



Full wwPDB EM Validation Report ⓘ

Oct 5, 2024 – 03:01 pm BST

PDB ID : 5N61
EMDB ID : EMD-3593
Title : RNA polymerase I initially transcribing complex
Authors : Engel, C.; Gubbey, T.; Neyer, S.; Sainsbury, S.; Oberthuer, C.; Baejen, C.; Bernecky, C.; Cramer, P.
Deposited on : 2017-02-14
Resolution : 3.40 Å(reported)

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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.dev113
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

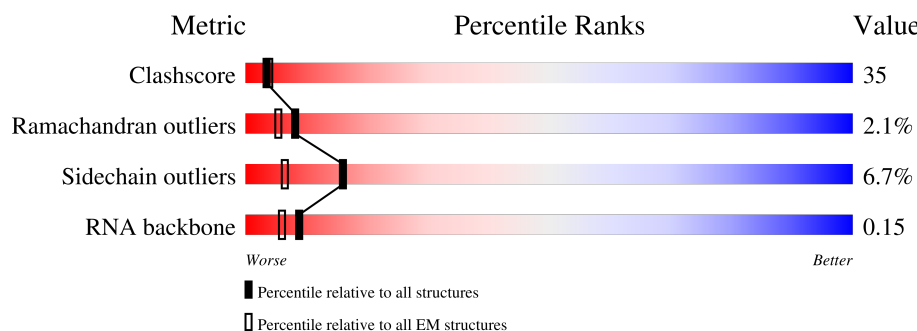
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	1664	
2	B	1203	
3	C	335	
4	D	137	
5	E	215	
6	F	155	
7	G	326	

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Mol	Chain	Length	Quality of chain
8	H	146	
9	I	125	
10	J	70	
11	K	142	
12	L	70	
13	M	415	
14	N	233	
15	O	627	
16	P	894	
17	Q	514	
18	R	507	
19	S	5	
20	T	47	
21	U	47	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	SO4	B	1301	-	-	X	-

2 Entry composition

There are 24 unique types of molecules in this entry. The entry contains 48547 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 I subunit RPA190.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1459	Total	C	N	O	S	0	0
			11526	7281	2004	2180	61		

- Molecule 2 is a protein called DNA-directed RNA polymerase I subunit RPA135.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1177	Total	C	N	O	S	0	0
			9350	5913	1639	1747	51		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	305	Total	C	N	O	S	0	0
			2423	1539	416	460	8		

- Molecule 4 is a protein called DNA-directed RNA polymerase I subunit RPA14.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	54	Total	C	N	O	0	0
			431	270	73	88		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	212	Total	C	N	O	S	0	0
			1735	1102	306	316	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	100	Total	C	N	O	S	0	0
			823	522	144	154	3		

- Molecule 7 is a protein called DNA-directed RNA polymerase I subunit RPA43.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	193	Total	C	N	O	S	0	0
			1526	985	262	274	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	131	Total	C	N	O	S	0	0
			1052	664	176	208	4		

- Molecule 9 is a protein called DNA-directed RNA polymerase I subunit RPA12.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	63	Total	C	N	O	S	0	0
			466	292	77	93	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	69	Total	C	N	O	S	0	0
			569	362	101	100	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
			793	496	130	162	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	44	Total	C	N	O	S	0	0
			352	217	70	61	4		

- Molecule 13 is a protein called DNA-directed RNA polymerase I subunit RPA49.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	108	Total	C	N	O		0	0
			856	543	142	171			

- Molecule 14 is a protein called DNA-directed RNA polymerase I subunit RPA34.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	129	Total	C	N	O	S	0	0
			1029	665	170	191	3		

- Molecule 15 is a protein called RNA polymerase I-specific transcription initiation factor RRN3.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	463	Total	C	N	O	S	0	0
			3811	2473	623	694	21		

- Molecule 16 is a protein called RNA polymerase I-specific transcription initiation factor RRN6.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	587	Total	C	N	O	S	0	0
			4764	3030	811	912	11		

- Molecule 17 is a protein called RNA polymerase I-specific transcription initiation factor RRN7.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	389	Total	C	N	O	S	0	0
			3254	2110	552	572	20		

- Molecule 18 is a protein called RNA polymerase I-specific transcription initiation factor RRN11.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	303	Total	C	N	O	S	0	0
			2535	1634	456	434	11		

- Molecule 19 is a RNA chain called product RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	5	Total	C	N	O	P	0	0
			108	48	21	34	5		

- Molecule 20 is a DNA chain called template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	41	Total	C	N	O	P	0	0
			641	304	66	231	40		

- Molecule 21 is a DNA chain called non-template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	33	Total	C	N	O	P	0	0
			490	228	55	174	33		

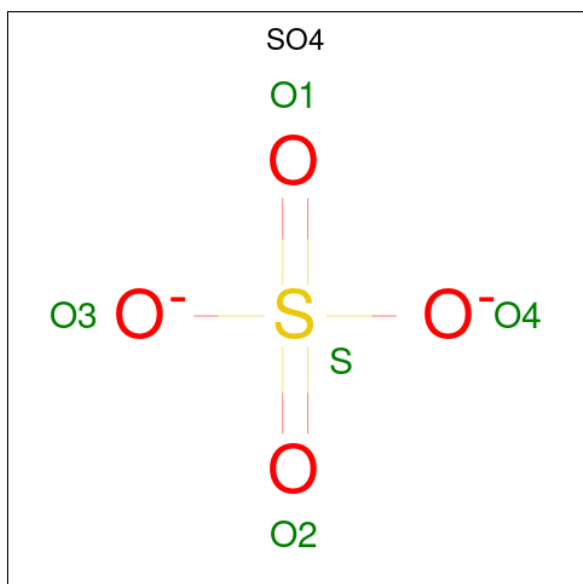
- Molecule 22 is ZINC ION (three-letter code: ZN) (formula: Zn).

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	
22	Q	1	Total	Zn	0
			1	1	

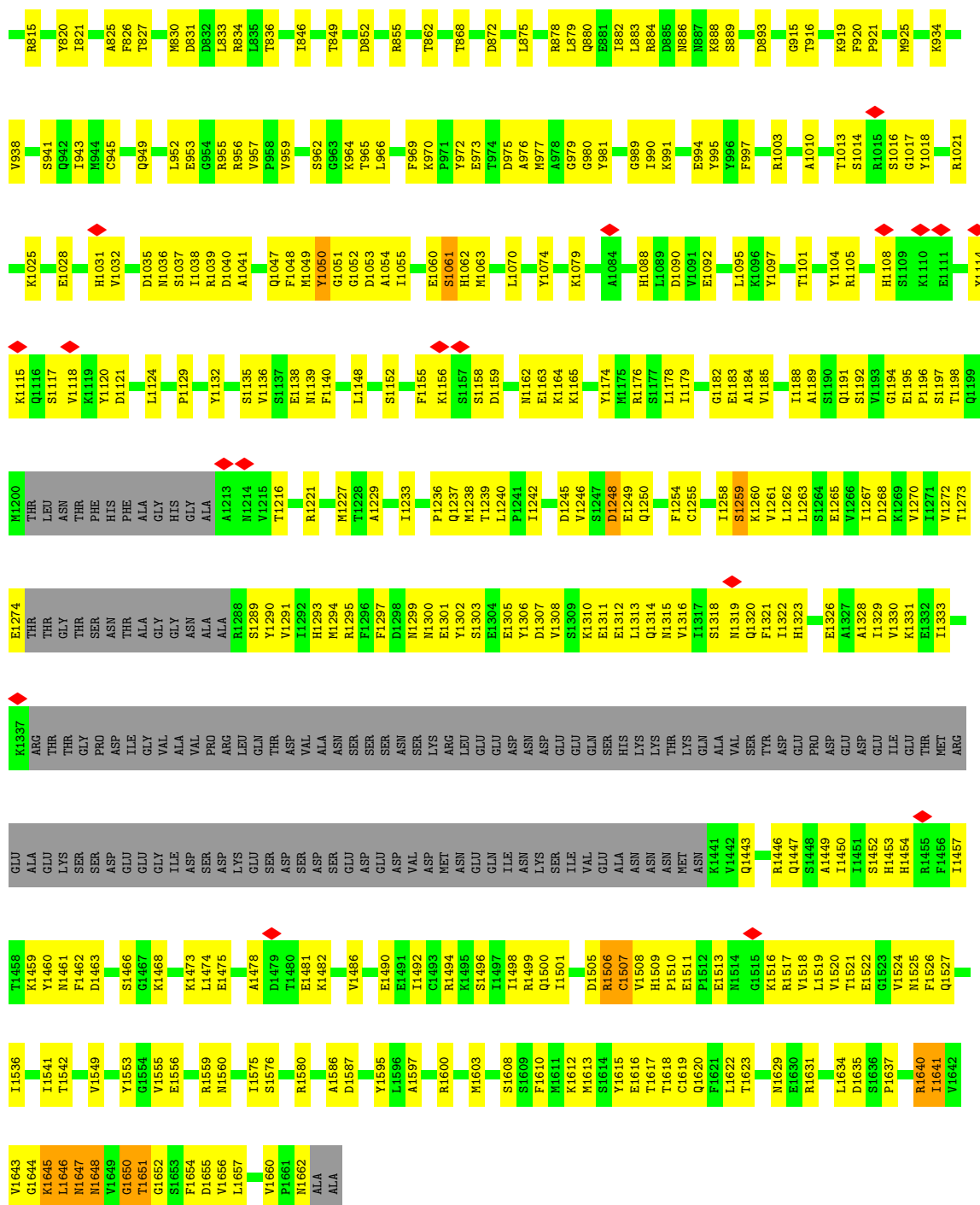
- Molecule 23 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
23	A	1	Total	Mg	0
			1	1	

- Molecule 24 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			AltConf
24	B	1	Total	O	S	0
			5	4	1	

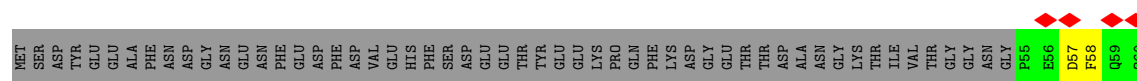


• Molecule 2: DNA-directed RNA polymerase I subunit RPA135

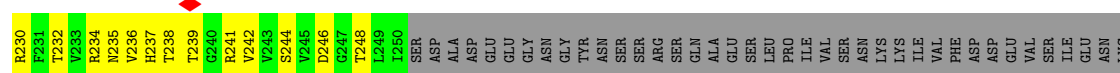
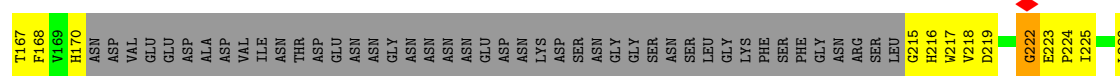
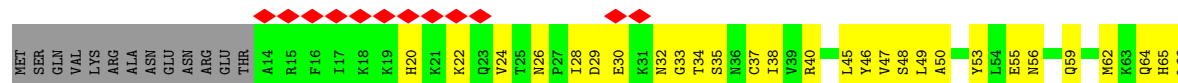
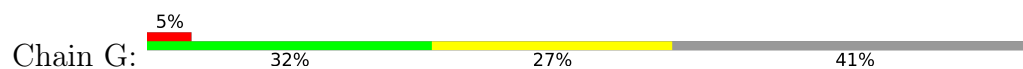
Chain B: 50% 46%

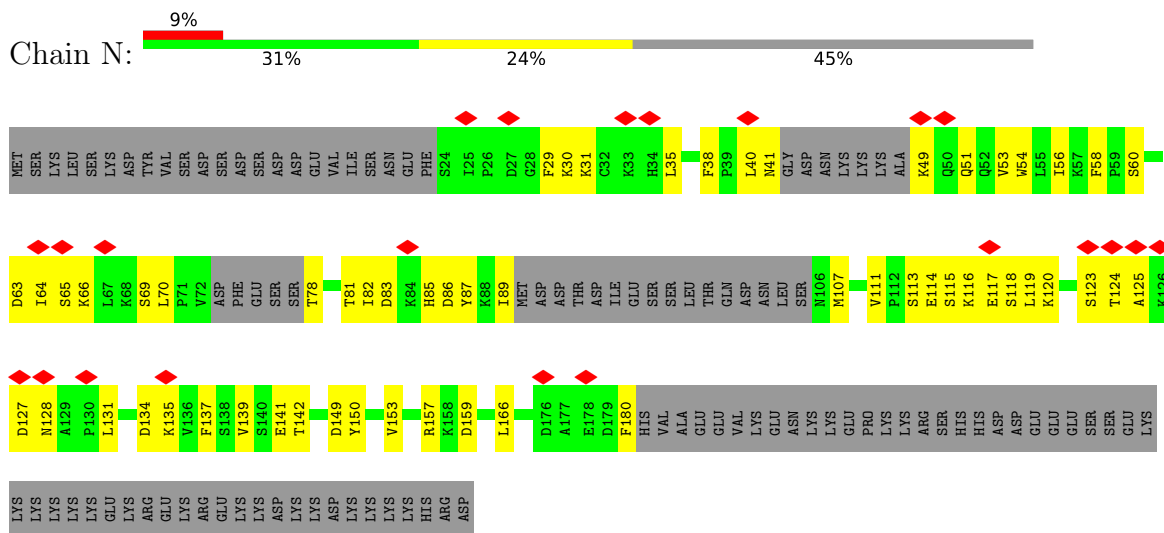




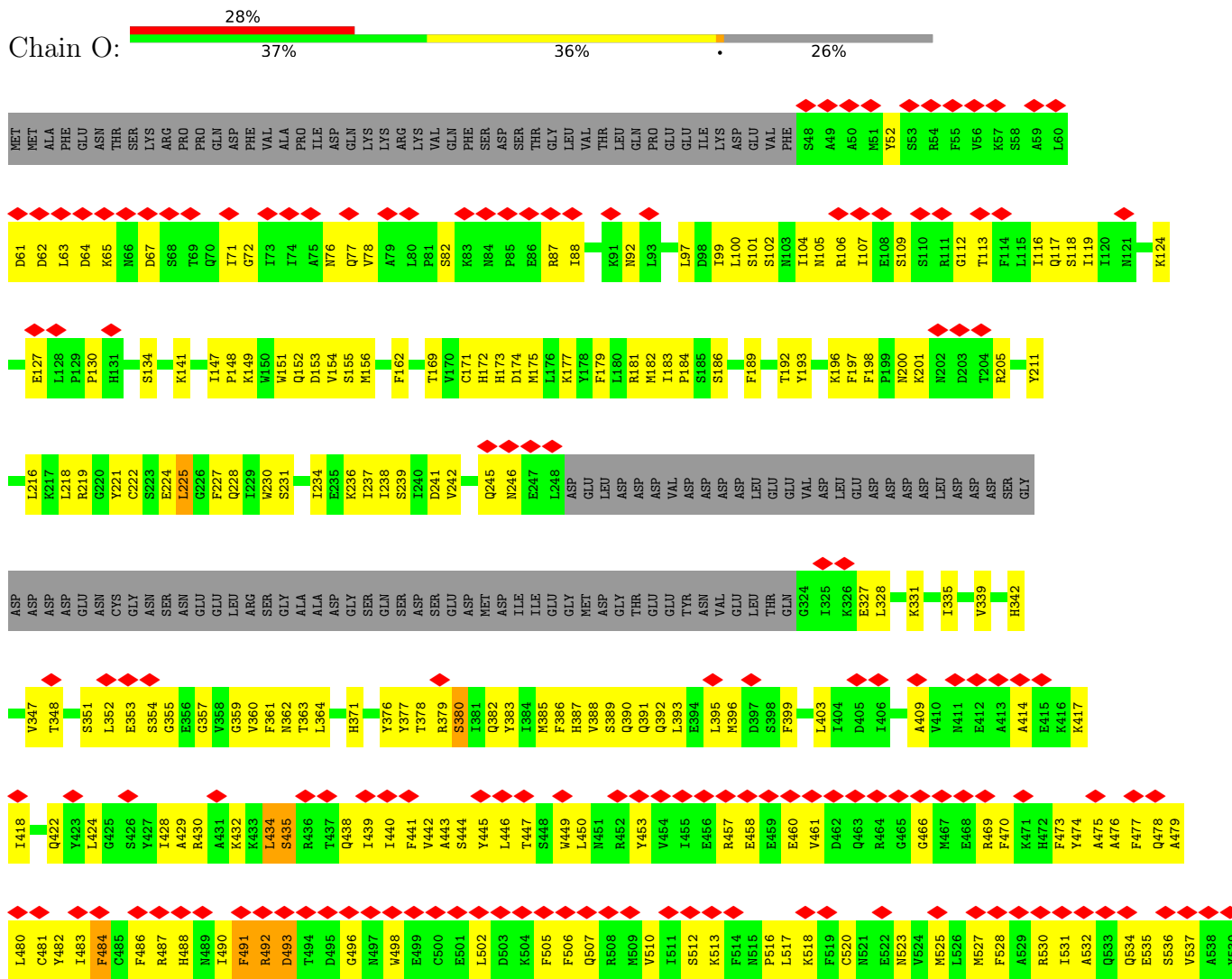


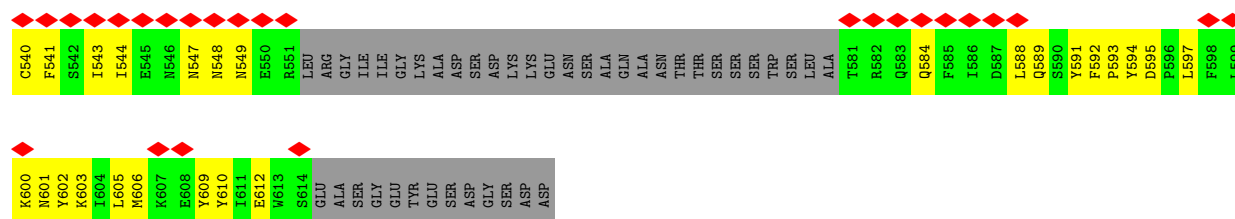
• Molecule 7: DNA-directed RNA polymerase I subunit RPA43



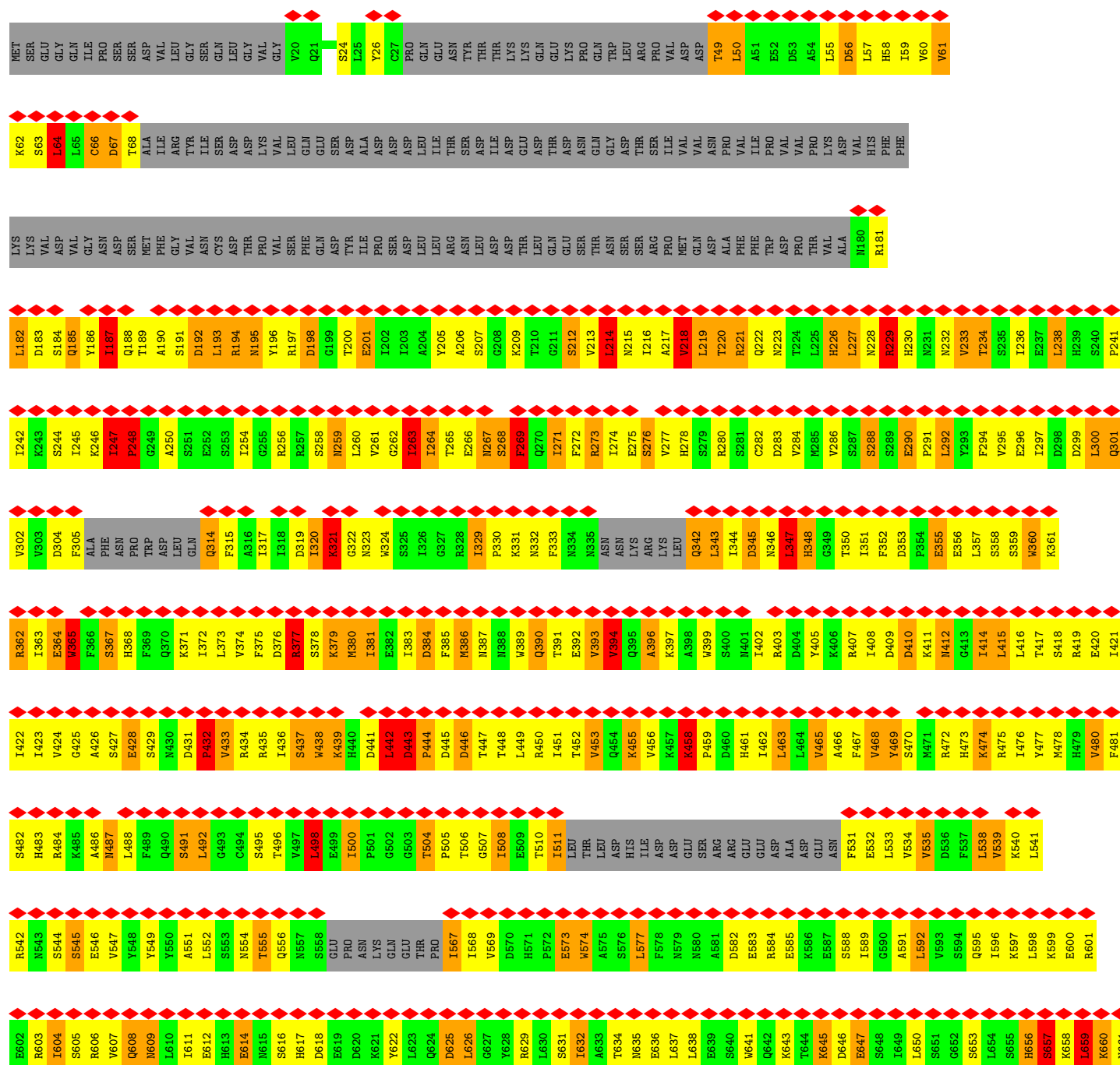


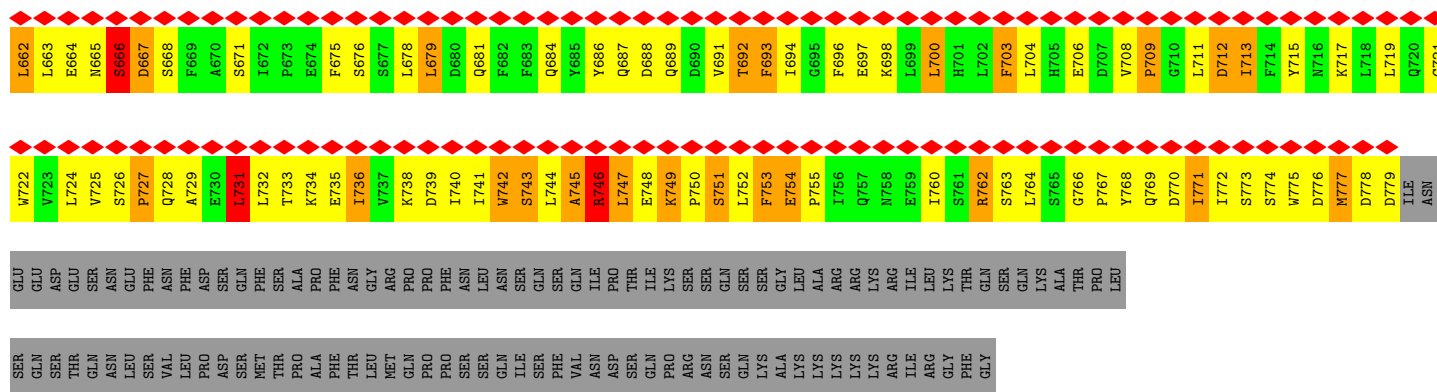
- Molecule 15: RNA polymerase I-specific transcription initiation factor RRN3



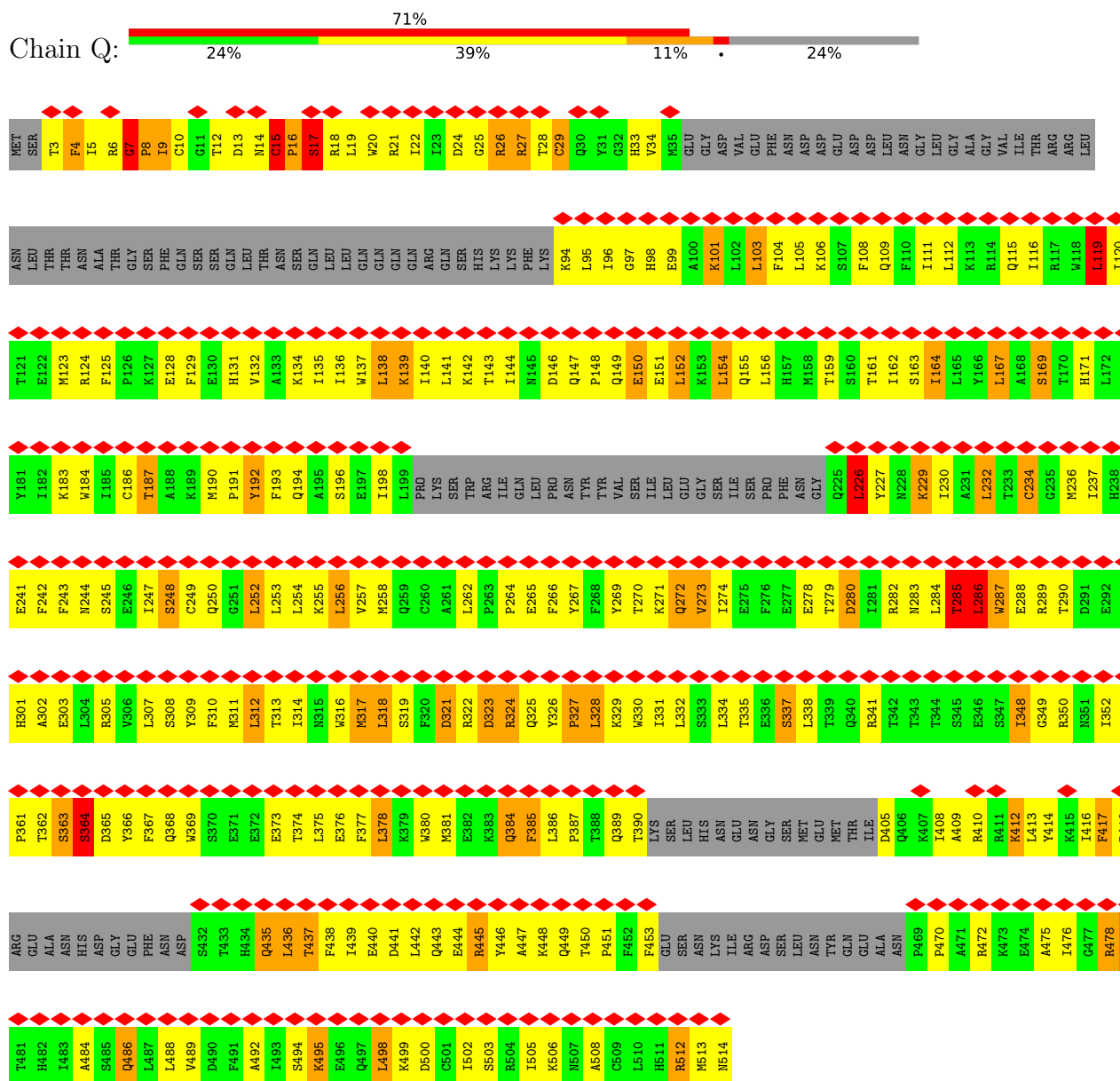


• Molecule 16: RNA polymerase I-specific transcription initiation factor RRN6

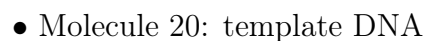
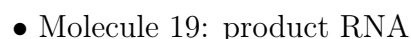


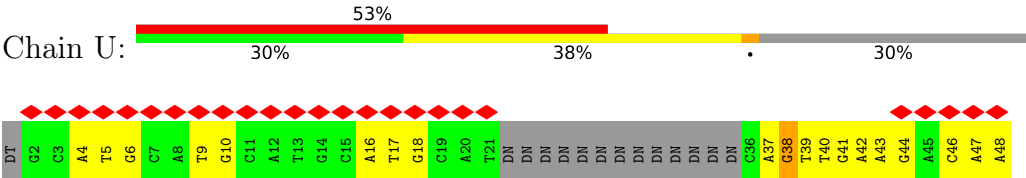


• Molecule 17: RNA polymerase I-specific transcription initiation factor RRN7



• Molecule 18: RNA polymerase I-specific transcription initiation factor RRN11





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	345000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.407	Depositor
Minimum map value	-0.199	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.065	Depositor
Map size (\AA)	372.9, 372.9, 372.9	wwPDB
Map dimensions	330, 330, 330	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.13, 1.13, 1.13	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, SO4, MG

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	0.48	0/11738	0.53	0/15851
2	B	0.52	0/9557	0.59	1/12918 (0.0%)
3	C	0.53	0/2475	0.54	0/3354
4	D	0.36	0/436	0.45	0/591
5	E	0.45	0/1771	0.49	0/2383
6	F	0.49	0/838	0.54	0/1129
7	G	0.42	0/1564	0.51	1/2127 (0.0%)
8	H	0.54	0/1070	0.55	0/1449
9	I	0.38	0/472	0.56	0/639
10	J	0.56	0/578	0.57	0/775
11	K	0.53	0/804	0.55	0/1083
12	L	0.52	0/354	0.57	0/468
13	M	0.41	0/872	0.51	0/1170
14	N	0.35	0/1049	0.50	0/1411
15	O	0.34	0/3897	0.44	0/5268
16	P	0.61	1/4857 (0.0%)	0.88	12/6572 (0.2%)
17	Q	0.65	2/3330 (0.1%)	0.91	9/4492 (0.2%)
18	R	0.52	0/2591	0.75	2/3483 (0.1%)
19	S	0.28	0/120	0.61	0/185
20	T	0.53	0/707	0.83	0/1076
21	U	0.67	1/543 (0.2%)	0.95	0/823
All	All	0.51	4/49623 (0.0%)	0.63	25/67247 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
16	P	0	18
17	Q	0	11

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Mol	Chain	#Chirality outliers	#Planarity outliers
18	R	0	10
All	All	0	39

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	Q	323	ASP	C-N	19.90	1.79	1.34
17	Q	356	VAL	C-N	-7.09	1.17	1.34
21	U	38	DG	C1'-N9	-6.35	1.38	1.47
16	P	247	ILE	C-N	5.97	1.45	1.34

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	819	ASP	C-N-CD	-28.25	58.44	120.60
17	Q	323	ASP	O-C-N	21.78	157.54	122.70
17	Q	323	ASP	CA-C-N	-17.00	79.80	117.20
17	Q	7	GLY	C-N-CD	-15.29	86.97	120.60
17	Q	323	ASP	C-N-CA	-14.08	86.50	121.70
16	P	431	ASP	C-N-CD	-8.77	101.30	120.60
16	P	747	LEU	CA-CB-CG	8.59	135.06	115.30
17	Q	119	LEU	CA-CB-CG	7.56	132.69	115.30
16	P	443	ASP	CB-CG-OD1	6.52	124.17	118.30
17	Q	226	LEU	CA-CB-CG	-6.43	100.51	115.30
17	Q	419	LEU	CA-CB-CG	6.25	129.67	115.30
17	Q	338	LEU	CA-CB-CG	5.67	128.33	115.30
16	P	347	LEU	CA-CB-CG	5.64	128.28	115.30
18	R	198	LEU	CA-CB-CG	5.57	128.11	115.30
16	P	214	LEU	CA-CB-CG	5.47	127.88	115.30
18	R	178	LEU	CA-CB-CG	5.45	127.83	115.30
16	P	415	LEU	CA-CB-CG	5.35	127.60	115.30
16	P	431	ASP	C-N-CA	5.24	144.01	122.00
16	P	64	LEU	CA-CB-CG	5.23	127.33	115.30
16	P	498	LEU	CA-CB-CG	5.21	127.28	115.30
7	G	222	GLY	C-N-CA	-5.13	108.86	121.70
16	P	498	LEU	CB-CG-CD2	5.12	119.70	111.00
17	Q	286	LEU	CA-CB-CG	5.10	127.04	115.30
16	P	347	LEU	CB-CG-CD1	5.04	119.56	111.00
16	P	731	LEU	CA-CB-CG	5.03	126.87	115.30

There are no chirality outliers.

All (39) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	P	218	VAL	Peptide
16	P	234	THR	Peptide
16	P	247	ILE	Peptide
16	P	256	ARG	Peptide
16	P	258	SER	Peptide
16	P	331	LYS	Peptide
16	P	333	PHE	Peptide
16	P	386	MET	Peptide
16	P	396	ALA	Peptide
16	P	432	PRO	Peptide
16	P	442	LEU	Peptide
16	P	498	LEU	Peptide
16	P	661	ASN	Peptide
16	P	666	SER	Peptide
16	P	667	ASP	Peptide
16	P	688	ASP	Peptide
16	P	727	PRO	Peptide
16	P	767	PRO	Peptide
17	Q	15	CYS	Peptide
17	Q	17	SER	Peptide
17	Q	194	GLN	Peptide
17	Q	25	GLY	Peptide
17	Q	285	THR	Peptide
17	Q	287	TRP	Peptide
17	Q	29	CYS	Peptide
17	Q	298	VAL	Peptide
17	Q	385	PHE	Peptide
17	Q	4	PHE	Peptide
17	Q	417	PHE	Peptide
18	R	10	ASN	Peptide
18	R	149	LYS	Peptide
18	R	294	VAL	Peptide
18	R	295	PRO	Peptide
18	R	303	THR	Peptide
18	R	304	HIS	Peptide
18	R	352	TRP	Peptide
18	R	357	PRO	Peptide
18	R	424	PHE	Peptide
18	R	426	VAL	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11526	0	11612	862	0
2	B	9350	0	9231	839	0
3	C	2423	0	2412	122	0
4	D	431	0	428	16	0
5	E	1735	0	1764	70	0
6	F	823	0	841	52	0
7	G	1526	0	1540	73	0
8	H	1052	0	1021	42	0
9	I	466	0	466	55	0
10	J	569	0	585	45	0
11	K	793	0	790	41	0
12	L	352	0	375	22	0
13	M	856	0	855	46	0
14	N	1029	0	1061	57	0
15	O	3811	0	3802	243	0
16	P	4764	0	4711	528	0
17	Q	3254	0	3296	484	0
18	R	2535	0	2594	459	0
19	S	108	0	53	19	0
20	T	641	0	362	130	0
21	U	490	0	267	45	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	Q	1	0	0	0	0
23	A	1	0	0	0	0
24	B	5	0	0	2	0
All	All	48547	0	48066	3403	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 35.

All (3403) 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)
17:Q:20:TRP:CZ3	17:Q:22:ILE:CG2	1.76	1.66
2:B:116:ALA:H	18:R:282:SER:CB	1.05	1.65
17:Q:12:THR:HG21	17:Q:33:HIS:CE1	1.12	1.62
16:P:725:VAL:HG21	17:Q:446:TYR:CD1	1.14	1.60
17:Q:356:VAL:HG21	18:R:208:TYR:CD2	1.09	1.59
17:Q:356:VAL:CG2	18:R:208:TYR:CD2	1.85	1.58
17:Q:356:VAL:HG21	18:R:208:TYR:CE2	1.05	1.55
17:Q:12:THR:CG2	17:Q:33:HIS:HE1	1.10	1.53
17:Q:20:TRP:HZ3	17:Q:22:ILE:CG2	1.10	1.53
1:A:672:ASP:H	2:B:783:MET:CE	1.21	1.50
17:Q:356:VAL:HG11	18:R:208:TYR:CD1	1.43	1.50
17:Q:366:TYR:CD1	18:R:215:THR:HG23	1.43	1.49
2:B:815:ARG:NH2	2:B:821:ILE:CG1	1.72	1.48
1:A:474:LYS:HD3	2:B:1096:SER:CB	1.39	1.47
2:B:101:GLN:NE2	18:R:359:MET:HE1	1.17	1.47
2:B:1084:THR:O	2:B:1088:LEU:CG	1.64	1.45
2:B:116:ALA:H	18:R:282:SER:CA	1.28	1.44
1:A:628:PHE:HD2	2:B:784:ASP:CB	1.32	1.43
1:A:1018:TYR:CD1	20:T:16:DT:H5"	1.55	1.42
1:A:1014:SER:HA	20:T:17:DT:C6	1.54	1.41
2:B:117:VAL:CG2	18:R:276:GLN:HG3	1.49	1.39
1:A:1238:MET:CB	1:A:1521:THR:OG1	1.68	1.39
15:O:492:ARG:CG	15:O:496:GLY:HA2	1.50	1.38
1:A:1654:PHE:CZ	6:F:89:GLU:HA	1.58	1.38
17:Q:386:LEU:HA	18:R:241:ARG:NH2	1.10	1.38
17:Q:186:CYS:HB3	18:R:208:TYR:CE2	1.60	1.36
1:A:672:ASP:OD1	2:B:952:HIS:CD2	1.79	1.36
1:A:1018:TYR:CE1	20:T:16:DT:OP1	1.78	1.36
1:A:672:ASP:N	2:B:783:MET:CE	1.83	1.34
1:A:651:ALA:CB	2:B:1084:THR:HG23	1.54	1.34
17:Q:356:VAL:CG2	18:R:208:TYR:CE2	1.95	1.33
17:Q:360:LYS:NZ	18:R:211:ARG:HH22	1.24	1.33
1:A:651:ALA:HB3	2:B:1084:THR:CG2	1.56	1.32
19:S:5:G:N2	20:T:19:DC:O2	1.60	1.32
17:Q:323:ASP:C	17:Q:324:ARG:N	1.79	1.31
2:B:931:TRP:HB3	2:B:936:MET:CE	1.61	1.31
16:P:389:TRP:HZ2	18:R:146:SER:C	1.32	1.31
16:P:725:VAL:CG2	17:Q:446:TYR:CD1	2.11	1.31
1:A:1238:MET:HB2	1:A:1521:THR:OG1	1.12	1.30
17:Q:26:ARG:HB3	17:Q:34:VAL:CG1	1.61	1.29
17:Q:356:VAL:HG11	18:R:208:TYR:CE1	1.69	1.28
1:A:474:LYS:CD	2:B:1096:SER:CB	2.10	1.27

