72	2.38	0.59
1:A:920:GLY:O	1:A:1083:LEU:N	2.30	0.59
2:B:722:ASP:OD1	2:B:723:THR:N	2.35	0.59
7:G:45:CYS:SG	7:G:46:ILE:N	2.75	0.59
11:K:69:ASP:OD1	11:K:70:HIS:N	2.32	0.59
14:N:371:LEU:HD13	14:N:384:LYS:HZ2	1.68	0.59
15:O:338:ASP:H	15:O:342:ALA:HB2	1.68	0.59
1:A:252:ARG:HH21	15:O:44:PRO:CD	2.12	0.59
1:A:956:PRO:HG2	1:A:1031:LEU:HD11	1.85	0.59
3:C:153:PRO:HA	3:C:156:LEU:HB2	1.85	0.59
6:F:75:PRO:HG2	6:F:78:GLN:HG2	1.83	0.59
7:G:13:ILE:HD11	7:G:66:SER:HB3	1.84	0.59
8:H:80:ARG:HA	11:K:108:TYR:OH	2.03	0.59
13:M:133:LYS:O	13:M:137:GLU:N	2.33	0.59
14:N:287:HIS:O	14:N:291:LEU:CB	2.51	0.59
15:O:583:TRP:O	15:O:587:ASN:ND2	2.36	0.59
16:P:206:VAL:HB	16:P:210:PRO:HB3	1.83	0.59
18:R:22:ASP:OD2	18:R:31:VAL:CG1	2.37	0.59
1:A:372:ARG:CB	2:B:1050:PRO:HG2	2.32	0.59
1:A:723:LEU:O	1:A:727:LYS:CB	2.51	0.59
1:A:1124:PRO:O	1:A:1127:LYS:HB2	2.03	0.59
1:A:1202:ILE:O	1:A:1205:ILE:HG13	2.02	0.59
2:B:536:LEU:HD22	2:B:571:PHE:HD1	1.68	0.59
2:B:944:MET:CG	2:B:945:ASN:H	2.15	0.59
2:B:1082:ARG:HG3	2:B:1083:LEU:HD12	1.84	0.59
9:I:13:LEU:HD21	9:I:27:ARG:HB2	1.85	0.59
16:P:254:GLU:O	16:P:261:TYR:HA	2.03	0.59
18:R:392:THR:O	18:R:488:GLY:HA2	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:545:GLN:HB3	18:R:548:GLU:HG3	1.85	0.59
1:A:38:ASP:HB3	1:A:290:THR:OG1	2.02	0.58
1:A:666:LYS:HG2	1:A:667:SER:H	1.68	0.58
3:C:256:ILE:HA	3:C:268:LYS:H	1.68	0.58
7:G:203:ASP:HB3	7:G:211:TRP:HE1	1.68	0.58
8:H:24:CYS:SG	8:H:25:ARG:N	2.75	0.58
15:O:190:LEU:O	15:O:194:LEU:HG	2.03	0.58
15:O:529:LYS:HE2	15:O:531:LYS:HB2	1.85	0.58
16:P:53:GLN:HE22	19:S:363:GLN:HA	1.68	0.58
1:A:204:VAL:CG2	15:O:517:VAL:HA	2.31	0.58
1:A:222:LEU:HA	1:A:226:LYS:HD2	1.83	0.58
1:A:914:PHE:CZ	5:E:211:TYR:HB2	2.38	0.58
1:A:1071:LEU:O	1:A:1074:ALA:HB3	2.02	0.58
6:F:136:ARG:O	6:F:143:PHE:O	2.20	0.58
14:N:315:ALA:HB2	14:N:375:ILE:HG22	1.85	0.58
18:R:91:SER:HB2	18:R:96:ILE:HD11	1.83	0.58
2:B:877:GLU:CG	2:B:878:PRO:HD2	2.33	0.58
2:B:1038:ARG:HE	2:B:1041:GLY:H	1.50	0.58
3:C:116:VAL:HA	3:C:130:ASN:HD21	1.67	0.58
15:O:255:LYS:HB3	15:O:256:PRO:HD3	1.85	0.58
16:P:190:THR:HA	16:P:215:TYR:HE1	1.67	0.58
1:A:541:LEU:HD11	1:A:694:MET:HE1	1.85	0.58
1:A:555:GLN:HG2	1:A:800:LYS:HD3	1.84	0.58
4:D:119:GLU:HA	4:D:122:GLN:HB3	1.85	0.58
6:F:79:ARG:HD2	6:F:146:TRP:CZ2	2.38	0.58
16:P:128:LEU:HA	16:P:131:GLN:HB2	1.85	0.58
1:A:148:CYS:SG	1:A:149:LYS:N	2.76	0.58
1:A:678:PHE:CE2	1:A:694:MET:HG2	2.37	0.58
1:A:753:GLN:O	1:A:755:GLY:N	2.33	0.58
1:A:1380:ARG:HH11	1:A:1385:GLN:NE2	2.00	0.58
3:C:285:PHE:HA	3:C:288:LYS:HZ3	1.68	0.58
16:P:295:ASN:HD21	16:P:298:LYS:HB3	1.68	0.58
20:X:14:DT:H2"	20:X:15:DT:C6	2.38	0.58
1:A:525:GLU:OE1	6:F:99:LEU:CA	2.40	0.58
5:E:6:GLU:O	5:E:10:SER:HB2	2.03	0.58
5:E:12:LEU:O	5:E:16:PHE:HB2	2.03	0.58
9:I:34:PRO:O	9:I:35:ILE:HG13	2.03	0.58
15:O:326:ILE:O	15:O:329:PRO:HD3	2.03	0.58
18:R:512:GLU:OE1	18:R:512:GLU:N	2.37	0.58
21:Y:10:DC:N3	21:Y:11:DA:N6	2.52	0.58
1:A:204:VAL:HG21	15:O:516:LEU:O	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:953:GLY:HA2	1:A:1063:SER:HB2	1.85	0.58
1:A:1171:PHE:HB3	1:A:1187:ARG:O	2.04	0.58
1:A:1272:VAL:HG13	1:A:1273:LYS:H	1.67	0.58
2:B:1038:ARG:NH2	2:B:1050:PRO:HA	2.18	0.58
15:O:259:LEU:HD21	15:O:261:GLN:HB2	1.85	0.58
18:R:258:ARG:HA	18:R:261:GLU:HB3	1.85	0.58
1:A:1343:MET:HE1	1:A:1355:ILE:HG13	1.85	0.58
2:B:264:SER:C	2:B:266:LEU:H	2.12	0.58
2:B:794:VAL:HG23	2:B:895:LEU:CD2	2.33	0.58
3:C:91:VAL:HG23	3:C:200:GLN:HE22	1.69	0.58
8:H:5:LEU:HD13	8:H:60:ALA:HA	1.86	0.58
1:A:18:PHE:CD1	2:B:1139:PRO:CA	2.85	0.58
1:A:372:ARG:HB3	2:B:1050:PRO:HG2	1.85	0.58
2:B:311:THR:HG23	2:B:313:ARG:H	1.69	0.58
3:C:84:TYR:CD2	3:C:207:HIS:CE1	2.91	0.58
3:C:324:LYS:HD3	11:K:68:GLU:OE2	2.03	0.58
4:D:11:LEU:HB3	7:G:3:ILE:HA	1.85	0.58
7:G:94:ALA:O	7:G:128:TRP:NE1	2.35	0.58
15:O:37:LEU:O	15:O:40:ARG:C	2.47	0.58
15:O:40:ARG:HH22	16:P:314:GLU:HB2	1.68	0.58
18:R:142:MET:HE2	18:R:219:ARG:HD2	1.85	0.58
18:R:195:LYS:O	18:R:199:VAL:N	2.35	0.58
1:A:37:ARG:HB3	1:A:39:LEU:HG	1.85	0.58
1:A:467:GLU:N	1:A:470:ASP:OD2	2.27	0.58
1:A:520:HIS:CE1	2:B:1062:LEU:HD21	2.35	0.58
1:A:665:ASP:CG	1:A:798:GLY:H	2.12	0.58
16:P:95:SER:HA	16:P:98:GLU:HG2	1.86	0.58
2:B:911:LYS:HD3	2:B:1029:HIS:HB2	1.86	0.57
9:I:33:PHE:CE2	9:I:35:ILE:HA	2.39	0.57
13:M:134:ASP:O	13:M:138:SER:N	2.37	0.57
15:O:36:SER:O	15:O:40:ARG:N	2.37	0.57
15:O:122:TYR:CD2	15:O:124:GLU:O	2.56	0.57
15:O:506:ARG:NH2	15:O:527:LEU:HB3	2.19	0.57
2:B:616:SER:HB2	2:B:621:ARG:HE	1.70	0.57
15:O:629:MET:O	15:O:633:ARG:HB2	2.04	0.57
18:R:178:PRO:HA	18:R:181:PHE:HD2	1.68	0.57
18:R:485:ASN:OD1	18:R:486:ILE:N	2.37	0.57
1:A:347:VAL:HG12	1:A:349:PRO:HG2	1.86	0.57
1:A:502:GLU:OE1	1:A:557:PHE:CZ	2.57	0.57
2:B:916:HIS:CD2	2:B:957:LYS:HB2	2.39	0.57
4:D:63:VAL:HG22	4:D:67:SER:HB2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:53:ALA:HB1	11:K:104:ARG:HH12	1.69	0.57
18:R:191:LEU:HD12	18:R:239:ARG:NH2	2.18	0.57
18:R:401:THR:N	18:R:479:THR:O	2.36	0.57
1:A:226:LYS:O	1:A:230:LEU:HB2	2.03	0.57
1:A:477:GLN:NE2	1:A:518:ASN:ND2	2.52	0.57
2:B:128:PRO:HA	2:B:151:ARG:HA	1.85	0.57
2:B:630:LEU:HB2	2:B:635:LEU:HD22	1.86	0.57
3:C:66:ALA:O	3:C:70:ILE:HG22	2.03	0.57
3:C:152:ASP:O	3:C:154:LYS:N	2.32	0.57
3:C:225:ALA:HB2	3:C:302:VAL:HG23	1.84	0.57
3:C:285:PHE:HA	3:C:288:LYS:NZ	2.19	0.57
4:D:5:GLU:HB3	7:G:6:LYS:HB3	1.87	0.57
5:E:25:ASP:OD1	5:E:25:ASP:N	2.32	0.57
13:M:72:GLU:HB2	14:N:364:ARG:HE	1.68	0.57
13:M:190:ASN:O	13:M:193:ARG:N	2.29	0.57
1:A:723:LEU:O	1:A:727:LYS:HB2	2.05	0.57
2:B:1004:LEU:HD12	2:B:1017:ILE:HD12	1.85	0.57
2:B:1036:HIS:CG	2:B:1054:ARG:HG3	2.40	0.57
7:G:98:LYS:HA	7:G:109:PHE:HA	1.86	0.57
9:I:8:CYS:CB	9:I:29:CYS:SG	2.93	0.57
10:J:45:CYS:O	10:J:48:ARG:HG2	2.03	0.57
13:M:165:ASP:OD1	14:N:300:LYS:NZ	2.37	0.57
1:A:185:TRP:O	1:A:186:VAL:HG22	2.04	0.57
1:A:287:VAL:O	1:A:290:THR:HG22	2.05	0.57
1:A:328:ASN:CG	1:A:329:SER:H	2.10	0.57
1:A:549:PRO:HG3	1:A:679:TYR:HB2	1.86	0.57
1:A:1151:GLU:HG3	1:A:1152:ARG:HG3	1.86	0.57
3:C:86:PHE:HD2	3:C:203:SER:OG	1.88	0.57
5:E:199:ILE:HG13	5:E:209:ALA:HB2	1.86	0.57
7:G:207:LEU:HD22	7:G:210:TRP:CD1	2.40	0.57
13:M:121:ILE:O	13:M:148:LEU:HB2	2.04	0.57
18:R:510:SER:HB3	18:R:520:ILE:HB	1.85	0.57
1:A:88:LEU:HD22	1:A:316:TRP:CD1	2.40	0.57
1:A:135:LEU:O	1:A:138:MET:N	2.38	0.57
1:A:1340:ASN:HA	1:A:1343:MET:HE2	1.86	0.57
14:N:364:ARG:HH11	14:N:365:VAL:H	1.52	0.57
15:O:185:TYR:N	15:O:185:TYR:CD1	2.73	0.57
15:O:587:ASN:O	15:O:590:PHE:HB2	2.04	0.57
15:O:630:VAL:O	15:O:634:GLU:HG2	2.05	0.57
18:R:171:THR:HG23	18:R:172:GLU:H	1.69	0.57
19:S:450:SER:N	19:S:453:GLN:OE1	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:Y:44:DT:H2'	21:Y:45:DT:H2'	1.87	0.57
1:A:572:ASP:O	1:A:576:LEU:N	2.35	0.57
1:A:926:MET:SD	1:A:930:ALA:HA	2.44	0.57
3:C:100:ARG:HH12	10:J:2:ILE:HG21	1.69	0.57
15:O:633:ARG:NH2	16:P:308:GLU:HG2	2.20	0.57
16:P:14:ASN:O	16:P:18:LEU:HB2	2.04	0.57
19:S:426:ILE:HA	19:S:429:TYR:HD2	1.69	0.57
2:B:424:VAL:HG23	18:R:89:ALA:C	2.30	0.57
2:B:526:GLU:O	2:B:529:ILE:HG22	2.05	0.57
3:C:88:ASN:CG	3:C:202:ILE:HG12	2.30	0.57
13:M:77:LYS:NZ	13:M:262:GLU:HB2	2.20	0.57
15:O:122:TYR:CE2	15:O:124:GLU:O	2.58	0.57
1:A:37:ARG:HA	1:A:293:VAL:HG11	1.86	0.57
1:A:269:ARG:HG3	1:A:285:LEU:HD22	1.86	0.57
1:A:482:ARG:HD3	1:A:544:PRO:CG	2.32	0.57
1:A:803:THR:O	1:A:807:SER:HB2	2.04	0.57
1:A:995:VAL:HG23	1:A:996:ASP:H	1.70	0.57
5:E:112:TYR:CG	5:E:116:ILE:HG12	2.40	0.57
6:F:101:ILE:HG21	6:F:120:ILE:HD11	1.87	0.57
15:O:211:ILE:O	15:O:214:LEU:HG	2.04	0.57
21:Y:43:DA:C8	21:Y:43:DA:H5'	2.39	0.57
1:A:443:ASN:OD1	1:A:444:LEU:N	2.38	0.56
1:A:560:GLY:HA3	1:A:701:CYS:SG	2.45	0.56
2:B:727:LEU:HD11	2:B:786:GLU:HB2	1.87	0.56
2:B:1088:ASP:OD2	2:B:1123:TYR:N	2.38	0.56
5:E:46:TYR:CZ	5:E:58:MET:HA	2.40	0.56
6:F:76:LYS:HD2	6:F:79:ARG:HE	1.69	0.56
18:R:144:ILE:HD12	18:R:154:VAL:HG21	1.87	0.56
18:R:273:GLN:HB2	19:S:277:UNK:N	2.20	0.56
18:R:505:HIS:O	18:R:508:PHE:N	2.38	0.56
18:R:607:ASP:OD1	18:R:610:LEU:N	2.38	0.56
19:S:527:ASP:O	19:S:531:GLN:HG3	2.05	0.56
21:Y:53:DT:H2'	21:Y:54:DA:H8	1.70	0.56
2:B:143:MET:SD	19:S:399:GLU:HB2	2.45	0.56
3:C:169:PHE:HB3	3:C:184:VAL:HG21	1.87	0.56
16:P:265:LEU:C	16:P:267:SER:H	2.12	0.56
18:R:478:PHE:O	18:R:599:PRO:HB3	2.04	0.56
1:A:363:ARG:NH1	2:B:1127:LEU:CD2	2.69	0.56
1:A:935:PHE:HE2	1:A:1008:LEU:HD13	1.70	0.56
1:A:1148:ASP:HB2	1:A:1290:LYS:HA	1.87	0.56
1:A:1302:ASP:O	1:A:1306:THR:N	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:412:ARG:NH2	2:B:416:TYR:OH	2.29	0.56
2:B:528:PRO:O	2:B:532:LEU:CB	2.54	0.56
2:B:772:VAL:HG23	2:B:924:ILE:O	2.05	0.56
3:C:100:ARG:NH2	3:C:192:LEU:O	2.38	0.56
3:C:238:PRO:O	3:C:239:ILE:HG13	2.06	0.56
5:E:87:SER:HA	5:E:115:ASN:HB3	1.88	0.56
15:O:34:ILE:HD11	16:P:307:LYS:HD2	1.87	0.56
15:O:203:ILE:HA	15:O:207:HIS:CD2	2.40	0.56
15:O:584:ASN:O	15:O:588:LEU:N	2.34	0.56
16:P:311:TYR:H	16:P:314:GLU:CD	2.12	0.56
17:Q:59:ILE:O	17:Q:62:GLY:N	2.39	0.56
18:R:237:LEU:HD13	18:R:239:ARG:CG	2.33	0.56
21:Y:52:DA:H2''	21:Y:53:DT:O5'	2.05	0.56
1:A:406:GLU:HB3	1:A:462:VAL:O	2.06	0.56
1:A:997:GLN:C	1:A:999:ASP:H	2.13	0.56
2:B:842:TYR:CE2	2:B:873:TYR:HB2	2.41	0.56
2:B:1047:THR:HB	2:B:1049:GLN:HG2	1.87	0.56
3:C:67:PHE:CE1	3:C:318:VAL:HG22	2.41	0.56
7:G:10:LEU:HA	7:G:69:ASN:HA	1.87	0.56
7:G:39:ILE:HG22	7:G:43:GLY:O	2.04	0.56
15:O:303:ARG:HD2	15:O:467:PHE:HE1	1.69	0.56
18:R:186:ALA:HA	18:R:189:LEU:HD12	1.88	0.56
18:R:501:LEU:O	18:R:505:HIS:N	2.35	0.56
19:S:451:ARG:HG3	19:S:452:LYS:H	1.70	0.56
21:Y:47:DC:H2'	21:Y:48:DT:C5	2.40	0.56
1:A:222:LEU:HG	1:A:226:LYS:HD2	1.87	0.56
1:A:387:LEU:HD11	1:A:391:GLU:HB2	1.87	0.56
1:A:390:ASP:HA	1:A:488:HIS:ND1	2.19	0.56
1:A:705:LEU:O	1:A:709:GLY:N	2.36	0.56
14:N:305:MET:HG2	14:N:414:GLY:HA3	1.87	0.56
1:A:82:GLY:O	1:A:263:ALA:N	2.32	0.56
1:A:347:VAL:O	1:A:348:LYS:HG3	2.06	0.56
1:A:363:ARG:NH1	2:B:1127:LEU:HD21	2.21	0.56
1:A:1222:VAL:HA	1:A:1231:ALA:O	2.05	0.56
2:B:203:ASN:ND2	2:B:221:THR:OG1	2.38	0.56
2:B:489:LEU:HG	2:B:493:GLN:OE1	2.06	0.56
2:B:521:THR:HB	2:B:587:PHE:HD2	1.68	0.56
2:B:657:SER:OG	2:B:672:HIS:ND1	2.31	0.56
2:B:1045:VAL:HA	18:R:37:ILE:HG23	1.86	0.56
3:C:59:ILE:HD13	3:C:63:ILE:HD11	1.88	0.56
5:E:9:ILE:HG22	5:E:53:PRO:HG3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:106:TRP:CD1	16:P:145:ARG:HA	2.41	0.56
2:B:961:LEU:HB2	2:B:1022:ILE:HD11	1.87	0.56
3:C:6:GLY:HA3	3:C:13:THR:HB	1.87	0.56
5:E:31:THR:HG23	5:E:34:GLU:H	1.71	0.56
5:E:118:PRO:O	5:E:122:LYS:N	2.39	0.56
14:N:308:GLN:HB2	14:N:417:VAL:HG12	1.88	0.56
15:O:58:GLY:HA2	15:O:62:ALA:HB2	1.88	0.56
15:O:200:LEU:C	15:O:201:ILE:HG13	2.22	0.56
16:P:218:THR:HG21	16:P:259:ASP:HB3	1.87	0.56
18:R:129:CYS:O	18:R:132:VAL:HG22	2.05	0.56
18:R:140:HIS:ND1	18:R:140:HIS:O	2.38	0.56
18:R:431:ARG:HG2	18:R:438:THR:HG23	1.87	0.56
13:M:116:SER:HB2	13:M:118:LEU:HD13	1.88	0.56
18:R:6:ASN:O	18:R:8:HIS:ND1	2.39	0.56
1:A:38:ASP:CG	1:A:39:LEU:H	2.14	0.56
1:A:870:GLU:O	1:A:874:ASP:CB	2.52	0.56
2:B:993:ASP:OD1	2:B:994:GLN:N	2.39	0.56
2:B:1096:ASP:HB3	2:B:1115:ASN:HD21	1.70	0.56
7:G:9:ASP:OD1	7:G:10:LEU:N	2.31	0.56
7:G:44:LEU:HD12	7:G:44:LEU:O	2.06	0.56
8:H:99:GLY:HA3	8:H:118:PHE:CD1	2.41	0.56
13:M:160:ALA:HB3	13:M:171:VAL:HB	1.88	0.56
15:O:588:LEU:O	15:O:591:LYS:N	2.39	0.56
19:S:444:GLN:NE2	19:S:490:LYS:HE3	2.20	0.56
1:A:13:ILE:HD11	2:B:1119:MET:HE1	1.88	0.56
1:A:816:GLN:HG2	1:A:864:HIS:HA	1.88	0.56
2:B:217:GLN:NE2	2:B:232:TYR:HB3	2.20	0.56
12:L:65:VAL:HG22	12:L:66:GLN:H	1.71	0.56
15:O:470:GLU:N	15:O:479:PRO:HD3	2.20	0.56
16:P:151:TYR:OH	18:R:647:ALA:O	2.24	0.56
1:A:1385:GLN:OE1	1:A:1412:SER:OG	2.23	0.55
2:B:1093:ASP:OD2	2:B:1104:SER:N	2.38	0.55
4:D:126:GLN:HG3	4:D:127:LEU:HD23	1.88	0.55
7:G:47:THR:O	7:G:75:VAL:HB	2.05	0.55
15:O:60:ARG:HD3	15:O:90:SER:HB3	1.88	0.55
17:Q:55:ALA:O	17:Q:58:TYR:HB3	2.06	0.55
18:R:123:GLN:HG2	18:R:150:LEU:HD21	1.87	0.55
18:R:216:GLU:HG2	18:R:534:VAL:HG21	1.88	0.55
1:A:285:LEU:HD21	1:A:353:PHE:CD1	2.42	0.55
1:A:653:ILE:HG23	1:A:660:LEU:HB2	1.87	0.55
1:A:1311:GLY:O	5:E:147:HIS:NE2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1101:MET:SD	2:B:1126:LYS:HG3	2.46	0.55
3:C:21:PRO:HB2	3:C:27:ALA:HB1	1.87	0.55
5:E:26:ARG:NH1	5:E:188:LEU:O	2.39	0.55
15:O:163:VAL:O	15:O:167:GLY:N	2.38	0.55
18:R:416:ARG:N	18:R:613:HIS:O	2.29	0.55
18:R:441:ILE:HD12	18:R:447:MET:HB3	1.88	0.55
1:A:15:GLY:H	1:A:1408:VAL:HG12	1.70	0.55
1:A:231:PHE:HA	1:A:234:ILE:HD12	1.89	0.55
1:A:449:ARG:O	1:A:452:LEU:N	2.35	0.55
1:A:1394:ASP:O	1:A:1398:ASP:CB	2.54	0.55
2:B:427:ASN:HA	2:B:430:THR:H	1.70	0.55
2:B:544:ILE:HD11	2:B:563:GLY:HA2	1.88	0.55
2:B:1038:ARG:HH22	2:B:1050:PRO:HA	1.72	0.55
3:C:34:GLU:HA	3:C:37:LYS:HB3	1.88	0.55
4:D:126:GLN:O	4:D:127:LEU:CG	2.46	0.55
5:E:1:MET:HG3	5:E:3:GLN:H	1.71	0.55
15:O:292:ARG:HB3	15:O:325:LYS:NZ	2.21	0.55
1:A:1373:ARG:HA	1:A:1376:LEU:CD1	2.34	0.55
1:A:1376:LEU:HD21	1:A:1389:PHE:CZ	2.41	0.55
2:B:84:LEU:HD23	19:S:384:HIS:NE2	2.22	0.55
2:B:427:ASN:O	2:B:431:SER:N	2.39	0.55
7:G:41:ASN:HA	7:G:155:PHE:CG	2.41	0.55
13:M:80:GLY:HA3	13:M:261:LYS:HE2	1.87	0.55
15:O:94:THR:O	15:O:98:LEU:HG	2.07	0.55
15:O:364:ILE:HA	15:O:476:TYR:CZ	2.41	0.55
1:A:123:PHE:CD2	1:A:144:ILE:HD13	2.42	0.55
1:A:153:ARG:NH2	15:O:337:GLN:O	2.36	0.55
2:B:462:SER:HG	2:B:465:SER:H	1.54	0.55
3:C:31:TRP:CZ2	11:K:123:ASP:HB3	2.42	0.55
3:C:85:PHE:HA	3:C:204:LEU:HA	1.87	0.55
15:O:471:THR:OG1	15:O:475:VAL:O	2.23	0.55
18:R:551:GLN:O	18:R:555:ALA:CB	2.54	0.55
19:S:425:MET:O	19:S:428:PHE:HB3	2.07	0.55
1:A:351:ARG:HB3	1:A:355:GLN:CD	2.31	0.55
1:A:904:VAL:HG13	1:A:912:VAL:HG23	1.89	0.55
2:B:141:ILE:HG23	2:B:142:ILE:N	2.21	0.55
2:B:354:ARG:HD2	2:B:549:LEU:HD13	1.89	0.55
2:B:638:ASP:HA	2:B:641:LEU:HD13	1.87	0.55
3:C:12:VAL:CG1	3:C:13:THR:N	2.69	0.55
3:C:222:VAL:HG13	3:C:303:GLU:O	2.06	0.55
9:I:8:CYS:SG	9:I:10:ASN:HB2	2.45	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:200:LEU:HA	15:O:281:THR:C	2.32	0.55
15:O:482:LYS:C	15:O:485:PRO:HD2	2.31	0.55
1:A:17:GLU:O	2:B:1139:PRO:HA	2.06	0.55
1:A:395:PRO:HB3	1:A:497:THR:H	1.72	0.55
1:A:606:GLY:HA2	1:A:609:VAL:HG12	1.89	0.55
1:A:727:LYS:O	1:A:731:VAL:N	2.33	0.55
1:A:791:PRO:O	1:A:795:ALA:N	2.33	0.55
2:B:253:ILE:O	2:B:256:VAL:N	2.39	0.55
2:B:658:TYR:HD2	2:B:670:MET:HA	1.72	0.55
13:M:87:VAL:HA	14:N:396:ALA:HA	1.88	0.55
15:O:188:SER:C	15:O:190:LEU:N	2.59	0.55
15:O:496:ILE:HA	15:O:499:THR:HB	1.88	0.55
15:O:580:ASN:HA	15:O:583:TRP:HB2	1.89	0.55
15:O:585:MET:HE1	15:O:648:TRP:HB2	1.88	0.55
15:O:595:LEU:HD22	15:O:633:ARG:HG2	1.88	0.55
1:A:786:ASP:OD1	1:A:787:ASN:N	2.40	0.55
1:A:1065:LYS:HA	1:A:1068:ARG:HB2	1.87	0.55
4:D:58:ILE:O	4:D:62:VAL:N	2.29	0.55
8:H:47:PHE:HZ	8:H:146:ARG:HG3	1.71	0.55
15:O:125:GLU:CB	15:O:128:HIS:HB2	2.37	0.55
15:O:203:ILE:HG22	15:O:207:HIS:HD2	1.71	0.55
1:A:746:ASN:OD1	1:A:747:LYS:N	2.39	0.55
1:A:770:LEU:O	1:A:774:ARG:HB2	2.06	0.55
1:A:1202:ILE:HG21	1:A:1224:ILE:HG21	1.88	0.55
2:B:481:ARG:HH22	21:Y:21:DG:H2'	1.72	0.55
3:C:83:VAL:HG11	3:C:85:PHE:HZ	1.59	0.55
3:C:88:ASN:O	12:L:60:ARG:HD3	2.06	0.55
13:M:71:ILE:HG23	13:M:72:GLU:OE1	2.07	0.55
13:M:148:LEU:HA	13:M:181:PRO:HA	1.87	0.55
15:O:128:HIS:CE1	15:O:132:TYR:CE2	2.94	0.55
15:O:140:ILE:HD11	15:O:160:VAL:HG21	1.89	0.55
16:P:106:TRP:CG	16:P:107:SER:H	2.25	0.55
18:R:408:LEU:HD13	18:R:427:ALA:HA	1.89	0.55
1:A:447:GLY:O	1:A:448:ASP:HB2	2.07	0.55
1:A:777:VAL:O	1:A:781:CYS:HB2	2.07	0.55
1:A:1299:GLY:C	1:A:1301:ARG:H	2.15	0.55
2:B:556:TYR:CE1	2:B:561:LEU:HB2	2.42	0.55
2:B:566:ARG:NH2	14:N:282:LEU:HD23	2.22	0.55
2:B:1007:GLY:O	3:C:69:ARG:NH1	2.40	0.55
3:C:31:TRP:CG	3:C:32:ASN:N	2.72	0.55
5:E:176:PRO:HB2	5:E:212:ARG:HG2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:95:TYR:N	8:H:144:ILE:O	2.40	0.55
15:O:124:GLU:HG3	15:O:125:GLU:OE1	2.07	0.55
15:O:170:THR:HG22	15:O:279:SER:N	2.22	0.55
16:P:254:GLU:CB	16:P:262:ARG:O	2.54	0.55
1:A:390:ASP:OD2	1:A:538:LYS:NZ	2.28	0.54
2:B:464:ILE:HD11	2:B:746:TYR:CE1	2.38	0.54
10:J:2:ILE:O	10:J:53:HIS:NE2	2.40	0.54
13:M:72:GLU:N	14:N:364:ARG:HG2	2.22	0.54
13:M:106:PHE:O	13:M:107:ILE:HG22	2.06	0.54
15:O:124:GLU:CG	15:O:125:GLU:N	2.16	0.54
1:A:136:ARG:HH21	1:A:140:ILE:HD11	1.72	0.54
1:A:310:ASN:HA	15:O:564:PHE:HE2	1.72	0.54
1:A:352:GLY:O	1:A:356:ARG:HB2	2.07	0.54
1:A:577:THR:HA	11:K:88:PHE:CE2	2.42	0.54
2:B:167:ASP:C	2:B:169:SER:H	2.16	0.54
2:B:1057:ASP:OD1	2:B:1058:GLY:N	2.40	0.54
5:E:112:TYR:CZ	5:E:116:ILE:HG23	2.42	0.54
13:M:86:HIS:HD2	13:M:175:ARG:HB2	1.72	0.54
15:O:484:MET:HB2	15:O:485:PRO:HD3	1.89	0.54
16:P:55:LEU:O	16:P:60:LEU:N	2.40	0.54
16:P:266:GLU:O	16:P:270:GLN:N	2.37	0.54
2:B:555:VAL:O	2:B:561:LEU:HA	2.06	0.54
16:P:304:LYS:HG3	16:P:305:HIS:CD2	2.42	0.54
19:S:312:UNK:O	19:S:316:UNK:N	2.40	0.54
20:X:11:DA:H2"	20:X:12:DT:C6	2.43	0.54
20:X:47:DA:H2"	20:X:48:DT:H71	1.88	0.54
1:A:323:VAL:O	1:A:326:TYR:HB3	2.07	0.54
1:A:599:LYS:HB3	1:A:600:PRO:HD3	1.90	0.54
1:A:623:VAL:N	1:A:685:TYR:OH	2.39	0.54
2:B:579:ARG:NH1	2:B:647:GLU:HG3	2.18	0.54
2:B:860:VAL:HG13	2:B:861:ASN:H	1.72	0.54
9:I:7:SER:OG	9:I:8:CYS:N	2.38	0.54
13:M:140:TRP:HB2	13:M:185:TYR:CD1	2.43	0.54
15:O:342:ALA:O	15:O:346:GLN:HB2	2.07	0.54
15:O:506:ARG:HH22	15:O:527:LEU:HB3	1.72	0.54
16:P:247:LEU:HA	16:P:250:ASP:HB2	1.89	0.54
18:R:84:ARG:O	18:R:88:ARG:N	2.32	0.54
1:A:1420:THR:HA	2:B:1080:LEU:HD11	1.90	0.54
1:A:1449:GLU:OE2	4:D:10:PHE:N	2.41	0.54
2:B:68:PHE:CE1	2:B:385:SER:OG	2.60	0.54
2:B:68:PHE:HD1	2:B:385:SER:HG	1.52	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:303:GLU:O	2:B:307:ALA:CB	2.56	0.54
2:B:1095:CYS:SG	2:B:1115:ASN:HB3	2.47	0.54
15:O:132:TYR:HE1	15:O:645:LEU:HD21	1.72	0.54
15:O:220:GLU:HG2	15:O:221:LYS:H	1.72	0.54
16:P:106:TRP:CZ3	16:P:108:LYS:HB3	2.42	0.54
16:P:135:LYS:HD3	16:P:151:TYR:HD1	1.72	0.54
16:P:216:SER:OG	16:P:261:TYR:N	2.26	0.54
18:R:137:GLU:O	18:R:138:LYS:HG2	2.07	0.54
18:R:468:ILE:HA	18:R:610:LEU:HD21	1.88	0.54
1:A:378:ARG:CD	2:B:1060:LEU:CD2	2.66	0.54
5:E:200:ARG:HD2	5:E:208:TYR:CZ	2.42	0.54
1:A:57:LYS:HA	1:A:68:ALA:HB3	1.89	0.54
1:A:200:GLU:O	15:O:516:LEU:HD21	2.06	0.54
1:A:205:LEU:O	1:A:209:PRO:HG3	2.08	0.54
1:A:687:PRO:HA	1:A:690:ALA:HB3	1.90	0.54
1:A:1059:LEU:HD23	1:A:1060:TYR:CD2	2.43	0.54
2:B:247:ILE:HG13	2:B:248:ALA:H	1.71	0.54
2:B:775:LYS:HG3	2:B:925:ILE:HG22	1.89	0.54
3:C:235:ILE:HG22	3:C:289:VAL:HG22	1.90	0.54
3:C:238:PRO:C	3:C:239:ILE:HG13	2.33	0.54
9:I:21:VAL:C	9:I:23:THR:H	2.14	0.54
10:J:36:LEU:HD22	10:J:47:ARG:HG3	1.89	0.54
13:M:86:HIS:CD2	13:M:175:ARG:HB2	2.43	0.54
13:M:113:LYS:NZ	13:M:237:ALA:O	2.39	0.54
18:R:273:GLN:HB2	19:S:277:UNK:H	1.72	0.54
1:A:22:SER:HG	1:A:25:ASP:H	1.55	0.54
1:A:1259:ARG:O	1:A:1263:LEU:HG	2.08	0.54
2:B:157:ARG:HD3	2:B:182:GLY:HA3	1.90	0.54
2:B:612:LEU:HA	2:B:675:ILE:HG23	1.89	0.54
6:F:136:ARG:O	6:F:143:PHE:C	2.51	0.54
7:G:55:GLU:OE2	7:G:69:ASN:N	2.41	0.54
15:O:55:ALA:HB2	15:O:593:GLU:HG3	1.90	0.54
15:O:125:GLU:HB2	15:O:128:HIS:CB	2.38	0.54
18:R:455:GLU:HG2	18:R:588:THR:HG23	1.90	0.54
19:S:381:VAL:HG22	19:S:383:ARG:H	1.72	0.54
1:A:235:LYS:NZ	15:O:44:PRO:HG2	2.23	0.54
2:B:356:VAL:O	2:B:360:MET:CB	2.55	0.54
2:B:710:ILE:HG12	2:B:1026:LYS:O	2.08	0.54
12:L:28:LYS:NZ	12:L:40:LEU:O	2.40	0.54
15:O:73:ARG:NH1	15:O:121:TYR:OH	2.34	0.54
15:O:229:ASN:HB3	15:O:237:LYS:HE3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:ASP:H	1:A:136:ARG:HB2	1.73	0.54
1:A:201:TRP:HB3	1:A:205:LEU:HD13	1.90	0.54
1:A:383:PRO:HG2	2:B:765:TYR:O	2.08	0.54
1:A:610:PHE:CZ	1:A:697:MET:HE1	2.40	0.54
2:B:1036:HIS:CD2	2:B:1054:ARG:HG3	2.43	0.54
2:B:1096:ASP:HB3	2:B:1115:ASN:ND2	2.23	0.54
4:D:157:ILE:O	4:D:161:ALA:N	2.41	0.54
5:E:6:GLU:O	5:E:10:SER:CB	2.56	0.54
8:H:138:GLU:OE1	8:H:138:GLU:N	2.39	0.54
9:I:15:THR:HG22	9:I:24:LEU:HA	1.90	0.54
13:M:164:LYS:HG3	14:N:300:LYS:HD3	1.89	0.54
15:O:200:LEU:CD2	15:O:282:ILE:H	2.19	0.54
15:O:581:LEU:HA	15:O:585:MET:SD	2.48	0.54
16:P:136:SER:HA	16:P:148:TYR:CE1	2.42	0.54
18:R:267:ALA:O	18:R:271:SER:OG	2.21	0.54
18:R:395:ASN:OD1	18:R:452:ALA:N	2.41	0.54
18:R:433:ARG:HD3	19:S:473:LEU:HD23	1.89	0.54
1:A:37:ARG:HD2	1:A:39:LEU:HD21	1.90	0.53
1:A:41:ASP:OD1	1:A:49:LYS:N	2.41	0.53
1:A:559:THR:HG21	2:B:947:HIS:NE2	2.22	0.53
1:A:1441:LEU:HG	7:G:52:LEU:HA	1.89	0.53
2:B:77:ILE:HG21	2:B:98:ILE:HD11	1.90	0.53
2:B:131:VAL:HG23	2:B:147:VAL:HB	1.88	0.53
2:B:593:ASN:OD1	2:B:594:SER:N	2.40	0.53
11:K:62:SER:OG	11:K:104:ARG:NH1	2.40	0.53
15:O:163:VAL:HG22	15:O:169:LEU:HD22	1.90	0.53
18:R:440:LEU:O	18:R:447:MET:HB2	2.08	0.53
1:A:196:ILE:O	1:A:200:GLU:HG3	2.07	0.53
1:A:210:GLU:N	1:A:212:GLU:OE1	2.41	0.53
2:B:357:VAL:HA	2:B:360:MET:HB3	1.90	0.53
6:F:115:THR:O	6:F:120:ILE:HG23	2.08	0.53
7:G:97:ILE:HG21	7:G:140:PHE:HZ	1.72	0.53
20:X:48:DT:C4	20:X:49:DA:N6	2.76	0.53
1:A:248:VAL:HG23	1:A:249:PRO:HD2	0.60	0.53
1:A:1003:ASP:O	1:A:1007:SER:HB3	2.08	0.53
1:A:1372:THR:C	1:A:1376:LEU:CD2	2.81	0.53
2:B:691:PRO:HA	2:B:694:ASN:ND2	2.24	0.53
3:C:1:MET:H2	3:C:295:ARG:HH22	1.55	0.53
3:C:173:GLY:C	3:C:175:GLN:H	2.16	0.53
12:L:29:TYR:OH	12:L:40:LEU:HB2	2.08	0.53
15:O:248:ASP:O	15:O:252:ILE:HG12	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:492:TYR:O	15:O:495:VAL:HG23	2.07	0.53
18:R:12:PHE:CD1	18:R:25:CYS:HB3	2.44	0.53
18:R:132:VAL:HG12	18:R:161:PHE:HE1	1.73	0.53
1:A:232:LYS:O	15:O:579:GLN:NE2	2.41	0.53
1:A:248:VAL:O	1:A:251:GLY:N	2.40	0.53
1:A:525:GLU:CD	6:F:102:SER:HB2	2.30	0.53
1:A:1225:ILE:HG22	1:A:1229:ARG:HE	1.74	0.53
2:B:38:ILE:HG13	2:B:43:ASP:HB3	1.89	0.53
2:B:412:ARG:HH12	2:B:416:TYR:HE2	1.56	0.53
2:B:615:VAL:HG22	2:B:671:THR:O	2.08	0.53
2:B:735:MET:HE2	2:B:754:ASN:ND2	2.23	0.53
3:C:33:VAL:HG12	3:C:34:GLU:N	2.24	0.53
3:C:70:ILE:O	3:C:75:VAL:HG13	2.08	0.53
3:C:172:GLN:N	3:C:175:GLN:HB3	2.21	0.53
15:O:46:LEU:HA	15:O:49:TYR:CD1	2.42	0.53
15:O:138:ASP:HA	15:O:141:ILE:HG12	1.90	0.53
15:O:195:CYS:SG	15:O:263:LEU:HG	2.48	0.53
15:O:543:TYR:CE2	16:P:312:PHE:HZ	2.18	0.53
1:A:249:PRO:C	1:A:251:GLY:N	2.65	0.53
1:A:302:GLY:O	1:A:303:LEU:HB3	2.08	0.53
1:A:310:ASN:HA	15:O:564:PHE:CE2	2.43	0.53
1:A:905:ARG:NH1	6:F:139:PRO:HG2	2.24	0.53
1:A:967:LEU:HD13	1:A:1009:ARG:HD3	1.89	0.53
1:A:1421:MET:HG2	1:A:1423:ILE:H	1.74	0.53
2:B:554:GLY:O	2:B:599:VAL:HG12	2.09	0.53
2:B:739:LYS:CD	2:B:977:THR:HG21	2.36	0.53
15:O:36:SER:OG	15:O:39:GLN:HB3	2.09	0.53
15:O:204:SER:H	15:O:207:HIS:HB2	1.72	0.53
15:O:581:LEU:HD22	15:O:648:TRP:CZ2	2.44	0.53
1:A:221:ASP:O	1:A:226:LYS:NZ	2.40	0.53
5:E:29:PHE:N	5:E:63:ASN:O	2.37	0.53
15:O:507:LEU:HD12	15:O:508:SER:N	2.24	0.53
1:A:370:GLY:O	2:B:1061:ARG:NH1	2.41	0.53
1:A:483:LEU:HD13	1:A:550:ILE:HG21	1.90	0.53
1:A:976:ARG:HG2	1:A:1002:ARG:NH2	2.24	0.53
1:A:1305:CYS:SG	5:E:141:VAL:HG11	2.49	0.53
2:B:987:MET:HA	2:B:990:ILE:HD12	1.90	0.53
14:N:280:LEU:O	14:N:283:LEU:HB2	2.08	0.53
15:O:553:ARG:NH1	15:O:554:THR:HB	2.22	0.53
1:A:366:GLY:O	2:B:1061:ARG:NH2	2.42	0.53
1:A:1266:ALA:O	1:A:1269:ASP:OD2	2.27	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:299:GLN:O	2:B:300:GLN:C	2.51	0.53
2:B:493:GLN:HG3	2:B:497:LEU:HD12	1.90	0.53
2:B:621:ARG:HG3	2:B:645:LEU:HG	1.89	0.53
3:C:120:LEU:N	3:C:121:PRO:HD3	2.23	0.53
8:H:43:ASN:ND2	8:H:46:LEU:HD13	2.23	0.53
14:N:394:VAL:HB	14:N:412:VAL:HB	1.89	0.53
18:R:431:ARG:NH2	19:S:437:THR:HB	2.15	0.53
18:R:506:GLY:HA2	18:R:509:SER:HB2	1.90	0.53
1:A:164:VAL:HA	1:A:179:ILE:O	2.08	0.53
1:A:601:TYR:HD1	3:C:24:SER:HG	1.54	0.53
2:B:68:PHE:HD1	2:B:385:SER:OG	1.92	0.53
2:B:320:LEU:HD23	2:B:324:ILE:HD12	1.90	0.53
2:B:574:GLN:HE22	14:N:422:ILE:HG12	1.74	0.53
2:B:888:VAL:HG12	12:L:46:VAL:HG11	1.91	0.53
2:B:959:ILE:HG23	2:B:984:LEU:HD12	1.91	0.53
2:B:1022:ILE:HG22	2:B:1023:TYR:N	2.12	0.53
3:C:117:ASP:CB	3:C:120:LEU:CD2	2.81	0.53
7:G:27:THR:HG22	7:G:31:ASN:HD21	1.73	0.53
8:H:59:ILE:HA	8:H:141:TYR:O	2.09	0.53
8:H:106:GLU:OE1	8:H:106:GLU:N	2.42	0.53
15:O:200:LEU:HD13	15:O:280:LEU:O	2.08	0.53
15:O:498:SER:HB3	16:P:296:TYR:CD1	2.44	0.53
15:O:570:GLU:HB2	15:O:574:TYR:CE2	2.43	0.53
1:A:154:CYS:SG	1:A:155:LEU:N	2.82	0.53
1:A:330:ASP:O	1:A:351:ARG:NH2	2.42	0.53
1:A:504:VAL:C	1:A:507:PRO:HD2	2.34	0.53
1:A:722:ASP:O	1:A:725:GLN:N	2.42	0.53
1:A:890:MET:HG2	1:A:894:GLU:HB2	1.91	0.53
1:A:1189:ASP:OD2	1:A:1192:THR:N	2.41	0.53
2:B:217:GLN:HG2	2:B:232:TYR:O	2.08	0.53
3:C:117:ASP:CG	3:C:120:LEU:HD21	2.34	0.53
3:C:218:LYS:HE2	12:L:70:ARG:HA	1.90	0.53
7:G:53:THR:CG2	7:G:71:THR:HG22	2.38	0.53
12:L:51:CYS:C	12:L:53:HIS:H	2.16	0.53
16:P:203:LYS:O	16:P:206:VAL:N	2.42	0.53
16:P:217:THR:O	16:P:218:THR:HG22	2.09	0.53
2:B:197:GLN:NE2	2:B:476:GLN:OE1	2.41	0.52
3:C:86:PHE:CD2	3:C:203:SER:OG	2.62	0.52
3:C:117:ASP:OD2	3:C:120:LEU:HD21	2.09	0.52
3:C:255:VAL:HG22	3:C:256:ILE:HG13	1.91	0.52
7:G:207:LEU:HD23	7:G:209:SER:H	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:63:LEU:HD13	8:H:141:TYR:CG	2.44	0.52
11:K:132:GLU:O	11:K:136:THR:HG22	2.09	0.52
15:O:106:TYR:HB3	15:O:208:TYR:CE2	2.43	0.52
15:O:588:LEU:HD11	15:O:637:VAL:HG23	1.91	0.52
15:O:635:LEU:HD22	17:Q:52:ARG:HG2	1.91	0.52
16:P:292:SER:OG	16:P:293:ILE:N	2.41	0.52
18:R:401:THR:HG23	18:R:446:LYS:HG2	1.91	0.52
21:Y:46:DA:H2'	21:Y:47:DC:C6	2.45	0.52
1:A:665:ASP:OD1	1:A:797:CYS:HB3	2.09	0.52
1:A:773:VAL:O	1:A:777:VAL:HG23	2.09	0.52
1:A:979:ASN:ND2	5:E:160:GLU:OE2	2.42	0.52
1:A:1164:THR:OG1	1:A:1272:VAL:HG12	2.09	0.52
2:B:95:TYR:OH	2:B:396:ASN:ND2	2.43	0.52
2:B:177:CYS:HB2	2:B:716:ASN:H	1.74	0.52
2:B:358:MET:O	2:B:361:TYR:HB3	2.08	0.52
4:D:102:SER:HA	4:D:105:GLU:HB2	1.90	0.52
5:E:115:ASN:OD1	5:E:116:ILE:N	2.42	0.52
6:F:100:GLN:O	6:F:103:MET:N	2.43	0.52
9:I:24:LEU:HG	9:I:33:PHE:CG	2.45	0.52
18:R:14:ARG:HA	18:R:23:LEU:HA	1.90	0.52
18:R:73:LEU:HB2	21:Y:32:DA:N1	2.24	0.52
1:A:18:PHE:HA	2:B:1138:ALA:O	2.09	0.52
1:A:644:GLU:OE1	8:H:102:TYR:OH	2.22	0.52
1:A:832:LEU:HD21	1:A:862:LEU:HD23	1.91	0.52
2:B:279:TYR:CE1	2:B:358:MET:HA	2.38	0.52
2:B:297:THR:CA	2:B:301:ALA:HB3	2.38	0.52
4:D:127:LEU:HB2	4:D:133:HIS:HB3	1.92	0.52
7:G:104:ILE:HG12	7:G:105:PHE:CD2	2.45	0.52
8:H:93:TYR:HB2	8:H:143:LEU:HD11	1.92	0.52
18:R:142:MET:O	18:R:146:PHE:N	2.28	0.52
18:R:219:ARG:HD3	18:R:220:PRO:HD2	1.90	0.52
1:A:416:LEU:HA	1:A:419:LEU:HB3	1.91	0.52
1:A:534:LEU:O	1:A:540:ASN:ND2	2.34	0.52
1:A:601:TYR:CD1	3:C:23:PHE:CD2	2.97	0.52
1:A:881:GLU:OE2	1:A:1127:LYS:NZ	2.36	0.52
1:A:1156:VAL:O	1:A:1159:GLY:N	2.41	0.52
1:A:1202:ILE:HD13	1:A:1224:ILE:HB	1.90	0.52
1:A:1392:THR:O	1:A:1392:THR:CG2	2.55	0.52
2:B:225:HIS:HB2	2:B:446:ARG:HH21	1.75	0.52
2:B:300:GLN:O	2:B:304:TYR:N	2.42	0.52
2:B:782:PHE:HD1	10:J:8:PHE:CD2	2.27	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:842:TYR:HE2	2:B:873:TYR:HB2	1.73	0.52
7:G:86:THR:HG23	7:G:145:LYS:HA	1.90	0.52
15:O:73:ARG:HA	15:O:121:TYR:HE1	1.73	0.52
15:O:362:ASN:HD21	15:O:478:VAL:HG23	1.74	0.52
20:X:57:DT:H2"	20:X:58:DC:C5	2.45	0.52
1:A:395:PRO:O	1:A:398:VAL:HG22	2.10	0.52
1:A:631:LYS:HE3	1:A:666:LYS:HD3	1.91	0.52
2:B:73:LEU:HB3	2:B:98:ILE:HG21	1.90	0.52
2:B:376:ARG:HH21	2:B:607:ARG:NH1	2.02	0.52
2:B:460:ARG:CZ	2:B:720:ARG:HH12	2.21	0.52
2:B:497:LEU:HD13	2:B:512:LYS:HD3	1.92	0.52
2:B:625:ILE:HD11	2:B:628:ARG:HE	1.74	0.52
2:B:698:ARG:HE	2:B:952:ARG:HG2	1.75	0.52
2:B:890:ASP:OD1	2:B:891:ASN:N	2.43	0.52
2:B:1043:ARG:O	18:R:37:ILE:HA	2.10	0.52
3:C:110:PRO:C	3:C:112:MET:H	2.17	0.52
3:C:231:PRO:HG2	3:C:271:ARG:H	1.73	0.52
5:E:1:MET:HB3	5:E:4:GLU:HG2	1.92	0.52
7:G:2:PHE:HE2	7:G:79:PRO:HB3	1.75	0.52
8:H:36:CYS:HA	8:H:126:GLU:HG3	1.92	0.52
10:J:56:LEU:O	10:J:59:LYS:N	2.43	0.52
15:O:201:ILE:H	15:O:281:THR:H	1.56	0.52
15:O:635:LEU:HB3	17:Q:47:ILE:HG21	1.91	0.52
18:R:93:ALA:CB	18:R:149:ARG:HH21	2.18	0.52
18:R:213:TRP:HH2	18:R:497:ARG:CB	2.22	0.52
18:R:468:ILE:HG13	18:R:610:LEU:HD11	1.91	0.52
3:C:12:VAL:HG12	3:C:13:THR:H	1.74	0.52
15:O:361:PHE:HB3	15:O:480:TYR:HE2	1.75	0.52
16:P:241:ARG:O	16:P:245:GLU:HG2	2.10	0.52
16:P:297:PHE:O	16:P:299:MET:HG2	2.09	0.52
16:P:311:TYR:O	17:Q:41:LEU:HD13	2.10	0.52
18:R:439:ALA:HA	18:R:450:THR:H	1.75	0.52
1:A:200:GLU:HA	15:O:515:LYS:CD	2.40	0.52
1:A:997:GLN:O	1:A:999:ASP:N	2.43	0.52
2:B:493:GLN:HG3	2:B:497:LEU:HB2	1.92	0.52
2:B:568:PRO:O	2:B:571:PHE:HB3	2.10	0.52
2:B:587:PHE:CD1	2:B:588:ILE:N	2.78	0.52
7:G:111:PRO:O	7:G:199:SER:OG	2.28	0.52
8:H:11:GLN:O	8:H:29:ALA:N	2.42	0.52
10:J:36:LEU:HD21	10:J:50:ILE:HB	1.90	0.52
14:N:385:GLY:O	14:N:416:ILE:HA	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:241:ALA:O	15:O:245:ALA:N	2.34	0.52
16:P:217:THR:O	16:P:219:GLN:N	2.42	0.52
1:A:268:ILE:HG22	1:A:269:ARG:HG2	1.91	0.52
1:A:848:VAL:HG22	1:A:850:ASN:H	1.75	0.52
1:A:1229:ARG:HH12	1:A:1231:ALA:HB2	1.74	0.52
1:A:1431:VAL:HG13	7:G:57:GLY:O	2.10	0.52
2:B:45:TRP:NE1	2:B:739:LYS:HD3	2.24	0.52
2:B:986:ASP:OD1	2:B:987:MET:N	2.43	0.52
10:J:53:HIS:ND1	10:J:53:HIS:O	2.43	0.52
13:M:148:LEU:HG	13:M:181:PRO:HB3	1.92	0.52
18:R:499:GLU:OE1	18:R:499:GLU:N	2.37	0.52
18:R:610:LEU:HA	18:R:613:HIS:CD2	2.45	0.52
21:Y:11:DA:C5	21:Y:12:DT:C4	2.98	0.52
21:Y:40:DA:H2"	21:Y:41:DG:C8	2.45	0.52
1:A:473:LEU:HG	1:A:520:HIS:HB2	1.92	0.52
