Full wwPDB EM Validation Report ⓘ

Feb 26, 2024 – 03:44 PM EST

PDB ID	:	8G9U
EMDB ID	:	EMD-29879
Title	:	Exploiting Activation and Inactivation Mechanisms in Type I-C CRISPR-Cas3 for Genome Editing Applications
Authors	:	Hu, C.; Nam, K.H.; Ke, A.
Deposited on	:	2023-02-22
Resolution	:	3.00 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

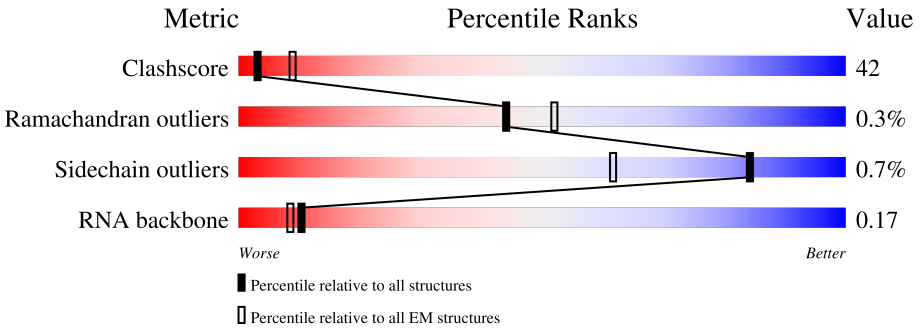
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	P	771	39% 58%
2	A	283	40% 58%
2	B	283	35% 63%
2	C	283	31% 68%
2	D	283	35% 64%
2	E	283	38% 61%
2	F	283	42% 53%

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Mol	Chain	Length	Quality of chain
2	M	283	35% 58% 7%
3	G	124	31% 62% 6%
3	I	124	31% 64% 6%
3	J	124	31% 64% 6%
4	H	582	38% 60%
5	K	43	19% 72% 9%
6	L	53	26% 72%
7	N	205	36% 63%
8	O	20	20% 80%
9	Q	20	35% 65%

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
11	PO4	P	803	-	-	X	-
11	PO4	P	804	-	-	X	-
11	PO4	Q	101	-	-	X	-

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 33546 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 Cas3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	P	757	Total	C	N	O	S	1	0
			5855	3716	1037	1084	18		

- Molecule 2 is a protein called CRISPR-associated protein, Csd2 family.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	283	Total	C	N	O	S	0	0
			2261	1408	406	436	11		
2	B	283	Total	C	N	O	S	0	0
			2261	1408	406	436	11		
2	D	283	Total	C	N	O	S	0	0
			2261	1408	406	436	11		
2	C	283	Total	C	N	O	S	0	0
			2261	1408	406	436	11		
2	E	283	Total	C	N	O	S	0	0
			2261	1408	406	436	11		
2	F	271	Total	C	N	O	S	0	0
			2173	1360	391	411	11		
2	M	264	Total	C	N	O	S	0	0
			2110	1318	379	402	11		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	284	GLY	-	expression tag	UNP D0W8X6
B	284	GLY	-	expression tag	UNP D0W8X6
D	284	GLY	-	expression tag	UNP D0W8X6
C	284	GLY	-	expression tag	UNP D0W8X6
E	284	GLY	-	expression tag	UNP D0W8X6
F	284	GLY	-	expression tag	UNP D0W8X6
M	284	GLY	-	expression tag	UNP D0W8X6

- Molecule 3 is a protein called Phage associated protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	124	Total	C	N	O	S	0	0
			1007	646	180	179	2		
3	G	124	Total	C	N	O	S	0	0
			1007	646	180	179	2		
3	J	124	Total	C	N	O	S	0	0
			1007	646	180	179	2		

- Molecule 4 is a protein called CRISPR-associated protein, Csd1 family.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	582	Total	C	N	O	S	0	0
			4555	2889	800	849	17		

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	190	ALA	VAL	conflict	UNP D0W8X5
H	239	ALA	ILE	conflict	UNP D0W8X5
H	242	ILE	VAL	conflict	UNP D0W8X5
H	260	GLY	SER	conflict	UNP D0W8X5
H	271	THR	ALA	conflict	UNP D0W8X5
H	296	ASN	LYS	conflict	UNP D0W8X5
H	299	ALA	GLU	conflict	UNP D0W8X5
H	306	ALA	THR	conflict	UNP D0W8X5
H	317	CYS	GLN	conflict	UNP D0W8X5
H	322	GLU	LYS	conflict	UNP D0W8X5
H	323	ASP	GLU	conflict	UNP D0W8X5

- Molecule 5 is a RNA chain called crRNA (43-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	K	43	Total	C	N	O	P	0	0
			916	408	161	304	43		

- Molecule 6 is a DNA chain called Traget strand DNA (53-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	L	53	Total	C	N	O	P	0	0
			1093	515	211	314	53		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	7	DA	-	expression tag	GB 1394359882
L	8	DG	-	expression tag	GB 1394359882

- Molecule 7 is a protein called pre-crRNA processing endonuclease.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	N	205	Total	C	N	O	S	0	0
			1674	1067	289	306	12		

- Molecule 8 is a DNA chain called proximal nontarget strand DNA (5'-D(P*AP*TP*GP*AP*AP*CP*TP*TP*CP*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
8	O	20	Total	C	N	O	P	0	0
			414	198	87	109	20		

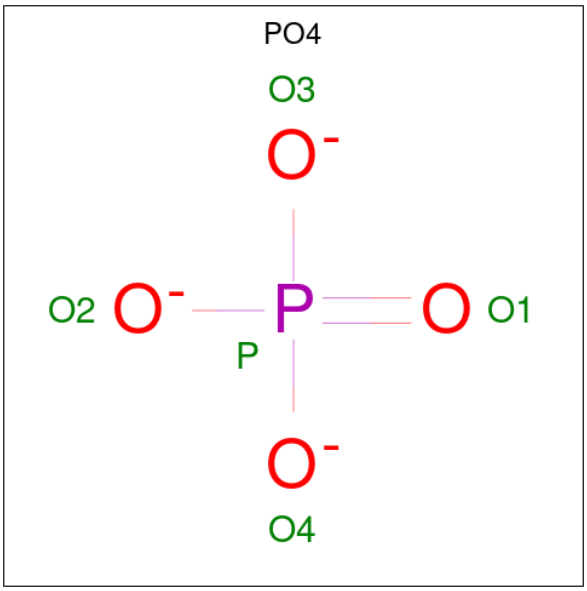
- Molecule 9 is a DNA chain called Distal nontarget DNA (5'-D(P*TP*TP*AP*TP*AP*TP*TP*AP*AP*TP*AP*TP*TP*AP*TP*AP*TP*TP*TP*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
9	Q	20	Total	C	N	O	P	0	0
			408	200	64	124	20		

- Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
10	P	2	Total	Mg	0
			2	2	

- Molecule 11 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P) (labeled as "Ligand of Interest" by depositor).



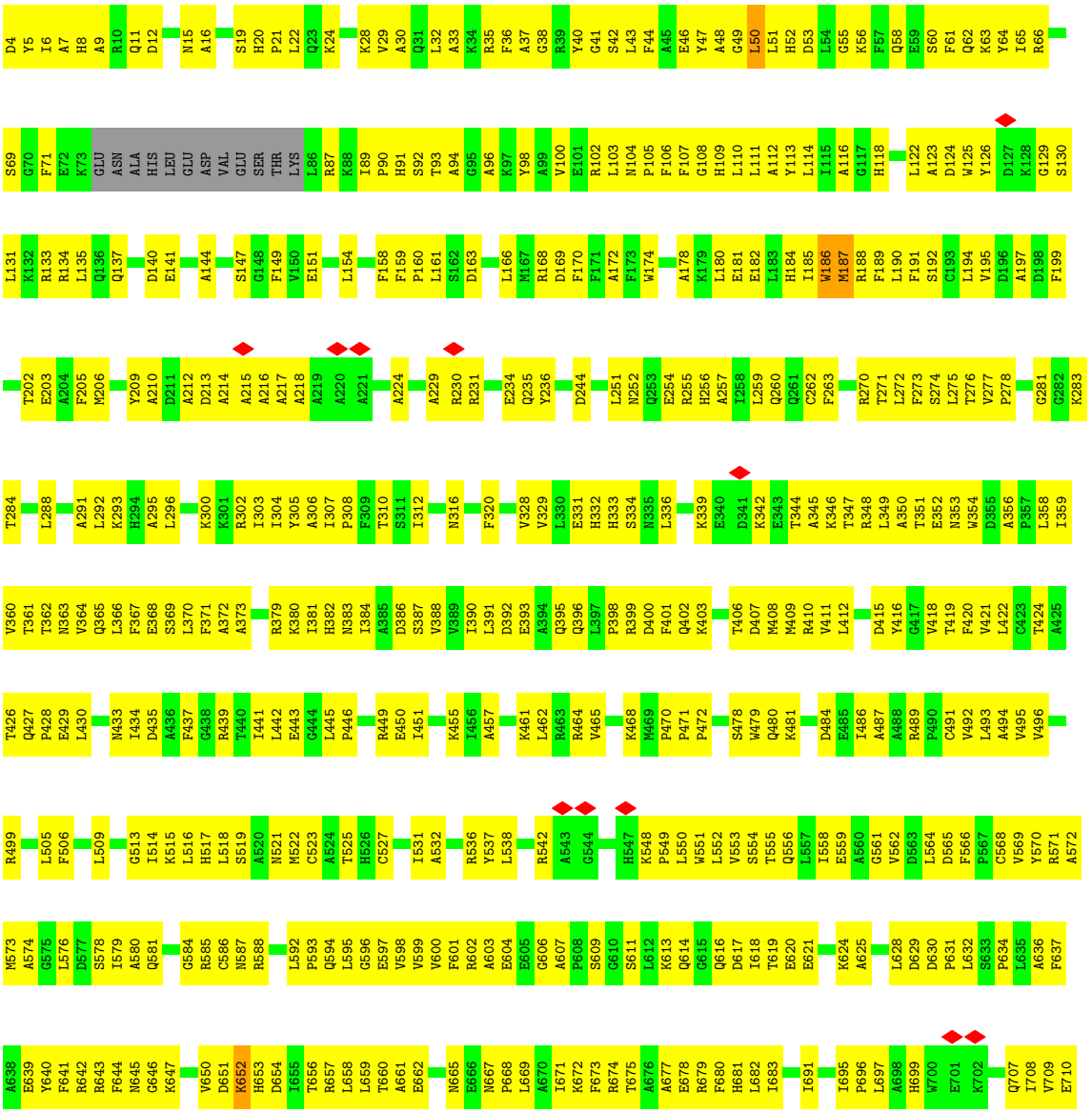
Mol	Chain	Residues	Atoms	AltConf
11	P	1	Total O P 5 4 1	0
11	P	1	Total O P 5 4 1	0
11	O	1	Total O P 5 4 1	0
11	Q	1	Total O P 5 4 1	0

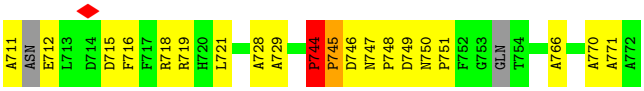
3 Residue-property plots (i)

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

- Molecule 1: Cas3

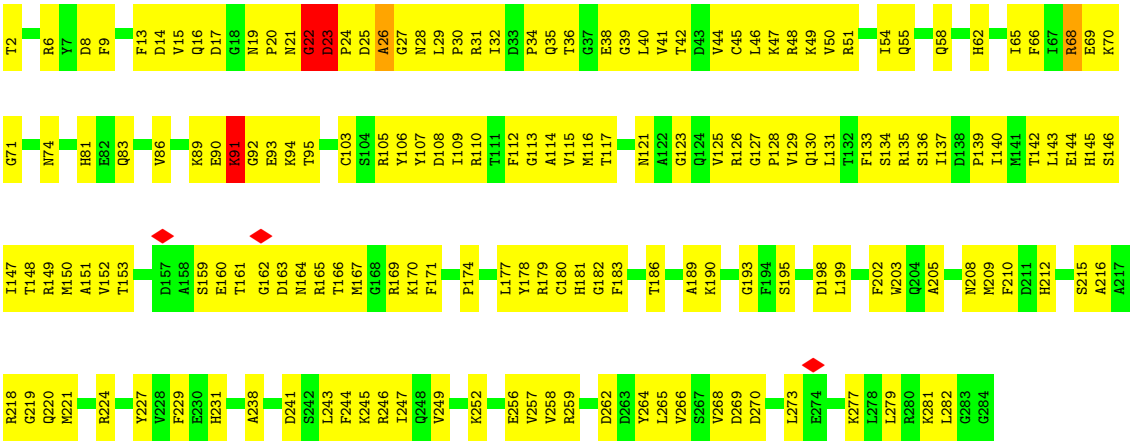
Chain P:





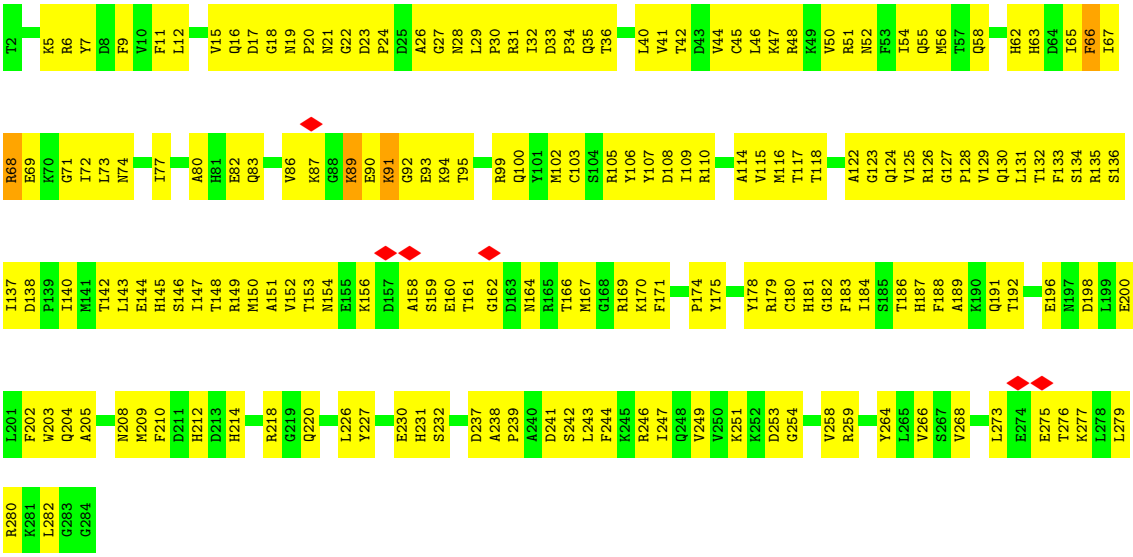
• Molecule 2: CRISPR-associated protein, Csd2 family

Chain A:



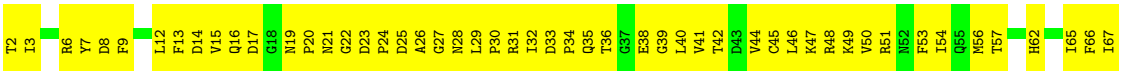
• Molecule 2: CRISPR-associated protein, Csd2 family

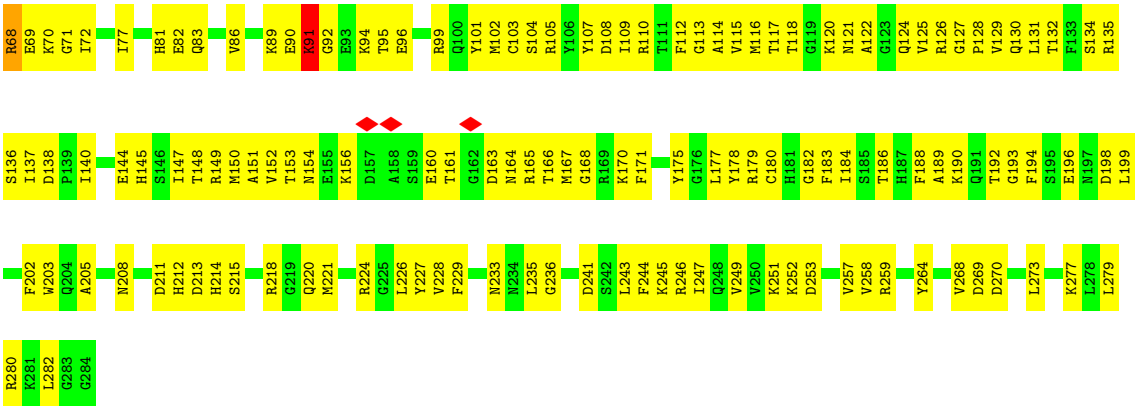
Chain B:



• Molecule 2: CRISPR-associated protein, Csd2 family

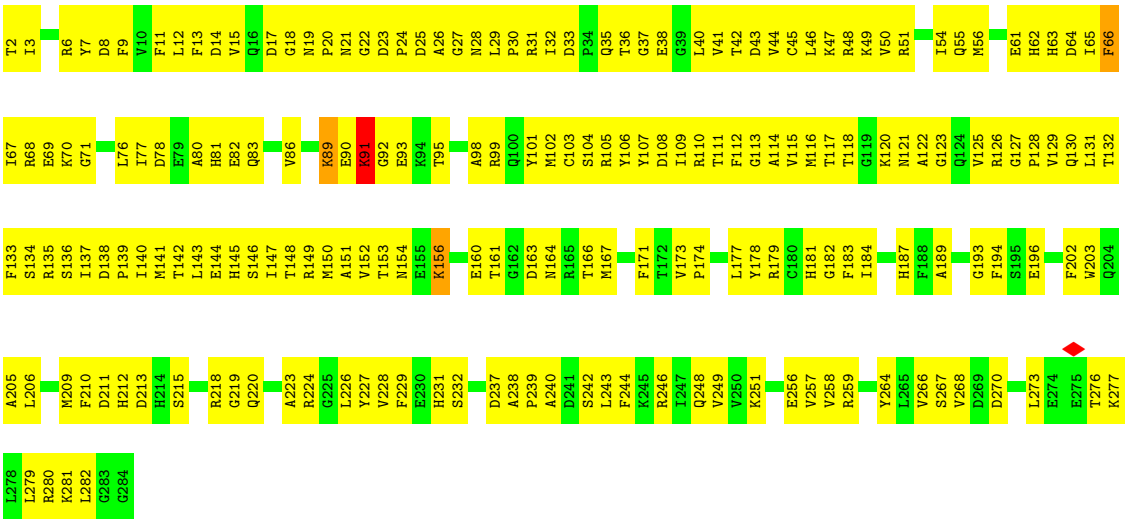
Chain D:





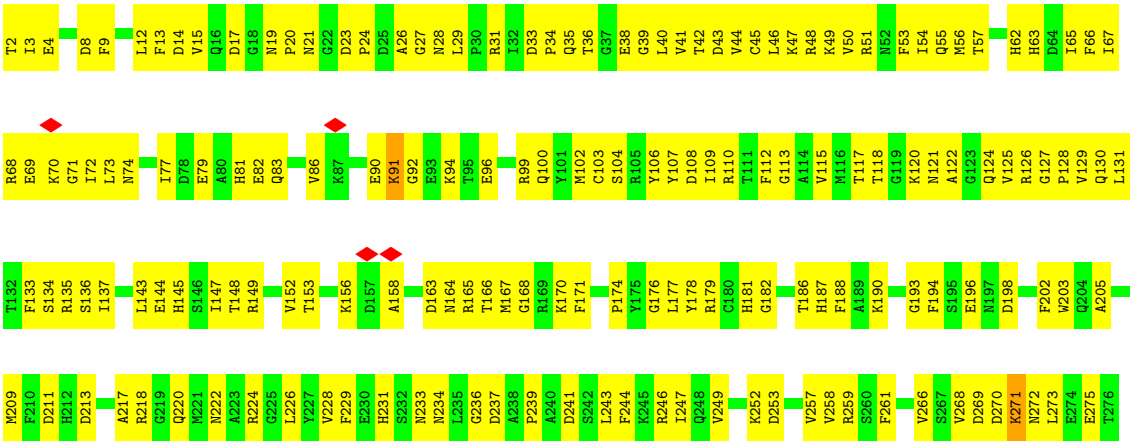
• Molecule 2: CRISPR-associated protein, Csd2 family

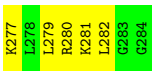
Chain C:



• Molecule 2: CRISPR-associated protein, Csd2 family

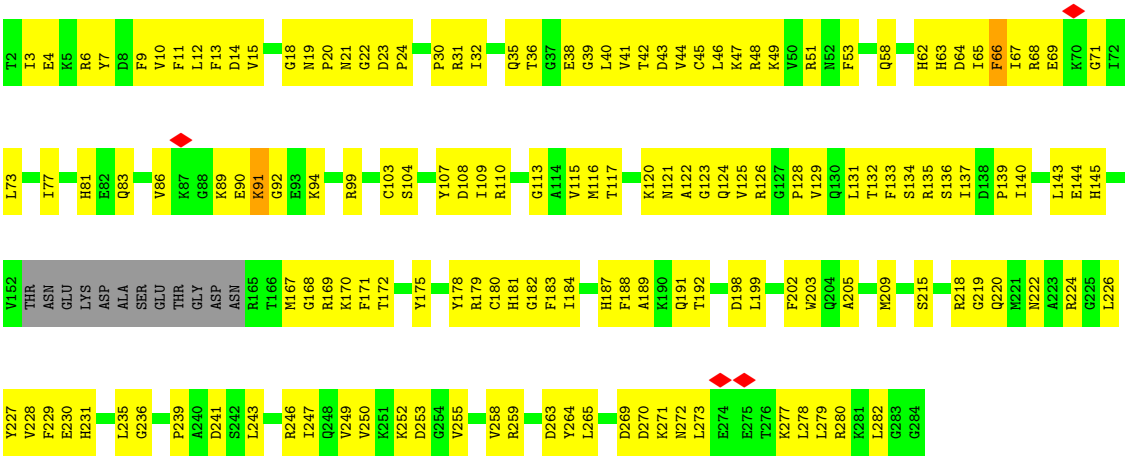
Chain E:





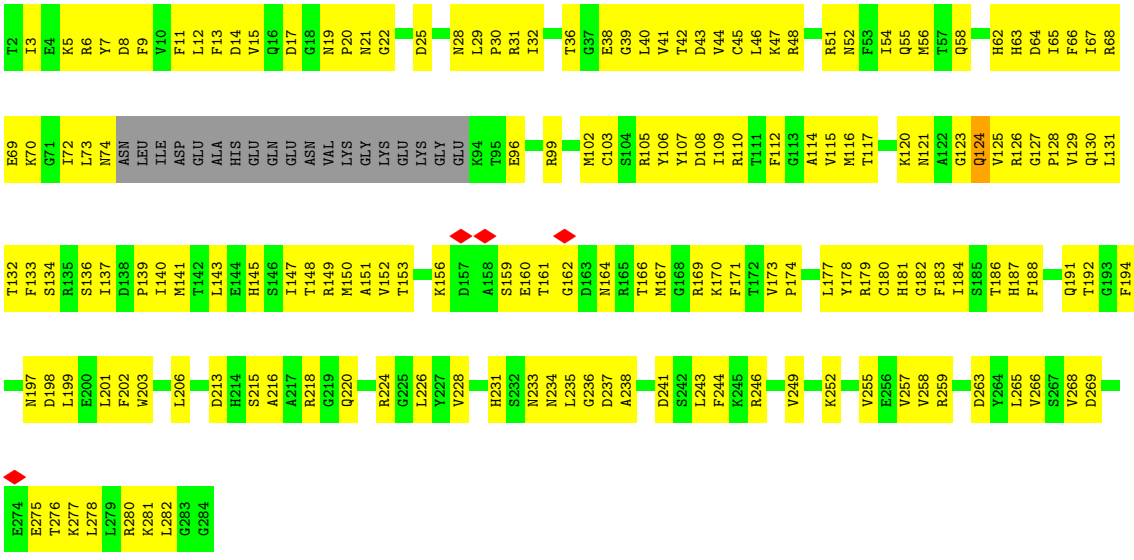
• Molecule 2: CRISPR-associated protein, Csd2 family

Chain F:



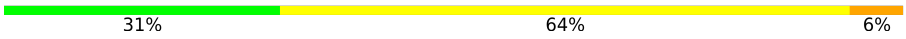
• Molecule 2: CRISPR-associated protein, Csd2 family

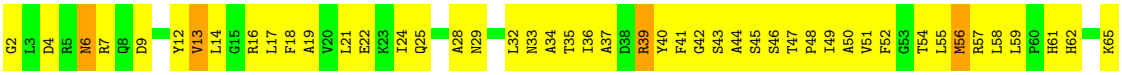
Chain M:



• Molecule 3: Phage associated protein

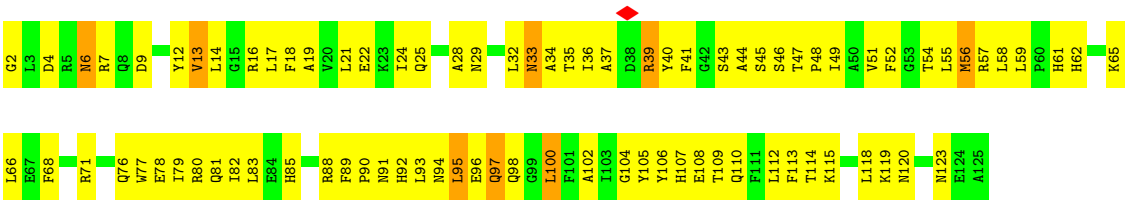
Chain I:





• Molecule 3: Phage associated protein

Chain G:

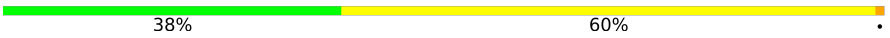


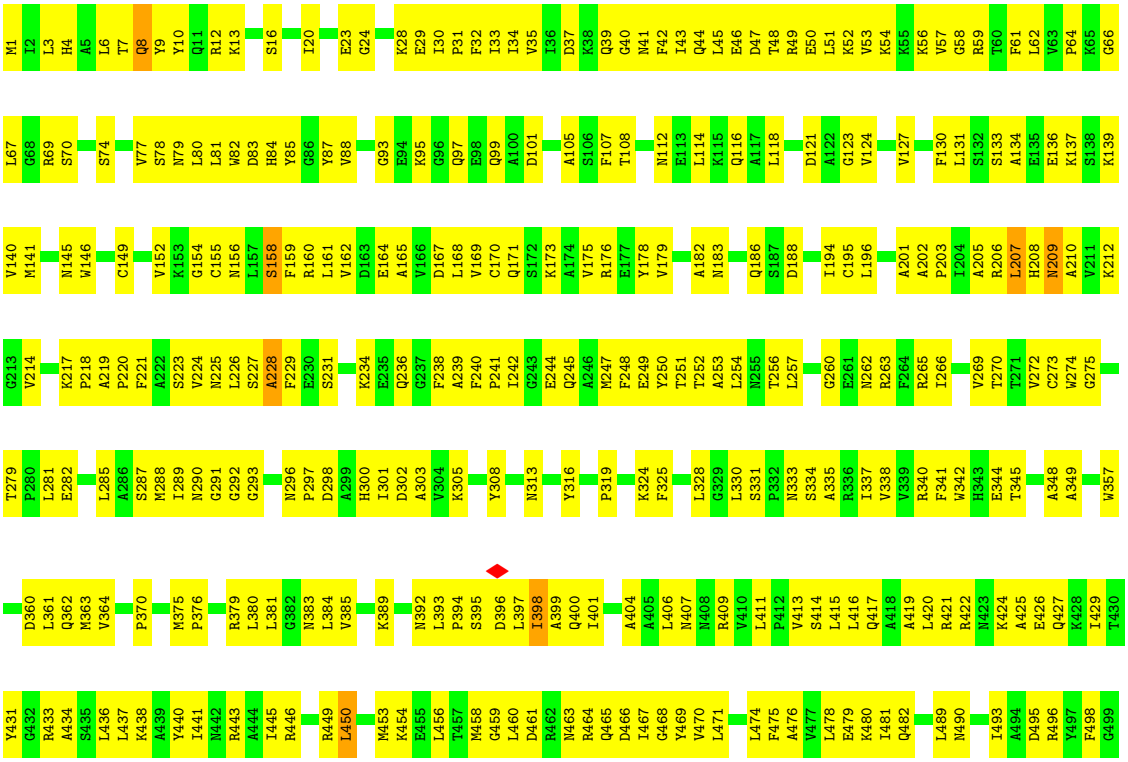
• Molecule 3: Phage associated protein

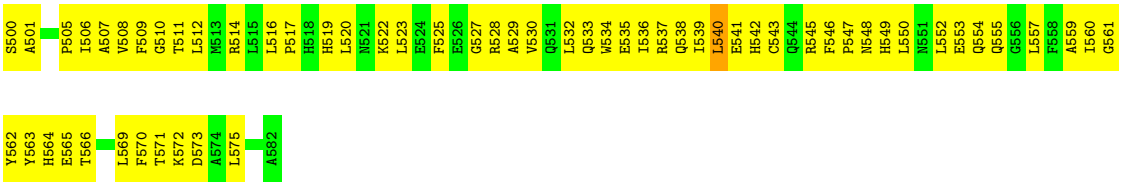
Chain J:

• Molecule 4: CRISPR-associated protein, Csd1 family

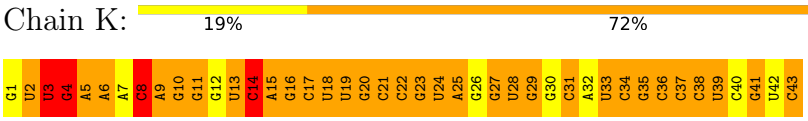
Chain H:



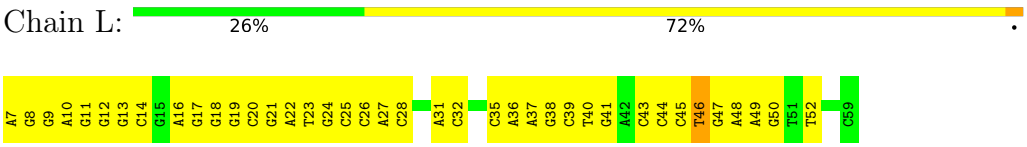




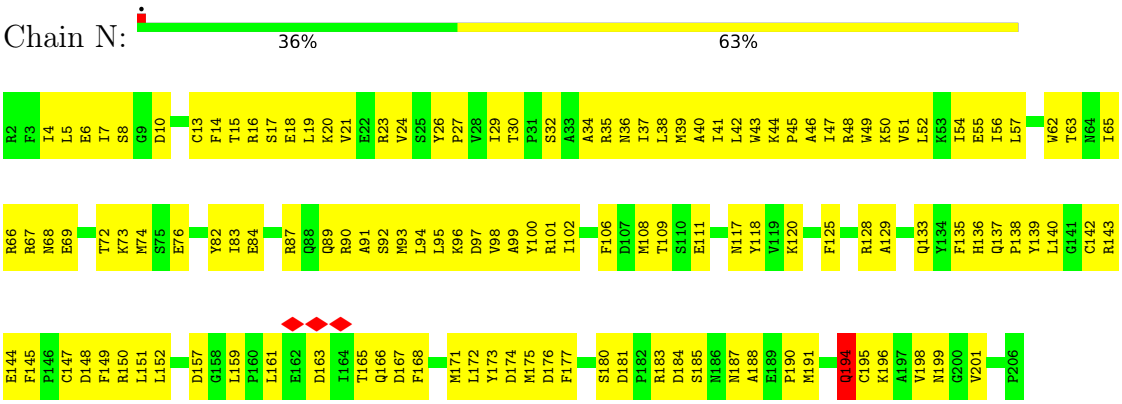
• Molecule 5: crRNA (43-MER)



• Molecule 6: Traget strand DNA (53-MER)



• Molecule 7: pre-crRNA processing endonuclease



• Molecule 8: proximal nontarget strand DNA (5'-D(P*AP*TP*GP*AP*AP*CP*TP*TP*CP*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')

• Molecule 9: Distal nontarget DNA (5'-D(P*TP*TP*AP*TP*AP*TP*TP*AP*AP*TP*AP*TP*TP*AP*TP*AP*TP*TP*TP*A)-3')

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	307088	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	67000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.947	Depositor
Minimum map value	-0.276	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.026	Depositor
Recommended contour level	0.111	Depositor
Map size (Å)	381.30002, 381.30002, 381.30002	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.271, 1.271, 1.271	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, 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	P	0.38	1/5983 (0.0%)	0.56	2/8111 (0.0%)
2	A	0.63	0/2303	0.69	2/3101 (0.1%)
2	B	0.61	0/2303	0.65	0/3101
2	C	0.61	0/2303	0.63	0/3101
2	D	0.62	0/2303	0.65	0/3101
2	E	0.55	0/2303	0.62	0/3101
2	F	0.40	0/2214	0.56	0/2979
2	M	0.58	0/2150	0.61	0/2896
3	G	0.58	0/1030	0.67	1/1392 (0.1%)
3	I	0.58	0/1030	0.67	1/1392 (0.1%)
3	J	0.58	0/1030	0.67	1/1392 (0.1%)
4	H	0.53	0/4644	0.64	2/6277 (0.0%)
5	K	1.20	0/1022	1.17	9/1591 (0.6%)
6	L	1.26	1/1228 (0.1%)	0.91	0/1894
7	N	0.51	0/1712	0.64	1/2307 (0.0%)
8	O	0.78	0/468	0.83	0/719
9	Q	0.78	0/455	1.04	0/700
All	All	0.61	2/34481 (0.0%)	0.68	19/47155 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	P	0	4
2	A	0	2
2	B	0	2
2	C	0	2
2	D	0	1
2	E	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	F	0	1
2	M	0	1
3	G	0	1
3	I	0	1
3	J	0	1
4	H	0	5
7	N	0	1
All	All	0	23

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	186	TRP	CB-CG	-5.91	1.39	1.50
6	L	46	DT	C3'-O3'	-5.64	1.36	1.44

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	22	GLY	C-N-CA	-7.91	101.94	121.70
5	K	14	C	N1-C2-O2	7.54	123.42	118.90
2	A	23	ASP	CB-CG-OD2	7.07	124.66	118.30
5	K	28	U	O5'-P-OP2	-7.00	99.40	105.70
5	K	8	C	N1-C2-O2	6.99	123.09	118.90
5	K	14	C	N3-C2-O2	-6.74	117.18	121.90
5	K	8	C	N3-C2-O2	-6.47	117.37	121.90
4	H	540	LEU	CB-CG-CD1	-6.21	100.44	111.00
5	K	3	U	N3-C2-O2	-6.16	117.89	122.20
5	K	3	U	C2-N1-C1'	6.08	125.00	117.70
1	P	187	MET	CG-SD-CE	-5.92	90.72	100.20
5	K	4	G	P-O3'-C3'	5.80	126.66	119.70
4	H	207	LEU	CB-CG-CD1	-5.72	101.28	111.00
7	N	195	CYS	N-CA-C	-5.62	95.83	111.00
5	K	3	U	N1-C2-O2	5.61	126.72	122.80
1	P	50	LEU	CA-CB-CG	5.55	128.06	115.30
3	J	95	LEU	CB-CG-CD2	-5.08	102.37	111.00
3	I	95	LEU	CB-CG-CD2	-5.08	102.37	111.00
3	G	95	LEU	CB-CG-CD2	-5.07	102.38	111.00

There are no chirality outliers.

All (23) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	22	GLY	Peptide
2	A	26	ALA	Peptide
2	B	66	PHE	Peptide
2	B	89	LYS	Peptide
2	C	66	PHE	Peptide
2	C	89	LYS	Peptide
2	D	66	PHE	Peptide
2	E	66	PHE	Peptide
2	F	66	PHE	Peptide
3	G	56	MET	Peptide
4	H	158	SER	Peptide
4	H	209	ASN	Peptide
4	H	228	ALA	Peptide
4	H	450	LEU	Peptide
4	H	8	GLN	Peptide
3	I	56	MET	Peptide
3	J	56	MET	Peptide
2	M	124	GLN	Peptide
7	N	194	GLN	Peptide
1	P	606	GLY	Peptide
1	P	652	LYS	Peptide
1	P	654	ASP	Peptide
1	P	744	PRO	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	P	5855	0	5783	460	0
2	A	2261	0	2193	229	0
2	B	2261	0	2193	228	0
2	C	2261	0	2193	233	0
2	D	2261	0	2193	227	0
2	E	2261	0	2193	212	0
2	F	2173	0	2120	161	0
2	M	2110	0	2050	220	0
3	G	1007	0	992	112	0
3	I	1007	0	992	126	0
3	J	1007	0	992	138	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	4555	0	4558	418	0
5	K	916	0	464	172	0
6	L	1093	0	592	96	0
7	N	1674	0	1663	173	0
8	O	414	0	224	24	0
9	Q	408	0	233	20	0
10	P	2	0	0	0	0
11	O	5	0	0	1	0
11	P	10	0	0	14	0
11	Q	5	0	0	2	0
All	All	33546	0	31628	2726	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 42.