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:628:PHE:CD2	2:B:784:ASP:HB2	1.68	1.27
20:T:4:DG:N2	21:U:46:DC:O2	1.67	1.27
2:B:817:ARG:CB	21:U:17:DT:H5'	1.63	1.26
2:B:1096:SER:O	2:B:1097:ASP:CG	1.75	1.25
1:A:672:ASP:N	2:B:783:MET:HE3	1.40	1.25
2:B:101:GLN:NE2	18:R:359:MET:CE	1.99	1.25
2:B:116:ALA:N	18:R:282:SER:CB	1.79	1.24
1:A:474:LYS:CD	2:B:1096:SER:HB3	1.69	1.23
1:A:640:ASN:ND2	2:B:1090:ASP:OD2	1.71	1.23
15:O:200:ASN:CB	17:Q:14:ASN:HB2	1.69	1.23
1:A:1018:TYR:CE1	20:T:16:DT:H5''	1.73	1.23
2:B:113:VAL:CG1	20:T:39:DT:H4'	1.67	1.22
17:Q:366:TYR:CG	18:R:215:THR:HG23	1.73	1.22
2:B:894:LYS:HE3	17:Q:405:ASP:OD2	1.35	1.22
2:B:1079:LEU:CD2	2:B:1088:LEU:HB3	1.69	1.22
17:Q:12:THR:CG2	17:Q:33:HIS:CE1	1.95	1.22
2:B:115:SER:O	18:R:280:SER:HB2	1.38	1.22
2:B:115:SER:C	18:R:280:SER:HB2	1.50	1.21
15:O:200:ASN:CA	17:Q:14:ASN:HB2	1.69	1.21
1:A:1018:TYR:HE1	20:T:16:DT:OP1	0.88	1.20
16:P:443:ASP:HB3	18:R:3:GLU:N	1.57	1.20
16:P:725:VAL:HG21	17:Q:446:TYR:CG	1.77	1.20
2:B:1093:LEU:CD1	2:B:1098:TYR:HB2	1.70	1.20
17:Q:386:LEU:CA	18:R:241:ARG:NH2	2.03	1.19
17:Q:20:TRP:CZ3	17:Q:22:ILE:HG23	1.48	1.19
1:A:511:VAL:HG12	1:A:575:LYS:O	1.04	1.18
1:A:1238:MET:CA	1:A:1521:THR:OG1	1.92	1.18
2:B:117:VAL:HG21	18:R:276:GLN:CB	1.50	1.18
16:P:55:LEU:HB3	18:R:227:HIS:ND1	1.56	1.18
1:A:70:LYS:NZ	17:Q:27:ARG:HH12	1.39	1.18
17:Q:378:LEU:CD1	18:R:231:LEU:HD21	1.74	1.18
1:A:511:VAL:CG1	1:A:575:LYS:O	1.92	1.17
2:B:817:ARG:CB	21:U:17:DT:C5'	2.22	1.17
16:P:389:TRP:NE1	18:R:146:SER:HB2	1.58	1.17
17:Q:356:VAL:HG13	18:R:212:HIS:CE1	1.80	1.17
2:B:117:VAL:CG2	18:R:276:GLN:CG	2.23	1.17
2:B:116:ALA:HB2	18:R:282:SER:O	1.01	1.16
2:B:117:VAL:HG21	18:R:276:GLN:CG	1.75	1.16
2:B:1078:ALA:O	2:B:1082:HIS:N	1.75	1.16
1:A:646:GLU:HG3	1:A:650:LEU:HD12	1.21	1.16
1:A:547:ILE:CD1	17:Q:26:ARG:HH22	1.59	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:817:ARG:HB3	21:U:17:DT:H5'	1.20	1.15
16:P:389:TRP:CE2	18:R:146:SER:HB2	1.82	1.15
20:T:9:DC:N4	21:U:41:DG:H1	1.41	1.15
16:P:389:TRP:CZ2	18:R:146:SER:C	2.19	1.15
20:T:9:DC:N4	21:U:41:DG:N1	1.92	1.15
2:B:1079:LEU:HD23	2:B:1088:LEU:CB	1.77	1.15
2:B:817:ARG:HB3	21:U:17:DT:C5'	1.77	1.15
1:A:628:PHE:CD2	2:B:784:ASP:CB	2.24	1.14
17:Q:22:ILE:CD1	17:Q:24:ASP:OD1	1.96	1.13
2:B:116:ALA:N	18:R:282:SER:CA	2.01	1.13
1:A:476:VAL:HA	2:B:1095:SER:O	1.47	1.12
1:A:1238:MET:HB2	1:A:1521:THR:CB	1.79	1.12
2:B:1079:LEU:HG	2:B:1088:LEU:HD22	1.19	1.12
17:Q:386:LEU:CA	18:R:241:ARG:HH22	1.59	1.12
2:B:113:VAL:O	18:R:282:SER:HA	1.49	1.12
17:Q:366:TYR:CD2	18:R:215:THR:OG1	2.00	1.12
17:Q:360:LYS:NZ	18:R:211:ARG:NH2	1.96	1.12
2:B:931:TRP:HB3	2:B:936:MET:HE3	1.17	1.11
16:P:435:ARG:NH2	18:R:140:ILE:CD1	2.14	1.11
1:A:508:PRO:HA	1:A:577:VAL:O	1.46	1.11
2:B:116:ALA:N	18:R:282:SER:HB3	1.41	1.11
17:Q:20:TRP:CZ3	17:Q:22:ILE:HG22	1.58	1.11
2:B:116:ALA:CB	18:R:282:SER:O	1.97	1.11
17:Q:134:LYS:O	17:Q:138:LEU:HB2	1.50	1.11
16:P:358:SER:OG	18:R:196:GLU:OE1	1.67	1.10
17:Q:356:VAL:HB	18:R:208:TYR:HA	1.22	1.10
2:B:114:SER:HB3	18:R:282:SER:HA	1.34	1.10
15:O:200:ASN:CB	17:Q:14:ASN:CB	2.28	1.10
2:B:815:ARG:NH2	2:B:821:ILE:HG12	0.77	1.10
17:Q:356:VAL:CG1	18:R:208:TYR:CD1	2.33	1.10
17:Q:26:ARG:HB3	17:Q:34:VAL:HG13	1.12	1.09
17:Q:323:ASP:CA	17:Q:324:ARG:N	2.14	1.09
19:S:3:G:N2	20:T:21:DC:O2	1.84	1.09
1:A:597:LYS:HB2	2:B:1082:HIS:HA	1.33	1.09
16:P:420:GLU:OE2	18:R:3:GLU:OE2	1.68	1.09
16:P:477:TYR:CE2	18:R:2:PHE:CE2	2.40	1.09
1:A:543:LEU:CD2	1:A:578:TYR:OH	2.00	1.09
1:A:651:ALA:HB2	2:B:1084:THR:HG23	1.33	1.09
1:A:1014:SER:HB3	20:T:17:DT:C7	1.83	1.08
17:Q:355:VAL:CG1	18:R:212:HIS:HA	1.82	1.08
15:O:200:ASN:HA	17:Q:14:ASN:HB2	1.24	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1240:LEU:HD11	1:A:1521:THR:CG2	1.84	1.08
15:O:241:ASP:OD1	15:O:380:SER:HB2	1.50	1.08
17:Q:9:ILE:HG13	17:Q:10:CYS:H	1.06	1.08
17:Q:258:MET:HE2	17:Q:438:PHE:HE2	1.16	1.08
17:Q:17:SER:O	17:Q:29:CYS:HB2	1.55	1.07
2:B:1093:LEU:HD12	2:B:1098:TYR:HB2	1.36	1.06
1:A:627:ASP:HA	2:B:784:ASP:OD1	1.54	1.06
1:A:1654:PHE:CE2	6:F:89:GLU:HA	1.90	1.06
15:O:491:PHE:HE2	15:O:502:LEU:HD11	1.19	1.06
16:P:477:TYR:HE2	18:R:2:PHE:CE2	1.72	1.06
2:B:113:VAL:HG11	20:T:39:DT:H4'	1.06	1.06
2:B:115:SER:O	18:R:280:SER:CB	2.02	1.06
17:Q:366:TYR:CD1	18:R:215:THR:CG2	2.38	1.06
2:B:320:LEU:HD23	2:B:325:GLN:HB3	1.31	1.06
16:P:189:THR:HG22	16:P:247:ILE:HG23	1.34	1.06
1:A:651:ALA:HB3	2:B:1084:THR:HG21	1.30	1.05
2:B:1084:THR:HB	2:B:1087:LEU:CD2	1.85	1.05
16:P:435:ARG:NH2	18:R:140:ILE:HD13	1.68	1.05
2:B:815:ARG:HH12	2:B:899:GLN:HG3	1.21	1.05
17:Q:366:TYR:CG	18:R:215:THR:CG2	2.38	1.05
1:A:628:PHE:HD2	2:B:784:ASP:HB2	0.91	1.05
16:P:55:LEU:HB3	18:R:227:HIS:CE1	1.90	1.05
16:P:389:TRP:CZ2	18:R:147:GLN:N	2.24	1.05
17:Q:15:CYS:HB3	17:Q:17:SER:N	1.70	1.05
1:A:628:PHE:HB2	2:B:785:ASP:H	1.12	1.05
18:R:350:SER:O	18:R:354:LEU:HB2	1.56	1.05
1:A:543:LEU:HD21	1:A:578:TYR:OH	1.57	1.04
15:O:491:PHE:HB3	15:O:498:TRP:HZ3	1.20	1.04
17:Q:5:ILE:O	17:Q:19:LEU:O	1.74	1.04
2:B:113:VAL:HG11	20:T:39:DT:C4'	1.87	1.04
15:O:492:ARG:HG2	15:O:496:GLY:CA	1.86	1.04
17:Q:186:CYS:CB	18:R:208:TYR:CE2	2.41	1.04
2:B:116:ALA:HB2	18:R:282:SER:C	1.76	1.04
16:P:389:TRP:HZ2	18:R:146:SER:CA	1.68	1.04
17:Q:186:CYS:HB3	18:R:208:TYR:CZ	1.93	1.04
17:Q:323:ASP:C	17:Q:324:ARG:CA	2.24	1.04
2:B:117:VAL:HG22	18:R:276:GLN:HG3	1.08	1.04
15:O:492:ARG:CG	15:O:496:GLY:CA	2.34	1.04
19:S:5:G:N2	20:T:19:DC:C2	2.26	1.03
2:B:1063:ARG:HG3	20:T:22:DG:OP2	1.57	1.03
15:O:492:ARG:HG3	15:O:496:GLY:O	1.57	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:356:VAL:CB	18:R:208:TYR:CD2	2.39	1.03
17:Q:386:LEU:HD12	18:R:241:ARG:NH2	1.73	1.03
17:Q:356:VAL:HG11	18:R:208:TYR:CG	1.94	1.02
2:B:1079:LEU:HG	2:B:1088:LEU:CD2	1.84	1.02
2:B:1096:SER:O	2:B:1097:ASP:CB	2.06	1.02
1:A:651:ALA:CB	2:B:1084:THR:CG2	2.25	1.02
1:A:672:ASP:N	2:B:783:MET:HE1	1.74	1.02
1:A:953:GLU:OE2	2:B:519:LYS:NZ	1.93	1.02
17:Q:357:TYR:CD2	17:Q:489:VAL:HG22	1.93	1.02
2:B:321:GLN:N	2:B:325:GLN:OE1	1.92	1.01
1:A:1014:SER:CA	20:T:17:DT:C6	2.43	1.01
2:B:114:SER:HB3	18:R:282:SER:CA	1.89	1.01
2:B:1084:THR:C	2:B:1088:LEU:HG	1.80	1.01
16:P:435:ARG:HH21	18:R:140:ILE:CD1	1.69	1.01
16:P:443:ASP:HB2	18:R:2:PHE:HB3	1.42	1.01
16:P:389:TRP:CZ2	18:R:146:SER:CB	2.44	1.01
1:A:547:ILE:HD12	17:Q:26:ARG:HH22	1.20	1.00
2:B:1068:GLY:O	2:B:1069:ILE:HD13	1.59	1.00
2:B:116:ALA:N	18:R:282:SER:N	2.07	1.00
2:B:785:ASP:OD2	2:B:926:VAL:HB	1.62	1.00
2:B:817:ARG:HB2	21:U:17:DT:C5'	1.90	1.00
2:B:1084:THR:OG1	2:B:1088:LEU:HD21	1.61	1.00
16:P:443:ASP:CB	18:R:3:GLU:N	2.18	1.00
16:P:625:ASP:O	16:P:629:ARG:HB2	1.61	1.00
17:Q:378:LEU:HD11	18:R:231:LEU:HD21	1.02	1.00
2:B:115:SER:C	18:R:280:SER:CB	2.27	1.00
17:Q:9:ILE:HG13	17:Q:10:CYS:N	1.77	1.00
20:T:11:DA:C2	20:T:12:DC:C2	2.50	1.00
1:A:672:ASP:CB	2:B:783:MET:CE	2.40	1.00
17:Q:22:ILE:CD1	17:Q:26:ARG:NE	2.25	1.00
1:A:1506:ARG:O	1:A:1522:GLU:HG3	1.61	0.99
1:A:672:ASP:HB2	2:B:783:MET:HE1	1.41	0.99
17:Q:12:THR:CB	17:Q:33:HIS:CE1	2.44	0.99
2:B:1079:LEU:HD23	2:B:1088:LEU:HB3	1.00	0.99
17:Q:9:ILE:HB	17:Q:16:PRO:HB2	1.43	0.99
16:P:186:TYR:HB3	18:R:198:LEU:CD2	1.93	0.98
17:Q:360:LYS:HZ3	18:R:211:ARG:NH2	1.56	0.98
1:A:511:VAL:O	1:A:574:ASN:ND2	1.96	0.98
1:A:672:ASP:HB2	2:B:783:MET:CE	1.94	0.97
17:Q:356:VAL:CB	18:R:208:TYR:CG	2.46	0.97
17:Q:366:TYR:CE2	18:R:215:THR:OG1	2.11	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:9:DC:H2''	20:T:10:DA:H8	1.28	0.97
1:A:511:VAL:HG13	1:A:574:ASN:HB2	1.47	0.97
1:A:1654:PHE:HB2	6:F:134:ILE:HG23	1.47	0.97
1:A:1021:ARG:NH2	20:T:16:DT:OP1	1.98	0.96
15:O:491:PHE:HE2	15:O:502:LEU:CD1	1.77	0.96
1:A:1641:ILE:H	1:A:1641:ILE:HD12	1.29	0.96
1:A:463:LYS:NZ	20:T:16:DT:H6	1.63	0.96
17:Q:15:CYS:SG	17:Q:17:SER:HB2	2.05	0.96
1:A:642:ASN:HB3	2:B:1086:PHE:CD2	2.00	0.96
1:A:671:GLN:HB2	2:B:783:MET:HE2	1.47	0.96
1:A:1018:TYR:CE1	20:T:16:DT:C5'	2.48	0.96
2:B:114:SER:CB	18:R:282:SER:CA	2.44	0.96
17:Q:356:VAL:HB	18:R:208:TYR:CA	1.94	0.96
11:K:104:ARG:HH21	11:K:106:GLN:HE21	1.13	0.96
1:A:628:PHE:HB3	2:B:785:ASP:CG	1.86	0.95
2:B:894:LYS:HZ2	17:Q:405:ASP:HB3	1.31	0.95
2:B:817:ARG:HB2	21:U:17:DT:H5''	1.46	0.95
2:B:929:ARG:HH12	11:K:96:PRO:HB2	1.30	0.95
16:P:477:TYR:CE2	18:R:2:PHE:HE2	1.83	0.95
1:A:712:ILE:H	11:K:106:GLN:HE22	1.15	0.95
2:B:101:GLN:HE21	18:R:359:MET:CE	1.70	0.95
17:Q:22:ILE:HD11	17:Q:26:ARG:NE	1.81	0.95
1:A:1014:SER:HB3	20:T:17:DT:C5	2.02	0.94
16:P:389:TRP:CZ2	18:R:146:SER:HB2	2.01	0.94
17:Q:366:TYR:CE1	18:R:215:THR:HA	2.03	0.94
1:A:475:ARG:O	2:B:1095:SER:O	1.86	0.94
1:A:672:ASP:CB	2:B:783:MET:HE1	1.96	0.94
2:B:320:LEU:HD21	2:B:325:GLN:C	1.87	0.94
17:Q:381:MET:HG3	18:R:238:THR:HG21	1.48	0.94
1:A:1240:LEU:CD1	1:A:1521:THR:HG23	1.98	0.94
2:B:320:LEU:CD2	2:B:325:GLN:HB3	1.98	0.94
2:B:1104:CYS:CB	2:B:1107:CYS:SG	2.55	0.93
16:P:725:VAL:CG2	17:Q:446:TYR:CG	2.42	0.93
17:Q:356:VAL:CB	18:R:208:TYR:HA	1.99	0.93
2:B:1058:GLN:HG2	2:B:1096:SER:O	1.67	0.93
17:Q:9:ILE:CG1	17:Q:10:CYS:H	1.79	0.93
1:A:1018:TYR:CD1	20:T:16:DT:C5'	2.51	0.93
2:B:1104:CYS:HB3	2:B:1107:CYS:SG	2.08	0.93
17:Q:386:LEU:HA	18:R:241:ARG:CZ	1.98	0.93
2:B:213:HIS:CD2	2:B:643:PHE:HZ	1.87	0.93
1:A:618:TYR:CE1	2:B:783:MET:HB3	2.03	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:386:LEU:CB	18:R:241:ARG:HH22	1.80	0.92
16:P:389:TRP:CZ2	18:R:146:SER:CA	2.52	0.92
1:A:1654:PHE:CZ	6:F:89:GLU:CA	2.52	0.92
17:Q:15:CYS:CB	17:Q:16:PRO:HA	1.99	0.92
18:R:168:ILE:HG23	18:R:169:PRO:HD3	1.52	0.92
15:O:491:PHE:HB3	15:O:498:TRP:CZ3	2.04	0.92
17:Q:155:GLN:HA	20:T:49:DC:H2"	1.53	0.91
1:A:70:LYS:NZ	17:Q:27:ARG:NH1	2.18	0.91
2:B:320:LEU:CD2	2:B:325:GLN:CB	2.48	0.91
17:Q:356:VAL:HB	18:R:208:TYR:CG	2.05	0.91
17:Q:356:VAL:CG1	18:R:208:TYR:CG	2.52	0.91
17:Q:357:TYR:CD2	17:Q:489:VAL:HA	2.05	0.91
17:Q:378:LEU:HD11	18:R:231:LEU:CD2	1.97	0.91
17:Q:186:CYS:HB3	18:R:208:TYR:HE2	1.29	0.91
2:B:117:VAL:CG1	18:R:277:ILE:HA	2.01	0.91
16:P:389:TRP:HE1	18:R:146:SER:HB2	1.29	0.91
17:Q:15:CYS:HB3	17:Q:16:PRO:CA	2.00	0.91
1:A:672:ASP:OD1	2:B:952:HIS:HD2	1.54	0.91
2:B:115:SER:O	18:R:280:SER:CA	2.17	0.91
2:B:894:LYS:NZ	17:Q:405:ASP:CB	2.34	0.91
16:P:662:LEU:HB3	16:P:665:ASN:HB2	1.52	0.91
1:A:1240:LEU:HD11	1:A:1521:THR:HG21	1.51	0.91
17:Q:22:ILE:HD12	17:Q:24:ASP:OD1	1.68	0.91
17:Q:353:VAL:HG12	17:Q:489:VAL:CG1	2.00	0.91
2:B:101:GLN:HE22	18:R:359:MET:CE	1.80	0.90
17:Q:26:ARG:CB	17:Q:34:VAL:HG13	1.99	0.90
1:A:637:PHE:H	2:B:1091:ARG:HH22	1.14	0.90
2:B:1084:THR:HB	2:B:1087:LEU:HD22	1.49	0.90
1:A:628:PHE:HD2	2:B:784:ASP:HB3	1.35	0.90
2:B:114:SER:HB3	18:R:282:SER:C	1.91	0.90
16:P:477:TYR:CE2	18:R:2:PHE:CZ	2.58	0.90
2:B:950:ASN:OD1	2:B:952:HIS:HD2	1.54	0.90
17:Q:19:LEU:HD11	17:Q:27:ARG:HB3	1.54	0.90
17:Q:262:LEU:O	17:Q:446:TYR:OH	1.90	0.90
16:P:532:GLU:HA	16:P:554:ASN:HD22	1.37	0.89
16:P:358:SER:HB3	16:P:377:ARG:HD3	1.55	0.89
20:T:11:DA:C6	20:T:12:DC:C4	2.60	0.89
1:A:354:SER:OG	1:A:355:PHE:CD1	2.25	0.89
17:Q:350:ARG:CD	17:Q:486:GLN:HG2	2.03	0.89
2:B:1084:THR:HB	2:B:1087:LEU:HD23	1.53	0.89
17:Q:20:TRP:CZ3	17:Q:22:ILE:HG21	2.08	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:350:ARG:NH1	17:Q:486:GLN:OE1	2.05	0.89
2:B:950:ASN:OD1	2:B:952:HIS:CD2	2.26	0.89
15:O:527:MET:SD	15:O:530:ARG:NH2	2.46	0.89
16:P:55:LEU:CB	18:R:227:HIS:CE1	2.55	0.89
17:Q:313:THR:O	17:Q:317:MET:HB2	1.71	0.89
2:B:776:ILE:C	2:B:951:PRO:HD3	1.93	0.89
1:A:1014:SER:CB	20:T:17:DT:C7	2.50	0.88
17:Q:3:THR:HG22	17:Q:20:TRP:HB2	1.53	0.88
17:Q:258:MET:CE	17:Q:438:PHE:HE2	1.85	0.88
2:B:284:SER:HB2	9:I:14:GLY:HA3	1.55	0.88
20:T:9:DC:H2''	20:T:10:DA:C8	2.08	0.88
20:T:9:DC:N4	21:U:41:DG:C6	2.40	0.88
2:B:711:GLN:HG2	2:B:713:PRO:HD2	1.55	0.88
2:B:1084:THR:O	2:B:1088:LEU:HG	0.71	0.88
1:A:1637:PRO:CB	1:A:1647:ASN:HD21	1.87	0.88
2:B:114:SER:CB	18:R:282:SER:C	2.42	0.88
1:A:646:GLU:CG	1:A:650:LEU:HD12	2.02	0.88
15:O:491:PHE:CE2	15:O:502:LEU:HD11	2.08	0.88
1:A:70:LYS:HZ3	17:Q:27:ARG:HH12	0.88	0.87
16:P:186:TYR:HB3	18:R:198:LEU:HD23	1.54	0.87
1:A:1486:VAL:HG23	9:I:51:THR:HG22	1.57	0.87
1:A:1654:PHE:CE2	6:F:89:GLU:CA	2.55	0.87
17:Q:20:TRP:CH2	17:Q:22:ILE:CG2	2.56	0.87
1:A:1506:ARG:O	1:A:1522:GLU:CG	2.23	0.87
2:B:776:ILE:O	2:B:951:PRO:HD3	1.75	0.87
15:O:492:ARG:HG2	15:O:496:GLY:HA2	0.89	0.87
17:Q:360:LYS:HZ1	18:R:211:ARG:NH2	1.69	0.87
1:A:672:ASP:OD1	2:B:952:HIS:NE2	2.07	0.87
17:Q:29:CYS:SG	17:Q:33:HIS:HB2	2.15	0.87
2:B:320:LEU:HD13	2:B:326:VAL:HG22	1.57	0.86
16:P:196:TYR:O	16:P:197:ARG:NH1	2.07	0.86
17:Q:12:THR:CB	17:Q:33:HIS:ND1	2.37	0.86
1:A:672:ASP:CA	2:B:783:MET:HE1	2.04	0.86
1:A:707:THR:HG22	1:A:709:ARG:H	1.40	0.86
1:A:618:TYR:CE1	2:B:783:MET:CB	2.58	0.86
1:A:1014:SER:CB	20:T:17:DT:C5	2.57	0.86
1:A:508:PRO:CA	1:A:577:VAL:O	2.23	0.86
2:B:1096:SER:O	2:B:1097:ASP:OD1	1.91	0.86
13:M:38:PHE:HB3	13:M:53:LEU:HD11	1.55	0.86
2:B:816:ASN:HB3	21:U:18:DG:OP1	1.76	0.86
1:A:637:PHE:N	2:B:1091:ARG:HH22	1.72	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:CYS:HB3	1:A:75:HIS:NE2	1.91	0.85
17:Q:258:MET:HE2	17:Q:438:PHE:CE2	2.09	0.85
16:P:55:LEU:CB	18:R:227:HIS:ND1	2.38	0.85
1:A:672:ASP:CA	2:B:783:MET:CE	2.55	0.85
2:B:320:LEU:HD23	2:B:325:GLN:CB	2.05	0.85
19:S:5:G:N1	20:T:19:DC:N3	2.23	0.85
1:A:700:ILE:O	1:A:706:HIS:ND1	2.09	0.85
16:P:725:VAL:CG2	17:Q:446:TYR:CB	2.54	0.85
1:A:628:PHE:HB2	2:B:785:ASP:N	1.90	0.85
16:P:725:VAL:CG2	17:Q:446:TYR:HB3	2.07	0.85
17:Q:350:ARG:HD3	17:Q:486:GLN:HG2	1.56	0.85
17:Q:385:PHE:O	18:R:241:ARG:CZ	2.25	0.85
16:P:725:VAL:HG21	17:Q:446:TYR:HD1	1.02	0.84
2:B:894:LYS:NZ	17:Q:405:ASP:HB3	1.91	0.84
1:A:70:LYS:HZ3	17:Q:27:ARG:NH1	1.72	0.84
2:B:894:LYS:CE	17:Q:405:ASP:OD2	2.21	0.84
16:P:389:TRP:CE2	18:R:146:SER:CB	2.60	0.84
15:O:200:ASN:CA	17:Q:14:ASN:CB	2.54	0.84
15:O:488:HIS:HB2	15:O:531:ILE:HG21	1.59	0.84
1:A:1637:PRO:CG	1:A:1647:ASN:HD21	1.90	0.84
17:Q:353:VAL:HG12	17:Q:489:VAL:HG13	1.59	0.84
17:Q:381:MET:HG3	18:R:238:THR:CG2	2.07	0.84
1:A:597:LYS:HB2	2:B:1082:HIS:CA	2.07	0.84
16:P:446:ASP:HA	18:R:200:THR:HG22	1.60	0.84
17:Q:15:CYS:HB3	17:Q:16:PRO:C	1.98	0.84
1:A:463:LYS:NZ	20:T:16:DT:C6	2.41	0.84
1:A:1238:MET:O	1:A:1521:THR:OG1	1.96	0.83
1:A:1013:THR:HB	20:T:17:DT:H3	1.42	0.83
1:A:1014:SER:O	20:T:17:DT:H5'	1.78	0.83
2:B:213:HIS:CD2	2:B:643:PHE:CZ	2.67	0.83
15:O:491:PHE:HD2	15:O:498:TRP:HE3	1.25	0.83
16:P:55:LEU:HG	18:R:227:HIS:CB	2.07	0.83
16:P:443:ASP:HB2	18:R:2:PHE:CB	2.08	0.83
20:T:11:DA:C6	20:T:12:DC:N4	2.46	0.83
2:B:1063:ARG:CG	20:T:22:DG:OP2	2.27	0.83
1:A:1637:PRO:HG3	1:A:1647:ASN:ND2	1.93	0.83
2:B:931:TRP:CB	2:B:936:MET:CE	2.53	0.83
16:P:725:VAL:HG23	17:Q:446:TYR:HB3	1.58	0.82
18:R:373:LEU:HD12	18:R:411:VAL:HG21	1.61	0.82
13:M:38:PHE:HB2	14:N:119:LEU:HB2	1.58	0.82
2:B:518:ARG:HB3	2:B:540:GLY:HA3	1.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:200:ASN:HA	17:Q:14:ASN:CB	2.08	0.82
1:A:486:PRO:HG2	2:B:781:TYR:O	1.78	0.82
1:A:547:ILE:HD12	17:Q:26:ARG:NH2	1.92	0.82
2:B:117:VAL:HG12	18:R:277:ILE:HA	1.59	0.82
17:Q:15:CYS:HB3	17:Q:16:PRO:HA	1.60	0.82
2:B:116:ALA:H	18:R:282:SER:HB3	1.07	0.82
17:Q:20:TRP:CE3	17:Q:22:ILE:HG23	2.15	0.82
2:B:815:ARG:HH12	2:B:899:GLN:CG	1.92	0.82
17:Q:26:ARG:CB	17:Q:34:VAL:CG1	2.53	0.82
1:A:628:PHE:CD2	2:B:784:ASP:HB3	2.09	0.82
17:Q:350:ARG:NE	17:Q:486:GLN:HG2	1.93	0.82
18:R:171:ARG:O	18:R:174:GLU:N	2.11	0.82
1:A:1246:VAL:HG13	1:A:1250:GLN:HB3	1.61	0.82
2:B:894:LYS:HZ1	17:Q:405:ASP:CG	1.81	0.82
1:A:1014:SER:HA	20:T:17:DT:N1	1.94	0.81
2:B:818:GLY:O	2:B:820:PRO:CD	2.28	0.81
17:Q:20:TRP:HZ3	17:Q:22:ILE:HG22	0.65	0.81
16:P:188:GLN:HG2	16:P:360:TRP:HB3	1.61	0.81
16:P:662:LEU:HB2	16:P:665:ASN:HD22	1.45	0.81
17:Q:357:TYR:CG	17:Q:489:VAL:HG22	2.15	0.81
1:A:550:SER:H	1:A:553:GLN:HE22	1.28	0.81
1:A:1637:PRO:HG3	1:A:1647:ASN:HD21	1.42	0.81
16:P:346:ASN:OD1	16:P:347:LEU:N	2.12	0.81
1:A:477:ASN:H	2:B:1095:SER:CB	1.91	0.81
1:A:628:PHE:HB2	2:B:784:ASP:HB3	1.61	0.81
1:A:1654:PHE:CD2	6:F:89:GLU:HG2	2.15	0.81
2:B:817:ARG:CB	21:U:17:DT:H5"	2.04	0.81
15:O:491:PHE:HD2	15:O:498:TRP:CE3	1.98	0.81
17:Q:350:ARG:CZ	17:Q:486:GLN:OE1	2.29	0.81
1:A:597:LYS:O	2:B:1082:HIS:NE2	2.13	0.81
1:A:1031:HIS:N	1:A:1039:ARG:O	2.11	0.81
2:B:1096:SER:C	2:B:1097:ASP:OD1	2.19	0.81
16:P:355:GLU:HB3	18:R:24:ILE:HD12	1.62	0.81
1:A:1014:SER:HA	20:T:17:DT:C5	2.13	0.81
1:A:642:ASN:ND2	2:B:1086:PHE:HE2	1.77	0.80
16:P:487:ASN:HB3	18:R:138:PHE:CZ	2.13	0.80
16:P:245:ILE:HD12	16:P:269:PHE:HD2	1.43	0.80
1:A:597:LYS:CB	2:B:1082:HIS:HA	2.12	0.80
1:A:1240:LEU:CD1	1:A:1521:THR:CG2	2.57	0.80
16:P:435:ARG:HH21	18:R:140:ILE:HD11	1.43	0.80
18:R:250:LEU:HD21	18:R:307:LYS:HG2	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:LEU:HD12	1:A:82:PRO:HD2	1.63	0.80
1:A:600:MET:HB3	2:B:1082:HIS:HD2	1.44	0.80
1:A:1654:PHE:CD2	6:F:89:GLU:CG	2.65	0.80
1:A:1014:SER:CA	20:T:17:DT:C5	2.65	0.80
12:L:48:CYS:HB3	12:L:52:GLY:H	1.45	0.80
19:S:4:C:O2	20:T:20:DG:N2	2.14	0.80
1:A:102:CYS:SG	1:A:105:CYS:N	2.54	0.80
1:A:587:VAL:HG12	1:A:637:PHE:HD1	1.47	0.80
1:A:600:MET:HB3	2:B:1082:HIS:CD2	2.17	0.80
1:A:638:PRO:CG	2:B:1087:LEU:CD1	2.60	0.80
2:B:1093:LEU:HD11	2:B:1098:TYR:HB2	1.64	0.80
15:O:492:ARG:HG3	15:O:496:GLY:C	2.03	0.80
1:A:527:PRO:HD3	1:A:554:ARG:HH12	1.46	0.79
1:A:547:ILE:HD11	17:Q:26:ARG:HH22	1.46	0.79
2:B:1049:THR:OG1	17:Q:24:ASP:HB2	1.82	0.79
6:F:99:LEU:HD23	7:G:112:PRO:HD3	1.64	0.79
18:R:11:ARG:NH1	21:U:4:DA:P	2.51	0.79
1:A:646:GLU:HG3	1:A:650:LEU:CD1	2.08	0.79
2:B:1079:LEU:CG	2:B:1088:LEU:HB3	2.07	0.79
20:T:11:DA:N1	20:T:12:DC:N3	2.31	0.79
1:A:1014:SER:HB3	20:T:17:DT:H73	1.64	0.79
2:B:954:PHE:O	2:B:956:SER:N	2.15	0.79
2:B:1075:GLU:O	2:B:1079:LEU:HD13	1.81	0.79
18:R:78:ARG:NH2	20:T:43:DT:H5"	1.97	0.79
21:U:38:DG:C2	21:U:39:DT:O2	2.35	0.79
16:P:375:PHE:HD2	16:P:402:ILE:HD13	1.48	0.79
16:P:389:TRP:CH2	18:R:147:GLN:N	2.50	0.79
16:P:577:LEU:O	17:Q:506:LYS:NZ	2.15	0.79
18:R:26:TYR:HB3	18:R:169:PRO:HB3	1.63	0.79
1:A:354:SER:OG	1:A:355:PHE:HD1	1.63	0.79
1:A:1322:ILE:HG21	1:A:1457:ILE:HD11	1.62	0.79
16:P:477:TYR:HE2	18:R:2:PHE:CZ	1.98	0.79
1:A:1238:MET:C	1:A:1521:THR:OG1	2.22	0.79
15:O:491:PHE:CE2	15:O:502:LEU:CD1	2.66	0.79
2:B:492:ASN:ND2	2:B:722:GLY:O	2.16	0.78
2:B:816:ASN:CB	21:U:18:DG:OP1	2.31	0.78
17:Q:192:TYR:HD1	17:Q:193:PHE:H	1.29	0.78
1:A:1038:ILE:HB	1:A:1047:GLN:H	1.48	0.78
1:A:1303:SER:HA	1:A:1308:VAL:H	1.48	0.78
15:O:434:LEU:HD22	15:O:439:ILE:HD11	1.65	0.78
17:Q:366:TYR:CZ	18:R:215:THR:HA	2.17	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:511:VAL:HG12	1:A:575:LYS:C	2.02	0.78
16:P:484:ARG:HB2	16:P:488:LEU:HB3	1.64	0.78
20:T:8:DT:H2'	20:T:9:DC:C6	2.17	0.78
1:A:1013:THR:HB	20:T:17:DT:N3	1.98	0.78
2:B:1086:PHE:HZ	7:G:109:PRO:O	1.67	0.78
17:Q:17:SER:O	17:Q:29:CYS:CB	2.30	0.78
17:Q:323:ASP:C	17:Q:324:ARG:HA	2.04	0.78
18:R:11:ARG:NH1	21:U:4:DA:OP2	2.17	0.78
1:A:321:LYS:HE3	1:A:325:ASP:OD2	1.84	0.78
16:P:245:ILE:HD12	16:P:269:PHE:CD2	2.19	0.78
19:S:4:C:O2	20:T:20:DG:N1	2.17	0.78
1:A:1258:ILE:HD11	1:A:1507:CYS:SG	2.23	0.78
7:G:237:HIS:HB2	7:G:244:SER:HB3	1.66	0.78
1:A:642:ASN:CG	2:B:1086:PHE:HE2	1.87	0.77
16:P:247:ILE:HG22	16:P:248:PRO:HD3	1.64	0.77
16:P:443:ASP:HB3	18:R:3:GLU:HB3	1.66	0.77
16:P:596:ILE:HA	16:P:599:LYS:HB3	1.65	0.77
18:R:158:THR:HG23	18:R:161:ASN:HB3	1.66	0.77
1:A:1014:SER:CB	20:T:17:DT:H71	2.14	0.77
9:I:28:VAL:N	9:I:37:TYR:O	2.16	0.77
2:B:641:TYR:HB3	2:B:643:PHE:CE1	2.19	0.77
2:B:818:GLY:O	2:B:820:PRO:HD3	1.85	0.77
16:P:389:TRP:HH2	18:R:149:LYS:H	1.31	0.77
17:Q:12:THR:OG1	17:Q:33:HIS:ND1	2.17	0.77
7:G:140:GLN:NE2	7:G:225:ILE:O	2.18	0.77
16:P:585:GLU:HA	16:P:588:SER:HB3	1.66	0.77
2:B:818:GLY:O	2:B:820:PRO:N	2.18	0.77
17:Q:355:VAL:C	18:R:212:HIS:CE1	2.58	0.77
15:O:492:ARG:NH2	15:O:535:GLU:OE1	2.17	0.77
18:R:248:LYS:HA	18:R:298:GLN:NE2	2.00	0.77
9:I:53:ASP:O	9:I:61:ARG:NH2	2.18	0.77
16:P:263:ILE:HG21	16:P:276:SER:HA	1.65	0.77
17:Q:378:LEU:CD1	18:R:231:LEU:CD2	2.57	0.77
1:A:638:PRO:HG3	2:B:1087:LEU:HD11	1.67	0.76
20:T:4:DG:N2	21:U:46:DC:C2	2.33	0.76
2:B:113:VAL:O	18:R:282:SER:CA	2.30	0.76
16:P:214:LEU:HB2	16:P:222:GLN:NE2	1.99	0.76
20:T:11:DA:C2	20:T:12:DC:N3	2.52	0.76
17:Q:386:LEU:CD1	18:R:241:ARG:NH2	2.48	0.76
1:A:1506:ARG:O	1:A:1522:GLU:CD	2.24	0.76
1:A:474:LYS:HD2	2:B:1096:SER:CB	2.14	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:26:ILE:HD12	8:H:42:ILE:HD12	1.65	0.76
16:P:218:VAL:HG23	16:P:219:LEU:HB3	1.68	0.76
16:P:477:TYR:CD2	18:R:2:PHE:CZ	2.73	0.76
17:Q:356:VAL:HG13	18:R:212:HIS:NE2	2.01	0.76
1:A:90:PHE:O	1:A:92:ASN:N	2.19	0.76
2:B:883:GLU:OE1	2:B:906:ARG:NH1	2.19	0.76
2:B:954:PHE:O	2:B:957:ARG:N	2.19	0.76
15:O:392:GLN:HB2	15:O:395:LEU:HD13	1.66	0.76
17:Q:331:ILE:HG22	17:Q:475:ALA:HB1	1.68	0.76
1:A:606:ARG:NH2	11:K:98:GLU:OE2	2.19	0.75
7:G:56:ASN:HB3	7:G:59:GLN:HB3	1.68	0.75
2:B:921:HIS:NE2	2:B:965:GLU:OE1	2.19	0.75
7:G:26:ASN:ND2	7:G:37:CYS:SG	2.58	0.75
7:G:140:GLN:HB3	7:G:217:TRP:HD1	1.49	0.75
1:A:543:LEU:HD22	1:A:578:TYR:OH	1.83	0.75
1:A:642:ASN:HB3	2:B:1086:PHE:HD2	1.48	0.75
18:R:9:THR:HG21	18:R:13:PHE:CD2	2.21	0.75
1:A:545:SER:HB2	17:Q:34:VAL:HG21	1.68	0.75
16:P:357:LEU:HB3	18:R:191:ILE:O	1.85	0.75
1:A:618:TYR:OH	2:B:780:GLY:O	2.03	0.75
2:B:320:LEU:CD2	2:B:325:GLN:C	2.55	0.75
17:Q:357:TYR:HD2	17:Q:489:VAL:HA	1.51	0.75
1:A:1237:GLN:HA	1:A:1521:THR:O	1.87	0.75
1:A:1238:MET:N	1:A:1521:THR:OG1	2.19	0.75
8:H:63:LEU:HB3	8:H:88:SER:HB2	1.67	0.75
17:Q:15:CYS:CB	17:Q:16:PRO:CA	2.62	0.75
9:I:33:CYS:O	13:M:59:ARG:NH1	2.20	0.75
15:O:383:TYR:OH	15:O:595:ASP:N	2.20	0.75
16:P:462:ILE:HB	16:P:483:HIS:HB3	1.69	0.75
1:A:509:GLU:CD	1:A:579:ARG:HE	1.90	0.75
17:Q:22:ILE:HD11	17:Q:24:ASP:OD1	1.86	0.75
2:B:816:ASN:OD1	21:U:18:DG:OP1	2.04	0.75
2:B:1060:VAL:O	2:B:1067:GLY:HA3	1.86	0.75
15:O:241:ASP:CG	15:O:380:SER:HB2	2.07	0.75
17:Q:22:ILE:CG1	17:Q:24:ASP:OD1	2.34	0.75
17:Q:386:LEU:HA	18:R:241:ARG:HH22	0.94	0.75
15:O:492:ARG:O	15:O:493:ASP:O	2.05	0.74
16:P:625:ASP:O	16:P:629:ARG:CB	2.34	0.74
1:A:637:PHE:N	2:B:1091:ARG:NH2	2.33	0.74
17:Q:3:THR:O	17:Q:20:TRP:HB3	1.87	0.74
17:Q:357:TYR:CD2	17:Q:489:VAL:CG2	2.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:815:ARG:NH1	2:B:899:GLN:HG3	2.00	0.74
16:P:358:SER:CB	18:R:196:GLU:OE1	2.35	0.74
1:A:1637:PRO:O	1:A:1641:ILE:N	2.18	0.74
2:B:143:TRP:HB3	2:B:152:LEU:HB2	1.68	0.74
17:Q:378:LEU:HD21	18:R:235:ILE:HD13	1.68	0.74
1:A:672:ASP:H	2:B:783:MET:HE3	0.59	0.74
17:Q:355:VAL:O	18:R:211:ARG:HB3	1.86	0.74
1:A:464:GLU:HB3	1:A:469:LYS:HB2	1.70	0.74
2:B:935:ASP:OD1	3:C:69:ARG:NH1	2.21	0.74
9:I:2:SER:O	9:I:9:PHE:N	2.21	0.74
17:Q:22:ILE:CD1	17:Q:26:ARG:CZ	2.65	0.74
1:A:771:PHE:HE1	1:A:776:LEU:HD13	1.53	0.74
2:B:465:LEU:HA	2:B:485:THR:HG21	1.68	0.74
8:H:106:GLU:HG2	8:H:112:ILE:HG12	1.68	0.74
15:O:444:SER:O	15:O:447:THR:OG1	2.06	0.74
16:P:420:GLU:CD	18:R:3:GLU:OE2	2.26	0.74
2:B:891:GLU:HG2	2:B:892:SER:H	1.52	0.73
16:P:597:LYS:HE3	17:Q:323:ASP:HB3	1.68	0.73
17:Q:155:GLN:HA	20:T:49:DC:C2'	2.18	0.73
17:Q:186:CYS:O	18:R:208:TYR:OH	2.03	0.73
17:Q:323:ASP:HA	17:Q:324:ARG:N	2.01	0.73
17:Q:356:VAL:CG1	18:R:208:TYR:CE1	2.61	0.73
1:A:489:ASN:ND2	2:B:781:TYR:OH	2.21	0.73
1:A:526:GLY:HA2	1:A:554:ARG:CZ	2.18	0.73
1:A:618:TYR:CZ	2:B:783:MET:HB2	2.23	0.73
1:A:637:PHE:O	2:B:1091:ARG:NH1	2.21	0.73
2:B:335:ARG:HG3	2:B:340:ALA:HB3	1.70	0.73
2:B:1079:LEU:HD23	2:B:1088:LEU:CA	2.18	0.73
15:O:181:ARG:HH22	15:O:222:CYS:HA	1.52	0.73
16:P:67:ASP:HA	16:P:545:SER:O	1.88	0.73
18:R:253:ILE:O	18:R:256:GLU:N	2.22	0.73
14:N:157:ARG:NH1	14:N:159:ASP:OD1	2.21	0.73
16:P:435:ARG:NH2	18:R:140:ILE:HD11	1.98	0.73
1:A:550:SER:N	1:A:553:GLN:HE22	1.85	0.73
2:B:1084:THR:OG1	2:B:1088:LEU:CD2	2.36	0.73
3:C:229:LEU:HB2	3:C:293:ARG:HD2	1.69	0.73
15:O:200:ASN:CG	17:Q:14:ASN:HB2	2.09	0.73
1:A:94:LEU:HB2	1:A:355:PHE:CD2	2.23	0.73
3:C:91:VAL:HG21	10:J:60:PHE:HB3	1.69	0.73
20:T:14:DG:N2	21:U:37:DA:C2	2.56	0.73
2:B:212:ASN:HB3	2:B:589:ASP:O	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:626:LEU:HD21	16:P:665:ASN:HA	1.70	0.73
1:A:591:ARG:NH2	19:S:6:A:H1'	2.04	0.73
1:A:636:HIS:HB3	2:B:1091:ARG:HH21	1.54	0.73
2:B:114:SER:OG	18:R:282:SER:C	2.26	0.73
2:B:213:HIS:HD2	2:B:643:PHE:HZ	1.33	0.73
16:P:264:ILE:HG22	16:P:275:GLU:HB2	1.71	0.73
17:Q:258:MET:CE	17:Q:438:PHE:CE2	2.70	0.72
1:A:646:GLU:OE1	1:A:1651:THR:HG21	1.89	0.72
2:B:212:ASN:HB3	2:B:589:ASP:C	2.09	0.72
15:O:492:ARG:HG3	15:O:496:GLY:CA	2.10	0.72
14:N:81:THR:HA	14:N:86:ASP:HA	1.72	0.72
3:C:241:GLY:N	3:C:263:ASP:OD2	2.17	0.72
1:A:597:LYS:O	2:B:1082:HIS:CD2	2.42	0.72
1:A:1319:ASN:O	1:A:1323:HIS:ND1	2.18	0.72
1:A:10:GLU:OE2	1:A:1645:LYS:HG3	1.88	0.72
1:A:637:PHE:H	2:B:1091:ARG:NH2	1.85	0.72
1:A:834:ARG:HH12	2:B:1007:TYR:HE2	1.35	0.72
1:A:1541:ILE:O	5:E:147:HIS:NE2	2.23	0.72
2:B:1017:ALA:O	3:C:65:ASN:ND2	2.22	0.72
9:I:23:VAL:O	9:I:39:LYS:NZ	2.22	0.72
16:P:302:VAL:HG11	16:P:362:ARG:HH11	1.55	0.72
16:P:442:LEU:HA	16:P:443:ASP:OD1	1.90	0.72
16:P:446:ASP:CA	18:R:200:THR:HG22	2.19	0.72
17:Q:12:THR:OG1	17:Q:33:HIS:CE1	2.42	0.72
18:R:252:GLY:O	18:R:256:GLU:HB2	1.89	0.72
1:A:1654:PHE:HB2	6:F:134:ILE:CG2	2.19	0.72
2:B:745:GLN:OE1	3:C:93:GLN:NE2	2.23	0.72
2:B:894:LYS:NZ	17:Q:405:ASP:CG	2.42	0.72
17:Q:356:VAL:HB	18:R:208:TYR:CB	2.20	0.72
1:A:1014:SER:HB2	20:T:17:DT:H71	1.69	0.72
2:B:168:ASN:HA	2:B:173:ASN:HD22	1.53	0.72
8:H:48:PRO:O	8:H:146:ARG:NH2	2.22	0.72
16:P:230:HIS:O	16:P:232:ASN:ND2	2.23	0.72
20:T:11:DA:C5	20:T:12:DC:C4	2.77	0.72
1:A:671:GLN:HB2	2:B:783:MET:CE	2.18	0.72
1:A:672:ASP:HB2	2:B:783:MET:SD	2.28	0.72
18:R:162:PHE:HA	18:R:165:ILE:HD12	1.72	0.72
2:B:1050:GLY:HA2	17:Q:24:ASP:HA	1.71	0.71
16:P:659:LEU:H	16:P:659:LEU:HD13	1.54	0.71
18:R:414:PHE:HA	18:R:417:ILE:HG22	1.70	0.71
1:A:1613:MET:HE3	1:A:1622:LEU:HD13	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:939:SER:HA	2:B:1013:MET:HG2	1.72	0.71
3:C:278:GLU:OE2	3:C:281:ARG:NH1	2.22	0.71
17:Q:322:ARG:O	17:Q:324:ARG:N	2.22	0.71
1:A:474:LYS:HD3	2:B:1096:SER:HB3	0.75	0.71
1:A:1306:TYR:O	1:A:1499:ARG:NH2	2.22	0.71
16:P:420:GLU:O	16:P:441:ASP:HA	1.88	0.71
18:R:303:THR:HA	18:R:358:PHE:CZ	2.25	0.71
7:G:32:ASN:ND2	7:G:34:THR:OG1	2.24	0.71
15:O:389:SER:HA	15:O:395:LEU:HB3	1.71	0.71
1:A:706:HIS:CE1	1:A:815:ARG:HH12	2.09	0.71
1:A:80:GLU:HA	1:A:359:VAL:HG12	1.71	0.71
1:A:642:ASN:HB3	2:B:1086:PHE:CE2	2.25	0.71
2:B:134:ARG:HD3	2:B:160:GLY:HA3	1.72	0.71
2:B:1084:THR:CB	2:B:1087:LEU:HD23	2.20	0.71
3:C:60:ASP:OD2	11:K:78:TYR:OH	2.04	0.71
4:D:47:LYS:NZ	7:G:84:TYR:OH	2.23	0.71
16:P:443:ASP:HB3	18:R:3:GLU:CA	2.21	0.71
1:A:1301:GLU:O	1:A:1305:GLU:N	2.21	0.71
2:B:505:ARG:HB3	2:B:509:PHE:HD2	1.54	0.71
16:P:622:TYR:O	16:P:626:LEU:HB2	1.90	0.71
1:A:973:GLU:HG3	1:A:975:ASP:H	1.55	0.71
1:A:1654:PHE:CE2	6:F:89:GLU:CG	2.74	0.71
2:B:184:LYS:HD2	2:B:735:HIS:CD2	2.25	0.71
3:C:65:ASN:OD1	3:C:68:ARG:NH2	2.24	0.71
1:A:1184:ALA:O	1:A:1188:ILE:HG12	1.91	0.70
2:B:547:HIS:HD1	2:B:760:TYR:HH	1.37	0.70
2:B:1084:THR:CB	2:B:1087:LEU:CD2	2.65	0.70
13:M:40:LEU:HD11	13:M:51:PHE:HB3	1.72	0.70
16:P:315:PHE:HB3	16:P:317:ILE:HD11	1.73	0.70
17:Q:386:LEU:CD1	18:R:241:ARG:HH22	2.03	0.70
20:T:11:DA:C4	20:T:12:DC:C5	2.79	0.70
20:T:12:DC:H2''	20:T:13:DT:H5'	1.72	0.70
2:B:894:LYS:HZ2	17:Q:405:ASP:CB	1.96	0.70
7:G:149:ILE:HB	7:G:153:PHE:HB2	1.73	0.70
15:O:225:LEU:HD11	15:O:228:GLN:HB2	1.73	0.70
15:O:379:ARG:HA	15:O:382:GLN:NE2	2.06	0.70
2:B:17:ARG:NH1	2:B:758:ASP:OD2	2.25	0.70
2:B:213:HIS:HD2	2:B:643:PHE:CZ	2.08	0.70
2:B:1127:CYS:SG	2:B:1171:ASN:ND2	2.63	0.70
17:Q:22:ILE:HD12	17:Q:24:ASP:CG	2.11	0.70
17:Q:350:ARG:CZ	17:Q:486:GLN:CD	2.60	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1641:ILE:HD12	1:A:1641:ILE:N	2.05	0.70
2:B:812:ALA:CB	2:B:815:ARG:HH11	2.04	0.70
16:P:435:ARG:HH21	18:R:140:ILE:HD13	1.33	0.70
2:B:817:ARG:NE	21:U:16:DA:O3'	2.24	0.70
2:B:1075:GLU:O	2:B:1079:LEU:CD1	2.39	0.70
3:C:227:TYR:HB3	3:C:300:PHE:CD1	2.27	0.70
17:Q:355:VAL:CG1	18:R:212:HIS:CA	2.64	0.70
1:A:1248:ASP:N	1:A:1248:ASP:OD1	2.23	0.70
16:P:389:TRP:NE1	18:R:146:SER:CB	2.49	0.70
16:P:719:LEU:HD13	16:P:733:THR:HG21	1.73	0.70
15:O:100:LEU:HD22	15:O:107:ILE:HD11	1.72	0.70
16:P:182:LEU:HD13	16:P:184:SER:H	1.56	0.70
16:P:567:ILE:HB	16:P:569:VAL:HG23	1.74	0.70
1:A:512:THR:HG21	1:A:514:TYR:CE2	2.27	0.70
1:A:526:GLY:HA2	1:A:554:ARG:NH2	2.06	0.70
1:A:627:ASP:CA	2:B:784:ASP:OD1	2.35	0.70
15:O:104:ILE:HD12	15:O:107:ILE:HD12	1.72	0.70
1:A:403:LEU:HB2	1:A:419:ILE:HG21	1.74	0.70
16:P:355:GLU:HA	18:R:24:ILE:HD12	1.74	0.70
17:Q:286:LEU:HB3	17:Q:300:ASN:HB3	1.73	0.70
1:A:7:VAL:HG21	2:B:1177:ALA:HB2	1.73	0.69
1:A:1047:GLN:NE2	1:A:1587:ASP:OD2	2.25	0.69
2:B:731:VAL:HA	10:J:60:PHE:HE1	1.55	0.69
2:B:895:PHE:CE2	20:T:39:DT:OP1	2.45	0.69
5:E:17:ARG:HH12	5:E:36:GLU:HA	1.55	0.69
17:Q:245:SER:HB3	17:Q:284:LEU:HD13	1.73	0.69
1:A:1641:ILE:H	1:A:1641:ILE:CD1	1.98	0.69
17:Q:192:TYR:HD1	17:Q:193:PHE:N	1.89	0.69
1:A:30:LYS:NZ	1:A:51:ASP:OD2	2.25	0.69
1:A:647:ALA:O	1:A:652:ASN:ND2	2.26	0.69
17:Q:186:CYS:SG	18:R:208:TYR:CE2	2.85	0.69
17:Q:322:ARG:C	17:Q:324:ARG:N	2.46	0.69
1:A:597:LYS:HD3	2:B:1081:GLY:O	1.92	0.69
2:B:117:VAL:HB	18:R:277:ILE:CA	2.14	0.69
2:B:1065:ARG:O	2:B:1066:HIS:HB2	1.92	0.69
17:Q:22:ILE:HG13	17:Q:24:ASP:OD1	1.92	0.69
1:A:597:LYS:HD2	2:B:1082:HIS:HA	1.74	0.69
2:B:795:GLU:OE1	3:C:217:ALA:N	2.24	0.69
2:B:816:ASN:CG	21:U:18:DG:OP1	2.31	0.69
1:A:527:PRO:HD3	1:A:554:ARG:HH22	1.57	0.69
2:B:116:ALA:N	18:R:282:SER:C	2.45	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:274:ILE:HD13	16:P:305:PHE:HE2	1.58	0.69
1:A:638:PRO:HG3	2:B:1087:LEU:CD1	2.22	0.69
1:A:646:GLU:CD	1:A:1651:THR:HG21	2.13	0.69
1:A:1259:SER:OG	1:A:1260:LYS:N	2.22	0.69
9:I:26:SER:HA	9:I:39:LYS:HE2	1.73	0.69
16:P:405:TYR:HB2	16:P:416:LEU:HD12	1.75	0.69
16:P:487:ASN:HB3	18:R:138:PHE:CE1	2.27	0.69
17:Q:183:LYS:O	17:Q:187:THR:OG1	2.11	0.69
2:B:480:GLN:OE1	2:B:507:SER:N	2.24	0.69
2:B:1060:VAL:O	2:B:1067:GLY:CA	2.41	0.69
16:P:186:TYR:CB	18:R:198:LEU:HD23	2.21	0.69
16:P:446:ASP:N	18:R:200:THR:CG2	2.55	0.69
16:P:473:HIS:NE2	18:R:1:MET:HB2	2.08	0.69
1:A:593:PRO:HD3	19:S:6:A:H2	1.58	0.69
1:A:641:GLU:HB2	6:F:99:LEU:HD12	1.75	0.69
16:P:446:ASP:N	18:R:200:THR:HG22	2.08	0.69
17:Q:360:LYS:HZ3	18:R:211:ARG:HH22	0.71	0.69
16:P:275:GLU:HG3	16:P:288:SER:HA	1.76	0.68
16:P:675:PHE:HE2	16:P:741:ILE:HG21	1.57	0.68
1:A:587:VAL:HG12	1:A:637:PHE:CD1	2.27	0.68
1:A:1619:CYS:O	1:A:1623:THR:N	2.19	0.68
2:B:698:SER:O	2:B:702:ASN:ND2	2.25	0.68
9:I:28:VAL:HG23	9:I:39:LYS:HA	1.74	0.68
16:P:218:VAL:HB	16:P:245:ILE:HG23	1.76	0.68
18:R:349:ILE:O	18:R:353:VAL:HB	1.93	0.68
1:A:628:PHE:CB	2:B:785:ASP:H	2.00	0.68
8:H:8:ASP:OD1	8:H:9:ILE:N	2.25	0.68
16:P:592:LEU:HA	16:P:595:GLN:HB2	1.74	0.68
18:R:264:SER:O	18:R:266:SER:OG	2.09	0.68
18:R:365:TRP:HB3	18:R:418:CYS:HB2	1.76	0.68
2:B:1107:CYS:O	2:B:1195:ARG:NH2	2.25	0.68
3:C:216:HIS:ND1	3:C:218:LYS:HG2	2.09	0.68
3:C:232:GLN:N	3:C:292:GLY:O	2.27	0.68
1:A:65:CYS:CB	1:A:75:HIS:NE2	2.54	0.68
1:A:407:GLN:O	1:A:411:VAL:N	2.25	0.68
1:A:511:VAL:HG11	1:A:575:LYS:N	2.08	0.68
2:B:924:LYS:NZ	19:S:6:A:OP1	2.25	0.68
2:B:934:ILE:HB	3:C:69:ARG:HD2	1.73	0.68
2:B:1189:LEU:HD12	2:B:1196:LEU:HD11	1.74	0.68
6:F:58:PHE:HA	6:F:61:HIS:CE1	2.28	0.68
17:Q:353:VAL:CG1	17:Q:489:VAL:CG1	2.71	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:356:VAL:HG11	18:R:208:TYR:CZ	2.27	0.68
15:O:461:VAL:HG11	15:O:513:LYS:HB3	1.75	0.68
1:A:862:THR:O	1:A:878:ARG:NH1	2.26	0.68
2:B:1093:LEU:CD1	2:B:1098:TYR:CB	2.62	0.68
2:B:1105:ARG:NH1	2:B:1172:GLU:OE1	2.26	0.68
9:I:3:VAL:HG22	9:I:8:ILE:HG23	1.75	0.68
1:A:1003:ARG:NH2	2:B:540:GLY:HA2	2.09	0.68
15:O:487:ARG:HH21	15:O:502:LEU:HD13	1.57	0.68
17:Q:162:ILE:HG21	17:Q:226:LEU:HD11	1.73	0.68
2:B:895:PHE:HE2	20:T:39:DT:OP1	1.75	0.68
16:P:363:ILE:HG23	16:P:374:VAL:HG13	1.76	0.68
16:P:393:VAL:HG23	16:P:394:VAL:H	1.59	0.68
17:Q:8:PRO:HG2	17:Q:19:LEU:HD23	1.75	0.68
20:T:9:DC:C2'	20:T:10:DA:C8	2.76	0.68
2:B:841:ASP:N	2:B:845:LEU:O	2.20	0.68
18:R:361:ASP:O	18:R:364:VAL:HG22	1.94	0.68
1:A:1242:ILE:HG22	1:A:1536:ILE:HG22	1.74	0.67
2:B:1079:LEU:CD2	2:B:1088:LEU:CB	2.55	0.67
3:C:32:ASN:OD1	3:C:33:VAL:N	2.27	0.67
16:P:480:VAL:HG23	16:P:492:LEU:HD21	1.76	0.67
17:Q:22:ILE:CD1	17:Q:26:ARG:HE	2.04	0.67
1:A:672:ASP:OD2	2:B:783:MET:SD	2.53	0.67
1:A:1654:PHE:CD2	6:F:89:GLU:HG3	2.28	0.67
2:B:894:LYS:HZ1	17:Q:405:ASP:CB	2.04	0.67
2:B:1047:ARG:CZ	2:B:1049:THR:HG22	2.24	0.67
2:B:1078:ALA:O	2:B:1082:HIS:HB2	1.93	0.67
14:N:85:HIS:HE1	14:N:141:GLU:HG3	1.58	0.67
16:P:357:LEU:O	18:R:194:GLY:HA2	1.93	0.67
3:C:127:THR:H	3:C:130:ASN:HB2	1.60	0.67
15:O:506:PHE:O	15:O:510:VAL:N	2.23	0.67
17:Q:356:VAL:CG2	18:R:208:TYR:HD2	1.97	0.67
21:U:38:DG:C2	21:U:39:DT:C2	2.82	0.67
1:A:355:PHE:HD1	1:A:355:PHE:H	1.39	0.67
2:B:480:GLN:O	2:B:484:TYR:OH	2.12	0.67
2:B:1096:SER:O	2:B:1097:ASP:HB3	1.93	0.67
1:A:70:LYS:HZ2	17:Q:27:ARG:NH1	1.92	0.67
1:A:1260:LYS:NZ	1:A:1500:GLN:OE1	2.27	0.67
16:P:229:ARG:HG3	16:P:230:HIS:H	1.57	0.67
17:Q:386:LEU:HD12	18:R:241:ARG:HH22	1.58	0.67
1:A:509:GLU:OE2	1:A:584:ARG:NH2	2.28	0.67
1:A:1600:ARG:NH2	1:A:1620:GLN:OE1	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:511:VAL:CG1	1:A:575:LYS:N	2.58	0.67
1:A:543:LEU:HD21	1:A:578:TYR:HH	1.57	0.67
16:P:238:LEU:HD11	16:P:284:VAL:HB	1.74	0.67
16:P:367:SER:OG	16:P:368:HIS:N	2.28	0.67
16:P:384:ASP:HB3	16:P:389:TRP:HB3	1.76	0.67
2:B:213:HIS:HB2	2:B:643:PHE:HE2	1.58	0.67
15:O:189:PHE:O	15:O:192:THR:OG1	2.11	0.67
1:A:855:ARG:NH1	1:A:868:THR:O	2.26	0.67
2:B:184:LYS:NZ	10:J:69:ARG:HH22	1.92	0.67
1:A:652:ASN:HB2	1:A:655:SER:HB2	1.77	0.67
2:B:113:VAL:C	18:R:282:SER:HA	2.15	0.67
5:E:17:ARG:NH1	5:E:35:VAL:O	2.27	0.67
16:P:468:VAL:HG22	16:P:477:TYR:HB3	1.76	0.67
18:R:236:PHE:O	18:R:240:ILE:HG22	1.94	0.67
18:R:361:ASP:HB2	18:R:364:VAL:HG13	1.77	0.67
15:O:453:TYR:CE2	15:O:473:PHE:HB2	2.29	0.66
16:P:506:THR:HG23	16:P:542:ARG:HD3	1.78	0.66
17:Q:232:LEU:HA	17:Q:287:TRP:CD1	2.30	0.66
1:A:512:THR:HG22	1:A:513:ALA:N	2.10	0.66
2:B:1014:TYR:HD1	2:B:1021:GLU:HA	1.60	0.66
15:O:446:LEU:O	15:O:450:LEU:N	2.26	0.66
16:P:362:ARG:HH22	16:P:364:GLU:HG3	1.61	0.66
16:P:498:LEU:HD13	17:Q:368:GLN:HE21	1.59	0.66
17:Q:361:PRO:O	17:Q:363:SER:N	2.28	0.66
1:A:1148:LEU:HG	1:A:1155:PHE:HE2	1.60	0.66
9:I:26:SER:O	9:I:39:LYS:N	2.27	0.66
15:O:379:ARG:CA	15:O:382:GLN:HE22	2.09	0.66
5:E:88:VAL:HB	5:E:116:ILE:HA	1.78	0.66
1:A:690:GLU:HB3	11:K:77:ARG:HH22	1.61	0.66
2:B:116:ALA:CB	18:R:282:SER:C	2.51	0.66
2:B:564:ILE:O	2:B:567:SER:OG	2.14	0.66
2:B:843:ASP:OD2	12:L:29:TYR:OH	2.13	0.66
17:Q:15:CYS:HB2	17:Q:16:PRO:HA	1.77	0.66
17:Q:355:VAL:CA	18:R:212:HIS:HE1	2.04	0.66
2:B:107:PRO:O	2:B:171:HIS:NE2	2.21	0.66
2:B:1107:CYS:HB2	2:B:1130:ARG:HH11	1.61	0.66
5:E:55:ARG:HG3	5:E:84:ASP:HA	1.77	0.66
17:Q:104:PHE:CZ	17:Q:156:LEU:HB2	2.31	0.66
17:Q:412:LYS:O	17:Q:416:ILE:HG13	1.96	0.66
2:B:974:LEU:O	10:J:47:ARG:NH2	2.29	0.66
11:K:54:THR:HG22	11:K:61:ALA:HA	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:200:ASN:CG	17:Q:14:ASN:CB	2.64	0.66
16:P:355:GLU:CB	18:R:24:ILE:HD12	2.25	0.66
2:B:815:ARG:NH2	2:B:821:ILE:CB	2.58	0.66
2:B:1092:LEU:HD23	2:B:1092:LEU:C	2.16	0.66
9:I:38:PRO:HD2	9:I:41:GLN:HE21	1.61	0.66
14:N:63:ASP:OD2	14:N:66:LYS:NZ	2.25	0.66
16:P:443:ASP:HB3	18:R:3:GLU:CB	2.26	0.66
18:R:250:LEU:HB2	18:R:270:PHE:HE2	1.60	0.66
2:B:144:SER:HA	2:B:151:ASN:HA	1.76	0.66
2:B:916:LYS:HD3	2:B:924:LYS:HD2	1.77	0.66
7:G:28:ILE:HD13	7:G:35:SER:HB3	1.78	0.66
11:K:60:SER:OG	11:K:104:ARG:NH2	2.29	0.65
1:A:1037:SER:OG	1:A:1039:ARG:NE	2.25	0.65
15:O:179:PHE:O	15:O:183:ILE:N	2.22	0.65
16:P:419:ARG:HG2	16:P:420:GLU:N	2.10	0.65
16:P:555:THR:HG22	16:P:556:GLN:HG2	1.78	0.65
16:P:724:LEU:CD1	17:Q:443:GLN:HG2	2.26	0.65
17:Q:15:CYS:SG	17:Q:17:SER:CB	2.83	0.65
1:A:385:LEU:HD23	1:A:437:PHE:HA	1.77	0.65
1:A:504:LYS:O	1:A:506:THR:HG23	1.96	0.65
2:B:115:SER:O	18:R:280:SER:N	2.29	0.65
2:B:731:VAL:HG13	10:J:60:PHE:CD1	2.32	0.65
3:C:64:ALA:O	3:C:68:ARG:N	2.21	0.65
3:C:85:PHE:HE1	3:C:204:LEU:HD22	1.60	0.65
15:O:466:GLY:O	15:O:469:ARG:NE	2.29	0.65
19:S:4:C:O5'	19:S:4:C:H6	1.79	0.65
3:C:212:ILE:HG13	3:C:215:ASP:H	1.61	0.65
17:Q:355:VAL:HG11	18:R:212:HIS:HA	1.76	0.65
1:A:372:LYS:HA	1:A:377:VAL:HA	1.78	0.65
2:B:954:PHE:O	2:B:955:PRO:C	2.33	0.65
9:I:10:CYS:HB3	9:I:13:CYS:SG	2.37	0.65
15:O:487:ARG:HA	15:O:491:PHE:HB2	1.78	0.65
18:R:6:ILE:HG22	18:R:245:VAL:HA	1.78	0.65
18:R:417:ILE:O	18:R:420:ASP:HB2	1.96	0.65
1:A:1302:TYR:HA	1:A:1305:GLU:HB3	1.77	0.65
1:A:1640:ARG:NH1	1:A:1640:ARG:HG2	2.11	0.65
16:P:420:GLU:HB2	16:P:442:LEU:N	2.12	0.65
17:Q:409:ALA:O	17:Q:413:LEU:HB2	1.97	0.65
3:C:222:VAL:C	3:C:224:THR:H	2.00	0.65
15:O:327:GLU:HB3	15:O:331:LYS:HE3	1.77	0.65
1:A:1162:ASN:HB3	1:A:1165:LYS:HG2	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1461:ASN:OD1	1:A:1462:PHE:N	2.29	0.65
2:B:1050:GLY:CA	17:Q:24:ASP:HA	2.27	0.65
16:P:458:LYS:HD3	16:P:459:PRO:HD3	1.78	0.65
16:P:662:LEU:CB	16:P:665:ASN:HB2	2.26	0.65
17:Q:366:TYR:HA	17:Q:369:TRP:NE1	2.12	0.65
1:A:474:LYS:CD	2:B:1096:SER:HB2	2.21	0.65
2:B:115:SER:C	18:R:282:SER:HB3	2.16	0.65
2:B:662:ASP:OD1	2:B:663:ILE:N	2.30	0.65
2:B:1079:LEU:CG	2:B:1088:LEU:HD22	2.12	0.65
16:P:355:GLU:HA	18:R:24:ILE:CD1	2.27	0.65
17:Q:288:GLU:O	17:Q:290:THR:N	2.30	0.65
18:R:217:THR:HG22	18:R:239:LEU:HD21	1.77	0.65
1:A:672:ASP:CA	2:B:783:MET:HE3	2.24	0.65
2:B:143:TRP:O	2:B:152:LEU:N	2.28	0.65
9:I:8:ILE:HG22	9:I:17:LEU:HD12	1.79	0.65
1:A:339:PHE:O	1:A:1629:ASN:ND2	2.30	0.64
1:A:568:VAL:O	1:A:571:HIS:ND1	2.25	0.64
1:A:916:THR:O	1:A:919:LYS:NZ	2.28	0.64
1:A:1185:VAL:HA	1:A:1188:ILE:HB	1.79	0.64
1:A:1258:ILE:HD12	1:A:1258:ILE:O	1.96	0.64
16:P:315:PHE:HB3	16:P:317:ILE:CD1	2.27	0.64
17:Q:104:PHE:CE1	20:T:49:DC:OP1	2.51	0.64
1:A:1326:GLU:HA	1:A:1329:ILE:HD12	1.78	0.64