1:A:1224:ILE:HD12	1:A:1228:ASP:HA	1.91	0.52
1:A:1406:ASP:CG	1:A:1407:ALA:H	2.17	0.52
2:B:417:ASP:CG	2:B:419:LEU:HB2	2.35	0.52
3:C:30:GLU:HG3	11:K:84:PRO:HG3	1.92	0.52
8:H:107:VAL:N	8:H:111:LEU:O	2.42	0.52
13:M:96:LEU:HB2	13:M:101:PRO:HA	1.92	0.52
15:O:356:THR:HB	15:O:357:PRO:HD3	1.92	0.52
16:P:266:GLU:OE1	16:P:269:LEU:HB2	2.09	0.52
18:R:241:HIS:CD2	18:R:255:LEU:HD23	2.43	0.52
18:R:267:ALA:HA	18:R:270:LEU:HB3	1.92	0.52
1:A:240:GLU:C	1:A:243:GLY:H	2.18	0.52
1:A:329:SER:HB2	1:A:351:ARG:CZ	2.40	0.52
1:A:906:THR:OG1	1:A:907:SER:N	2.43	0.52
1:A:1177:TYR:HD1	1:A:1183:PHE:H	1.57	0.52
2:B:324:ILE:HG23	2:B:325:GLU:N	2.25	0.52
2:B:586:GLU:HG2	2:B:587:PHE:H	1.74	0.52
15:O:221:LYS:N	15:O:224:LYS:HB3	2.25	0.52
16:P:265:LEU:O	16:P:265:LEU:HG	2.10	0.52
16:P:267:SER:O	16:P:270:GLN:HB3	2.10	0.52
18:R:269:LYS:HA	18:R:272:VAL:HB	1.92	0.52
18:R:470:GLN:HG2	18:R:475:ALA:O	2.10	0.52
1:A:18:PHE:HD1	2:B:1139:PRO:CA	2.17	0.51
1:A:115:LEU:HD22	1:A:147:GLN:HG2	1.90	0.51
1:A:203:GLU:O	1:A:207:HIS:N	2.43	0.51
1:A:250:SER:HB3	1:A:1403:MET:CE	2.39	0.51
1:A:429:GLY:O	1:A:465:HIS:ND1	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1203:GLU:HA	1:A:1206:ALA:HB3	1.92	0.51
1:A:1325:VAL:HG23	1:A:1326:LEU:H	1.75	0.51
2:B:399:PHE:N	2:B:425:HIS:HE1	2.08	0.51
2:B:538:VAL:HA	2:B:565:ILE:HD12	1.92	0.51
2:B:811:VAL:HA	2:B:817:PRO:HA	1.91	0.51
2:B:1088:ASP:OD2	2:B:1124:ALA:N	2.33	0.51
3:C:190:ASP:O	3:C:191:ILE:HG13	2.09	0.51
7:G:17:GLN:OE1	7:G:17:GLN:N	2.42	0.51
13:M:147:THR:C	13:M:148:LEU:HD12	2.35	0.51
15:O:159:ILE:HG13	15:O:188:SER:HB3	1.92	0.51
15:O:186:THR:O	15:O:187:ILE:C	2.52	0.51
15:O:338:ASP:CG	15:O:340:GLU:H	2.17	0.51
18:R:467:ARG:HD3	18:R:602:LEU:HG	1.91	0.51
18:R:488:GLY:O	18:R:540:LEU:N	2.35	0.51
1:A:134:ASN:OD1	1:A:1404:LYS:NZ	2.43	0.51
2:B:241:TYR:HB3	2:B:250:GLU:HA	1.93	0.51
2:B:383:LEU:HB3	2:B:442:TRP:CZ3	2.44	0.51
2:B:1061:ARG:NE	21:Y:24:DT:OP2	2.32	0.51
3:C:77:SER:HB2	3:C:219:PHE:O	2.11	0.51
5:E:26:ARG:HH12	5:E:189:GLY:HA3	1.75	0.51
5:E:83:CYS:SG	5:E:84:ASP:N	2.84	0.51
14:N:306:VAL:O	14:N:415:LYS:HA	2.09	0.51
15:O:262:ILE:O	15:O:275:LYS:N	2.43	0.51
15:O:641:LEU:HA	15:O:644:LEU:HB2	1.92	0.51
18:R:2:PRO:HG2	18:R:12:PHE:HE2	1.75	0.51
18:R:621:LYS:O	18:R:625:ARG:N	2.42	0.51
1:A:292:ILE:HA	1:A:295:THR:HG22	1.92	0.51
1:A:379:THR:HG22	1:A:380:VAL:N	2.23	0.51
2:B:390:ASP:O	2:B:393:LYS:HB3	2.11	0.51
2:B:831:GLU:OE2	12:L:61:THR:N	2.44	0.51
6:F:81:THR:HG22	6:F:82:THR:N	2.25	0.51
20:X:47:DA:H2"	20:X:48:DT:OP2	2.09	0.51
1:A:785:LEU:HG	1:A:789:ASN:HD22	1.76	0.51
2:B:297:THR:HG1	2:B:301:ALA:HB3	1.73	0.51
2:B:882:ASP:OD1	2:B:882:ASP:N	2.43	0.51
15:O:80:VAL:HG11	15:O:87:ASP:HB2	1.92	0.51
15:O:87:ASP:C	15:O:89:ASP:H	2.17	0.51
15:O:132:TYR:CE1	15:O:645:LEU:HD21	2.45	0.51
15:O:507:LEU:O	15:O:511:ILE:N	2.39	0.51
15:O:537:LEU:O	15:O:541:ILE:HG22	2.10	0.51
18:R:406:LEU:HD13	18:R:411:VAL:HG21	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:516:PHE:HB2	20:X:13:DA:H5'	1.91	0.51
2:B:155:MET:HB2	2:B:185:PHE:CE1	2.46	0.51
2:B:248:ALA:O	2:B:249:GLU:HG3	2.10	0.51
2:B:553:TYR:HA	2:B:597:MET:HB3	1.93	0.51
2:B:767:ILE:HG13	2:B:768:GLU:N	2.25	0.51
5:E:53:PRO:HB2	5:E:55:ARG:HH12	1.76	0.51
5:E:82:PHE:HA	5:E:110:PHE:HB2	1.91	0.51
1:A:26:ILE:HG23	1:A:262:PRO:HG3	1.92	0.51
2:B:217:GLN:OE1	2:B:356:VAL:HG11	2.11	0.51
2:B:695:GLN:NE2	2:B:697:PRO:HB2	2.26	0.51
3:C:2:SER:O	3:C:4:ILE:HG13	2.10	0.51
3:C:40:PHE:CZ	3:C:56:LEU:HD11	2.46	0.51
5:E:153:HIS:HB3	5:E:196:VAL:HG21	1.93	0.51
15:O:200:LEU:HD22	15:O:282:ILE:N	2.17	0.51
15:O:583:TRP:NE1	16:P:314:GLU:OE2	2.43	0.51
18:R:489:SER:HA	18:R:539:VAL:HA	1.93	0.51
20:X:23:DC:H2''	20:X:24:DT:C6	2.46	0.51
21:Y:25:DC:H2''	21:Y:26:DA:H8	1.74	0.51
21:Y:39:DA:C6	21:Y:40:DA:C6	2.99	0.51
1:A:1347:GLY:O	1:A:1348:MET:HG2	2.11	0.51
2:B:584:VAL:CB	2:B:588:ILE:HD12	2.32	0.51
2:B:817:PRO:HG2	2:B:822:GLN:HG3	1.93	0.51
13:M:77:LYS:HA	14:N:360:VAL:HG22	1.91	0.51
13:M:230:SER:O	13:M:234:HIS:N	2.39	0.51
16:P:52:VAL:HA	16:P:61:ILE:HD11	1.91	0.51
18:R:137:GLU:C	18:R:138:LYS:HG2	2.36	0.51
18:R:617:GLU:HG2	18:R:621:LYS:HE2	1.91	0.51
1:A:433:LEU:N	1:A:442:ARG:O	2.41	0.51
1:A:448:ASP:OD2	1:A:452:LEU:CD1	2.59	0.51
1:A:1059:LEU:HD23	1:A:1060:TYR:HD2	1.74	0.51
2:B:137:ARG:HG2	2:B:141:ILE:HG12	1.93	0.51
9:I:4:PHE:O	9:I:6:PRO:HD3	2.11	0.51
15:O:536:THR:O	15:O:540:LEU:N	2.43	0.51
18:R:398:ALA:HB3	18:R:449:VAL:HB	1.92	0.51
1:A:8:GLU:OE1	1:A:8:GLU:N	2.43	0.51
1:A:383:PRO:HG3	1:A:512:PHE:CZ	2.46	0.51
1:A:853:PHE:HE1	2:B:984:LEU:HD13	1.76	0.51
1:A:1317:ASN:O	1:A:1318:HIS:ND1	2.44	0.51
2:B:1008:ILE:O	3:C:65:ASN:ND2	2.37	0.51
5:E:79:TRP:NE1	5:E:81:GLU:HB3	2.26	0.51
5:E:157:SER:HB2	5:E:160:GLU:HG3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:89:GLU:HG2	6:F:93:ILE:HG13	1.92	0.51
10:J:48:ARG:O	10:J:52:THR:N	2.44	0.51
11:K:85:ASP:OD2	11:K:111:THR:HB	2.10	0.51
15:O:68:LEU:O	15:O:72:GLY:N	2.38	0.51
15:O:498:SER:HB3	16:P:296:TYR:HD1	1.74	0.51
15:O:500:LEU:HD21	15:O:539:SER:OG	2.11	0.51
16:P:107:SER:O	16:P:110:ILE:HG22	2.10	0.51
16:P:121:VAL:O	16:P:125:LEU:HG	2.11	0.51
16:P:265:LEU:C	16:P:267:SER:N	2.67	0.51
20:X:16:DA:H5'	20:X:17:DG:OP2	2.10	0.51
1:A:99:THR:O	1:A:102:ILE:HG22	2.10	0.51
1:A:352:GLY:HA2	1:A:355:GLN:HB2	1.93	0.51
1:A:625:ASN:HA	1:A:654:ILE:O	2.11	0.51
1:A:822:ARG:NE	1:A:845:LYS:HB2	2.26	0.51
1:A:935:PHE:CE2	1:A:1008:LEU:HD13	2.46	0.51
2:B:59:LYS:HZ1	2:B:519:HIS:HA	1.75	0.51
2:B:122:ASP:HA	2:B:189:GLY:CA	2.41	0.51
3:C:12:VAL:CG1	3:C:13:THR:H	2.24	0.51
3:C:255:VAL:HG22	3:C:256:ILE:N	2.19	0.51
6:F:85:MET:HE3	6:F:153:VAL:HG12	1.93	0.51
9:I:35:ILE:HD12	9:I:36:GLU:HG2	1.92	0.51
15:O:643:ARG:NH1	16:P:293:ILE:O	2.31	0.51
18:R:135:ARG:HB3	18:R:174:PRO:HB3	1.92	0.51
20:X:10:DT:C4	20:X:11:DA:N6	2.79	0.51
1:A:37:ARG:HG2	1:A:38:ASP:H	1.76	0.50
1:A:717:VAL:HA	1:A:810:VAL:HG22	1.92	0.50
1:A:948:ASN:OD1	1:A:949:ASN:N	2.44	0.50
2:B:306:GLY:CA	2:B:325:GLU:HB2	2.40	0.50
2:B:636:ASP:OD1	2:B:637:PHE:N	2.44	0.50
2:B:762:TYR:OH	2:B:930:ASP:HB3	2.11	0.50
3:C:67:PHE:O	3:C:71:MET:HB2	2.11	0.50
13:M:77:LYS:HG2	14:N:360:VAL:N	2.25	0.50
13:M:248:ALA:N	14:N:406:ALA:O	2.38	0.50
15:O:349:ALA:O	15:O:352:VAL:HG12	2.11	0.50
1:A:713:GLY:O	1:A:716:ASP:HB2	2.11	0.50
1:A:768:GLY:O	1:A:772:LYS:CB	2.60	0.50
1:A:891:LYS:NZ	1:A:1389:PHE:HA	2.25	0.50
2:B:1062:LEU:HD22	2:B:1066:GLU:CD	2.36	0.50
5:E:191:LYS:H	5:E:194:GLU:CD	2.20	0.50
14:N:363:ILE:HA	14:N:372:SER:O	2.12	0.50
16:P:311:TYR:HD2	16:P:314:GLU:HB3	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:51:PHE:HD1	2:B:637:PHE:CE2	2.28	0.50
2:B:194:ILE:HA	2:B:455:THR:HG22	1.92	0.50
3:C:120:LEU:HD12	3:C:120:LEU:O	2.11	0.50
5:E:171:LYS:H	5:E:174:GLN:NE2	2.09	0.50
7:G:7:ILE:C	7:G:71:THR:HG1	2.18	0.50
8:H:137:GLN:HB3	8:H:139:ASN:OD1	2.11	0.50
14:N:364:ARG:O	14:N:371:LEU:HA	2.11	0.50
21:Y:19:DT:H2'	21:Y:20:DT:C2	2.47	0.50
1:A:11:LYS:HG3	2:B:1117:ILE:HD13	1.93	0.50
1:A:360:LYS:HB3	1:A:361:GLN:OE1	2.11	0.50
1:A:944:ASN:OD1	1:A:945:ILE:N	2.45	0.50
1:A:1376:LEU:CD2	1:A:1389:PHE:CZ	2.95	0.50
2:B:137:ARG:HG2	2:B:141:ILE:HG21	1.92	0.50
2:B:257:LEU:O	2:B:260:CYS:HB2	2.11	0.50
2:B:475:SER:HB3	2:B:510:LEU:H	1.77	0.50
2:B:501:ASP:HB3	2:B:703:CYS:CB	2.41	0.50
2:B:949:PHE:CE1	2:B:957:LYS:HD3	2.47	0.50
2:B:1043:ARG:NH1	2:B:1049:GLN:HA	2.26	0.50
8:H:128:ASN:CG	8:H:129:TYR:N	2.69	0.50
15:O:128:HIS:HA	15:O:131:LEU:CD2	2.41	0.50
15:O:593:GLU:HA	15:O:596:LYS:HG2	1.93	0.50
16:P:228:ALA:HA	16:P:232:ASN:HD21	1.76	0.50
18:R:84:ARG:HG3	18:R:105:PHE:CE1	2.46	0.50
18:R:152:VAL:HG22	18:R:154:VAL:N	2.21	0.50
18:R:399:THR:O	18:R:481:PHE:HA	2.11	0.50
1:A:99:THR:HA	1:A:102:ILE:HG22	1.94	0.50
1:A:415:LYS:O	1:A:419:LEU:N	2.41	0.50
1:A:676:SER:HB2	1:A:679:TYR:HB3	1.93	0.50
1:A:1166:LEU:HA	1:A:1169:VAL:HB	1.93	0.50
1:A:1456:ALA:HB2	4:D:116:PHE:HA	1.94	0.50
2:B:289:GLU:HA	2:B:292:LYS:HG2	1.94	0.50
2:B:681:LEU:HD23	2:B:685:ALA:HB1	1.93	0.50
2:B:848:PRO:O	2:B:851:SER:OG	2.22	0.50
3:C:64:ALA:HA	3:C:67:PHE:HD2	1.77	0.50
5:E:106:GLN:O	5:E:131:THR:N	2.41	0.50
13:M:92:ASN:HD21	13:M:181:PRO:HD3	1.77	0.50
15:O:159:ILE:CD1	15:O:188:SER:OG	2.60	0.50
15:O:159:ILE:HD11	15:O:188:SER:OG	2.11	0.50
15:O:472:LYS:HB3	15:O:475:VAL:HG12	1.93	0.50
16:P:183:TRP:HD1	16:P:247:LEU:HD23	1.77	0.50
20:X:26:DT:C6	20:X:27:DT:H72	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:X:44:DA:N6	21:Y:20:DT:O4	2.44	0.50
1:A:110:CYS:HB2	1:A:156:HIS:CE1	2.32	0.50
1:A:186:VAL:HG21	1:A:189:LYS:HB3	1.92	0.50
1:A:368:LEU:O	1:A:371:LYS:HG3	2.11	0.50
1:A:1449:GLU:O	4:D:117:LYS:NZ	2.37	0.50
2:B:234:ILE:HD11	2:B:238:GLY:H	1.76	0.50
2:B:431:SER:HA	2:B:434:ASN:HD22	1.76	0.50
2:B:737:LYS:HE2	2:B:973:LEU:HB3	1.93	0.50
2:B:961:LEU:HD12	2:B:1022:ILE:HD11	1.93	0.50
5:E:118:PRO:HA	5:E:121:MET:HB2	1.93	0.50
10:J:33:GLY:O	10:J:37:SER:N	2.41	0.50
15:O:108:GLN:N	15:O:108:GLN:OE1	2.44	0.50
15:O:292:ARG:O	15:O:296:LEU:HG	2.11	0.50
16:P:45:LEU:HG	19:S:372:MET:HE2	1.94	0.50
16:P:131:GLN:HB3	16:P:133:TYR:CD2	2.41	0.50
18:R:213:TRP:CH2	18:R:497:ARG:HB3	2.46	0.50
1:A:502:GLU:OE1	1:A:557:PHE:CE2	2.64	0.50
1:A:580:LEU:HD21	1:A:590:PHE:CG	2.46	0.50
1:A:1058:GLN:HB2	8:H:104:PHE:HD2	1.77	0.50
3:C:56:LEU:O	3:C:297:HIS:HD2	1.94	0.50
5:E:185:ALA:HA	5:E:190:LEU:HD13	1.93	0.50
7:G:89:ILE:HG23	7:G:142:VAL:HG12	1.94	0.50
8:H:12:VAL:HB	8:H:53:ASP:H	1.76	0.50
9:I:33:PHE:CD1	9:I:34:PRO:HD2	2.47	0.50
13:M:229:GLY:O	13:M:232:LEU:HB3	2.11	0.50
15:O:297:ILE:HD13	15:O:313:LYS:HG3	1.93	0.50
15:O:511:ILE:HA	15:O:514:ASN:OD1	2.12	0.50
20:X:10:DT:H2"	20:X:11:DA:C8	2.47	0.50
1:A:427:HIS:HB3	1:A:428:PRO:HD3	1.93	0.50
1:A:573:ARG:HB2	1:A:604:TRP:HZ3	1.77	0.50
1:A:580:LEU:HB3	11:K:88:PHE:CE2	2.47	0.50
1:A:803:THR:O	1:A:807:SER:CB	2.60	0.50
1:A:829:ASP:OD1	1:A:838:ASN:ND2	2.45	0.50
1:A:1235:PHE:HB2	1:A:1236:PRO:HD2	1.93	0.50
1:A:1330:ALA:HB2	5:E:150:VAL:HG22	1.94	0.50
1:A:1387:ALA:HB2	1:A:1392:THR:HG23	1.92	0.50
2:B:422:ILE:O	2:B:426:SER:HB3	2.12	0.50
2:B:458:LEU:HA	2:B:469:MET:SD	2.52	0.50
5:E:66:GLU:HG3	5:E:67:GLU:H	1.75	0.50
13:M:72:GLU:OE1	14:N:364:ARG:NE	2.43	0.50
13:M:113:LYS:HE2	13:M:118:LEU:HB2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:483:GLU:O	19:S:487:GLU:HB3	2.12	0.50
20:X:7:DA:H4'	20:X:8:DC:OP1	2.12	0.50
1:A:895:ASP:OD2	1:A:1410:GLY:HA2	2.11	0.50
1:A:1175:ASP:OD1	1:A:1185:GLN:N	2.42	0.50
3:C:251:PHE:HB2	3:C:255:VAL:CG2	2.42	0.50
7:G:34:PHE:O	7:G:37:LYS:HB2	2.12	0.50
7:G:105:PHE:CD1	7:G:107:ASP:HB2	2.47	0.50
7:G:112:GLN:HE22	7:G:128:TRP:HD1	1.57	0.50
7:G:121:TYR:HD1	7:G:127:ALA:O	1.94	0.50
15:O:286:ARG:HH21	15:O:321:GLN:HE21	1.60	0.50
17:Q:63:LYS:O	17:Q:67:ASP:N	2.39	0.50
1:A:528:ARG:O	1:A:532:ILE:HG22	2.11	0.49
1:A:1050:ASP:O	1:A:1053:LYS:N	2.35	0.49
2:B:128:PRO:HA	2:B:151:ARG:HG2	1.94	0.49
2:B:393:LYS:NZ	2:B:397:ASN:HD21	2.10	0.49
3:C:152:ASP:C	3:C:154:LYS:H	2.16	0.49
3:C:327:TYR:OH	11:K:43:ASP:OD2	2.30	0.49
7:G:84:ILE:HA	7:G:148:PHE:O	2.12	0.49
9:I:24:LEU:HG	9:I:33:PHE:HB2	1.93	0.49
15:O:210:PRO:HB2	15:O:213:ASP:HB3	1.92	0.49
15:O:267:PRO:HG2	15:O:270:SER:HB2	1.94	0.49
16:P:10:GLN:HB3	16:P:13:ASP:HB3	1.93	0.49
16:P:55:LEU:HD22	16:P:60:LEU:HB2	1.94	0.49
16:P:198:PHE:HE2	16:P:204:LYS:HZ3	1.60	0.49
18:R:235:ASN:ND2	18:R:237:LEU:HD23	2.26	0.49
1:A:1393:THR:HG23	1:A:1397:PHE:HE2	1.78	0.49
2:B:204:ARG:HH21	2:B:558:ASN:C	2.19	0.49
3:C:88:ASN:HB3	12:L:60:ARG:HH12	1.76	0.49
3:C:142:ARG:HA	3:C:157:TYR:HD1	1.76	0.49
4:D:146:ASP:O	4:D:150:ILE:HG12	2.12	0.49
5:E:40:GLU:HA	5:E:43:LYS:HE2	1.94	0.49
5:E:151:PRO:HB3	5:E:200:ARG:HA	1.94	0.49
7:G:147:ARG:NH2	7:G:211:TRP:HB2	2.27	0.49
13:M:117:HIS:HD1	13:M:119:TRP:CG	2.30	0.49
15:O:101:LEU:HD21	15:O:130:LEU:HD21	1.93	0.49
15:O:263:LEU:HA	15:O:274:VAL:HG12	1.93	0.49
15:O:581:LEU:O	15:O:585:MET:HB2	2.11	0.49
15:O:590:PHE:C	15:O:594:LYS:HG2	2.37	0.49
19:S:523:ALA:HA	19:S:526:GLU:HB3	1.94	0.49
21:Y:1:DC:H1'	21:Y:2:DC:C2	2.47	0.49
1:A:227:THR:HA	1:A:230:LEU:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:418:GLU:O	1:A:421:VAL:HG12	2.11	0.49
1:A:1451:LEU:HG	4:D:107:MET:SD	2.52	0.49
2:B:48:LEU:HD22	2:B:743:LEU:HD23	1.93	0.49
2:B:234:ILE:HD11	2:B:238:GLY:N	2.27	0.49
2:B:627:LEU:HA	2:B:630:LEU:HB3	1.95	0.49
2:B:880:HIS:CE1	12:L:67:PHE:HE1	2.30	0.49
3:C:7:ILE:HG12	3:C:292:GLY:HA2	1.94	0.49
3:C:162:VAL:HG23	3:C:193:LEU:HB2	1.93	0.49
3:C:256:ILE:HG22	3:C:267:VAL:HA	1.94	0.49
6:F:74:ILE:HG23	6:F:78:GLN:HE21	1.78	0.49
7:G:49:TYR:HB2	7:G:75:VAL:HG23	1.94	0.49
14:N:307:PHE:CG	14:N:416:ILE:HG22	2.46	0.49
16:P:184:ARG:O	16:P:187:SER:OG	2.25	0.49
18:R:137:GLU:O	18:R:138:LYS:CG	2.59	0.49
18:R:196:ILE:O	18:R:199:VAL:HB	2.12	0.49
18:R:213:TRP:HH2	18:R:497:ARG:HB3	1.78	0.49
1:A:493:ARG:HB2	1:A:499:ARG:NH2	2.26	0.49
2:B:181:PRO:HB2	2:B:470:MET:HE1	1.94	0.49
2:B:658:TYR:HE2	2:B:670:MET:HG2	1.75	0.49
2:B:914:SER:C	2:B:916:HIS:N	2.70	0.49
2:B:961:LEU:HD11	2:B:1020:GLY:N	2.26	0.49
6:F:89:GLU:O	6:F:93:ILE:HB	2.12	0.49
7:G:48:ILE:HD12	7:G:72:PHE:CE1	2.47	0.49
9:I:34:PRO:C	9:I:35:ILE:HG13	2.37	0.49
13:M:93:ARG:HH12	13:M:123:ILE:HD13	1.77	0.49
13:M:147:THR:HB	13:M:182:PHE:O	2.12	0.49
13:M:149:LYS:HB3	13:M:182:PHE:HE1	1.77	0.49
15:O:312:TYR:O	15:O:316:LEU:HD13	2.12	0.49
18:R:121:ARG:HB2	18:R:124:ASN:HD22	1.76	0.49
1:A:364:PHE:HD2	1:A:365:ARG:NE	2.09	0.49
1:A:482:ARG:CD	1:A:544:PRO:HG3	2.36	0.49
1:A:1329:GLU:OE2	5:E:200:ARG:NH2	2.41	0.49
1:A:1362:MET:HG3	1:A:1369:LEU:O	2.13	0.49
2:B:143:MET:HE3	19:S:397:VAL:HG13	1.94	0.49
2:B:235:THR:HG22	2:B:236:LYS:HG3	1.94	0.49
2:B:521:THR:CG2	2:B:609:CYS:SG	3.01	0.49
2:B:698:ARG:HH21	2:B:952:ARG:HG3	1.77	0.49
3:C:83:VAL:HG21	3:C:98:ALA:HB1	1.94	0.49
3:C:88:ASN:OD1	3:C:89:THR:N	2.45	0.49
14:N:365:VAL:HG13	14:N:370:LYS:N	2.25	0.49
15:O:300:ALA:O	15:O:304:VAL:HG22	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:106:TRP:CG	16:P:107:SER:N	2.80	0.49
1:A:126:GLU:OE1	1:A:127:LEU:HD12	2.13	0.49
1:A:319:LEU:C	1:A:322:THR:HG22	2.31	0.49
1:A:590:PHE:HA	1:A:617:ASN:OD1	2.13	0.49
1:A:921:LEU:HD23	1:A:932:PRO:HG2	1.95	0.49
1:A:1058:GLN:HB2	8:H:104:PHE:CD2	2.47	0.49
1:A:1072:GLU:O	1:A:1076:PHE:N	2.41	0.49
2:B:93:LEU:HA	2:B:135:TYR:HB2	1.95	0.49
2:B:264:SER:OG	2:B:267:GLU:N	2.45	0.49
2:B:1011:GLU:OE1	2:B:1011:GLU:N	2.46	0.49
5:E:94:LYS:O	5:E:98:ILE:HG12	2.12	0.49
5:E:156:LEU:HD11	5:E:195:VAL:HB	1.94	0.49
15:O:546:VAL:HB	15:O:548:ILE:HG13	1.94	0.49
18:R:627:TRP:O	18:R:631:ASN:ND2	2.30	0.49
21:Y:26:DA:C8	21:Y:27:DC:C4	3.00	0.49
21:Y:26:DA:N7	21:Y:27:DC:N4	2.60	0.49
1:A:223:ASN:HD22	1:A:225:LEU:HB3	1.77	0.49
1:A:595:PRO:HA	1:A:604:TRP:CE2	2.48	0.49
1:A:645:MET:HE2	8:H:122:LEU:HB3	1.95	0.49
1:A:789:ASN:C	1:A:791:PRO:HD2	2.34	0.49
1:A:1257:PHE:HA	1:A:1260:MET:HB3	1.95	0.49
2:B:138:GLY:O	2:B:141:ILE:HG22	2.12	0.49
2:B:531:LYS:O	2:B:535:VAL:HG23	2.12	0.49
2:B:765:TYR:OH	11:K:96:PRO:HD2	2.13	0.49
2:B:916:HIS:NE2	2:B:954:THR:OG1	2.46	0.49
2:B:948:GLY:O	2:B:952:ARG:HB3	2.12	0.49
3:C:216:HIS:CG	3:C:218:LYS:HE3	2.48	0.49
7:G:149:ARG:HD3	7:G:201:GLN:HE22	1.78	0.49
12:L:40:LEU:HG	12:L:41:SER:O	2.13	0.49
12:L:47:ARG:NH1	12:L:52:GLY:O	2.45	0.49
13:M:117:HIS:HB2	13:M:119:TRP:NE1	2.28	0.49
13:M:259:ILE:O	13:M:262:GLU:HG2	2.13	0.49
15:O:284:LEU:HD22	15:O:288:MET:HE2	1.94	0.49
16:P:20:SER:HA	16:P:23:MET:HG2	1.95	0.49
18:R:219:ARG:HG3	18:R:221:ALA:H	1.78	0.49
20:X:57:DT:H2"	20:X:58:DC:H5	1.77	0.49
1:A:543:THR:HG22	1:A:548:GLU:O	2.13	0.49
1:A:1391:LYS:HB2	1:A:1395:HIS:CE1	2.47	0.49
2:B:529:ILE:HD11	2:B:575:PHE:HE1	1.78	0.49
2:B:1091:GLU:HA	2:B:1119:MET:O	2.12	0.49
2:B:1104:SER:OG	2:B:1105:GLY:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:117:ASP:HB3	3:C:120:LEU:CG	2.42	0.49
7:G:96:GLY:HA2	7:G:112:GLN:HG3	1.93	0.49
14:N:364:ARG:HG3	14:N:365:VAL:N	2.27	0.49
15:O:128:HIS:CE1	15:O:132:TYR:HE2	2.30	0.49
15:O:134:GLY:O	15:O:137:ILE:HB	2.13	0.49
15:O:564:PHE:C	15:O:565:LEU:HD12	2.38	0.49
16:P:31:PHE:CE2	16:P:72:PHE:HB2	2.47	0.49
16:P:53:GLN:NE2	19:S:364:LEU:HG	2.27	0.49
18:R:218:ARG:HH11	18:R:258:ARG:NH2	2.11	0.49
18:R:639:GLU:HG3	18:R:642:ARG:HH21	1.77	0.49
1:A:231:PHE:CD1	1:A:234:ILE:HD12	2.47	0.49
1:A:476:ARG:NH1	1:A:510:ALA:HA	2.28	0.49
1:A:637:LYS:NZ	1:A:647:GLN:HE21	2.11	0.49
2:B:98:ILE:HD13	2:B:131:VAL:HG12	1.95	0.49
2:B:501:ASP:HB3	2:B:703:CYS:HB2	1.94	0.49
4:D:155:GLU:O	4:D:158:SER:OG	2.24	0.49
13:M:237:ALA:HA	13:M:240:GLU:HB2	1.95	0.49
15:O:37:LEU:O	15:O:41:THR:N	2.45	0.49
16:P:313:ASP:CG	16:P:314:GLU:H	2.21	0.49
18:R:463:ARG:NH1	18:R:601:ASN:O	2.45	0.49
19:S:521:ASN:HA	19:S:524:LYS:HB3	1.95	0.49
1:A:27:VAL:HG23	1:A:83:HIS:CD2	2.48	0.49
1:A:30:SER:OG	1:A:82:GLY:HA2	2.11	0.49
1:A:57:LYS:HB2	1:A:69:THR:HG23	1.93	0.49
1:A:347:VAL:CG1	1:A:349:PRO:CD	2.80	0.49
1:A:371:LYS:HE3	2:B:1087:SER:HB3	1.95	0.49
1:A:481:HIS:CD2	1:A:483:LEU:H	2.31	0.49
1:A:533:ASN:O	1:A:539:ASN:ND2	2.46	0.49
1:A:866:ILE:HD12	2:B:489:LEU:O	2.13	0.49
3:C:84:TYR:HD2	3:C:207:HIS:HE1	1.55	0.49
3:C:143:ASN:N	3:C:156:LEU:O	2.46	0.49
3:C:235:ILE:C	3:C:236:LEU:HD12	2.38	0.49
9:I:28:SER:HA	13:M:135:LYS:HZ1	1.78	0.49
15:O:151:GLU:O	15:O:155:LEU:N	2.39	0.49
15:O:200:LEU:HD23	15:O:281:THR:C	2.30	0.49
15:O:538:ALA:O	15:O:541:ILE:HG23	2.13	0.49
15:O:650:VAL:HG13	15:O:651:PHE:H	1.78	0.49
18:R:498:LEU:HD22	18:R:532:ILE:HG22	1.94	0.49
1:A:185:TRP:C	1:A:187:GLY:H	2.21	0.48
1:A:329:SER:HB2	1:A:351:ARG:NH1	2.27	0.48
1:A:464:ARG:HB3	1:A:467:GLU:OE2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:770:LEU:O	1:A:774:ARG:CB	2.61	0.48
1:A:1365:LYS:O	5:E:177:ARG:HB2	2.12	0.48
2:B:698:ARG:NH2	2:B:952:ARG:HG3	2.27	0.48
3:C:278:GLU:O	3:C:281:ARG:HG2	2.13	0.48
5:E:101:GLN:O	5:E:104:ASN:ND2	2.46	0.48
8:H:9:ILE:O	8:H:31:THR:HG22	2.13	0.48
8:H:18:GLY:C	8:H:20:TYR:H	2.21	0.48
9:I:5:CYS:HB3	9:I:10:ASN:H	1.78	0.48
13:M:94:PRO:HA	14:N:391:LEU:O	2.12	0.48
15:O:123:ASN:O	15:O:126:GLY:N	2.46	0.48
15:O:519:GLU:HG3	15:O:534:ARG:NH2	2.28	0.48
15:O:647:LEU:O	15:O:650:VAL:HG12	2.13	0.48
1:A:942:ALA:O	1:A:946:THR:HG22	2.12	0.48
1:A:993:GLU:O	5:E:197:LYS:NZ	2.46	0.48
2:B:142:ILE:HD11	19:S:395:GLU:C	2.38	0.48
2:B:649:LEU:HB3	2:B:653:GLU:OE1	2.13	0.48
2:B:782:PHE:O	2:B:784:ARG:HG3	2.13	0.48
2:B:813:GLU:C	2:B:815:GLY:H	2.20	0.48
2:B:1147:PHE:HD2	7:G:10:LEU:HD11	1.78	0.48
3:C:270:ALA:C	3:C:272:LYS:H	2.21	0.48
5:E:112:TYR:CD1	5:E:116:ILE:HG12	2.48	0.48
5:E:177:ARG:O	5:E:212:ARG:HD3	2.13	0.48
8:H:112:ILE:O	8:H:126:GLU:HA	2.14	0.48
10:J:48:ARG:HG3	10:J:49:MET:N	2.28	0.48
18:R:231:ALA:HA	18:R:234:MET:HB3	1.95	0.48
18:R:607:ASP:C	18:R:609:GLU:H	2.22	0.48
18:R:626:ILE:O	18:R:629:GLY:N	2.46	0.48
1:A:815:GLN:HE21	1:A:847:PHE:HB2	1.78	0.48
1:A:1318:HIS:CD2	1:A:1321:GLU:HB2	2.48	0.48
2:B:612:LEU:HD21	2:B:659:ILE:HD13	1.94	0.48
2:B:757:VAL:O	2:B:1019:PHE:HB2	2.13	0.48
2:B:780:ARG:HE	3:C:217:ALA:HB1	1.78	0.48
2:B:1107:CYS:HB3	2:B:1110:CYS:SG	2.54	0.48
3:C:40:PHE:HZ	3:C:56:LEU:HD11	1.78	0.48
3:C:270:ALA:O	3:C:271:ARG:HG2	2.14	0.48
3:C:285:PHE:HD1	3:C:288:LYS:HZ1	1.59	0.48
5:E:88:VAL:HG21	5:E:112:TYR:HE1	1.76	0.48
6:F:85:MET:HA	6:F:151:LEU:HD21	1.95	0.48
15:O:201:ILE:N	15:O:280:LEU:HB3	2.25	0.48
16:P:89:GLU:O	16:P:93:VAL:N	2.36	0.48
16:P:135:LYS:HG3	16:P:136:SER:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:508:PHE:O	18:R:522:ARG:N	2.30	0.48
1:A:64:SER:OG	1:A:65:LEU:N	2.46	0.48
1:A:73:ASN:OD1	1:A:74:LEU:N	2.47	0.48
1:A:363:ARG:HD3	1:A:363:ARG:HA	1.54	0.48
1:A:791:PRO:CB	1:A:806:VAL:HG21	2.43	0.48
1:A:1075:LEU:HA	1:A:1078:TYR:HB3	1.95	0.48
1:A:1209:ILE:O	1:A:1213:SER:N	2.43	0.48
2:B:623:LYS:O	2:B:625:ILE:N	2.46	0.48
5:E:153:HIS:CE1	5:E:184:VAL:HG11	2.49	0.48
18:R:116:PHE:CE2	18:R:164:MET:HB3	2.48	0.48
18:R:467:ARG:CZ	18:R:603:GLU:HG3	2.44	0.48
1:A:1318:HIS:NE2	1:A:1321:GLU:HB2	2.28	0.48
2:B:372:VAL:HG11	2:B:608:ILE:HD12	1.95	0.48
2:B:639:ASP:O	2:B:643:LEU:HB2	2.13	0.48
2:B:737:LYS:HD3	2:B:973:LEU:HD23	1.96	0.48
2:B:790:LYS:HA	2:B:899:LEU:HA	1.95	0.48
2:B:989:LYS:HA	2:B:992:VAL:HG12	1.95	0.48
2:B:1022:ILE:CG2	2:B:1023:TYR:H	2.15	0.48
2:B:1080:LEU:O	2:B:1085:ILE:HD12	2.13	0.48
3:C:89:THR:HG22	3:C:201:GLU:H	1.78	0.48
8:H:57:VAL:HG22	8:H:144:ILE:HG12	1.95	0.48
16:P:203:LYS:HB2	16:P:206:VAL:HG22	1.95	0.48
19:S:461:GLU:HG3	19:S:465:ARG:HH21	1.78	0.48
1:A:235:LYS:NZ	1:A:254:GLU:OE2	2.45	0.48
2:B:651:VAL:HG23	2:B:652:ASN:N	2.26	0.48
2:B:692:HIS:CE1	2:B:979:PHE:H	2.32	0.48
6:F:135:ARG:HA	6:F:144:GLU:O	2.14	0.48
13:M:255:PHE:O	13:M:259:ILE:HG12	2.14	0.48
15:O:223:TYR:HE1	15:O:238:ARG:HA	1.79	0.48
15:O:496:ILE:O	15:O:500:LEU:N	2.43	0.48
15:O:538:ALA:HA	15:O:541:ILE:CG2	2.43	0.48
16:P:175:ILE:O	16:P:178:LEU:HG	2.12	0.48
18:R:391:PRO:HD2	18:R:550:TYR:CE1	2.49	0.48
18:R:521:TYR:HD2	18:R:530:LEU:HD13	1.78	0.48
1:A:17:GLU:O	2:B:1140:ARG:N	2.46	0.48
1:A:404:TYR:O	1:A:463:GLU:HA	2.14	0.48
1:A:506:THR:OG1	1:A:507:PRO:HD3	2.14	0.48
1:A:731:VAL:HG12	1:A:735:TYR:CE2	2.49	0.48
2:B:180:ASP:OD2	2:B:184:TYR:OH	2.26	0.48
2:B:710:ILE:HG13	2:B:728:MET:HE3	1.95	0.48
3:C:85:PHE:HD1	3:C:204:LEU:HB3	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:154:LYS:HG3	3:C:155:GLU:H	1.77	0.48
7:G:147:ARG:HH22	7:G:204:GLY:HA3	1.79	0.48
10:J:7:CYS:SG	10:J:10:CYS:N	2.86	0.48
13:M:112:TYR:HA	13:M:119:TRP:CD1	2.49	0.48
13:M:159:TYR:CD1	13:M:172:PRO:HA	2.48	0.48
15:O:583:TRP:HZ2	16:P:312:PHE:C	2.22	0.48
18:R:521:TYR:HE2	18:R:523:MET:HB2	1.78	0.48
19:S:498:PHE:HA	19:S:501:LYS:HB3	1.95	0.48
1:A:121:ARG:HE	15:O:73:ARG:NH1	2.12	0.48
1:A:687:PRO:O	1:A:690:ALA:N	2.46	0.48
1:A:702:ALA:HA	2:B:764:GLY:HA3	1.95	0.48
1:A:1145:LEU:HD23	1:A:1146:VAL:HG23	1.95	0.48
2:B:77:ILE:HG13	2:B:78:LYS:N	2.28	0.48
1:A:362:GLY:O	1:A:367:ASN:N	2.47	0.48
1:A:384:ASP:O	1:A:387:LEU:HB3	2.14	0.48
1:A:409:THR:H	1:A:412:ASN:ND2	2.12	0.48
1:A:601:TYR:CD1	3:C:24:SER:OG	2.67	0.48
1:A:968:GLY:O	1:A:972:GLU:HG2	2.12	0.48
1:A:1272:VAL:HG13	1:A:1273:LYS:N	2.29	0.48
2:B:798:TYR:O	2:B:801:HIS:N	2.41	0.48
3:C:20:PHE:HD1	3:C:22:GLY:H	1.61	0.48
19:S:407:ASN:HD21	21:Y:55:DT:H3'	1.77	0.48
19:S:507:ASN:HA	19:S:510:LYS:HB3	1.95	0.48
1:A:610:PHE:O	1:A:613:LEU:HB3	2.13	0.48
1:A:1267:LEU:O	1:A:1269:ASP:N	2.35	0.48
2:B:1078:LEU:O	2:B:1082:ARG:HB2	2.14	0.48
3:C:33:VAL:O	3:C:35:LYS:N	2.40	0.48
5:E:88:VAL:HG21	5:E:112:TYR:CE1	2.49	0.48
13:M:162:PHE:CE1	13:M:169:TYR:HB2	2.49	0.48
15:O:200:LEU:HD13	15:O:280:LEU:C	2.38	0.48
16:P:183:TRP:CD1	16:P:252:LYS:HB3	2.49	0.48
18:R:219:ARG:CZ	18:R:514:GLU:HB3	2.44	0.48
18:R:419:GLU:HB2	18:R:429:ILE:HD13	1.95	0.48
18:R:633:ASP:HA	18:R:636:LEU:HB3	1.95	0.48
1:A:338:PRO:HB2	1:A:342:ASN:HD22	1.80	0.47
1:A:407:LYS:HB2	6:F:102:SER:OG	2.12	0.47
1:A:656:GLY:O	1:A:657:SER:OG	2.27	0.47
1:A:893:LEU:HD23	1:A:1094:ALA:HB2	1.96	0.47
1:A:949:ASN:OD1	1:A:950:GLN:N	2.47	0.47
2:B:426:SER:O	2:B:428:ASN:N	2.43	0.47
2:B:695:GLN:HE21	2:B:698:ARG:CZ	2.24	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:877:GLU:HG2	2:B:878:PRO:N	2.27	0.47
2:B:944:MET:HG2	2:B:945:ASN:N	2.20	0.47
3:C:5:VAL:HG22	3:C:293:ARG:N	2.26	0.47
3:C:104:VAL:HG23	3:C:191:ILE:HD12	1.96	0.47
3:C:252:PRO:O	3:C:255:VAL:HB	2.12	0.47
15:O:59:GLU:HG3	15:O:61:ALA:H	1.77	0.47
15:O:67:MET:HG2	15:O:83:ILE:HD11	1.96	0.47
18:R:492:VAL:HG21	18:R:496:ILE:HD11	1.96	0.47
18:R:499:GLU:O	18:R:503:PHE:N	2.36	0.47
18:R:532:ILE:HA	18:R:538:ILE:HD12	1.94	0.47
19:S:450:SER:H	19:S:453:GLN:CD	2.20	0.47
21:Y:26:DA:C8	21:Y:27:DC:N4	2.82	0.47
1:A:33:GLU:HG3	1:A:83:HIS:CD2	2.49	0.47
1:A:347:VAL:CG1	1:A:349:PRO:HG2	2.44	0.47
1:A:1202:ILE:HG23	1:A:1203:GLU:H	1.78	0.47
1:A:1217:ILE:HG22	1:A:1218:GLN:N	2.29	0.47
1:A:1365:LYS:HE2	1:A:1379:MET:HB2	1.96	0.47
2:B:61:HIS:O	2:B:155:MET:HE1	2.14	0.47
2:B:81:GLN:N	2:B:81:GLN:OE1	2.47	0.47
2:B:478:GLU:OE1	2:B:486:PRO:HB3	2.14	0.47
2:B:1045:VAL:HG13	18:R:38:VAL:C	2.39	0.47
3:C:70:ILE:HG23	3:C:317:SER:OG	2.14	0.47
5:E:97:VAL:HA	5:E:100:ILE:HG12	1.96	0.47
8:H:8:ASP:HB3	8:H:10:PHE:CE1	2.50	0.47
15:O:87:ASP:O	15:O:88:VAL:HG12	2.13	0.47
15:O:273:ILE:HG12	15:O:274:VAL:N	2.29	0.47
15:O:572:HIS:O	15:O:576:PHE:N	2.44	0.47
18:R:512:GLU:HA	18:R:513:PRO:HD2	1.67	0.47
1:A:933:VAL:HG11	1:A:935:PHE:CD2	2.50	0.47
2:B:209:ALA:HA	2:B:215:ILE:HG23	1.96	0.47
2:B:554:GLY:HA2	2:B:564:SER:CB	2.45	0.47
2:B:848:PRO:HG3	2:B:866:TYR:CE1	2.49	0.47
3:C:178:THR:HG23	3:C:179:PHE:CD2	2.48	0.47
5:E:99:HIS:O	5:E:103:LYS:CB	2.56	0.47
6:F:75:PRO:HD2	6:F:78:GLN:NE2	2.29	0.47
8:H:135:LEU:HB2	8:H:137:GLN:NE2	2.29	0.47
13:M:154:GLU:OE1	13:M:175:ARG:HG2	2.15	0.47
15:O:152:HIS:HA	15:O:155:LEU:HD12	1.95	0.47
16:P:183:TRP:NE1	16:P:252:LYS:HB3	2.29	0.47
1:A:433:LEU:O	1:A:442:ARG:N	2.33	0.47
1:A:827:PHE:HB2	1:A:830:ARG:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:978:ASP:HB2	1:A:984:VAL:N	2.28	0.47
1:A:1128:GLU:OE1	1:A:1136:ILE:HG13	2.15	0.47
2:B:809:MET:HE1	2:B:826:PRO:HA	1.96	0.47
8:H:97:MET:SD	8:H:121:LEU:HD13	2.54	0.47
10:J:7:CYS:HA	10:J:49:MET:SD	2.54	0.47
15:O:260:SER:O	15:O:264:THR:N	2.47	0.47
16:P:135:LYS:HB2	16:P:151:TYR:CD1	2.45	0.47
18:R:413:LEU:O	18:R:615:LEU:HD11	2.15	0.47
19:S:363:GLN:HB2	19:S:378:THR:HG21	1.95	0.47
1:A:43:GLU:C	1:A:45:ASP:H	2.22	0.47
1:A:546:SER:OG	1:A:1349:SER:O	2.32	0.47
1:A:768:GLY:O	1:A:772:LYS:HB2	2.14	0.47
1:A:891:LYS:HZ3	1:A:1389:PHE:HA	1.79	0.47
1:A:964:ASN:HA	1:A:967:LEU:HB2	1.96	0.47
2:B:39:ASN:O	2:B:43:ASP:N	2.34	0.47
2:B:112:LEU:HD23	2:B:113:THR:N	2.30	0.47
2:B:262:ILE:HA	13:M:180:LYS:NZ	2.29	0.47
2:B:754:ASN:O	10:J:48:ARG:NH1	2.48	0.47
2:B:1006:SER:HB3	2:B:1010:GLY:N	2.29	0.47
3:C:132:ILE:HG23	3:C:169:PHE:CE1	2.49	0.47
8:H:6:PHE:CZ	8:H:8:ASP:HB2	2.50	0.47
9:I:28:SER:HA	13:M:135:LYS:NZ	2.29	0.47
13:M:190:ASN:OD1	13:M:194:LYS:HB2	2.15	0.47
15:O:550:GLU:N	15:O:550:GLU:OE1	2.47	0.47
18:R:522:ARG:HD3	18:R:529:VAL:HG22	1.97	0.47
1:A:363:ARG:HH12	2:B:1127:LEU:HD21	1.79	0.47
1:A:577:THR:HG23	11:K:88:PHE:CD2	2.49	0.47
2:B:148:GLU:OE1	2:B:148:GLU:N	2.48	0.47
2:B:494:PHE:CE1	2:B:680:ILE:HD12	2.50	0.47
3:C:227:TYR:HB3	3:C:300:PHE:CD1	2.31	0.47
3:C:317:SER:HA	3:C:320:ILE:HD12	1.97	0.47
5:E:82:PHE:CD1	5:E:111:VAL:HB	2.48	0.47
15:O:191:PHE:HD2	15:O:192:VAL:HG13	1.79	0.47
19:S:413:ARG:NH1	20:X:11:DA:H3'	2.29	0.47
1:A:3:GLU:HB3	7:G:37:LYS:HG3	1.96	0.47
1:A:37:ARG:HE	1:A:294:TRP:HE3	1.63	0.47
1:A:136:ARG:O	1:A:140:ILE:CB	2.56	0.47
1:A:207:HIS:O	1:A:209:PRO:HD3	2.15	0.47
1:A:207:HIS:CE1	15:O:521:ILE:CD1	2.98	0.47
1:A:608:GLN:O	1:A:611:SER:HB3	2.15	0.47
1:A:675:HIS:HB3	1:A:937:ARG:HH22	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:706:GLY:CA	2:B:762:TYR:HA	2.45	0.47
1:A:1173:VAL:HG13	1:A:1186:VAL:HG12	1.95	0.47
1:A:1452:SER:HB2	4:D:117:LYS:NZ	2.29	0.47
2:B:51:PHE:CD2	2:B:517:MET:HE3	2.50	0.47
2:B:60:GLN:OE1	2:B:60:GLN:N	2.43	0.47
2:B:92:TYR:H	2:B:136:THR:HB	1.79	0.47
2:B:129:ILE:HB	2:B:149:ILE:HG13	1.96	0.47
2:B:177:CYS:SG	2:B:714:ALA:HB1	2.55	0.47
2:B:244:HIS:O	2:B:247:ILE:HG22	2.14	0.47
2:B:524:ASP:CB	2:B:587:PHE:HE1	2.28	0.47
2:B:590:ILE:HD12	2:B:601:ILE:HD11	1.96	0.47
2:B:640:PHE:O	2:B:644:GLY:N	2.48	0.47
2:B:766:ASP:C	2:B:767:ILE:HG22	2.39	0.47
2:B:767:ILE:O	2:B:945:ASN:ND2	2.47	0.47
2:B:889:SER:OG	2:B:891:ASN:OD1	2.33	0.47
2:B:1057:ASP:CG	2:B:1058:GLY:H	2.22	0.47
3:C:136:LEU:HD12	3:C:167:LEU:HA	1.96	0.47
4:D:54:GLU:OE2	7:G:36:ASN:ND2	2.47	0.47
5:E:165:LEU:HB3	5:E:170:LEU:O	2.13	0.47
7:G:15:PRO:HA	7:G:18:PHE:CE2	2.50	0.47
7:G:51:LEU:HD12	7:G:72:PHE:HB3	1.96	0.47
7:G:190:LYS:C	7:G:192:PRO:HD3	2.40	0.47
8:H:7:ASP:HA	8:H:57:VAL:O	2.14	0.47
15:O:52:LEU:O	15:O:56:HIS:HB3	2.15	0.47
15:O:536:THR:HA	15:O:539:SER:HB3	1.97	0.47
15:O:546:VAL:HG23	15:O:547:GLU:H	1.80	0.47
15:O:591:LYS:O	15:O:633:ARG:NH2	2.47	0.47
16:P:217:THR:C	16:P:219:GLN:N	2.71	0.47
18:R:213:TRP:CH2	18:R:497:ARG:HA	2.50	0.47
18:R:636:LEU:HD22	19:S:502:LEU:HD21	1.96	0.47
19:S:427:LYS:HA	19:S:430:LYS:HB2	1.96	0.47
19:S:451:ARG:HG3	19:S:452:LYS:N	2.28	0.47
19:S:471:LEU:O	19:S:475:SER:N	2.46	0.47
19:S:509:HIS:O	19:S:513:MET:HG3	2.15	0.47
20:X:9:DA:C5	20:X:10:DT:C4	3.03	0.47
20:X:62:DG:C2	21:Y:3:DA:N1	2.83	0.47
1:A:496:ARG:O	1:A:497:THR:HB	2.15	0.47
1:A:959:ILE:HG22	1:A:960:MET:HE2	1.96	0.47
1:A:1374:PHE:O	1:A:1377:SER:O	2.32	0.47
2:B:611:PRO:HG3	2:B:648:TYR:CD1	2.50	0.47
2:B:841:ILE:HD13	2:B:872:ILE:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1132:LEU:HB3	2:B:1137:ILE:HG23	1.97	0.47
5:E:26:ARG:NH2	5:E:187:TYR:O	2.48	0.47
8:H:79:TRP:CH2	8:H:81:PRO:HA	2.50	0.47
13:M:148:LEU:HD23	13:M:179:LEU:HG	1.97	0.47
14:N:290:ILE:O	14:N:294:LEU:HB3	2.11	0.47
15:O:124:GLU:HG2	15:O:126:GLY:H	1.80	0.47
1:A:15:GLY:C	1:A:16:LEU:HD12	2.40	0.47
1:A:70:CYS:HB3	2:B:1103:TYR:CE2	2.50	0.47
1:A:214:TYR:CD2	1:A:215:VAL:HG13	2.50	0.47
1:A:338:PRO:HG2	1:A:342:ASN:HD22	1.80	0.47
1:A:546:SER:O	1:A:674:LYS:HE2	2.15	0.47
1:A:595:PRO:HD3	8:H:79:TRP:CD2	2.50	0.47
1:A:1099:GLU:OE1	1:A:1099:GLU:N	2.42	0.47
2:B:86:ASP:HA	19:S:383:ARG:NH2	2.30	0.47
2:B:86:ASP:HB2	16:P:117:HIS:NE2	2.30	0.47
2:B:758:ALA:HA	2:B:1019:PHE:HB2	1.96	0.47
2:B:832:VAL:HB	12:L:60:ARG:HA	1.97	0.47