All (2726) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:56:LYS:HZ3	11:P:804:PO4:P	1.75	1.08
4:H:370:PRO:HB2	11:Q:101:PO4:O2	1.52	1.08
1:P:56:LYS:NZ	11:P:804:PO4:O1	1.94	0.99
1:P:180:LEU:HD21	4:H:289:ILE:HG23	1.46	0.96
2:C:126:ARG:HH21	5:K:14:C:H41	1.13	0.95
2:E:51:ARG:NE	2:E:108:ASP:OD1	1.99	0.94
2:E:205:ALA:O	2:E:209:MET:HB3	1.67	0.94
1:P:69:SER:OG	11:P:803:PO4:O4	1.83	0.93
3:I:113:PHE:HB2	3:J:80:ARG:HH12	1.32	0.93
1:P:56:LYS:NZ	11:P:804:PO4:P	2.40	0.93
1:P:56:LYS:NZ	11:P:804:PO4:O4	2.01	0.93
3:I:80:ARG:HH12	3:G:113:PHE:HB2	1.35	0.91
2:F:205:ALA:O	2:F:209:MET:HB3	1.70	0.90
4:H:422:ARG:NH1	6:L:36:DA:OP1	2.04	0.90
4:H:67:LEU:H	4:H:79:ASN:HD21	1.16	0.88
2:A:15:VAL:HG11	2:A:20:PRO:HG3	1.55	0.88
4:H:385:VAL:HG11	4:H:389:LYS:HA	1.55	0.88
2:B:129:VAL:HG22	2:B:184:ILE:HG12	1.55	0.88
4:H:231:SER:HB3	7:N:20:LYS:HE3	1.56	0.88
2:B:205:ALA:O	2:B:209:MET:HB3	1.75	0.87
1:P:65:ILE:HD11	11:P:803:PO4:O1	1.73	0.87
5:K:27:G:N2	6:L:28:DC:O2	2.08	0.87
2:E:15:VAL:HG11	2:E:20:PRO:HG3	1.56	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:45:CYS:SG	2:E:49:LYS:NZ	2.48	0.87
2:D:68:ARG:HD3	2:D:69:GLU:H	1.40	0.86
3:J:33:ASN:HD21	6:L:26:DC:H3'	1.38	0.86
2:D:110:ARG:NE	2:D:198:ASP:OD2	2.08	0.85
2:E:246:ARG:HE	2:E:273:LEU:HD23	1.39	0.85
5:K:15:A:N6	6:L:40:DT:O4	2.09	0.85
2:F:24:PRO:HB3	2:F:31:ARG:HG3	1.56	0.85
2:D:15:VAL:HG11	2:D:20:PRO:HG3	1.58	0.85
2:D:21:ASN:ND2	5:K:33:U:OP1	2.10	0.85
2:C:205:ALA:O	2:C:209:MET:HB3	1.74	0.85
2:B:68:ARG:HG3	2:B:69:GLU:H	1.38	0.85
2:C:32:ILE:HD12	3:J:95:LEU:HD21	1.58	0.85
2:D:257:VAL:HG21	2:E:35:GLN:HB3	1.58	0.84
4:H:540:LEU:HD23	3:J:106:TYR:HB2	1.59	0.84
2:M:69:GLU:HG3	2:M:72:ILE:HD12	1.59	0.84
4:H:370:PRO:CB	11:Q:101:PO4:O2	2.26	0.83
3:J:34:ALA:O	3:J:39:ARG:NH2	2.12	0.83
2:B:149:ARG:NH2	2:B:153:THR:OG1	2.11	0.83
3:I:7:ARG:HG2	3:I:12:TYR:HD2	1.44	0.83
3:G:34:ALA:O	3:G:39:ARG:NH2	2.12	0.83
3:G:7:ARG:HG2	3:G:12:TYR:HD2	1.44	0.82
2:F:48:ARG:HA	2:F:51:ARG:HD2	1.61	0.82
2:C:218:ARG:NH1	5:K:23:G:OP1	2.12	0.82
3:J:7:ARG:HG2	3:J:12:TYR:HD2	1.44	0.82
2:C:62:HIS:O	2:C:110:ARG:NH1	2.13	0.81
3:I:14:LEU:HD11	3:I:90:PRO:HD2	1.61	0.81
3:I:34:ALA:O	3:I:39:ARG:NH2	2.12	0.81
2:M:149:ARG:HH21	2:M:166:THR:HG21	1.45	0.81
3:G:14:LEU:HD11	3:G:90:PRO:HD2	1.61	0.81
3:J:14:LEU:HD11	3:J:90:PRO:HD2	1.61	0.81
2:A:149:ARG:HH21	6:L:24:DG:H21	1.25	0.81
1:P:744:PRO:O	1:P:746:ASP:N	2.13	0.81
2:F:68:ARG:HD3	2:F:69:GLU:H	1.46	0.81
1:P:493:LEU:HB3	1:P:569:VAL:HG22	1.62	0.81
2:B:22:GLY:N	5:K:16:G:OP2	2.14	0.81
2:D:19:ASN:ND2	2:D:28:ASN:O	2.10	0.80
2:B:179:ARG:NH1	2:B:244:PHE:O	2.15	0.80
2:D:149:ARG:NH2	2:D:153:THR:OG1	2.14	0.80
2:E:258:VAL:O	2:E:259:ARG:NH2	2.13	0.80
5:K:4:G:OP2	7:N:36:ASN:ND2	2.15	0.80
1:P:48:ALA:HB1	1:P:194:LEU:HD21	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:206:MET:CE	11:P:803:PO4:O2	2.29	0.80
4:H:228:ALA:HB2	7:N:73:LYS:HG2	1.62	0.79
4:H:514:ARG:HH22	3:J:46:SER:HB3	1.45	0.79
2:A:21:ASN:HD22	2:A:42:THR:H	1.28	0.79
1:P:4:ASP:OD1	1:P:66:ARG:NH2	2.15	0.79
2:D:51:ARG:NH2	5:K:31:C:OP1	2.14	0.79
3:J:54:THR:HA	3:J:57:ARG:HD3	1.63	0.79
1:P:468:LYS:HB3	1:P:599:VAL:HG22	1.65	0.79
3:I:54:THR:HA	3:I:57:ARG:HD3	1.64	0.79
4:H:422:ARG:HB2	4:H:433:ARG:HD3	1.63	0.79
1:P:206:MET:HE1	11:P:803:PO4:O2	1.83	0.78
2:A:51:ARG:NH2	5:K:25:A:OP1	2.15	0.78
2:C:15:VAL:HG11	2:C:20:PRO:HG3	1.63	0.78
2:C:68:ARG:HE	2:C:69:GLU:H	1.30	0.78
4:H:404:ALA:O	4:H:443:ARG:NH2	2.16	0.78
4:H:397:LEU:O	4:H:400:GLN:N	2.13	0.78
3:G:54:THR:HA	3:G:57:ARG:HD3	1.63	0.78
3:G:119:LYS:O	3:G:123:ASN:ND2	2.17	0.78
4:H:168:LEU:HB2	4:H:171:GLN:HG2	1.65	0.78
4:H:416:LEU:O	4:H:420:LEU:HB2	1.84	0.78
2:M:179:ARG:NH1	2:M:244:PHE:O	2.17	0.78
2:A:27:GLY:HA2	3:J:40:TYR:CD1	2.19	0.78
3:G:94:ASN:O	3:G:98:GLN:N	2.17	0.78
2:B:187:HIS:NE2	2:M:72:ILE:O	2.15	0.77
3:I:107:HIS:NE2	3:J:83:LEU:O	2.17	0.77
4:H:69:ARG:NH1	4:H:79:ASN:OD1	2.17	0.77
2:M:126:ARG:O	7:N:143:ARG:NH2	2.18	0.77
4:H:511:THR:HA	4:H:514:ARG:HE	1.48	0.77
3:I:83:LEU:O	3:G:107:HIS:NE2	2.18	0.77
2:M:117:THR:N	7:N:74:MET:O	2.17	0.77
7:N:37:ILE:HG23	7:N:138:PRO:HB3	1.67	0.77
3:I:119:LYS:O	3:I:123:ASN:ND2	2.17	0.77
3:J:94:ASN:O	3:J:98:GLN:N	2.17	0.77
4:H:6:LEU:HD23	4:H:9:TYR:HE1	1.49	0.77
2:D:243:LEU:HD21	2:D:277:LYS:HE3	1.67	0.76
2:C:55:GLN:HB2	2:C:65:ILE:HG13	1.66	0.76
3:J:119:LYS:O	3:J:123:ASN:ND2	2.17	0.76
2:A:62:HIS:O	2:A:110:ARG:NH1	2.19	0.76
2:C:127:GLY:O	2:C:130:GLN:NE2	2.17	0.76
6:L:36:DA:H2"	6:L:37:DA:H5'	1.67	0.76
1:P:184:HIS:HD2	1:P:188:ARG:HH22	1.33	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:353:ASN:O	1:P:383:ASN:ND2	2.19	0.76
3:I:94:ASN:O	3:I:98:GLN:N	2.17	0.76
1:P:643:ARG:HG2	4:H:165:ALA:HB1	1.68	0.76
2:C:8:ASP:OD2	2:C:231:HIS:NE2	2.19	0.76
2:M:67:ILE:HD11	7:N:74:MET:SD	2.26	0.75
7:N:138:PRO:HB2	7:N:147:CYS:HB2	1.67	0.75
1:P:53:ASP:OD1	1:P:118:HIS:NE2	2.18	0.75
1:P:609:SER:HA	1:P:613:LYS:HE2	1.68	0.75
2:D:136:SER:HA	2:D:178:TYR:HA	1.69	0.75
1:P:295:ALA:HB2	1:P:303:ILE:HD11	1.67	0.75
2:B:74:ASN:ND2	2:B:118:THR:OG1	2.20	0.75
2:B:91:LYS:HA	2:B:94:LYS:HB3	1.67	0.75
2:D:27:GLY:HA2	3:I:39:ARG:HG3	1.68	0.75
4:H:381:LEU:HD13	4:H:398:ILE:HG22	1.68	0.75
4:H:385:VAL:HG12	4:H:392:ASN:HB2	1.69	0.75
1:P:212:ALA:HA	1:P:217:ALA:HB3	1.68	0.74
2:C:152:VAL:HG12	2:C:166:THR:HG23	1.69	0.74
3:G:22:GLU:OE1	3:G:105:TYR:OH	2.04	0.74
1:P:209:TYR:HB3	1:P:216:ALA:HB1	1.67	0.74
2:A:150:MET:SD	2:D:48:ARG:HD3	2.27	0.74
2:F:255:VAL:HG11	2:F:263:ASP:HB3	1.69	0.74
2:C:136:SER:HA	2:C:178:TYR:HA	1.69	0.74
2:D:51:ARG:NH1	2:D:108:ASP:OD2	2.21	0.74
6:L:19:DG:H2"	6:L:20:DC:H5'	1.69	0.74
2:A:150:MET:HE2	2:D:68:ARG:HG2	1.70	0.74
2:A:160:GLU:HG3	2:A:161:THR:H	1.53	0.74
2:A:41:VAL:HB	2:A:134:SER:HB2	1.69	0.74
2:A:270:ASP:HB3	2:A:279:LEU:HD23	1.70	0.74
4:H:506:ILE:HG12	4:H:548:ASN:HA	1.70	0.74
3:J:6:ASN:HA	3:J:85:HIS:CE1	2.23	0.74
2:B:156:LYS:HE2	6:L:37:DA:H5"	1.69	0.74
1:P:6:ILE:N	1:P:62:GLN:OE1	2.20	0.73
3:G:58:LEU:HG	3:G:62:HIS:CE1	2.23	0.73
1:P:410:ARG:NH1	1:P:443:GLU:O	2.21	0.73
3:I:33:ASN:HD21	6:L:20:DC:H3'	1.54	0.73
3:I:58:LEU:HG	3:I:62:HIS:CE1	2.23	0.73
2:E:156:LYS:HG3	2:E:158:ALA:H	1.52	0.73
1:P:531:ILE:HG23	1:P:564:LEU:HD21	1.70	0.73
2:E:117:THR:OG1	6:L:20:DC:O2	2.04	0.73
3:I:6:ASN:HA	3:I:85:HIS:CE1	2.23	0.73
1:P:114:LEU:HD23	1:P:194:LEU:HD13	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:37:DA:H2"	6:L:38:DG:H5'	1.71	0.73
3:G:6:ASN:HA	3:G:85:HIS:CE1	2.23	0.73
1:P:472:PRO:O	1:P:624:LYS:NZ	2.19	0.73
2:C:27:GLY:HA2	4:H:496:ARG:HG2	1.70	0.73
1:P:429:GLU:O	1:P:645:ASN:ND2	2.20	0.73
4:H:445:ILE:HD13	4:H:450:LEU:HB3	1.70	0.73
2:M:41:VAL:HB	2:M:134:SER:HB2	1.70	0.73
2:D:241:ASP:OD2	2:D:245:LYS:NZ	2.22	0.73
2:M:235:LEU:HB3	7:N:133:GLN:HB3	1.68	0.73
1:P:331:GLU:OE1	1:P:365:GLN:NE2	2.21	0.72
2:B:51:ARG:HH22	5:K:13:U:P	2.11	0.72
3:J:58:LEU:HG	3:J:62:HIS:CE1	2.23	0.72
2:A:130:GLN:NE2	5:K:24:U:OP1	2.22	0.72
2:D:160:GLU:HG3	2:D:161:THR:H	1.54	0.72
2:B:132:THR:HG21	2:M:220:GLN:HB2	1.69	0.72
3:I:17:LEU:HD21	3:I:56:MET:HE1	1.70	0.72
2:B:133:PHE:HB2	2:M:17:ASP:HB3	1.71	0.72
3:J:32:LEU:HD11	6:L:24:DG:H5"	1.71	0.72
2:A:179:ARG:NH1	2:A:244:PHE:O	2.23	0.72