2:B:817:ARG:CG	21:U:17:DT:H5'	2.25	0.64
2:B:1051:PRO:HD3	2:B:1066:HIS:O	1.97	0.64
2:B:1098:TYR:CE1	2:B:1177:ALA:HB1	2.33	0.64
16:P:446:ASP:HA	18:R:200:THR:CG2	2.27	0.64
1:A:872:ASP:OD2	1:A:875:LEU:N	2.30	0.64
1:A:1104:TYR:HB3	1:A:1120:TYR:HE2	1.63	0.64
2:B:812:ALA:HA	2:B:815:ARG:HD2	1.79	0.64
18:R:206:ARG:C	18:R:207:ASN:HB2	2.17	0.64
18:R:427:PRO:HG2	18:R:429:ARG:HH21	1.63	0.64
17:Q:355:VAL:HG13	18:R:212:HIS:HA	1.79	0.64
17:Q:356:VAL:CG1	18:R:212:HIS:CE1	2.69	0.64
1:A:358:ASP:OD1	1:A:358:ASP:N	2.31	0.64
4:D:39:PHE:HZ	7:G:83:GLY:HA3	1.62	0.64
15:O:600:LYS:HG3	15:O:601:ASN:H	1.62	0.64
16:P:729:ALA:O	16:P:733:THR:HG22	1.96	0.64
1:A:827:THR:HG21	2:B:1026:ILE:HA	1.78	0.64
1:A:1018:TYR:CE1	20:T:16:DT:P	2.89	0.64
1:A:1299:ASN:HA	1:A:1302:TYR:CZ	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:63:LEU:HB2	15:O:71:ILE:HG13	1.79	0.64
16:P:487:ASN:HB3	18:R:138:PHE:HZ	1.60	0.64
16:P:658:LYS:O	16:P:747:LEU:HG	1.97	0.64
16:P:698:LYS:HE2	17:Q:124:ARG:HH21	1.62	0.64
3:C:69:ARG:NE	11:K:71:THR:OG1	2.23	0.64
15:O:186:SER:HA	15:O:189:PHE:CE2	2.33	0.64
16:P:421:ILE:HG22	16:P:423:ILE:HG13	1.79	0.64
2:B:936:MET:CG	2:B:948:ILE:HD11	2.27	0.64
15:O:446:LEU:HD11	15:O:476:ALA:HB1	1.80	0.64
16:P:62:LYS:HG2	16:P:63:SER:N	2.13	0.64
16:P:658:LYS:HB3	16:P:660:LYS:H	1.62	0.64
1:A:95:TYR:OH	1:A:99:ARG:NH1	2.31	0.64
1:A:1654:PHE:CE2	6:F:89:GLU:HG3	2.33	0.64
3:C:89:THR:OG1	3:C:201:GLU:N	2.17	0.64
13:M:36:THR:HG21	13:M:62:TYR:HE2	1.63	0.64
13:M:57:ASN:HD21	13:M:60:LEU:HB2	1.62	0.64
15:O:218:LEU:HD12	15:O:221:TYR:HB2	1.79	0.64
15:O:430:ARG:HG2	15:O:482:TYR:OH	1.97	0.64
16:P:221:ARG:HH12	16:P:264:ILE:HG21	1.63	0.64
1:A:109:ARG:NH1	1:A:230:ARG:O	2.30	0.64
1:A:1651:THR:HG21	2:B:1086:PHE:HB2	1.80	0.64
2:B:709:PHE:HE2	2:B:992:PRO:HG2	1.63	0.64
15:O:440:ILE:O	15:O:444:SER:N	2.31	0.64
1:A:527:PRO:HD3	1:A:554:ARG:NH1	2.13	0.63
1:A:879:LEU:HA	1:A:882:ILE:HG22	1.80	0.63
16:P:380:MET:HB3	16:P:393:VAL:HG21	1.79	0.63
16:P:592:LEU:O	16:P:596:ILE:HG22	1.98	0.63
17:Q:19:LEU:HD11	17:Q:27:ARG:CB	2.27	0.63
17:Q:198:ILE:HD12	17:Q:390:THR:HA	1.81	0.63
17:Q:356:VAL:HG12	18:R:208:TYR:O	1.98	0.63
1:A:368:ARG:HA	1:A:380:ASN:HD22	1.63	0.63
1:A:638:PRO:CG	2:B:1087:LEU:HD11	2.26	0.63
1:A:1013:THR:CB	20:T:17:DT:N3	2.61	0.63
17:Q:22:ILE:HD11	17:Q:26:ARG:HE	1.62	0.63
17:Q:101:LYS:HE3	17:Q:154:LEU:HD12	1.79	0.63
1:A:552:GLU:O	15:O:246:ASN:ND2	2.31	0.63
1:A:628:PHE:HB3	2:B:785:ASP:OD1	1.99	0.63
1:A:880:GLN:NE2	2:B:633:THR:H	1.96	0.63
7:G:167:THR:O	7:G:218:VAL:N	2.29	0.63
13:M:61:GLU:N	13:M:101:VAL:O	2.25	0.63
17:Q:337:SER:HB2	17:Q:448:LYS:HD3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:646:GLU:OE2	6:F:91:ALA:HB1	1.98	0.63
1:A:672:ASP:CG	2:B:783:MET:SD	2.76	0.63
2:B:307:GLU:HB2	9:I:7:LEU:HD11	1.80	0.63
2:B:787:MET:HG3	2:B:928:SER:N	2.12	0.63
1:A:852:ASP:OD1	1:A:855:ARG:NE	2.29	0.63
1:A:882:ILE:O	1:A:889:SER:OG	2.17	0.63
1:A:1139:ASN:ND2	5:E:204:THR:O	2.31	0.63
2:B:674:ILE:HG12	2:B:688:HIS:HB2	1.79	0.63
2:B:1117:VAL:HG21	2:B:1162:GLY:HA2	1.79	0.63
11:K:64:GLN:HE21	11:K:100:LEU:HD22	1.63	0.63
1:A:1105:ARG:NH1	1:A:1138:GLU:HG2	2.14	0.63
2:B:145:VAL:N	2:B:150:GLU:O	2.23	0.63
3:C:150:SER:OG	3:C:155:GLU:OE2	2.17	0.63
6:F:83:PRO:HB2	6:F:152:ILE:HD13	1.80	0.63
16:P:697:GLU:OE1	16:P:697:GLU:N	2.25	0.63
1:A:618:TYR:CE1	2:B:783:MET:HB2	2.33	0.63
2:B:216:ALA:HA	2:B:234:ILE:HD13	1.80	0.63
2:B:366:GLY:O	2:B:370:LYS:N	2.24	0.63
15:O:61:ASP:OD1	15:O:106:ARG:NH2	2.31	0.63
16:P:596:ILE:HD13	17:Q:272:GLN:NE2	2.14	0.63
16:P:760:ILE:HA	16:P:763:SER:HB3	1.81	0.63
1:A:1634:LEU:O	1:A:1640:ARG:NH1	2.31	0.63
1:A:1635:ASP:O	1:A:1640:ARG:HD2	1.99	0.63
2:B:225:ARG:NH2	2:B:268:GLU:OE1	2.24	0.63
2:B:731:VAL:HG13	10:J:60:PHE:HD1	1.63	0.63
17:Q:12:THR:HG1	17:Q:33:HIS:CE1	2.15	0.63
17:Q:278:GLU:O	17:Q:279:THR:OG1	2.14	0.63
19:S:3:G:C2	20:T:21:DC:O2	2.52	0.63
1:A:833:LEU:HD22	1:A:943:ILE:HG21	1.81	0.63
1:A:956:ARG:NH2	1:A:979:GLY:HA3	2.13	0.63
2:B:532:HIS:ND1	24:B:1301:SO4:O4	2.31	0.63
2:B:790:ASN:HA	2:B:936:MET:SD	2.39	0.63
3:C:89:THR:HG1	3:C:201:GLU:H	1.45	0.63
9:I:60:LEU:O	9:I:64:LYS:N	2.31	0.63
17:Q:6:ARG:O	17:Q:7:GLY:O	2.17	0.63
17:Q:8:PRO:HB2	17:Q:19:LEU:HD23	1.79	0.63
18:R:346:ILE:HB	18:R:375:LYS:HE2	1.80	0.63
1:A:1032:VAL:HG22	1:A:1038:ILE:HD13	1.81	0.62
2:B:96:SER:HB2	2:B:144:SER:HB3	1.80	0.62
10:J:18:TRP:NE1	10:J:55:ASP:OD2	2.32	0.62
16:P:384:ASP:OD2	16:P:387:ASN:HB2	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:435:ARG:HH22	18:R:140:ILE:CD1	2.09	0.62
1:A:964:LYS:NZ	2:B:672:MET:O	2.32	0.62
2:B:158:CYS:O	2:B:457:ILE:N	2.32	0.62
2:B:320:LEU:HD21	2:B:325:GLN:O	1.98	0.62
2:B:534:PRO:HG3	2:B:542:LEU:HD12	1.81	0.62
2:B:1137:ASP:HA	2:B:1140:LYS:HD2	1.80	0.62
16:P:420:GLU:HA	16:P:442:LEU:O	1.99	0.62
16:P:700:LEU:HD12	16:P:703:PHE:HD2	1.64	0.62
16:P:721:CYS:SG	17:Q:442:LEU:HD23	2.39	0.62
17:Q:355:VAL:HG12	18:R:212:HIS:CA	2.26	0.62
1:A:373:LEU:N	1:A:376:GLU:O	2.32	0.62
1:A:1262:LEU:HB2	1:A:1265:GLU:HG3	1.80	0.62
1:A:1646:LEU:HD11	2:B:1086:PHE:CE1	2.33	0.62
2:B:811:LEU:HD13	2:B:823:GLN:HB2	1.80	0.62
16:P:305:PHE:HE1	16:P:314:GLN:HG3	1.64	0.62
17:Q:10:CYS:CB	17:Q:17:SER:H	2.12	0.62
17:Q:329:LYS:HA	17:Q:332:LEU:HD23	1.80	0.62
17:Q:386:LEU:CG	18:R:241:ARG:HH22	2.11	0.62
2:B:1063:ARG:NE	20:T:22:DG:OP2	2.31	0.62
3:C:58:ASN:HA	3:C:296:ASN:ND2	2.15	0.62
5:E:100:ILE:HG23	5:E:105:PHE:HB2	1.81	0.62
16:P:603:ARG:O	16:P:607:VAL:HG23	1.99	0.62
17:Q:3:THR:HG22	17:Q:20:TRP:CB	2.29	0.62
17:Q:356:VAL:HG22	18:R:208:TYR:CE2	2.24	0.62
17:Q:410:ARG:HA	17:Q:413:LEU:HB3	1.80	0.62
1:A:520:ARG:HH21	1:A:559:ASN:HD21	1.48	0.62
6:F:61:HIS:HA	6:F:64:ILE:HB	1.81	0.62
16:P:209:LYS:NZ	16:P:277:VAL:HG11	2.14	0.62
16:P:405:TYR:HE2	16:P:414:ILE:HG13	1.64	0.62
16:P:722:TRP:CD1	17:Q:264:PRO:HD3	2.34	0.62
20:T:21:DC:O5'	20:T:21:DC:H6	1.81	0.62
1:A:15:ASP:HB2	2:B:1197:ARG:HB3	1.79	0.62
1:A:1603:MET:HG2	1:A:1612:LYS:HG2	1.81	0.62
16:P:345:ASP:OD1	16:P:345:ASP:N	2.32	0.62
16:P:414:ILE:HG12	16:P:425:GLY:H	1.62	0.62
16:P:442:LEU:HB3	16:P:477:TYR:CZ	2.34	0.62
18:R:173:MET:O	18:R:177:LEU:HB2	2.00	0.62
1:A:1258:ILE:HB	1:A:1501:ILE:CD1	2.29	0.62
2:B:314:LYS:O	2:B:315:LYS:HG2	1.99	0.62
2:B:1105:ARG:HH21	2:B:1174:THR:HG22	1.64	0.62
8:H:103:LYS:HB3	8:H:115:TYR:HD2	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:357:TYR:CE2	17:Q:489:VAL:HA	2.34	0.62
1:A:70:LYS:HZ2	17:Q:27:ARG:HH12	1.40	0.62
1:A:512:THR:HG22	1:A:513:ALA:H	1.65	0.62
1:A:782:ASP:OD1	1:A:783:LYS:N	2.33	0.62
1:A:1507:CYS:HB3	1:A:1520:VAL:O	1.99	0.62
5:E:26:ARG:NH1	5:E:133:GLU:OE1	2.29	0.62
8:H:115:TYR:HE1	8:H:124:ARG:HG3	1.65	0.62
17:Q:318:LEU:HB3	17:Q:476:ILE:HD12	1.82	0.62
18:R:273:TRP:O	18:R:277:ILE:HG22	1.99	0.62
2:B:302:LEU:HD13	2:B:379:ARG:NH1	2.14	0.62
16:P:356:GLU:OE1	16:P:377:ARG:NE	2.33	0.62
17:Q:274:ILE:HD13	17:Q:282:ARG:HH12	1.64	0.62
20:T:7:DT:H3	21:U:43:DA:H61	1.46	0.62
1:A:511:VAL:HG13	1:A:574:ASN:CB	2.25	0.62
1:A:1240:LEU:HD12	1:A:1521:THR:HG23	1.78	0.62
2:B:815:ARG:NH1	2:B:899:GLN:CD	2.53	0.62
15:O:393:LEU:HD21	15:O:438:GLN:HE22	1.64	0.62
16:P:631:SER:O	16:P:686:TYR:OH	2.17	0.62
16:P:721:CYS:SG	17:Q:439:ILE:HG22	2.39	0.62
18:R:361:ASP:OD1	18:R:361:ASP:N	2.25	0.62
1:A:17:GLY:O	2:B:1195:ARG:N	2.33	0.61
2:B:70:GLU:HA	2:B:98:SER:HB3	1.82	0.61
2:B:302:LEU:HD13	2:B:379:ARG:HH12	1.65	0.61
16:P:622:TYR:OH	16:P:665:ASN:O	2.16	0.61
17:Q:299:SER:O	17:Q:299:SER:OG	2.11	0.61
18:R:160:HIS:HA	18:R:163:LYS:HE2	1.81	0.61
18:R:242:ILE:HG22	18:R:245:VAL:HG22	1.81	0.61
1:A:547:ILE:CD1	17:Q:26:ARG:NH2	2.45	0.61
1:A:1176:ARG:NH2	6:F:154:ASP:O	2.32	0.61
2:B:1053:ASN:N	2:B:1058:GLN:O	2.29	0.61
7:G:141:SER:O	7:G:217:TRP:NE1	2.34	0.61
16:P:596:ILE:HD13	17:Q:272:GLN:CD	2.20	0.61
1:A:702:PRO:HD3	1:A:712:ILE:HD11	1.82	0.61
1:A:1510:PRO:HG3	1:A:1520:VAL:HG23	1.81	0.61
2:B:368:GLN:HG3	2:B:372:ARG:HH12	1.65	0.61
3:C:69:ARG:HH21	11:K:71:THR:H	1.47	0.61
15:O:403:LEU:HB3	15:O:424:LEU:HB2	1.81	0.61
16:P:434:ARG:HB3	18:R:143:THR:HG21	1.81	0.61
16:P:584:ARG:O	16:P:588:SER:HB2	2.00	0.61
18:R:75:GLN:HA	18:R:78:ARG:HE	1.64	0.61
2:B:796:ARG:HD2	10:J:8:PHE:HA	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:812:ALA:HB1	2:B:815:ARG:HH11	1.66	0.61
3:C:84:TYR:HB3	12:L:64:LEU:HD11	1.82	0.61
16:P:376:ASP:O	16:P:378:SER:N	2.33	0.61
17:Q:324:ARG:NE	17:Q:324:ARG:O	2.33	0.61
1:A:94:LEU:HB2	1:A:355:PHE:HD2	1.63	0.61
2:B:651:ARG:NH2	2:B:690:GLU:OE2	2.23	0.61
12:L:68:GLU:HG2	12:L:70:ARG:H	1.65	0.61
16:P:629:ARG:NH2	16:P:662:LEU:HD21	2.14	0.61
17:Q:230:ILE:O	17:Q:234:CYS:HB2	2.00	0.61
17:Q:265:GLU:OE1	17:Q:265:GLU:N	2.31	0.61
1:A:638:PRO:CG	2:B:1087:LEU:HD12	2.29	0.61
1:A:1300:ASN:OD1	1:A:1301:GLU:N	2.33	0.61
1:A:1307:ASP:HB3	1:A:1499:ARG:HH12	1.64	0.61
2:B:234:ILE:HG12	2:B:381:LEU:HD13	1.81	0.61
2:B:324:THR:HG23	2:B:347:LEU:HD13	1.81	0.61
2:B:547:HIS:ND1	2:B:760:TYR:OH	2.26	0.61
15:O:205:ARG:HD3	15:O:331:LYS:HA	1.82	0.61
15:O:379:ARG:CB	15:O:591:TYR:OH	2.49	0.61
17:Q:115:GLN:NE2	17:Q:191:PRO:O	2.27	0.61
19:S:4:C:O2	20:T:20:DG:C2	2.53	0.61
1:A:1640:ARG:HG2	1:A:1640:ARG:HH11	1.66	0.61
1:A:1650:GLY:C	1:A:1652:GLY:H	2.02	0.61
2:B:114:SER:CB	18:R:282:SER:HA	1.97	0.61
5:E:47:CYS:HA	5:E:53:PRO:HA	1.81	0.61
13:M:34:SER:OG	14:N:128:ASN:ND2	2.33	0.61
15:O:383:TYR:O	15:O:387:HIS:N	2.32	0.61
17:Q:356:VAL:HB	18:R:208:TYR:CD2	2.23	0.61
1:A:952:LEU:HD12	1:A:957:VAL:HA	1.83	0.61
2:B:838:GLU:O	12:L:63:ARG:NH2	2.34	0.61
3:C:164:ALA:HB2	3:C:191:ILE:HB	1.83	0.61
14:N:89:ILE:HG12	14:N:139:VAL:HG22	1.83	0.61
16:P:55:LEU:CA	18:R:227:HIS:CE1	2.84	0.61
20:T:4:DG:H8	20:T:4:DG:O5'	1.82	0.61
1:A:597:LYS:O	2:B:1082:HIS:CE1	2.53	0.61
1:A:729:LYS:HD2	8:H:120:GLY:HA3	1.82	0.61
1:A:1654:PHE:CE2	6:F:89:GLU:N	2.69	0.61
11:K:88:PHE:HB3	11:K:106:GLN:HB2	1.81	0.61
13:M:51:PHE:HD2	13:M:94:PRO:HG3	1.65	0.61
18:R:295:PRO:O	18:R:297:PHE:N	2.33	0.61
2:B:910:THR:O	2:B:1035:ARG:NH2	2.33	0.61
5:E:200:ARG:O	5:E:208:TYR:N	2.32	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:113:SER:HG	14:N:115:SER:HG	1.46	0.61
15:O:152:GLN:O	15:O:155:SER:OG	2.16	0.61
15:O:442:VAL:O	15:O:446:LEU:N	2.29	0.61
16:P:290:GLU:O	16:P:343:LEU:HD21	2.00	0.61
16:P:486:ALA:HB1	18:R:137:SER:OG	2.01	0.61
1:A:638:PRO:HG2	2:B:1087:LEU:CD1	2.31	0.60
1:A:1450:ILE:HA	1:A:1453:HIS:HD2	1.65	0.60
16:P:221:ARG:NH1	16:P:264:ILE:HG21	2.16	0.60
16:P:724:LEU:HD12	17:Q:443:GLN:HA	1.83	0.60
1:A:1459:LYS:HD3	1:A:1473:LYS:HD3	1.83	0.60
2:B:931:TRP:CB	2:B:936:MET:HE3	2.11	0.60
3:C:227:TYR:HB3	3:C:300:PHE:HD1	1.66	0.60
15:O:379:ARG:HA	15:O:382:GLN:CD	2.21	0.60
16:P:475:ARG:H	16:P:475:ARG:HD2	1.65	0.60
17:Q:232:LEU:HD22	17:Q:287:TRP:CD1	2.36	0.60
18:R:26:TYR:CB	18:R:169:PRO:HB3	2.31	0.60
1:A:1302:TYR:O	1:A:1306:TYR:N	2.33	0.60
2:B:494:TYR:HB3	2:B:700:LEU:HD11	1.82	0.60
3:C:57:ILE:HG13	3:C:297:HIS:CD2	2.36	0.60
6:F:66:ARG:O	6:F:70:LYS:N	2.32	0.60
15:O:353:GLU:HG3	15:O:354:SER:H	1.65	0.60
16:P:220:THR:HG22	16:P:241:PRO:HB3	1.82	0.60
1:A:925:MET:SD	2:B:955:PRO:HB3	2.41	0.60
1:A:1643:VAL:O	2:B:1179:PRO:HD2	2.00	0.60
2:B:929:ARG:NH1	11:K:96:PRO:HB2	2.10	0.60
15:O:458:GLU:HB3	15:O:513:LYS:HD2	1.82	0.60
16:P:687:GLN:O	16:P:689:GLN:NE2	2.35	0.60
5:E:176:PRO:HB2	5:E:212:ARG:HD3	1.83	0.60
16:P:477:TYR:CE2	18:R:2:PHE:HZ	2.19	0.60
16:P:477:TYR:HE2	18:R:2:PHE:HE2	1.19	0.60
4:D:47:LYS:HB3	4:D:82:LEU:HD21	1.83	0.60
15:O:328:LEU:HA	15:O:331:LYS:HB2	1.82	0.60
18:R:257:ILE:CG2	18:R:267:GLY:H	2.13	0.60
1:A:260:GLN:O	1:A:264:ASN:N	2.27	0.60
3:C:132:ILE:HB	3:C:208:CYS:HB2	1.84	0.60
15:O:62:ASP:O	15:O:67:ASP:N	2.35	0.60
16:P:55:LEU:HA	18:R:227:HIS:CE1	2.36	0.60
17:Q:15:CYS:HB3	17:Q:17:SER:H	1.62	0.60
18:R:412:ARG:NE	18:R:432:GLU:OE2	2.28	0.60
1:A:216:ARG:NH2	1:A:338:VAL:O	2.34	0.60
1:A:709:ARG:NH1	1:A:737:LEU:O	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1640:ARG:HH11	1:A:1640:ARG:CG	2.15	0.60
2:B:320:LEU:CD2	2:B:325:GLN:HB2	2.30	0.60
2:B:815:ARG:NH1	2:B:899:GLN:CG	2.62	0.60
2:B:1087:LEU:HD23	2:B:1088:LEU:HD23	1.83	0.60
3:C:236:LEU:HD11	3:C:290:LYS:HG3	1.83	0.60
7:G:22:LYS:NZ	7:G:77:VAL:O	2.33	0.60
14:N:40:LEU:HA	14:N:51:GLN:HE22	1.66	0.60
16:P:446:ASP:CA	18:R:200:THR:CG2	2.80	0.60
1:A:597:LYS:CD	2:B:1081:GLY:O	2.50	0.60
2:B:987:ASN:OD1	2:B:990:ASP:N	2.24	0.60
3:C:77:SER:OG	3:C:219:PHE:O	2.20	0.60
16:P:608:GLN:HA	16:P:611:ILE:HD12	1.83	0.60
17:Q:154:LEU:H	17:Q:154:LEU:HD22	1.66	0.60
1:A:1188:ILE:O	1:A:1192:SER:N	2.30	0.60
2:B:296:ASP:OD2	2:B:379:ARG:NH2	2.34	0.60
2:B:420:TYR:HE1	2:B:455:GLU:HB3	1.65	0.60
9:I:2:SER:HB2	9:I:11:LEU:HD21	1.83	0.60
16:P:320:ILE:O	16:P:320:ILE:HG12	2.01	0.60
16:P:657:SER:HA	16:P:747:LEU:O	2.02	0.60
2:B:1161:ASP:OD1	2:B:1165:ASN:N	2.28	0.59
5:E:88:VAL:HG21	5:E:116:ILE:HG12	1.82	0.59
16:P:473:HIS:CE1	18:R:1:MET:SD	2.95	0.59
17:Q:378:LEU:HD21	18:R:235:ILE:CD1	2.32	0.59
1:A:719:ILE:O	1:A:724:PRO:HA	2.02	0.59
15:O:447:THR:HB	15:O:505:PHE:CZ	2.37	0.59
17:Q:366:TYR:CB	18:R:215:THR:CG2	2.80	0.59
18:R:177:LEU:HD21	18:R:185:LYS:HA	1.84	0.59
1:A:1194:GLY:O	1:A:1197:SER:OG	2.20	0.59
1:A:1654:PHE:HZ	6:F:89:GLU:HA	1.56	0.59
2:B:311:ARG:HE	9:I:16:LEU:HG	1.66	0.59
9:I:12:ASP:OD2	13:M:59:ARG:NH2	2.36	0.59
15:O:352:LEU:HD11	15:O:392:GLN:HG3	1.84	0.59
1:A:195:LYS:O	1:A:198:SER:OG	2.14	0.59
2:B:790:ASN:HA	2:B:936:MET:CE	2.33	0.59
16:P:60:VAL:O	16:P:61:VAL:HG23	2.02	0.59
16:P:355:GLU:HB3	18:R:24:ILE:HG23	1.83	0.59
17:Q:12:THR:HB	17:Q:33:HIS:ND1	2.18	0.59
17:Q:389:GLN:O	18:R:243:PRO:HG3	2.01	0.59
20:T:19:DC:H2'	20:T:20:DG:C8	2.37	0.59
1:A:91:PHE:O	1:A:95:TYR:N	2.24	0.59
2:B:1058:GLN:CG	2:B:1096:SER:O	2.45	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:136:LEU:HB3	3:C:204:LEU:HG	1.84	0.59
15:O:484:PHE:CE1	15:O:528:PHE:HA	2.36	0.59
1:A:1035:ASP:OD2	1:A:1039:ARG:NH2	2.33	0.59
2:B:396:ALA:HB1	2:B:523:GLU:OE1	2.02	0.59
2:B:931:TRP:HB3	2:B:936:MET:HE2	1.74	0.59
3:C:243:SER:OG	3:C:246:ARG:NH2	2.36	0.59
17:Q:139:LYS:HG2	17:Q:237:ILE:HG12	1.85	0.59
18:R:78:ARG:HH21	20:T:43:DT:H5''	1.64	0.59
1:A:1105:ARG:HH12	1:A:1138:GLU:HG2	1.66	0.59
1:A:1508:VAL:O	1:A:1508:VAL:HG12	2.00	0.59
1:A:1619:CYS:HA	1:A:1622:LEU:HB3	1.85	0.59
1:A:1651:THR:O	1:A:1651:THR:HG22	2.01	0.59
2:B:117:VAL:CB	18:R:277:ILE:HA	2.31	0.59
5:E:9:ILE:HG22	5:E:39:LEU:HD11	1.85	0.59
15:O:61:ASP:HA	15:O:64:ASP:HB2	1.84	0.59
1:A:513:ALA:O	1:A:516:ILE:HG22	2.02	0.59
1:A:552:GLU:HG2	1:A:553:GLN:H	1.67	0.59
1:A:1289:SER:HB3	1:A:1475:GLU:HG2	1.85	0.59
16:P:362:ARG:NH2	16:P:364:GLU:HG3	2.18	0.59
1:A:642:ASN:CB	2:B:1086:PHE:CE2	2.85	0.59
3:C:131:THR:O	3:C:175:GLN:NE2	2.34	0.59
6:F:106:PRO:HG2	7:G:55:GLU:HG2	1.84	0.59
17:Q:186:CYS:CB	18:R:208:TYR:HE2	1.95	0.59
17:Q:227:TYR:O	17:Q:230:ILE:HG13	2.03	0.59
18:R:299:THR:CG2	18:R:305:THR:HA	2.33	0.59
18:R:314:TRP:NE1	18:R:363:GLU:OE2	2.35	0.59
1:A:1013:THR:C	20:T:17:DT:C2	2.76	0.59
2:B:420:TYR:CE1	2:B:455:GLU:HB3	2.37	0.59
2:B:560:ARG:O	2:B:563:SER:OG	2.16	0.59
8:H:93:TYR:HA	8:H:145:ARG:HB3	1.84	0.59
16:P:477:TYR:CD2	18:R:2:PHE:HZ	2.19	0.59
2:B:116:ALA:CA	18:R:282:SER:C	2.71	0.58
2:B:299:ASP:OD1	2:B:301:PHE:N	2.35	0.58
2:B:1074:MET:CE	20:T:18:DT:H4'	2.33	0.58
9:I:19:ASN:HB3	9:I:22:ALA:HB2	1.85	0.58
15:O:422:GLN:NE2	15:O:591:TYR:O	2.36	0.58
1:A:464:GLU:HB2	1:A:465:GLY:HA2	1.85	0.58
1:A:591:ARG:HH21	19:S:6:A:H1'	1.67	0.58
16:P:197:ARG:HD2	16:P:262:GLY:N	2.18	0.58
17:Q:350:ARG:NE	17:Q:486:GLN:CG	2.64	0.58
1:A:596:HIS:CD2	1:A:598:ALA:HB3	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:671:GLN:CB	2:B:783:MET:CE	2.80	0.58
1:A:1316:VAL:HG13	1:A:1320:GLN:HE21	1.68	0.58
3:C:86:PHE:HE2	3:C:205:LYS:HG3	1.69	0.58
15:O:446:LEU:O	15:O:450:LEU:HG	2.03	0.58
16:P:59:ILE:O	16:P:552:LEU:HA	2.04	0.58
17:Q:9:ILE:HB	17:Q:16:PRO:CB	2.26	0.58
17:Q:20:TRP:CH2	17:Q:22:ILE:HG21	2.29	0.58
18:R:11:ARG:HG3	18:R:12:LYS:H	1.68	0.58
2:B:1119:ARG:NH2	2:B:1160:GLU:OE2	2.36	0.58
3:C:311:GLU:OE1	3:C:311:GLU:N	2.34	0.58
7:G:140:GLN:HB3	7:G:217:TRP:CD1	2.36	0.58
15:O:130:PRO:O	15:O:134:SER:N	2.25	0.58
16:P:458:LYS:HZ3	16:P:458:LYS:HA	1.68	0.58
17:Q:22:ILE:HD11	17:Q:26:ARG:CD	2.33	0.58
17:Q:375:LEU:HA	17:Q:378:LEU:HD12	1.84	0.58
18:R:362:ALA:O	18:R:365:TRP:HB2	2.02	0.58
1:A:582:LYS:HE3	1:A:584:ARG:HE	1.67	0.58
1:A:793:ILE:HG23	1:A:794:VAL:H	1.68	0.58
1:A:1258:ILE:HB	1:A:1501:ILE:HD12	1.83	0.58
8:H:110:ASP:O	8:H:129:TYR:N	2.36	0.58
17:Q:10:CYS:HB2	17:Q:17:SER:H	1.67	0.58
17:Q:249:CYS:SG	17:Q:282:ARG:NH1	2.77	0.58
1:A:53:ALA:HA	1:A:63:SER:HB2	1.85	0.58
1:A:65:CYS:HB3	1:A:75:HIS:CE1	2.38	0.58
1:A:411:VAL:HG11	1:A:416:ARG:HE	1.68	0.58
1:A:474:LYS:HD2	2:B:1096:SER:HB2	1.83	0.58
1:A:1637:PRO:CA	1:A:1647:ASN:HD21	2.16	0.58
2:B:1105:ARG:NH2	2:B:1173:THR:O	2.36	0.58
2:B:1134:ARG:HD3	2:B:1167:PHE:HE1	1.67	0.58
4:D:89:LEU:HD23	4:D:92:ILE:HD12	1.86	0.58
16:P:443:ASP:CB	18:R:3:GLU:HB3	2.31	0.58
17:Q:8:PRO:O	17:Q:9:ILE:C	2.42	0.58
17:Q:26:ARG:HB3	17:Q:34:VAL:HG11	1.75	0.58
17:Q:142:LYS:NZ	17:Q:146:ASP:OD2	2.25	0.58
18:R:257:ILE:HG23	18:R:266:SER:HB3	1.86	0.58
1:A:62:CYS:SG	1:A:65:CYS:N	2.75	0.58
2:B:280:LEU:HD23	2:B:354:LEU:HD13	1.85	0.58
2:B:464:PHE:O	2:B:468:GLY:N	2.31	0.58
2:B:1093:LEU:HD13	2:B:1093:LEU:O	2.04	0.58
15:O:445:TYR:O	15:O:449:TRP:N	2.23	0.58
18:R:168:ILE:HG12	18:R:169:PRO:N	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:ALA:O	1:A:196:ALA:N	2.29	0.58
1:A:628:PHE:CB	2:B:784:ASP:HB3	2.34	0.58
1:A:628:PHE:CB	2:B:785:ASP:CG	2.67	0.58
5:E:14:ARG:HD2	5:E:141:VAL:HG13	1.86	0.58
5:E:165:LEU:O	5:E:169:ARG:N	2.36	0.58
16:P:428:GLU:N	16:P:433:VAL:HG11	2.18	0.58
16:P:622:TYR:CZ	16:P:668:SER:HB3	2.38	0.58
20:T:14:DG:H8	20:T:14:DG:O5'	1.85	0.58
1:A:1155:PHE:CD2	1:A:1163:GLU:HG2	2.38	0.58
1:A:1274:GLU:HA	1:A:1290:TYR:HB3	1.85	0.58
2:B:211:ARG:HD2	2:B:239:VAL:HG11	1.85	0.58
2:B:504:HIS:CD2	2:B:506:GLY:H	2.21	0.58
3:C:40:PHE:HA	3:C:58:ASN:HB2	1.85	0.58
16:P:436:ILE:CG2	18:R:141:TRP:O	2.52	0.58
16:P:739:ASP:OD2	17:Q:271:LYS:HE2	2.04	0.58
1:A:469:LYS:O	2:B:1070:ARG:NH1	2.30	0.58
1:A:638:PRO:HB3	2:B:1087:LEU:HD12	1.86	0.58
1:A:672:ASP:CB	2:B:783:MET:SD	2.91	0.58
2:B:841:ASP:HA	2:B:847:TYR:CZ	2.39	0.58
2:B:893:ASN:OD1	20:T:39:DT:OP1	2.21	0.58
15:O:387:HIS:ND1	15:O:606:MET:SD	2.76	0.58
1:A:671:GLN:CB	2:B:783:MET:HE2	2.29	0.57
1:A:1447:GLN:HG3	1:A:1460:TYR:HB3	1.85	0.57
1:A:355:PHE:CD1	1:A:355:PHE:N	2.73	0.57
1:A:537:GLN:HB2	1:A:578:TYR:OH	2.04	0.57
1:A:642:ASN:CG	2:B:1086:PHE:CE2	2.73	0.57
14:N:123:SER:HA	14:N:131:LEU:H	1.69	0.57
15:O:391:GLN:NE2	15:O:609:TYR:OH	2.36	0.57
16:P:535:VAL:HG12	16:P:552:LEU:HB2	1.85	0.57
17:Q:24:ASP:OD2	17:Q:26:ARG:NH1	2.31	0.57
1:A:1258:ILE:HD12	1:A:1258:ILE:C	2.24	0.57
2:B:1063:ARG:CD	20:T:22:DG:OP2	2.51	0.57
2:B:1063:ARG:HD3	20:T:22:DG:OP1	2.04	0.57
13:M:81:PHE:HB2	13:M:88:ILE:HD12	1.85	0.57
16:P:329:ILE:HD12	16:P:330:PRO:HD2	1.86	0.57
17:Q:355:VAL:C	18:R:212:HIS:ND1	2.57	0.57
17:Q:366:TYR:HA	17:Q:369:TRP:CD1	2.39	0.57
17:Q:378:LEU:CD2	18:R:235:ILE:HD13	2.34	0.57
20:T:11:DA:N1	20:T:12:DC:C4	2.71	0.57
1:A:1559:ARG:HD2	1:A:1587:ASP:OD1	2.04	0.57
7:G:232:THR:O	7:G:248:THR:N	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:41:TYR:HB3	14:N:29:PHE:HB3	1.86	0.57
15:O:390:GLN:HE21	15:O:432:LYS:H	1.52	0.57
15:O:480:LEU:HA	15:O:483:ILE:HD12	1.86	0.57
16:P:391:THR:OG1	18:R:146:SER:HB3	2.04	0.57
16:P:419:ARG:CG	16:P:420:GLU:H	2.17	0.57
16:P:422:ILE:HG13	16:P:442:LEU:HD11	1.87	0.57
17:Q:441:ASP:O	17:Q:445:ARG:HG2	2.04	0.57
18:R:175:ILE:O	18:R:178:LEU:HB3	2.04	0.57
20:T:8:DT:H2'	20:T:9:DC:H6	1.68	0.57
1:A:1050:TYR:HB3	1:A:1054:ALA:HA	1.86	0.57
1:A:1311:GLU:OE1	1:A:1311:GLU:N	2.36	0.57
12:L:32:ALA:HB3	12:L:55:ILE:HG23	1.87	0.57
13:M:13:GLU:HG3	13:M:87:SER:HB2	1.86	0.57
15:O:484:PHE:CB	15:O:528:PHE:HD1	2.17	0.57
15:O:484:PHE:HB2	15:O:528:PHE:HD1	1.68	0.57
16:P:186:TYR:CD1	18:R:198:LEU:HB3	2.40	0.57
1:A:579:ARG:NH2	1:A:585:ASP:OD1	2.34	0.57
1:A:755:ILE:HD12	1:A:780:ILE:HD11	1.87	0.57
1:A:1053:ASP:OD2	1:A:1580:ARG:NH2	2.37	0.57
1:A:1246:VAL:O	1:A:1517:ARG:NH2	2.38	0.57
1:A:1310:LYS:HA	1:A:1313:LEU:HB3	1.86	0.57
2:B:117:VAL:HB	18:R:277:ILE:HA	1.86	0.57
2:B:1155:ASP:OD2	7:G:239:THR:N	2.37	0.57
7:G:147:LEU:HB2	7:G:155:ALA:HB3	1.86	0.57
15:O:379:ARG:CB	15:O:382:GLN:HE22	2.17	0.57
17:Q:140:ILE:HG22	17:Q:236:MET:HG2	1.85	0.57
1:A:581:ILE:HD11	1:A:605:VAL:HG21	1.87	0.57
1:A:1010:ALA:O	1:A:1013:THR:OG1	2.23	0.57
16:P:355:GLU:CA	18:R:24:ILE:HD12	2.34	0.57
16:P:422:ILE:CG1	16:P:442:LEU:HD11	2.35	0.57
16:P:732:LEU:O	16:P:735:GLU:N	2.37	0.57
17:Q:22:ILE:HD12	17:Q:24:ASP:OD2	2.04	0.57
17:Q:186:CYS:HB3	18:R:208:TYR:OH	2.05	0.57
18:R:138:PHE:CE2	18:R:140:ILE:HD11	2.38	0.57
1:A:477:ASN:H	2:B:1095:SER:HB2	1.70	0.57
1:A:493:ASN:HA	1:A:653:THR:HG21	1.86	0.57
1:A:1262:LEU:H	1:A:1265:GLU:CD	2.07	0.57
2:B:1084:THR:O	2:B:1088:LEU:CB	2.48	0.57
15:O:422:GLN:NE2	15:O:589:GLN:O	2.38	0.57
16:P:391:THR:HG23	18:R:149:LYS:HD3	1.86	0.57
17:Q:366:TYR:CB	18:R:215:THR:HG21	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:LEU:HD12	1:A:241:PRO:HD2	1.87	0.57
2:B:114:SER:O	18:R:281:LYS:CA	2.25	0.57
2:B:117:VAL:CG1	18:R:277:ILE:CA	2.80	0.57
2:B:627:GLY:N	2:B:641:TYR:O	2.34	0.57
10:J:9:SER:HB2	10:J:45:CYS:SG	2.45	0.57
15:O:385:MET:HA	15:O:388:VAL:HG12	1.87	0.57
16:P:384:ASP:HB3	16:P:389:TRP:CD1	2.39	0.57
18:R:177:LEU:CD2	18:R:185:LYS:HA	2.34	0.57
1:A:87:ASN:N	1:A:355:PHE:O	2.32	0.57
1:A:371:SER:O	1:A:378:HIS:N	2.37	0.57
1:A:747:ILE:HG22	1:A:774:GLY:HA2	1.87	0.57
16:P:376:ASP:C	16:P:378:SER:H	2.09	0.57
16:P:419:ARG:HG2	16:P:420:GLU:H	1.67	0.57
16:P:725:VAL:HG23	17:Q:446:TYR:CG	2.35	0.57
17:Q:286:LEU:HD13	17:Q:286:LEU:H	1.69	0.57
18:R:354:LEU:HG	18:R:368:TYR:OH	2.04	0.57
2:B:156:ARG:HH21	2:B:450:LEU:HD12	1.70	0.56
2:B:709:PHE:CE2	2:B:992:PRO:HG2	2.39	0.56
2:B:817:ARG:HB3	21:U:17:DT:C4'	2.35	0.56
3:C:160:ALA:O	3:C:196:LEU:N	2.36	0.56
17:Q:20:TRP:CE2	17:Q:28:THR:HB	2.39	0.56
17:Q:436:LEU:HD12	17:Q:436:LEU:H	1.70	0.56
1:A:618:TYR:HE1	2:B:783:MET:HB3	1.65	0.56
2:B:117:VAL:HG21	18:R:276:GLN:HB3	1.75	0.56
2:B:379:ARG:HE	2:B:580:GLY:HA2	1.69	0.56
2:B:752:VAL:HG21	2:B:965:GLU:HG3	1.88	0.56
2:B:812:ALA:HB2	2:B:815:ARG:HH11	1.70	0.56
2:B:1099:THR:OG1	2:B:1100:GLN:N	2.38	0.56
8:H:25:ARG:NH1	8:H:27:GLU:OE2	2.32	0.56
9:I:15:ASP:OD2	9:I:32:GLN:N	2.36	0.56
15:O:487:ARG:HE	15:O:502:LEU:HD13	1.69	0.56
17:Q:328:LEU:HD22	17:Q:328:LEU:H	1.69	0.56
17:Q:366:TYR:HB2	18:R:215:THR:HG21	1.87	0.56
18:R:299:THR:HG21	18:R:305:THR:HA	1.86	0.56
1:A:556:ALA:HA	15:O:242:VAL:HG12	1.87	0.56
1:A:831:ASP:OD2	2:B:1010:ASN:ND2	2.37	0.56
1:A:1013:THR:CB	20:T:17:DT:H3	2.15	0.56
2:B:212:ASN:HD22	2:B:212:ASN:N	2.02	0.56
2:B:894:LYS:HE3	17:Q:405:ASP:CG	2.21	0.56
16:P:24:SER:OG	18:R:321:GLN:OE1	2.22	0.56
16:P:68:THR:HB	16:P:545:SER:HB3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:320:ILE:O	16:P:322:GLY:N	2.38	0.56
16:P:629:ARG:HH22	16:P:662:LEU:HD21	1.70	0.56
17:Q:22:ILE:HD12	17:Q:26:ARG:NE	2.18	0.56
1:A:593:PRO:HB3	20:T:18:DT:H1'	1.86	0.56
1:A:1016:SER:OG	1:A:1197:SER:OG	2.19	0.56
1:A:1182:GLY:O	1:A:1650:GLY:CA	2.54	0.56
2:B:60:LEU:O	2:B:64:GLY:N	2.37	0.56
2:B:338:PHE:HZ	2:B:357:ILE:HD11	1.69	0.56
2:B:705:PRO:HG2	2:B:921:HIS:CE1	2.40	0.56
6:F:140:ASP:OD1	6:F:142:SER:N	2.35	0.56
7:G:37:CYS:HB2	7:G:125:TRP:NE1	2.20	0.56
9:I:30:CYS:HB3	9:I:35:ALA:H	1.70	0.56
1:A:509:GLU:CG	1:A:579:ARG:HE	2.18	0.56
2:B:247:THR:OG1	2:B:477:ASP:OD1	2.21	0.56
2:B:320:LEU:HD11	2:B:326:VAL:HA	1.87	0.56
2:B:714:ARG:HG2	2:B:959:THR:HG22	1.86	0.56
2:B:753:LYS:O	2:B:981:SER:N	2.24	0.56
2:B:768:GLY:N	2:B:1032:TYR:OH	2.38	0.56
5:E:40:GLU:O	5:E:44:ALA:N	2.27	0.56
5:E:183:PRO:O	5:E:187:TYR:N	2.34	0.56
15:O:379:ARG:HA	15:O:382:GLN:OE1	2.05	0.56
15:O:457:ARG:O	15:O:460:GLU:N	2.38	0.56
16:P:209:LYS:HZ1	16:P:277:VAL:HG11	1.69	0.56
18:R:309:ALA:O	18:R:313:LEU:HB2	2.05	0.56
1:A:320:VAL:HA	1:A:323:ILE:HD12	1.88	0.56
2:B:264:TRP:CD1	2:B:265:ARG:HG2	2.40	0.56
7:G:29:ASP:OD1	7:G:30:GLU:N	2.36	0.56
8:H:3:ASN:OD1	8:H:4:THR:N	2.38	0.56
16:P:290:GLU:HB3	16:P:342:GLN:HB3	1.86	0.56
19:S:5:G:C2	20:T:19:DC:N3	2.74	0.56
1:A:1088:HIS:CG	6:F:152:ILE:HD11	2.41	0.56
2:B:913:ILE:HD11	2:B:930:LYS:H	1.71	0.56
14:N:85:HIS:CE1	14:N:141:GLU:HG3	2.40	0.56
15:O:442:VAL:HA	15:O:445:TYR:HB3	1.87	0.56
16:P:273:ARG:HG2	16:P:291:PRO:HB3	1.87	0.56
16:P:450:ARG:NH2	16:P:506:THR:O	2.38	0.56
16:P:657:SER:O	16:P:657:SER:OG	2.19	0.56
17:Q:96:ILE:HD12	17:Q:103:LEU:HD12	1.87	0.56
1:A:653:THR:OG1	1:A:654:ASP:N	2.39	0.56
2:B:566:TYR:HB3	13:M:74:ASN:OD1	2.06	0.56
2:B:1074:MET:HE1	20:T:18:DT:C4'	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1084:THR:O	2:B:1088:LEU:CD2	2.49	0.56
7:G:234:ARG:N	7:G:246:ASP:O	2.37	0.56
16:P:428:GLU:HB3	16:P:433:VAL:HG21	1.87	0.56
17:Q:495:LYS:HD2	17:Q:499:LYS:HZ2	1.71	0.56
18:R:222:LEU:O	18:R:226:ARG:HG3	2.06	0.56
18:R:294:VAL:HB	18:R:295:PRO:CD	2.36	0.56
1:A:1463:ASP:OD2	1:A:1468:LYS:N	2.35	0.56
2:B:714:ARG:HG2	2:B:959:THR:CG2	2.36	0.56
7:G:82:LEU:HD11	7:G:125:TRP:HB2	1.87	0.56
10:J:45:CYS:O	10:J:48:ARG:HG2	2.06	0.56
13:M:75:GLN:O	14:N:58:PHE:N	2.39	0.56
1:A:512:THR:HG21	1:A:514:TYR:HE2	1.70	0.56
11:K:50:LEU:HD11	11:K:64:GLN:HB2	1.87	0.56
16:P:666:SER:HB3	16:P:742:TRP:NE1	2.21	0.56
16:P:713:ILE:O	16:P:717:LYS:HG2	2.06	0.56
18:R:171:ARG:O	18:R:174:GLU:HB3	2.05	0.56
1:A:117:ARG:HB3	1:A:185:ARG:NH1	2.20	0.55
1:A:880:GLN:HG3	1:A:972:TYR:OH	2.06	0.55
2:B:1093:LEU:HD11	2:B:1098:TYR:CB	2.33	0.55
6:F:99:LEU:O	6:F:102:SER:OG	2.15	0.55
6:F:147:SER:N	6:F:150:GLU:OE2	2.35	0.55
13:M:36:THR:HG21	13:M:62:TYR:CE2	2.41	0.55
16:P:185:GLN:C	18:R:198:LEU:HD23	2.27	0.55
16:P:300:LEU:HA	16:P:320:ILE:HA	1.87	0.55
16:P:697:GLU:HG2	16:P:698:LYS:H	1.70	0.55
16:P:725:VAL:CG2	17:Q:446:TYR:HD1	1.81	0.55
17:Q:410:ARG:HE	17:Q:413:LEU:HD13	1.71	0.55
1:A:36:THR:HG22	1:A:45:VAL:HG21	1.86	0.55
1:A:37:VAL:HG12	1:A:38:LEU:HG	1.88	0.55
1:A:1179:ILE:HD11	1:A:1183:GLU:OE2	2.07	0.55
2:B:17:ARG:O	2:B:21:ARG:N	2.30	0.55
15:O:491:PHE:CD2	15:O:498:TRP:CE3	2.88	0.55
16:P:724:LEU:HD11	17:Q:443:GLN:HG2	1.88	0.55
1:A:543:LEU:HB2	17:Q:34:VAL:O	2.06	0.55
1:A:666:VAL:HG23	1:A:667:ARG:HG3	1.87	0.55
2:B:20:GLU:OE2	2:B:24:ARG:NH1	2.33	0.55
2:B:321:GLN:O	2:B:322:ASN:HB2	2.06	0.55
2:B:1061:LYS:O	2:B:1067:GLY:HA3	2.05	0.55
2:B:1078:ALA:C	2:B:1082:HIS:HB2	2.26	0.55
8:H:21:ASN:OD1	8:H:22:LYS:N	2.39	0.55
15:O:379:ARG:HA	15:O:382:GLN:HE22	1.69	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:194:ARG:HG2	16:P:538:LEU:HD11	1.87	0.55
16:P:420:GLU:O	16:P:442:LEU:HD22	2.07	0.55
16:P:760:ILE:O	16:P:764:LEU:HG	2.06	0.55
1:A:527:PRO:HD3	1:A:554:ARG:NH2	2.20	0.55
1:A:882:ILE:HG13	1:A:888:LYS:HB3	1.88	0.55
1:A:959:VAL:HG22	1:A:965:THR:HG22	1.88	0.55
2:B:132:SER:OG	2:B:462:GLN:NE2	2.39	0.55
7:G:40:ARG:HB2	7:G:123:TYR:HE1	1.70	0.55
15:O:498:TRP:HB3	15:O:502:LEU:HD12	1.88	0.55
16:P:301:GLN:HG3	16:P:361:LYS:H	1.70	0.55
18:R:408:ILE:HG23	18:R:435:LEU:HD13	1.87	0.55
1:A:1238:MET:HE2	1:A:1525:ASN:N	2.22	0.55
2:B:816:ASN:HB3	21:U:18:DG:P	2.46	0.55
16:P:254:ILE:HD11	16:P:365:TRP:HD1	1.71	0.55
18:R:253:ILE:HA	18:R:256:GLU:HB3	1.89	0.55
1:A:1637:PRO:CB	1:A:1647:ASN:ND2	2.64	0.55
3:C:69:ARG:NH2	11:K:70:HIS:HB2	2.21	0.55
16:P:323:ASN:HA	16:P:350:THR:HA	1.88	0.55
17:Q:131:HIS:O	17:Q:135:ILE:HG12	2.05	0.55
17:Q:308:SER:O	17:Q:312:LEU:HD22	2.05	0.55
17:Q:505:ILE:HA	17:Q:508:ALA:HB3	1.88	0.55
18:R:16:ARG:HG3	18:R:184:ASN:ND2	2.22	0.55
18:R:222:LEU:HD23	18:R:226:ARG:NH2	2.20	0.55
18:R:412:ARG:NH2	18:R:439:GLU:OE2	2.35	0.55
20:T:11:DA:C5	20:T:12:DC:N4	2.75	0.55
1:A:588:LEU:HD22	2:B:1087:LEU:HD21	1.88	0.55
2:B:186:GLU:CD	2:B:731:VAL:H	2.10	0.55
2:B:728:THR:HG21	10:J:56:LEU:HD21	1.88	0.55
2:B:731:VAL:HG11	10:J:59:LYS:HB3	1.88	0.55
2:B:818:GLY:C	2:B:820:PRO:N	2.59	0.55
2:B:851:TYR:HD1	2:B:881:TYR:CE1	2.24	0.55
15:O:173:HIS:HB3	15:O:221:TYR:CE2	2.41	0.55
15:O:359:GLY:HA2	15:O:362:ASN:HD22	1.72	0.55
15:O:383:TYR:OH	15:O:595:ASP:O	2.16	0.55
16:P:353:ASP:OD1	16:P:355:GLU:HG3	2.06	0.55
17:Q:104:PHE:HZ	17:Q:156:LEU:HB2	1.72	0.55
17:Q:310:PHE:O	17:Q:314:ILE:HG13	2.06	0.55
17:Q:331:ILE:CG2	17:Q:475:ALA:HB1	2.36	0.55
18:R:83:HIS:O	18:R:85:ARG:N	2.39	0.55
1:A:463:LYS:HZ1	20:T:16:DT:H2'	1.72	0.55
1:A:938:VAL:O	1:A:941:SER:OG	2.16	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1104:TYR:HB3	1:A:1120:TYR:CE2	2.42	0.55
2:B:74:PHE:HE1	2:B:94:LYS:HG3	1.70	0.55
2:B:894:LYS:CE	17:Q:405:ASP:CG	2.75	0.55
3:C:95:GLU:OE1	3:C:95:GLU:N	2.39	0.55
3:C:172:GLN:H	3:C:175:GLN:HB2	1.70	0.55
16:P:762:ARG:HA	16:P:762:ARG:HE	1.71	0.55
1:A:487:ASP:OD2	11:K:95:HIS:NE2	2.30	0.55
1:A:642:ASN:ND2	2:B:1086:PHE:CE2	2.68	0.55
1:A:1182:GLY:O	1:A:1650:GLY:HA2	2.06	0.55
1:A:1297:PHE:CE2	9:I:58:SER:HB2	2.42	0.55
1:A:1660:VAL:O	7:G:102:GLU:HA	2.07	0.55
2:B:936:MET:HG2	2:B:948:ILE:HD11	1.88	0.55
3:C:218:LYS:HG3	3:C:218:LYS:O	2.06	0.55
5:E:78:LEU:HD12	5:E:107:THR:O	2.07	0.55
8:H:115:TYR:CE1	8:H:124:ARG:HG3	2.42	0.55
16:P:371:LYS:HD2	16:P:432:PRO:HB3	1.89	0.55
20:T:11:DA:C2	20:T:12:DC:C4	2.95	0.55
1:A:553:GLN:N	1:A:553:GLN:OE1	2.40	0.55
3:C:253:PRO:HD2	14:N:180:PHE:HB3	1.88	0.55
4:D:19:PRO:HA	7:G:47:VAL:HG12	1.89	0.55
15:O:443:ALA:O	15:O:446:LEU:HB3	2.07	0.55
16:P:348:HIS:HE1	18:R:154:LYS:HD3	1.72	0.55
16:P:614:GLU:OE2	16:P:734:LYS:NZ	2.26	0.55
17:Q:177:TYR:OH	17:Q:248:SER:O	2.11	0.55
18:R:23:TYR:HD1	18:R:173:MET:HG3	1.71	0.55
1:A:1238:MET:HE3	1:A:1526:PHE:HA	1.90	0.54
7:G:138:PHE:CZ	7:G:146:GLY:HA3	2.42	0.54
16:P:443:ASP:HB2	18:R:2:PHE:CA	2.37	0.54
16:P:486:ALA:O	18:R:138:PHE:CE1	2.59	0.54
2:B:641:TYR:CB	2:B:643:PHE:CE1	2.89	0.54
16:P:182:LEU:CD1	16:P:185:GLN:HG2	2.36	0.54
16:P:348:HIS:HE1	18:R:154:LYS:CD	2.21	0.54
16:P:743:SER:OG	17:Q:250:GLN:HG3	2.07	0.54
17:Q:8:PRO:HB2	17:Q:19:LEU:CD2	2.36	0.54
18:R:301:SER:O	18:R:303:THR:N	2.35	0.54
1:A:527:PRO:CD	1:A:554:ARG:HH12	2.19	0.54
1:A:1018:TYR:HB2	20:T:17:DT:H5"	1.89	0.54
2:B:115:SER:O	18:R:280:SER:C	2.33	0.54
2:B:320:LEU:HD22	2:B:325:GLN:HB2	1.87	0.54
7:G:74:ASN:OD1	7:G:75:ASN:N	2.41	0.54
18:R:246:GLN:NE2	18:R:247:ILE:HD12	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1014:SER:O	20:T:17:DT:O4'	2.25	0.54
2:B:71:LYS:N	2:B:97:VAL:O	2.40	0.54
2:B:265:ARG:O	2:B:267:ASN:ND2	2.39	0.54
2:B:1105:ARG:HG2	2:B:1172:GLU:HB3	1.90	0.54
7:G:235:ASN:H	7:G:246:ASP:HB3	1.72	0.54
16:P:229:ARG:HG3	16:P:230:HIS:N	2.21	0.54
17:Q:186:CYS:O	18:R:208:TYR:CZ	2.61	0.54
18:R:357:PRO:HB3	18:R:359:MET:SD	2.48	0.54
2:B:99:VAL:HG12	2:B:100:GLU:H	1.72	0.54
13:M:43:LYS:HB2	14:N:29:PHE:CD1	2.43	0.54
14:N:54:TRP:CD1	14:N:135:LYS:HB2	2.42	0.54
17:Q:6:ARG:HA	17:Q:18:ARG:HD2	1.88	0.54
1:A:111:LYS:HD2	1:A:114:GLU:HG2	1.88	0.54
2:B:683:ASN:HA	14:N:150:TYR:CE1	2.42	0.54
2:B:1074:MET:CE	20:T:18:DT:C4'	2.86	0.54
3:C:105:PRO:HB2	3:C:187:ALA:HB3	1.88	0.54
7:G:235:ASN:HD22	7:G:237:HIS:CE1	2.26	0.54
10:J:31:ASP:OD1	10:J:34:THR:N	2.29	0.54
14:N:125:ALA:C	14:N:127:ASP:H	2.11	0.54
15:O:441:PHE:O	15:O:445:TYR:N	2.28	0.54
16:P:598:LEU:HA	16:P:601:ARG:HG3	1.89	0.54
17:Q:136:ILE:HG12	17:Q:243:PHE:CZ	2.42	0.54
2:B:1114:GLN:OE1	2:B:1129:ARG:NH2	2.38	0.54
16:P:185:GLN:C	18:R:198:LEU:CD2	2.76	0.54
16:P:194:ARG:CZ	16:P:511:ILE:HG12	2.38	0.54
17:Q:366:TYR:HA	17:Q:369:TRP:CE2	2.43	0.54
18:R:427:PRO:HG2	18:R:429:ARG:NH2	2.23	0.54
20:T:7:DT:H3	21:U:43:DA:N6	2.06	0.54
1:A:321:LYS:CE	1:A:325:ASP:OD2	2.56	0.54
2:B:832:TRP:CZ3	2:B:834:LYS:HA	2.43	0.54
2:B:1065:ARG:O	2:B:1066:HIS:CB	2.56	0.54
3:C:134:LEU:HD23	3:C:169:PHE:HA	1.89	0.54
3:C:157:TYR:HB2	3:C:160:ALA:HB2	1.90	0.54
17:Q:314:ILE:O	17:Q:318:LEU:HB2	2.08	0.54
17:Q:323:ASP:N	17:Q:324:ARG:N	2.55	0.54
19:S:5:G:H8	19:S:5:G:O5'	1.90	0.54
1:A:435:ASN:O	1:A:439:ASP:N	2.41	0.54
1:A:578:TYR:N	1:A:578:TYR:CD1	2.75	0.54
1:A:627:ASP:N	1:A:631:ASP:OD2	2.41	0.54
1:A:1018:TYR:HE1	20:T:16:DT:P	2.14	0.54
2:B:101:GLN:HE21	18:R:359:MET:HE1	0.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:396:ALA:HA	2:B:521:LEU:CD1	2.37	0.54
2:B:432:ILE:O	2:B:435:GLY:N	2.31	0.54
2:B:492:ASN:OD1	2:B:495:ARG:N	2.30	0.54
8:H:29:ALA:HA	8:H:37:LYS:HA	1.90	0.54
17:Q:366:TYR:HB2	18:R:215:THR:CG2	2.38	0.54
18:R:252:GLY:O	18:R:256:GLU:CB	2.56	0.54
1:A:462:LYS:O	1:A:464:GLU:N	2.38	0.54
1:A:1443:GLN:HG2	1:A:1446:ARG:NH2	2.23	0.54
2:B:566:TYR:HE1	2:B:572:PRO:HA	1.72	0.54
5:E:185:ALA:O	5:E:189:GLY:N	2.40	0.54
15:O:360:VAL:HA	15:O:363:THR:HG22	1.89	0.54
15:O:532:ALA:O	15:O:536:SER:N	2.41	0.54
16:P:384:ASP:HB3	16:P:389:TRP:HD1	1.71	0.54
17:Q:356:VAL:HG23	18:R:208:TYR:CD2	2.24	0.54
17:Q:374:THR:HG23	18:R:219:LEU:HD13	1.90	0.54
1:A:457:LYS:HG3	1:A:1619:CYS:SG	2.48	0.53
1:A:591:ARG:HB2	1:A:633:MET:HG2	1.90	0.53
1:A:1328:ALA:HA	1:A:1331:LYS:HB3	1.90	0.53
2:B:114:SER:O	18:R:280:SER:O	2.25	0.53
2:B:1051:PRO:HG2	2:B:1059:PRO:HA	1.90	0.53
7:G:45:LEU:HD13	7:G:47:VAL:HG13	1.90	0.53
9:I:11:LEU:N	9:I:37:TYR:OH	2.37	0.53
15:O:361:PHE:HZ	15:O:399:PHE:HB2	1.73	0.53
17:Q:22:ILE:HD12	17:Q:26:ARG:NH1	2.24	0.53
17:Q:330:TRP:O	17:Q:334:LEU:HB2	2.08	0.53
18:R:250:LEU:O	18:R:253:ILE:N	2.40	0.53
2:B:792:SER:O	2:B:796:ARG:HG3	2.08	0.53
3:C:81:GLU:O	12:L:69:ALA:N	2.32	0.53
7:G:170:HIS:HA	7:G:215:GLY:HA3	1.90	0.53
16:P:383:ILE:HG12	16:P:390:GLN:HG2	1.89	0.53
16:P:411:LYS:HB2	16:P:412:ASN:OD1	2.08	0.53
1:A:672:ASP:CG	2:B:783:MET:CE	2.77	0.53
2:B:101:GLN:HE22	18:R:359:MET:HE3	1.71	0.53
5:E:26:ARG:HH21	5:E:187:TYR:C	2.12	0.53
16:P:577:LEU:HD21	17:Q:499:LYS:HB2	1.89	0.53
18:R:231:LEU:O	18:R:235:ILE:HG12	2.08	0.53
18:R:416:LYS:O	18:R:419:LEU:N	2.41	0.53
1:A:1513:GLU:O	1:A:1516:LYS:N	2.37	0.53
2:B:45:HIS:O	2:B:48:SER:OG	2.18	0.53
2:B:994:ASP:HA	2:B:1007:TYR:OH	2.09	0.53
15:O:200:ASN:OD1	17:Q:14:ASN:HB2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:254:ILE:HD11	16:P:365:TRP:CD1	2.43	0.53
16:P:421:ILE:CG2	16:P:423:ILE:HG13	2.38	0.53
16:P:452:THR:HG21	16:P:508:ILE:HG22	1.90	0.53
16:P:778:ASP:OD1	16:P:779:ASP:N	2.42	0.53
1:A:520:ARG:HH21	1:A:559:ASN:ND2	2.06	0.53
1:A:949:GLN:HA	1:A:981:TYR:HA	1.90	0.53
1:A:962:SER:HB3	2:B:670:VAL:HG12	1.90	0.53
1:A:1637:PRO:HB3	1:A:1647:ASN:ND2	2.23	0.53
3:C:43:ASN:O	3:C:55:ASP:N	2.37	0.53
9:I:35:ALA:HB2	13:M:59:ARG:HH22	1.72	0.53
15:O:484:PHE:CZ	15:O:528:PHE:HA	2.43	0.53
16:P:185:GLN:O	18:R:198:LEU:HD21	2.08	0.53
1:A:1136:VAL:HG11	1:A:1140:PHE:HD2	1.74	0.53
1:A:1238:MET:HE1	1:A:1524:VAL:HG13	1.90	0.53
1:A:1239:THR:HG23	1:A:1518:VAL:HG11	1.89	0.53
2:B:650:LEU:HB3	2:B:663:ILE:CG2	2.39	0.53
5:E:83:CYS:HB2	5:E:110:PHE:CZ	2.43	0.53
15:O:487:ARG:NH2	15:O:502:LEU:HD13	2.22	0.53
16:P:436:ILE:HG21	18:R:141:TRP:O	2.09	0.53
1:A:1506:ARG:O	1:A:1522:GLU:OE1	2.26	0.53
2:B:731:VAL:HA	10:J:60:PHE:CE1	2.42	0.53
15:O:434:LEU:HD22	15:O:439:ILE:CD1	2.35	0.53
16:P:186:TYR:CD1	18:R:198:LEU:HD23	2.44	0.53
16:P:715:TYR:CE1	16:P:733:THR:HG23	2.44	0.53
17:Q:350:ARG:CD	17:Q:486:GLN:CG	2.83	0.53
18:R:250:LEU:HD23	18:R:251:TRP:H	1.72	0.53
20:T:17:DT:H6	20:T:17:DT:O5'	1.92	0.53
1:A:646:GLU:OE2	6:F:91:ALA:CB	2.57	0.53
13:M:60:LEU:HA	13:M:102:SER:HA	1.90	0.53
15:O:418:ILE:HG12	15:O:475:ALA:HB2	1.91	0.53
16:P:433:VAL:HG23	16:P:434:ARG:O	2.08	0.53
16:P:470:SER:O	16:P:505:PRO:HD2	2.08	0.53
2:B:75:ASP:OD1	2:B:93:ASN:N	2.42	0.53
2:B:320:LEU:CD2	2:B:326:VAL:N	2.71	0.53
2:B:1106:GLU:O	2:B:1197:ARG:NH2	2.38	0.53
8:H:101:ALA:HB2	8:H:116:TYR:CE2	2.44	0.53
9:I:46:LYS:HE3	9:I:48:VAL:HG23	1.91	0.53
15:O:352:LEU:HD21	15:O:395:LEU:HD11	1.91	0.53
16:P:302:VAL:HG21	16:P:362:ARG:HD2	1.91	0.53
16:P:455:LYS:H	16:P:455:LYS:HD2	1.74	0.53
2:B:954:PHE:CB	2:B:955:PRO:CD	2.87	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1074:MET:HE1	20:T:18:DT:O4'	2.09	0.53
7:G:47:VAL:HB	7:G:65:HIS:CD2	2.44	0.53
15:O:484:PHE:CD1	15:O:528:PHE:HA	2.43	0.53
16:P:215:ASN:N	16:P:220:THR:OG1	2.42	0.53
18:R:209:ARG:H	18:R:209:ARG:HD3	1.74	0.53
1:A:797:LEU:HD23	1:A:809:VAL:HG21	1.91	0.52
1:A:1060:GLU:OE1	1:A:1580:ARG:NH1	2.43	0.52
1:A:1637:PRO:HB3	1:A:1647:ASN:HD21	1.70	0.52
2:B:778:TYR:CE2	2:B:937:PRO:HD3	2.44	0.52
2:B:841:ASP:OD2	12:L:58:LYS:NZ	2.35	0.52
2:B:916:LYS:NZ	19:S:5:G:H4'	2.24	0.52
20:T:14:DG:H2'	20:T:15:DC:C6	2.44	0.52
1:A:1049:MET:HB2	1:A:1052:GLY:HA2	1.92	0.52
2:B:691:PHE:HB2	2:B:695:ASN:HD21	1.73	0.52
2:B:828:GLY:HA3	2:B:862:PHE:CD1	2.43	0.52
2:B:916:LYS:HZ2	19:S:5:G:H4'	1.73	0.52
6:F:137:TYR:CD1	6:F:143:PHE:HB3	2.44	0.52
7:G:219:ASP:OD1	7:G:222:GLY:N	2.42	0.52
15:O:62:ASP:HB3	15:O:67:ASP:HB3	1.91	0.52
15:O:473:PHE:O	15:O:477:PHE:N	2.40	0.52
16:P:261:VAL:HG22	16:P:262:GLY:H	1.74	0.52
1:A:836:THR:N	1:A:915:GLY:O	2.22	0.52
16:P:261:VAL:HG22	16:P:262:GLY:N	2.24	0.52
16:P:681:GLN:HA	16:P:684:GLN:HB2	1.92	0.52
2:B:211:ARG:NH2	2:B:645:GLY:HA3	2.24	0.52
2:B:403:LEU:HD11	2:B:411:MET:HE3	1.91	0.52
2:B:755:ASN:ND2	2:B:980:ASP:OD1	2.43	0.52
4:D:43:PHE:O	4:D:47:LYS:HG2	2.10	0.52
7:G:20:HIS:ND1	7:G:20:HIS:O	2.43	0.52
15:O:78:VAL:HG23	15:O:118:SER:HB3	1.91	0.52
16:P:358:SER:HB3	16:P:377:ARG:CD	2.34	0.52
16:P:544:SER:O	16:P:546:GLU:N	2.40	0.52
17:Q:364:SER:O	17:Q:367:PHE:HB2	2.10	0.52
1:A:50:TYR:OH	1:A:383:ASN:ND2	2.43	0.52
1:A:600:MET:CB	2:B:1082:HIS:CD2	2.91	0.52
1:A:1238:MET:CE	1:A:1525:ASN:C	2.78	0.52
1:A:1297:PHE:HB3	1:A:1301:GLU:OE1	2.10	0.52
1:A:1656:VAL:HG11	6:F:96:THR:HG21	1.89	0.52
2:B:216:ALA:HB1	2:B:384:LEU:HD22	1.90	0.52
2:B:643:PHE:N	2:B:643:PHE:CD1	2.77	0.52
2:B:788:ILE:HB	2:B:948:ILE:HB	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:124:VAL:HB	5:E:125:PRO:HD3	1.91	0.52
6:F:89:GLU:OE2	6:F:136:ARG:NE	2.41	0.52
13:M:81:PHE:HD1	13:M:88:ILE:HB	1.74	0.52
15:O:435:SER:HB3	15:O:438:GLN:HG3	1.91	0.52
16:P:242:ILE:HD13	16:P:273:ARG:HE	1.75	0.52
16:P:314:GLN:OE1	16:P:314:GLN:HA	2.09	0.52
16:P:776:ASP:O	16:P:777:MET:HG2	2.10	0.52