2:B:1006:SER:OG	2:B:1009:THR:N	2.45	0.47
3:C:33:VAL:C	3:C:35:LYS:H	2.22	0.47
3:C:88:ASN:ND2	3:C:202:ILE:HG12	2.30	0.47
8:H:42:ILE:HG13	8:H:97:MET:HE2	1.96	0.47
16:P:14:ASN:HA	16:P:17:THR:HG22	1.95	0.47
16:P:190:THR:HG21	16:P:263:VAL:HB	1.96	0.47
16:P:253:LEU:HD13	16:P:261:TYR:HB3	1.96	0.47
18:R:416:ARG:HE	18:R:615:LEU:HA	1.80	0.47
1:A:787:ASN:HA	1:A:792:LEU:HD13	1.97	0.47
1:A:809:MET:HE1	2:B:950:PRO:HA	1.96	0.47
1:A:828:GLN:NE2	2:B:595:HIS:H	2.13	0.47
3:C:57:ILE:HG13	3:C:58:ASN:CG	2.40	0.47
3:C:89:THR:CG2	3:C:200:GLN:HA	2.45	0.47
3:C:137:ASN:HA	3:C:202:ILE:O	2.14	0.47
6:F:143:PHE:O	6:F:144:GLU:HB2	2.14	0.47
7:G:87:GLY:HA3	7:G:148:PHE:CE2	2.46	0.47
11:K:87:GLU:N	11:K:106:GLN:O	2.38	0.47
15:O:479:PRO:O	15:O:483:LEU:HB2	2.14	0.47
16:P:26:GLY:O	16:P:31:PHE:HB2	2.15	0.47
18:R:11:GLU:N	18:R:11:GLU:OE1	2.48	0.47
18:R:272:VAL:HG11	19:S:280:UNK:HA	1.97	0.47
19:S:429:TYR:CE1	19:S:468:LEU:HD23	2.50	0.47
21:Y:53:DT:C2'	21:Y:54:DA:H8	2.28	0.47
1:A:38:ASP:C	1:A:40:PHE:N	2.71	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:677:VAL:O	1:A:681:ILE:HG13	2.15	0.46
1:A:988:ASP:HA	1:A:991:LYS:CB	2.38	0.46
2:B:48:LEU:HB3	2:B:49:PRO:HD3	1.96	0.46
2:B:240:ILE:HD11	2:B:286:ASN:HD22	1.80	0.46
4:D:127:LEU:HD12	4:D:127:LEU:O	2.15	0.46
5:E:76:GLY:H	5:E:106:GLN:NE2	2.12	0.46
13:M:122:ASP:HB3	13:M:145:VAL:CG2	2.45	0.46
18:R:219:ARG:N	21:Y:54:DA:OP1	2.46	0.46
18:R:391:PRO:HD2	18:R:550:TYR:HE1	1.80	0.46
18:R:409:LYS:O	18:R:413:LEU:HG	2.15	0.46
18:R:472:ILE:HD11	18:R:614:LEU:HB3	1.97	0.46
18:R:523:MET:O	18:R:527:LYS:HA	2.16	0.46
1:A:124:LEU:HD22	1:A:128:ARG:HH12	1.79	0.46
1:A:545:LYS:HG3	1:A:546:SER:N	2.28	0.46
1:A:556:ASP:O	1:A:560:GLY:N	2.23	0.46
1:A:790:ALA:H	1:A:791:PRO:HD2	1.73	0.46
1:A:1166:LEU:O	1:A:1170:ALA:N	2.48	0.46
2:B:536:LEU:HD23	2:B:536:LEU:O	2.16	0.46
2:B:757:VAL:HG23	2:B:942:ILE:O	2.15	0.46
2:B:766:ASP:O	2:B:770:ALA:HB3	2.15	0.46
2:B:1045:VAL:HG13	18:R:38:VAL:O	2.15	0.46
3:C:55:ASP:OD1	3:C:56:LEU:N	2.48	0.46
3:C:89:THR:HG21	3:C:200:GLN:HA	1.96	0.46
6:F:86:THR:HG22	6:F:88:TYR:H	1.80	0.46
7:G:89:ILE:HB	7:G:140:PHE:HE1	1.80	0.46
11:K:72:LEU:O	11:K:75:ALA:N	2.49	0.46
13:M:88:PHE:HB2	14:N:395:ILE:CG2	2.45	0.46
15:O:131:LEU:C	15:O:131:LEU:CD1	2.88	0.46
15:O:240:GLN:O	15:O:243:MET:HB2	2.14	0.46
16:P:86:MET:HB3	16:P:90:GLU:HB2	1.96	0.46
18:R:208:ARG:O	18:R:212:ASP:N	2.46	0.46
18:R:528:ILE:HG22	18:R:530:LEU:HD12	1.97	0.46
20:X:55:DA:H1'	20:X:56:DC:H5'	1.98	0.46
1:A:200:GLU:HB3	15:O:516:LEU:HD23	1.93	0.46
1:A:269:ARG:HH11	1:A:356:ARG:HH12	1.60	0.46
1:A:671:ASP:CG	1:A:672:GLY:H	2.23	0.46
1:A:846:GLY:HA2	1:A:863:PHE:CD2	2.50	0.46
1:A:957:TYR:HD1	1:A:1031:LEU:HD13	1.80	0.46
2:B:131:VAL:O	2:B:147:VAL:N	2.46	0.46
2:B:723:THR:HG23	2:B:724:LEU:H	1.80	0.46
2:B:888:VAL:HG23	2:B:893:GLN:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1114:GLU:HG3	2:B:1115:ASN:N	2.30	0.46
4:D:110:LEU:HB3	4:D:120:LYS:CE	2.42	0.46
5:E:59:SER:HA	5:E:81:GLU:HA	1.97	0.46
5:E:200:ARG:HD2	5:E:208:TYR:OH	2.15	0.46
15:O:200:LEU:CA	15:O:281:THR:O	2.63	0.46
15:O:338:ASP:OD1	15:O:339:LEU:N	2.48	0.46
15:O:570:GLU:OE1	15:O:570:GLU:N	2.47	0.46
1:A:1431:VAL:HB	6:F:133:VAL:HG13	1.96	0.46
2:B:337:VAL:HG23	2:B:338:GLU:H	1.80	0.46
2:B:588:ILE:O	2:B:588:ILE:HG22	2.15	0.46
2:B:1050:PRO:O	2:B:1051:THR:C	2.58	0.46
3:C:325:ALA:O	3:C:328:LEU:N	2.47	0.46
9:I:5:CYS:O	9:I:9:ASN:HA	2.14	0.46
11:K:87:GLU:HG2	11:K:107:THR:CA	2.46	0.46
13:M:164:LYS:HD2	13:M:259:ILE:HD11	1.97	0.46
14:N:313:LEU:HB3	14:N:318:ARG:HH21	1.80	0.46
14:N:366:HIS:H	14:N:370:LYS:HB2	1.80	0.46
18:R:97:PRO:HG2	18:R:100:ILE:HD12	1.98	0.46
18:R:510:SER:N	18:R:520:ILE:O	2.29	0.46
21:Y:49:DA:H1'	21:Y:50:DA:C4	2.51	0.46
1:A:387:LEU:HD21	1:A:391:GLU:O	2.15	0.46
3:C:103:LEU:HD21	10:J:6:ARG:CD	2.45	0.46
3:C:136:LEU:O	3:C:203:SER:HA	2.16	0.46
8:H:3:ASN:ND2	8:H:62:SER:OG	2.48	0.46
13:M:241:ALA:O	13:M:242:ASN:CB	2.48	0.46
18:R:413:LEU:HB3	18:R:620:SER:OG	2.16	0.46
19:S:509:HIS:CE1	19:S:512:HIS:HD2	2.33	0.46
20:X:12:DT:H2''	20:X:13:DA:H8	1.80	0.46
1:A:372:ARG:C	2:B:1050:PRO:CG	2.88	0.46
1:A:429:GLY:C	1:A:465:HIS:HD1	2.24	0.46
1:A:599:LYS:HG2	8:H:94:ASP:O	2.15	0.46
1:A:693:ALA:O	1:A:696:ARG:N	2.49	0.46
1:A:730:LEU:HB3	1:A:777:VAL:HG22	1.97	0.46
2:B:1049:GLN:CB	2:B:1050:PRO:HD2	2.26	0.46
5:E:112:TYR:HB2	5:E:136:ASN:HA	1.97	0.46
15:O:222:HIS:HB3	15:O:241:ALA:HB1	1.96	0.46
15:O:358:GLY:HA2	15:O:361:PHE:HB2	1.97	0.46
15:O:538:ALA:HA	15:O:541:ILE:HG22	1.97	0.46
18:R:218:ARG:HD3	18:R:258:ARG:NE	2.30	0.46
1:A:408:VAL:HG12	1:A:460:ASP:O	2.16	0.46
1:A:498:PHE:CE1	1:A:519:LEU:HD22	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:527:ALA:O	1:A:530:GLU:HB3	2.15	0.46
1:A:557:PHE:HA	1:A:701:CYS:SG	2.56	0.46
1:A:1332:ARG:HH21	5:E:200:ARG:CZ	2.29	0.46
2:B:77:ILE:HD13	2:B:98:ILE:HG12	1.98	0.46
2:B:327:ILE:HD13	13:M:230:SER:OG	2.16	0.46
2:B:611:PRO:HG3	2:B:648:TYR:HE1	1.78	0.46
2:B:660:ALA:HB2	2:B:670:MET:SD	2.56	0.46
2:B:1097:LYS:H	2:B:1115:ASN:ND2	2.14	0.46
13:M:140:TRP:CG	13:M:185:TYR:HB3	2.51	0.46
15:O:133:SER:O	15:O:136:ILE:N	2.35	0.46
15:O:199:TYR:HD2	15:O:200:LEU:H	1.54	0.46
15:O:200:LEU:HD23	15:O:282:ILE:HG13	1.97	0.46
15:O:223:TYR:CE1	15:O:238:ARG:HA	2.51	0.46
16:P:207:PHE:CG	16:P:208:TYR:N	2.82	0.46
21:Y:12:DT:H2"	21:Y:13:DT:C7	2.46	0.46
1:A:624:ILE:H	1:A:657:SER:HB3	1.81	0.46
1:A:822:ARG:CZ	1:A:845:LYS:HB2	2.45	0.46
1:A:1152:ARG:O	1:A:1155:ARG:N	2.48	0.46
1:A:1153:ALA:O	1:A:1157:VAL:HG22	2.15	0.46
1:A:1201:THR:H	1:A:1204:ASP:HB2	1.81	0.46
2:B:776:SER:OG	2:B:928:GLN:NE2	2.49	0.46
2:B:877:GLU:CG	2:B:878:PRO:N	2.79	0.46
2:B:916:HIS:CG	2:B:957:LYS:HB2	2.51	0.46
2:B:1095:CYS:O	2:B:1099:GLY:HA2	2.16	0.46
4:D:61:ASN:ND2	7:G:103:GLY:O	2.49	0.46
5:E:190:LEU:HA	5:E:194:GLU:OE1	2.16	0.46
15:O:43:ASN:CB	15:O:47:PHE:HB2	2.44	0.46
15:O:128:HIS:HA	15:O:131:LEU:HG	1.98	0.46
15:O:284:LEU:O	15:O:284:LEU:HD23	2.16	0.46
15:O:291:ARG:HG3	15:O:292:ARG:N	2.31	0.46
18:R:274:LYS:O	18:R:275:PHE:CG	2.69	0.46
18:R:409:LYS:HE2	18:R:413:LEU:HD21	1.98	0.46
18:R:415:ALA:HA	18:R:614:LEU:HA	1.98	0.46
1:A:436:ARG:HH11	1:A:459:GLY:HA3	1.80	0.46
1:A:598:MET:HA	1:A:602:TYR:CD1	2.51	0.46
1:A:815:GLN:HA	1:A:846:GLY:O	2.16	0.46
2:B:135:TYR:O	2:B:142:ILE:HA	2.16	0.46
2:B:383:LEU:HB3	2:B:442:TRP:CH2	2.51	0.46
2:B:540:ASP:OD1	2:B:541:ILE:N	2.49	0.46
2:B:618:GLY:HA2	2:B:668:PRO:HA	1.97	0.46
2:B:623:LYS:C	2:B:625:ILE:H	2.24	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:721:ILE:HG12	2:B:899:LEU:CD2	2.46	0.46
3:C:321:LEU:HD21	11:K:124:LEU:HD21	1.98	0.46
7:G:15:PRO:HA	7:G:18:PHE:CZ	2.51	0.46
15:O:40:ARG:HG2	15:O:587:ASN:CG	2.41	0.46
15:O:170:THR:HG22	15:O:278:VAL:C	2.41	0.46
15:O:289:LYS:CD	15:O:325:LYS:HZ2	2.26	0.46
18:R:218:ARG:NH1	21:Y:53:DT:H5'	2.31	0.46
18:R:467:ARG:O	18:R:471:LYS:HB2	2.16	0.46
1:A:69:THR:OG1	1:A:80:HIS:NE2	2.44	0.46
1:A:1022:LEU:HA	1:A:1025:SER:HB3	1.98	0.46
1:A:1063:SER:N	1:A:1066:SER:OG	2.42	0.46
1:A:1067:VAL:HG12	1:A:1071:LEU:HG	1.98	0.46
1:A:1373:ARG:N	1:A:1376:LEU:HD21	2.31	0.46
2:B:324:ILE:HG23	2:B:325:GLU:H	1.80	0.46
2:B:369:ARG:HG3	2:B:369:ARG:O	2.15	0.46
2:B:422:ILE:O	2:B:426:SER:N	2.49	0.46
2:B:483:VAL:HG12	2:B:485:GLY:H	1.81	0.46
2:B:698:ARG:HE	2:B:952:ARG:CG	2.28	0.46
4:D:17:LEU:HA	4:D:20:LEU:HD12	1.98	0.46
7:G:115:LEU:H	7:G:199:SER:HB3	1.81	0.46
7:G:203:ASP:OD1	7:G:204:GLY:N	2.41	0.46
15:O:204:SER:H	15:O:207:HIS:CB	2.29	0.46
16:P:220:GLU:O	16:P:223:GLU:HB2	2.16	0.46
18:R:77:GLU:HA	18:R:80:LEU:HD12	1.98	0.46
19:S:484:TYR:CE1	19:S:488:ILE:HD13	2.51	0.46
1:A:1123:VAL:N	1:A:1124:PRO:HD2	2.30	0.45
2:B:84:LEU:HG	2:B:85:SER:O	2.16	0.45
2:B:204:ARG:HH21	2:B:558:ASN:CA	2.29	0.45
2:B:244:HIS:HE1	2:B:332:ILE:O	1.98	0.45
2:B:533:CYS:SG	2:B:538:VAL:HG11	2.56	0.45
2:B:824:LEU:O	2:B:831:GLU:HB2	2.16	0.45
3:C:216:HIS:CD2	3:C:218:LYS:HE3	2.51	0.45
10:J:6:ARG:HD3	10:J:11:GLY:O	2.16	0.45
10:J:36:LEU:CD2	10:J:47:ARG:HG3	2.46	0.45
11:K:91:TYR:HA	11:K:102:ASN:O	2.16	0.45
13:M:187:ASP:O	13:M:191:VAL:HG23	2.15	0.45
15:O:37:LEU:O	15:O:41:THR:OG1	2.34	0.45
15:O:352:VAL:O	15:O:357:PRO:HD2	2.15	0.45
15:O:645:LEU:O	15:O:649:GLU:HG3	2.16	0.45
16:P:93:VAL:HG11	16:P:124:CYS:SG	2.56	0.45
16:P:141:LYS:HG2	16:P:142:PHE:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:48:THR:O	17:Q:52:ARG:HG3	2.16	0.45
18:R:397:VAL:HG12	18:R:484:GLN:HB2	1.98	0.45
18:R:512:GLU:HB3	18:R:515:LEU:HB3	1.98	0.45
20:X:24:DT:H2''	20:X:25:DT:H6	1.81	0.45
1:A:392:VAL:HG23	1:A:488:HIS:CD2	2.51	0.45
1:A:730:LEU:O	1:A:733:ILE:HG22	2.16	0.45
1:A:1299:GLY:O	1:A:1301:ARG:N	2.50	0.45
1:A:1452:SER:C	4:D:117:LYS:HZ2	2.24	0.45
2:B:65:PHE:HZ	2:B:154:ILE:HA	1.81	0.45
2:B:131:VAL:HG21	2:B:149:ILE:HG23	1.98	0.45
2:B:137:ARG:H	2:B:141:ILE:CG2	2.26	0.45
2:B:539:GLU:CD	2:B:539:GLU:H	2.25	0.45
8:H:130:ARG:O	8:H:130:ARG:HG3	2.14	0.45
12:L:61:THR:HG21	12:L:63:ARG:HB3	1.98	0.45
14:N:383:GLY:O	14:N:384:LYS:HD2	2.16	0.45
18:R:239:ARG:NH1	19:S:291:UNK:O	2.49	0.45
18:R:269:LYS:O	18:R:272:VAL:HG12	2.17	0.45
19:S:382:ASP:C	19:S:384:HIS:H	2.24	0.45
21:Y:8:DG:H2'	21:Y:9:DT:H71	1.98	0.45
1:A:183:PHE:CG	1:A:184:ARG:N	2.84	0.45
1:A:1453:ASN:HA	4:D:117:LYS:HD3	1.97	0.45
2:B:572:VAL:HG22	2:B:590:ILE:HD11	1.97	0.45
2:B:628:ARG:HA	2:B:631:LEU:HG	1.97	0.45
2:B:658:TYR:O	2:B:671:THR:OG1	2.35	0.45
5:E:62:ALA:O	5:E:77:SER:HB2	2.17	0.45
15:O:516:LEU:HD12	15:O:565:LEU:HD23	1.98	0.45
15:O:583:TRP:NE1	16:P:311:TYR:O	2.49	0.45
18:R:99:TYR:HD2	18:R:100:ILE:HG13	1.82	0.45
1:A:404:TYR:CD1	1:A:405:PRO:HD2	2.51	0.45
1:A:409:THR:H	1:A:412:ASN:HD22	1.64	0.45
1:A:413:ARG:O	1:A:417:GLN:HG2	2.16	0.45
1:A:857:SER:O	1:A:860:GLU:HG2	2.16	0.45
1:A:912:VAL:HG12	1:A:1364:TYR:CD1	2.51	0.45
1:A:1211:ARG:HA	1:A:1214:LYS:NZ	2.31	0.45
1:A:1300:LEU:HD23	1:A:1325:VAL:HG21	1.99	0.45
1:A:1360:ASP:O	1:A:1363:THR:N	2.49	0.45
2:B:207:VAL:HG11	2:B:356:VAL:HG12	1.98	0.45
2:B:659:ILE:HG23	2:B:673:LEU:HA	1.97	0.45
2:B:758:ALA:O	2:B:943:ILE:HD12	2.16	0.45
2:B:988:SER:OG	2:B:998:TYR:HB2	2.15	0.45
2:B:1147:PHE:CE2	7:G:67:TYR:CG	3.04	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:544:ASN:OD1	15:O:545:SER:N	2.50	0.45
15:O:573:SER:C	15:O:575:ASN:N	2.74	0.45
16:P:201:GLY:N	16:P:202:PRO:HD2	2.31	0.45
18:R:153:SER:C	18:R:155:TYR:H	2.24	0.45
18:R:198:VAL:HG13	18:R:231:ALA:HB1	1.99	0.45
18:R:478:PHE:HB3	18:R:599:PRO:HA	1.98	0.45
18:R:521:TYR:CE2	18:R:523:MET:HB2	2.52	0.45
21:Y:58:DT:H4'	21:Y:59:DG:H5'	1.98	0.45
1:A:252:ARG:O	1:A:254:GLU:N	2.45	0.45
1:A:636:PRO:HG3	1:A:646:SER:HB3	1.98	0.45
1:A:1144:VAL:HG22	1:A:1313:ARG:O	2.17	0.45
2:B:230:LYS:HD3	2:B:333:ALA:HB2	1.98	0.45
2:B:347:LEU:O	2:B:351:MET:HG2	2.16	0.45
2:B:415:GLU:C	2:B:417:ASP:H	2.24	0.45
2:B:666:ILE:HA	2:B:670:MET:SD	2.57	0.45
2:B:811:VAL:HG22	2:B:817:PRO:HB3	1.98	0.45
2:B:877:GLU:CG	2:B:878:PRO:CD	2.94	0.45
18:R:516:PHE:CD1	18:R:517:PRO:HD2	2.51	0.45
1:A:332:VAL:HG13	1:A:333:ASN:H	1.81	0.45
1:A:1206:ALA:HB1	1:A:1222:VAL:HG11	1.99	0.45
2:B:253:ILE:HG23	2:B:254:ALA:N	2.31	0.45
2:B:574:GLN:NE2	14:N:422:ILE:HG12	2.31	0.45
2:B:579:ARG:HD2	2:B:587:PHE:O	2.17	0.45
3:C:88:ASN:OD1	3:C:90:SER:N	2.29	0.45
15:O:260:SER:HA	15:O:263:LEU:HB2	1.97	0.45
18:R:111:ALA:HB1	18:R:116:PHE:HB3	1.98	0.45
21:Y:48:DT:H2'	21:Y:49:DA:C8	2.51	0.45
1:A:308:SER:HA	15:O:534:ARG:CD	2.47	0.45
1:A:367:ASN:O	1:A:371:LYS:HA	2.16	0.45
1:A:689:GLU:O	1:A:692:ASN:HB3	2.16	0.45
1:A:694:MET:O	1:A:697:MET:HB3	2.17	0.45
1:A:738:CYS:HA	1:A:741:LEU:HD12	1.99	0.45
1:A:834:HIS:ND1	2:B:659:ILE:O	2.46	0.45
1:A:1095:GLN:NE2	2:B:1068:ASP:OD2	2.49	0.45
2:B:67:TYR:CZ	2:B:71:THR:HG21	2.52	0.45
2:B:217:GLN:CD	2:B:232:TYR:HB3	2.42	0.45
2:B:232:TYR:CD1	2:B:242:LEU:HD23	2.48	0.45
2:B:421:SER:HA	2:B:424:VAL:HG12	1.98	0.45
2:B:766:ASP:O	2:B:767:ILE:CG2	2.63	0.45
3:C:140:CYS:HB3	3:C:198:PRO:HA	1.98	0.45
13:M:125:LEU:HD13	13:M:144:ASN:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:104:VAL:C	15:O:123:ASN:HB2	2.42	0.45
15:O:200:LEU:HB3	15:O:281:THR:H	1.76	0.45
15:O:331:THR:HB	15:O:335:LEU:HD21	1.98	0.45
15:O:471:THR:HA	15:O:477:TYR:HD2	1.82	0.45
15:O:590:PHE:O	15:O:593:GLU:N	2.49	0.45
18:R:401:THR:HB	18:R:480:ASP:HB2	1.98	0.45
18:R:430:MET:HE3	18:R:441:ILE:HB	1.98	0.45
1:A:387:LEU:HD22	1:A:393:ALA:HB2	1.98	0.45
1:A:432:TYR:HD1	1:A:443:ASN:HA	1.80	0.45
1:A:634:VAL:HG21	1:A:648:ASN:HD21	1.81	0.45
2:B:912:PHE:HE1	2:B:1026:LYS:HD2	1.81	0.45
2:B:1006:SER:HB3	2:B:1010:GLY:H	1.82	0.45
3:C:121:PRO:O	3:C:122:ASP:CG	2.60	0.45
4:D:58:ILE:HG23	7:G:36:ASN:OD1	2.17	0.45
7:G:51:LEU:HD11	7:G:70:VAL:HG21	1.98	0.45
7:G:207:LEU:HB3	7:G:210:TRP:CE2	2.52	0.45
15:O:262:ILE:HA	15:O:275:LYS:HB2	1.97	0.45
15:O:599:ASN:O	15:O:603:LEU:HG	2.17	0.45
18:R:396:ILE:HG13	18:R:486:ILE:HG23	1.98	0.45
19:S:487:GLU:HG2	19:S:488:ILE:HD12	1.99	0.45
1:A:1278:ILE:HG12	1:A:1297:GLY:HA3	1.99	0.45
2:B:48:LEU:HD22	2:B:743:LEU:CD2	2.47	0.45
2:B:490:GLN:H	2:B:490:GLN:CD	2.24	0.45
2:B:874:ARG:HG2	18:R:16:LEU:HD13	1.98	0.45
4:D:126:GLN:HE21	7:G:85:VAL:HA	1.82	0.45
15:O:593:GLU:OE1	15:O:596:LYS:HG3	2.17	0.45
15:O:650:VAL:HG13	15:O:651:PHE:N	2.31	0.45
19:S:425:MET:HE2	19:S:457:LYS:NZ	2.32	0.45
1:A:273:MET:HE3	18:R:39:SER:HB3	1.98	0.45
1:A:407:LYS:O	1:A:412:ASN:ND2	2.50	0.45
1:A:678:PHE:CZ	1:A:694:MET:HG2	2.52	0.45
1:A:712:ILE:HG22	1:A:713:GLY:H	1.81	0.45
1:A:897:SER:OG	1:A:898:CYS:N	2.50	0.45
1:A:1022:LEU:HD23	1:A:1059:LEU:HD11	1.99	0.45
2:B:129:ILE:HG22	2:B:131:VAL:HG13	1.98	0.45
2:B:475:SER:HB3	2:B:510:LEU:N	2.32	0.45
2:B:587:PHE:HD1	2:B:588:ILE:N	2.15	0.45
7:G:84:ILE:CG2	7:G:147:ARG:HB3	2.47	0.45
7:G:105:PHE:HD1	7:G:107:ASP:H	1.65	0.45
7:G:115:LEU:HA	7:G:200:CYS:O	2.17	0.45
8:H:80:ARG:HG3	11:K:108:TYR:CZ	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:71:ILE:HG22	14:N:366:HIS:HA	1.99	0.45
15:O:283:ASN:OD1	15:O:284:LEU:N	2.49	0.45
16:P:178:LEU:HD12	16:P:179:LEU:HD12	1.97	0.45
16:P:246:VAL:HG12	16:P:250:ASP:OD2	2.17	0.45
18:R:14:ARG:HB2	18:R:23:LEU:HD13	1.98	0.45
18:R:182:ILE:HD13	18:R:199:VAL:HG13	1.98	0.45
18:R:387:SER:HA	18:R:579:PRO:HA	1.99	0.45
18:R:490:CYS:N	18:R:538:ILE:O	2.46	0.45
18:R:500:GLY:HA2	18:R:503:PHE:HB3	1.98	0.45
18:R:545:GLN:HG3	18:R:547:GLU:H	1.81	0.45
20:X:24:DT:O2	21:Y:41:DG:N2	2.50	0.45
1:A:90:VAL:HG13	1:A:258:TRP:HB2	1.99	0.44
1:A:95:TYR:CE1	1:A:1397:PHE:HD1	2.36	0.44
1:A:269:ARG:HB3	1:A:283:ASP:OD2	2.16	0.44
1:A:383:PRO:HG3	1:A:512:PHE:CE1	2.51	0.44
1:A:559:THR:HB	1:A:799:SER:HB3	1.99	0.44
1:A:573:ARG:HH21	11:K:87:GLU:HA	1.81	0.44
1:A:627:ASP:HB3	1:A:653:ILE:HG13	1.99	0.44
1:A:828:GLN:HE22	2:B:594:SER:H	1.64	0.44
2:B:907:GLU:OE2	2:B:908:LEU:HB3	2.18	0.44
3:C:129:GLU:OE1	3:C:129:GLU:N	2.43	0.44
3:C:255:VAL:HG13	3:C:256:ILE:O	2.17	0.44
5:E:1:MET:HG3	5:E:3:GLN:N	2.32	0.44
7:G:55:GLU:N	7:G:55:GLU:OE1	2.50	0.44
9:I:20:GLY:C	9:I:22:TYR:H	2.25	0.44
13:M:251:THR:HG21	13:M:255:PHE:CE2	2.52	0.44
15:O:98:LEU:HB3	15:O:103:CYS:HB2	1.98	0.44
15:O:105:LYS:HB2	15:O:121:TYR:H	1.81	0.44
15:O:197:MET:HA	15:O:321:GLN:HE22	1.82	0.44
15:O:341:GLU:HA	15:O:344:SER:HB2	1.98	0.44
16:P:266:GLU:CG	16:P:269:LEU:HD13	2.43	0.44
16:P:267:SER:HA	16:P:270:GLN:HB3	1.99	0.44
21:Y:18:DC:H1'	21:Y:19:DT:N1	2.33	0.44
21:Y:49:DA:H2''	21:Y:50:DA:C8	2.52	0.44
1:A:147:GLN:NE2	1:A:150:LYS:HD2	2.32	0.44
1:A:625:ASN:HD21	1:A:941:HIS:HA	1.82	0.44
1:A:792:LEU:O	1:A:796:THR:HB	2.17	0.44
1:A:808:GLN:HB3	1:A:813:VAL:HG22	1.99	0.44
1:A:815:GLN:NE2	1:A:847:PHE:HB2	2.31	0.44
1:A:1163:LYS:HD3	1:A:1278:ILE:O	2.17	0.44
2:B:51:PHE:CG	2:B:517:MET:HE3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:495:GLY:HA3	2:B:610:ARG:NH1	2.32	0.44
2:B:520:ILE:HA	2:B:607:ARG:O	2.16	0.44
2:B:794:VAL:HA	2:B:895:LEU:CD2	2.46	0.44
2:B:806:ILE:HG13	12:L:42:ARG:NH2	2.32	0.44
9:I:6:PRO:C	9:I:7:SER:HG	2.25	0.44
11:K:59:THR:O	11:K:107:THR:HG22	2.17	0.44
13:M:77:LYS:HZ1	13:M:262:GLU:HB2	1.82	0.44
13:M:85:LEU:HD21	14:N:409:LEU:HD22	1.99	0.44
15:O:197:MET:HB2	15:O:286:ARG:NE	2.29	0.44
15:O:239:SER:O	15:O:243:MET:HG2	2.17	0.44
15:O:307:VAL:O	15:O:311:VAL:HG23	2.17	0.44
15:O:348:GLU:HA	15:O:351:LEU:HG	2.00	0.44
15:O:457:LEU:HD21	15:O:476:TYR:OH	2.17	0.44
16:P:14:ASN:O	16:P:18:LEU:HB3	2.16	0.44
18:R:159:ALA:O	18:R:163:LYS:HG2	2.16	0.44
19:S:388:SER:O	19:S:392:GLU:HG3	2.17	0.44
19:S:407:ASN:HB2	21:Y:55:DT:OP1	2.17	0.44
1:A:408:VAL:CA	1:A:412:ASN:HD22	2.27	0.44
1:A:625:ASN:HD21	1:A:940:ASP:C	2.24	0.44
1:A:671:ASP:OD1	1:A:672:GLY:N	2.48	0.44
1:A:1391:LYS:CD	21:Y:19:DT:H4'	2.46	0.44
2:B:156:LEU:HD22	2:B:184:TYR:CZ	2.52	0.44
2:B:248:ALA:HB3	2:B:308:LYS:HG2	1.98	0.44
2:B:521:THR:HG21	2:B:586:GLU:HG2	1.99	0.44
2:B:553:TYR:CE2	2:B:568:PRO:HG3	2.51	0.44
2:B:914:SER:HB2	2:B:918:GLN:HB2	1.98	0.44
2:B:1067:ARG:O	2:B:1070:VAL:HG22	2.16	0.44
6:F:94:LEU:HD11	6:F:125:LEU:HD13	1.99	0.44
13:M:148:LEU:HB3	13:M:179:LEU:HD11	2.00	0.44
15:O:588:LEU:O	15:O:589:LEU:C	2.60	0.44
18:R:287:PRO:HD2	18:R:290:PHE:HE2	1.81	0.44
18:R:500:GLY:O	18:R:504:SER:N	2.50	0.44
18:R:547:GLU:OE1	18:R:547:GLU:N	2.50	0.44
19:S:408:TYR:HD2	21:Y:55:DT:OP1	2.01	0.44
19:S:450:SER:HB3	19:S:453:GLN:HG3	1.99	0.44
1:A:48:PRO:C	1:A:49:LYS:HG2	2.42	0.44
1:A:192:PRO:O	1:A:196:ILE:HG12	2.17	0.44
1:A:204:VAL:HG12	1:A:212:GLU:OE2	2.17	0.44
1:A:314:GLU:HA	1:A:317:ASP:HB3	2.00	0.44
1:A:353:PHE:O	1:A:356:ARG:HB3	2.17	0.44
1:A:376:SER:HB2	2:B:1060:LEU:HD12	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:540:ASN:OD1	2:B:1073:TYR:HE1	2.01	0.44
1:A:999:ASP:HA	1:A:1002:ARG:HB2	2.00	0.44
2:B:97:ASP:OD1	2:B:98:ILE:N	2.51	0.44
2:B:145:LYS:HD3	19:S:399:GLU:HG2	1.99	0.44
2:B:234:ILE:HA	2:B:240:ILE:HA	1.99	0.44
2:B:667:VAL:HG23	2:B:670:MET:HE3	1.99	0.44
2:B:695:GLN:HG3	2:B:697:PRO:CG	2.43	0.44
2:B:913:SER:OG	2:B:914:SER:N	2.51	0.44
3:C:58:ASN:H	3:C:296:ASN:HB3	1.83	0.44
5:E:32:GLN:O	5:E:36:GLU:N	2.50	0.44
8:H:56:THR:HB	8:H:145:ARG:HG2	1.99	0.44
11:K:122:LYS:O	11:K:125:MET:HB2	2.18	0.44
16:P:22:MET:HB3	16:P:74:GLY:H	1.82	0.44
16:P:235:LEU:HD23	16:P:236:THR:O	2.18	0.44
1:A:129:ARG:O	1:A:132:VAL:HG23	2.17	0.44
1:A:185:TRP:HE1	1:A:219:MET:HE1	1.82	0.44
1:A:348:LYS:HB2	1:A:349:PRO:HD3	2.00	0.44
1:A:379:THR:HB	1:A:498:PHE:CD2	2.52	0.44
1:A:408:VAL:HG21	1:A:456:LEU:HD11	1.99	0.44
1:A:882:THR:O	1:A:885:MET:HB3	2.18	0.44
1:A:967:LEU:HA	1:A:970:LEU:HD12	2.00	0.44
1:A:1078:TYR:O	1:A:1081:ALA:N	2.50	0.44
2:B:353:THR:O	2:B:356:VAL:HG22	2.17	0.44
2:B:1038:ARG:NH2	2:B:1042:PRO:O	2.49	0.44
4:D:29:TRP:CZ3	4:D:32:LYS:HB2	2.52	0.44
6:F:101:ILE:HD12	6:F:107:VAL:HG12	1.99	0.44
10:J:8:PHE:H	10:J:49:MET:HE1	1.82	0.44
18:R:213:TRP:O	18:R:213:TRP:CD1	2.70	0.44
18:R:630:LEU:HD11	19:S:444:GLN:CD	2.42	0.44
18:R:646:GLU:OE1	19:S:510:LYS:HG3	2.18	0.44
1:A:204:VAL:HA	1:A:207:HIS:HB3	1.99	0.44
1:A:614:ILE:HG21	1:A:624:ILE:HD12	1.99	0.44
1:A:712:ILE:HG22	1:A:713:GLY:N	2.31	0.44
1:A:789:ASN:HB3	1:A:791:PRO:CD	2.42	0.44
1:A:834:HIS:HA	2:B:659:ILE:O	2.18	0.44
1:A:968:GLY:C	1:A:970:LEU:H	2.26	0.44
1:A:999:ASP:OD1	1:A:999:ASP:O	2.35	0.44
1:A:1163:LYS:HB2	1:A:1279:SER:O	2.16	0.44
2:B:262:ILE:HA	13:M:180:LYS:HZ3	1.82	0.44
2:B:987:MET:O	2:B:990:ILE:HB	2.17	0.44
3:C:59:ILE:HD12	3:C:60:ASP:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:63:ILE:O	3:C:66:ALA:HB3	2.17	0.44
4:D:25:LYS:HA	4:D:29:TRP:HB2	1.99	0.44
5:E:123:LEU:HD21	5:E:126:SER:HA	1.99	0.44
5:E:200:ARG:HH11	5:E:208:TYR:HE2	1.65	0.44
11:K:53:ALA:HB1	11:K:104:ARG:NH1	2.33	0.44
13:M:230:SER:C	13:M:234:HIS:HD1	2.25	0.44
14:N:396:ALA:C	14:N:397:LEU:HD12	2.43	0.44
15:O:40:ARG:HG2	15:O:587:ASN:OD1	2.17	0.44
18:R:148:SER:O	18:R:148:SER:OG	2.33	0.44
18:R:492:VAL:HG22	18:R:536:GLY:CA	2.48	0.44
18:R:537:LYS:HD3	21:Y:52:DA:OP1	2.17	0.44
19:S:430:LYS:O	19:S:434:MET:HG2	2.17	0.44
1:A:42:LEU:HA	1:A:48:PRO:HD2	1.99	0.44
1:A:683:ARG:HG3	1:A:1077:LYS:HE2	2.00	0.44
2:B:72:ASP:O	2:B:76:ILE:HG12	2.18	0.44
2:B:117:GLU:HG3	12:L:53:HIS:NE2	2.33	0.44
3:C:101:ILE:O	3:C:104:VAL:HG12	2.18	0.44
3:C:236:LEU:O	3:C:288:LYS:HB2	2.17	0.44
7:G:82:GLY:HA2	7:G:150:ILE:O	2.17	0.44
8:H:107:VAL:O	8:H:111:LEU:HB2	2.17	0.44
9:I:8:CYS:HB2	9:I:29:CYS:CB	2.47	0.44
10:J:16:ASP:OD1	10:J:17:LYS:HG3	2.17	0.44
10:J:17:LYS:HB3	10:J:39:LEU:HD21	1.99	0.44
13:M:83:GLU:C	13:M:84:SER:O	2.61	0.44
15:O:49:TYR:O	15:O:52:LEU:HB2	2.17	0.44
15:O:53:VAL:O	15:O:58:GLY:N	2.51	0.44
15:O:287:PHE:CE2	15:O:291:ARG:HD3	2.52	0.44
15:O:325:LYS:HG3	15:O:326:ILE:H	1.83	0.44
16:P:118:GLN:O	16:P:122:LEU:HG	2.18	0.44
1:A:363:ARG:NH1	2:B:1131:GLU:OE2	2.51	0.44
1:A:730:LEU:HD13	1:A:777:VAL:HG22	1.99	0.44
1:A:1217:ILE:H	1:A:1217:ILE:HD12	1.82	0.44
2:B:102:LYS:NZ	2:B:106:SER:O	2.40	0.44
2:B:186:ILE:HG13	2:B:190:THR:O	2.17	0.44
2:B:640:PHE:HB3	2:B:645:LEU:HB2	1.99	0.44
3:C:74:GLU:HA	3:C:212:ILE:HD11	2.00	0.44
3:C:123:ASP:OD1	3:C:124:GLU:N	2.50	0.44
7:G:137:LYS:HE3	7:G:210:TRP:CD1	2.53	0.44
13:M:88:PHE:HB2	14:N:395:ILE:HG23	2.00	0.44
13:M:115:LYS:HG2	13:M:116:SER:H	1.82	0.44
15:O:286:ARG:HH21	15:O:321:GLN:NE2	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:258:ARG:HH22	21:Y:53:DT:H3'	1.83	0.44
19:S:439:PHE:O	19:S:442:ILE:N	2.51	0.44
1:A:579:LEU:O	1:A:582:MET:N	2.50	0.44
1:A:637:LYS:HZ3	1:A:647:GLN:HE21	1.66	0.44
1:A:923:PRO:HA	1:A:926:MET:HE2	1.99	0.44
2:B:89:PRO:HA	19:S:383:ARG:HH11	1.83	0.44
2:B:285:VAL:O	2:B:288:GLU:HB3	2.17	0.44
2:B:987:MET:HA	2:B:990:ILE:HB	1.99	0.44
6:F:86:THR:C	6:F:88:TYR:H	2.26	0.44
11:K:60:SER:OG	11:K:106:GLN:HG3	2.18	0.44
13:M:160:ALA:HB2	14:N:306:VAL:HG12	1.99	0.44
16:P:209:ALA:O	16:P:212:VAL:HG12	2.18	0.44
19:S:426:ILE:O	19:S:430:LYS:HG3	2.18	0.44
21:Y:3:DA:H1'	21:Y:4:DT:C2	2.53	0.44
1:A:106:ILE:HG13	1:A:112:ALA:C	2.43	0.43
1:A:596:ALA:HB2	1:A:608:GLN:OE1	2.18	0.43
1:A:609:VAL:HG13	1:A:610:PHE:N	2.32	0.43
2:B:405:LYS:HG2	2:B:408:LYS:CE	2.48	0.43
2:B:534:TYR:HA	2:B:538:VAL:HG22	2.00	0.43
2:B:591:TYR:CG	2:B:652:ASN:HB3	2.53	0.43
2:B:650:ASP:OD1	2:B:651:VAL:HG22	2.18	0.43
2:B:1103:TYR:C	2:B:1104:SER:HG	2.24	0.43
3:C:309:THR:OG1	3:C:311:GLU:HG2	2.18	0.43
7:G:203:ASP:HB3	7:G:211:TRP:NE1	2.32	0.43
8:H:109:LYS:NZ	8:H:110:ASP:OD2	2.48	0.43
16:P:31:PHE:O	16:P:71:LYS:HA	2.17	0.43
18:R:524:VAL:HA	18:R:527:LYS:HA	2.00	0.43
21:Y:48:DT:C4	21:Y:49:DA:N6	2.85	0.43
1:A:114:LEU:HD12	1:A:115:LEU:N	2.32	0.43
1:A:704:PHE:O	1:A:707:ASN:N	2.51	0.43
1:A:911:ILE:HD11	1:A:914:PHE:HA	2.00	0.43
2:B:619:GLN:OE1	2:B:619:GLN:N	2.52	0.43
2:B:786:GLU:OE2	3:C:93:GLN:HG3	2.17	0.43
7:G:110:ILE:O	7:G:110:ILE:HG13	2.18	0.43
7:G:207:LEU:HD23	7:G:209:SER:N	2.33	0.43
10:J:8:PHE:HB2	10:J:48:ARG:NH2	2.33	0.43
15:O:292:ARG:HB3	15:O:325:LYS:HZ3	1.81	0.43
15:O:532:ASP:O	15:O:535:SER:N	2.50	0.43
15:O:635:LEU:HD22	17:Q:47:ILE:HD13	1.99	0.43
16:P:98:GLU:HB2	16:P:150:LEU:HD11	2.00	0.43
16:P:296:TYR:CD1	17:Q:42:PRO:HG3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:610:LEU:HA	18:R:613:HIS:HB2	2.00	0.43
21:Y:9:DT:H2"	21:Y:10:DC:C6	2.54	0.43
1:A:84:LEU:HB3	1:A:261:LEU:HB3	2.00	0.43
1:A:119:ASP:O	1:A:122:GLN:HB3	2.17	0.43
1:A:600:PRO:O	1:A:601:TYR:CB	2.58	0.43
1:A:1120:THR:OG1	1:A:1125:ARG:HD2	2.17	0.43
1:A:1177:TYR:CD1	1:A:1182:SER:HA	2.53	0.43
1:A:1319:VAL:O	1:A:1322:VAL:N	2.52	0.43
2:B:296:TYR:HE2	9:I:28:SER:OG	2.01	0.43
2:B:305:ILE:CB	2:B:325:GLU:HG2	2.46	0.43
2:B:1043:ARG:HB3	2:B:1048:ARG:CA	2.41	0.43
7:G:22:THR:O	7:G:26:ILE:HG12	2.18	0.43
7:G:115:LEU:N	7:G:199:SER:HB3	2.33	0.43
11:K:107:THR:HG23	11:K:108:TYR:O	2.18	0.43
13:M:115:LYS:NZ	13:M:233:ALA:HA	2.33	0.43
15:O:132:TYR:CD1	15:O:645:LEU:HD11	2.53	0.43
15:O:200:LEU:HD21	15:O:282:ILE:HD12	2.00	0.43
15:O:553:ARG:H	15:O:562:ALA:HA	1.83	0.43
16:P:179:LEU:HD11	16:P:243:LEU:HG	2.00	0.43
18:R:428:VAL:O	18:R:441:ILE:HG22	2.19	0.43
21:Y:20:DT:C5	21:Y:21:DG:C6	3.07	0.43
1:A:147:GLN:HE22	1:A:150:LYS:HD2	1.83	0.43
1:A:970:LEU:HB3	1:A:1005:TYR:CE2	2.53	0.43
1:A:1188:ILE:H	1:A:1228:ASP:HB2	1.83	0.43
1:A:1396:LEU:HD23	1:A:1396:LEU:HA	1.83	0.43
2:B:58:VAL:HA	2:B:60:GLN:OE1	2.18	0.43
2:B:574:GLN:O	2:B:577:HIS:HB3	2.18	0.43
2:B:715:TYR:C	2:B:717:GLN:H	2.27	0.43
2:B:777:SER:O	2:B:781:GLY:N	2.51	0.43
2:B:929:GLU:CD	3:C:69:ARG:HB3	2.44	0.43
2:B:1008:ILE:HG23	11:K:70:HIS:CG	2.52	0.43
3:C:3:ASN:HB2	3:C:294:VAL:HG23	2.00	0.43
3:C:33:VAL:HB	3:C:34:GLU:CD	2.43	0.43
13:M:146:GLN:HG2	13:M:147:THR:H	1.82	0.43
15:O:105:LYS:HB3	15:O:210:PRO:HD3	2.01	0.43
15:O:233:SER:O	15:O:236:LYS:HG2	2.19	0.43
15:O:352:VAL:HG13	15:O:353:GLU:N	2.34	0.43
16:P:22:MET:HB3	16:P:74:GLY:N	2.34	0.43
16:P:108:LYS:HA	16:P:111:LYS:HE2	2.00	0.43
16:P:135:LYS:HD3	16:P:151:TYR:CE1	2.52	0.43
18:R:268:ALA:O	18:R:272:VAL:HB	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:467:ARG:HB3	18:R:610:LEU:HD13	2.01	0.43
20:X:4:DT:H2"	20:X:5:DC:OP2	2.17	0.43
1:A:239:CYS:O	1:A:242:LEU:N	2.51	0.43
2:B:184:TYR:CB	2:B:193:VAL:HG22	2.48	0.43
2:B:416:TYR:C	2:B:418:ALA:H	2.26	0.43
2:B:622:VAL:HG22	2:B:645:LEU:HD23	2.00	0.43
2:B:714:ALA:O	2:B:717:GLN:HB2	2.18	0.43
5:E:50:MET:HB3	5:E:52:ARG:HH11	1.83	0.43
5:E:53:PRO:HB2	5:E:55:ARG:NH1	2.33	0.43
10:J:2:ILE:C	10:J:53:HIS:NE2	2.76	0.43
11:K:103:ILE:HG12	11:K:105:ILE:HD11	2.00	0.43
13:M:174:GLU:HG2	13:M:175:ARG:CG	2.40	0.43
13:M:246:THR:N	14:N:404:SER:HA	2.27	0.43
14:N:306:VAL:HG23	14:N:415:LYS:HD3	2.00	0.43
14:N:364:ARG:O	14:N:371:LEU:HD12	2.18	0.43
14:N:366:HIS:HB3	14:N:370:LYS:HB2	1.99	0.43
15:O:638:PHE:O	15:O:641:LEU:N	2.51	0.43
16:P:215:TYR:O	16:P:216:SER:OG	2.33	0.43
18:R:282:ASP:OD1	18:R:283:GLY:N	2.51	0.43
19:S:425:MET:HG2	19:S:429:TYR:CE2	2.53	0.43
1:A:46:ARG:NH2	2:B:852:ALA:HB1	2.34	0.43
1:A:329:SER:HB3	1:A:355:GLN:HE21	1.84	0.43
1:A:472:VAL:HG13	1:A:520:HIS:O	2.18	0.43
1:A:476:ARG:HB2	1:A:517:MET:SD	2.59	0.43
1:A:517:MET:O	1:A:518:ASN:OD1	2.37	0.43
1:A:916:TYR:CG	1:A:1083:LEU:HD11	2.54	0.43
1:A:1380:ARG:NH1	1:A:1385:GLN:HE22	2.07	0.43
2:B:128:PRO:CA	2:B:151:ARG:HG2	2.48	0.43
2:B:305:ILE:CG2	2:B:325:GLU:HG2	2.49	0.43
2:B:440:GLY:C	2:B:454:VAL:HG12	2.44	0.43
2:B:566:ARG:HG3	2:B:567:PHE:CD1	2.53	0.43
2:B:838:SER:HA	2:B:873:TYR:O	2.18	0.43
2:B:1047:THR:HB	2:B:1049:GLN:CG	2.47	0.43
8:H:89:LEU:HD23	8:H:90:ALA:HB2	2.01	0.43
8:H:95:TYR:O	8:H:144:ILE:N	2.49	0.43
13:M:96:LEU:H	13:M:101:PRO:CA	2.30	0.43
15:O:53:VAL:HG23	15:O:57:LEU:HB2	2.00	0.43
15:O:190:LEU:O	15:O:194:LEU:N	2.51	0.43
15:O:311:VAL:HG11	15:O:459:ILE:HG21	2.00	0.43
15:O:629:MET:O	15:O:633:ARG:CB	2.66	0.43
16:P:117:HIS:H	16:P:120:VAL:CG2	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:244:CYS:SG	16:P:253:LEU:HD11	2.58	0.43
21:Y:48:DT:H2''	21:Y:49:DA:O4'	2.18	0.43
1:A:106:ILE:HG13	1:A:112:ALA:O	2.18	0.43
1:A:232:LYS:HD3	16:P:315:TRP:CH2	2.48	0.43
1:A:323:VAL:HA	1:A:326:TYR:HB3	2.00	0.43
1:A:327:ILE:O	1:A:354:CYS:N	2.44	0.43
1:A:442:ARG:HA	18:R:29:GLY:O	2.17	0.43
1:A:580:LEU:HB3	11:K:88:PHE:HE2	1.83	0.43
1:A:654:ILE:HA	1:A:660:LEU:HD13	2.00	0.43
1:A:887:ARG:O	1:A:890:MET:HB3	2.19	0.43
1:A:1145:LEU:HG	1:A:1309:VAL:HG12	1.99	0.43
2:B:354:ARG:O	2:B:358:MET:HG3	2.19	0.43
2:B:427:ASN:HA	2:B:430:THR:HB	2.01	0.43
2:B:757:VAL:HG11	2:B:1022:ILE:HD12	2.00	0.43
2:B:801:HIS:CE1	18:R:136:LYS:HD3	2.54	0.43
5:E:2:ASP:O	5:E:6:GLU:HG2	2.19	0.43
7:G:157:ASP:CG	7:G:158:VAL:H	2.25	0.43
16:P:15:ALA:HA	16:P:55:LEU:HD11	2.00	0.43
16:P:128:LEU:HB3	16:P:134:VAL:HG12	2.00	0.43
18:R:127:ALA:HB1	18:R:146:PHE:HE2	1.83	0.43
20:X:19:DA:H4'	20:X:20:DA:OP1	2.19	0.43
21:Y:43:DA:H5'	21:Y:43:DA:H8	1.81	0.43
1:A:653:ILE:O	1:A:660:LEU:HB2	2.18	0.43
2:B:97:ASP:HB3	2:B:132:ASP:HB2	2.00	0.43
4:D:135:TYR:HA	4:D:141:CYS:SG	2.59	0.43
5:E:13:TRP:HD1	5:E:42:PHE:CG	2.36	0.43
9:I:24:LEU:H	9:I:33:PHE:HB3	1.83	0.43
15:O:490:SER:O	15:O:493:GLU:HG2	2.19	0.43
15:O:648:TRP:NE1	15:O:652:GLN:OE1	2.52	0.43
16:P:25:LYS:HG3	16:P:26:GLY:N	2.34	0.43
16:P:31:PHE:CD2	16:P:72:PHE:HB2	2.53	0.43
18:R:442:PHE:HD2	18:R:446:LYS:HB2	1.84	0.43
19:S:418:ASP:HB3	19:S:449:ARG:NH1	2.33	0.43
1:A:114:LEU:HD21	1:A:148:CYS:HB2	2.00	0.43
1:A:308:SER:HA	15:O:534:ARG:HD2	1.99	0.43
1:A:321:LEU:O	1:A:324:ALA:HB3	2.18	0.43
1:A:733:ILE:HD12	1:A:736:HIS:NE2	2.33	0.43
1:A:818:ILE:HD11	1:A:824:PRO:HD2	2.01	0.43
1:A:1173:VAL:HG22	1:A:1186:VAL:HG12	2.01	0.43
1:A:1193:ILE:O	1:A:1197:GLN:HA	2.18	0.43
1:A:1373:ARG:HA	1:A:1376:LEU:HD21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:72:ASP:O	2:B:76:ILE:N	2.46	0.43
2:B:281:ASP:OD1	2:B:282:ILE:HG13	2.19	0.43
2:B:539:GLU:OE2	2:B:565:ILE:HA	2.18	0.43
2:B:721:ILE:HG12	2:B:899:LEU:HD23	2.01	0.43
5:E:82:PHE:HZ	5:E:113:GLN:HA	1.84	0.43
6:F:79:ARG:NH1	6:F:144:GLU:OE2	2.39	0.43
15:O:201:ILE:HA	15:O:280:LEU:HD23	2.00	0.43
15:O:253:ILE:O	15:O:256:PRO:HD2	2.19	0.43
16:P:313:ASP:C	16:P:315:TRP:N	2.72	0.43
17:Q:48:THR:O	17:Q:51:GLU:HB3	2.19	0.43
18:R:273:GLN:H	18:R:273:GLN:CD	2.26	0.43
18:R:275:PHE:HB2	18:R:278:ASN:OD1	2.19	0.43
20:X:24:DT:H2''	20:X:25:DT:C6	2.54	0.43
1:A:18:PHE:CD1	2:B:1139:PRO:CB	3.02	0.43
1:A:32:VAL:C	1:A:83:HIS:CE1	2.97	0.43
1:A:101:GLN:O	1:A:104:GLN:N	2.49	0.43
1:A:448:ASP:O	1:A:450:MET:HE2	2.19	0.43
1:A:487:SER:OG	1:A:536:GLY:HA2	2.19	0.43