2:D:273:LEU:HD21	2:D:279:LEU:HB2	1.71	0.72
2:M:213:ASP:HB3	2:M:218:ARG:HH12	1.54	0.72
2:M:114:ALA:N	2:M:125:VAL:O	2.19	0.72
2:B:51:ARG:NE	2:B:108:ASP:OD1	2.23	0.72
2:C:129:VAL:HG22	2:C:184:ILE:HD12	1.70	0.72
3:G:17:LEU:HD21	3:G:56:MET:HE1	1.71	0.72
1:P:401:PHE:HE2	1:P:680:PHE:HA	1.55	0.72
3:I:22:GLU:OE1	3:I:105:TYR:OH	2.04	0.72
4:H:20:ILE:HG13	4:H:256:THR:HG21	1.72	0.72
2:B:35:GLN:NE2	4:H:449:ARG:O	2.20	0.71
2:E:68:ARG:HD3	2:E:69:GLU:H	1.55	0.71
3:J:17:LEU:HD21	3:J:56:MET:HE1	1.70	0.71
2:M:66:PHE:CE2	7:N:74:MET:HB3	2.24	0.71
2:B:179:ARG:NH1	2:B:247:ILE:O	2.22	0.71
2:A:22:GLY:N	5:K:28:U:OP2	2.23	0.71
2:D:28:ASN:OD1	5:K:33:U:O2'	2.06	0.71
2:M:7:TYR:HB2	2:M:184:ILE:HB	1.72	0.71
4:H:522:LYS:NZ	6:L:28:DC:OP1	2.22	0.71
2:D:179:ARG:NH1	2:D:244:PHE:O	2.23	0.71
2:E:28:ASN:OD1	5:K:39:U:O2'	2.08	0.71
7:N:7:ILE:HD12	7:N:147:CYS:HB3	1.71	0.71
2:A:23:ASP:OD1	2:A:30:PRO:HA	1.88	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:51:ARG:HE	2:C:108:ASP:CG	1.94	0.71
2:E:27:GLY:HA2	3:G:39:ARG:HG3	1.72	0.71
2:E:257:VAL:HG21	2:F:35:GLN:HB3	1.72	0.71
2:F:51:ARG:NH2	5:K:43:C:OP1	2.24	0.71
4:H:23:GLU:O	4:H:183:ASN:ND2	2.20	0.71
5:K:12:G:OP2	2:M:215:SER:OG	2.07	0.71
2:D:125:VAL:O	5:K:29:G:O2'	2.08	0.71
6:L:24:DG:H2"	6:L:25:DC:H5'	1.73	0.71
2:B:160:GLU:HG3	2:B:161:THR:HG23	1.72	0.71
2:F:269:ASP:OD2	2:F:271:LYS:NZ	2.23	0.71
2:A:163:ASP:OD2	2:A:165:ARG:NE	2.23	0.71
2:B:51:ARG:NH2	5:K:13:U:OP1	2.18	0.70
2:E:68:ARG:NH2	2:E:69:GLU:OE1	2.24	0.70
1:P:284:THR:OG1	1:P:316:ASN:OD1	2.06	0.70
2:D:14:ASP:OD2	2:D:224:ARG:NE	2.17	0.70
2:A:143:LEU:HG	2:A:174:PRO:HG3	1.73	0.70
7:N:67:ARG:NE	7:N:69:GLU:OE2	2.22	0.70
3:I:80:ARG:NH2	9:Q:11:DT:O2	2.25	0.70
1:P:607:ALA:HB1	1:P:613:LYS:HA	1.74	0.70
4:H:124:VAL:HA	4:H:127:VAL:HG12	1.73	0.70
1:P:399:ARG:HA	1:P:402:GLN:HB2	1.74	0.70
2:E:57:THR:HG22	2:F:235:LEU:HD11	1.72	0.70
7:N:198:VAL:HG23	7:N:199:ASN:H	1.56	0.70
4:H:12:ARG:NH2	4:H:275:GLY:O	2.25	0.70
4:H:397:LEU:O	4:H:399:ALA:N	2.25	0.70
7:N:68:ASN:ND2	7:N:89:GLN:OE1	2.25	0.70
2:A:51:ARG:NH1	2:A:108:ASP:OD2	2.24	0.70
2:B:169:ARG:NH1	4:H:424:LYS:O	2.24	0.70
3:G:32:LEU:HD23	3:G:35:THR:HG22	1.74	0.70
2:D:2:THR:HG21	2:D:190:LYS:HA	1.72	0.69
4:H:266:ILE:HG22	4:H:406:LEU:HD13	1.74	0.69
2:B:28:ASN:OD1	5:K:15:A:O2'	2.08	0.69
4:H:220:PRO:HB2	4:H:223:SER:HB3	1.73	0.69
7:N:35:ARG:NE	7:N:174:ASP:OD2	2.25	0.69
2:C:113:GLY:HA3	5:K:18:U:H5"	1.75	0.69
4:H:429:ILE:HD13	4:H:559:ALA:HA	1.74	0.69
4:H:510:GLY:O	4:H:514:ARG:NE	2.25	0.69
3:J:32:LEU:HD23	3:J:35:THR:HG22	1.74	0.69
1:P:398:PRO:HG2	1:P:682:LEU:HG	1.74	0.69
2:E:19:ASN:ND2	2:E:28:ASN:O	2.26	0.69
2:M:121:ASN:HB2	2:M:124:GLN:HG2	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:39:GLY:N	2:E:136:SER:OG	2.24	0.69
3:I:32:LEU:HD23	3:I:35:THR:HG22	1.74	0.69
3:J:43:SER:O	3:J:47:THR:N	2.23	0.69
4:H:206:ARG:HG2	4:H:207:LEU:HD23	1.73	0.69
3:J:6:ASN:HA	3:J:85:HIS:HE1	1.58	0.69
1:P:558:ILE:HD12	1:P:564:LEU:HD11	1.74	0.68
2:B:80:ALA:HB2	2:B:102:MET:SD	2.33	0.68
2:C:77:ILE:HG23	2:C:122:ALA:HB2	1.76	0.68
2:F:64:ASP:O	2:F:107:TYR:N	2.25	0.68
3:J:51:VAL:O	3:J:54:THR:N	2.27	0.68
1:P:33:ALA:HA	1:P:36:PHE:HB2	1.75	0.68
1:P:295:ALA:HA	1:P:300:LYS:HB2	1.74	0.68
2:D:117:THR:OG1	6:L:26:DC:O2	2.10	0.68
2:F:21:ASN:HD22	2:F:42:THR:H	1.40	0.68
2:M:258:VAL:O	2:M:259:ARG:NH2	2.25	0.68
1:P:187:MET:HE1	1:P:669:LEU:HD11	1.76	0.68
1:P:291:ALA:HB1	1:P:303:ILE:HD12	1.74	0.68
1:P:628:LEU:HB3	1:P:631:PRO:HG3	1.76	0.68
2:B:259:ARG:NH1	2:C:35:GLN:HE21	1.91	0.68
2:F:7:TYR:HB2	2:F:184:ILE:HD13	1.76	0.68
4:H:527:GLY:HA3	9:Q:-1:DA:H2"	1.74	0.68
7:N:194:GLN:HG3	7:N:201:VAL:HG21	1.75	0.68
1:P:168:ARG:O	1:P:172:ALA:N	2.23	0.68
2:B:126:ARG:O	2:B:130:GLN:NE2	2.27	0.68
2:B:204:GLN:O	2:B:208:ASN:ND2	2.27	0.68
2:B:26:ALA:HB1	2:B:29:LEU:HD12	1.75	0.68
2:D:27:GLY:HA3	3:I:40:TYR:HE1	1.57	0.68
3:I:6:ASN:HA	3:I:85:HIS:HE1	1.58	0.68
4:H:69:ARG:HG2	4:H:77:VAL:HB	1.76	0.68
2:M:109:ILE:HG23	2:M:114:ALA:HB2	1.74	0.68
3:G:6:ASN:HA	3:G:85:HIS:HE1	1.58	0.68
2:M:43:ASP:HB2	2:M:131:LEU:HB3	1.75	0.68
1:P:536:ARG:HB3	1:P:721:LEU:HD21	1.75	0.68
2:A:220:GLN:HB2	2:D:132:THR:HG21	1.76	0.68
3:I:51:VAL:O	3:I:54:THR:N	2.27	0.68
3:J:59:LEU:HD21	3:J:79:ILE:HD13	1.76	0.68
2:B:24:PRO:HG2	2:M:167:MET:HE1	1.75	0.68
2:B:31:ARG:O	2:B:40:LEU:N	2.26	0.68
2:B:220:GLN:HB2	2:C:132:THR:HG21	1.74	0.68
3:J:93:LEU:HD22	3:J:97:GLN:HB3	1.75	0.68
2:A:224:ARG:NH1	2:D:241:ASP:OD2	2.22	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:259:ARG:NH2	2:D:35:GLN:OE1	2.27	0.67
7:N:140:LEU:HG	7:N:147:CYS:SG	2.35	0.67
1:P:536:ARG:HD3	1:P:716:PHE:HB3	1.77	0.67
2:B:77:ILE:HG23	2:B:122:ALA:HB2	1.75	0.67
3:G:51:VAL:O	3:G:54:THR:N	2.27	0.67
1:P:94:ALA:HB2	1:P:141:GLU:HG2	1.74	0.67
1:P:278:PRO:HD2	1:P:462:LEU:HD23	1.75	0.67
1:P:486:ILE:HD11	1:P:509:LEU:HD21	1.77	0.67
3:I:93:LEU:HD22	3:I:97:GLN:HB3	1.75	0.67
4:H:51:LEU:HD23	4:H:56:LYS:HD2	1.77	0.67
2:C:251:LYS:NZ	2:C:256:GLU:O	2.27	0.67
4:H:490:ASN:N	6:L:31:DA:OP1	2.22	0.67
6:L:13:DG:H2"	6:L:14:DC:H5'	1.76	0.67
4:H:134:ALA:H	4:H:137:LYS:HZ3	1.42	0.67
2:B:125:VAL:O	5:K:11:G:O2'	2.11	0.67
7:N:63:THR:HG23	7:N:96:LYS:HB2	1.75	0.67
1:P:521:ASN:HB3	1:P:771:ALA:H	1.60	0.67
1:P:542:ARG:NH2	1:P:565:ASP:OD2	2.28	0.67
3:G:93:LEU:HD22	3:G:97:GLN:HB3	1.75	0.67
3:J:77:TRP:HD1	3:J:80:ARG:HH21	1.43	0.67
1:P:412:LEU:HA	1:P:416:TYR:HD2	1.60	0.67
2:B:109:ILE:HG23	2:B:125:VAL:HG21	1.75	0.67
3:G:43:SER:O	3:G:47:THR:N	2.23	0.67
3:G:59:LEU:HD21	3:G:79:ILE:HD13	1.76	0.67
4:H:67:LEU:N	4:H:79:ASN:HD21	1.92	0.67
2:E:33:ASP:OD2	2:E:135:ARG:NH1	2.28	0.66
4:H:69:ARG:NH1	4:H:83:ASP:OD1	2.28	0.66
4:H:108:THR:HA	4:H:131:LEU:HD23	1.78	0.66
4:H:383:ASN:HB3	4:H:433:ARG:HG3	1.76	0.66
3:J:33:ASN:N	6:L:25:DC:OP1	2.27	0.66
2:M:268:VAL:HG21	2:M:281:LYS:HE3	1.77	0.66
2:E:9:PHE:CZ	2:E:182:GLY:HA3	2.30	0.66
3:I:46:SER:HB3	3:J:57:ARG:NH2	2.10	0.66
1:P:494:ALA:HA	1:P:570:TYR:O	1.96	0.66
2:B:152:VAL:HA	2:B:166:THR:HG23	1.78	0.66
3:I:59:LEU:HD21	3:I:79:ILE:HD13	1.76	0.66
4:H:245:GLN:NE2	4:H:249:GLU:OE2	2.27	0.66
2:D:96:GLU:OE1	2:D:99:ARG:NH1	2.28	0.66
2:C:148:THR:HA	2:C:167:MET:HA	1.76	0.66
3:G:77:TRP:HD1	3:G:80:ARG:HH21	1.43	0.66
1:P:302:ARG:HD2	1:P:383:ASN:HB3	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:571:ARG:HH22	1:P:574:ALA:HB3	1.59	0.66
3:G:58:LEU:HG	3:G:62:HIS:HE1	1.61	0.66
2:C:45:CYS:SG	2:C:49:LYS:NZ	2.68	0.66
4:H:9:TYR:CZ	4:H:253:ALA:HB1	2.31	0.66
2:M:6:ARG:NH1	2:M:8:ASP:OD2	2.28	0.66
2:A:24:PRO:C	2:A:26:ALA:H	1.98	0.66
1:P:328:VAL:HG22	1:P:358:LEU:HD23	1.78	0.66
2:A:183:PHE:HZ	2:C:220:GLN:HG3	1.59	0.66
2:F:68:ARG:HD3	2:F:69:GLU:N	2.11	0.66
2:F:258:VAL:HG13	2:F:263:ASP:HB2	1.77	0.66
4:H:454:LYS:HE2	4:H:464:ARG:HD2	1.77	0.66
7:N:167:ASP:HB2	7:N:196:LYS:HG3	1.77	0.66
2:B:169:ARG:NH2	2:C:25:ASP:OD2	2.29	0.65
3:I:58:LEU:HG	3:I:62:HIS:HE1	1.61	0.65
2:B:161:THR:O	2:C:70:LYS:NZ	2.27	0.65
2:D:147:ILE:HD13	2:D:170:LYS:HB2	1.79	0.65
3:I:77:TRP:HD1	3:I:80:ARG:HH21	1.43	0.65
7:N:6:GLU:HA	7:N:101:ARG:HA	1.77	0.65
2:B:33:ASP:OD2	2:B:135:ARG:NH1	2.28	0.65
2:M:170:LYS:HZ3	2:M:216:ALA:HB1	1.62	0.65