17:Q:159:THR:O	17:Q:163:SER:OG	2.16	0.52
1:A:223:PHE:CE2	1:A:227:LEU:HD11	2.45	0.52
1:A:463:LYS:HZ2	20:T:16:DT:H71	1.73	0.52
1:A:1645:LYS:NZ	1:A:1645:LYS:CB	2.73	0.52
2:B:37:LEU:HD12	2:B:759:ASP:HB3	1.91	0.52
2:B:110:ASN:HA	2:B:118:GLU:HG2	1.92	0.52
8:H:39:THR:HB	8:H:124:ARG:HB3	1.91	0.52
10:J:8:PHE:HB2	10:J:48:ARG:HH22	1.73	0.52
15:O:584:GLN:O	15:O:588:LEU:HG	2.09	0.52
15:O:602:TYR:HA	15:O:605:LEU:HD12	1.92	0.52
16:P:433:VAL:HG23	16:P:434:ARG:N	2.24	0.52
1:A:93:GLN:HB2	1:A:355:PHE:HE2	1.75	0.52
1:A:130:ILE:O	1:A:133:SER:OG	2.22	0.52
1:A:638:PRO:CB	2:B:1087:LEU:HD12	2.39	0.52
1:A:1640:ARG:NH1	1:A:1640:ARG:CG	2.73	0.52
2:B:516:THR:HA	2:B:519:LYS:HE2	1.91	0.52
2:B:773:VAL:HG21	2:B:1033:TYR:HE1	1.73	0.52
2:B:841:ASP:OD1	2:B:842:GLU:N	2.38	0.52
3:C:116:VAL:HG22	3:C:130:ASN:HB3	1.92	0.52
6:F:117:PRO:HA	6:F:120:ILE:HD12	1.91	0.52
9:I:29:GLU:HA	9:I:36:ILE:HA	1.91	0.52
15:O:78:VAL:HG12	15:O:88:ILE:HG21	1.91	0.52
16:P:389:TRP:CH2	18:R:149:LYS:CG	2.93	0.52
18:R:303:THR:HG22	18:R:304:HIS:H	1.75	0.52
1:A:1303:SER:O	1:A:1307:ASP:HA	2.10	0.52
1:A:1654:PHE:HE2	6:F:89:GLU:N	2.07	0.52
2:B:135:GLY:O	2:B:161:LEU:N	2.25	0.52
2:B:368:GLN:O	2:B:372:ARG:NH1	2.43	0.52
10:J:7:CYS:HA	10:J:49:MET:HG3	1.92	0.52
15:O:169:THR:HA	15:O:172:HIS:ND1	2.25	0.52
15:O:477:PHE:HE2	15:O:525:MET:HE1	1.74	0.52
16:P:473:HIS:N	16:P:504:THR:HG21	2.24	0.52
16:P:585:GLU:O	16:P:589:ILE:HG13	2.10	0.52
16:P:622:TYR:O	16:P:626:LEU:CB	2.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:706:GLU:O	16:P:708:VAL:HG23	2.10	0.52
17:Q:101:LYS:O	17:Q:105:LEU:HG	2.09	0.52
17:Q:414:TYR:CE2	17:Q:419:LEU:HB3	2.45	0.52
18:R:346:ILE:HD11	18:R:374:LEU:HD12	1.91	0.52
18:R:436:LYS:HA	18:R:439:GLU:HB2	1.92	0.52
1:A:464:GLU:HB2	1:A:465:GLY:CA	2.40	0.52
1:A:552:GLU:HG2	1:A:553:GLN:N	2.25	0.52
1:A:1238:MET:HB2	1:A:1521:THR:HB	1.84	0.52
2:B:338:PHE:CE2	2:B:353:VAL:HG22	2.45	0.52
2:B:658:LEU:HD23	2:B:660:LYS:HD3	1.91	0.52
15:O:200:ASN:OD1	17:Q:14:ASN:CG	2.48	0.52
15:O:357:GLY:HA2	15:O:360:VAL:HB	1.91	0.52
16:P:419:ARG:CG	16:P:420:GLU:N	2.73	0.52
17:Q:8:PRO:CB	17:Q:19:LEU:HD23	2.39	0.52
18:R:153:ASN:OD1	18:R:154:LYS:N	2.43	0.52
1:A:462:LYS:C	1:A:464:GLU:H	2.13	0.52
1:A:526:GLY:HA2	1:A:554:ARG:NH1	2.25	0.52
1:A:581:ILE:HD12	1:A:637:PHE:CE1	2.45	0.52
2:B:120:LYS:HE2	18:R:352:TRP:CH2	2.45	0.52
7:G:149:ILE:HG22	7:G:150:HIS:ND1	2.25	0.52
15:O:491:PHE:CB	15:O:498:TRP:HZ3	2.07	0.52
1:A:584:ARG:HD2	6:F:116:ASP:HB2	1.92	0.51
1:A:846:ILE:O	1:A:849:THR:OG1	2.21	0.51
2:B:322:ASN:HB3	2:B:325:GLN:HG3	1.92	0.51
2:B:939:SER:HG	2:B:943:ILE:H	1.55	0.51
2:B:1019:GLY:HA3	3:C:65:ASN:HB2	1.92	0.51
2:B:1063:ARG:CG	20:T:22:DG:P	2.98	0.51
9:I:37:TYR:HB3	9:I:41:GLN:NE2	2.25	0.51
10:J:34:THR:O	10:J:38:ARG:N	2.36	0.51
16:P:532:GLU:HA	16:P:554:ASN:ND2	2.17	0.51
16:P:724:LEU:HD12	17:Q:443:GLN:CA	2.39	0.51
16:P:748:GLU:HG2	16:P:749:LYS:HG3	1.91	0.51
17:Q:355:VAL:HG12	18:R:212:HIS:HA	1.72	0.51
1:A:81:LEU:HD12	1:A:82:PRO:CD	2.37	0.51
1:A:244:ARG:HH22	1:A:312:SER:HA	1.75	0.51
1:A:477:ASN:HB3	2:B:1047:ARG:NH1	2.25	0.51
1:A:480:ALA:HB2	2:B:1046:VAL:HG23	1.92	0.51
1:A:594:THR:HG23	1:A:599:SER:HB2	1.91	0.51
1:A:772:LYS:HE3	8:H:137:GLN:HE21	1.76	0.51
2:B:119:ARG:NH2	2:B:125:GLU:OE2	2.36	0.51
2:B:1104:CYS:HB2	2:B:1128:CYS:SG	2.49	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:243:SER:HA	3:C:246:ARG:HE	1.75	0.51
5:E:64:PRO:HB2	5:E:69:ILE:HG13	1.91	0.51
7:G:40:ARG:HB2	7:G:123:TYR:CE1	2.44	0.51
14:N:113:SER:OG	14:N:115:SER:OG	2.22	0.51
17:Q:8:PRO:CG	17:Q:19:LEU:HD23	2.40	0.51
1:A:1650:GLY:O	1:A:1652:GLY:N	2.44	0.51
2:B:819:ASP:O	2:B:820:PRO:O	2.27	0.51
16:P:712:ASP:OD1	16:P:712:ASP:N	2.44	0.51
16:P:762:ARG:HG3	17:Q:139:LYS:CE	2.40	0.51
1:A:368:ARG:HA	1:A:380:ASN:ND2	2.24	0.51
1:A:1608:SER:O	1:A:1612:LYS:NZ	2.41	0.51
2:B:807:GLU:O	2:B:903:ILE:N	2.38	0.51
7:G:216:HIS:ND1	7:G:224:PRO:HB3	2.25	0.51
13:M:55:GLY:N	13:M:62:TYR:O	2.36	0.51
14:N:85:HIS:CD2	14:N:86:ASP:H	2.28	0.51
16:P:362:ARG:HG3	16:P:363:ILE:N	2.24	0.51
18:R:314:TRP:CD1	18:R:367:ILE:HD11	2.45	0.51
1:A:440:SER:N	1:A:458:GLN:HE22	2.08	0.51
1:A:579:ARG:NH1	1:A:585:ASP:OD2	2.29	0.51
1:A:1651:THR:CG2	2:B:1086:PHE:HB2	2.41	0.51
2:B:757:TYR:CE1	2:B:762:MET:HB2	2.46	0.51
3:C:224:THR:HG21	10:J:43:ARG:NH2	2.25	0.51
16:P:66:CYS:HB2	16:P:547:VAL:HB	1.92	0.51
16:P:389:TRP:CZ2	18:R:147:GLN:CA	2.94	0.51
16:P:389:TRP:CH2	18:R:147:GLN:CA	2.94	0.51
1:A:401:ASP:O	1:A:404:SER:OG	2.24	0.51
1:A:535:GLN:HB2	1:A:578:TYR:CD1	2.46	0.51
2:B:777:SER:OG	2:B:951:PRO:HD2	2.11	0.51
3:C:227:TYR:HB3	3:C:300:PHE:CE1	2.45	0.51
16:P:299:ASP:O	16:P:320:ILE:HB	2.10	0.51
16:P:389:TRP:CZ3	18:R:149:LYS:HB2	2.45	0.51
16:P:417:THR:OG1	16:P:451:ILE:HB	2.10	0.51
1:A:636:HIS:HB3	2:B:1091:ARG:HD2	1.93	0.51
1:A:1516:LYS:HG3	1:A:1518:VAL:HG23	1.92	0.51
2:B:736:ARG:O	2:B:904:LYS:NZ	2.26	0.51
8:H:10:PHE:CD1	8:H:30:SER:HA	2.46	0.51
8:H:112:ILE:HD11	8:H:129:TYR:CD1	2.46	0.51
9:I:31:SER:O	9:I:34:LYS:NZ	2.37	0.51
13:M:57:ASN:ND2	13:M:60:LEU:HB2	2.25	0.51
16:P:704:LEU:HD23	17:Q:258:MET:HE3	1.93	0.51
18:R:173:MET:O	18:R:176:PRO:HD2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:PHE:CE2	1:A:444:GLN:HG2	2.46	0.51
2:B:240:ARG:HG2	2:B:360:VAL:HB	1.93	0.51
3:C:128:ASP:O	3:C:175:GLN:NE2	2.44	0.51
3:C:237:GLN:HE21	3:C:288:LYS:HG2	1.75	0.51
16:P:186:TYR:HD1	18:R:198:LEU:HB3	1.74	0.51
16:P:267:ASN:OD1	16:P:268:SER:N	2.43	0.51
16:P:378:SER:OG	16:P:379:LYS:HD2	2.11	0.51
16:P:474:LYS:H	16:P:474:LYS:CD	2.23	0.51
17:Q:97:GLY:O	17:Q:99:GLU:N	2.39	0.51
17:Q:186:CYS:SG	18:R:208:TYR:HE2	2.31	0.51
17:Q:192:TYR:CD1	17:Q:193:PHE:N	2.76	0.51
17:Q:366:TYR:CG	18:R:215:THR:HG21	2.42	0.51
1:A:409:ASP:OD1	1:A:410:LYS:N	2.42	0.51
1:A:1268:ASP:N	1:A:1295:ARG:O	2.42	0.51
1:A:1272:VAL:O	9:I:49:THR:N	2.38	0.51
8:H:127:GLY:N	8:H:132:LEU:HD11	2.26	0.51
9:I:9:PHE:HA	9:I:15:ASP:O	2.10	0.51
11:K:66:VAL:O	11:K:68:GLU:HG2	2.11	0.51
16:P:233:VAL:HG12	16:P:234:THR:H	1.75	0.51
16:P:405:TYR:HE2	16:P:414:ILE:CG1	2.24	0.51
16:P:438:TRP:HE3	16:P:439:LYS:O	1.93	0.51
18:R:12:LYS:O	18:R:15:GLN:N	2.44	0.51
18:R:406:LYS:O	18:R:410:TYR:HB2	2.11	0.51
1:A:463:LYS:NZ	20:T:16:DT:C7	2.74	0.51
1:A:941:SER:O	1:A:945:CYS:N	2.39	0.51
1:A:991:LYS:N	1:A:994:GLU:OE1	2.43	0.51
1:A:1316:VAL:HG13	1:A:1320:GLN:NE2	2.25	0.51
1:A:1450:ILE:HA	1:A:1453:HIS:CD2	2.46	0.51
2:B:173:ASN:OD1	2:B:174:LYS:N	2.44	0.51
5:E:91:LYS:O	5:E:95:THR:N	2.27	0.51
15:O:52:TYR:CZ	15:O:92:ASN:HB3	2.46	0.51
16:P:330:PRO:HG3	16:P:342:GLN:CG	2.41	0.51
16:P:634:THR:HG22	16:P:686:TYR:CE2	2.46	0.51
17:Q:381:MET:CG	18:R:238:THR:HG21	2.32	0.51
18:R:189:GLN:O	18:R:192:SER:OG	2.29	0.51
1:A:748:ASN:OD1	1:A:773:ASP:N	2.37	0.50
2:B:1078:ALA:O	2:B:1082:HIS:CB	2.59	0.50
5:E:26:ARG:NH2	5:E:187:TYR:O	2.39	0.50
13:M:22:ALA:HA	13:M:94:PRO:HD2	1.93	0.50
16:P:188:GLN:HG2	16:P:360:TRP:CB	2.37	0.50
16:P:380:MET:HB3	16:P:393:VAL:CG2	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:658:LYS:HB3	16:P:659:LEU:HD22	1.93	0.50
17:Q:24:ASP:CG	17:Q:26:ARG:HE	2.14	0.50
17:Q:270:THR:HA	17:Q:273:VAL:HG23	1.92	0.50
17:Q:349:GLY:O	17:Q:352:ILE:N	2.44	0.50
18:R:291:ARG:NH2	20:T:42:DA:OP2	2.43	0.50
1:A:1449:ALA:O	1:A:1452:SER:OG	2.17	0.50
2:B:143:TRP:CD1	2:B:152:LEU:HD12	2.45	0.50
2:B:816:ASN:O	21:U:17:DT:H4'	2.11	0.50
2:B:1079:LEU:CG	2:B:1088:LEU:CB	2.74	0.50
8:H:11:GLN:HA	8:H:54:SER:HA	1.91	0.50
8:H:102:TYR:CZ	8:H:115:TYR:HB3	2.45	0.50
15:O:245:GLN:HG2	15:O:377:TYR:O	2.10	0.50
16:P:272:PHE:HB2	16:P:300:LEU:HD11	1.93	0.50
16:P:658:LYS:C	16:P:660:LYS:N	2.64	0.50
17:Q:378:LEU:HD13	18:R:231:LEU:CD2	2.40	0.50
21:U:40:DT:H6	21:U:40:DT:H5''	1.75	0.50
1:A:1003:ARG:HD3	2:B:520:LEU:HD22	1.92	0.50
1:A:1645:LYS:NZ	1:A:1645:LYS:HB3	2.26	0.50
2:B:731:VAL:HG12	10:J:63:TYR:CE2	2.46	0.50
2:B:1103:VAL:HG12	2:B:1110:ILE:HG22	1.92	0.50
9:I:32:GLN:OE1	13:M:105:SER:HB2	2.11	0.50
15:O:477:PHE:HA	15:O:480:LEU:HG	1.93	0.50
16:P:227:LEU:HD23	16:P:227:LEU:H	1.75	0.50
16:P:408:ILE:HD12	16:P:409:ASP:H	1.76	0.50
16:P:410:ASP:O	16:P:411:LYS:HD3	2.10	0.50
16:P:762:ARG:HG3	17:Q:139:LYS:NZ	2.27	0.50
17:Q:447:ALA:HA	17:Q:450:THR:HB	1.93	0.50
18:R:11:ARG:CZ	21:U:4:DA:O5'	2.45	0.50
1:A:95:TYR:CD1	1:A:245:LYS:HD3	2.47	0.50
1:A:102:CYS:HB3	1:A:107:HIS:H	1.76	0.50
1:A:416:ARG:O	1:A:420:PHE:N	2.45	0.50
1:A:509:GLU:CD	1:A:579:ARG:NE	2.63	0.50
1:A:519:LEU:HA	1:A:522:ALA:HB3	1.92	0.50
1:A:1261:VAL:HG12	1:A:1498:ILE:HB	1.93	0.50
1:A:1648:ASN:OD1	1:A:1648:ASN:N	2.39	0.50
2:B:168:ASN:OD1	2:B:169:ARG:HG2	2.11	0.50
2:B:328:GLN:NE2	13:M:110:GLY:O	2.45	0.50
2:B:428:VAL:O	2:B:432:ILE:N	2.43	0.50
2:B:985:ILE:O	14:N:157:ARG:NH2	2.45	0.50
2:B:1093:LEU:HD11	2:B:1098:TYR:HD1	1.76	0.50
3:C:65:ASN:O	3:C:68:ARG:HB3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:34:CYS:HB3	12:L:51:CYS:SG	2.51	0.50
16:P:446:ASP:N	18:R:200:THR:HG21	2.25	0.50
17:Q:353:VAL:CG1	17:Q:489:VAL:HG12	2.39	0.50
18:R:361:ASP:HB2	18:R:364:VAL:CG1	2.42	0.50
1:A:39:ASP:OD1	1:A:43:HIS:N	2.44	0.50
1:A:56:ALA:HB3	1:A:69:GLU:HA	1.93	0.50
1:A:419:ILE:O	1:A:422:ARG:N	2.43	0.50
1:A:880:GLN:HE21	2:B:633:THR:H	1.59	0.50
1:A:975:ASP:OD1	1:A:976:ALA:N	2.45	0.50
2:B:279:ALA:HB1	2:B:354:LEU:HD11	1.93	0.50
2:B:1093:LEU:HD12	2:B:1098:TYR:CB	2.25	0.50
2:B:1093:LEU:HD11	2:B:1098:TYR:CD1	2.46	0.50
3:C:308:MET:SD	3:C:316:LYS:NZ	2.70	0.50
9:I:6:SER:H	9:I:45:LEU:HD11	1.76	0.50
11:K:104:ARG:NH2	11:K:106:GLN:HE21	1.95	0.50
14:N:124:THR:H	14:N:131:LEU:HB2	1.75	0.50
16:P:50:LEU:HD11	18:R:259:ASP:OD1	2.11	0.50
16:P:444:PRO:HG3	16:P:449:LEU:HD11	1.93	0.50
18:R:257:ILE:HG23	18:R:267:GLY:H	1.75	0.50
18:R:320:CYS:O	18:R:323:SER:HB3	2.11	0.50
1:A:4:SER:HB3	1:A:576:LYS:NZ	2.26	0.50
1:A:618:TYR:OH	2:B:783:MET:HB2	2.11	0.50
2:B:641:TYR:CB	2:B:643:PHE:HE1	2.25	0.50
2:B:790:ASN:HB2	2:B:936:MET:SD	2.51	0.50
9:I:58:SER:HG	9:I:62:ALA:H	1.59	0.50
15:O:198:PHE:CE1	15:O:236:LYS:HG3	2.47	0.50
16:P:190:ALA:O	16:P:248:PRO:HA	2.12	0.50
16:P:262:GLY:C	16:P:263:ILE:HG12	2.31	0.50
16:P:487:ASN:CB	18:R:138:PHE:CE1	2.94	0.50
17:Q:356:VAL:CG1	18:R:208:TYR:CD2	2.90	0.50
17:Q:357:TYR:OH	17:Q:488:LEU:HB3	2.12	0.50
21:U:38:DG:H2''	21:U:39:DT:O4'	2.12	0.50
1:A:804:GLU:H	1:A:804:GLU:CD	2.15	0.50
1:A:1040:ASP:OD1	1:A:1041:ALA:N	2.41	0.50
2:B:532:HIS:CD2	2:B:719:CYS:HB3	2.46	0.50
4:D:80:THR:HG21	15:O:227:PHE:CD2	2.46	0.50
16:P:414:ILE:CD1	16:P:425:GLY:HA3	2.41	0.50
16:P:443:ASP:CB	18:R:2:PHE:HB3	2.30	0.50
16:P:725:VAL:HG23	17:Q:446:TYR:CB	2.26	0.50
17:Q:119:LEU:HD13	17:Q:125:PHE:CG	2.47	0.50
1:A:44:PRO:HG2	1:A:52:LEU:HD21	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:ILE:O	1:A:140:THR:OG1	2.29	0.50
1:A:264:ASN:O	1:A:268:GLY:N	2.44	0.50
1:A:543:LEU:HD22	1:A:578:TYR:CZ	2.47	0.50
1:A:1459:LYS:HB2	1:A:1473:LYS:HB3	1.94	0.50
1:A:1646:LEU:HD11	2:B:1086:PHE:CD1	2.47	0.50
2:B:399:HIS:O	2:B:400:GLN:HG3	2.11	0.50
2:B:717:TYR:O	2:B:721:MET:N	2.41	0.50
2:B:790:ASN:CA	2:B:936:MET:SD	3.00	0.50
10:J:53:HIS:NE2	10:J:55:ASP:OD1	2.39	0.50
13:M:44:LYS:NZ	13:M:47:GLU:O	2.40	0.50
15:O:99:ILE:O	15:O:102:SER:OG	2.19	0.50
17:Q:10:CYS:HB2	17:Q:17:SER:N	2.25	0.50
17:Q:10:CYS:SG	17:Q:29:CYS:SG	3.07	0.50
17:Q:326:TYR:HB3	17:Q:330:TRP:CZ3	2.47	0.50
17:Q:374:THR:O	17:Q:377:PHE:HB3	2.12	0.50
18:R:302:ARG:O	18:R:303:THR:OG1	2.21	0.50
1:A:535:GLN:O	1:A:578:TYR:HD1	1.95	0.50
1:A:652:ASN:HB2	1:A:655:SER:CB	2.39	0.50
2:B:396:ALA:HA	2:B:521:LEU:HD12	1.93	0.50
2:B:599:GLU:H	2:B:599:GLU:CD	2.16	0.50
2:B:795:GLU:HB3	3:C:216:HIS:CE1	2.46	0.50
5:E:16:PHE:CZ	5:E:20:LYS:HE3	2.46	0.50
7:G:37:CYS:HB2	7:G:125:TRP:CD1	2.47	0.50
15:O:478:GLN:OE1	15:O:520:CYS:HB3	2.12	0.50
16:P:319:ASP:OD1	16:P:324:TRP:HB3	2.12	0.50
16:P:762:ARG:HG3	17:Q:139:LYS:HE3	1.93	0.50
17:Q:162:ILE:HG22	17:Q:226:LEU:HD21	1.94	0.50
21:U:38:DG:C6	21:U:39:DT:N3	2.80	0.50
1:A:545:SER:CB	17:Q:34:VAL:HG21	2.39	0.49
2:B:216:ALA:HB2	2:B:380:LYS:HE2	1.94	0.49
2:B:954:PHE:HB2	2:B:955:PRO:CD	2.41	0.49
6:F:66:ARG:HH22	7:G:90:LEU:HD13	1.76	0.49
15:O:197:PHE:O	15:O:211:TYR:OH	2.21	0.49
16:P:609:ASN:O	16:P:612:GLU:HB2	2.12	0.49
17:Q:109:GLN:CD	17:Q:137:TRP:HE1	2.16	0.49
1:A:19:LEU:N	2:B:1193:GLY:O	2.35	0.49
1:A:95:TYR:CG	1:A:245:LYS:HD3	2.47	0.49
1:A:621:THR:O	1:A:625:ASN:N	2.45	0.49
1:A:671:GLN:OE1	2:B:783:MET:O	2.29	0.49
1:A:1654:PHE:CB	6:F:134:ILE:HG23	2.33	0.49
2:B:1075:GLU:OE1	2:B:1075:GLU:N	2.40	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1116:SER:N	2:B:1125:THR:O	2.44	0.49
3:C:237:GLN:HE21	3:C:288:LYS:HE3	1.78	0.49
6:F:77:ASP:OD1	6:F:78:GLN:N	2.44	0.49
7:G:38:ILE:HG13	7:G:125:TRP:HD1	1.77	0.49
14:N:35:LEU:N	14:N:116:LYS:O	2.35	0.49
16:P:549:TYR:HE1	16:P:551:ALA:HB2	1.76	0.49
16:P:551:ALA:C	16:P:552:LEU:HD23	2.32	0.49
18:R:299:THR:OG1	18:R:300:GLY:N	2.45	0.49
1:A:1242:ILE:HA	1:A:1536:ILE:HA	1.94	0.49
2:B:1154:ASP:HB3	2:B:1157:GLN:HG2	1.94	0.49
5:E:41:ASP:HA	5:E:44:ALA:HB3	1.94	0.49
8:H:100:THR:OG1	8:H:139:ASN:OD1	2.21	0.49
13:M:57:ASN:O	13:M:103:LYS:NZ	2.23	0.49
15:O:429:ALA:HB3	15:O:482:TYR:CE2	2.47	0.49
16:P:405:TYR:OH	16:P:414:ILE:HB	2.12	0.49
18:R:85:ARG:HG2	18:R:85:ARG:HH11	1.77	0.49
18:R:362:ALA:O	18:R:365:TRP:N	2.46	0.49
21:U:38:DG:N2	21:U:39:DT:O2	2.45	0.49
1:A:1246:VAL:HA	1:A:1250:GLN:OE1	2.13	0.49
2:B:1102:SER:HA	2:B:1174:THR:O	2.12	0.49
15:O:351:SER:HA	15:O:355:GLY:HA3	1.93	0.49
15:O:507:GLN:HE22	15:O:543:ILE:HD11	1.78	0.49
16:P:193:LEU:HG	16:P:250:ALA:HA	1.95	0.49
16:P:353:ASP:OD2	16:P:379:LYS:NZ	2.46	0.49
16:P:426:ALA:O	16:P:433:VAL:HG22	2.12	0.49
17:Q:198:ILE:HG21	17:Q:390:THR:H	1.77	0.49
17:Q:232:LEU:HD13	17:Q:287:TRP:HE1	1.77	0.49
17:Q:356:VAL:N	18:R:212:HIS:CE1	2.80	0.49
18:R:23:TYR:CD1	18:R:173:MET:HG3	2.47	0.49
18:R:274:MET:HB3	18:R:308:PHE:HB3	1.94	0.49
18:R:282:SER:O	18:R:282:SER:OG	2.27	0.49
20:T:7:DT:O2	21:U:44:DG:N2	2.46	0.49
1:A:831:ASP:HB3	2:B:1008:HIS:CG	2.47	0.49
1:A:1185:VAL:O	1:A:1189:ALA:N	2.36	0.49
1:A:1191:GLN:HE22	2:B:1078:ALA:HA	1.77	0.49
1:A:1650:GLY:C	1:A:1652:GLY:N	2.66	0.49
15:O:219:ARG:HE	15:O:230:TRP:HE1	1.61	0.49
17:Q:335:THR:HG21	17:Q:478:ARG:HD2	1.95	0.49
17:Q:357:TYR:HE2	17:Q:488:LEU:C	2.16	0.49
18:R:160:HIS:O	18:R:164:LYS:HG3	2.13	0.49
20:T:11:DA:N6	20:T:12:DC:N4	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:990:ILE:HD11	1:A:995:TYR:HD1	1.77	0.49
1:A:1114:TYR:CD1	5:E:146:HIS:HA	2.48	0.49
1:A:1238:MET:HG2	1:A:1524:VAL:HG22	1.94	0.49
1:A:1299:ASN:HA	1:A:1302:TYR:CE2	2.48	0.49
1:A:1657:LEU:O	6:F:133:VAL:N	2.45	0.49
2:B:31:ASP:OD1	2:B:32:LYS:N	2.40	0.49
2:B:1163:GLN:OE1	2:B:1163:GLN:N	2.46	0.49
15:O:116:ILE:HA	15:O:119:ILE:HD12	1.94	0.49
15:O:487:ARG:NH2	15:O:506:PHE:CE2	2.81	0.49
16:P:196:TYR:HB3	16:P:206:ALA:HB1	1.93	0.49
16:P:357:LEU:CD1	18:R:191:ILE:HD12	2.43	0.49
16:P:722:TRP:CZ3	16:P:736:ILE:HD12	2.47	0.49
18:R:206:ARG:C	18:R:207:ASN:CB	2.80	0.49
1:A:1055:ILE:HB	1:A:1580:ARG:HH21	1.77	0.49
1:A:1097:TYR:O	1:A:1101:THR:HG23	2.11	0.49
2:B:42:VAL:HG21	2:B:190:ILE:HD12	1.94	0.49
7:G:90:LEU:HD11	7:G:119:HIS:NE2	2.28	0.49
15:O:474:TYR:O	15:O:478:GLN:N	2.24	0.49
16:P:408:ILE:HB	16:P:453:VAL:HG21	1.95	0.49
17:Q:274:ILE:HG12	17:Q:282:ARG:HH22	1.77	0.49
1:A:129:LEU:HB3	1:A:132:GLU:OE1	2.12	0.49
1:A:1508:VAL:O	1:A:1510:PRO:HD3	2.12	0.49
2:B:368:GLN:HG3	2:B:372:ARG:NH1	2.27	0.49
2:B:398:GLN:NE2	2:B:636:GLN:OE1	2.42	0.49
8:H:38:LEU:HD11	8:H:123:MET:HG3	1.95	0.49
9:I:54:ASP:OD1	9:I:55:ALA:N	2.45	0.49
14:N:114:GLU:HG2	14:N:120:LYS:NZ	2.28	0.49
16:P:274:ILE:CD1	16:P:305:PHE:HE2	2.25	0.49
16:P:305:PHE:HZ	16:P:329:ILE:HG21	1.76	0.49
16:P:357:LEU:HD12	18:R:191:ILE:HD12	1.94	0.49
16:P:458:LYS:HA	16:P:458:LYS:NZ	2.28	0.49
16:P:693:PHE:HA	16:P:746:ARG:NE	2.28	0.49
17:Q:141:LEU:O	17:Q:144:ILE:HG13	2.12	0.49
17:Q:247:ILE:HD12	17:Q:248:SER:H	1.77	0.49
1:A:354:SER:OG	1:A:355:PHE:CE1	2.61	0.49
1:A:552:GLU:OE1	1:A:552:GLU:N	2.38	0.49
1:A:1014:SER:CB	20:T:17:DT:C6	2.91	0.49
1:A:1090:ASP:HB3	1:A:1132:TYR:HD1	1.76	0.49
1:A:1443:GLN:NE2	1:A:1461:ASN:OD1	2.46	0.49
2:B:1079:LEU:H	2:B:1079:LEU:HD12	1.77	0.49
3:C:113:LEU:HD23	3:C:210:LEU:HG	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:315:PHE:HE1	11:K:135:PHE:HD2	1.61	0.49
5:E:107:THR:HG23	5:E:131:THR:HG23	1.95	0.49
8:H:124:ARG:NH1	8:H:126:GLU:OE1	2.27	0.49
15:O:205:ARG:HB2	15:O:331:LYS:HG2	1.95	0.49
16:P:405:TYR:CE2	16:P:414:ILE:HB	2.48	0.49
16:P:458:LYS:HD3	16:P:459:PRO:CD	2.43	0.49
16:P:573:GLU:HB2	17:Q:499:LYS:NZ	2.27	0.49
17:Q:22:ILE:HD12	17:Q:26:ARG:CZ	2.40	0.49
17:Q:356:VAL:HG11	18:R:208:TYR:CD2	2.46	0.49
17:Q:386:LEU:CA	18:R:241:ARG:CZ	2.74	0.49
1:A:257:ASN:O	1:A:261:ILE:HD12	2.13	0.49
1:A:1050:TYR:CE2	1:A:1580:ARG:HD3	2.47	0.49
1:A:1447:GLN:NE2	1:A:1460:TYR:H	2.10	0.49
1:A:1575:ILE:HG22	1:A:1576:SER:H	1.77	0.49
3:C:297:HIS:CD2	3:C:298:PHE:H	2.30	0.49
5:E:28:TYR:HA	5:E:64:PRO:HA	1.95	0.49
15:O:592:PHE:O	15:O:594:TYR:N	2.45	0.49
16:P:274:ILE:HD13	16:P:305:PHE:CE2	2.43	0.49
16:P:319:ASP:HB2	16:P:363:ILE:CG1	2.43	0.49
16:P:319:ASP:HB2	16:P:363:ILE:HG13	1.95	0.49
1:A:1227:MET:O	1:A:1597:ALA:HB1	2.13	0.48
2:B:887:LEU:N	12:L:56:LEU:O	2.42	0.48
2:B:1114:GLN:HE21	2:B:1159:TRP:HZ3	1.61	0.48
7:G:49:LEU:HD11	7:G:53:TYR:HB2	1.95	0.48
15:O:383:TYR:HA	15:O:386:PHE:HB3	1.95	0.48
16:P:300:LEU:N	16:P:300:LEU:HD23	2.27	0.48
16:P:414:ILE:HG12	16:P:425:GLY:N	2.28	0.48
17:Q:352:ILE:HD12	17:Q:380:TRP:CE3	2.48	0.48
17:Q:363:SER:C	17:Q:365:ASP:N	2.65	0.48
17:Q:385:PHE:O	18:R:241:ARG:NE	2.45	0.48
18:R:304:HIS:NE2	18:R:361:ASP:HB3	2.28	0.48
1:A:248:PHE:CD2	1:A:444:GLN:HG2	2.49	0.48
1:A:332:GLN:NE2	1:A:349:LEU:HB3	2.28	0.48
1:A:492:THR:HB	1:A:667:ARG:NH2	2.28	0.48
1:A:646:GLU:OE1	2:B:1086:PHE:CB	2.61	0.48
1:A:651:ALA:H	2:B:1084:THR:CG2	2.27	0.48
1:A:656:GLN:HE22	2:B:1082:HIS:HD1	1.61	0.48
2:B:752:VAL:HB	2:B:920:ARG:HH22	1.78	0.48
8:H:103:LYS:HD2	8:H:115:TYR:CE2	2.47	0.48
15:O:141:LYS:HA	15:O:179:PHE:HZ	1.78	0.48
16:P:61:VAL:HB	16:P:551:ALA:HB3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:347:LEU:HD22	16:P:385:PHE:HD2	1.78	0.48
17:Q:266:PHE:HA	17:Q:269:TYR:HB2	1.94	0.48
1:A:482:SER:OG	1:A:483:VAL:N	2.45	0.48
1:A:1290:TYR:CE1	1:A:1474:LEU:HB2	2.48	0.48
2:B:184:LYS:HZ2	10:J:69:ARG:HH22	1.60	0.48
2:B:402:VAL:O	2:B:647:SER:HB3	2.13	0.48
2:B:747:GLY:HA3	2:B:766:PRO:HB2	1.96	0.48
7:G:24:VAL:O	7:G:128:GLN:NE2	2.36	0.48
11:K:77:ARG:HD2	11:K:91:TYR:HD1	1.77	0.48
13:M:83:PRO:HG2	14:N:49:LYS:HE3	1.94	0.48
16:P:56:ASP:O	16:P:57:LEU:HD23	2.12	0.48
16:P:223:ASN:HD22	16:P:286:VAL:HG11	1.78	0.48
17:Q:10:CYS:HB3	17:Q:16:PRO:HA	1.93	0.48
17:Q:239:PHE:HB2	17:Q:245:SER:OG	2.13	0.48
18:R:15:GLN:OE1	18:R:181:THR:HG23	2.12	0.48
18:R:23:TYR:CE1	18:R:170:LEU:HD23	2.49	0.48
1:A:512:THR:CG2	1:A:513:ALA:H	2.24	0.48
1:A:1025:LYS:HG2	1:A:1615:TYR:CD1	2.48	0.48
1:A:1229:ALA:HB3	1:A:1597:ALA:HB2	1.94	0.48
2:B:129:ARG:HH22	2:B:890:ASP:HA	1.78	0.48
2:B:320:LEU:HD22	2:B:326:VAL:N	2.28	0.48
2:B:736:ARG:HD3	2:B:738:ASP:OD2	2.13	0.48
5:E:67:GLU:H	5:E:67:GLU:CD	2.16	0.48
12:L:48:CYS:HB3	12:L:52:GLY:N	2.22	0.48
13:M:80:LEU:HD21	14:N:38:PHE:CZ	2.49	0.48
15:O:179:PHE:HD2	15:O:183:ILE:HD12	1.78	0.48
15:O:484:PHE:HB2	15:O:528:PHE:CD1	2.48	0.48
1:A:418:VAL:HG13	1:A:419:ILE:HG13	1.94	0.48
1:A:552:GLU:H	1:A:552:GLU:CD	2.16	0.48
1:A:734:THR:O	1:A:738:ASN:ND2	2.46	0.48
2:B:585:CYS:HB2	2:B:595:TRP:CZ3	2.49	0.48
2:B:745:GLN:NE2	10:J:1:MET:SD	2.81	0.48
2:B:1087:LEU:CD2	2:B:1088:LEU:HD23	2.43	0.48
16:P:194:ARG:O	16:P:195:ASN:ND2	2.46	0.48
16:P:238:LEU:HD21	16:P:284:VAL:HG23	1.96	0.48
17:Q:350:ARG:NE	17:Q:486:GLN:CD	2.66	0.48
1:A:463:LYS:NZ	20:T:16:DT:H71	2.27	0.48
1:A:966:LEU:HB3	1:A:969:PHE:CD2	2.49	0.48
5:E:76:GLY:HA3	5:E:106:GLN:HB2	1.96	0.48
15:O:532:ALA:HB1	15:O:537:VAL:HB	1.95	0.48
16:P:294:PHE:CE2	16:P:299:ASP:HA	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:751:SER:O	16:P:753:PHE:N	2.46	0.48
17:Q:22:ILE:HD11	17:Q:26:ARG:CG	2.44	0.48
17:Q:140:ILE:O	17:Q:143:THR:HG22	2.14	0.48
1:A:219:LEU:O	1:A:223:PHE:N	2.32	0.48
1:A:1311:GLU:O	1:A:1314:GLN:HB3	2.13	0.48
2:B:985:ILE:HG13	2:B:986:PHE:CD2	2.48	0.48
2:B:1138:ALA:HB1	2:B:1153:ILE:HG13	1.95	0.48
8:H:103:LYS:HD2	8:H:115:TYR:CD2	2.48	0.48
14:N:56:ILE:HG12	14:N:137:PHE:HB2	1.94	0.48
16:P:348:HIS:CE1	18:R:154:LYS:HE2	2.49	0.48
16:P:475:ARG:HD2	16:P:475:ARG:N	2.28	0.48
1:A:232:LYS:HE2	1:A:239:PHE:CZ	2.48	0.48
1:A:613:THR:OG1	1:A:615:ARG:NH2	2.46	0.48
1:A:647:ALA:HB2	2:B:1087:LEU:HD13	1.94	0.48
1:A:1003:ARG:HD3	2:B:520:LEU:HB2	1.95	0.48
1:A:1013:THR:O	20:T:17:DT:C2	2.67	0.48
1:A:1490:GLU:HB3	1:A:1494:ARG:HH12	1.79	0.48
1:A:1610:PHE:HA	1:A:1613:MET:HB3	1.96	0.48
2:B:18:THR:O	2:B:21:ARG:HB3	2.14	0.48
2:B:52:LEU:HD23	2:B:60:LEU:HD12	1.95	0.48
2:B:211:ARG:HB3	2:B:401:GLU:OE2	2.13	0.48
2:B:1064:LYS:HE2	2:B:1064:LYS:HB3	1.62	0.48
15:O:162:PHE:O	15:O:211:TYR:HA	2.14	0.48
15:O:498:TRP:CZ2	15:O:535:GLU:HB3	2.48	0.48
16:P:60:VAL:HG12	16:P:61:VAL:H	1.78	0.48
16:P:182:LEU:HD12	16:P:185:GLN:HG2	1.95	0.48
16:P:300:LEU:HB3	16:P:320:ILE:HG22	1.96	0.48
16:P:422:ILE:O	16:P:439:LYS:HB3	2.14	0.48
16:P:436:ILE:HG23	18:R:141:TRP:HB2	1.95	0.48
17:Q:234:CYS:SG	17:Q:284:LEU:HB3	2.53	0.48
18:R:368:TYR:CE2	18:R:414:PHE:CZ	3.02	0.48
18:R:402:ASN:O	18:R:406:LYS:HG2	2.14	0.48
2:B:299:ASP:OD1	2:B:300:SER:N	2.47	0.48
2:B:943:ILE:HD11	10:J:43:ARG:HB3	1.96	0.48
2:B:1064:LYS:HD2	2:B:1064:LYS:O	2.13	0.48
2:B:1187:SER:O	2:B:1190:SER:OG	2.27	0.48
3:C:57:ILE:HG22	3:C:58:ASN:ND2	2.29	0.48
7:G:134:GLU:HA	7:G:229:LEU:O	2.14	0.48
15:O:348:THR:HG23	15:O:351:SER:H	1.78	0.48
16:P:463:LEU:HA	16:P:482:SER:HA	1.96	0.48
17:Q:417:PHE:HE1	18:R:265:SER:O	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:158:THR:OG1	18:R:159:TYR:N	2.46	0.48
21:U:39:DT:H2"	21:U:40:DT:H5"	1.96	0.48
1:A:371:SER:N	1:A:378:HIS:O	2.31	0.48
1:A:830:MET:HG3	2:B:967:LEU:HD11	1.95	0.48
2:B:939:SER:OG	2:B:942:GLY:N	2.46	0.48
2:B:1159:TRP:O	2:B:1167:PHE:N	2.40	0.48
12:L:34:CYS:HB3	12:L:51:CYS:HG	1.78	0.48
15:O:61:ASP:O	15:O:65:LYS:N	2.44	0.48
16:P:475:ARG:HH21	17:Q:364:SER:HA	1.78	0.48
16:P:533:LEU:H	16:P:554:ASN:HB2	1.78	0.48
16:P:658:LYS:C	16:P:660:LYS:H	2.17	0.48
16:P:678:LEU:HD22	16:P:679:LEU:HD13	1.96	0.48
17:Q:355:VAL:CA	18:R:212:HIS:CE1	2.60	0.48
18:R:4:VAL:HG13	18:R:6:ILE:H	1.78	0.48
18:R:82:ARG:HD2	18:R:82:ARG:O	2.14	0.48
1:A:15:ASP:OD1	1:A:1631:ARG:HG3	2.13	0.47
1:A:244:ARG:O	1:A:252:PHE:N	2.25	0.47
1:A:367:PHE:CD1	2:B:1184:TYR:HD1	2.31	0.47
1:A:920:PHE:CD1	1:A:921:PRO:HA	2.49	0.47
1:A:1261:VAL:HB	1:A:1499:ARG:H	1.79	0.47
2:B:301:PHE:CE2	2:B:386:ALA:HB2	2.49	0.47
2:B:826:GLY:N	2:B:860:ALA:O	2.46	0.47
2:B:954:PHE:CZ	2:B:963:PHE:CE1	3.03	0.47
2:B:1097:ASP:O	2:B:1179:PRO:HA	2.14	0.47
7:G:74:ASN:HB3	7:G:77:VAL:HG22	1.96	0.47
16:P:389:TRP:HZ2	18:R:147:GLN:N	1.71	0.47
17:Q:15:CYS:CB	17:Q:17:SER:N	2.60	0.47
1:A:511:VAL:CG1	1:A:575:LYS:C	2.74	0.47
1:A:537:GLN:HE21	1:A:541:GLY:HA2	1.78	0.47
1:A:546:LEU:HB3	1:A:554:ARG:CZ	2.44	0.47
1:A:771:PHE:HA	1:A:775:ALA:O	2.15	0.47
1:A:966:LEU:HD11	2:B:525:TRP:CE3	2.49	0.47
1:A:1240:LEU:HB2	1:A:1519:LEU:HB2	1.95	0.47
1:A:1312:GLU:O	1:A:1316:VAL:N	2.26	0.47
9:I:30:CYS:HB3	9:I:35:ALA:N	2.29	0.47
15:O:109:SER:O	15:O:113:THR:OG1	2.29	0.47
16:P:66:CYS:HB2	16:P:547:VAL:CG2	2.44	0.47
16:P:412:ASN:OD1	16:P:412:ASN:N	2.45	0.47
17:Q:123:MET:HE1	17:Q:184:TRP:HE1	1.78	0.47
17:Q:499:LYS:HE3	17:Q:499:LYS:HB3	1.59	0.47
18:R:275:CYS:SG	18:R:309:ALA:HA	2.54	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:468:ARG:NH2	1:A:1615:TYR:O	2.46	0.47
1:A:1013:THR:HB	20:T:17:DT:C2	2.49	0.47
2:B:113:VAL:O	18:R:282:SER:HB2	2.13	0.47
2:B:1128:CYS:N	2:B:1170:GLY:O	2.30	0.47
6:F:83:PRO:HB2	6:F:152:ILE:CD1	2.44	0.47
6:F:137:TYR:HD1	6:F:143:PHE:HB3	1.78	0.47
14:N:53:VAL:O	14:N:134:ASP:HB2	2.14	0.47
15:O:72:GLY:O	15:O:76:ASN:N	2.45	0.47
15:O:192:THR:O	15:O:196:LYS:N	2.27	0.47
15:O:228:GLN:HA	15:O:231:SER:HB2	1.96	0.47
15:O:478:GLN:NE2	15:O:481:CYS:SG	2.87	0.47
18:R:200:THR:H	18:R:203:SER:HB3	1.79	0.47
18:R:250:LEU:HG	18:R:307:LYS:HZ2	1.79	0.47
1:A:248:PHE:O	1:A:249:THR:OG1	2.30	0.47
1:A:597:LYS:CD	2:B:1082:HIS:HA	2.41	0.47
1:A:1460:TYR:OH	1:A:1462:PHE:HB2	2.14	0.47
2:B:207:ILE:HB	2:B:505:ARG:HD2	1.96	0.47
2:B:314:LYS:C	2:B:316:ARG:H	2.18	0.47
2:B:975:HIS:CG	14:N:166:LEU:HD22	2.50	0.47
2:B:1120:ILE:HD12	15:O:117:GLN:HE21	1.79	0.47
3:C:71:MET:HB2	3:C:317:SER:OG	2.15	0.47
9:I:38:PRO:CD	9:I:41:GLN:HE21	2.26	0.47
10:J:68:LYS:HE2	12:L:34:CYS:HB2	1.97	0.47
15:O:63:LEU:HD11	15:O:112:GLY:N	2.28	0.47
15:O:518:LYS:HB2	15:O:547:ASN:ND2	2.29	0.47
17:Q:161:THR:OG1	17:Q:162:ILE:N	2.47	0.47
1:A:440:SER:H	1:A:458:GLN:HE22	1.61	0.47
1:A:597:LYS:HD2	2:B:1082:HIS:CA	2.44	0.47
1:A:672:ASP:CG	2:B:950:ASN:HD21	2.18	0.47
2:B:48:SER:HB3	2:B:404:LEU:HD13	1.96	0.47
2:B:107:PRO:HG2	2:B:133:TYR:CE2	2.49	0.47
2:B:492:ASN:HD21	2:B:723:LYS:HA	1.79	0.47
2:B:1084:THR:CB	2:B:1087:LEU:HD22	2.33	0.47
15:O:390:GLN:OE1	15:O:609:TYR:HB3	2.14	0.47
15:O:602:TYR:O	15:O:606:MET:HG2	2.14	0.47
16:P:271:ILE:HG12	16:P:272:PHE:N	2.29	0.47
16:P:477:TYR:HD2	18:R:2:PHE:CZ	2.30	0.47
16:P:582:ASP:N	16:P:585:GLU:HB2	2.29	0.47
18:R:250:LEU:HD11	18:R:307:LYS:HG3	1.96	0.47
18:R:440:SER:O	18:R:440:SER:OG	2.31	0.47
7:G:48:SER:HB3	7:G:115:PHE:CE1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:302:VAL:O	16:P:363:ILE:HD11	2.13	0.47
16:P:397:LYS:O	16:P:397:LYS:HG2	2.14	0.47
17:Q:319:SER:O	17:Q:319:SER:OG	2.30	0.47
18:R:12:LYS:O	18:R:14:ALA:N	2.47	0.47
1:A:507:TYR:CE1	1:A:639:GLN:O	2.68	0.47
1:A:657:TYR:CZ	1:A:665:PRO:HB3	2.50	0.47
1:A:1114:TYR:CE2	1:A:1115:LYS:HG2	2.49	0.47
1:A:1555:VAL:HG21	5:E:212:ARG:HH12	1.80	0.47
2:B:656:LEU:HD22	14:N:153:VAL:HG21	1.97	0.47
2:B:787:MET:HB2	2:B:927:CYS:HA	1.92	0.47
2:B:963:PHE:O	2:B:1027:TYR:OH	2.31	0.47
2:B:1074:MET:CE	20:T:18:DT:O4'	2.62	0.47
3:C:105:PRO:HG2	10:J:13:VAL:HG21	1.95	0.47
3:C:316:LYS:HA	3:C:319:ARG:HB3	1.97	0.47
5:E:50:MET:HG2	5:E:52:ARG:HB2	1.96	0.47
11:K:50:LEU:O	11:K:54:THR:HG23	2.14	0.47
16:P:465:VAL:HG13	16:P:480:VAL:HG13	1.96	0.47
16:P:498:LEU:CD1	17:Q:368:GLN:HE21	2.26	0.47
16:P:775:TRP:O	17:Q:109:GLN:NE2	2.47	0.47
17:Q:135:ILE:O	17:Q:139:LYS:HD2	2.15	0.47
17:Q:274:ILE:HG23	17:Q:282:ARG:NH2	2.30	0.47
20:T:2:DT:H3	21:U:48:DA:H61	1.61	0.47
20:T:11:DA:C4	20:T:12:DC:C4	3.02	0.47
1:A:407:GLN:H	1:A:410:LYS:HE2	1.80	0.47
2:B:113:VAL:O	18:R:282:SER:CB	2.63	0.47
2:B:938:PHE:CE2	2:B:1014:TYR:HD2	2.32	0.47
3:C:90:SER:HB3	3:C:202:ILE:HD11	1.97	0.47
5:E:110:PHE:O	5:E:134:THR:HA	2.15	0.47
6:F:76:LYS:HA	6:F:79:ARG:NH1	2.29	0.47
7:G:92:ALA:HB3	7:G:104:LEU:HB2	1.97	0.47
14:N:41:ASN:HD22	14:N:51:GLN:CD	2.18	0.47
15:O:548:ASN:OD1	15:O:549:ASN:N	2.48	0.47
1:A:597:LYS:HE3	1:A:660:PRO:HG2	1.97	0.47
1:A:1637:PRO:CG	1:A:1647:ASN:ND2	2.62	0.47
2:B:372:ARG:HH21	2:B:574:SER:HA	1.80	0.47
2:B:541:LEU:O	2:B:543:ASN:ND2	2.47	0.47
2:B:823:GLN:HG2	2:B:863:ASP:HA	1.97	0.47
6:F:140:ASP:OD1	6:F:141:GLY:N	2.47	0.47
7:G:241:ARG:HG2	15:O:189:PHE:CD2	2.49	0.47
1:A:1238:MET:SD	1:A:1526:PHE:CE1	3.08	0.47
1:A:1511:GLU:O	1:A:1513:GLU:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:219:ARG:HG2	2:B:221:SER:H	1.79	0.47
2:B:992:PRO:HA	2:B:995:TYR:HB3	1.97	0.47
9:I:30:CYS:N	9:I:35:ALA:O	2.38	0.47
15:O:201:LYS:HD3	15:O:239:SER:OG	2.15	0.47
16:P:186:TYR:HE1	16:P:447:THR:OG1	1.98	0.47
16:P:263:ILE:CG2	16:P:277:VAL:HG12	2.44	0.47
16:P:363:ILE:HA	16:P:373:LEU:O	2.14	0.47
16:P:428:GLU:HG3	16:P:429:SER:N	2.29	0.47
18:R:320:CYS:SG	18:R:346:ILE:HG13	2.55	0.47
21:U:42:DA:H1'	21:U:43:DA:H5'	1.97	0.47
1:A:239:PHE:HE2	1:A:263:ASN:HD22	1.63	0.46
1:A:440:SER:H	1:A:458:GLN:NE2	2.12	0.46
1:A:970:LYS:HE2	1:A:973:GLU:OE1	2.15	0.46
1:A:1052:GLY:HA2	5:E:208:TYR:CE1	2.51	0.46
2:B:264:TRP:NE1	2:B:265:ARG:HG2	2.30	0.46
2:B:504:HIS:HB3	2:B:542:LEU:HD23	1.97	0.46
3:C:64:ALA:HA	3:C:67:PHE:HB3	1.97	0.46
3:C:87:ASN:OD1	3:C:88:ASN:N	2.48	0.46
11:K:55:SER:OG	11:K:57:ASP:OD1	2.21	0.46
15:O:174:ASP:HA	15:O:177:LYS:HE2	1.97	0.46
15:O:477:PHE:O	15:O:480:LEU:HG	2.15	0.46
16:P:304:ASP:HB2	16:P:363:ILE:O	2.15	0.46
16:P:416:LEU:HD23	16:P:423:ILE:HD12	1.97	0.46
17:Q:129:PHE:HE1	17:Q:169:SER:N	2.12	0.46
1:A:202:THR:HG22	1:A:203:THR:O	2.16	0.46
5:E:91:LYS:HA	5:E:94:LYS:HB3	1.97	0.46
15:O:77:GLN:HE21	15:O:88:ILE:HA	1.80	0.46
15:O:396:MET:HG3	15:O:434:LEU:HD11	1.54	0.46
16:P:363:ILE:HG22	16:P:374:VAL:HG22	1.98	0.46
17:Q:283:ASN:C	17:Q:284:LEU:HD12	2.36	0.46
17:Q:327:PRO:HG2	17:Q:330:TRP:H	1.80	0.46
18:R:356:PRO:CB	18:R:357:PRO:HA	2.45	0.46
20:T:12:DC:C2'	20:T:13:DT:H5'	2.44	0.46
1:A:831:ASP:N	1:A:831:ASP:OD1	2.48	0.46
1:A:1092:GLU:O	1:A:1095:LEU:N	2.48	0.46
2:B:54:GLU:O	2:B:59:GLY:HA2	2.15	0.46
15:O:216:LEU:HB3	15:O:342:HIS:CD2	2.50	0.46
15:O:434:LEU:CD2	15:O:439:ILE:HD11	2.39	0.46
15:O:487:ARG:HG2	15:O:491:PHE:CG	2.50	0.46
16:P:265:THR:HG23	16:P:274:ILE:HG12	1.97	0.46
16:P:322:GLY:N	16:P:361:LYS:HD3	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:436:ILE:CG2	18:R:141:TRP:HB2	2.45	0.46
16:P:442:LEU:N	16:P:442:LEU:HD13	2.31	0.46
16:P:463:LEU:H	16:P:463:LEU:HD22	1.81	0.46
16:P:540:LYS:O	16:P:541:LEU:HD13	2.16	0.46
16:P:573:GLU:HB2	17:Q:499:LYS:HZ1	1.79	0.46
16:P:724:LEU:HD12	17:Q:443:GLN:HG2	1.98	0.46
18:R:200:THR:O	18:R:204:GLU:HG2	2.15	0.46
1:A:590:ASN:HD21	2:B:1075:GLU:HG2	1.81	0.46
2:B:273:VAL:HG21	2:B:378:ILE:HD11	1.98	0.46
2:B:442:ASP:HB3	2:B:445:TYR:HB3	1.97	0.46
2:B:794:ASP:HA	2:B:798:PHE:HB3	1.97	0.46
16:P:361:LYS:HA	16:P:375:PHE:O	2.16	0.46
16:P:751:SER:O	16:P:754:GLU:N	2.44	0.46
18:R:253:ILE:HD13	18:R:257:ILE:HD12	1.97	0.46
1:A:461:GLU:HG2	1:A:1618:THR:HB	1.98	0.46
1:A:535:GLN:NE2	17:Q:26:ARG:HD3	2.31	0.46
1:A:564:PRO:HD2	15:O:371:HIS:HA	1.96	0.46
1:A:812:VAL:HA	1:A:815:ARG:HH21	1.80	0.46
2:B:1104:CYS:SG	2:B:1107:CYS:N	2.70	0.46
15:O:225:LEU:O	15:O:227:PHE:N	2.49	0.46
15:O:241:ASP:OD2	15:O:378:THR:HG22	2.15	0.46
16:P:394:VAL:HG12	16:P:434:ARG:NH1	2.30	0.46
17:Q:128:GLU:O	17:Q:132:VAL:HG23	2.15	0.46
17:Q:384:GLN:HA	17:Q:387:PRO:HD2	1.96	0.46
19:S:3:G:N1	20:T:21:DC:N3	2.51	0.46
1:A:81:LEU:CD2	1:A:85:CYS:SG	3.04	0.46
1:A:1314:GLN:O	1:A:1318:SER:N	2.49	0.46
2:B:212:ASN:CB	2:B:589:ASP:O	2.62	0.46
2:B:517:VAL:HG23	2:B:518:ARG:HG3	1.96	0.46
2:B:679:GLN:OE1	2:B:679:GLN:N	2.38	0.46
2:B:887:LEU:HB2	12:L:56:LEU:HB2	1.97	0.46
4:D:28:PRO:HD2	7:G:24:VAL:HG11	1.97	0.46
15:O:531:ILE:HA	15:O:534:GLN:HB2	1.97	0.46
16:P:659:LEU:HD12	16:P:742:TRP:CD1	2.50	0.46
18:R:171:ARG:C	18:R:174:GLU:H	2.18	0.46
18:R:250:LEU:HD21	18:R:307:LYS:CG	2.41	0.46
18:R:250:LEU:HB2	18:R:270:PHE:CE2	2.45	0.46
21:U:9:DT:H2''	21:U:10:DG:H5'	1.97	0.46
1:A:707:THR:HG22	1:A:709:ARG:N	2.21	0.46
1:A:1038:ILE:N	1:A:1047:GLN:O	2.43	0.46
4:D:86:ILE:HA	4:D:89:LEU:HD12	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:70:HIS:CE1	11:K:93:ILE:HD12	2.50	0.46
11:K:122:LYS:NZ	11:K:126:ASP:OD2	2.49	0.46
15:O:453:TYR:CZ	15:O:473:PHE:HB2	2.51	0.46
16:P:481:PHE:CE1	16:P:491:SER:HB2	2.50	0.46
16:P:604:ILE:HG22	16:P:605:SER:N	2.31	0.46
16:P:724:LEU:HB2	17:Q:446:TYR:HB3	1.96	0.46
17:Q:283:ASN:CG	17:Q:284:LEU:H	2.18	0.46
17:Q:410:ARG:HA	17:Q:413:LEU:CB	2.45	0.46
21:U:5:DT:H2''	21:U:6:DG:H5'	1.98	0.46
1:A:1104:TYR:CZ	1:A:1108:HIS:HD2	2.34	0.46
2:B:71:LYS:HG3	2:B:421:LEU:HB3	1.97	0.46
2:B:215:MET:HE2	2:B:217:ILE:HD11	1.97	0.46
2:B:729:PRO:HG2	2:B:733:LEU:HD21	1.98	0.46
2:B:912:GLN:N	2:B:915:ASP:OD2	2.48	0.46
5:E:43:LYS:O	5:E:47:CYS:HB2	2.15	0.46
15:O:540:CYS:O	15:O:544:ILE:N	2.40	0.46
16:P:288:SER:O	16:P:288:SER:OG	2.31	0.46
16:P:315:PHE:O	16:P:317:ILE:HD12	2.16	0.46
17:Q:139:LYS:HZ3	17:Q:139:LYS:N	2.14	0.46
17:Q:152:LEU:HB2	17:Q:154:LEU:HD13	1.97	0.46
17:Q:282:ARG:HG2	17:Q:302:ALA:HB1	1.98	0.46
17:Q:350:ARG:HD3	17:Q:486:GLN:CG	2.38	0.46
18:R:354:LEU:C	18:R:356:PRO:HD3	2.37	0.46
20:T:11:DA:C5	20:T:12:DC:C5	3.04	0.46
20:T:19:DC:H2'	20:T:20:DG:H8	1.81	0.46
1:A:1018:TYR:N	20:T:17:DT:H4'	2.31	0.46
1:A:1245:ASP:OD1	1:A:1246:VAL:N	2.41	0.46
1:A:1254:PHE:CE1	1:A:1258:ILE:HG21	2.51	0.46
1:A:1270:VAL:HG22	1:A:1294:MET:HG2	1.98	0.46
2:B:204:ARG:HH11	2:B:502:MET:HE1	1.81	0.46
2:B:770:ASN:O	10:J:48:ARG:NH1	2.48	0.46
2:B:815:ARG:HE	2:B:821:ILE:HA	1.80	0.46
2:B:881:TYR:CZ	12:L:67:PHE:HE1	2.34	0.46
2:B:954:PHE:CE1	2:B:963:PHE:CE1	3.04	0.46
3:C:243:SER:O	3:C:247:PHE:N	2.27	0.46
15:O:147:ILE:O	15:O:149:LYS:N	2.47	0.46
16:P:290:GLU:OE2	16:P:291:PRO:HD2	2.16	0.46
1:A:488:PRO:HB3	1:A:618:TYR:HE2	1.80	0.46
1:A:495:ILE:HG22	1:A:604:LYS:O	2.15	0.46
1:A:717:PRO:HG2	1:A:720:PHE:CD1	2.50	0.46
1:A:1238:MET:CE	1:A:1524:VAL:HG13	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:894:LYS:C	2:B:896:GLN:H	2.17	0.46
15:O:147:ILE:C	15:O:149:LYS:H	2.18	0.46
16:P:768:TYR:HB3	16:P:769:GLN:H	1.35	0.46
1:A:643:ALA:CA	2:B:1087:LEU:HB2	2.46	0.45
1:A:1038:ILE:CG1	1:A:1047:GLN:HB2	2.46	0.45
1:A:1297:PHE:HE2	9:I:58:SER:HB2	1.81	0.45
1:A:1556:GLU:O	1:A:1560:ASN:ND2	2.49	0.45
2:B:527:PHE:O	2:B:546:ALA:N	2.32	0.45
2:B:529:CYS:SG	2:B:698:SER:N	2.86	0.45
2:B:966:SER:OG	2:B:1029:GLY:HA3	2.16	0.45
9:I:37:TYR:HB3	9:I:41:GLN:HE22	1.80	0.45
11:K:77:ARG:HD2	11:K:91:TYR:CD1	2.51	0.45
13:M:102:SER:HB3	13:M:105:SER:OG	2.16	0.45
15:O:478:GLN:HA	15:O:481:CYS:SG	2.56	0.45
16:P:182:LEU:HA	16:P:182:LEU:HD22	1.51	0.45
16:P:190:ALA:O	16:P:247:ILE:O	2.34	0.45
16:P:215:ASN:OD1	16:P:218:VAL:HA	2.16	0.45
16:P:475:ARG:C	16:P:476:ILE:HD13	2.36	0.45
1:A:241:PRO:HB2	1:A:254:THR:O	2.16	0.45
1:A:771:PHE:CE1	1:A:776:LEU:HD13	2.43	0.45
1:A:1662:ASN:HB3	7:G:101:SER:HA	1.97	0.45
2:B:99:VAL:HG12	2:B:100:GLU:N	2.31	0.45
2:B:302:LEU:O	2:B:306:LEU:N	2.43	0.45
2:B:679:GLN:HE21	14:N:157:ARG:HA	1.81	0.45
2:B:683:ASN:HA	14:N:150:TYR:CZ	2.50	0.45
2:B:946:ASP:OD2	10:J:48:ARG:NH2	2.48	0.45
3:C:127:THR:OG1	3:C:130:ASN:N	2.47	0.45
3:C:232:GLN:HG2	3:C:232:GLN:O	2.16	0.45
9:I:6:SER:N	9:I:45:LEU:HD11	2.31	0.45
10:J:16:ASP:OD1	10:J:17:LYS:HG3	2.16	0.45
13:M:75:GLN:HB2	14:N:60:SER:HA	1.98	0.45
16:P:301:GLN:N	16:P:319:ASP:O	2.49	0.45
18:R:207:ASN:HD21	18:R:209:ARG:HH21	1.63	0.45
18:R:304:HIS:CD2	18:R:361:ASP:HB3	2.50	0.45
20:T:39:DT:H2''	20:T:40:DG:H5'	1.98	0.45
1:A:262:THR:O	1:A:266:VAL:HG23	2.17	0.45
1:A:643:ALA:HB1	2:B:1087:LEU:HD12	1.98	0.45
1:A:1293:HIS:CD2	1:A:1295:ARG:HH22	2.34	0.45
2:B:554:GLN:HA	2:B:646:HIS:CD2	2.51	0.45
2:B:1062:GLY:HA2	2:B:1067:GLY:H	1.81	0.45
2:B:1104:CYS:HA	2:B:1172:GLU:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1110:ILE:HG13	2:B:1111:LEU:HG	1.98	0.45
2:B:1134:ARG:HH12	2:B:1165:ASN:ND2	2.15	0.45
3:C:121:PRO:O	3:C:125:LYS:N	2.49	0.45
5:E:22:MET:O	5:E:26:ARG:N	2.34	0.45
12:L:68:GLU:OE2	12:L:70:ARG:HD3	2.17	0.45
13:M:58:GLU:O	13:M:103:LYS:NZ	2.49	0.45
15:O:477:PHE:HD2	15:O:520:CYS:SG	2.40	0.45
18:R:240:ILE:O	18:R:240:ILE:HG13	2.15	0.45
1:A:63:SER:O	2:B:1162:GLY:HA3	2.16	0.45
1:A:590:ASN:HD21	2:B:1075:GLU:CG	2.29	0.45
2:B:71:LYS:HB3	2:B:425:ILE:HG13	1.97	0.45
2:B:320:LEU:HD21	2:B:326:VAL:N	2.30	0.45
2:B:335:ARG:NH2	2:B:342:PRO:O	2.49	0.45
2:B:782:ASP:HB3	2:B:788:ILE:HG12	1.98	0.45
3:C:222:VAL:HB	3:C:224:THR:O	2.16	0.45
13:M:56:GLU:OE2	13:M:103:LYS:NZ	2.49	0.45
14:N:38:PHE:CE2	14:N:40:LEU:HB2	2.52	0.45
14:N:54:TRP:NE1	14:N:135:LYS:HD2	2.31	0.45
15:O:189:PHE:HD1	15:O:193:TYR:CE2	2.33	0.45
16:P:194:ARG:CZ	16:P:511:ILE:CG1	2.95	0.45
16:P:198:ASP:CB	16:P:261:VAL:HG23	2.46	0.45
16:P:574:TRP:O	16:P:577:LEU:HB2	2.17	0.45
17:Q:253:LEU:HD11	17:Q:270:THR:CG2	2.46	0.45
17:Q:366:TYR:CG	18:R:215:THR:CB	3.00	0.45
18:R:207:ASN:HD21	18:R:209:ARG:NH2	2.14	0.45
18:R:435:LEU:O	18:R:439:GLU:HG3	2.16	0.45
20:T:31:DT:H2''	20:T:32:DG:H5'	1.99	0.45
1:A:643:ALA:CB	2:B:1087:LEU:HA	2.46	0.45
1:A:1274:GLU:HB2	9:I:47:VAL:HB	1.99	0.45
1:A:1615:TYR:CD2	1:A:1616:GLU:HG3	2.51	0.45
2:B:252:TYR:HB2	2:B:381:LEU:HD21	1.99	0.45
2:B:726:MET:HG3	2:B:742:TYR:HB3	1.98	0.45
2:B:1074:MET:HE2	20:T:18:DT:H4'	1.97	0.45
3:C:273:ASP:CG	3:C:275:VAL:H	2.19	0.45
8:H:90:ALA:HB1	8:H:96:VAL:HG21	1.99	0.45
11:K:116:ALA:O	11:K:120:GLY:N	2.36	0.45
17:Q:360:LYS:HZ1	18:R:211:ARG:HH21	1.58	0.45
1:A:590:ASN:O	1:A:634:ASN:N	2.43	0.45
1:A:1070:LEU:HD13	1:A:1155:PHE:HE1	1.81	0.45
2:B:57:ASP:OD1	2:B:57:ASP:N	2.46	0.45
2:B:134:ARG:HD3	2:B:160:GLY:CA	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:372:ARG:NH2	2:B:574:SER:HA	2.31	0.45
2:B:1058:GLN:HG2	2:B:1096:SER:C	2.33	0.45
2:B:1060:VAL:O	2:B:1068:GLY:N	2.50	0.45
2:B:1079:LEU:CD1	2:B:1079:LEU:H	2.30	0.45
2:B:1093:LEU:HD13	2:B:1093:LEU:C	2.37	0.45
13:M:77:VAL:HG11	13:M:90:LEU:HB3	1.98	0.45
16:P:344:ILE:HG22	16:P:345:ASP:H	1.81	0.45
17:Q:341:ARG:HD3	17:Q:373:GLU:OE1	2.16	0.45
20:T:13:DT:H3	21:U:37:DA:H61	1.65	0.45
21:U:17:DT:H2''	21:U:18:DG:H5'	1.98	0.45
1:A:31:GLN:HB2	1:A:78:HIS:CE1	2.51	0.45
1:A:94:LEU:N	1:A:355:PHE:CE2	2.85	0.45
1:A:782:ASP:H	1:A:785:GLN:HB2	1.81	0.45
1:A:1136:VAL:HA	1:A:1174:TYR:CE2	2.52	0.45
1:A:1299:ASN:HB2	1:A:1466:SER:O	2.17	0.45
2:B:320:LEU:CD1	2:B:326:VAL:HA	2.46	0.45
2:B:600:GLN:HG3	2:B:604:ILE:HD11	1.99	0.45
7:G:62:MET:HA	7:G:66:LEU:HB2	1.99	0.45
11:K:60:SER:OG	11:K:106:GLN:HG2	2.17	0.45
15:O:540:CYS:O	15:O:543:ILE:N	2.50	0.45
16:P:727:PRO:HA	16:P:729:ALA:H	1.82	0.45
17:Q:408:ILE:HG13	17:Q:412:LYS:HD3	1.97	0.45
18:R:25:ASN:HD21	18:R:81:GLU:HG3	0.67	0.45
1:A:628:PHE:CB	2:B:785:ASP:OD1	2.64	0.45
1:A:646:GLU:OE1	2:B:1086:PHE:HB3	2.16	0.45
1:A:1039:ARG:CZ	6:F:139:PRO:HG2	2.47	0.45
1:A:1239:THR:HB	1:A:1542:THR:OG1	2.17	0.45
2:B:575:HIS:HB2	14:N:107:MET:HE2	1.99	0.45
4:D:19:PRO:HG2	4:D:22:ILE:HD11	1.99	0.45
15:O:477:PHE:CE1	15:O:480:LEU:HD11	2.52	0.45
17:Q:361:PRO:C	17:Q:363:SER:H	2.20	0.45
1:A:474:LYS:HD2	2:B:1092:LEU:HD21	1.98	0.45
1:A:557:LEU:O	1:A:561:LEU:N	2.49	0.45
2:B:545:PHE:HB3	2:B:549:CYS:HB3	1.98	0.45