1:A:571:TYR:HD1	1:A:575:THR:HG21	1.84	0.43
1:A:770:LEU:HD22	1:A:847:PHE:CE1	2.53	0.43
1:A:890:MET:O	1:A:894:GLU:N	2.52	0.43
1:A:974:LEU:HD21	1:A:998:TYR:CB	2.47	0.43
1:A:998:TYR:O	1:A:1002:ARG:HG3	2.18	0.43
1:A:1004:PHE:CZ	1:A:1078:TYR:HB2	2.54	0.43
1:A:1029:LEU:HD12	1:A:1029:LEU:O	2.19	0.43
2:B:204:ARG:HH21	2:B:558:ASN:HA	1.84	0.43
2:B:264:SER:C	2:B:266:LEU:N	2.76	0.43
2:B:297:THR:OG1	2:B:302:LEU:HG	2.19	0.43
2:B:1055:SER:O	2:B:1056:ARG:C	2.62	0.43
3:C:1:MET:N	3:C:14:ASN:HD21	2.17	0.43
3:C:116:VAL:CA	3:C:130:ASN:HD21	2.32	0.43
5:E:14:ARG:HG3	5:E:141:VAL:O	2.19	0.43
5:E:55:ARG:HD2	5:E:82:PHE:CE2	2.53	0.43
7:G:2:PHE:N	7:G:77:PHE:HA	2.34	0.43
7:G:130:TRP:HB2	7:G:137:LYS:N	2.34	0.43
8:H:7:ASP:OD1	8:H:7:ASP:O	2.36	0.43
9:I:18:ASP:O	9:I:19:SER:OG	2.29	0.43
11:K:77:ARG:HG3	11:K:78:TYR:N	2.33	0.43
11:K:85:ASP:C	11:K:107:THR:HG1	2.17	0.43
12:L:61:THR:OG1	12:L:62:LYS:N	2.52	0.43
16:P:63:LEU:HD11	16:P:70:LEU:HD13	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:139:SER:OG	16:P:140:VAL:N	2.51	0.43
16:P:221:ILE:HG21	16:P:240:ILE:HD12	2.01	0.43
18:R:213:TRP:HZ2	18:R:496:ILE:O	2.01	0.43
18:R:497:ARG:HD3	18:R:565:LYS:HE2	2.01	0.43
19:S:420:TRP:HE3	19:S:424:GLU:HG2	1.84	0.43
20:X:58:DC:C4	20:X:59:DC:N4	2.86	0.43
21:Y:23:DG:C2	21:Y:24:DT:C2	3.07	0.43
1:A:57:LYS:HA	1:A:67:CYS:O	2.18	0.42
1:A:305:LYS:HG3	1:A:306:GLY:N	2.34	0.42
2:B:281:ASP:OD1	2:B:281:ASP:N	2.50	0.42
2:B:405:LYS:HA	2:B:408:LYS:HG3	2.01	0.42
2:B:857:PRO:HB3	18:R:107:TRP:HH2	1.84	0.42
2:B:961:LEU:HD21	2:B:1019:PHE:C	2.44	0.42
2:B:1121:ILE:HG12	2:B:1125:ALA:HB3	2.01	0.42
3:C:67:PHE:O	3:C:71:MET:CB	2.67	0.42
4:D:29:TRP:HB3	4:D:33:SER:OG	2.19	0.42
5:E:60:PHE:CZ	5:E:80:VAL:HG11	2.54	0.42
5:E:156:LEU:HD21	5:E:195:VAL:HG12	2.01	0.42
6:F:151:LEU:HD23	6:F:152:ILE:N	2.34	0.42
9:I:5:CYS:CB	9:I:10:ASN:H	2.31	0.42
13:M:131:TYR:OH	13:M:136:ALA:HB2	2.19	0.42
13:M:135:LYS:NZ	13:M:140:TRP:HZ2	2.17	0.42
13:M:135:LYS:O	13:M:138:SER:OG	2.24	0.42
15:O:240:GLN:HG2	15:O:244:ASN:OD1	2.18	0.42
15:O:583:TRP:CZ2	16:P:312:PHE:C	2.97	0.42
15:O:588:LEU:CD1	15:O:637:VAL:HG23	2.49	0.42
1:A:16:LEU:HD11	1:A:1417:LEU:HD11	2.01	0.42
1:A:36:THR:OG1	1:A:52:GLY:HA2	2.19	0.42
1:A:76:SER:OG	1:A:77:CYS:N	2.52	0.42
1:A:204:VAL:CG2	15:O:516:LEU:O	2.66	0.42
1:A:235:LYS:HD3	1:A:235:LYS:HA	1.77	0.42
1:A:1124:PRO:HA	1:A:1127:LYS:HD3	2.01	0.42
2:B:392:PHE:O	2:B:395:PHE:HB3	2.20	0.42
2:B:417:ASP:OD1	2:B:418:ALA:N	2.52	0.42
2:B:441:ASN:HD22	2:B:452:ALA:HA	1.84	0.42
2:B:503:PRO:HG2	2:B:511:VAL:HG21	2.01	0.42
2:B:908:LEU:HD13	2:B:923:GLY:C	2.44	0.42
5:E:97:VAL:O	5:E:100:ILE:HB	2.19	0.42
6:F:92:ARG:HH12	7:G:61:PRO:HB3	1.83	0.42
7:G:203:ASP:O	7:G:205:MET:HG2	2.18	0.42
8:H:112:ILE:N	8:H:127:GLY:O	2.43	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:41:LEU:HD23	10:J:47:ARG:HA	2.01	0.42
11:K:48:LYS:HE2	11:K:64:GLN:NE2	2.34	0.42
11:K:110:GLU:O	11:K:111:THR:C	2.62	0.42
13:M:254:GLN:NE2	14:N:302:GLU:OE2	2.52	0.42
15:O:132:TYR:O	15:O:133:SER:C	2.62	0.42
15:O:159:ILE:HD13	15:O:174:TYR:OH	2.19	0.42
15:O:163:VAL:HA	15:O:169:LEU:HD13	2.01	0.42
15:O:196:GLU:HG3	15:O:197:MET:N	2.34	0.42
15:O:312:TYR:CD1	15:O:468:LEU:HD21	2.54	0.42
15:O:503:SER:O	15:O:506:ARG:HG2	2.19	0.42
16:P:126:LYS:O	16:P:129:GLU:HB3	2.19	0.42
1:A:444:LEU:CD2	1:A:449:ARG:CD	2.81	0.42
1:A:912:VAL:HG23	1:A:913:GLN:H	1.83	0.42
1:A:956:PRO:HG2	1:A:1031:LEU:HD21	2.01	0.42
1:A:998:TYR:O	1:A:1002:ARG:N	2.34	0.42
2:B:1130:GLN:O	2:B:1134:SER:N	2.48	0.42
3:C:103:LEU:HD22	10:J:5:VAL:CG2	2.48	0.42
3:C:278:GLU:OE1	3:C:278:GLU:N	2.52	0.42
7:G:142:VAL:C	7:G:144:GLU:H	2.26	0.42
15:O:46:LEU:O	15:O:49:TYR:N	2.51	0.42
15:O:156:VAL:HA	15:O:159:ILE:CG1	2.49	0.42
15:O:199:TYR:CD2	15:O:200:LEU:CB	2.99	0.42
15:O:364:ILE:HA	15:O:476:TYR:CE2	2.54	0.42
16:P:177:SER:O	16:P:181:ILE:HG12	2.19	0.42
18:R:289:SER:HB2	18:R:535:SER:HB3	2.00	0.42
21:Y:18:DC:H1'	21:Y:19:DT:C2	2.54	0.42
21:Y:25:DC:C2	21:Y:26:DA:N7	2.88	0.42
1:A:314:GLU:OE1	1:A:314:GLU:N	2.47	0.42
1:A:347:VAL:C	1:A:349:PRO:HD2	2.42	0.42
1:A:717:VAL:HG21	2:B:958:MET:HE1	2.00	0.42
1:A:723:LEU:O	1:A:727:LYS:HB3	2.19	0.42
1:A:905:ARG:HA	1:A:910:GLY:O	2.19	0.42
1:A:1122:GLY:C	1:A:1124:PRO:HD2	2.43	0.42
2:B:82:LEU:HD21	2:B:94:LYS:HE2	2.01	0.42
2:B:471:THR:HG23	2:B:514:LEU:HD12	2.01	0.42
2:B:566:ARG:HG3	2:B:567:PHE:CG	2.54	0.42
2:B:667:VAL:HB	2:B:670:MET:HG3	2.01	0.42
2:B:785:CYS:O	2:B:903:ASN:HA	2.20	0.42
3:C:117:ASP:HB2	3:C:120:LEU:HD21	1.94	0.42
6:F:135:ARG:HH12	7:G:58:GLN:NE2	2.16	0.42
7:G:98:LYS:HB2	7:G:109:PHE:HD1	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:156:VAL:HG23	7:G:193:ALA:HA	2.00	0.42
8:H:61:SER:OG	8:H:139:ASN:ND2	2.52	0.42
15:O:365:ASP:H	15:O:476:TYR:HH	1.60	0.42
15:O:497:ALA:HB3	16:P:296:TYR:CE2	2.54	0.42
15:O:595:LEU:CD2	15:O:633:ARG:HG2	2.49	0.42
15:O:630:VAL:O	15:O:633:ARG:HB3	2.20	0.42
16:P:128:LEU:O	16:P:132:ARG:N	2.51	0.42
17:Q:1079:UNK:O	17:Q:1083:UNK:N	2.52	0.42
18:R:161:PHE:O	18:R:165:VAL:HG23	2.20	0.42
18:R:470:GLN:NE2	18:R:477:LYS:HA	2.34	0.42
18:R:583:HIS:HE1	18:R:587:THR:HG22	1.84	0.42
21:Y:26:DA:H2"	21:Y:27:DC:C6	2.55	0.42
1:A:378:ARG:HG3	2:B:1060:LEU:CD1	2.38	0.42
1:A:573:ARG:O	1:A:577:THR:OG1	2.21	0.42
1:A:668:VAL:HG23	1:A:669:LEU:H	1.85	0.42
1:A:880:ALA:HA	21:Y:22:DT:C2	2.54	0.42
1:A:1145:LEU:HD11	1:A:1157:VAL:CG2	2.47	0.42
1:A:1302:ASP:OD1	1:A:1302:ASP:N	2.52	0.42
2:B:798:TYR:O	18:R:99:TYR:OH	2.37	0.42
2:B:860:VAL:HG13	2:B:861:ASN:N	2.33	0.42
2:B:877:GLU:HG2	2:B:878:PRO:O	2.19	0.42
3:C:3:ASN:HD22	3:C:296:ASN:ND2	2.18	0.42
5:E:85:GLU:CD	5:E:86:PRO:HD2	2.45	0.42
7:G:68:ILE:HG22	7:G:70:VAL:HG13	2.01	0.42
8:H:26:ILE:HG23	8:H:40:LEU:HB3	2.02	0.42
8:H:131:ASN:CA	8:H:134:ASN:HD22	2.32	0.42
10:J:24:LEU:O	10:J:24:LEU:HD23	2.19	0.42
13:M:183:PHE:HB3	13:M:185:TYR:HB2	2.00	0.42
15:O:61:ALA:HA	15:O:94:THR:HG22	2.01	0.42
15:O:200:LEU:HD21	15:O:282:ILE:CD1	2.50	0.42
18:R:149:ARG:HG2	18:R:149:ARG:HH11	1.84	0.42
18:R:470:GLN:OE1	18:R:602:LEU:HD22	2.19	0.42
1:A:611:SER:OG	1:A:658:GLN:HA	2.19	0.42
1:A:912:VAL:HG23	1:A:913:GLN:N	2.35	0.42
1:A:933:VAL:HG12	1:A:935:PHE:N	2.34	0.42
1:A:1086:GLY:O	1:A:1424:GLY:HA2	2.18	0.42
1:A:1207:VAL:O	1:A:1211:ARG:HG2	2.19	0.42
3:C:101:ILE:HD12	3:C:101:ILE:H	1.85	0.42
3:C:113:LEU:HD11	3:C:132:ILE:HD11	2.02	0.42
4:D:130:ASN:HA	4:D:154:LEU:HD11	2.02	0.42
8:H:99:GLY:HA3	8:H:118:PHE:HD1	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:6:ARG:HD3	10:J:11:GLY:C	2.44	0.42
13:M:144:ASN:CG	13:M:145:VAL:H	2.27	0.42
14:N:313:LEU:HD22	14:N:318:ARG:HE	1.85	0.42
14:N:315:ALA:CB	14:N:375:ILE:HG22	2.49	0.42
15:O:288:MET:HA	15:O:291:ARG:NE	2.34	0.42
15:O:478:VAL:HG12	15:O:479:PRO:O	2.20	0.42
16:P:62:LYS:HD3	16:P:83:LYS:HE2	2.01	0.42
17:Q:48:THR:O	17:Q:52:ARG:N	2.42	0.42
17:Q:1076:UNK:O	17:Q:1078:UNK:N	2.52	0.42
18:R:135:ARG:NH2	18:R:174:PRO:O	2.53	0.42
18:R:147:SER:C	18:R:152:VAL:HG11	2.44	0.42
18:R:434:GLU:HA	18:R:435:PRO:HA	1.85	0.42
21:Y:42:DT:H2'	21:Y:43:DA:C8	2.55	0.42
1:A:18:PHE:CE1	2:B:1139:PRO:CA	3.02	0.42
1:A:25:ASP:HA	1:A:28:ALA:HB3	2.01	0.42
1:A:591:ASP:OD1	1:A:591:ASP:N	2.52	0.42
1:A:988:ASP:OD2	1:A:994:TYR:N	2.42	0.42
1:A:1027:GLY:C	1:A:1028:MET:HE2	2.44	0.42
1:A:1319:VAL:HA	1:A:1322:VAL:HG23	2.01	0.42
1:A:1328:ILE:O	1:A:1331:ALA:N	2.52	0.42
2:B:287:LEU:O	2:B:291:SER:N	2.48	0.42
2:B:956:GLY:O	2:B:960:GLU:HB2	2.20	0.42
3:C:21:PRO:HD3	3:C:29:ASN:O	2.20	0.42
4:D:126:GLN:HG2	7:G:84:ILE:O	2.20	0.42
6:F:143:PHE:CG	6:F:144:GLU:N	2.88	0.42
7:G:3:ILE:HG12	7:G:78:LYS:HB3	2.00	0.42
8:H:95:TYR:HB3	8:H:144:ILE:HB	2.01	0.42
10:J:17:LYS:HD3	10:J:39:LEU:CD2	2.49	0.42
12:L:29:TYR:HB2	12:L:57:LEU:O	2.19	0.42
13:M:227:LEU:HG	13:M:232:LEU:HA	2.00	0.42
15:O:55:ALA:CB	15:O:593:GLU:HG3	2.50	0.42
15:O:312:TYR:CZ	15:O:316:LEU:HD11	2.54	0.42
15:O:553:ARG:HB3	15:O:562:ALA:HA	2.02	0.42
15:O:554:THR:HG23	15:O:561:ARG:HD2	2.02	0.42
16:P:59:ASN:OD1	16:P:80:ALA:HB1	2.20	0.42
21:Y:20:DT:H2'	21:Y:21:DG:C4	2.55	0.42
21:Y:38:DA:C6	21:Y:39:DA:N6	2.88	0.42
1:A:332:VAL:HG13	1:A:333:ASN:N	2.35	0.42
1:A:481:HIS:NE2	1:A:483:LEU:HB2	2.35	0.42
1:A:792:LEU:C	1:A:794:MET:H	2.28	0.42
1:A:919:ASP:CG	1:A:921:LEU:HB2	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1279:SER:HB2	1:A:1296:GLU:HB2	2.02	0.42
1:A:1310:ILE:HG12	1:A:1312:SER:H	1.84	0.42
2:B:232:TYR:CD2	2:B:233:VAL:N	2.87	0.42
2:B:263:LEU:HD21	2:B:296:TYR:HE1	1.84	0.42
2:B:401:LEU:HA	2:B:404:ASP:OD2	2.20	0.42
2:B:401:LEU:O	2:B:404:ASP:HB2	2.20	0.42
2:B:568:PRO:O	2:B:572:VAL:HG23	2.19	0.42
2:B:591:TYR:CD2	2:B:652:ASN:HB3	2.55	0.42
2:B:723:THR:HG23	2:B:724:LEU:N	2.35	0.42
2:B:780:ARG:HE	3:C:217:ALA:CB	2.32	0.42
2:B:961:LEU:HD22	2:B:1018:PHE:CE1	2.54	0.42
2:B:969:LEU:C	2:B:971:GLY:N	2.77	0.42
2:B:1038:ARG:HD2	2:B:1058:GLY:C	2.45	0.42
3:C:103:LEU:HD21	10:J:6:ARG:HD2	2.00	0.42
3:C:128:ASP:HB3	3:C:129:GLU:OE1	2.19	0.42
5:E:170:LEU:HB3	5:E:174:GLN:HE21	1.85	0.42
8:H:128:ASN:OD1	8:H:129:TYR:N	2.48	0.42
9:I:9:ASN:ND2	13:M:91:ALA:O	2.53	0.42
11:K:110:GLU:OE2	11:K:111:THR:OG1	2.36	0.42
13:M:236:VAL:O	13:M:240:GLU:N	2.47	0.42
15:O:131:LEU:HD12	15:O:132:TYR:N	2.35	0.42
15:O:455:SER:O	15:O:458:LYS:HB2	2.20	0.42
15:O:471:THR:HA	15:O:477:TYR:HB3	2.00	0.42
16:P:98:GLU:HB3	16:P:150:LEU:HD21	2.01	0.42
19:S:418:ASP:C	19:S:449:ARG:HH12	2.21	0.42
1:A:474:PHE:CZ	1:A:517:MET:HG3	2.55	0.42
1:A:548:GLU:OE2	1:A:672:GLY:N	2.52	0.42
1:A:553:ALA:HB1	1:A:557:PHE:HB2	2.02	0.42
1:A:600:PRO:HB2	8:H:46:LEU:HD23	2.01	0.42
1:A:897:SER:O	1:A:904:VAL:HG23	2.20	0.42
1:A:956:PRO:CG	1:A:1031:LEU:HD11	2.48	0.42
2:B:831:GLU:HG3	2:B:832:VAL:O	2.19	0.42
2:B:1001:LYS:HE3	2:B:1016:TYR:HB2	2.01	0.42
3:C:96:VAL:O	3:C:100:ARG:HG2	2.20	0.42
3:C:195:LYS:HD2	10:J:57:ILE:HG21	2.02	0.42
4:D:58:ILE:HD13	7:G:46:ILE:HG23	2.01	0.42
7:G:104:ILE:HG23	7:G:105:PHE:N	2.30	0.42
13:M:159:TYR:HB3	13:M:170:LEU:HD21	2.01	0.42
15:O:98:LEU:O	15:O:102:ARG:N	2.53	0.42
15:O:200:LEU:HB3	15:O:280:LEU:C	2.41	0.42
15:O:266:ASP:HA	15:O:272:ARG:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:235:LEU:CD2	16:P:239:ASN:HB3	2.48	0.42
18:R:84:ARG:HD2	18:R:88:ARG:NH2	2.34	0.42
18:R:87:LEU:HD12	18:R:126:ILE:HD11	2.02	0.42
18:R:215:PHE:CD1	18:R:223:ILE:HD13	2.51	0.42
18:R:511:TYR:CE2	18:R:513:PRO:HA	2.55	0.42
21:Y:27:DC:H1'	21:Y:28:DT:H5'	2.02	0.42
1:A:296:SER:O	1:A:299:ILE:N	2.53	0.42
1:A:314:GLU:O	1:A:318:TYR:N	2.30	0.42
1:A:386:ASN:HA	1:A:699:LYS:HG2	2.01	0.42
1:A:467:GLU:OE1	1:A:467:GLU:N	2.53	0.42
1:A:481:HIS:HA	1:A:1095:GLN:OE1	2.20	0.42
1:A:898:CYS:O	1:A:1086:GLY:N	2.38	0.42
1:A:984:VAL:HG21	1:A:988:ASP:HB3	2.02	0.42
1:A:1023:ARG:HG2	1:A:1028:MET:HB2	2.02	0.42
2:B:118:CYS:SG	2:B:123:MET:HB2	2.60	0.42
2:B:376:ARG:HE	2:B:607:ARG:NH1	2.18	0.42
2:B:504:GLU:C	2:B:506:GLU:H	2.28	0.42
2:B:587:PHE:HD1	2:B:588:ILE:H	1.68	0.42
2:B:588:ILE:HA	2:B:602:ALA:O	2.20	0.42
2:B:637:PHE:C	2:B:639:ASP:H	2.27	0.42
2:B:760:MET:O	2:B:946:PRO:HD3	2.19	0.42
2:B:784:ARG:HA	2:B:906:PRO:HD3	2.00	0.42
2:B:1045:VAL:HA	18:R:37:ILE:CG2	2.48	0.42
3:C:117:ASP:CG	3:C:120:LEU:CD2	2.91	0.42
3:C:256:ILE:HB	3:C:266:TYR:O	2.20	0.42
3:C:316:LYS:O	3:C:319:ARG:N	2.53	0.42
6:F:89:GLU:OE1	6:F:90:ARG:N	2.53	0.42
7:G:41:ASN:HA	7:G:155:PHE:CD2	2.55	0.42
15:O:159:ILE:HG13	15:O:188:SER:CB	2.50	0.42
18:R:501:LEU:HG	18:R:505:HIS:HD2	1.85	0.42
1:A:96:PHE:HZ	1:A:166:LYS:HG3	1.84	0.41
1:A:106:ILE:HD13	1:A:234:ILE:HG12	2.02	0.41
1:A:150:LYS:O	1:A:152:ARG:NH1	2.53	0.41
1:A:299:ILE:O	1:A:303:LEU:HB3	2.20	0.41
1:A:716:ASP:HB3	1:A:791:PRO:HD3	2.01	0.41
1:A:792:LEU:C	1:A:794:MET:N	2.78	0.41
1:A:809:MET:O	1:A:851:SER:HB3	2.20	0.41
1:A:978:ASP:HB3	1:A:982:CYS:HB2	2.01	0.41
1:A:1077:LYS:O	1:A:1081:ALA:N	2.49	0.41
2:B:265:ASP:N	2:B:268:ILE:HD12	2.32	0.41
2:B:276:ASP:HA	2:B:280:GLN:NE2	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:328:ALA:HB1	2:B:332:ILE:HG23	2.02	0.41
2:B:385:SER:O	2:B:386:LEU:C	2.62	0.41
3:C:33:VAL:C	3:C:35:LYS:N	2.78	0.41
3:C:43:ASN:O	3:C:54:PHE:HB2	2.19	0.41
3:C:230:LEU:HD13	3:C:297:HIS:CE1	2.55	0.41
3:C:239:ILE:O	3:C:244:ALA:HB2	2.19	0.41
5:E:21:GLU:OE2	5:E:143:ASN:ND2	2.53	0.41
5:E:123:LEU:HG	5:E:125:PRO:HD2	2.01	0.41
8:H:116:TYR:HB3	8:H:118:PHE:CE1	2.54	0.41
12:L:65:VAL:HG22	12:L:66:GLN:N	2.34	0.41
13:M:131:TYR:OH	13:M:143:VAL:N	2.53	0.41
13:M:257:ASP:HA	13:M:260:VAL:HG22	2.01	0.41
15:O:482:LYS:HG2	15:O:486:VAL:HG13	2.01	0.41
15:O:568:CYS:SG	15:O:569:LYS:N	2.93	0.41
15:O:620:LEU:O	15:O:624:LEU:HD13	2.20	0.41
16:P:62:LYS:HB2	16:P:73:GLN:HG2	2.02	0.41
18:R:132:VAL:HG12	18:R:161:PHE:CE1	2.52	0.41
18:R:257:GLN:O	18:R:261:GLU:HB2	2.19	0.41
18:R:417:ASN:ND2	18:R:431:ARG:O	2.53	0.41
1:A:193:GLU:HA	1:A:196:ILE:HB	2.01	0.41
1:A:535:MET:HE3	2:B:1073:TYR:CD2	2.55	0.41
1:A:540:ASN:OD1	2:B:1073:TYR:CE1	2.73	0.41
1:A:617:ASN:O	1:A:620:SER:OG	2.20	0.41
1:A:721:ASP:CG	1:A:722:ASP:H	2.28	0.41
1:A:864:HIS:HE2	2:B:695:GLN:HB2	1.85	0.41
1:A:1260:MET:HA	1:A:1263:LEU:HD12	2.02	0.41
1:A:1333:TYR:HE1	5:E:202:SER:HB2	1.85	0.41
1:A:1378:LYS:HG3	1:A:1379:MET:N	2.17	0.41
2:B:66:ASN:O	2:B:69:VAL:HG22	2.19	0.41
2:B:125:TYR:HB3	2:B:186:ILE:HG23	2.01	0.41
2:B:593:ASN:ND2	2:B:596:GLN:HB3	2.35	0.41
2:B:612:LEU:CD1	2:B:672:HIS:HB3	2.50	0.41
2:B:613:ILE:HG13	2:B:675:ILE:HG22	2.02	0.41
2:B:733:GLN:HG3	10:J:54:VAL:HG13	2.01	0.41
2:B:1054:ARG:C	2:B:1055:SER:HG	2.18	0.41
4:D:134:LEU:HD12	4:D:135:TYR:N	2.34	0.41
5:E:155:ARG:HB2	5:E:188:LEU:CD2	2.48	0.41
7:G:138:LEU:H	7:G:210:TRP:HZ2	1.68	0.41
13:M:89:GLN:HG3	13:M:178:GLN:OE1	2.20	0.41
13:M:247:TRP:HA	14:N:406:ALA:HB3	2.01	0.41
14:N:311:THR:O	14:N:314:PRO:HD3	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:464:ASN:HA	15:O:469:ASN:ND2	2.34	0.41
15:O:632:GLU:HA	15:O:635:LEU:HD12	2.01	0.41
1:A:13:ILE:H	1:A:13:ILE:HD12	1.84	0.41
1:A:507:PRO:HG3	1:A:550:ILE:HG23	2.01	0.41
1:A:565:SER:HB2	1:A:664:MET:HE2	2.02	0.41
1:A:940:ASP:O	1:A:943:TYR:N	2.53	0.41
1:A:1202:ILE:HD13	1:A:1224:ILE:HD12	2.02	0.41
2:B:540:ASP:OD1	2:B:541:ILE:HG22	2.19	0.41
2:B:758:ALA:HA	2:B:1019:PHE:CB	2.50	0.41
2:B:846:SER:OG	2:B:866:TYR:HB3	2.20	0.41
2:B:932:PRO:HG3	2:B:1004:LEU:HD13	2.02	0.41
3:C:55:ASP:OD2	3:C:297:HIS:NE2	2.53	0.41
4:D:17:LEU:HD13	4:D:62:VAL:HG12	2.03	0.41
4:D:127:LEU:O	4:D:129:ALA:N	2.47	0.41
13:M:106:PHE:CG	13:M:107:ILE:N	2.88	0.41
15:O:203:ILE:HG22	15:O:207:HIS:CD2	2.53	0.41
16:P:111:LYS:O	16:P:115:ASN:N	2.52	0.41
18:R:14:ARG:CZ	18:R:23:LEU:HB2	2.50	0.41
18:R:492:VAL:HG22	18:R:536:GLY:HA3	2.03	0.41
21:Y:53:DT:C2	21:Y:54:DA:C8	3.09	0.41
1:A:163:VAL:O	1:A:180:HIS:HA	2.21	0.41
1:A:232:LYS:HA	1:A:254:GLU:OE2	2.21	0.41
1:A:409:THR:O	1:A:410:ARG:C	2.63	0.41
1:A:574:ALA:O	1:A:577:THR:HB	2.19	0.41
1:A:716:ASP:CG	1:A:790:ALA:H	2.28	0.41
1:A:943:TYR:O	1:A:947:PHE:HB2	2.20	0.41
1:A:1079:ARG:HH21	6:F:83:PRO:HD2	1.85	0.41
1:A:1373:ARG:HA	1:A:1376:LEU:CG	2.50	0.41
1:A:1376:LEU:HG	1:A:1376:LEU:H	1.64	0.41
2:B:330:THR:HA	2:B:345:LYS:HE3	2.02	0.41
2:B:579:ARG:HA	2:B:583:LYS:O	2.19	0.41
2:B:914:SER:CB	2:B:918:GLN:HB2	2.50	0.41
4:D:58:ILE:H	4:D:58:ILE:HG13	1.69	0.41
7:G:111:PRO:HD2	7:G:198:GLY:H	1.85	0.41
10:J:6:ARG:HA	10:J:14:VAL:HG23	2.02	0.41
15:O:222:HIS:CE1	15:O:244:ASN:HB3	2.56	0.41
15:O:580:ASN:O	15:O:583:TRP:HB3	2.20	0.41
16:P:151:TYR:CZ	18:R:650:ALA:HB3	2.56	0.41
18:R:214:MET:HE1	18:R:286:ARG:C	2.45	0.41
18:R:623:LYS:HZ3	19:S:435:TRP:HB3	1.84	0.41
20:X:48:DT:O4	20:X:49:DA:N6	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:HIS:ND1	2:B:1090:PHE:HZ	2.19	0.41
1:A:89:PRO:HG3	1:A:225:LEU:HA	2.01	0.41
1:A:252:ARG:C	1:A:254:GLU:H	2.27	0.41
1:A:401:VAL:O	2:B:1039:ALA:HB2	2.21	0.41
1:A:454:LYS:HE3	1:A:454:LYS:HB3	1.81	0.41
1:A:542:LEU:HG	1:A:548:GLU:C	2.45	0.41
1:A:609:VAL:HG13	1:A:610:PHE:H	1.85	0.41
1:A:869:ARG:NH2	2:B:700:THR:OG1	2.53	0.41
1:A:1143:ALA:HA	1:A:1314:THR:HG22	2.02	0.41
2:B:64:SER:HB3	2:B:381:GLY:H	1.84	0.41
2:B:241:TYR:HE1	2:B:252:PRO:HG3	1.86	0.41
2:B:319:ILE:HD11	13:M:231:LEU:HD22	2.02	0.41
5:E:13:TRP:CD2	5:E:39:LEU:HD13	2.56	0.41
7:G:38:ILE:HG13	7:G:44:LEU:HB3	2.02	0.41
7:G:52:LEU:HD12	7:G:53:THR:HG22	2.01	0.41
10:J:16:ASP:CG	10:J:17:LYS:HG3	2.46	0.41
14:N:280:LEU:HA	14:N:283:LEU:HD12	2.01	0.41
15:O:87:ASP:O	15:O:89:ASP:N	2.52	0.41
15:O:104:VAL:CA	15:O:123:ASN:H	2.28	0.41
15:O:190:LEU:HA	15:O:193:GLN:HB2	2.03	0.41
15:O:200:LEU:CD2	15:O:281:THR:CA	2.77	0.41
16:P:154:GLN:N	16:P:155:PRO:HD3	2.35	0.41
16:P:201:GLY:HA2	16:P:204:LYS:HE2	2.02	0.41
18:R:274:LYS:HB3	18:R:275:PHE:H	1.71	0.41
18:R:274:LYS:HD3	19:S:277:UNK:N	2.34	0.41
21:Y:42:DT:C4	21:Y:43:DA:N6	2.88	0.41
1:A:123:PHE:CG	1:A:144:ILE:HD13	2.56	0.41
1:A:676:SER:HB2	1:A:679:TYR:CB	2.50	0.41
1:A:935:PHE:HB3	1:A:1011:TYR:CE2	2.55	0.41
1:A:962:THR:O	1:A:965:GLU:HB3	2.20	0.41
2:B:276:ASP:OD1	2:B:280:GLN:NE2	2.52	0.41
2:B:649:LEU:HD22	2:B:653:GLU:CD	2.46	0.41
2:B:813:GLU:C	2:B:815:GLY:N	2.77	0.41
2:B:916:HIS:CE1	2:B:956:GLY:HA3	2.56	0.41
8:H:18:GLY:O	8:H:20:TYR:N	2.53	0.41
8:H:65:LEU:HA	8:H:89:LEU:HD12	2.02	0.41
8:H:83:GLN:HB3	8:H:84:ALA:H	1.62	0.41
12:L:31:CYS:CB	12:L:34:CYS:HB2	2.51	0.41
13:M:90:TYR:HD1	13:M:92:ASN:H	1.68	0.41
13:M:158:GLN:C	13:M:173:ILE:HD12	2.45	0.41
15:O:68:LEU:HD21	15:O:121:TYR:C	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:199:TYR:CE2	15:O:200:LEU:CB	2.91	0.41
15:O:325:LYS:HG3	15:O:326:ILE:HG12	2.03	0.41
15:O:528:MET:HB2	15:O:533:ILE:HD11	2.02	0.41
15:O:623:GLU:O	15:O:627:LEU:HG	2.20	0.41
16:P:205:ASN:O	16:P:210:PRO:HD3	2.21	0.41
20:X:3:DT:H2''	20:X:4:DT:C6	2.56	0.41
1:A:92:HIS:CE1	1:A:95:TYR:H	2.38	0.41
1:A:311:ASN:HA	1:A:314:GLU:OE2	2.21	0.41
1:A:668:VAL:HG23	1:A:669:LEU:N	2.36	0.41
1:A:830:ARG:NH2	1:A:833:PRO:O	2.54	0.41
1:A:994:TYR:C	5:E:197:LYS:HZ1	2.28	0.41
1:A:1371:ILE:O	1:A:1371:ILE:HG22	2.21	0.41
2:B:48:LEU:HG	2:B:517:MET:SD	2.60	0.41
2:B:287:LEU:HA	2:B:290:SER:HB3	2.03	0.41
2:B:532:LEU:O	2:B:535:VAL:HB	2.20	0.41
2:B:639:ASP:OD1	2:B:643:LEU:HD13	2.20	0.41
4:D:14:TYR:CZ	4:D:103:PHE:HB2	2.55	0.41
4:D:65:TYR:OH	4:D:69:ASN:ND2	2.54	0.41
5:E:64:PRO:HD3	5:E:77:SER:CA	2.47	0.41
6:F:135:ARG:NE	6:F:143:PHE:CE1	2.89	0.41
7:G:97:ILE:HD13	7:G:140:PHE:CZ	2.55	0.41
10:J:31:ASP:HB2	10:J:34:THR:OG1	2.21	0.41
11:K:63:PHE:HB2	11:K:103:ILE:HG23	2.01	0.41
13:M:174:GLU:CG	13:M:175:ARG:N	2.63	0.41
15:O:51:GLU:OE2	15:O:590:PHE:HA	2.21	0.41
16:P:52:VAL:HG13	16:P:61:ILE:HD11	2.03	0.41
18:R:136:LYS:HE2	18:R:173:LEU:CD1	2.47	0.41
18:R:460:LEU:CD2	18:R:464:LYS:HE2	2.51	0.41
18:R:533:PHE:CZ	21:Y:51:DT:H1'	2.56	0.41
18:R:549:ILE:O	18:R:553:PHE:HB2	2.20	0.41
20:X:61:DT:C2	21:Y:3:DA:C2	3.09	0.41
21:Y:35:DG:H1'	21:Y:36:DA:H5'	2.02	0.41
21:Y:56:DG:C4	21:Y:57:DT:C4	3.09	0.41
1:A:301:ALA:O	1:A:304:ASP:HB3	2.21	0.41
1:A:585:ASP:OD1	1:A:585:ASP:N	2.54	0.41
3:C:117:ASP:HB3	3:C:120:LEU:HD11	2.02	0.41
4:D:126:GLN:NE2	7:G:85:VAL:HA	2.35	0.41
7:G:9:ASP:OD2	7:G:33:LYS:HE2	2.20	0.41
7:G:49:TYR:HB2	7:G:75:VAL:CG2	2.50	0.41
12:L:33:GLU:HG3	12:L:53:HIS:CE1	2.56	0.41
13:M:87:VAL:HG13	13:M:176:VAL:HG13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:352:VAL:HG13	15:O:353:GLU:HG2	2.02	0.41
15:O:519:GLU:HG2	15:O:520:LYS:N	2.36	0.41
16:P:48:LEU:HA	16:P:51:ILE:HG22	2.01	0.41
18:R:1:MET:N	18:R:2:PRO:HD2	2.36	0.41
18:R:468:ILE:O	18:R:472:ILE:N	2.41	0.41
18:R:516:PHE:CB	20:X:13:DA:H5'	2.49	0.41
21:Y:6:DG:C6	21:Y:7:DA:C6	3.08	0.41
21:Y:15:DT:C4	21:Y:16:DA:N6	2.89	0.41
21:Y:50:DA:H2'	21:Y:51:DT:C2	2.56	0.41
21:Y:58:DT:C4'	21:Y:59:DG:H5'	2.50	0.41
1:A:4:VAL:HA	7:G:38:ILE:HG23	2.02	0.41
1:A:124:LEU:HB3	1:A:128:ARG:HH12	1.86	0.41
1:A:291:GLU:O	1:A:294:TRP:N	2.54	0.41
1:A:408:VAL:HG11	1:A:460:ASP:HB2	2.03	0.41
1:A:412:ASN:O	1:A:413:ARG:C	2.63	0.41
1:A:544:PRO:HB2	1:A:1092:ILE:HG23	2.02	0.41
1:A:563:LEU:HD13	1:A:708:ARG:NH1	2.36	0.41
1:A:830:ARG:HH22	2:B:658:TYR:HA	1.86	0.41
1:A:832:LEU:HD11	2:B:491:PRO:HB3	2.02	0.41
1:A:925:GLU:OE2	1:A:1081:ALA:HA	2.21	0.41
1:A:1054:THR:O	1:A:1058:GLN:HG2	2.21	0.41
1:A:1205:ILE:O	1:A:1209:ILE:HG12	2.21	0.41
1:A:1302:ASP:OD1	1:A:1303:VAL:N	2.51	0.41
2:B:234:ILE:HB	2:B:240:ILE:HG22	2.03	0.41
2:B:403:ILE:O	2:B:406:VAL:HB	2.21	0.41
2:B:427:ASN:ND2	18:R:92:TYR:HE2	2.19	0.41
2:B:610:ARG:HA	2:B:611:PRO:HD3	1.96	0.41
3:C:19:ASP:HB2	3:C:29:ASN:HD22	1.86	0.41
3:C:41:GLU:HB2	3:C:57:ILE:HG21	2.02	0.41
3:C:103:LEU:HD23	3:C:103:LEU:O	2.21	0.41
3:C:244:ALA:O	3:C:247:PHE:HB3	2.20	0.41
5:E:82:PHE:CE1	5:E:111:VAL:HB	2.56	0.41
7:G:14:PRO:HB2	7:G:17:GLN:OE1	2.21	0.41
7:G:57:GLY:HA2	7:G:68:ILE:HG12	2.03	0.41
7:G:88:TRP:CG	7:G:143:ASN:H	2.39	0.41
8:H:76:THR:C	8:H:78:SER:H	2.29	0.41
13:M:131:TYR:CE2	13:M:133:LYS:HA	2.55	0.41
15:O:52:LEU:HD13	15:O:127:ILE:HG22	2.01	0.41
15:O:88:VAL:HA	15:O:91:VAL:HB	2.02	0.41
15:O:150:GLU:O	15:O:153:LYS:HB3	2.21	0.41
15:O:152:HIS:O	15:O:156:VAL:HG22	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:169:LEU:O	15:O:279:SER:HA	2.20	0.41
15:O:200:LEU:CD2	15:O:282:ILE:HD12	2.51	0.41
15:O:312:TYR:CE1	15:O:468:LEU:HD21	2.55	0.41
15:O:338:ASP:HB3	15:O:341:GLU:N	2.35	0.41
16:P:110:ILE:O	16:P:114:THR:HG22	2.21	0.41
16:P:312:PHE:N	17:Q:39:ILE:O	2.36	0.41
18:R:74:GLU:HB2	18:R:77:GLU:HB2	2.03	0.41
18:R:99:TYR:CD2	18:R:100:ILE:HG13	2.56	0.41
18:R:177:ASP:OD1	18:R:180:LEU:HD13	2.20	0.41
18:R:485:ASN:ND2	20:X:15:DT:O4'	2.53	0.41
19:S:461:GLU:OE1	19:S:465:ARG:NE	2.54	0.41
1:A:197:TRP:O	1:A:200:GLU:HB2	2.21	0.41
1:A:232:LYS:HB3	15:O:579:GLN:HE21	1.86	0.41
1:A:496:ARG:HB2	2:B:1035:MET:SD	2.61	0.41
1:A:537:VAL:O	1:A:540:ASN:N	2.52	0.41
1:A:580:LEU:HD21	1:A:590:PHE:CD1	2.55	0.41
1:A:660:LEU:HG	8:H:117:SER:OG	2.21	0.41
1:A:790:ALA:HB3	1:A:791:PRO:HD3	2.03	0.41
2:B:334:HIS:NE2	2:B:348:TYR:HE2	2.19	0.41
2:B:481:ARG:NH2	21:Y:21:DG:H2'	2.35	0.41
2:B:572:VAL:HG13	2:B:590:ILE:HD13	2.03	0.41
2:B:794:VAL:HA	2:B:895:LEU:HD23	2.03	0.41
3:C:86:PHE:N	3:C:203:SER:O	2.49	0.41
3:C:328:LEU:HD11	11:K:47:ILE:HD11	2.03	0.41
8:H:131:ASN:OD1	8:H:131:ASN:N	2.54	0.41
13:M:171:VAL:HG12	13:M:172:PRO:O	2.21	0.41
15:O:200:LEU:C	15:O:281:THR:O	2.64	0.41
15:O:358:GLY:HA2	15:O:361:PHE:CD2	2.56	0.41
15:O:471:THR:OG1	15:O:477:TYR:HB3	2.21	0.41
15:O:484:MET:O	15:O:487:LEU:HB3	2.21	0.41
18:R:13:GLU:OE2	18:R:26:LYS:HE2	2.21	0.41
19:S:423:GLU:HA	19:S:426:ILE:HG12	2.03	0.41
20:X:7:DA:P	20:X:7:DA:H3'	2.61	0.41
1:A:136:ARG:HE	1:A:140:ILE:HD11	1.85	0.40
1:A:215:VAL:HG21	15:O:552:PRO:O	2.21	0.40
1:A:413:ARG:O	1:A:417:GLN:N	2.41	0.40
1:A:474:PHE:HD2	1:A:508:TYR:CZ	2.39	0.40
1:A:574:ALA:HA	11:K:81:MET:HE3	2.03	0.40
1:A:911:ILE:HG22	5:E:174:GLN:O	2.21	0.40
1:A:919:ASP:OD1	1:A:921:LEU:HD13	2.21	0.40
1:A:1176:VAL:HG12	1:A:1177:TYR:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1225:ILE:H	1:A:1229:ARG:NE	2.10	0.40
2:B:191:GLU:OE2	2:B:458:LEU:HD13	2.22	0.40
2:B:205:ILE:HG12	2:B:219:SER:HB2	2.03	0.40
2:B:316:LYS:NZ	13:M:226:ARG:HH21	2.19	0.40
2:B:787:THR:O	2:B:901:ARG:HA	2.21	0.40
3:C:44:ILE:HA	3:C:54:PHE:HB2	2.03	0.40
3:C:195:LYS:HD2	10:J:57:ILE:CG2	2.51	0.40
8:H:65:LEU:HG	8:H:66:GLU:H	1.85	0.40
14:N:419:THR:HG23	14:N:420:PRO:HD2	2.02	0.40
15:O:202:GLN:OE1	15:O:278:VAL:HG11	2.21	0.40
15:O:478:VAL:HB	15:O:480:TYR:CZ	2.56	0.40
16:P:125:LEU:HD22	16:P:148:TYR:CD2	2.56	0.40
17:Q:52:ARG:O	17:Q:55:ALA:N	2.54	0.40
18:R:12:PHE:CE1	18:R:25:CYS:HB3	2.56	0.40
18:R:531:LEU:HB2	18:R:539:VAL:C	2.46	0.40
20:X:13:DA:H8	20:X:13:DA:O5'	2.04	0.40
1:A:384:ASP:HA	2:B:765:TYR:CD1	2.57	0.40
1:A:468:ASP:OD1	1:A:469:GLY:N	2.54	0.40
1:A:489:TYR:CE2	1:A:532:ILE:HD11	2.56	0.40
1:A:562:TYR:O	1:A:566:HIS:N	2.55	0.40
1:A:957:TYR:CE2	1:A:1035:PRO:HD3	2.56	0.40
1:A:1163:LYS:CG	1:A:1164:THR:H	2.25	0.40
1:A:1328:ILE:HG22	1:A:1329:GLU:N	2.36	0.40
2:B:217:GLN:CG	2:B:232:TYR:HB3	2.51	0.40
2:B:615:VAL:HG22	2:B:671:THR:C	2.46	0.40
2:B:640:PHE:CD1	2:B:645:LEU:HD22	2.56	0.40
2:B:822:GLN:O	2:B:824:LEU:N	2.53	0.40
2:B:887:SER:HB3	12:L:55:ILE:HG22	2.03	0.40
5:E:88:VAL:CG2	5:E:117:THR:H	2.34	0.40
5:E:147:HIS:ND1	5:E:148:GLU:N	2.69	0.40
5:E:150:VAL:HG12	5:E:151:PRO:O	2.21	0.40
6:F:97:ARG:O	6:F:101:ILE:HG12	2.21	0.40
9:I:21:VAL:O	9:I:23:THR:N	2.54	0.40
11:K:46:LYS:HD2	11:K:46:LYS:HA	1.86	0.40
12:L:31:CYS:HB2	12:L:35:SER:N	2.36	0.40
13:M:72:GLU:HB2	14:N:364:ARG:NE	2.33	0.40
13:M:115:LYS:NZ	13:M:236:VAL:HB	2.35	0.40
15:O:48:LEU:HG	15:O:52:LEU:HD11	2.04	0.40
15:O:201:ILE:N	15:O:281:THR:H	2.18	0.40
15:O:326:ILE:O	15:O:326:ILE:HG22	2.21	0.40
15:O:640:ARG:NH1	17:Q:44:ASN:HA	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:650:VAL:HG13	15:O:651:PHE:CD2	2.55	0.40
18:R:96:ILE:HG22	18:R:141:HIS:NE2	2.37	0.40
18:R:556:ILE:O	18:R:559:VAL:HB	2.20	0.40
1:A:9:THR:O	1:A:11:LYS:HG2	2.21	0.40
1:A:590:PHE:O	11:K:106:GLN:NE2	2.39	0.40
1:A:813:VAL:HG21	1:A:852:PHE:CE2	2.56	0.40
1:A:913:GLN:NE2	1:A:917:GLY:H	2.19	0.40
1:A:939:TRP:CE2	1:A:1015:LYS:HD3	2.57	0.40
1:A:1326:LEU:HG	5:E:144:ILE:HG23	2.04	0.40
1:A:1339:ILE:O	1:A:1343:MET:HB2	2.21	0.40
2:B:152:MET:SD	2:B:153:PRO:HD2	2.61	0.40
2:B:211:GLU:O	2:B:212:LYS:HG2	2.22	0.40
2:B:502:THR:HG23	2:B:511:VAL:O	2.22	0.40
2:B:800:ASN:HA	2:B:855:PRO:HB3	2.03	0.40
2:B:1039:ALA:HB3	18:R:20:ASN:OD1	2.21	0.40
3:C:294:VAL:HG13	3:C:297:HIS:HB3	2.04	0.40
7:G:88:TRP:HA	7:G:146:ILE:HD12	2.02	0.40
7:G:89:ILE:O	7:G:142:VAL:HG12	2.21	0.40
8:H:1:MET:HG2	8:H:3:ASN:ND2	2.36	0.40
11:K:69:ASP:OD1	11:K:93:ILE:HD11	2.21	0.40
13:M:117:HIS:CG	13:M:118:LEU:N	2.88	0.40
15:O:136:ILE:O	15:O:139:GLU:HB3	2.22	0.40
15:O:199:TYR:CZ	15:O:200:LEU:CD1	2.83	0.40
15:O:284:LEU:O	15:O:287:PHE:HB3	2.21	0.40
15:O:454:ASN:O	15:O:457:LEU:HB3	2.21	0.40
15:O:602:LEU:O	15:O:606:ALA:N	2.35	0.40
16:P:118:GLN:O	16:P:122:LEU:N	2.47	0.40
18:R:12:PHE:HD1	18:R:25:CYS:HB3	1.85	0.40
18:R:233:ARG:NH1	19:S:281:UNK:HA	2.37	0.40
19:S:433:SER:HA	19:S:476:LYS:HD2	2.03	0.40
1:A:362:GLY:O	1:A:367:ASN:HB2	2.12	0.40
1:A:396:ASP:OD1	1:A:397:ARG:N	2.55	0.40
1:A:473:LEU:HA	1:A:487:SER:HA	2.03	0.40
1:A:551:ILE:HD11	1:A:694:MET:HE1	2.04	0.40
1:A:562:TYR:HA	1:A:565:SER:HB3	2.04	0.40
1:A:577:THR:HG21	11:K:89:CYS:H	1.86	0.40
1:A:869:ARG:NH2	2:B:500:ALA:O	2.54	0.40
6:F:79:ARG:NH1	6:F:145:ASP:O	2.54	0.40
7:G:54:VAL:HA	7:G:70:VAL:CG1	2.50	0.40
10:J:17:LYS:HD3	10:J:39:LEU:HD21	2.03	0.40
11:K:87:GLU:HG2	11:K:107:THR:C	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:89:GLN:HB3	14:N:394:VAL:HG22	2.04	0.40
15:O:46:LEU:HD12	15:O:47:PHE:N	2.37	0.40
15:O:482:LYS:O	15:O:486:VAL:HG22	2.22	0.40
16:P:146:LYS:HD3	21:Y:37:DA:OP1	2.22	0.40
16:P:169:GLU:OE2	16:P:239:ASN:ND2	2.54	0.40
18:R:392:THR:O	18:R:488:GLY:CA	2.68	0.40
18:R:536:GLY:O	18:R:538:ILE:HG12	2.22	0.40
20:X:12:DT:H2''	20:X:13:DA:C8	2.56	0.40
20:X:46:DG:N2	21:Y:18:DC:C2	2.89	0.40
21:Y:10:DC:C2	21:Y:11:DA:N6	2.89	0.40
21:Y:35:DG:H1'	21:Y:36:DA:C5'	2.52	0.40
1:A:4:VAL:HA	7:G:38:ILE:O	2.22	0.40
1:A:164:VAL:HG21	1:A:178:ILE:HB	2.04	0.40
1:A:186:VAL:HG23	1:A:188:LYS:H	1.86	0.40
1:A:232:LYS:HB3	15:O:579:GLN:NE2	2.37	0.40
1:A:348:LYS:O	1:A:350:ILE:N	2.55	0.40
1:A:409:THR:N	1:A:412:ASN:HD22	2.19	0.40
2:B:279:TYR:O	2:B:280:GLN:C	2.64	0.40
2:B:355:ARG:NH2	2:B:367:ASP:OD2	2.54	0.40
2:B:417:ASP:OD1	2:B:417:ASP:C	2.64	0.40
2:B:475:SER:OG	2:B:476:GLN:N	2.55	0.40
2:B:536:LEU:HD22	2:B:571:PHE:CD1	2.53	0.40
2:B:908:LEU:HD13	2:B:923:GLY:O	2.21	0.40
3:C:310:PRO:HA	3:C:313:ILE:HB	2.04	0.40
4:D:130:ASN:O	4:D:133:HIS:HB2	2.21	0.40
5:E:81:GLU:HG3	5:E:110:PHE:HB3	2.02	0.40
7:G:195:ALA:C	7:G:196:LEU:HD12	2.47	0.40
14:N:291:LEU:O	14:N:294:LEU:HB3	2.21	0.40
15:O:259:LEU:CD2	15:O:261:GLN:HB2	2.50	0.40
15:O:316:LEU:HA	15:O:319:THR:HG22	2.04	0.40
15:O:516:LEU:CD1	15:O:565:LEU:HD23	2.52	0.40
15:O:637:VAL:O	15:O:640:ARG:HB3	2.21	0.40
15:O:639:ALA:HB1	17:Q:51:GLU:HG2	2.02	0.40
18:R:402:LEU:HA	18:R:477:LYS:O	2.21	0.40
18:R:521:TYR:HE2	18:R:523:MET:HE3	1.87	0.40
20:X:28:DT:C4	20:X:29:DC:N4	2.90	0.40
21:Y:42:DT:H2''	21:Y:43:DA:H8	1.86	0.40
21:Y:54:DA:H2'	21:Y:55:DT:H71	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1422/1460 (97%)	1110 (78%)	289 (20%)	23 (2%)	7	37
2	B	1112/1149 (97%)	890 (80%)	201 (18%)	21 (2%)	6	32
3	C	333/335 (99%)	281 (84%)	46 (14%)	6 (2%)	6	33
4	D	113/161 (70%)	84 (74%)	26 (23%)	3 (3%)	4	25
5	E	213/215 (99%)	186 (87%)	25 (12%)	2 (1%)	14	49
6	F	81/155 (52%)	67 (83%)	12 (15%)	2 (2%)	4	26
7	G	178/212 (84%)	147 (83%)	29 (16%)	2 (1%)	11	45
8	H	136/146 (93%)	112 (82%)	23 (17%)	1 (1%)	18	55
9	I	40/110 (36%)	30 (75%)	7 (18%)	3 (8%)	1	10
10	J	65/70 (93%)	55 (85%)	10 (15%)	0	100	100
11	K	99/142 (70%)	80 (81%)	19 (19%)	0	100	100
12	L	44/70 (63%)	37 (84%)	7 (16%)	0	100	100
13	M	160/282 (57%)	126 (79%)	31 (19%)	3 (2%)	6	32
14	N	106/422 (25%)	81 (76%)	25 (24%)	0	100	100
15	O	533/654 (82%)	401 (75%)	119 (22%)	13 (2%)	4	27
16	P	271/317 (86%)	225 (83%)	42 (16%)	4 (2%)	8	38
17	Q	33/251 (13%)	29 (88%)	4 (12%)	0	100	100
18	R	514/736 (70%)	435 (85%)	74 (14%)	5 (1%)	12	47
19	S	172/594 (29%)	149 (87%)	23 (13%)	0	100	100
All	All	5625/7481 (75%)	4525 (80%)	1012 (18%)	88 (2%)	10	37