2:B:259:ARG:HH12	2:C:35:GLN:HE21	1.42	0.65
2:D:6:ARG:HH11	2:D:236:GLY:HA3	1.61	0.65
2:E:149:ARG:NH2	2:E:153:THR:OG1	2.29	0.65
2:D:161:THR:HG22	2:F:91:LYS:HB2	1.79	0.65
2:E:168:GLY:HA3	6:L:12:DG:C5	2.32	0.65
2:M:69:GLU:HB2	2:M:72:ILE:HB	1.78	0.65
7:N:69:GLU:HG3	7:N:90:ARG:HD3	1.79	0.65
2:A:17:ASP:OD2	2:D:135:ARG:NH1	2.30	0.65
4:H:49:ARG:O	4:H:50:GLU:HG3	1.96	0.65
1:P:665:ASN:ND2	4:H:279:THR:OG1	2.28	0.65
2:D:47:LYS:O	2:D:51:ARG:HG2	1.97	0.65
2:M:121:ASN:HA	7:N:184:ASP:OD1	1.97	0.65
4:H:392:ASN:O	4:H:394:PRO:HD3	1.97	0.65
2:C:153:THR:OG1	6:L:31:DA:H4'	1.97	0.65
2:M:19:ASN:ND2	2:M:28:ASN:O	2.30	0.65
2:C:104:SER:O	2:C:110:ARG:NH1	2.27	0.65
4:H:196:LEU:HB3	4:H:242:ILE:HG12	1.78	0.65
2:M:55:GLN:NE2	2:M:68:ARG:HB2	2.12	0.65
4:H:214:VAL:HG21	4:H:337:ILE:HD13	1.80	0.64
2:M:55:GLN:HE22	2:M:68:ARG:HB2	1.62	0.64
1:P:272:LEU:HD21	1:P:445:LEU:HD22	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:339:LYS:O	1:P:344:THR:OG1	2.13	0.64
2:B:9:PHE:CZ	2:B:182:GLY:HA3	2.31	0.64
2:D:151:ALA:HB1	2:E:71:GLY:O	1.97	0.64
2:E:224:ARG:NH2	2:F:241:ASP:OD2	2.30	0.64
2:M:54:ILE:HB	2:M:65:ILE:HD11	1.79	0.64
3:G:77:TRP:HA	3:G:80:ARG:HE	1.63	0.64
4:H:262:ASN:ND2	4:H:273:CYS:O	2.21	0.64
2:M:21:ASN:HB2	2:M:41:VAL:HG13	1.78	0.64
1:P:561:GLY:H	1:P:585:ARG:HH21	1.46	0.64
2:F:229:PHE:HE1	2:F:279:LEU:HD22	1.63	0.64
2:A:210:PHE:HB3	2:A:221:MET:O	1.98	0.64
3:I:102:ALA:HB1	3:J:56:MET:SD	2.37	0.64
4:H:236:GLN:O	4:H:236:GLN:HG2	1.98	0.64
3:J:77:TRP:HA	3:J:80:ARG:HE	1.63	0.64
1:P:332:HIS:O	1:P:333:HIS:ND1	2.30	0.64
2:B:21:ASN:OD1	2:B:31:ARG:NE	2.28	0.64
2:B:156:LYS:HG3	2:B:158:ALA:H	1.63	0.64
2:E:31:ARG:O	2:E:40:LEU:N	2.24	0.64
4:H:464:ARG:NH2	4:H:466:ASP:OD2	2.31	0.64
1:P:369:SER:HA	1:P:372:ALA:HB2	1.79	0.63
3:J:58:LEU:HG	3:J:62:HIS:HE1	1.61	0.63
2:A:149:ARG:NH1	2:A:151:ALA:O	2.31	0.63
2:D:68:ARG:CD	2:D:69:GLU:H	2.11	0.63
4:H:194:ILE:HD13	4:H:201:ALA:HA	1.80	0.63
7:N:30:THR:HG22	7:N:32:SER:H	1.62	0.63
1:P:48:ALA:HB3	1:P:194:LEU:HD11	1.79	0.63
1:P:657:ARG:HH22	4:H:296:ASN:HB3	1.62	0.63
2:B:117:THR:OG1	6:L:44:DC:O2	2.12	0.63
2:C:32:ILE:HG22	2:C:140:ILE:HD11	1.79	0.63
1:P:56:LYS:HG3	1:P:61:PHE:CE2	2.33	0.63
3:I:77:TRP:HA	3:I:80:ARG:HE	1.63	0.63
3:I:80:ARG:HG2	3:G:106:TYR:HD1	1.62	0.63
3:J:80:ARG:NH2	9:Q:6:DT:O2	2.31	0.63
5:K:3:U:OP1	2:M:121:ASN:ND2	2.29	0.63
2:M:255:VAL:HG11	2:M:263:ASP:HB3	1.81	0.63
1:P:652:LYS:HG3	1:P:653:HIS:H	1.62	0.63
2:C:49:LYS:HB2	2:C:209:MET:CE	2.29	0.63
2:F:137:ILE:HG13	2:F:249:VAL:HG13	1.81	0.63
1:P:480:GLN:NE2	1:P:484:ASP:OD1	2.31	0.63
2:C:126:ARG:NH2	5:K:14:C:H41	1.91	0.63
2:E:40:LEU:HD23	2:E:133:PHE:HD2	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:11:PHE:HB3	2:F:180:CYS:HB3	1.79	0.63
3:G:45:SER:O	3:G:98:GLN:NE2	2.32	0.63
3:J:45:SER:O	3:J:98:GLN:NE2	2.32	0.63
2:B:35:GLN:NE2	2:M:141:MET:SD	2.63	0.63
2:C:148:THR:N	5:K:27:G:OP2	2.31	0.63
2:E:83:GLN:O	2:E:86:VAL:HG23	1.99	0.63
2:F:230:GLU:HB2	2:F:278:LEU:HB2	1.81	0.63
3:I:43:SER:O	3:I:47:THR:N	2.23	0.63
4:H:178:TYR:O	4:H:182:ALA:N	2.31	0.63
1:P:110:LEU:HG	1:P:187:MET:HE1	1.81	0.62
2:C:33:ASP:OD2	2:C:135:ARG:NE	2.32	0.62
2:F:258:VAL:O	2:F:259:ARG:NH2	2.28	0.62
4:H:85:TYR:HD2	4:H:155:CYS:HB3	1.64	0.62
4:H:525:PHE:HB3	9:Q:-1:DA:H1'	1.81	0.62
1:P:98:TYR:CZ	1:P:102:ARG:HD3	2.34	0.62
2:F:179:ARG:NH2	2:F:247:ILE:O	2.32	0.62
4:H:214:VAL:HG11	4:H:337:ILE:HG23	1.81	0.62
1:P:538:LEU:O	1:P:542:ARG:HG2	1.99	0.62
5:K:13:U:H1'	2:M:149:ARG:HB2	1.81	0.62
2:B:127:GLY:O	2:B:130:GLN:NE2	2.31	0.62
2:D:82:GLU:HA	2:D:86:VAL:HG12	1.81	0.62
2:D:95:THR:HG21	2:C:161:THR:HB	1.81	0.62
4:H:229:PHE:CE1	7:N:90:ARG:HD2	2.34	0.62
2:B:5:LYS:O	2:B:186:THR:OG1	2.17	0.62
2:C:144:GLU:HG2	2:C:171:PHE:HD1	1.63	0.62
4:H:34:ILE:HB	4:H:159:PHE:H	1.62	0.62
4:H:123:GLY:HA2	4:H:161:LEU:HD13	1.79	0.62
4:H:514:ARG:HD2	3:J:45:SER:CB	2.29	0.62
2:E:152:VAL:H	2:E:164:ASN:HB3	1.65	0.62
2:F:110:ARG:NE	2:F:198:ASP:OD2	2.32	0.62
3:I:46:SER:HB3	3:J:57:ARG:HH21	1.65	0.62
7:N:171:MET:HG3	7:N:194:GLN:HE22	1.64	0.62
1:P:331:GLU:H	1:P:361:THR:HG22	1.62	0.62
2:B:17:ASP:OD1	2:C:135:ARG:NH1	2.28	0.62
2:C:9:PHE:CZ	2:C:182:GLY:HA3	2.35	0.62
2:E:170:LYS:NZ	2:F:43:ASP:OD1	2.33	0.62
2:E:275:GLU:OE2	2:E:277:LYS:NZ	2.33	0.62
3:I:45:SER:O	3:I:98:GLN:NE2	2.32	0.62
4:H:208:HIS:HE1	4:H:242:ILE:HD12	1.65	0.62
4:H:42:PHE:HZ	4:H:45:LEU:HB2	1.64	0.62
2:C:80:ALA:HB2	2:C:102:MET:SD	2.40	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:154:ASN:O	2:C:156:LYS:N	2.29	0.62
2:E:148:THR:HA	2:E:167:MET:HB2	1.79	0.62
2:E:96:GLU:OE2	2:E:99:ARG:NH1	2.31	0.62
1:P:244:ASP:HA	1:P:252:ASN:HD21	1.65	0.61
2:A:128:PRO:HG3	2:A:189:ALA:HA	1.82	0.61
2:D:56:MET:HG2	2:E:187:HIS:CG	2.35	0.61
4:H:429:ILE:HD12	4:H:562:TYR:CD2	2.35	0.61
1:P:65:ILE:HD11	11:P:803:PO4:P	2.39	0.61
1:P:393:GLU:OE1	1:P:396:GLN:NE2	2.33	0.61
1:P:525:THR:OG1	1:P:747:ASN:OD1	2.12	0.61
2:A:136:SER:HA	2:A:178:TYR:HA	1.80	0.61
2:C:42:THR:HG22	2:C:133:PHE:CZ	2.35	0.61
4:H:6:LEU:HD23	4:H:9:TYR:CE1	2.34	0.61
4:H:541:GLU:HG3	3:J:2:GLY:HA3	1.82	0.61
2:M:21:ASN:HD22	2:M:42:THR:H	1.49	0.61
1:P:465:VAL:HG21	1:P:586:CYS:HB3	1.82	0.61
2:B:21:ASN:HD22	2:B:45:CYS:HB2	1.65	0.61
2:F:115:VAL:HG22	5:K:41:G:C4	2.36	0.61
1:P:625:ALA:HB1	4:H:162:VAL:HG11	1.82	0.61
2:A:21:ASN:ND2	2:A:42:THR:H	1.99	0.61
2:A:91:LYS:HB2	2:B:161:THR:HG22	1.82	0.61
3:I:12:TYR:OH	3:I:107:HIS:ND1	2.32	0.61
7:N:8:SER:O	7:N:148:ASP:N	2.33	0.61
7:N:69:GLU:HG3	7:N:90:ARG:HB2	1.82	0.61
2:D:51:ARG:HH22	5:K:31:C:H5”	1.63	0.61
2:F:42:THR:HG23	2:F:133:PHE:CZ	2.36	0.61
4:H:363:MET:HB3	4:H:431:TYR:CE2	2.35	0.61
4:H:468:GLY:HA3	4:H:554:GLN:HB3	1.82	0.61
2:M:114:ALA:HA	7:N:74:MET:CE	2.30	0.61
2:A:130:GLN:HE21	2:C:215:SER:HA	1.64	0.61
2:C:23:ASP:OD1	2:C:31:ARG:NH1	2.33	0.61
1:P:437:PHE:CD2	4:H:176:ARG:HD2	2.35	0.61
2:B:42:THR:HG22	2:B:133:PHE:CE2	2.36	0.61
2:D:65:ILE:HB	2:D:67:ILE:HG22	1.82	0.61
2:E:149:ARG:NH2	2:E:166:THR:OG1	2.33	0.61
3:J:22:GLU:OE1	3:J:105:TYR:OH	2.04	0.61
2:M:130:GLN:HB2	7:N:143:ARG:HH11	1.65	0.61
7:N:20:LYS:O	7:N:90:ARG:NH2	2.28	0.61
4:H:514:ARG:HD2	3:J:45:SER:HB3	1.83	0.61
1:P:41:GLY:HA3	1:P:190:LEU:HD21	1.83	0.61
2:B:174:PRO:HB2	2:B:259:ARG:HH22	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:259:ARG:HD2	2:C:36:THR:HB	1.82	0.61
2:C:19:ASN:ND2	2:C:28:ASN:O	2.25	0.61
4:H:188:ASP:HA	4:H:203:PRO:HG3	1.82	0.61
1:P:306:ALA:HB3	1:P:391:LEU:HD23	1.81	0.61
2:B:144:GLU:HG3	2:B:171:PHE:CD1	2.36	0.61
2:D:44:VAL:HG11	5:K:31:C:H2'	1.82	0.61
2:F:3:ILE:HG21	2:F:199:LEU:HD13	1.83	0.61
4:H:33:ILE:HG13	4:H:158:SER:O	2.01	0.61
2:M:132:THR:HB	2:M:181:HIS:H	1.64	0.61
7:N:10:ASP:O	7:N:97:ASP:N	2.30	0.61
2:A:91:LYS:HA	2:A:94:LYS:HB3	1.82	0.60
2:E:68:ARG:HD3	2:E:69:GLU:N	2.16	0.60
4:H:83:ASP:O	4:H:156:ASN:ND2	2.30	0.60
1:P:93:THR:HG22	1:P:134:ARG:HH21	1.67	0.60
1:P:306:ALA:HB1	1:P:363:ASN:HB3	1.83	0.60
1:P:426:THR:OG1	1:P:427:GLN:N	2.29	0.60
4:H:70:SER:HA	8:O:13:DC:H1'	1.83	0.60
4:H:228:ALA:HB2	7:N:73:LYS:CG	2.30	0.60
7:N:83:ILE:HD12	7:N:87:ARG:NH1	2.16	0.60
7:N:175:MET:HB3	7:N:187:ASN:HD22	1.66	0.60
1:P:44:PHE:CE2	1:P:110:LEU:HD22	2.36	0.60
1:P:556:GLN:O	1:P:559:GLU:HB2	2.02	0.60