5:E:100:ILE:O	5:E:104:ASN:N	2.50	0.45
11:K:46:LYS:NZ	11:K:67:GLU:HB2	2.32	0.45
15:O:388:VAL:HG22	15:O:395:LEU:HD23	1.99	0.45
15:O:399:PHE:CE2	15:O:403:LEU:HD11	2.51	0.45
18:R:75:GLN:HB2	20:T:43:DT:O3'	2.17	0.45
18:R:239:LEU:HD12	18:R:239:LEU:HA	1.74	0.45
20:T:3:DT:O2	21:U:47:DA:C2	2.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1048:PHE:CZ	5:E:211:TYR:HB2	2.52	0.45
1:A:1195:GLU:HB3	1:A:1196:PRO:HD3	1.98	0.45
2:B:262:PHE:CZ	2:B:269:TYR:HB2	2.51	0.45
2:B:890:ASP:O	12:L:54:ARG:HD3	2.17	0.45
3:C:123:ASP:OD1	3:C:124:GLU:N	2.48	0.45
3:C:230:LEU:HD22	3:C:231:PRO:HD2	1.97	0.45
3:C:277:ARG:HB3	3:C:280:LEU:HD12	1.98	0.45
3:C:309:THR:O	3:C:312:GLU:HB3	2.16	0.45
8:H:103:LYS:HB3	8:H:115:TYR:CD2	2.50	0.45
14:N:111:VAL:N	14:N:120:LYS:O	2.33	0.45
15:O:396:MET:HE1	15:O:434:LEU:HD12	0.99	0.45
15:O:610:TYR:CE2	15:O:612:GLU:HA	2.52	0.45
16:P:778:ASP:CG	16:P:779:ASP:H	2.19	0.45
18:R:34:ILE:HD12	18:R:34:ILE:HA	1.81	0.45
21:U:37:DA:C2	21:U:38:DG:C5	3.05	0.45
1:A:674:ILE:HA	1:A:786:TYR:OH	2.16	0.44
1:A:1258:ILE:CD1	1:A:1507:CYS:SG	3.00	0.44
2:B:459:SER:O	2:B:463:TYR:N	2.40	0.44
15:O:82:SER:HA	15:O:87:ARG:CZ	2.47	0.44
16:P:221:ARG:NH1	16:P:223:ASN:HD21	2.15	0.44
16:P:577:LEU:HD11	17:Q:503:SER:HB3	1.99	0.44
17:Q:150:GLU:OE1	17:Q:150:GLU:HA	2.17	0.44
18:R:365:TRP:HA	18:R:365:TRP:CE3	2.53	0.44
20:T:3:DT:H2"	20:T:4:DG:C8	2.51	0.44
1:A:537:GLN:HB3	1:A:576:LYS:HB2	2.00	0.44
1:A:547:ILE:HD11	17:Q:26:ARG:NH2	2.23	0.44
1:A:593:PRO:HD3	20:T:18:DT:O2	2.17	0.44
1:A:964:LYS:HE3	1:A:969:PHE:O	2.17	0.44
1:A:1118:VAL:O	1:A:1118:VAL:HG12	2.18	0.44
1:A:1158:SER:OG	1:A:1159:ASP:N	2.50	0.44
2:B:407:PHE:O	2:B:411:MET:HG3	2.18	0.44
2:B:974:LEU:HD23	10:J:44:TYR:HB3	1.99	0.44
2:B:1134:ARG:HH12	2:B:1165:ASN:HD22	1.66	0.44
3:C:74:GLU:HA	3:C:212:ILE:HB	1.99	0.44
10:J:16:ASP:OD1	10:J:17:LYS:N	2.50	0.44
11:K:66:VAL:HG12	11:K:67:GLU:N	2.32	0.44
15:O:124:LYS:HD3	15:O:127:GLU:OE1	2.17	0.44
16:P:399:TRP:CH2	18:R:294:VAL:HG23	2.52	0.44
18:R:157:MET:HG3	18:R:162:PHE:HB2	1.99	0.44
18:R:375:LYS:HA	18:R:375:LYS:HD3	1.57	0.44
1:A:81:LEU:HD23	1:A:85:CYS:SG	2.57	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:LYS:HG2	1:A:201:ARG:HH22	1.82	0.44
1:A:1090:ASP:HB3	1:A:1132:TYR:CD1	2.52	0.44
1:A:1303:SER:OG	1:A:1308:VAL:O	2.13	0.44
1:A:1320:GLN:HG3	1:A:1321:PHE:N	2.32	0.44
2:B:184:LYS:HZ3	10:J:69:ARG:HH22	1.65	0.44
2:B:996:PHE:O	2:B:999:GLN:N	2.51	0.44
2:B:1092:LEU:C	2:B:1092:LEU:CD2	2.85	0.44
5:E:13:TRP:HB2	5:E:42:PHE:CD2	2.53	0.44
8:H:116:TYR:HB2	8:H:123:MET:HB3	1.99	0.44
15:O:458:GLU:OE2	15:O:512:SER:HB2	2.18	0.44
15:O:479:ALA:O	15:O:483:ILE:HG13	2.17	0.44
16:P:186:TYR:CE1	16:P:448:THR:HG22	2.52	0.44
16:P:504:THR:HG22	16:P:505:PRO:HD3	2.00	0.44
17:Q:159:THR:HG22	17:Q:229:LYS:CB	2.46	0.44
17:Q:357:TYR:CD2	17:Q:489:VAL:CA	2.92	0.44
17:Q:366:TYR:CZ	18:R:215:THR:CA	2.95	0.44
17:Q:418:PRO:HD3	18:R:233:TYR:OH	2.18	0.44
18:R:15:GLN:HG3	18:R:184:ASN:HD22	1.83	0.44
1:A:564:PRO:HB2	15:O:371:HIS:NE2	2.33	0.44
1:A:697:TYR:CE1	1:A:701:ARG:HA	2.51	0.44
1:A:720:PHE:CE2	8:H:141:TYR:HE2	2.35	0.44
1:A:1136:VAL:HG22	1:A:1174:TYR:CD2	2.52	0.44
1:A:1196:PRO:HB3	1:A:1575:ILE:HG21	1.98	0.44
2:B:173:ASN:OD1	2:B:174:LYS:HG3	2.17	0.44
2:B:449:VAL:O	2:B:453:VAL:HG23	2.17	0.44
2:B:847:TYR:HB2	2:B:850:THR:OG1	2.18	0.44
2:B:908:ARG:HG2	3:C:95:GLU:HG3	1.99	0.44
2:B:949:ILE:CD1	2:B:954:PHE:CE2	3.00	0.44
5:E:76:GLY:H	5:E:106:GLN:HG2	1.82	0.44
5:E:177:ARG:NE	5:E:215:MET:HB2	2.32	0.44
11:K:64:GLN:NE2	11:K:100:LEU:HD13	2.32	0.44
13:M:42:LYS:O	14:N:30:LYS:N	2.46	0.44
15:O:328:LEU:HA	15:O:331:LYS:HD2	1.99	0.44
15:O:428:ILE:HD12	15:O:439:ILE:HD12	1.99	0.44
15:O:492:ARG:C	15:O:493:ASP:O	2.55	0.44
16:P:228:ASN:O	16:P:230:HIS:N	2.50	0.44
16:P:466:ALA:O	16:P:478:MET:HA	2.17	0.44
17:Q:283:ASN:OD1	17:Q:284:LEU:N	2.36	0.44
17:Q:309:TYR:O	17:Q:313:THR:OG1	2.30	0.44
1:A:93:GLN:CB	1:A:355:PHE:HE2	2.30	0.44
1:A:248:PHE:CZ	1:A:444:GLN:HA	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:956:ARG:HH21	1:A:979:GLY:HA3	1.82	0.44
1:A:1216:THR:HG22	1:A:1221:ARG:HB2	1.99	0.44
2:B:228:SER:O	2:B:254:ASN:ND2	2.50	0.44
2:B:649:MET:HE3	2:B:666:PRO:HG2	1.98	0.44
2:B:785:ASP:N	2:B:785:ASP:OD1	2.51	0.44
8:H:107:VAL:HB	8:H:111:LEU:CD1	2.47	0.44
15:O:447:THR:HA	15:O:450:LEU:HD12	2.00	0.44
15:O:477:PHE:CZ	15:O:516:PRO:HB2	2.53	0.44
16:P:214:LEU:HB2	16:P:222:GLN:CD	2.38	0.44
16:P:389:TRP:CH2	18:R:149:LYS:CB	3.00	0.44
16:P:436:ILE:HG23	16:P:436:ILE:O	2.18	0.44
16:P:451:ILE:HA	16:P:467:PHE:O	2.18	0.44
16:P:507:GLY:O	16:P:539:VAL:HA	2.17	0.44
16:P:738:LYS:HA	16:P:741:ILE:HG22	2.00	0.44
17:Q:19:LEU:CD1	17:Q:27:ARG:CB	2.94	0.44
17:Q:365:ASP:N	17:Q:365:ASP:OD1	2.50	0.44
18:R:76:LYS:O	18:R:80:ARG:HG3	2.17	0.44
18:R:350:SER:HB2	18:R:368:TYR:HE1	1.82	0.44
18:R:372:HIS:CD2	18:R:410:TYR:HB3	2.52	0.44
1:A:470:HIS:CD2	2:B:1056:THR:HG21	2.53	0.44
1:A:609:PRO:HB2	1:A:610:ASN:ND2	2.33	0.44
1:A:672:ASP:CB	2:B:783:MET:HE3	2.33	0.44
1:A:680:LEU:HD12	1:A:820:TYR:CG	2.53	0.44
1:A:683:LYS:HB2	8:H:20:TYR:CE1	2.53	0.44
1:A:1229:ALA:HB1	1:A:1595:TYR:CE2	2.53	0.44
1:A:1559:ARG:HG3	1:A:1586:ALA:HB1	2.00	0.44
2:B:65:VAL:CG2	2:B:99:VAL:HB	2.48	0.44
2:B:72:VAL:HG11	2:B:94:LYS:HE3	1.99	0.44
2:B:712:SER:HA	2:B:715:ASN:HD22	1.83	0.44
2:B:840:LEU:HA	2:B:846:PRO:HA	1.99	0.44
2:B:954:PHE:C	2:B:956:SER:N	2.70	0.44
2:B:1079:LEU:HD12	2:B:1079:LEU:N	2.33	0.44
3:C:31:TRP:HA	3:C:35:LYS:HD2	2.00	0.44
5:E:23:VAL:HG13	5:E:28:TYR:HD2	1.83	0.44
9:I:15:ASP:OD2	9:I:31:SER:OG	2.27	0.44
12:L:27:LEU:N	12:L:39:SER:HB2	2.32	0.44
15:O:541:PHE:HA	15:O:544:ILE:HB	2.00	0.44
16:P:343:LEU:N	16:P:343:LEU:HD23	2.32	0.44
16:P:582:ASP:H	16:P:585:GLU:HB2	1.82	0.44
17:Q:104:PHE:CD2	17:Q:105:LEU:HD23	2.53	0.44
17:Q:437:THR:OG1	17:Q:440:GLU:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:305:THR:HB	18:R:308:PHE:CE1	2.52	0.44
1:A:253:GLU:O	1:A:312:SER:N	2.51	0.44
1:A:559:ASN:HD22	15:O:376:TYR:HB2	1.83	0.44
1:A:584:ARG:NH1	1:A:644:ARG:HH12	2.15	0.44
1:A:654:ASP:N	1:A:654:ASP:OD1	2.47	0.44
1:A:672:ASP:CG	2:B:783:MET:HE3	2.38	0.44
1:A:1028:GLU:HG3	1:A:1637:PRO:HD2	1.99	0.44
1:A:1088:HIS:CD2	6:F:152:ILE:HD11	2.52	0.44
1:A:1508:VAL:O	1:A:1509:HIS:C	2.55	0.44
2:B:499:HIS:O	2:B:502:MET:HB3	2.18	0.44
2:B:822:THR:HG22	2:B:823:GLN:HG3	1.99	0.44
2:B:854:GLU:HA	2:B:874:TYR:HD2	1.83	0.44
2:B:916:LYS:HB3	2:B:1036:LEU:HD12	2.00	0.44
2:B:1093:LEU:CD1	2:B:1093:LEU:C	2.86	0.44
3:C:60:ASP:O	3:C:63:ILE:N	2.41	0.44
3:C:227:TYR:HA	3:C:299:ILE:O	2.17	0.44
5:E:205:SER:OG	5:E:206:GLY:N	2.51	0.44
9:I:8:ILE:O	9:I:17:LEU:N	2.50	0.44
13:M:77:VAL:HG21	14:N:64:ILE:HG21	2.00	0.44
15:O:153:ASP:HA	15:O:156:MET:HB3	2.00	0.44
15:O:357:GLY:O	15:O:361:PHE:N	2.27	0.44
16:P:283:ASP:OD1	16:P:284:VAL:N	2.50	0.44
17:Q:108:PHE:O	17:Q:111:ILE:HG22	2.18	0.44
18:R:408:ILE:HA	18:R:411:VAL:HG12	1.99	0.44
1:A:512:THR:CG2	1:A:514:TYR:CE2	2.99	0.44
1:A:584:ARG:HH12	1:A:644:ARG:HH12	1.65	0.44
1:A:793:ILE:O	1:A:796:SER:N	2.48	0.44
1:A:1654:PHE:CG	6:F:89:GLU:HG2	2.51	0.44
3:C:67:PHE:HE2	3:C:314:PHE:CZ	2.35	0.44
3:C:237:GLN:NE2	3:C:288:LYS:HG2	2.32	0.44
3:C:240:LYS:HB2	3:C:263:ASP:OD2	2.18	0.44
7:G:126:GLN:HG3	7:G:126:GLN:O	2.18	0.44
7:G:242:VAL:HG21	15:O:148:PRO:HB2	2.00	0.44
15:O:335:ILE:O	15:O:339:VAL:HG23	2.17	0.44
15:O:450:LEU:HD22	15:O:473:PHE:CE1	2.53	0.44
15:O:487:ARG:NE	15:O:502:LEU:HD13	2.31	0.44
16:P:55:LEU:HB3	18:R:227:HIS:HD1	1.67	0.44
16:P:389:TRP:HE1	18:R:146:SER:CB	2.13	0.44
16:P:632:ILE:O	16:P:636:GLU:HG3	2.18	0.44
17:Q:265:GLU:HB3	17:Q:269:TYR:CE1	2.52	0.44
1:A:530:TRP:CD1	1:A:531:PRO:HA	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:560:GLN:NE2	15:O:239:SER:HA	2.32	0.44
1:A:735:VAL:O	1:A:738:ASN:N	2.51	0.44
1:A:1311:GLU:O	1:A:1315:ASN:N	2.44	0.44
1:A:1492:ILE:O	1:A:1496:SER:N	2.49	0.44
1:A:1646:LEU:HD11	2:B:1086:PHE:HE1	1.79	0.44
2:B:25:PHE:CE1	10:J:59:LYS:HD2	2.53	0.44
2:B:289:PHE:HD1	2:B:306:LEU:HD22	1.83	0.44
2:B:822:THR:HG23	2:B:865:THR:HG23	2.00	0.44
3:C:86:PHE:HB3	12:L:62:LYS:HG3	2.00	0.44
16:P:330:PRO:HG3	16:P:342:GLN:HE21	1.82	0.44
16:P:658:LYS:CB	16:P:660:LYS:H	2.29	0.44
17:Q:22:ILE:HD13	17:Q:26:ARG:CZ	2.46	0.44
17:Q:381:MET:O	17:Q:385:PHE:HB2	2.18	0.44
17:Q:446:TYR:O	17:Q:449:GLN:HG2	2.18	0.44
1:A:263:ASN:HA	1:A:266:VAL:HB	1.99	0.43
1:A:1162:ASN:ND2	1:A:1164:LYS:HB2	2.33	0.43
2:B:174:LYS:NZ	18:R:351:GLU:OE2	2.41	0.43
2:B:292:ILE:O	2:B:579:ALA:HB3	2.18	0.43
2:B:374:LEU:HD12	2:B:374:LEU:HA	1.78	0.43
2:B:840:LEU:HD13	2:B:860:ALA:HB2	1.98	0.43
2:B:891:GLU:O	2:B:892:SER:OG	2.25	0.43
2:B:970:LYS:NZ	2:B:1011:GLU:OE2	2.39	0.43
10:J:14:VAL:CG2	10:J:50:ILE:HG12	2.48	0.43
14:N:87:TYR:HA	14:N:142:THR:HG22	2.00	0.43
15:O:361:PHE:CZ	15:O:399:PHE:HB2	2.53	0.43
16:P:186:TYR:N	18:R:198:LEU:HD23	2.33	0.43
16:P:187:ILE:HG22	16:P:188:GLN:H	1.83	0.43
17:Q:239:PHE:CG	17:Q:240:LYS:N	2.86	0.43
17:Q:334:LEU:HD12	17:Q:334:LEU:HA	1.76	0.43
18:R:161:ASN:O	18:R:164:LYS:HB2	2.18	0.43
20:T:9:DC:H2''	20:T:10:DA:O5'	2.18	0.43
1:A:413:LEU:HG	1:A:417:ARG:HH12	1.82	0.43
1:A:482:SER:HB3	1:A:614:LEU:HG	2.01	0.43
1:A:672:ASP:HA	2:B:952:HIS:NE2	2.33	0.43
1:A:753:ASN:HA	1:A:784:SER:OG	2.18	0.43
1:A:883:LEU:HD23	1:A:884:ARG:HH12	1.82	0.43
1:A:1182:GLY:O	1:A:1650:GLY:HA3	2.18	0.43
1:A:1305:GLU:HG2	9:I:59:SER:HB2	2.00	0.43
2:B:395:ASP:HA	2:B:505:ARG:HH12	1.82	0.43
2:B:881:TYR:HB2	2:B:906:ARG:HB3	1.98	0.43
3:C:67:PHE:HE2	3:C:314:PHE:CE1	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:78:LEU:HD21	5:E:109:ILE:HD12	1.99	0.43
16:P:49:THR:O	16:P:49:THR:OG1	2.35	0.43
16:P:227:LEU:HD21	16:P:234:THR:O	2.17	0.43
16:P:229:ARG:HE	16:P:230:HIS:CB	2.31	0.43
18:R:80:ARG:O	18:R:83:HIS:HB3	2.18	0.43
20:T:47:DT:H2''	20:T:48:DG:H5'	1.99	0.43
1:A:403:LEU:HD22	1:A:419:ILE:HG22	2.00	0.43
1:A:527:PRO:HD3	1:A:554:ARG:CZ	2.49	0.43
1:A:1017:GLY:HA3	20:T:17:DT:O4'	2.18	0.43
2:B:547:HIS:CG	2:B:760:TYR:HH	2.34	0.43
2:B:851:TYR:HD1	2:B:881:TYR:HE1	1.65	0.43
2:B:857:PRO:HG3	2:B:871:ILE:HD11	2.00	0.43
2:B:1063:ARG:CD	20:T:22:DG:P	3.06	0.43
3:C:80:ALA:HA	3:C:208:CYS:HA	2.00	0.43
3:C:165:ARG:HB3	3:C:189:PRO:HB3	2.00	0.43
3:C:334:THR:HG21	11:K:44:ARG:HB3	1.99	0.43
9:I:3:VAL:HA	9:I:7:LEU:O	2.18	0.43
15:O:241:ASP:CG	15:O:380:SER:CB	2.82	0.43
16:P:246:LYS:HD3	16:P:266:GLU:OE2	2.17	0.43
16:P:385:PHE:C	16:P:387:ASN:H	2.21	0.43
16:P:389:TRP:CH2	18:R:147:GLN:C	2.91	0.43
16:P:629:ARG:CZ	16:P:662:LEU:HD11	2.48	0.43
17:Q:356:VAL:CG1	18:R:208:TYR:CZ	2.97	0.43
1:A:481:ARG:NE	1:A:632:GLU:OE1	2.51	0.43
1:A:628:PHE:CB	2:B:785:ASP:CB	2.96	0.43
1:A:1258:ILE:O	1:A:1501:ILE:HD12	2.19	0.43
1:A:1617:THR:CG2	20:T:14:DG:H4'	2.48	0.43
2:B:229:TYR:HE1	2:B:253:LEU:HD11	1.83	0.43
2:B:1116:SER:O	2:B:1124:SER:OG	2.24	0.43
6:F:103:MET:O	6:F:104:ASN:HB2	2.18	0.43
15:O:591:TYR:CE2	15:O:593:PRO:HG3	2.53	0.43
15:O:600:LYS:HG3	15:O:601:ASN:N	2.32	0.43
16:P:389:TRP:CH2	18:R:149:LYS:N	2.79	0.43
16:P:696:PHE:HZ	16:P:745:ALA:HA	1.83	0.43
17:Q:178:THR:HG22	17:Q:303:GLU:OE2	2.18	0.43
17:Q:366:TYR:CG	18:R:215:THR:OG1	2.61	0.43
17:Q:366:TYR:OH	18:R:218:ASP:OD2	2.33	0.43
17:Q:472:ARG:O	17:Q:476:ILE:HG12	2.17	0.43
18:R:76:LYS:HA	18:R:79:ARG:HB2	2.01	0.43
1:A:449:GLY:C	1:A:451:VAL:H	2.21	0.43
1:A:1038:ILE:HG13	1:A:1047:GLN:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1245:ASP:OD1	1:A:1245:ASP:N	2.51	0.43
2:B:37:LEU:HB3	2:B:760:TYR:CE1	2.53	0.43
2:B:790:ASN:CB	2:B:936:MET:SD	3.06	0.43
7:G:45:LEU:HD13	7:G:47:VAL:CG1	2.48	0.43
12:L:33:GLU:HG2	12:L:53:HIS:NE2	2.34	0.43
14:N:149:ASP:O	14:N:153:VAL:HG12	2.19	0.43
15:O:446:LEU:HA	15:O:449:TRP:HB3	1.99	0.43
17:Q:484:ALA:O	17:Q:488:LEU:HG	2.18	0.43
18:R:248:LYS:HA	18:R:298:GLN:CD	2.39	0.43
1:A:109:ARG:HA	1:A:233:CYS:HA	2.01	0.43
2:B:225:ARG:HB2	2:B:229:TYR:CD2	2.53	0.43
2:B:832:TRP:HH2	2:B:837:LEU:HD21	1.83	0.43
7:G:168:PHE:HA	7:G:217:TRP:HA	2.00	0.43
13:M:67:ASP:HB3	13:M:70:SER:OG	2.18	0.43
15:O:600:LYS:O	15:O:603:LYS:HB3	2.19	0.43
16:P:329:ILE:HG13	16:P:330:PRO:O	2.18	0.43
16:P:365:TRP:CE3	16:P:372:ILE:HG22	2.54	0.43
16:P:675:PHE:HZ	16:P:742:TRP:CZ3	2.37	0.43
17:Q:120:ILE:HA	17:Q:125:PHE:HB2	2.00	0.43
17:Q:257:VAL:HG13	17:Q:262:LEU:HB2	2.00	0.43
17:Q:285:THR:OG1	17:Q:287:TRP:HB3	2.19	0.43
17:Q:323:ASP:C	17:Q:325:GLN:H	2.22	0.43
18:R:216:LEU:HD23	18:R:216:LEU:HA	1.91	0.43
18:R:415:LEU:HD21	18:R:428:SER:HB3	2.01	0.43
1:A:474:LYS:HD2	2:B:1092:LEU:CD2	2.48	0.43
1:A:966:LEU:HB3	1:A:969:PHE:HD2	1.84	0.43
1:A:1330:VAL:HA	1:A:1333:ILE:HD12	2.01	0.43
3:C:213:GLY:N	3:C:219:PHE:HB2	2.33	0.43
13:M:80:LEU:C	13:M:88:ILE:HG13	2.39	0.43
16:P:376:ASP:C	16:P:378:SER:N	2.72	0.43
16:P:641:TRP:CE3	16:P:750:PRO:HD3	2.54	0.43
17:Q:177:TYR:O	17:Q:180:ASP:HB2	2.19	0.43
20:T:35:DT:H2''	20:T:36:DG:H5'	1.99	0.43
1:A:194:ALA:O	1:A:198:SER:N	2.49	0.43
1:A:741:PRO:HD2	1:A:801:TYR:CD2	2.54	0.43
1:A:934:LYS:HG3	2:B:956:SER:OG	2.19	0.43
1:A:1074:TYR:OH	1:A:1159:ASP:OD2	2.24	0.43
1:A:1549:VAL:O	1:A:1553:TYR:N	2.51	0.43
1:A:1575:ILE:HG22	1:A:1576:SER:N	2.34	0.43
2:B:186:GLU:OE1	2:B:731:VAL:N	2.43	0.43
2:B:641:TYR:HB3	2:B:643:PHE:CZ	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:725:THR:HA	2:B:1036:LEU:HA	1.99	0.43
2:B:808:LYS:HA	2:B:902:SER:HA	1.99	0.43
2:B:916:LYS:O	2:B:917:PHE:HD1	2.02	0.43
3:C:161:HIS:CD2	3:C:195:LYS:HG2	2.53	0.43
6:F:57:ASP:OD1	6:F:58:PHE:N	2.51	0.43
10:J:7:CYS:HB2	10:J:46:CYS:SG	2.52	0.43
15:O:224:GLU:OE1	15:O:224:GLU:N	2.43	0.43
16:P:187:ILE:C	16:P:188:GLN:OE1	2.57	0.43
16:P:446:ASP:H	18:R:200:THR:HG21	1.82	0.43
16:P:745:ALA:O	16:P:747:LEU:N	2.44	0.43
17:Q:488:LEU:HD21	17:Q:498:LEU:HD12	2.01	0.43
18:R:307:LYS:HB3	18:R:308:PHE:H	1.66	0.43
1:A:646:GLU:OE1	2:B:1086:PHE:HB2	2.19	0.43
1:A:729:LYS:HE3	1:A:779:GLY:O	2.19	0.43
1:A:1291:VAL:HA	1:A:1473:LYS:HA	2.01	0.43
2:B:171:HIS:O	2:B:175:MET:HE3	2.19	0.43
2:B:335:ARG:HH21	2:B:342:PRO:HA	1.83	0.43
2:B:949:ILE:HD11	2:B:954:PHE:CE2	2.53	0.43
2:B:1013:MET:SD	2:B:1026:ILE:HD11	2.59	0.43
3:C:222:VAL:C	3:C:224:THR:N	2.69	0.43
3:C:241:GLY:O	3:C:245:ARG:NH1	2.52	0.43
3:C:294:VAL:CG2	3:C:297:HIS:HB3	2.49	0.43
15:O:383:TYR:CE2	15:O:594:TYR:HD1	2.37	0.43
16:P:226:HIS:NE2	16:P:232:ASN:HB3	2.34	0.43
16:P:358:SER:HB2	18:R:196:GLU:CD	2.40	0.43
16:P:650:LEU:HB3	17:Q:242:PHE:CD1	2.54	0.43
17:Q:171:HIS:HA	17:Q:244:ASN:O	2.19	0.43
17:Q:327:PRO:O	17:Q:331:ILE:HD13	2.18	0.43
19:S:6:A:H8	19:S:6:A:O5'	2.02	0.43
21:U:42:DA:H2''	21:U:43:DA:OP2	2.19	0.43
1:A:109:ARG:C	1:A:230:ARG:HG2	2.39	0.43
1:A:1060:GLU:HA	1:A:1063:MET:SD	2.59	0.43
2:B:524:SER:HB3	2:B:528:LEU:HB2	2.00	0.43
2:B:776:ILE:C	2:B:951:PRO:CD	2.77	0.43
3:C:169:PHE:CE2	3:C:171:PRO:HG3	2.54	0.43
3:C:226:SER:OG	3:C:227:TYR:N	2.52	0.43
5:E:114:ASN:OD1	5:E:115:ASN:N	2.48	0.43
5:E:154:ILE:HB	5:E:197:LYS:HB3	2.00	0.43
10:J:49:MET:O	10:J:53:HIS:HB2	2.19	0.43
10:J:53:HIS:CG	10:J:54:VAL:N	2.86	0.43
11:K:49:LEU:HD11	11:K:61:ALA:HB1	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:113:SER:N	14:N:118:SER:O	2.49	0.43
15:O:422:GLN:O	15:O:593:PRO:HD2	2.18	0.43
16:P:381:ILE:HA	16:P:391:THR:O	2.19	0.43
17:Q:177:TYR:OH	17:Q:252:LEU:N	2.52	0.43
17:Q:375:LEU:HA	17:Q:375:LEU:HD23	1.87	0.43
1:A:476:VAL:HG12	2:B:1095:SER:HB3	1.55	0.42
1:A:579:ARG:HH22	1:A:585:ASP:CG	2.22	0.42
1:A:808:LYS:O	1:A:812:VAL:HG23	2.19	0.42
1:A:1261:VAL:N	1:A:1499:ARG:O	2.52	0.42
1:A:1654:PHE:CE2	6:F:89:GLU:HG2	2.50	0.42
2:B:75:ASP:OD1	2:B:76:GLY:N	2.52	0.42
2:B:232:TYR:HD1	2:B:384:LEU:HG	1.83	0.42
2:B:572:PRO:HD2	2:B:575:HIS:CE1	2.54	0.42
2:B:929:ARG:HG2	2:B:930:LYS:O	2.18	0.42
2:B:986:PHE:CD2	2:B:992:PRO:HG3	2.54	0.42
3:C:42:VAL:HB	11:K:138:LYS:HG3	2.00	0.42
3:C:85:PHE:CE1	3:C:204:LEU:HD22	2.47	0.42
5:E:81:GLU:N	5:E:109:ILE:O	2.50	0.42
10:J:45:CYS:SG	10:J:46:CYS:N	2.92	0.42
16:P:192:ASP:OD1	16:P:212:SER:HA	2.19	0.42
16:P:197:ARG:HA	16:P:197:ARG:HD3	1.75	0.42
16:P:263:ILE:CG2	16:P:276:SER:HA	2.43	0.42
16:P:264:ILE:HD13	16:P:265:THR:H	1.84	0.42
16:P:458:LYS:HZ2	16:P:459:PRO:HD3	1.84	0.42
16:P:472:ARG:CZ	16:P:472:ARG:HB3	2.48	0.42
16:P:475:ARG:NH2	17:Q:364:SER:OG	2.52	0.42
18:R:301:SER:C	18:R:302:ARG:HG2	2.39	0.42
18:R:305:THR:O	18:R:306:ALA:C	2.57	0.42
18:R:366:PHE:CE2	18:R:425:ALA:HB2	2.54	0.42
1:A:120:CYS:HB3	1:A:189:VAL:HG21	2.01	0.42
1:A:1121:ASP:OD1	5:E:197:LYS:NZ	2.46	0.42
2:B:812:ALA:HB1	2:B:815:ARG:HD3	2.00	0.42
2:B:1078:ALA:O	2:B:1082:HIS:CA	2.63	0.42
5:E:7:ARG:O	5:E:11:ARG:N	2.36	0.42
10:J:8:PHE:HB2	10:J:48:ARG:NH2	2.34	0.42
14:N:69:SER:OG	14:N:70:LEU:N	2.52	0.42
14:N:82:ILE:HB	14:N:87:TYR:CE1	2.54	0.42
16:P:321:LYS:HB3	16:P:321:LYS:HE2	1.36	0.42
16:P:551:ALA:O	16:P:552:LEU:HD23	2.20	0.42
16:P:691:VAL:HG22	16:P:692:THR:O	2.19	0.42
17:Q:253:LEU:HB3	17:Q:267:TYR:CD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:269:TYR:HD2	17:Q:317:MET:HG3	1.84	0.42
18:R:242:ILE:HG13	18:R:243:PRO:HD2	2.01	0.42
1:A:651:ALA:H	2:B:1084:THR:HG22	1.84	0.42
1:A:1055:ILE:HD11	1:A:1174:TYR:CZ	2.54	0.42
1:A:1527:GLN:H	1:A:1527:GLN:CD	2.22	0.42
3:C:84:TYR:CE2	3:C:207:HIS:CD2	3.07	0.42
3:C:332:PRO:HG2	11:K:44:ARG:HG2	2.00	0.42
5:E:123:LEU:O	5:E:126:SER:HB3	2.18	0.42
14:N:78:THR:O	14:N:89:ILE:N	2.45	0.42
15:O:97:LEU:O	15:O:101:SER:N	2.42	0.42
15:O:409:ALA:O	15:O:417:LYS:HE2	2.19	0.42
16:P:236:ILE:HD13	16:P:236:ILE:HA	1.91	0.42
16:P:301:GLN:NE2	16:P:359:SER:O	2.52	0.42
18:R:4:VAL:CG1	18:R:6:ILE:HG12	2.49	0.42
18:R:162:PHE:HA	18:R:165:ILE:CD1	2.45	0.42
18:R:374:LEU:HD22	18:R:374:LEU:HA	1.84	0.42
1:A:325:ASP:O	1:A:329:ARG:HG3	2.19	0.42
1:A:1035:ASP:O	1:A:1036:ASN:HB2	2.18	0.42
1:A:1263:LEU:HG	1:A:1267:ILE:HD11	2.02	0.42
2:B:390:SER:HB3	2:B:634:ARG:O	2.20	0.42
2:B:393:ASN:HB3	2:B:396:ALA:HB2	2.01	0.42
2:B:936:MET:HG3	2:B:948:ILE:HD11	2.00	0.42
2:B:1011:GLU:N	2:B:1026:ILE:O	2.45	0.42
8:H:92:ASP:O	8:H:145:ARG:HD3	2.19	0.42
10:J:20:SER:O	10:J:24:LEU:HG	2.20	0.42
15:O:430:ARG:HD2	15:O:610:TYR:CE1	2.54	0.42
16:P:356:GLU:OE2	16:P:378:SER:HB3	2.18	0.42
16:P:715:TYR:HE1	16:P:733:THR:HG23	1.84	0.42
17:Q:167:LEU:HD22	17:Q:167:LEU:HA	1.90	0.42
17:Q:288:GLU:O	17:Q:290:THR:HG22	2.19	0.42
18:R:187:TYR:O	18:R:191:ILE:HG23	2.20	0.42
18:R:358:PHE:O	18:R:360:GLU:N	2.47	0.42
1:A:246:ASP:OD2	1:A:250:LYS:HB2	2.19	0.42
1:A:627:ASP:C	2:B:784:ASP:OD1	2.58	0.42
2:B:417:ILE:O	2:B:420:TYR:HB3	2.20	0.42
2:B:795:GLU:HB3	3:C:216:HIS:NE2	2.34	0.42
3:C:235:ILE:HG22	3:C:237:GLN:H	1.85	0.42
15:O:347:VAL:HG11	15:O:395:LEU:HD21	2.02	0.42
16:P:200:THR:OG1	16:P:280:ARG:NH1	2.53	0.42
16:P:330:PRO:HG3	16:P:342:GLN:HG3	2.00	0.42
16:P:422:ILE:HG12	16:P:442:LEU:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:6:ARG:HA	17:Q:18:ARG:CD	2.50	0.42
17:Q:115:GLN:HB3	17:Q:190:MET:HE3	2.00	0.42
17:Q:329:LYS:O	17:Q:332:LEU:HB2	2.19	0.42
17:Q:500:ASP:O	17:Q:503:SER:OG	2.36	0.42
18:R:30:ARG:NE	18:R:168:ILE:HD13	2.34	0.42
1:A:407:GLN:O	1:A:411:VAL:HG23	2.20	0.42
1:A:503:VAL:HG13	1:A:527:PRO:O	2.20	0.42
1:A:511:VAL:HG11	1:A:575:LYS:CA	2.49	0.42
1:A:671:GLN:CB	2:B:783:MET:HE3	2.48	0.42
1:A:690:GLU:OE1	1:A:690:GLU:N	2.46	0.42
1:A:826:PHE:O	2:B:776:ILE:HG13	2.19	0.42
1:A:975:ASP:OD2	1:A:977:MET:HB3	2.20	0.42
2:B:113:VAL:HB	18:R:281:LYS:HE3	2.01	0.42
2:B:314:LYS:O	2:B:316:ARG:N	2.49	0.42
2:B:1103:VAL:O	2:B:1173:THR:HA	2.18	0.42
3:C:100:ARG:NH1	10:J:3:VAL:O	2.47	0.42
5:E:96:PHE:O	5:E:99:HIS:HB3	2.20	0.42
14:N:35:LEU:O	14:N:116:LYS:HD3	2.19	0.42
15:O:82:SER:OG	15:O:87:ARG:NH1	2.53	0.42
16:P:442:LEU:HB3	16:P:477:TYR:OH	2.20	0.42
16:P:475:ARG:NH2	17:Q:364:SER:HA	2.34	0.42
17:Q:7:GLY:HA3	17:Q:8:PRO:HD2	1.45	0.42
17:Q:256:LEU:HG	17:Q:310:PHE:CE2	2.54	0.42
1:A:75:HIS:N	1:A:364:PRO:HB3	2.34	0.42
1:A:91:PHE:CE2	1:A:245:LYS:HD2	2.55	0.42
1:A:246:ASP:HB2	1:A:250:LYS:H	1.85	0.42
1:A:750:ILE:HG12	1:A:770:LEU:HD13	2.01	0.42
2:B:90:TYR:CE2	2:B:92:GLY:HA2	2.54	0.42
2:B:300:SER:O	2:B:303:THR:OG1	2.32	0.42
2:B:343:ASP:OD1	2:B:344:GLN:HG3	2.20	0.42
2:B:439:ASN:HB3	2:B:442:ASP:HB2	2.01	0.42
2:B:654:ARG:NH2	2:B:659:ASP:OD2	2.53	0.42
2:B:702:ASN:HB3	2:B:756:LEU:HD12	2.02	0.42
2:B:1049:THR:O	2:B:1052:VAL:HG13	2.20	0.42
3:C:233:ILE:HG12	3:C:291:LEU:HD22	2.01	0.42
5:E:200:ARG:N	5:E:208:TYR:O	2.36	0.42
8:H:62:SER:OG	8:H:63:LEU:N	2.53	0.42
16:P:426:ALA:HB3	16:P:435:ARG:HD2	2.02	0.42
16:P:473:HIS:CG	16:P:475:ARG:HD3	2.54	0.42
17:Q:356:VAL:CA	18:R:208:TYR:HA	2.49	0.42
17:Q:366:TYR:HE1	18:R:218:ASP:HB2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:GLU:OE2	1:A:1645:LYS:CG	2.63	0.42
1:A:477:ASN:HB3	2:B:1047:ARG:HH11	1.83	0.42
1:A:812:VAL:HG22	1:A:815:ARG:NH2	2.35	0.42
1:A:1238:MET:HE2	1:A:1525:ASN:H	1.83	0.42
2:B:328:GLN:O	2:B:346:ASP:HB3	2.19	0.42
2:B:648:ARG:NH1	2:B:650:LEU:HD21	2.34	0.42
2:B:853:GLU:HG2	2:B:856:ASP:OD2	2.19	0.42
3:C:69:ARG:HH21	11:K:71:THR:N	2.15	0.42
3:C:103:LEU:HD23	3:C:218:LYS:HB3	2.01	0.42
4:D:33:THR:O	4:D:37:LEU:N	2.32	0.42
5:E:68:SER:HB3	5:E:75:MET:SD	2.60	0.42
7:G:73:TYR:CZ	7:G:238:THR:HG21	2.55	0.42
11:K:62:SER:OG	11:K:104:ARG:NH1	2.41	0.42
16:P:324:TRP:CZ2	16:P:383:ILE:HG21	2.55	0.42
16:P:438:TRP:CE3	16:P:439:LYS:O	2.73	0.42
16:P:597:LYS:HD2	17:Q:321:ASP:OD1	2.19	0.42
16:P:740:ILE:O	16:P:744:LEU:HG	2.20	0.42
17:Q:297:ARG:HB2	17:Q:297:ARG:HH11	1.84	0.42
17:Q:302:ALA:O	17:Q:303:GLU:C	2.58	0.42
18:R:253:ILE:HG22	18:R:254:GLY:N	2.34	0.42
20:T:11:DA:N3	20:T:12:DC:C6	2.88	0.42
1:A:132:GLU:O	1:A:136:LEU:N	2.51	0.42
1:A:259:LYS:O	1:A:262:THR:HB	2.18	0.42
1:A:489:ASN:ND2	2:B:781:TYR:CZ	2.85	0.42
1:A:560:GLN:HE22	15:O:238:ILE:HG22	1.85	0.42
1:A:1051:GLY:CA	1:A:1580:ARG:HG2	2.49	0.42
1:A:1482:LYS:HD2	2:B:307:GLU:OE1	2.20	0.42
2:B:95:LEU:HD12	2:B:144:SER:O	2.20	0.42
2:B:561:ILE:HB	2:B:562:PRO:HD3	2.02	0.42
2:B:712:SER:N	2:B:713:PRO:HD2	2.35	0.42
2:B:789:ILE:HD12	2:B:927:CYS:SG	2.59	0.42
3:C:294:VAL:HG21	3:C:297:HIS:HB3	2.02	0.42
4:D:27:LEU:HA	4:D:28:PRO:HD3	1.91	0.42
4:D:89:LEU:HA	4:D:92:ILE:HD12	2.01	0.42
5:E:55:ARG:NE	5:E:113:GLN:HE21	2.18	0.42
7:G:33:GLY:HA3	7:G:230:ARG:HH22	1.85	0.42
7:G:127:PRO:HG2	7:G:236:VAL:HG21	2.01	0.42
9:I:29:GLU:HG3	9:I:36:ILE:HG13	2.01	0.42
9:I:30:CYS:O	9:I:34:LYS:HA	2.20	0.42
13:M:10:ILE:HB	14:N:70:LEU:HB3	2.01	0.42
15:O:474:TYR:HA	15:O:477:PHE:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:393:VAL:HG23	16:P:394:VAL:N	2.31	0.42
17:Q:147:GLN:N	17:Q:148:PRO:HD3	2.34	0.42
17:Q:323:ASP:C	17:Q:325:GLN:N	2.72	0.42
17:Q:439:ILE:H	17:Q:439:ILE:HG13	1.66	0.42
17:Q:512:ARG:HA	17:Q:512:ARG:HD3	1.84	0.42
18:R:426:VAL:HG23	18:R:427:PRO:HD2	2.02	0.42
1:A:821:ILE:O	1:A:825:ALA:N	2.38	0.42
1:A:1645:LYS:CB	1:A:1645:LYS:HZ2	2.33	0.42
2:B:909:ARG:NH2	2:B:1042:ASP:OD1	2.53	0.42
2:B:917:PHE:CE1	2:B:1035:ARG:HG3	2.55	0.42
5:E:50:MET:HB3	5:E:52:ARG:H	1.85	0.42
8:H:33:GLN:HB2	8:H:36:CYS:HB3	2.02	0.42
14:N:83:ASP:C	14:N:85:HIS:H	2.23	0.42
15:O:364:LEU:HB3	15:O:385:MET:HE3	2.02	0.42
16:P:473:HIS:HA	16:P:474:LYS:HE3	2.02	0.42
16:P:582:ASP:HB2	16:P:585:GLU:HG3	2.02	0.42
16:P:607:VAL:O	16:P:611:ILE:HG13	2.20	0.42
16:P:776:ASP:HB3	17:Q:134:LYS:HE3	2.02	0.42
17:Q:112:LEU:CD1	17:Q:164:ILE:HD11	2.50	0.42
17:Q:356:VAL:CB	18:R:208:TYR:CA	2.77	0.42
1:A:103:LEU:CD1	1:A:241:PRO:HD2	2.50	0.41
1:A:476:VAL:HA	2:B:1095:SER:C	2.17	0.41
1:A:525:ASN:ND2	1:A:531:PRO:O	2.36	0.41
1:A:535:GLN:C	1:A:578:TYR:CD1	2.93	0.41
1:A:1246:VAL:CG1	1:A:1250:GLN:HB3	2.41	0.41
1:A:1657:LEU:HD23	7:G:104:LEU:HB3	2.01	0.41
2:B:1087:LEU:HD23	2:B:1088:LEU:CD2	2.50	0.41
6:F:147:SER:O	6:F:150:GLU:HG2	2.19	0.41
11:K:83:ASN:ND2	11:K:119:LYS:HD3	2.35	0.41
13:M:10:ILE:O	14:N:69:SER:HA	2.20	0.41
16:P:473:HIS:ND1	16:P:473:HIS:O	2.53	0.41
16:P:492:LEU:HD22	16:P:492:LEU:N	2.35	0.41
16:P:697:GLU:HB3	16:P:709:PRO:O	2.20	0.41
16:P:768:TYR:O	16:P:771:ILE:N	2.53	0.41
18:R:8:LEU:HB2	18:R:9:THR:HG22	2.01	0.41
18:R:246:GLN:CD	18:R:247:ILE:HD12	2.40	0.41
18:R:372:HIS:CE1	18:R:410:TYR:CD2	3.08	0.41
1:A:1289:SER:CB	1:A:1475:GLU:HG2	2.49	0.41
2:B:527:PHE:HE2	2:B:669:GLN:OE1	2.03	0.41
2:B:565:LEU:HB3	2:B:570:VAL:HG21	2.01	0.41
2:B:612:LYS:CG	2:B:622:ILE:HA	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:146:ALA:HB1	3:C:156:LEU:HD23	2.02	0.41
7:G:65:HIS:O	7:G:68:PRO:HD2	2.20	0.41
8:H:30:SER:HB3	8:H:33:GLN:O	2.20	0.41
14:N:81:THR:HG22	14:N:86:ASP:HB3	2.02	0.41
15:O:502:LEU:HD22	15:O:506:PHE:CE2	2.55	0.41
16:P:300:LEU:HA	16:P:320:ILE:CA	2.48	0.41
16:P:504:THR:O	16:P:542:ARG:HG2	2.20	0.41
17:Q:22:ILE:HD12	17:Q:26:ARG:HE	1.78	0.41
17:Q:26:ARG:HD2	17:Q:34:VAL:HG11	2.02	0.41
18:R:75:GLN:HA	18:R:78:ARG:NE	2.32	0.41
1:A:76:GLN:HB3	1:A:364:PRO:HD3	2.02	0.41
1:A:461:GLU:O	1:A:465:GLY:N	2.54	0.41
1:A:597:LYS:HE3	1:A:660:PRO:CG	2.50	0.41
2:B:311:ARG:NH2	9:I:17:LEU:O	2.53	0.41
2:B:528:LEU:HA	2:B:528:LEU:HD23	1.86	0.41
2:B:775:VAL:HG12	2:B:951:PRO:HB3	2.03	0.41
2:B:929:ARG:HG2	2:B:930:LYS:N	2.34	0.41
2:B:1112:THR:OG1	2:B:1128:CYS:SG	2.64	0.41
3:C:128:ASP:HB2	3:C:175:GLN:HG3	2.02	0.41
4:D:88:GLN:HE21	15:O:184:PRO:HB2	1.84	0.41
7:G:47:VAL:HB	7:G:65:HIS:NE2	2.35	0.41
13:M:42:LYS:HG3	13:M:51:PHE:HE1	1.85	0.41
14:N:31:LYS:HE2	14:N:117:GLU:HG2	2.01	0.41
16:P:64:LEU:CD2	16:P:64:LEU:H	2.33	0.41
16:P:184:SER:C	18:R:198:LEU:HG	2.40	0.41
16:P:348:HIS:HE1	18:R:154:LYS:CE	2.33	0.41
16:P:358:SER:HB2	18:R:196:GLU:OE1	2.16	0.41
17:Q:4:PHE:HE2	17:Q:18:ARG:HH11	1.67	0.41
18:R:297:PHE:N	18:R:297:PHE:CD1	2.89	0.41
18:R:402:ASN:O	18:R:405:ILE:HB	2.20	0.41
1:A:407:GLN:HB2	1:A:410:LYS:HB3	2.01	0.41
1:A:582:LYS:CE	1:A:584:ARG:HE	2.33	0.41
1:A:733:THR:HG23	1:A:775:ALA:HA	2.02	0.41
1:A:1003:ARG:CD	2:B:520:LEU:HD22	2.49	0.41
1:A:1273:THR:HG22	9:I:48:VAL:HG13	2.02	0.41
3:C:128:ASP:OD1	3:C:129:GLU:N	2.53	0.41
5:E:33:GLU:OE1	5:E:33:GLU:N	2.42	0.41
8:H:115:TYR:HE1	8:H:124:ARG:CG	2.32	0.41
10:J:36:LEU:HD11	10:J:51:LEU:HD13	2.03	0.41
14:N:82:ILE:O	14:N:87:TYR:HE1	2.04	0.41
15:O:523:ASN:O	15:O:527:MET:N	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:611:ILE:CD1	16:P:731:LEU:HB2	2.50	0.41
16:P:755:PRO:HB3	17:Q:131:HIS:HB3	2.03	0.41
1:A:54:LEU:HA	1:A:54:LEU:HD23	1.85	0.41
1:A:632:GLU:OE2	2:B:1043:LYS:HB3	2.19	0.41
1:A:1129:PRO:HB2	1:A:1178:LEU:HD11	2.03	0.41
2:B:918:SER:HA	2:B:923:GLN:O	2.21	0.41
2:B:975:HIS:CE1	2:B:1003:ALA:HB2	2.56	0.41
5:E:112:TYR:CD2	5:E:116:ILE:HD11	2.55	0.41
7:G:158:LYS:HG2	15:O:105:ASN:OD1	2.21	0.41
7:G:216:HIS:HD1	7:G:224:PRO:HB3	1.85	0.41
10:J:30:LEU:HD11	10:J:38:ARG:NH1	2.34	0.41
13:M:67:ASP:OD1	13:M:68:SER:N	2.53	0.41
15:O:383:TYR:CE1	15:O:597:LEU:HD21	2.55	0.41
16:P:186:TYR:HD1	18:R:198:LEU:HD23	1.82	0.41
16:P:194:ARG:HA	16:P:209:LYS:O	2.20	0.41
16:P:540:LYS:HE2	16:P:544:SER:O	2.21	0.41
16:P:596:ILE:HB	17:Q:272:GLN:HG2	2.01	0.41
16:P:666:SER:HB3	16:P:742:TRP:CE2	2.54	0.41
16:P:697:GLU:HG2	16:P:698:LYS:N	2.34	0.41
17:Q:353:VAL:HG11	17:Q:489:VAL:HG12	2.01	0.41
18:R:165:ILE:H	18:R:165:ILE:HG13	1.49	0.41
18:R:216:LEU:HD13	18:R:239:LEU:HD13	2.02	0.41
20:T:14:DG:C2	21:U:37:DA:C2	3.09	0.41
1:A:2:ASP:OD2	1:A:4:SER:OG	2.37	0.41
1:A:67:LEU:HD11	2:B:1115:GLN:HG3	2.03	0.41
1:A:91:PHE:O	1:A:94:LEU:HB3	2.21	0.41
1:A:126:GLN:HB3	1:A:343:PRO:HD3	2.01	0.41
1:A:358:ASP:HB2	1:A:359:VAL:H	1.64	0.41
1:A:514:TYR:OH	6:F:102:SER:HA	2.21	0.41
1:A:518:GLU:OE1	1:A:582:LYS:NZ	2.54	0.41
1:A:539:GLU:HB3	1:A:570:THR:HB	2.02	0.41
1:A:581:ILE:CD1	1:A:637:PHE:CE1	3.03	0.41
1:A:772:LYS:HE3	8:H:137:GLN:NE2	2.35	0.41
1:A:934:LYS:HE2	2:B:956:SER:OG	2.21	0.41
1:A:989:GLY:HA3	2:B:709:PHE:HE1	1.85	0.41
1:A:1319:ASN:C	1:A:1323:HIS:HD1	2.16	0.41
2:B:117:VAL:HG23	18:R:276:GLN:HA	1.68	0.41
2:B:178:TYR:O	2:B:182:GLN:HG2	2.20	0.41
2:B:218:ILE:HG23	2:B:231:HIS:ND1	2.36	0.41
2:B:560:ARG:HH22	2:B:618:PRO:HB2	1.85	0.41
2:B:584:CYS:HB3	2:B:596:VAL:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:893:ASN:ND2	20:T:39:DT:H5"	2.36	0.41
2:B:1131:CYS:HB2	2:B:1170:GLY:HA2	2.02	0.41
3:C:44:ILE:HA	3:C:54:PHE:CB	2.51	0.41
9:I:19:ASN:OD1	9:I:21:ASN:N	2.48	0.41
12:L:50:ASP:HA	17:Q:412:LYS:NZ	2.36	0.41
14:N:63:ASP:OD1	14:N:65:SER:OG	2.32	0.41
15:O:457:ARG:HB3	15:O:470:PHE:HE1	1.85	0.41
17:Q:123:MET:HG2	17:Q:184:TRP:CZ2	2.56	0.41
18:R:231:LEU:HD23	18:R:231:LEU:HA	1.78	0.41
1:A:413:LEU:O	1:A:417:ARG:NH1	2.53	0.41
1:A:638:PRO:HB3	1:A:643:ALA:HB1	2.03	0.41
1:A:719:ILE:HG12	8:H:97:MET:HG2	2.02	0.41
1:A:800:VAL:O	1:A:1079:LYS:HD2	2.21	0.41
1:A:1478:ALA:O	9:I:19:ASN:ND2	2.53	0.41
1:A:1481:GLU:OE1	1:A:1481:GLU:N	2.49	0.41
2:B:135:GLY:N	2:B:161:LEU:O	2.52	0.41
2:B:781:TYR:OH	11:K:96:PRO:HD2	2.21	0.41
2:B:806:THR:OG1	2:B:904:LYS:HG2	2.21	0.41
2:B:913:ILE:HD12	2:B:929:ARG:HA	2.02	0.41
2:B:995:TYR:O	2:B:998:GLU:HB3	2.21	0.41
2:B:1061:LYS:HE2	20:T:21:DC:OP2	2.21	0.41
4:D:22:ILE:O	7:G:76:LYS:NZ	2.39	0.41
4:D:88:GLN:O	4:D:92:ILE:HG13	2.21	0.41
5:E:118:PRO:O	5:E:121:MET:HB2	2.20	0.41
7:G:138:PHE:CD1	15:O:182:MET:SD	3.14	0.41
15:O:181:ARG:NH2	15:O:221:TYR:O	2.54	0.41
15:O:200:ASN:OD1	17:Q:14:ASN:CB	2.66	0.41
18:R:219:LEU:O	18:R:223:ASN:ND2	2.51	0.41
1:A:571:HIS:CE1	1:A:572:THR:HG23	2.56	0.41
1:A:597:LYS:HB2	2:B:1082:HIS:CG	2.55	0.41
1:A:793:ILE:HG23	1:A:794:VAL:N	2.32	0.41
1:A:826:PHE:HB3	2:B:777:SER:HB2	2.03	0.41
1:A:886:ASN:OD1	1:A:955:ARG:NH1	2.32	0.41
1:A:1156:LYS:HE2	1:A:1156:LYS:HB2	1.91	0.41
1:A:1233:ILE:HD11	1:A:1236:PRO:HA	2.03	0.41
1:A:1314:GLN:O	1:A:1318:SER:OG	2.36	0.41
1:A:1655:ASP:HB2	6:F:135:ARG:HB3	2.03	0.41
2:B:127:ARG:NH2	2:B:193:TYR:OH	2.50	0.41
3:C:240:LYS:HA	3:C:244:ALA:HB2	2.02	0.41
5:E:39:LEU:O	5:E:42:PHE:HB3	2.21	0.41
5:E:191:LYS:HB2	5:E:194:GLU:OE2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:141:SER:HG	7:G:144:HIS:HD1	1.62	0.41
13:M:42:LYS:HG3	13:M:51:PHE:CE1	2.56	0.41
16:P:645:LYS:O	16:P:647:GLU:N	2.54	0.41
18:R:16:ARG:NH2	18:R:183:GLU:OE2	2.54	0.41
1:A:332:GLN:HG2	1:A:349:LEU:HD22	2.03	0.41
1:A:628:PHE:CG	2:B:784:ASP:HB3	2.54	0.41
1:A:810:LEU:HA	1:A:810:LEU:HD12	1.88	0.41
1:A:1644:GLY:HA3	2:B:1179:PRO:HD3	2.02	0.41
2:B:79:LEU:HB2	2:B:90:TYR:CE2	2.56	0.41
2:B:211:ARG:HH22	2:B:645:GLY:HA3	1.86	0.41
2:B:212:ASN:HD22	2:B:212:ASN:H	1.67	0.41
2:B:460:LYS:O	2:B:463:TYR:HB3	2.21	0.41
2:B:610:TYR:HE1	2:B:658:LEU:HD11	1.86	0.41
2:B:612:LYS:HG2	2:B:622:ILE:HA	2.03	0.41
2:B:1058:GLN:O	2:B:1059:PRO:O	2.39	0.41
2:B:1202:PRO:HG3	7:G:46:TYR:CD2	2.56	0.41
5:E:183:PRO:HA	5:E:186:LEU:HD12	2.03	0.41
11:K:79:VAL:HG21	11:K:124:LEU:HD13	2.02	0.41
14:N:82:ILE:HB	14:N:87:TYR:CD1	2.56	0.41
15:O:484:PHE:CZ	15:O:527:MET:O	2.74	0.41
15:O:487:ARG:HG2	15:O:491:PHE:CD2	2.56	0.41
15:O:606:MET:HA	15:O:609:TYR:CD2	2.56	0.41
15:O:606:MET:HA	15:O:609:TYR:HD2	1.84	0.41
16:P:220:THR:HB	16:P:222:GLN:HE22	1.86	0.41
16:P:329:ILE:HG13	16:P:330:PRO:N	2.33	0.41
16:P:351:ILE:O	16:P:352:PHE:HB2	2.21	0.41
16:P:414:ILE:HD13	16:P:425:GLY:HA3	2.03	0.41
16:P:420:GLU:HB2	16:P:442:LEU:H	1.82	0.41
16:P:484:ARG:HG3	16:P:488:LEU:HD23	2.02	0.41
16:P:510:THR:C	16:P:511:ILE:HG13	2.41	0.41
16:P:596:ILE:O	16:P:596:ILE:HD12	2.21	0.41
16:P:662:LEU:CB	16:P:665:ASN:HD22	2.25	0.41
16:P:732:LEU:O	16:P:733:THR:C	2.58	0.41
16:P:764:LEU:O	16:P:766:GLY:N	2.54	0.41
17:Q:15:CYS:CB	17:Q:17:SER:H	2.30	0.41
17:Q:178:THR:CG2	17:Q:303:GLU:OE1	2.69	0.41
17:Q:229:LYS:HA	17:Q:232:LEU:HB2	2.03	0.41
17:Q:307:LEU:O	17:Q:311:MET:HG2	2.21	0.41
17:Q:356:VAL:CG1	18:R:212:HIS:NE2	2.80	0.41
17:Q:441:ASP:OD2	17:Q:445:ARG:NH1	2.54	0.41
1:A:70:LYS:HZ2	17:Q:27:ARG:CZ	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:ARG:HA	1:A:369:LEU:HG	2.02	0.41
1:A:499:PRO:HG3	1:A:609:PRO:HA	2.03	0.41
1:A:893:ASP:OD2	1:A:955:ARG:HB3	2.21	0.41
1:A:1014:SER:O	20:T:17:DT:C5'	2.60	0.41
1:A:1031:HIS:O	1:A:1039:ARG:N	2.53	0.41
1:A:1104:TYR:OH	1:A:1117:SER:HB3	2.20	0.41
1:A:1152:SER:O	1:A:1156:LYS:NZ	2.53	0.41
1:A:1323:HIS:CE1	1:A:1454:HIS:NE2	2.89	0.41
2:B:461:MET:O	2:B:464:PHE:HB3	2.21	0.41
2:B:1136:GLU:O	2:B:1140:LYS:HG3	2.21	0.41
3:C:40:PHE:O	11:K:134:LYS:NZ	2.54	0.41
5:E:67:GLU:HA	5:E:70:SER:OG	2.20	0.41
7:G:48:SER:OG	7:G:64:GLN:NE2	2.54	0.41
7:G:50:ALA:HB3	7:G:53:TYR:HD2	1.86	0.41
15:O:234:ILE:HA	15:O:237:ILE:HB	2.03	0.41
16:P:450:ARG:O	16:P:468:VAL:HA	2.21	0.41
16:P:698:LYS:HB3	17:Q:124:ARG:HB3	2.03	0.41
17:Q:302:ALA:O	17:Q:305:ARG:N	2.53	0.41
17:Q:435:GLN:H	17:Q:435:GLN:HG3	1.42	0.41
18:R:9:THR:HG21	18:R:13:PHE:HD2	1.83	0.41
18:R:350:SER:HA	18:R:353:VAL:HB	2.03	0.41
1:A:81:LEU:HD11	1:A:430:ILE:HD11	2.01	0.40
1:A:447:THR:O	1:A:447:THR:HG22	2.21	0.40
1:A:511:VAL:HG11	1:A:575:LYS:H	1.85	0.40
1:A:553:GLN:O	1:A:556:ALA:HB3	2.22	0.40
1:A:633:MET:HB3	1:A:633:MET:HE2	1.85	0.40
1:A:701:ARG:NH2	1:A:704:ASP:OD2	2.54	0.40
1:A:718:THR:OG1	1:A:730:GLN:NE2	2.53	0.40
1:A:1061:SER:OG	1:A:1062:HIS:N	2.53	0.40
1:A:1238:MET:HE3	1:A:1525:ASN:C	2.42	0.40
1:A:1300:ASN:OD1	1:A:1301:GLU:HG3	2.20	0.40
1:A:1305:GLU:HG3	1:A:1306:TYR:CD1	2.56	0.40
1:A:1646:LEU:HD22	1:A:1646:LEU:HA	1.76	0.40
2:B:114:SER:O	18:R:281:LYS:HA	2.14	0.40
2:B:212:ASN:N	2:B:212:ASN:ND2	2.68	0.40
2:B:711:GLN:HB2	2:B:958:MET:HB2	2.03	0.40
2:B:792:SER:HA	3:C:217:ALA:HB2	2.03	0.40
2:B:874:TYR:CZ	2:B:876:SER:HB3	2.56	0.40
2:B:1007:TYR:HB3	3:C:281:ARG:HD2	2.03	0.40
5:E:22:MET:HB2	5:E:187:TYR:CE1	2.56	0.40
6:F:93:ILE:HD13	6:F:93:ILE:HA	1.91	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:113:SER:OG	14:N:116:LYS:N	2.54	0.40
15:O:236:LYS:HA	15:O:239:SER:HB3	2.03	0.40
15:O:403:LEU:HD13	15:O:424:LEU:HA	2.04	0.40
16:P:302:VAL:C	16:P:363:ILE:HD11	2.40	0.40
16:P:408:ILE:HD11	16:P:455:LYS:HG3	2.03	0.40
16:P:469:TYR:CE2	16:P:508:ILE:HB	2.56	0.40
17:Q:116:ILE:O	17:Q:120:ILE:HG13	2.21	0.40
17:Q:178:THR:HG22	17:Q:178:THR:H	1.63	0.40
17:Q:262:LEU:HA	17:Q:262:LEU:HD23	1.67	0.40
1:A:1124:LEU:HD23	1:A:1135:SER:OG	2.21	0.40
1:A:1559:ARG:NH2	5:E:200:ARG:HD3	2.36	0.40
2:B:26:ILE:HA	10:J:58:GLU:OE2	2.21	0.40
2:B:1093:LEU:CD1	2:B:1098:TYR:CD1	3.04	0.40
2:B:1158:ILE:HA	2:B:1167:PHE:O	2.20	0.40
5:E:9:ILE:HG21	5:E:43:LYS:HD3	2.03	0.40
13:M:55:GLY:HA3	13:M:62:TYR:HB2	2.03	0.40
16:P:198:ASP:HB3	16:P:261:VAL:HG23	2.02	0.40
16:P:272:PHE:HD2	16:P:292:LEU:HD11	1.85	0.40
16:P:656:HIS:CE1	16:P:748:GLU:HG3	2.56	0.40
17:Q:106:LYS:HB3	17:Q:106:LYS:HE3	1.81	0.40
17:Q:187:THR:HG22	17:Q:380:TRP:HE1	1.86	0.40
17:Q:366:TYR:OH	18:R:214:VAL:HG13	2.21	0.40
18:R:357:PRO:HB3	18:R:359:MET:HB3	2.02	0.40
1:A:81:LEU:CD1	1:A:82:PRO:HD2	2.45	0.40
1:A:659:THR:HG1	1:A:664:SER:H	1.64	0.40
1:A:1032:VAL:HG22	1:A:1038:ILE:CD1	2.48	0.40
1:A:1195:GLU:O	1:A:1198:THR:OG1	2.29	0.40
2:B:139:LEU:O	2:B:155:VAL:HA	2.21	0.40
2:B:387:GLY:O	2:B:634:ARG:NH1	2.54	0.40
2:B:883:GLU:HB3	2:B:904:LYS:CB	2.51	0.40
3:C:105:PRO:HG3	10:J:6:ARG:NH2	2.37	0.40
3:C:297:HIS:CD2	3:C:298:PHE:N	2.89	0.40
5:E:154:ILE:O	5:E:197:LYS:N	2.46	0.40
11:K:63:PHE:O	11:K:102:ASN:HA	2.21	0.40
13:M:8:SER:OG	13:M:9:GLU:N	2.53	0.40
14:N:111:VAL:O	14:N:120:LYS:N	2.34	0.40
15:O:151:TRP:HA	15:O:154:VAL:HB	2.04	0.40
15:O:171:CYS:O	15:O:175:MET:N	2.42	0.40
15:O:414:ALA:HA	15:O:417:LYS:HD2	2.02	0.40
15:O:487:ARG:HH21	15:O:502:LEU:CD1	2.29	0.40
15:O:510:VAL:HG13	15:O:517:LEU:HG	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:219:LEU:HB2	16:P:244:SER:O	2.21	0.40
16:P:358:SER:CB	18:R:196:GLU:CD	2.90	0.40
16:P:418:SER:O	16:P:419:ARG:HB3	2.21	0.40
16:P:437:SER:O	16:P:438:TRP:HD1	2.04	0.40
16:P:616:SER:OG	16:P:618:ASP:N	2.48	0.40
18:R:250:LEU:HD22	18:R:298:GLN:NE2	2.36	0.40
18:R:253:ILE:O	18:R:255:VAL:N	2.54	0.40
1:A:463:LYS:HD3	20:T:16:DT:C7	2.52	0.40
1:A:628:PHE:CE2	2:B:784:ASP:HB2	2.41	0.40
1:A:752:LYS:O	1:A:785:GLN:NE2	2.55	0.40
1:A:771:PHE:CD1	1:A:776:LEU:HA	2.56	0.40
2:B:119:ARG:HH22	2:B:125:GLU:CD	2.23	0.40
2:B:286:ARG:HD3	9:I:9:PHE:CD2	2.57	0.40
2:B:572:PRO:HG3	13:M:74:ASN:ND2	2.37	0.40
2:B:698:SER:HB3	24:B:1301:SO4:S	2.60	0.40
2:B:1114:GLN:HG3	2:B:1115:GLN:O	2.21	0.40
5:E:29:PHE:N	5:E:63:ASN:O	2.46	0.40
8:H:108:SER:OG	8:H:111:LEU:HG	2.21	0.40
9:I:12:ASP:HB2	9:I:33:CYS:SG	2.61	0.40
9:I:19:ASN:HB3	9:I:22:ALA:CB	2.51	0.40
10:J:69:ARG:NH2	12:L:33:GLU:OE2	2.54	0.40
16:P:68:THR:HG23	16:P:214:LEU:O	2.21	0.40
18:R:205:VAL:O	18:R:205:VAL:HG12	2.20	0.40
18:R:297:PHE:N	18:R:297:PHE:HD1	2.20	0.40
1:A:184:LYS:HA	1:A:187:GLU:OE2	2.22	0.40
1:A:510:PRO:HG2	6:F:102:SER:HB2	2.03	0.40
1:A:590:ASN:OD1	1:A:591:ARG:N	2.54	0.40
1:A:665:PRO:O	1:A:788:ALA:HB1	2.21	0.40
1:A:980:GLY:HA2	1:A:997:PHE:CD2	2.56	0.40
2:B:75:ASP:OD1	2:B:75:ASP:N	2.54	0.40
2:B:228:SER:O	2:B:254:ASN:N	2.35	0.40
2:B:338:PHE:HE2	2:B:353:VAL:HA	1.87	0.40
7:G:91:ASP:OD1	7:G:104:LEU:N	2.44	0.40
7:G:219:ASP:OD1	7:G:223:GLU:N	2.55	0.40
16:P:217:ALA:O	16:P:219:LEU:N	2.51	0.40
16:P:389:TRP:CZ3	18:R:149:LYS:N	2.89	0.40
16:P:773:SER:O	16:P:775:TRP:N	2.54	0.40
17:Q:6:ARG:HA	17:Q:18:ARG:HG3	2.02	0.40
17:Q:348:ILE:HG12	17:Q:376:GLU:HB3	2.04	0.40
18:R:219:LEU:HD23	18:R:219:LEU:HA	1.66	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	1447/1664 (87%)	1307 (90%)	131 (9%)	9 (1%)	22	50
2	B	1171/1203 (97%)	1094 (93%)	61 (5%)	16 (1%)	9	31
3	C	303/335 (90%)	276 (91%)	26 (9%)	1 (0%)	37	66
4	D	50/137 (36%)	48 (96%)	2 (4%)	0	100	100
5	E	210/215 (98%)	199 (95%)	11 (5%)	0	100	100
6	F	98/155 (63%)	92 (94%)	6 (6%)	0	100	100
7	G	189/326 (58%)	180 (95%)	9 (5%)	0	100	100
8	H	127/146 (87%)	123 (97%)	4 (3%)	0	100	100
9	I	61/125 (49%)	52 (85%)	8 (13%)	1 (2%)	8	29
10	J	67/70 (96%)	61 (91%)	6 (9%)	0	100	100
11	K	99/142 (70%)	94 (95%)	5 (5%)	0	100	100
12	L	42/70 (60%)	38 (90%)	4 (10%)	0	100	100
13	M	106/415 (26%)	101 (95%)	5 (5%)	0	100	100
14	N	121/233 (52%)	112 (93%)	9 (7%)	0	100	100
15	O	457/627 (73%)	418 (92%)	36 (8%)	3 (1%)	19	47
16	P	573/894 (64%)	414 (72%)	113 (20%)	46 (8%)	1	5
17	Q	377/514 (73%)	311 (82%)	49 (13%)	17 (4%)	2	13
18	R	289/507 (57%)	219 (76%)	41 (14%)	29 (10%)	0	3
All	All	5787/7778 (74%)	5139 (89%)	526 (9%)	122 (2%)	8	24