All (88) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	186	VAL
1	A	248	VAL

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Mol	Chain	Res	Type
1	A	251	GLY
1	A	277	SER
1	A	348	LYS
1	A	364	PHE
1	A	1371	ILE
2	B	300	GLN
2	B	587	PHE
2	B	975	TYR
2	B	1049	GLN
3	C	87	ASN
9	I	21	VAL
13	M	84	SER
13	M	107	ILE
15	O	88	VAL
15	O	146	VAL
15	O	189	SER
15	O	201	ILE
15	O	542	ARG
16	P	314	GLU
18	R	154	VAL
18	R	513	PRO
1	A	307	ILE
1	A	975	VAL
1	A	995	VAL
1	A	1269	ASP
2	B	87	VAL
3	C	25	LYS
3	C	255	VAL
8	H	130	ARG
13	M	242	ASN
15	O	126	GLY
15	O	583	TRP
18	R	149	ARG
1	A	349	PRO
1	A	448	ASP
1	A	455	ASN
2	B	168	GLU
2	B	764	GLY
6	F	144	GLU
7	G	191	PRO
9	I	35	ILE
15	O	497	ALA

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Mol	Chain	Res	Type
15	O	518	SER
15	O	543	TYR
18	R	274	LYS
1	A	587	ILE
1	A	601	TYR
1	A	1328	ILE
2	B	713	ILE
2	B	767	ILE
3	C	88	ASN
4	D	128	PRO
9	I	23	THR
1	A	39	LEU
1	A	998	TYR
1	A	1300	LEU
2	B	766	ASP
2	B	927	LYS
2	B	969	LEU
2	B	1048	ARG
2	B	1050	PRO
2	B	1051	THR
4	D	64	ASN
5	E	147	HIS
6	F	116	ASP
15	O	535	SER
16	P	218	THR
2	B	417	ASP
1	A	1033	GLU
2	B	215	ILE
1	A	558	ILE
3	C	33	VAL
5	E	30	ILE
16	P	309	VAL
2	B	811	VAL
15	O	91	VAL
16	P	206	VAL
2	B	783	GLY
2	B	1139	PRO
7	G	158	VAL
1	A	26	ILE
2	B	309	VAL
3	C	256	ILE
4	D	127	LEU