2:A:31:ARG:O	2:A:40:LEU:N	2.21	0.60
2:A:167:MET:H	6:L:22:DA:H2"	1.67	0.60
2:D:167:MET:HG3	6:L:16:DA:H2'	1.82	0.60
2:E:156:LYS:NZ	6:L:11:DG:OP1	2.27	0.60
3:G:24:ILE:HG23	3:G:66:LEU:HD11	1.84	0.60
4:H:31:PRO:HB3	4:H:57:VAL:HB	1.82	0.60
4:H:441:ILE:O	4:H:445:ILE:HG12	2.01	0.60
2:M:44:VAL:HA	2:M:47:LYS:HB2	1.82	0.60
1:P:110:LEU:HG	1:P:187:MET:CE	2.32	0.60
2:B:161:THR:OG1	2:B:162:GLY:N	2.34	0.60
2:D:9:PHE:CZ	2:D:182:GLY:HA3	2.36	0.60
3:J:2:GLY:O	3:J:107:HIS:ND1	2.35	0.60
2:A:103:CYS:O	2:A:110:ARG:HG3	2.02	0.60
2:A:183:PHE:CZ	2:C:220:GLN:HG3	2.36	0.60
4:H:52:LYS:HE2	4:H:53:VAL:HG22	1.82	0.60
4:H:411:LEU:HB3	4:H:415:LEU:HD12	1.82	0.60
1:P:100:VAL:HG11	1:P:135:LEU:HD13	1.84	0.60
1:P:305:TYR:CE2	1:P:307:ILE:HD11	2.36	0.60
2:A:152:VAL:HG12	2:A:164:ASN:HB3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:243:LEU:HD21	2:A:277:LYS:HG2	1.83	0.60
2:B:73:LEU:HB2	2:M:153:THR:HA	1.83	0.60
2:C:65:ILE:HB	2:C:67:ILE:HG22	1.83	0.60
2:C:98:ALA:O	2:C:102:MET:HG2	2.02	0.60
2:F:47:LYS:HG3	2:F:131:LEU:HD12	1.82	0.60
4:H:6:LEU:HD13	4:H:254:LEU:HD21	1.82	0.60
4:H:9:TYR:HH	4:H:257:LEU:HD13	1.66	0.60
4:H:208:HIS:CE1	4:H:242:ILE:HB	2.36	0.60
4:H:411:LEU:HD13	4:H:443:ARG:HD2	1.83	0.60
2:M:64:ASP:OD2	2:M:105:ARG:NH1	2.22	0.60
1:P:336:LEU:HD13	1:P:348:ARG:HH21	1.65	0.60
1:P:370:LEU:HG	1:P:408:MET:SD	2.42	0.60
1:P:617:ASP:OD1	4:H:44:GLN:NE2	2.29	0.60
2:A:45:CYS:SG	2:A:49:LYS:NZ	2.70	0.60
2:C:64:ASP:HB2	2:C:106:TYR:HD1	1.66	0.60
2:M:52:ASN:O	2:M:56:MET:HG3	2.01	0.60
2:E:21:ASN:HD22	2:E:45:CYS:HB2	1.66	0.60
2:F:103:CYS:O	2:F:110:ARG:HG3	2.01	0.60
3:G:48:PRO:O	3:G:52:PHE:HB2	2.02	0.60
2:B:164:ASN:HB2	2:C:69:GLU:O	2.02	0.60
2:D:19:ASN:H	2:D:218:ARG:HA	1.67	0.60
2:D:144:GLU:HA	2:D:171:PHE:HD1	1.67	0.60
2:E:3:ILE:HG23	2:E:186:THR:HG22	1.82	0.60
2:E:4:GLU:O	2:E:234:ASN:ND2	2.33	0.60
2:F:131:LEU:HB3	2:F:180:CYS:SG	2.42	0.60
3:I:2:GLY:O	3:I:107:HIS:ND1	2.35	0.60
4:H:256:THR:O	4:H:260:GLY:N	2.34	0.60
2:M:174:PRO:HB2	2:M:259:ARG:CZ	2.32	0.60
7:N:176:ASP:N	7:N:188:ALA:O	2.25	0.60
1:P:199:PHE:HA	1:P:202:THR:HG22	1.82	0.60
2:A:24:PRO:O	2:C:146:SER:HB3	2.02	0.60
2:A:27:GLY:N	3:J:39:ARG:O	2.21	0.60
5:K:4:G:OP2	7:N:139:TYR:OH	2.20	0.60
1:P:342:LYS:HD2	1:P:346:LYS:HB2	1.82	0.59
3:G:2:GLY:O	3:G:107:HIS:ND1	2.35	0.59
3:J:48:PRO:O	3:J:52:PHE:HB2	2.02	0.59
2:M:145:HIS:HB2	2:M:170:LYS:O	2.02	0.59
2:A:39:GLY:N	2:A:136:SER:OG	2.35	0.59
2:B:48:ARG:HD3	2:M:150:MET:SD	2.41	0.59
2:E:129:VAL:HG11	2:E:202:PHE:CZ	2.37	0.59
3:I:24:ILE:HG23	3:I:66:LEU:HD11	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:48:PRO:O	3:I:52:PHE:HB2	2.02	0.59
3:J:24:ILE:HG23	3:J:66:LEU:HD11	1.84	0.59
1:P:114:LEU:HB3	1:P:194:LEU:HD22	1.84	0.59
1:P:124:ASP:OD1	1:P:673:PHE:N	2.35	0.59
1:P:464:ARG:HB3	1:P:587:ASN:HD22	1.67	0.59
1:P:537:TYR:HB3	1:P:550:LEU:HD11	1.83	0.59
1:P:629:ASP:OD1	1:P:630:ASP:N	2.35	0.59
2:A:205:ALA:O	2:A:209:MET:HB3	2.03	0.59
2:B:21:ASN:ND2	2:B:45:CYS:HB2	2.17	0.59
2:D:90:GLU:O	2:D:92:GLY:N	2.35	0.59
2:E:270:ASP:HA	2:E:273:LEU:HD21	1.84	0.59
3:J:12:TYR:CE1	3:J:104:GLY:HA2	2.38	0.59
2:M:252:LYS:HG2	2:M:265:LEU:HG	1.83	0.59
4:H:67:LEU:H	4:H:79:ASN:ND2	1.95	0.59
4:H:393:LEU:HD22	6:L:41:DG:C6	2.37	0.59
9:Q:-4:DT:H2"	9:Q:-3:DA:H5'	1.84	0.59
2:B:147:ILE:HD13	2:B:170:LYS:HB2	1.85	0.59
2:D:77:ILE:HG23	2:D:122:ALA:HB2	1.85	0.59
4:H:470:VAL:HG23	4:H:471:LEU:HD12	1.83	0.59
6:L:50:DG:N2	8:O:11:DT:O2	2.34	0.59
2:A:90:GLU:O	2:A:92:GLY:N	2.36	0.59
2:E:91:LYS:HA	2:E:94:LYS:HB3	1.84	0.59
1:P:114:LEU:HD21	1:P:190:LEU:HB3	1.82	0.59
1:P:133:ARG:NH1	1:P:137:GLN:OE1	2.36	0.59
1:P:304:ILE:O	1:P:390:ILE:N	2.32	0.59
2:E:42:THR:HG22	2:E:133:PHE:CE2	2.38	0.59
2:E:126:ARG:HG3	5:K:35:G:H5'	1.84	0.59
3:J:12:TYR:OH	3:J:107:HIS:ND1	2.32	0.59
2:M:36:THR:HG23	2:M:38:GLU:H	1.67	0.59
2:C:270:ASP:HB3	2:C:279:LEU:HD23	1.85	0.59
2:E:165:ARG:HH12	6:L:9:DG:N2	2.00	0.59
3:G:12:TYR:OH	3:G:107:HIS:ND1	2.32	0.59
4:H:6:LEU:HD22	4:H:254:LEU:HD22	1.83	0.59
6:L:9:DG:N7	6:L:10:DA:N6	2.51	0.59
2:B:148:THR:N	5:K:21:C:OP2	2.28	0.59
2:D:203:TRP:HE1	2:D:280:ARG:HH12	1.51	0.59
2:D:229:PHE:CE2	2:D:279:LEU:HD12	2.38	0.59
2:D:247:ILE:HD11	2:D:279:LEU:HD11	1.85	0.59
2:M:9:PHE:CE2	2:M:182:GLY:HA3	2.37	0.59
2:M:102:MET:HE2	7:N:76:GLU:HA	1.85	0.59
1:P:395:GLN:NE2	1:P:581:GLN:OE1	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:143:LEU:HD21	2:E:174:PRO:HG3	1.84	0.58
2:B:220:GLN:HG3	2:C:183:PHE:HZ	1.68	0.58
2:C:152:VAL:HG13	2:C:164:ASN:HB3	1.85	0.58
2:E:51:ARG:NH2	5:K:37:C:OP1	2.35	0.58
2:A:164:ASN:HB2	2:D:69:GLU:O	2.03	0.58
2:B:17:ASP:HB3	2:C:133:PHE:HB2	1.85	0.58
2:B:99:ARG:HH21	2:B:125:VAL:HG12	1.68	0.58
2:B:100:GLN:NE2	2:B:191:GLN:O	2.26	0.58
2:C:32:ILE:HD12	3:J:95:LEU:CD2	2.33	0.58
2:C:68:ARG:HG3	2:C:69:GLU:HG2	1.85	0.58
2:F:116:MET:HB3	2:F:122:ALA:HB3	1.85	0.58
4:H:209:ASN:H	4:H:251:THR:HG21	1.67	0.58
4:H:401:ILE:HD12	4:H:415:LEU:HD11	1.85	0.58
4:H:464:ARG:O	4:H:466:ASP:N	2.37	0.58
4:H:523:LEU:HD12	4:H:529:ALA:HA	1.84	0.58
5:K:12:G:H21	2:M:149:ARG:HH12	1.51	0.58
2:D:34:PRO:HB3	3:I:47:THR:HG23	1.84	0.58
2:F:14:ASP:OD1	2:F:222:ASN:N	2.35	0.58
2:F:134:SER:OG	2:F:178:TYR:HB3	2.04	0.58
3:I:80:ARG:HG2	3:G:106:TYR:CD1	2.39	0.58
4:H:225:ASN:ND2	6:L:49:DA:H2'	2.18	0.58
7:N:5:LEU:HD22	7:N:38:LEU:HD21	1.84	0.58
2:A:47:LYS:HG2	2:A:112:PHE:CD1	2.38	0.58
2:F:19:ASN:HB3	2:F:22:GLY:HA3	1.85	0.58
2:F:91:LYS:HA	2:F:94:LYS:HB3	1.84	0.58
4:H:511:THR:HG22	4:H:514:ARG:HH11	1.68	0.58
3:J:33:ASN:ND2	6:L:26:DC:H5"	2.19	0.58
2:M:237:ASP:OD2	2:M:276:THR:OG1	2.13	0.58
7:N:47:ILE:HG13	7:N:106:PHE:CD2	2.38	0.58
1:P:364:VAL:HG11	1:P:683:ILE:HG13	1.85	0.58
1:P:571:ARG:NH2	1:P:574:ALA:HB3	2.18	0.58
1:P:744:PRO:HB2	1:P:745:PRO:CD	2.34	0.58
2:A:215:SER:OG	5:K:30:G:OP2	2.12	0.58
2:B:169:ARG:HH22	2:C:25:ASP:CG	2.06	0.58
2:D:134:SER:OG	2:D:178:TYR:HB3	2.03	0.58
2:C:95:THR:HG21	2:M:162:GLY:HA2	1.85	0.58
3:J:115:LYS:HA	9:Q:2:DA:H5"	1.85	0.58
2:A:30:PRO:O	2:A:32:ILE:HG23	2.03	0.58
3:I:17:LEU:HB2	3:I:82:ILE:HG21	1.86	0.58
3:G:12:TYR:CE1	3:G:104:GLY:HA2	2.38	0.58
4:H:514:ARG:HG2	3:J:42:GLY:HA2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:426:THR:O	1:P:427:GLN:HG2	2.04	0.58
5:K:16:G:N7	5:K:17:C:N4	2.51	0.58
2:M:110:ARG:NE	2:M:198:ASP:OD2	2.35	0.58
2:B:21:ASN:HD21	5:K:15:A:P	2.27	0.58
2:B:58:GLN:HG2	2:B:63:HIS:CG	2.39	0.58
2:D:83:GLN:O	2:D:86:VAL:HG13	2.03	0.58
2:C:83:GLN:O	2:C:86:VAL:HG13	2.03	0.58
2:C:91:LYS:HB2	2:M:161:THR:HG22	1.84	0.58
2:F:62:HIS:O	2:F:110:ARG:NH1	2.37	0.58
4:H:35:VAL:HA	4:H:160:ARG:O	2.03	0.58
4:H:83:ASP:HB3	4:H:87:TYR:HB2	1.86	0.58
2:A:66:PHE:CZ	2:A:109:ILE:HD11	2.39	0.58
2:F:38:GLU:HA	2:F:139:PRO:HA	1.85	0.58
3:I:12:TYR:CE1	3:I:104:GLY:HA2	2.38	0.58
1:P:573:MET:HB2	1:P:602:ARG:HA	1.86	0.57
1:P:672:LYS:HB3	1:P:675:THR:HB	1.86	0.57
1:P:745:PRO:O	1:P:748:PRO:HD3	2.04	0.57
2:A:32:ILE:HD12	3:I:95:LEU:HD21	1.86	0.57
2:A:249:VAL:HG13	2:A:266:VAL:HG22	1.85	0.57
2:C:25:ASP:HB3	4:H:500:SER:HB2	1.85	0.57
2:C:131:LEU:HD11	2:C:202:PHE:HZ	1.69	0.57
2:F:22:GLY:HA2	2:F:30:PRO:HA	1.85	0.57
2:F:134:SER:HG	2:F:178:TYR:HB3	1.69	0.57