All (122) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	819	ASP
2	B	820	PRO
2	B	954	PHE
2	B	1097	ASP

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Mol	Chain	Res	Type
15	O	493	ASP
16	P	218	VAL
16	P	229	ARG
16	P	248	PRO
16	P	271	ILE
16	P	321	LYS
16	P	332	ASN
16	P	393	VAL
16	P	432	PRO
16	P	444	PRO
16	P	743	SER
16	P	752	LEU
17	Q	8	PRO
17	Q	9	ILE
17	Q	15	CYS
17	Q	289	ARG
18	R	11	ARG
18	R	155	GLN
18	R	247	ILE
18	R	294	VAL
18	R	295	PRO
18	R	296	PRO
18	R	302	ARG
18	R	306	ALA
18	R	307	LYS
18	R	359	MET
18	R	427	PRO
1	A	90	PHE
1	A	91	PHE
1	A	358	ASP
1	A	1651	THR
2	B	955	PRO
2	B	1059	PRO
2	B	1066	HIS
15	O	492	ARG
16	P	61	VAL
16	P	67	ASP
16	P	216	ILE
16	P	259	ASN
16	P	377	ARG
16	P	396	ALA
16	P	657	SER

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Mol	Chain	Res	Type
16	P	659	LEU
16	P	726	SER
16	P	774	SER
17	Q	7	GLY
17	Q	196	SER
17	Q	280	ASP
17	Q	316	TRP
17	Q	317	MET
17	Q	362	THR
18	R	254	GLY
18	R	420	ASP
1	A	1259	SER
1	A	1505	ASP
2	B	322	ASN
2	B	784	ASP
2	B	1100	GLN
16	P	191	SER
16	P	201	GLU
16	P	269	PHE
16	P	301	GLN
16	P	365	TRP
16	P	437	SER
16	P	591	ALA
16	P	746	ARG
17	Q	364	SER
18	R	5	PRO
18	R	141	TRP
18	R	151	PRO
18	R	239	LEU
18	R	301	SER
18	R	323	SER
1	A	1650	GLY
2	B	815	ARG
16	P	263	ILE
16	P	290	GLU
16	P	394	VAL
16	P	446	ASP
16	P	545	SER
16	P	745	ALA
17	Q	13	ASP
17	Q	492	ALA
18	R	149	LYS