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Mol	Chain	Res	Type
15	O	517	VAL
18	R	435	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1232/1257 (98%)	1224 (99%)	8 (1%)	78	81
2	B	975/1006 (97%)	967 (99%)	8 (1%)	73	78
3	C	296/296 (100%)	293 (99%)	3 (1%)	68	76
4	D	110/145 (76%)	108 (98%)	2 (2%)	51	67
5	E	197/197 (100%)	196 (100%)	1 (0%)	81	82
6	F	73/137 (53%)	73 (100%)	0	100	100
7	G	164/190 (86%)	163 (99%)	1 (1%)	78	81
8	H	123/128 (96%)	123 (100%)	0	100	100
9	I	38/98 (39%)	38 (100%)	0	100	100
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%)	40 (100%)	0	100	100
13	M	142/249 (57%)	141 (99%)	1 (1%)	76	79
14	N	92/360 (26%)	92 (100%)	0	100	100
15	O	495/593 (84%)	487 (98%)	8 (2%)	55	69
16	P	255/285 (90%)	253 (99%)	2 (1%)	73	78
17	Q	31/195 (16%)	31 (100%)	0	100	100
18	R	450/623 (72%)	448 (100%)	2 (0%)	84	83
19	S	157/494 (32%)	157 (100%)	0	100	100
All	All	5023/6505 (77%)	4987 (99%)	36 (1%)	73	79

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	155	LEU
1	A	248	VAL
1	A	277	SER
1	A	350	ILE
1	A	363	ARG
1	A	365	ARG
1	A	1270	VAL
1	A	1376	LEU
2	B	694	ASN
2	B	695	GLN
2	B	741	ILE
2	B	772	VAL
2	B	877	GLU
2	B	969	LEU
2	B	1049	GLN
2	B	1085	ILE
3	C	59	ILE
3	C	120	LEU
3	C	294	VAL
4	D	58	ILE
4	D	127	LEU
5	E	109	ILE
7	G	42	VAL
13	M	85	LEU
15	O	41	THR
15	O	124	GLU
15	O	184	LYS
15	O	185	TYR
15	O	187	ILE
15	O	188	SER
15	O	516	LEU
15	O	541	ILE
16	P	265	LEU
16	P	266	GLU
18	R	149	ARG
18	R	191	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (102) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	147	GLN
1	A	156	HIS
1	A	320	GLN

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Mol	Chain	Res	Type
1	A	342	ASN
1	A	386	ASN
1	A	412	ASN
1	A	437	ASN
1	A	455	ASN
1	A	477	GLN
1	A	518	ASN
1	A	520	HIS
1	A	523	GLN
1	A	619	ASN
1	A	643	ASN
1	A	707	ASN
1	A	815	GLN
1	A	838	ASN
1	A	913	GLN
1	A	941	HIS
1	A	1040	GLN
1	A	1385	GLN
1	A	1419	GLN
2	B	46	HIS
2	B	116	HIS
2	B	175	ASN
2	B	197	GLN
2	B	203	ASN
2	B	275	ASN
2	B	280	GLN
2	B	286	ASN
2	B	396	ASN
2	B	397	ASN
2	B	425	HIS
2	B	441	ASN
2	B	552	ASN
2	B	626	HIS
2	B	693	HIS
2	B	695	GLN
2	B	754	ASN
2	B	774	ASN
2	B	803	GLN
2	B	821	HIS
2	B	893	GLN
2	B	902	GLN
2	B	928	GLN

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Mol	Chain	Res	Type
2	B	1115	ASN
2	B	1148	GLN
3	C	14	ASN
3	C	29	ASN
3	C	99	HIS
3	C	130	ASN
3	C	175	GLN
3	C	207	HIS
3	C	296	ASN
4	D	56	GLN
4	D	69	ASN
4	D	71	ASN
4	D	111	ASN
5	E	5	ASN
5	E	54	GLN
5	E	114	ASN
5	E	174	GLN
6	F	78	GLN
7	G	31	ASN
8	H	3	ASN
8	H	133	ASN
8	H	134	ASN
11	K	64	GLN
11	K	95	HIS
13	M	86	HIS
13	M	92	ASN
13	M	156	ASN
13	M	242	ASN
13	M	254	GLN
14	N	288	GLN
15	O	43	ASN
15	O	162	ASN
15	O	207	HIS
15	O	222	HIS
15	O	310	GLN
15	O	321	GLN
15	O	346	GLN
15	O	454	ASN
15	O	514	ASN
15	O	599	ASN
15	O	626	GLN
16	P	34	GLN

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Mol	Chain	Res	Type
16	P	53	GLN
16	P	119	HIS
16	P	239	ASN
16	P	305	HIS
18	R	35	ASN
18	R	184	HIS
18	R	235	ASN
18	R	241	HIS
18	R	256	GLN
18	R	505	HIS
18	R	613	HIS
19	S	386	ASN
19	S	444	GLN
19	S	506	GLN
19	S	509	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 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	37.39
1	Q	70:PHE	C	1070:UNK	N	14.81

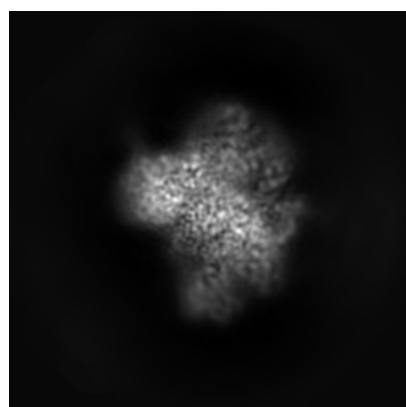
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7532. These allow visual inspection of the internal detail of the map and identification of artifacts.