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Mol	Chain	Res	Type
18	R	421	LYS
1	A	1050	TYR
1	A	1061	SER
2	B	786	ALA
2	B	1063	ARG
3	C	232	GLN
15	O	225	LEU
16	P	58	HIS
16	P	445	ASP
16	P	458	LYS
16	P	487	ASN
16	P	666	SER
17	Q	16	PRO
18	R	18	LYS
18	R	232	ALA
18	R	425	ALA
2	B	1052	VAL
16	P	187	ILE
16	P	297	ILE
16	P	500	ILE
18	R	262	SER
18	R	423	GLY
2	B	491	ILE
16	P	709	PRO
17	Q	451	PRO
17	Q	470	PRO
18	R	267	GLY
2	B	699	ILE
17	Q	327	PRO
9	I	47	VAL
16	P	233	VAL
18	R	293	ILE
16	P	568	ILE
18	R	357	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	1289/1465 (88%)	1271 (99%)	18 (1%)	62	77
2	B	1030/1053 (98%)	1017 (99%)	13 (1%)	65	78
3	C	269/296 (91%)	269 (100%)	0	100	100
4	D	52/116 (45%)	52 (100%)	0	100	100
5	E	194/197 (98%)	194 (100%)	0	100	100
6	F	90/137 (66%)	90 (100%)	0	100	100
7	G	171/291 (59%)	171 (100%)	0	100	100
8	H	115/128 (90%)	115 (100%)	0	100	100
9	I	55/110 (50%)	55 (100%)	0	100	100
10	J	64/65 (98%)	63 (98%)	1 (2%)	58	75
11	K	91/130 (70%)	91 (100%)	0	100	100
12	L	39/57 (68%)	39 (100%)	0	100	100
13	M	98/371 (26%)	98 (100%)	0	100	100
14	N	119/220 (54%)	119 (100%)	0	100	100
15	O	427/576 (74%)	420 (98%)	7 (2%)	58	75
16	P	543/828 (66%)	374 (69%)	169 (31%)	0	1
17	Q	364/476 (76%)	293 (80%)	71 (20%)	1	3
18	R	286/474 (60%)	209 (73%)	77 (27%)	0	1
All	All	5296/6990 (76%)	4940 (93%)	356 (7%)	16	38