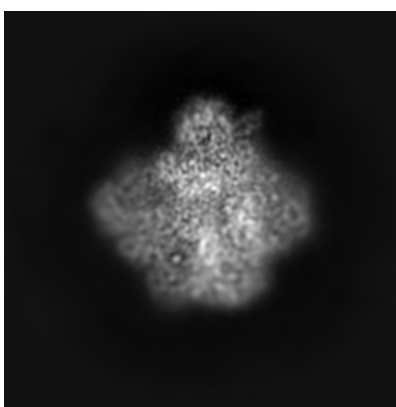
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

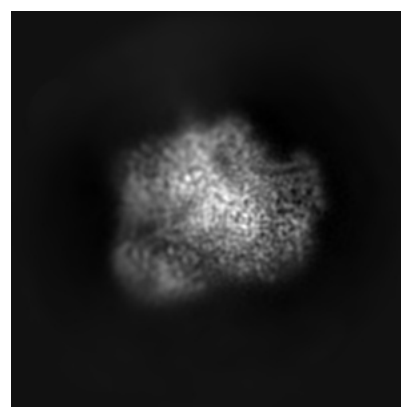
6.1.1 Primary map



X



Y

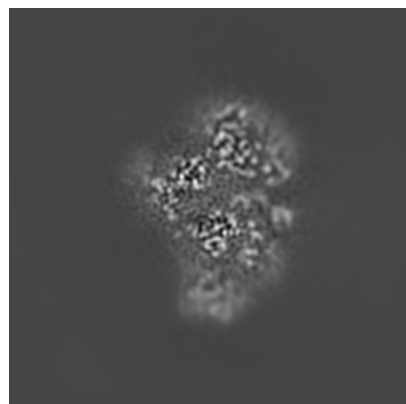


Z

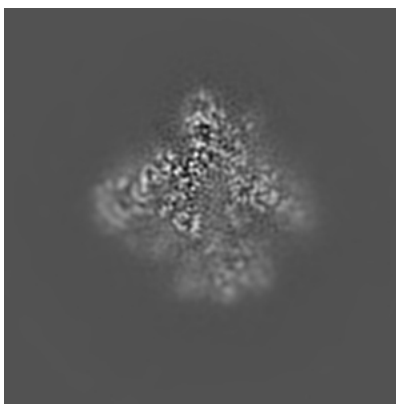
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

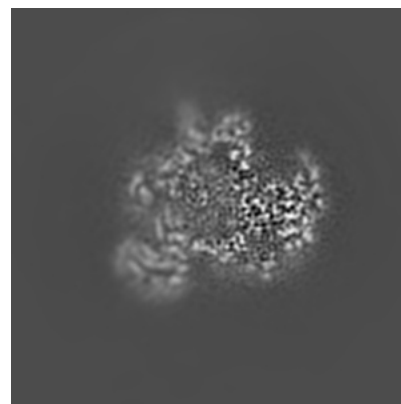
6.2.1 Primary map



X Index: 144



Y Index: 144

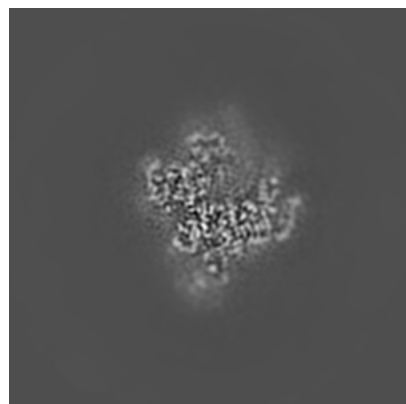


Z Index: 144

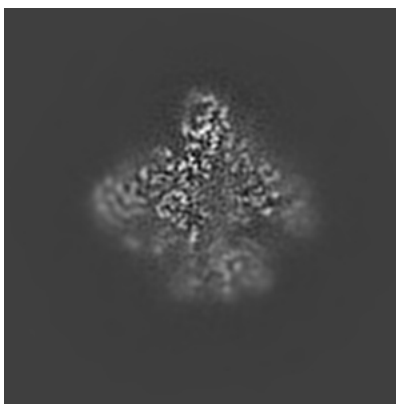
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

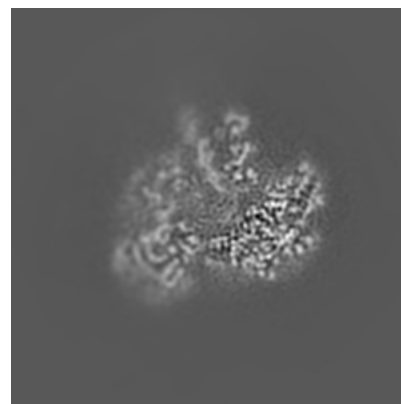
6.3.1 Primary map



X Index: 168



Y Index: 147

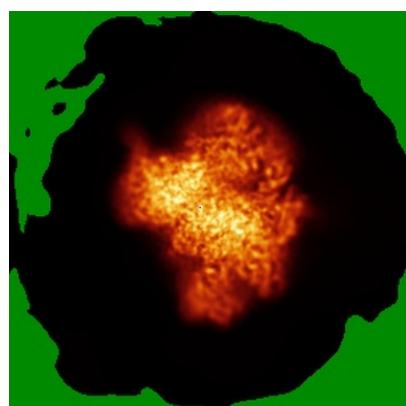


Z Index: 150

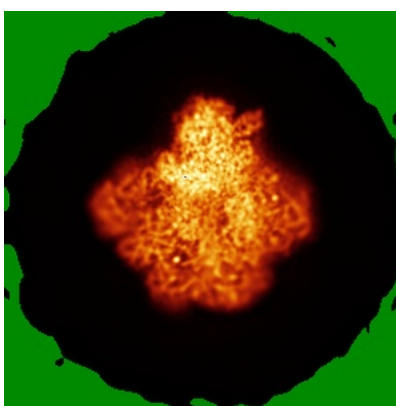
The images above show the largest variance slices of the map in three orthogonal directions.

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

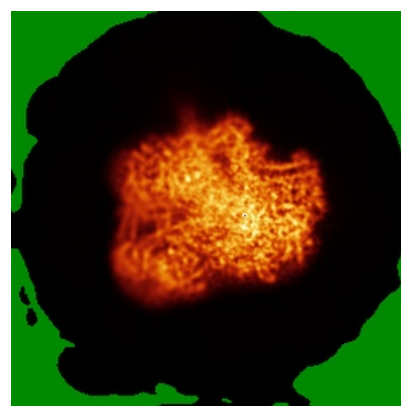
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.035. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

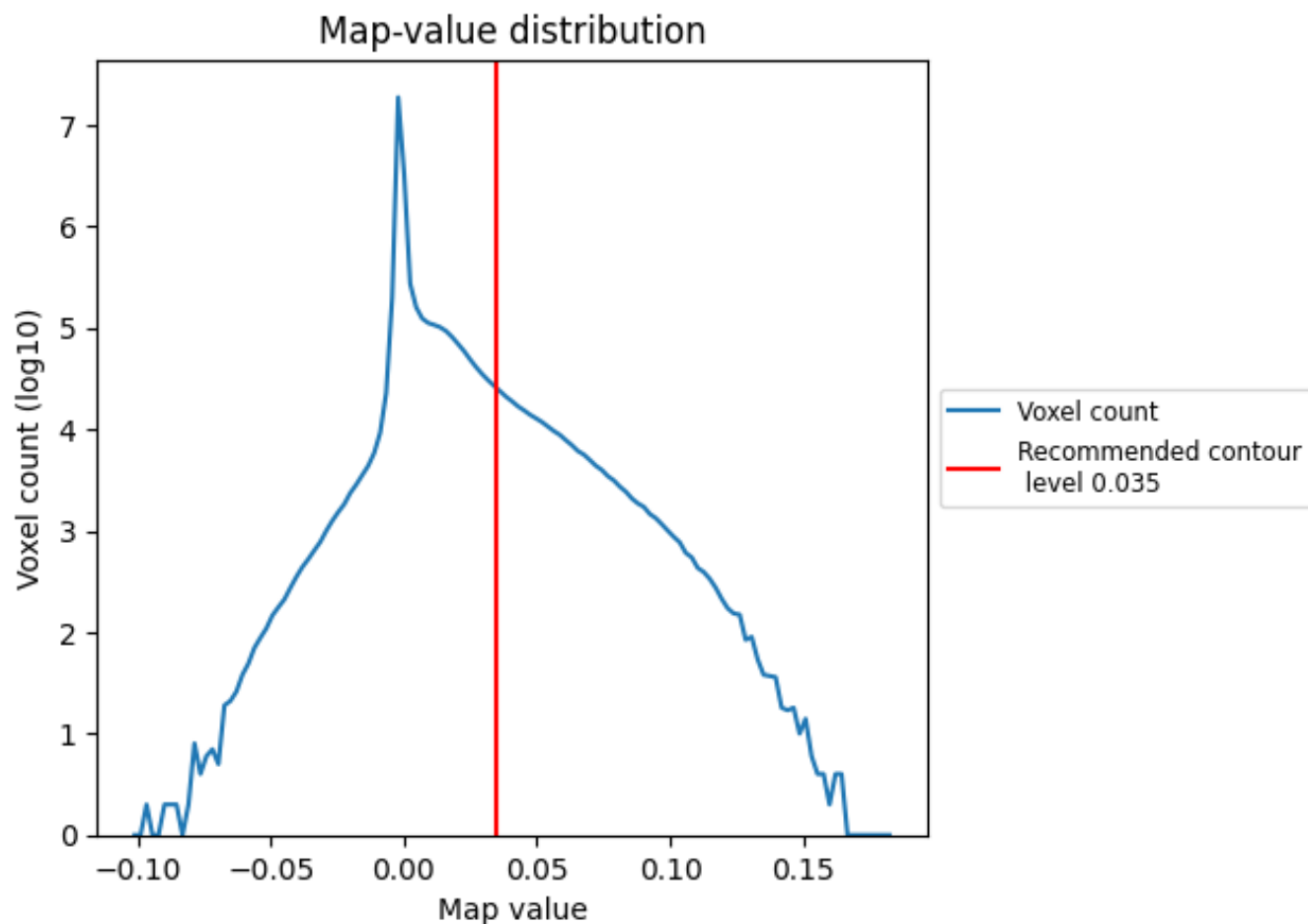
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

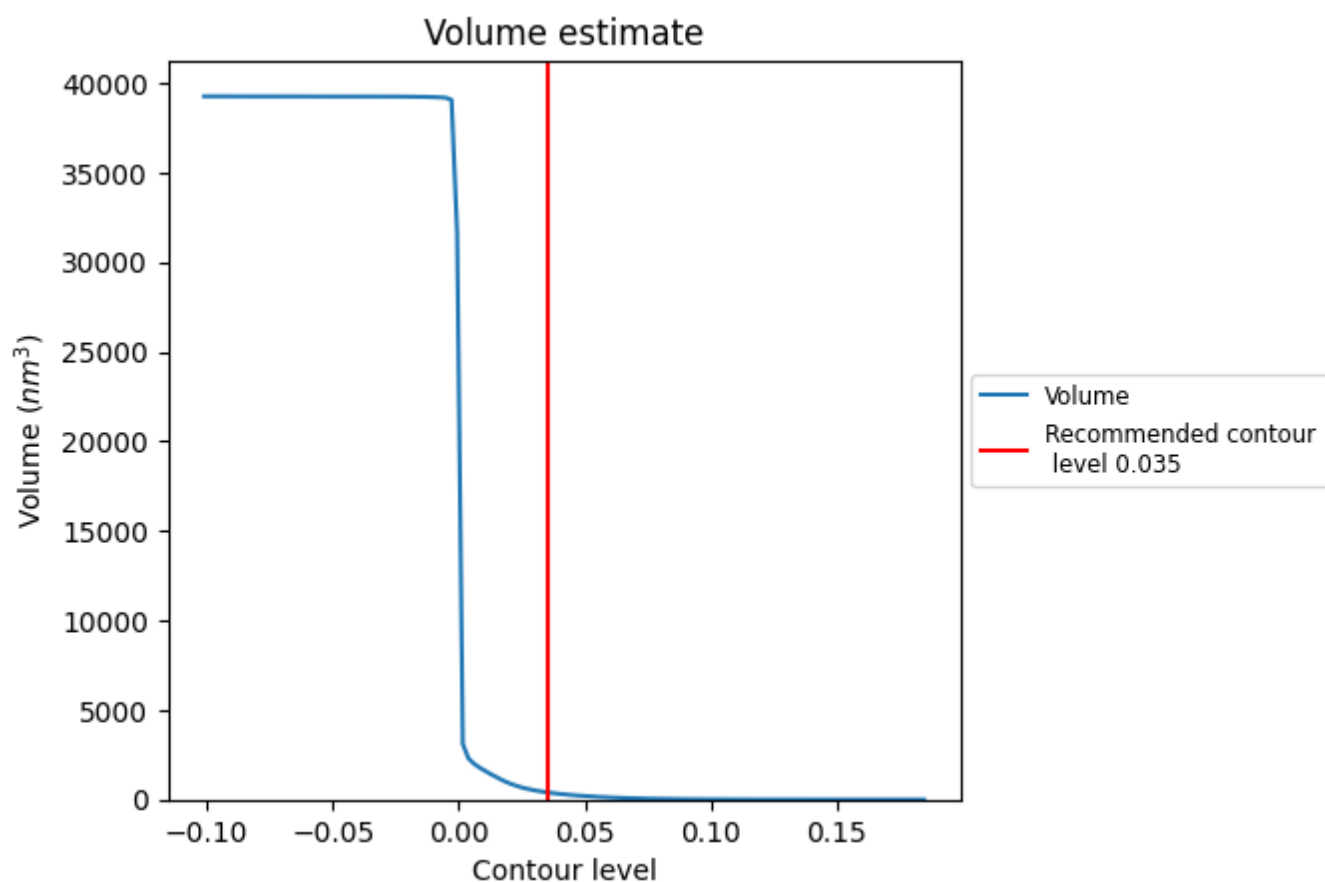
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

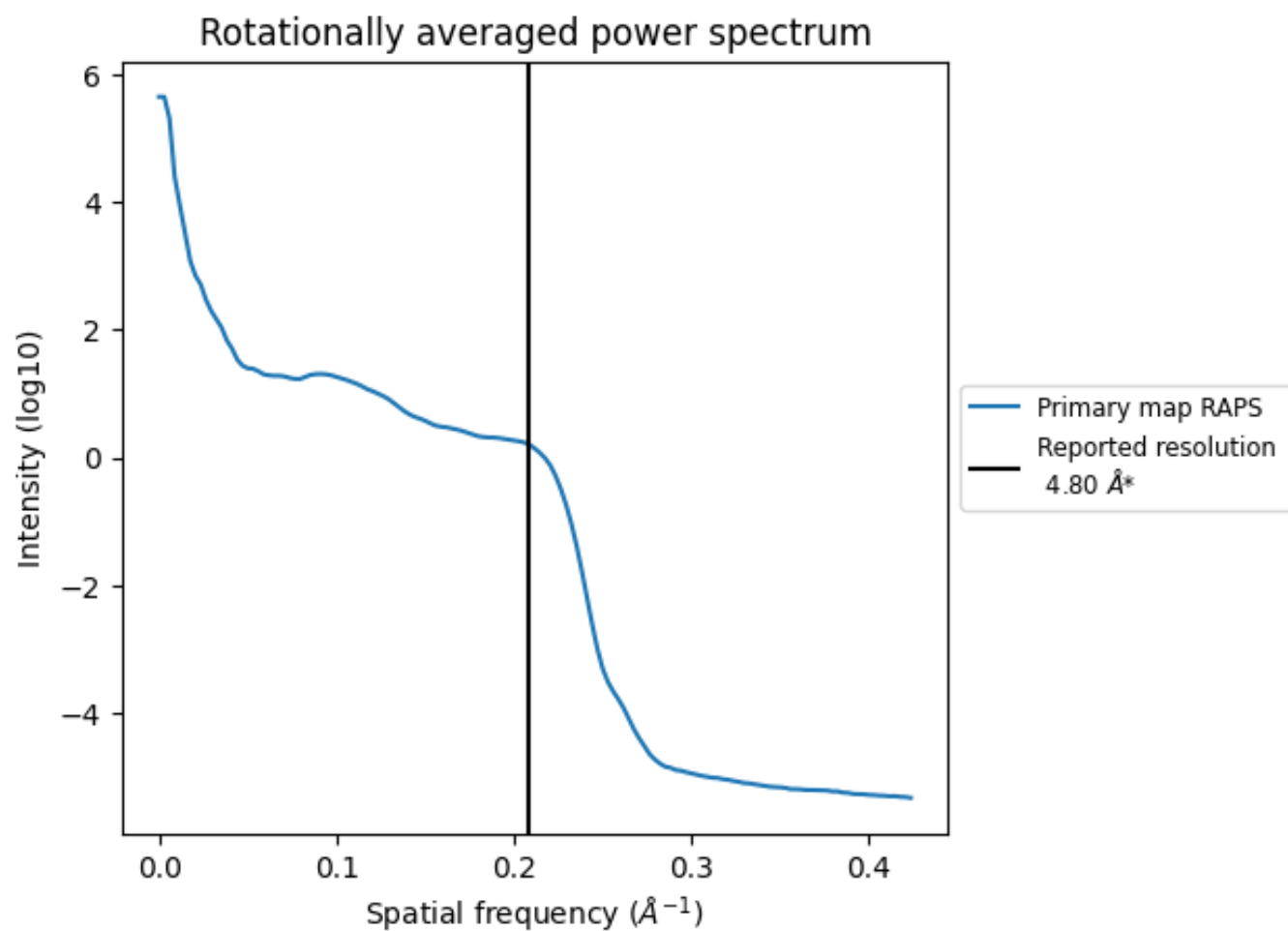
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 402 nm³; this corresponds to an approximate mass of 363 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

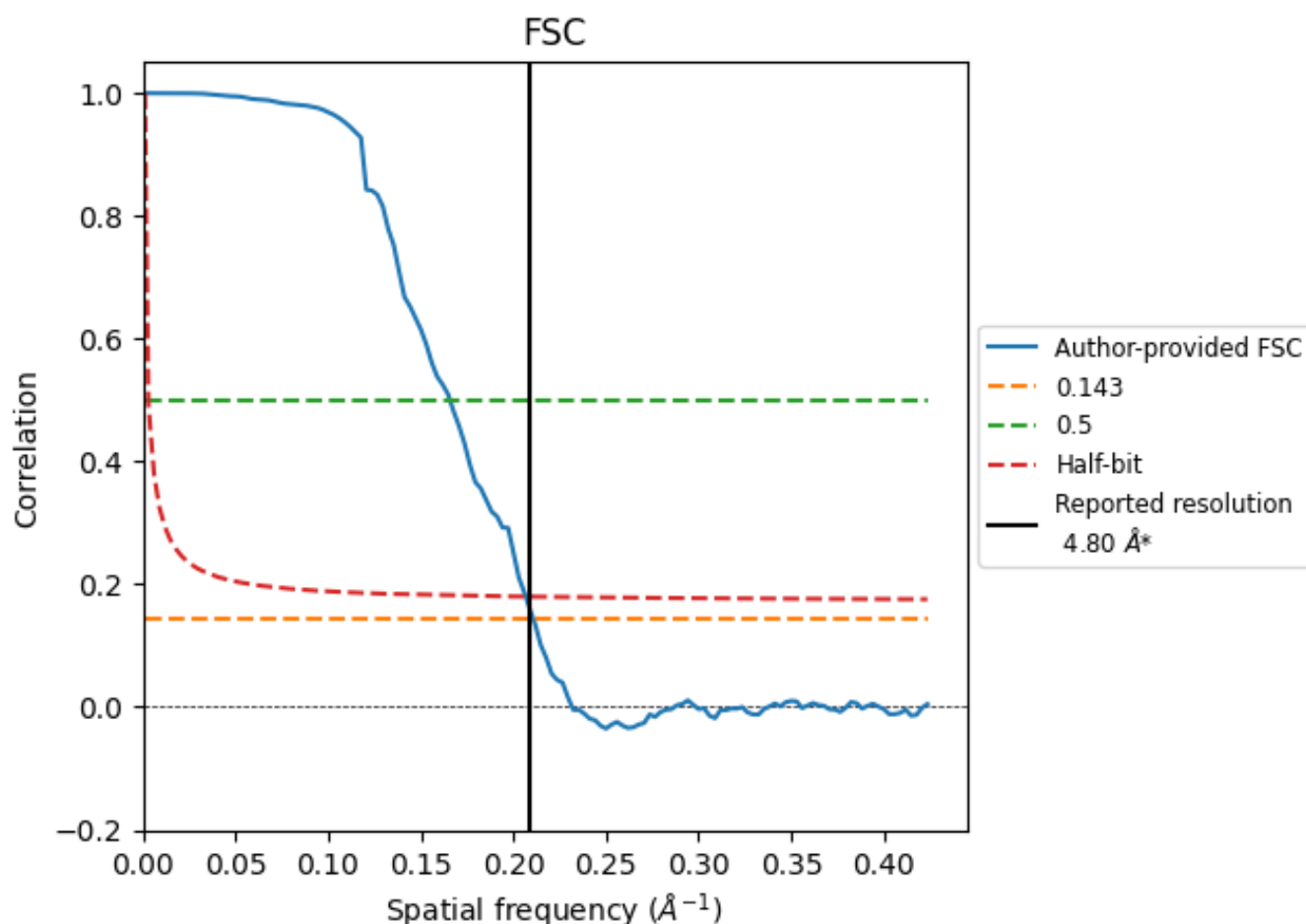


*Reported resolution corresponds to spatial frequency of 0.208 Å⁻¹

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 0.208 Å⁻¹

8.2 Resolution estimates [i](#)

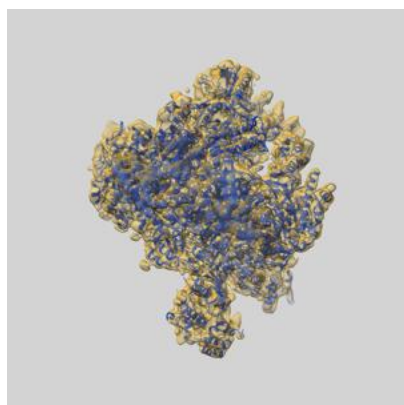
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.80	-	-
Author-provided FSC curve	4.74	6.03	4.84
Unmasked-calculated*	-	-	-

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

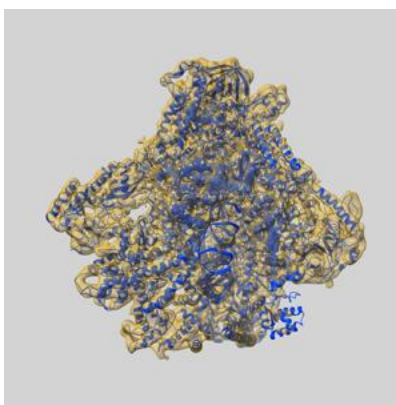
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-7532 and PDB model 6CND. Per-residue inclusion information can be found in [section 3](#) on [page 9](#).

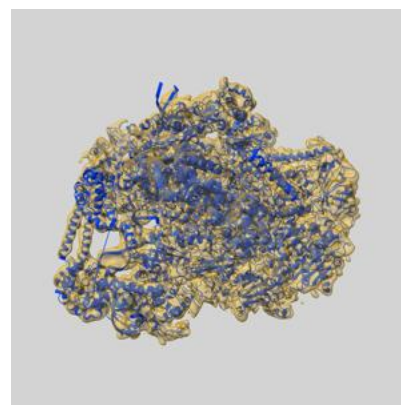
9.1 Map-model overlay [i](#)



X



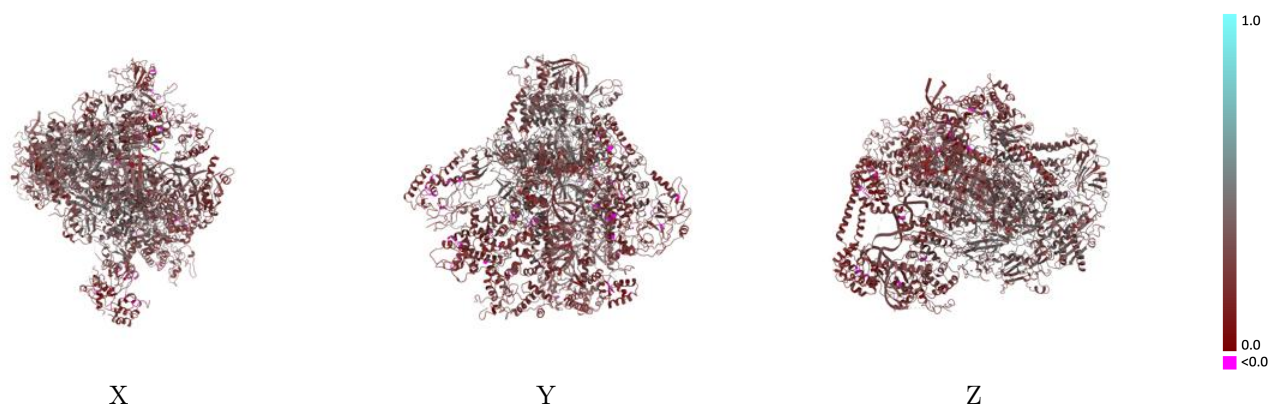
Y



Z

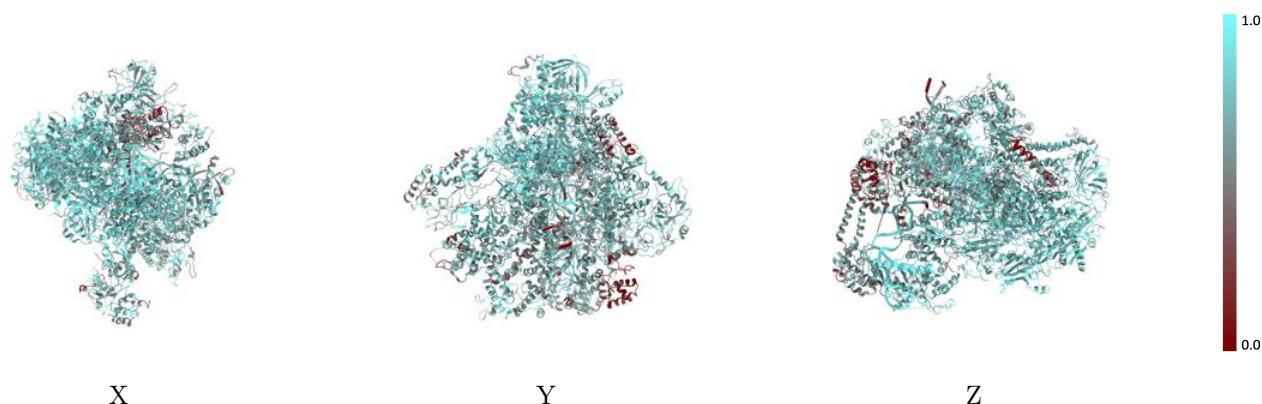
The images above show the 3D surface view of the map at the recommended contour level 0.035 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



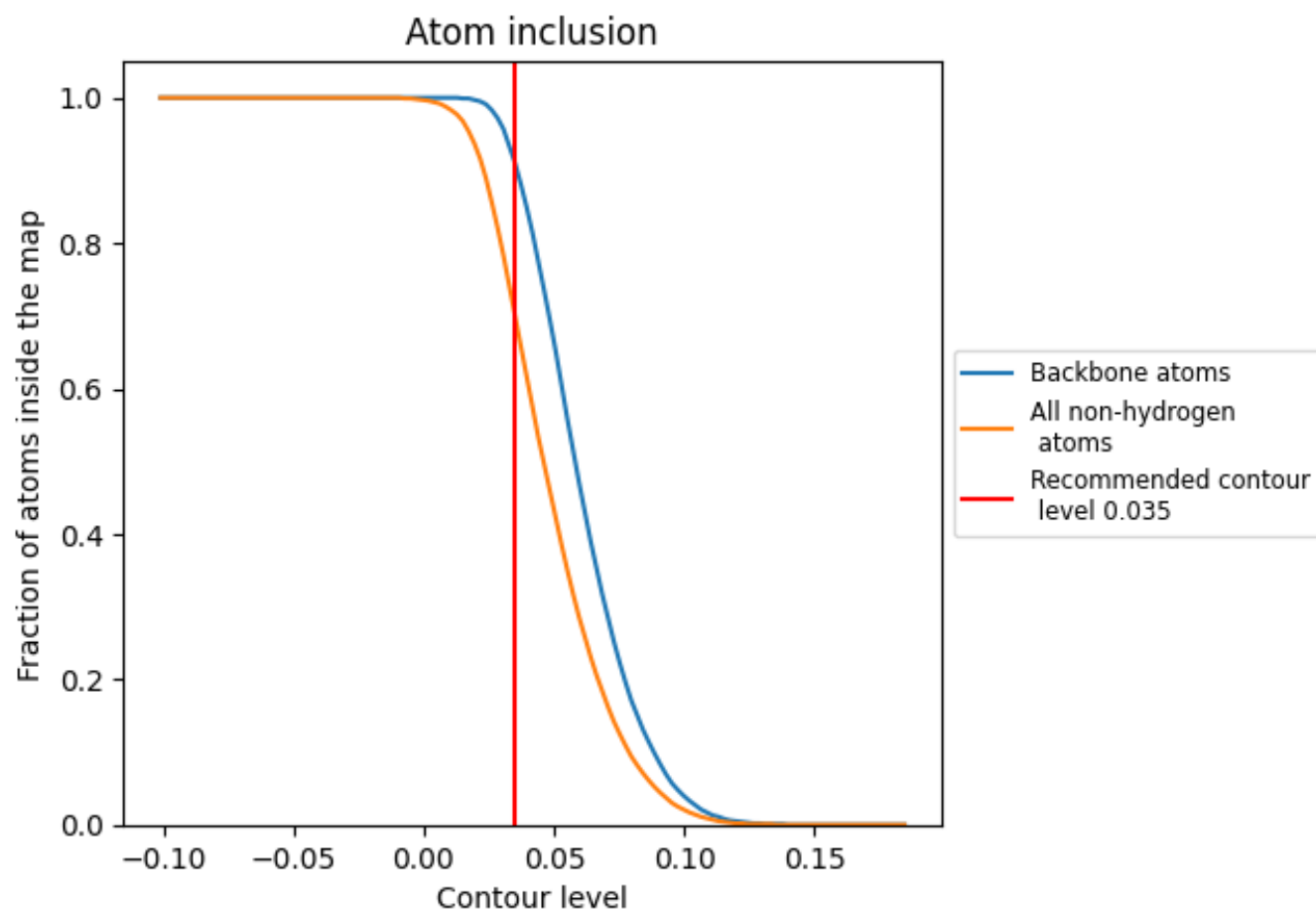
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.035).

9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 70% 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 (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7020	 0.2910
A	 0.7150	 0.3260
B	 0.7450	 0.3380
C	 0.8160	 0.3420
D	 0.6200	 0.1930
E	 0.7480	 0.2860
F	 0.8160	 0.3600
G	 0.6810	 0.2350
H	 0.7830	 0.3240
I	 0.7290	 0.2520
J	 0.8240	 0.3660
K	 0.7970	 0.3450
L	 0.8060	 0.3510
M	 0.6190	 0.2300
N	 0.6590	 0.2340
O	 0.6100	 0.2230
P	 0.5390	 0.2110
Q	 0.8220	 0.3060
R	 0.6500	 0.2350
S	 0.5470	 0.2340
X	 0.8140	 0.2880
Y	 0.7570	 0.3000