All (356) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	105	CYS
1	A	321	LYS
1	A	355	PHE
1	A	357	MET
1	A	358	ASP
1	A	578	TYR
1	A	646	GLU
1	A	1248	ASP
1	A	1249	GLU
1	A	1255	CYS
1	A	1506	ARG
1	A	1507	CYS
1	A	1640	ARG
1	A	1641	ILE

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Mol	Chain	Res	Type
1	A	1645	LYS
1	A	1646	LEU
1	A	1647	ASN
1	A	1648	ASN
2	B	784	ASP
2	B	787	MET
2	B	817	ARG
2	B	936	MET
2	B	949	ILE
2	B	1060	VAL
2	B	1064	LYS
2	B	1065	ARG
2	B	1086	PHE
2	B	1087	LEU
2	B	1091	ARG
2	B	1093	LEU
2	B	1096	SER
10	J	45	CYS
15	O	380	SER
15	O	434	LEU
15	O	435	SER
15	O	484	PHE
15	O	486	PHE
15	O	490	ILE
15	O	491	PHE
16	P	26	TYR
16	P	49	THR
16	P	50	LEU
16	P	56	ASP
16	P	64	LEU
16	P	66	CYS
16	P	181	ARG
16	P	182	LEU
16	P	183	ASP
16	P	185	GLN
16	P	187	ILE
16	P	192	ASP
16	P	193	LEU
16	P	194	ARG
16	P	195	ASN
16	P	198	ASP
16	P	201	GLU

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Mol	Chain	Res	Type
16	P	205	TYR
16	P	207	SER
16	P	212	SER
16	P	213	VAL
16	P	214	LEU
16	P	219	LEU
16	P	220	THR
16	P	221	ARG
16	P	226	HIS
16	P	227	LEU
16	P	229	ARG
16	P	238	LEU
16	P	247	ILE
16	P	248	PRO
16	P	259	ASN
16	P	260	LEU
16	P	263	ILE
16	P	264	ILE
16	P	267	ASN
16	P	268	SER
16	P	269	PHE
16	P	273	ARG
16	P	276	SER
16	P	278	HIS
16	P	282	CYS
16	P	288	SER
16	P	292	LEU
16	P	295	VAL
16	P	296	GLU
16	P	300	LEU
16	P	314	GLN
16	P	320	ILE
16	P	321	LYS
16	P	329	ILE
16	P	342	GLN
16	P	343	LEU
16	P	345	ASP
16	P	347	LEU
16	P	348	HIS
16	P	355	GLU
16	P	360	TRP
16	P	362	ARG

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Mol	Chain	Res	Type
16	P	364	GLU
16	P	365	TRP
16	P	367	SER
16	P	377	ARG
16	P	379	LYS
16	P	380	MET
16	P	381	ILE
16	P	384	ASP
16	P	386	MET
16	P	390	GLN
16	P	392	GLU
16	P	394	VAL
16	P	403	ARG
16	P	407	ARG
16	P	410	ASP
16	P	412	ASN
16	P	414	ILE
16	P	415	LEU
16	P	424	VAL
16	P	427	SER
16	P	428	GLU
16	P	433	VAL
16	P	438	TRP
16	P	439	LYS
16	P	442	LEU
16	P	443	ASP
16	P	453	VAL
16	P	455	LYS
16	P	456	VAL
16	P	458	LYS
16	P	461	HIS
16	P	463	LEU
16	P	465	VAL
16	P	468	VAL
16	P	469	TYR
16	P	474	LYS
16	P	480	VAL
16	P	491	SER
16	P	492	LEU
16	P	495	SER
16	P	496	THR
16	P	498	LEU

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Mol	Chain	Res	Type
16	P	500	ILE
16	P	504	THR
16	P	508	ILE
16	P	511	ILE
16	P	531	PHE
16	P	534	VAL
16	P	535	VAL
16	P	538	LEU
16	P	539	VAL
16	P	555	THR
16	P	567	ILE
16	P	573	GLU
16	P	574	TRP
16	P	577	LEU
16	P	583	GLU
16	P	592	LEU
16	P	600	GLU
16	P	604	ILE
16	P	606	ARG
16	P	608	GLN
16	P	609	ASN
16	P	614	GLU
16	P	617	HIS
16	P	625	ASP
16	P	626	LEU
16	P	632	ILE
16	P	635	ASN
16	P	637	LEU
16	P	638	LEU
16	P	643	LYS
16	P	645	LYS
16	P	646	ASP
16	P	647	GLU
16	P	653	SER
16	P	656	HIS
16	P	657	SER
16	P	659	LEU
16	P	660	LYS
16	P	662	LEU
16	P	663	LEU
16	P	664	GLU
16	P	666	SER

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Mol	Chain	Res	Type
16	P	667	ASP
16	P	671	SER
16	P	676	SER
16	P	679	LEU
16	P	692	THR
16	P	693	PHE
16	P	694	ILE
16	P	700	LEU
16	P	703	PHE
16	P	711	LEU
16	P	712	ASP
16	P	713	ILE
16	P	728	GLN
16	P	731	LEU
16	P	736	ILE
16	P	742	TRP
16	P	746	ARG
16	P	749	LYS
16	P	751	SER
16	P	753	PHE
16	P	754	GLU
16	P	762	ARG
16	P	770	ASP
16	P	771	ILE
16	P	772	ILE
16	P	777	MET
17	Q	17	SER
17	Q	21	ARG
17	Q	26	ARG
17	Q	27	ARG
17	Q	94	LYS
17	Q	95	LEU
17	Q	98	HIS
17	Q	101	LYS
17	Q	103	LEU
17	Q	119	LEU
17	Q	138	LEU
17	Q	139	LYS
17	Q	149	GLN
17	Q	150	GLU
17	Q	151	GLU
17	Q	152	LEU

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Mol	Chain	Res	Type
17	Q	154	LEU
17	Q	164	ILE
17	Q	167	LEU
17	Q	169	SER
17	Q	176	VAL
17	Q	178	THR
17	Q	187	THR
17	Q	192	TYR
17	Q	226	LEU
17	Q	229	LYS
17	Q	232	LEU
17	Q	234	CYS
17	Q	241	GLU
17	Q	248	SER
17	Q	252	LEU
17	Q	254	LEU
17	Q	255	LYS
17	Q	256	LEU
17	Q	272	GLN
17	Q	273	VAL
17	Q	280	ASP
17	Q	285	THR
17	Q	286	LEU
17	Q	295	THR
17	Q	297	ARG
17	Q	299	SER
17	Q	301	HIS
17	Q	312	LEU
17	Q	318	LEU
17	Q	321	ASP
17	Q	324	ARG
17	Q	328	LEU
17	Q	337	SER
17	Q	348	ILE
17	Q	363	SER
17	Q	364	SER
17	Q	378	LEU
17	Q	384	GLN
17	Q	412	LYS
17	Q	419	LEU
17	Q	435	GLN
17	Q	436	LEU

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Mol	Chain	Res	Type
17	Q	437	THR
17	Q	444	GLU
17	Q	445	ARG
17	Q	453	PHE
17	Q	478	ARG
17	Q	486	GLN
17	Q	494	SER
17	Q	495	LYS
17	Q	498	LEU
17	Q	502	ILE
17	Q	512	ARG
17	Q	513	MET
17	Q	514	ASN
18	R	1	MET
18	R	4	VAL
18	R	8	LEU
18	R	28	SER
18	R	74	GLN
18	R	80	ARG
18	R	84	TRP
18	R	85	ARG
18	R	87	VAL
18	R	143	THR
18	R	146	SER
18	R	149	LYS
18	R	156	LYS
18	R	158	THR
18	R	160	HIS
18	R	165	ILE
18	R	167	LYS
18	R	168	ILE
18	R	175	ILE
18	R	177	LEU
18	R	178	LEU
18	R	181	THR
18	R	182	LYS
18	R	189	GLN
18	R	202	THR
18	R	206	ARG
18	R	209	ARG
18	R	211	ARG
18	R	212	HIS

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Mol	Chain	Res	Type
18	R	214	VAL
18	R	216	LEU
18	R	230	SER
18	R	231	LEU
18	R	238	THR
18	R	240	ILE
18	R	242	ILE
18	R	245	VAL
18	R	246	GLN
18	R	247	ILE
18	R	249	SER
18	R	250	LEU
18	R	253	ILE
18	R	255	VAL
18	R	257	ILE
18	R	258	LEU
18	R	261	LEU
18	R	264	SER
18	R	272	GLN
18	R	275	CYS
18	R	276	GLN
18	R	282	SER
18	R	294	VAL
18	R	296	PRO
18	R	299	THR
18	R	307	LYS
18	R	308	PHE
18	R	324	MET
18	R	345	LEU
18	R	347	ASP
18	R	348	LYS
18	R	354	LEU
18	R	355	THR
18	R	361	ASP
18	R	365	TRP
18	R	373	LEU
18	R	374	LEU
18	R	375	LYS
18	R	403	GLN
18	R	409	HIS
18	R	410	TYR
18	R	411	VAL

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Mol	Chain	Res	Type
18	R	426	VAL
18	R	427	PRO
18	R	429	ARG
18	R	430	LEU
18	R	437	SER
18	R	440	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (77) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	107	HIS
1	A	383	ASN
1	A	458	GLN
1	A	470	HIS
1	A	489	ASN
1	A	537	GLN
1	A	559	ASN
1	A	560	GLN
1	A	610	ASN
1	A	639	GLN
1	A	730	GLN
1	A	880	GLN
1	A	949	GLN
1	A	1108	HIS
1	A	1314	GLN
1	A	1320	GLN
1	A	1443	GLN
1	A	1447	GLN
1	A	1453	HIS
1	A	1647	ASN
2	B	27	ASN
2	B	101	GLN
2	B	212	ASN
2	B	213	HIS
2	B	254	ASN
2	B	267	ASN
2	B	399	HIS
2	B	422	GLN
2	B	504	HIS
2	B	543	ASN
2	B	555	GLN
2	B	646	HIS

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Mol	Chain	Res	Type
2	B	695	ASN
2	B	816	ASN
2	B	952	HIS
2	B	1066	HIS
2	B	1157	GLN
2	B	1165	ASN
2	B	1171	ASN
3	C	161	HIS
3	C	237	GLN
3	C	297	HIS
4	D	88	GLN
7	G	26	ASN
7	G	32	ASN
7	G	237	HIS
8	H	11	GLN
8	H	52	GLN
9	I	44	ASN
11	K	64	GLN
11	K	106	GLN
12	L	53	HIS
14	N	41	ASN
14	N	51	GLN
14	N	85	HIS
14	N	128	ASN
15	O	77	GLN
15	O	117	GLN
15	O	173	HIS
15	O	362	ASN
15	O	391	GLN
15	O	438	GLN
15	O	472	HIS
15	O	507	GLN
16	P	222	GLN
16	P	223	ASN
16	P	348	HIS
16	P	554	ASN
16	P	665	ASN
17	Q	145	ASN
17	Q	157	HIS
17	Q	368	GLN
17	Q	507	ASN
18	R	25	ASN

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Mol	Chain	Res	Type
18	R	184	ASN
18	R	207	ASN
18	R	298	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
19	S	4/5 (80%)	1 (25%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
19	S	3	G

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 8 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
24	SO4	B	1301	-	4,4,4	0.17	0	6,6,6	0.07	0

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.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	B	1301	SO4	2	0

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
17	Q	2
18	R	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	R	206:ARG	C	207:ASN	N	2.76
1	Q	323:ASP	C	324:ARG	N	1.79
1	Q	356:VAL	C	357:TYR	N	1.17

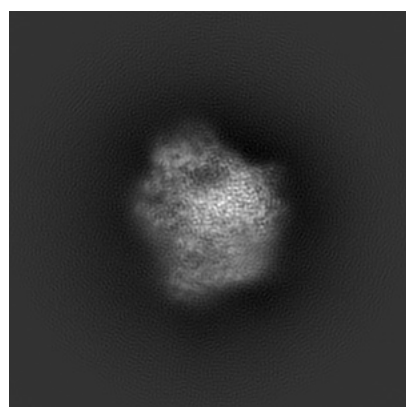
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3593. These allow visual inspection of the internal detail of the map and identification of artifacts.

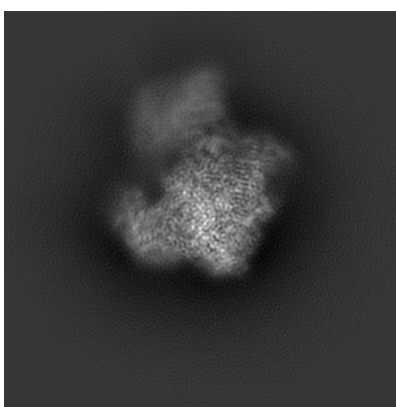
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

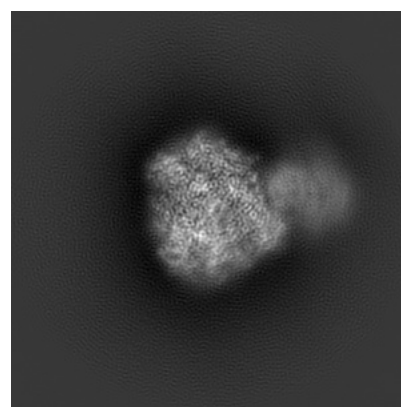
6.1.1 Primary map



X



Y

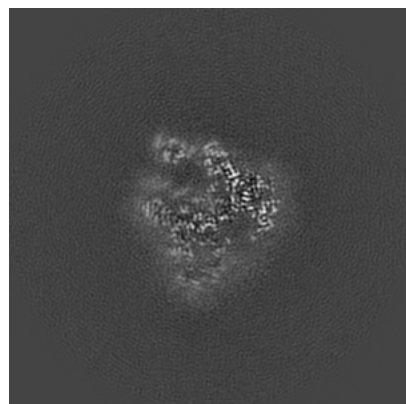


Z

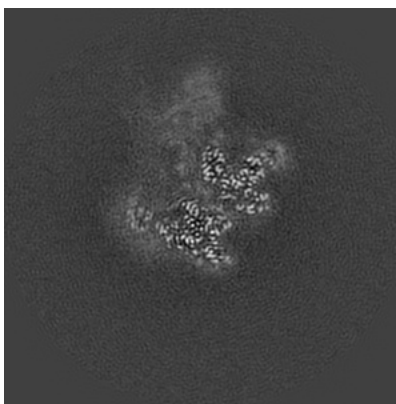
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

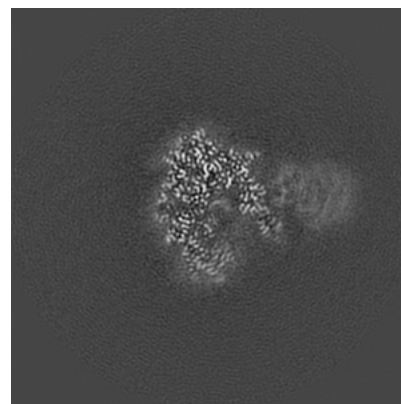
6.2.1 Primary map



X Index: 165



Y Index: 165

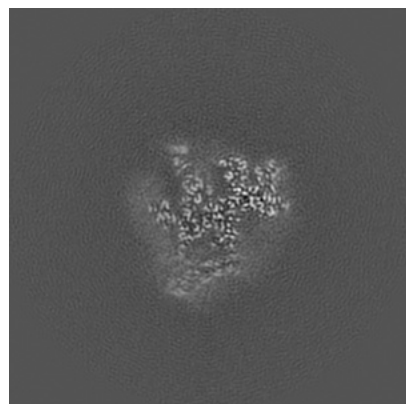


Z Index: 165

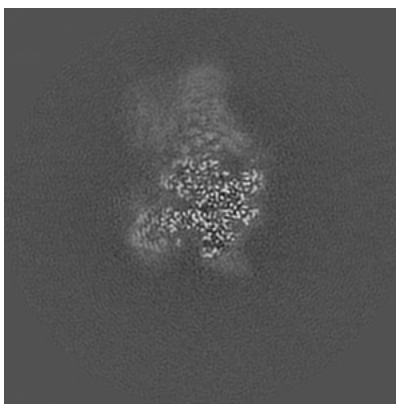
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

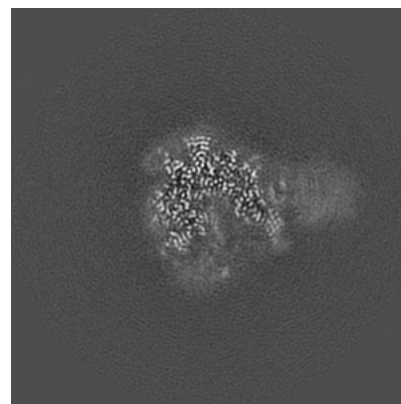
6.3.1 Primary map



X Index: 157



Y Index: 182

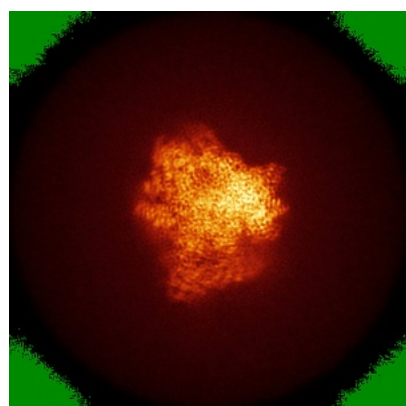


Z Index: 172

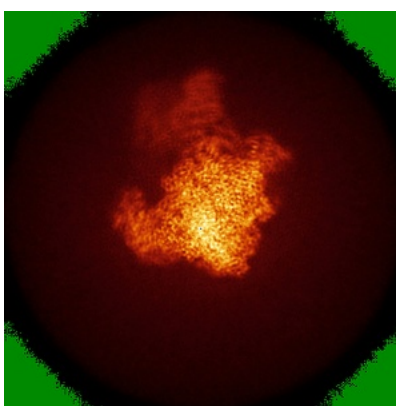
The images above show the largest variance slices of the map in three orthogonal directions.

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

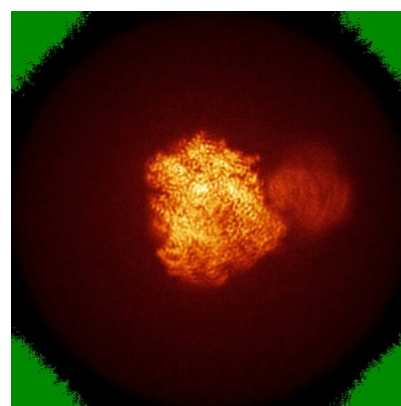
6.4.1 Primary map



X



Y

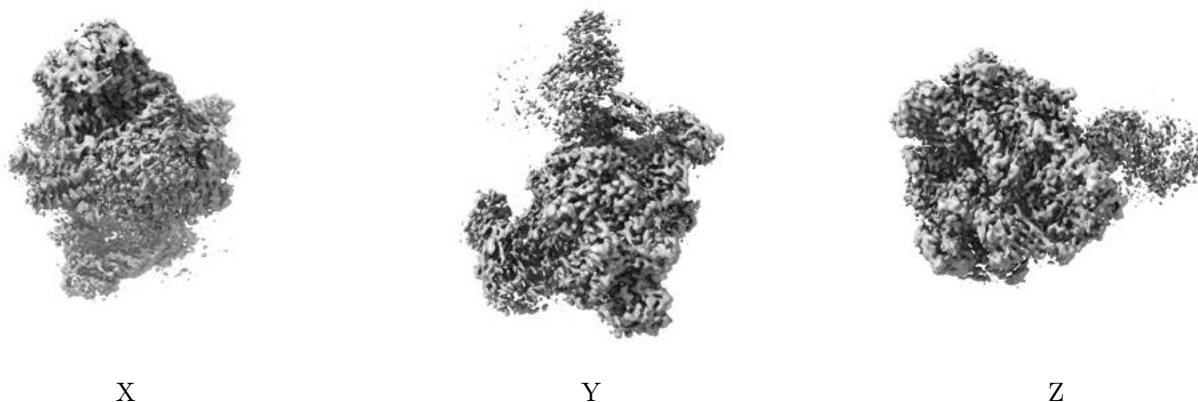


Z

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 0.065. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

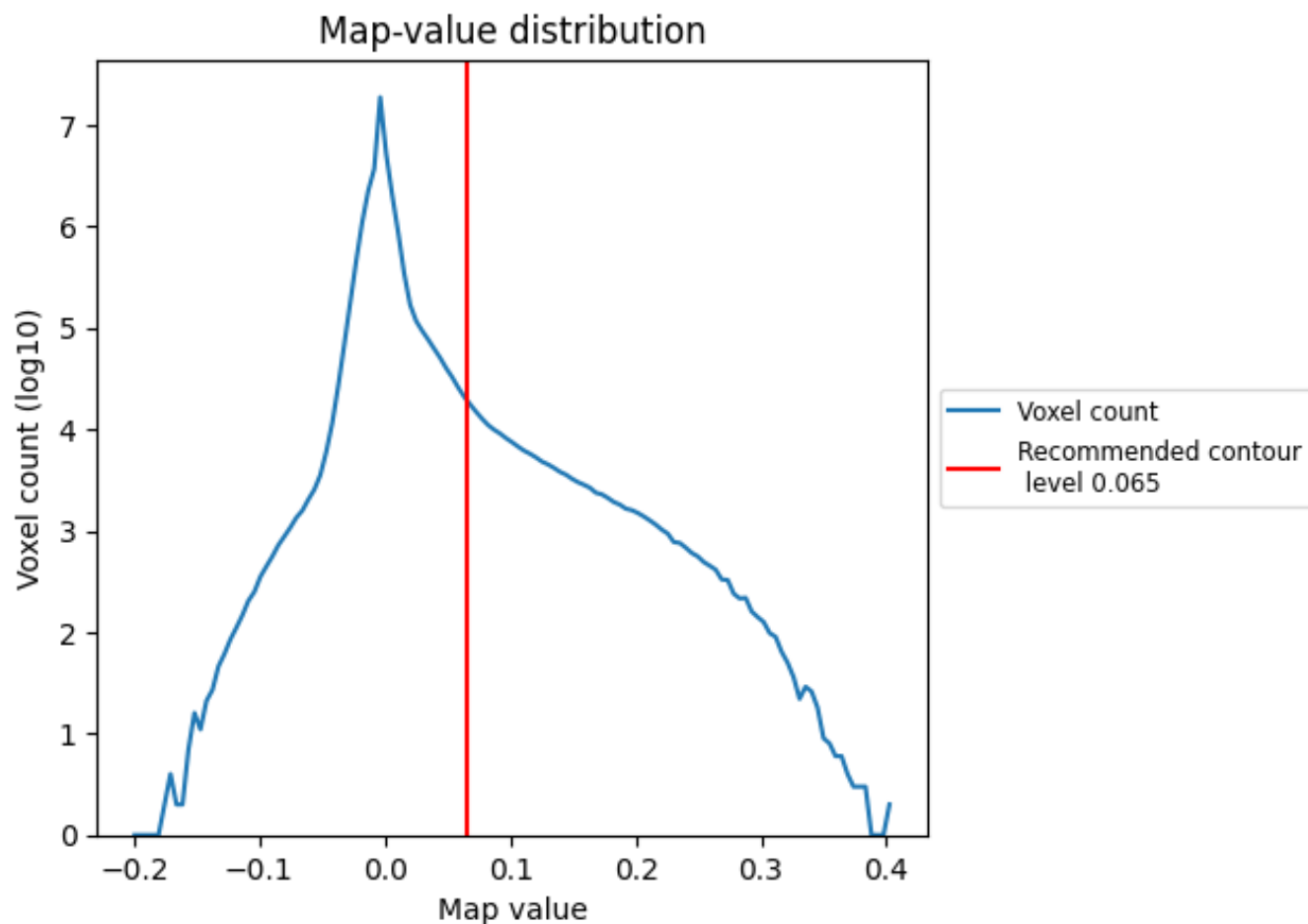
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

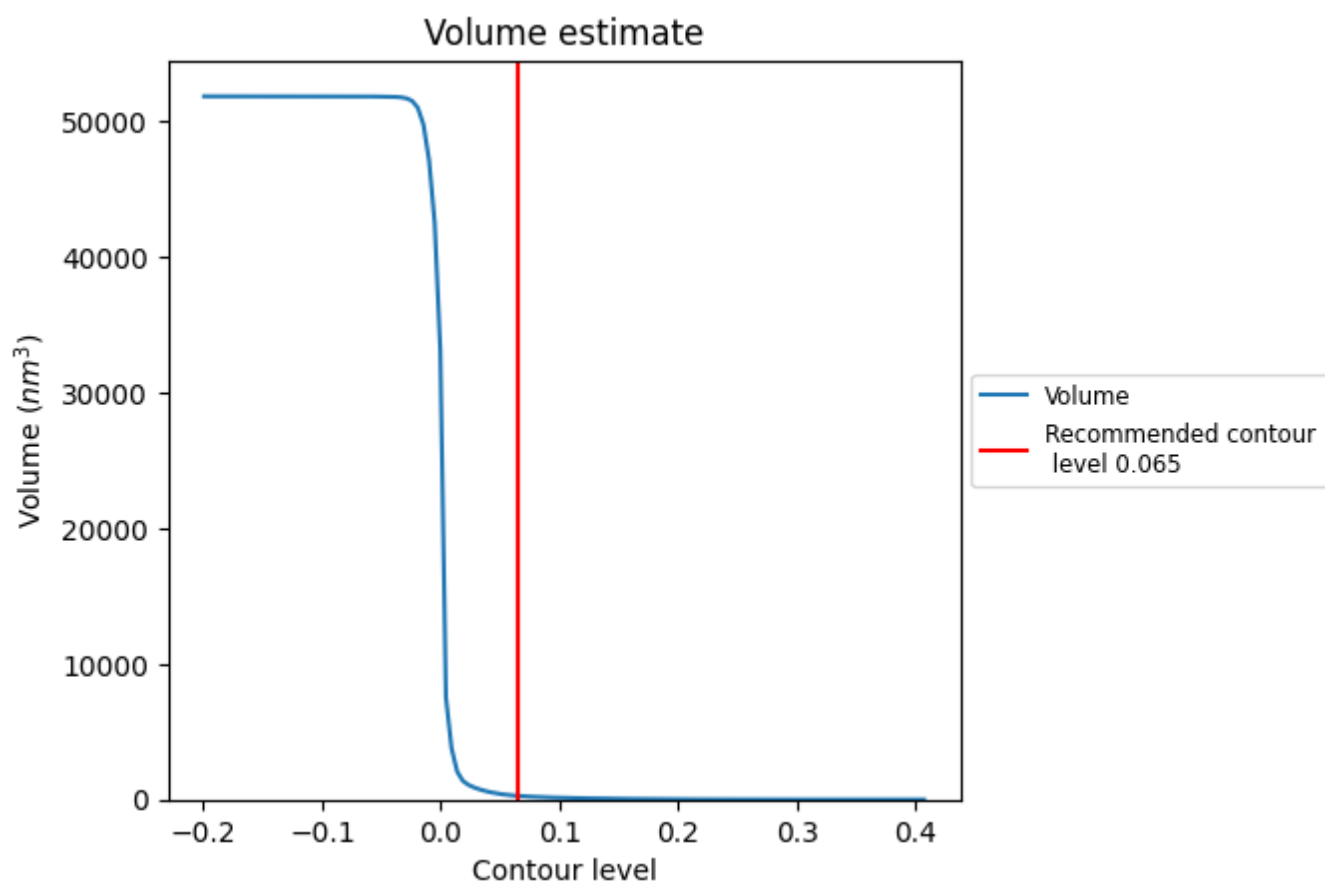
This section contains the results of statistical analysis of the map.

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.

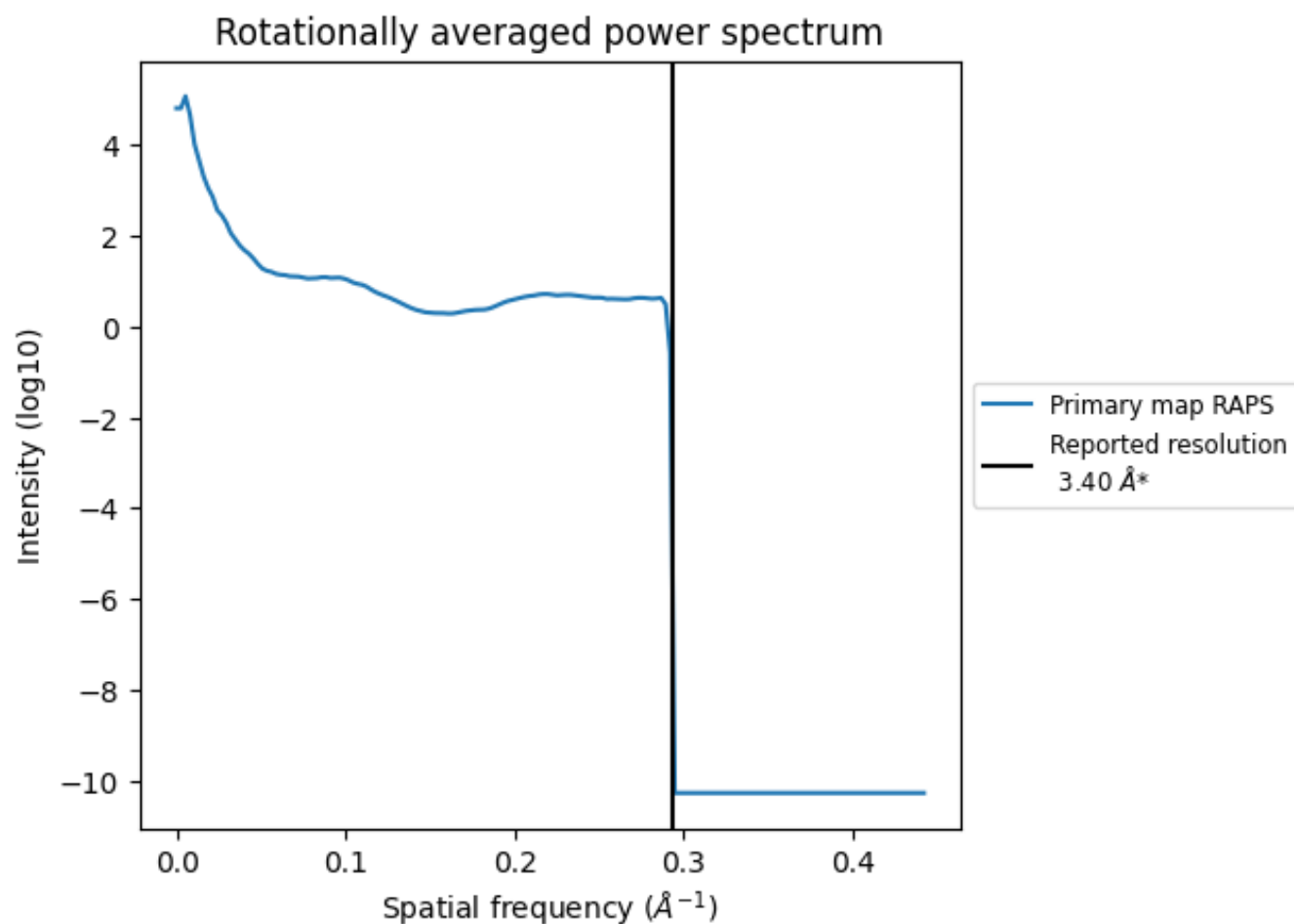
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 273 nm³; this corresponds to an approximate mass of 246 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 0.294 Å⁻¹

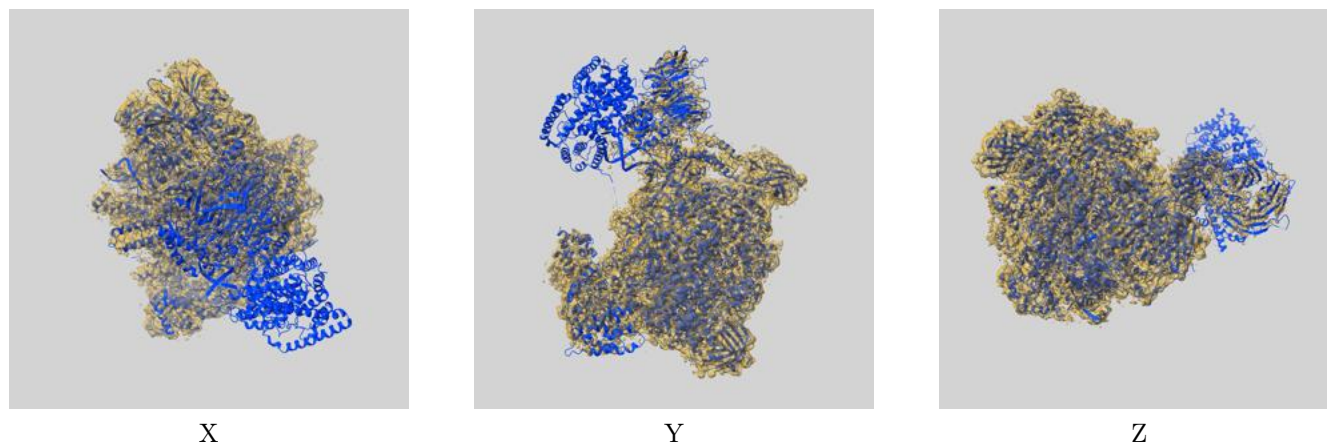
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

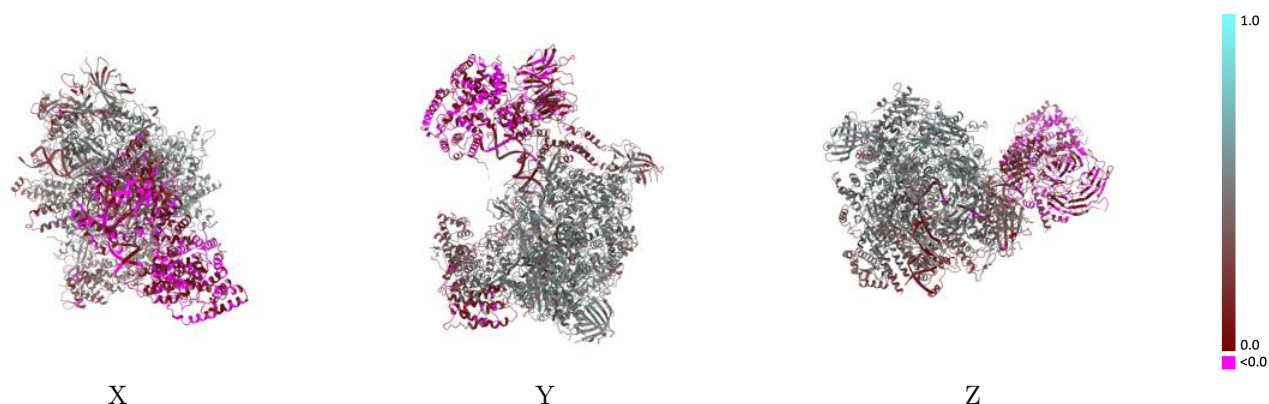
This section contains information regarding the fit between EMDB map EMD-3593 and PDB model 5N61. Per-residue inclusion information can be found in [section 3](#) on [page 9](#).

9.1 Map-model overlay [i](#)



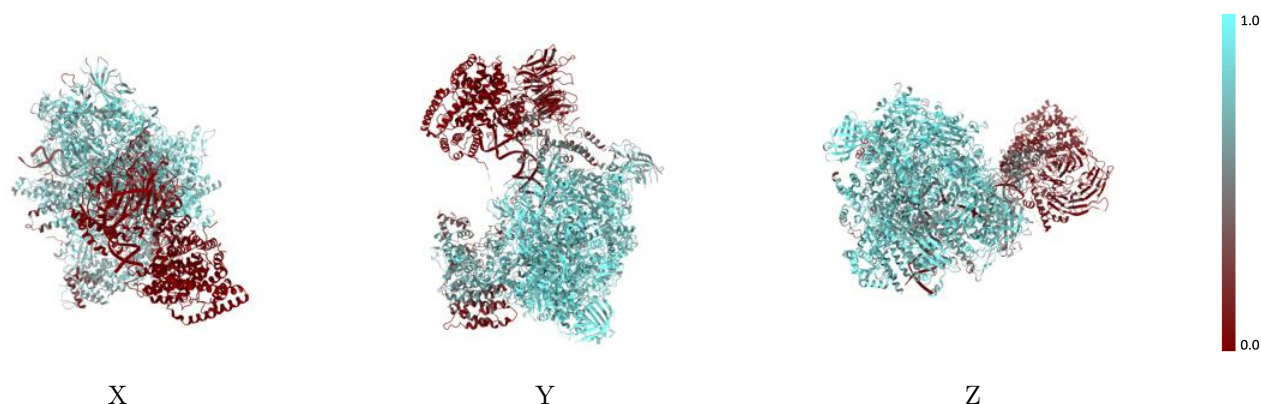
The images above show the 3D surface view of the map at the recommended contour level 0.065 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



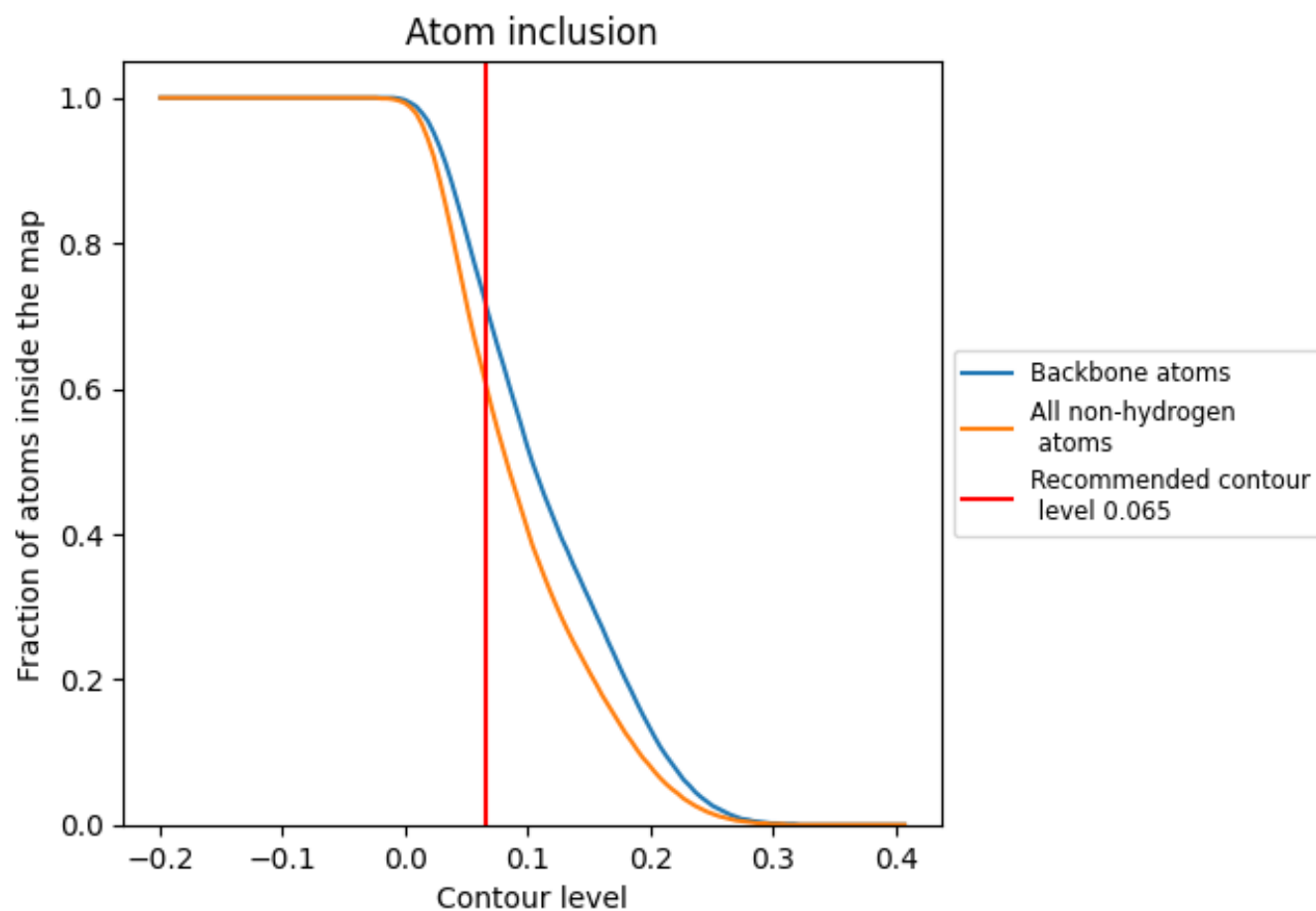
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.065).













































9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 61% 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 (0.065) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6110	 0.3430
A	 0.8020	 0.4510
B	 0.8260	 0.4740
C	 0.8760	 0.4830
D	 0.7380	 0.4080
E	 0.8300	 0.4280
F	 0.7960	 0.4770
G	 0.7100	 0.3960
H	 0.8800	 0.4860
I	 0.6880	 0.3020
J	 0.8970	 0.5110
K	 0.8430	 0.4840
L	 0.8380	 0.4670
M	 0.6350	 0.3390
N	 0.6270	 0.3470
O	 0.4820	 0.2610
P	 0.0550	 0.0410
Q	 0.0490	 0.0480
R	 0.2270	 0.1240
S	 0.4720	 0.2280
T	 0.2680	 0.1150
U	 0.2160	 0.1170