4:H:48:THR:HG21	4:H:61:PHE:HZ	1.69	0.57
2:M:114:ALA:HA	7:N:74:MET:HE3	1.86	0.57
1:P:662:GLU:O	4:H:300:HIS:NE2	2.37	0.57
2:B:227:TYR:HB3	2:B:279:LEU:HD11	1.86	0.57
4:H:170:CYS:HA	4:H:175:VAL:HG11	1.86	0.57
1:P:170:PHE:HA	1:P:186:TRP:HH2	1.68	0.57
1:P:514:ILE:HG23	1:P:548:LYS:HD3	1.85	0.57
2:B:62:HIS:HA	2:B:105:ARG:HA	1.87	0.57
2:E:233:ASN:OD1	2:E:234:ASN:N	2.37	0.57
2:F:63:HIS:HA	2:F:107:TYR:HB2	1.86	0.57
4:H:42:PHE:CD1	4:H:140:VAL:HG22	2.40	0.57
7:N:142:CYS:HB3	7:N:144:GLU:OE1	2.05	0.57
1:P:407:ASP:HA	1:P:410:ARG:NH1	2.19	0.57
1:P:570:TYR:CD1	1:P:599:VAL:HB	2.40	0.57
1:P:628:LEU:HD22	1:P:631:PRO:HB3	1.85	0.57
2:B:7:TYR:HB2	2:B:184:ILE:HB	1.85	0.57
2:B:68:ARG:CG	2:B:69:GLU:H	2.13	0.57
2:C:20:PRO:HD2	2:C:30:PRO:HB3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:143:LEU:CD2	2:E:174:PRO:HG3	2.35	0.57
5:K:32:A:H2'	5:K:33:U:H4'	1.86	0.57
5:K:38:C:N4	5:K:40:C:O2'	2.37	0.57
2:B:109:ILE:HD13	2:B:116:MET:HE3	1.87	0.57
2:E:47:LYS:HG2	2:E:112:PHE:CE1	2.39	0.57
2:F:246:ARG:HH22	2:F:272:ASN:H	1.53	0.57
4:H:545:ARG:NE	3:J:96:GLU:OE2	2.34	0.57
5:K:8:C:H1'	5:K:10:G:OP1	2.03	0.57
2:M:215:SER:OG	2:M:216:ALA:N	2.37	0.57
1:P:122:LEU:N	1:P:373:ALA:O	2.33	0.57
1:P:390:ILE:HG23	1:P:421:VAL:HB	1.84	0.57
2:D:68:ARG:HD3	2:D:69:GLU:N	2.14	0.57
2:D:258:VAL:O	2:D:259:ARG:NH2	2.36	0.57
2:C:51:ARG:NH2	2:C:108:ASP:OD1	2.37	0.57
3:I:42:GLY:HA2	3:J:57:ARG:HG3	1.86	0.57
1:P:412:LEU:HA	1:P:416:TYR:CD2	2.40	0.57
2:B:241:ASP:OD2	2:M:224:ARG:NH2	2.37	0.57
2:D:20:PRO:HD2	2:D:30:PRO:HB3	1.87	0.57
2:D:129:VAL:HG11	2:D:202:PHE:CZ	2.40	0.57
2:F:81:HIS:NE2	2:F:120:LYS:O	2.38	0.57
3:I:19:ALA:HB2	3:I:105:TYR:HA	1.86	0.57
3:I:115:LYS:HA	9:Q:7:DT:H5"	1.87	0.57
2:A:167:MET:HE1	6:L:22:DA:C2	2.39	0.57
2:A:179:ARG:NH1	2:A:247:ILE:O	2.38	0.57
2:B:142:THR:O	4:H:549:HIS:NE2	2.38	0.57
2:D:149:ARG:HB2	5:K:37:C:H1'	1.85	0.57
2:E:77:ILE:HG23	2:E:122:ALA:HB2	1.86	0.57
4:H:81:LEU:HB2	4:H:170:CYS:HB3	1.86	0.57
2:A:117:THR:OG1	6:L:32:DC:O2	2.22	0.57
2:C:21:ASN:ND2	2:C:45:CYS:SG	2.77	0.57
2:C:41:VAL:HB	2:C:134:SER:HB2	1.87	0.57
2:M:152:VAL:HG22	2:M:164:ASN:HB3	1.87	0.57
1:P:189:PHE:CD2	1:P:190:LEU:HD12	2.40	0.57
2:D:134:SER:HB2	2:D:180:CYS:HB2	1.86	0.57
2:C:47:LYS:HG2	2:C:112:PHE:CD1	2.40	0.57
2:E:17:ASP:HB3	2:F:133:PHE:HB2	1.87	0.57
4:H:361:LEU:HD21	4:H:380:LEU:HD22	1.87	0.57
3:J:17:LEU:HB2	3:J:82:ILE:HG21	1.86	0.57
1:P:744:PRO:HB2	1:P:745:PRO:HD3	1.86	0.56
2:A:29:LEU:HD13	3:J:54:THR:HG21	1.87	0.56
2:A:146:SER:O	2:D:31:ARG:NH2	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:12:LEU:HD12	2:C:227:TYR:HE2	1.69	0.56
3:G:19:ALA:HB2	3:G:105:TYR:HA	1.86	0.56
1:P:584:GLY:O	1:P:588:ARG:NH2	2.37	0.56
2:A:2:THR:HG22	2:A:193:GLY:HA2	1.87	0.56
2:A:55:GLN:HB2	2:A:65:ILE:HG13	1.87	0.56
2:A:148:THR:O	5:K:31:C:O2'	2.19	0.56
2:A:169:ARG:NH2	2:D:25:ASP:OD2	2.34	0.56
2:D:31:ARG:O	2:D:40:LEU:N	2.27	0.56
2:E:21:ASN:ND2	2:E:45:CYS:HB2	2.20	0.56
2:F:77:ILE:HG23	2:F:122:ALA:HB2	1.86	0.56
2:F:243:LEU:HD21	2:F:277:LYS:HZ3	1.70	0.56
4:H:88:VAL:HG13	4:H:159:PHE:CZ	2.40	0.56
4:H:501:ALA:HB2	4:H:508:VAL:HG11	1.87	0.56
3:J:19:ALA:HB2	3:J:105:TYR:HA	1.86	0.56
2:M:160:GLU:HG3	2:M:161:THR:HG23	1.86	0.56
1:P:8:HIS:HD2	1:P:20:HIS:HD1	1.53	0.56
1:P:65:ILE:CD1	11:P:803:PO4:O1	2.50	0.56
1:P:486:ILE:HG22	1:P:570:TYR:CD2	2.40	0.56
2:A:74:ASN:HD22	2:C:154:ASN:HB3	1.70	0.56
2:D:29:LEU:HD21	3:I:54:THR:HG21	1.88	0.56
2:D:144:GLU:OE1	3:I:57:ARG:NH2	2.39	0.56
2:C:9:PHE:HB3	2:C:228:VAL:HG22	1.86	0.56
2:C:64:ASP:HB2	2:C:106:TYR:CD1	2.39	0.56
2:E:271:LYS:HD2	2:E:272:ASN:HB2	1.86	0.56
1:P:11:GLN:NE2	1:P:15:ASN:HA	2.21	0.56
2:A:151:ALA:HB1	2:D:71:GLY:O	2.05	0.56
2:B:15:VAL:HG11	2:B:20:PRO:HG3	1.85	0.56
2:D:152:VAL:HG22	2:D:164:ASN:HB3	1.86	0.56
2:D:168:GLY:HA3	6:L:18:DG:C6	2.41	0.56
2:C:90:GLU:O	2:C:92:GLY:N	2.37	0.56
2:F:83:GLN:O	2:F:86:VAL:HG23	2.05	0.56
6:L:40:DT:H2"	6:L:41:DG:H5'	1.87	0.56
1:P:51:LEU:HD11	1:P:161:LEU:HD21	1.87	0.56
2:B:32:ILE:HD11	4:H:552:LEU:HD22	1.87	0.56
4:H:572:LYS:NZ	4:H:573:ASP:OD1	2.35	0.56
1:P:215:ALA:HA	1:P:218:ALA:HB3	1.87	0.56
1:P:561:GLY:H	1:P:585:ARG:NH2	2.02	0.56
2:A:51:ARG:NH1	5:K:25:A:H5"	2.20	0.56
2:A:152:VAL:HA	2:A:166:THR:OG1	2.06	0.56
3:I:56:MET:SD	3:G:102:ALA:HB1	2.45	0.56
4:H:87:TYR:HD2	4:H:107:PHE:HB2	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:66:PHE:HB2	2:M:106:TYR:CD1	2.39	0.56
1:P:43:LEU:HG	1:P:169:ASP:OD2	2.05	0.56
2:A:13:PHE:CE1	2:A:46:LEU:HD11	2.40	0.56
2:B:12:LEU:HD12	2:B:227:TYR:HE2	1.69	0.56
2:B:27:GLY:N	4:H:421:ARG:HD3	2.21	0.56
4:H:319:PRO:HG2	4:H:348:ALA:HA	1.88	0.56
4:H:476:ALA:HB3	4:H:565:GLU:HB3	1.88	0.56
2:M:15:VAL:HG11	2:M:20:PRO:HG3	1.86	0.56
1:P:170:PHE:CZ	1:P:178:ALA:HB2	2.41	0.56
1:P:406:THR:HA	1:P:409:MET:HG2	1.88	0.56
2:B:83:GLN:O	2:B:86:VAL:HG13	2.06	0.56
2:D:47:LYS:HG2	2:D:112:PHE:CE1	2.41	0.56
1:P:12:ASP:N	1:P:16:ALA:O	2.37	0.56
1:P:305:TYR:HB3	1:P:360:VAL:HG22	1.87	0.56
2:A:144:GLU:HG2	2:A:171:PHE:HD2	1.71	0.56
2:B:103:CYS:SG	2:B:125:VAL:HG11	2.46	0.56
2:F:31:ARG:O	2:F:40:LEU:N	2.32	0.56
4:H:205:ALA:HB2	4:H:244:GLU:HA	1.88	0.56
2:M:12:LEU:HD21	2:M:249:VAL:HG21	1.88	0.56
2:A:22:GLY:HA3	5:K:27:G:O2’	2.06	0.56
3:I:40:TYR:HD2	3:I:55:LEU:HD21	1.71	0.56
3:G:39:ARG:HG2	3:G:40:TYR:CD1	2.41	0.56
4:H:84:HIS:NE2	4:H:154:GLY:HA2	2.21	0.56
4:H:265:ARG:HH21	8:O:17:DA:H1’	1.69	0.56
4:H:380:LEU:HG	4:H:436:LEU:HD22	1.87	0.56
4:H:467:ILE:O	4:H:471:LEU:HD13	2.06	0.56
1:P:673:PHE:O	1:P:677:ALA:N	2.39	0.55
2:A:113:GLY:HA2	2:A:125:VAL:HG12	1.87	0.55
2:D:50:VAL:O	2:D:54:ILE:HG12	2.07	0.55
2:E:34:PRO:HB3	3:G:47:THR:HG23	1.87	0.55
3:I:77:TRP:HD1	3:I:80:ARG:NH2	2.04	0.55
3:G:17:LEU:HB2	3:G:82:ILE:HG21	1.86	0.55
6:L:47:DG:H2”	6:L:48:DA:C8	2.40	0.55
2:M:129:VAL:HG22	2:M:184:ILE:HG13	1.88	0.55
7:N:14:PHE:CE1	7:N:29:ILE:HG13	2.41	0.55
7:N:128:ARG:O	7:N:133:GLN:N	2.38	0.55
4:H:79:ASN:N	4:H:83:ASP:OD2	2.40	0.55
5:K:8:C:H5’	2:M:48:ARG:HB2	1.88	0.55
7:N:50:LYS:HE3	7:N:52:LEU:HD21	1.88	0.55
2:B:82:GLU:HA	2:B:86:VAL:HG12	1.88	0.55
3:I:24:ILE:HG22	3:I:62:HIS:HB3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:36:DA:C2'	6:L:37:DA:H5'	2.36	0.55
1:P:274:SER:HB2	1:P:422:LEU:HD12	1.88	0.55
2:D:20:PRO:HG2	2:D:178:TYR:OH	2.06	0.55
2:D:153:THR:HB	6:L:19:DG:H4'	1.88	0.55
4:H:48:THR:O	4:H:59:ARG:N	2.40	0.55
4:H:275:GLY:HA2	4:H:325:PHE:HD1	1.70	0.55
4:H:415:LEU:O	4:H:419:ALA:N	2.31	0.55
3:J:24:ILE:HG22	3:J:62:HIS:HB3	1.89	0.55
1:P:184:HIS:CD2	1:P:188:ARG:HH22	2.19	0.55
1:P:187:MET:O	1:P:191:PHE:HB2	2.07	0.55
1:P:402:GLN:HE21	1:P:430:LEU:HA	1.71	0.55
1:P:696:PRO:HD2	1:P:729:ALA:HB3	1.87	0.55
2:C:30:PRO:O	2:C:32:ILE:HG23	2.07	0.55
2:M:249:VAL:HG13	2:M:266:VAL:HG22	1.88	0.55
1:P:195:VAL:HG12	1:P:379:ARG:HG2	1.88	0.55
1:P:395:GLN:HB2	1:P:641:PHE:CZ	2.40	0.55
2:D:34:PRO:HA	3:I:49:ILE:HD11	1.89	0.55
2:D:224:ARG:NH2	2:E:241:ASP:OD2	2.32	0.55
3:G:24:ILE:HG22	3:G:62:HIS:HB3	1.89	0.55
4:H:425:ALA:O	6:L:35:DC:H2'	2.06	0.55
7:N:181:ASP:OD1	7:N:185:SER:OG	2.22	0.55
1:P:187:MET:HG3	1:P:671:ILE:HD12	1.89	0.55
1:P:348:ARG:HA	1:P:351:THR:HG22	1.89	0.55
1:P:695:ILE:HB	1:P:728:ALA:HA	1.88	0.55
2:A:29:LEU:HD23	2:A:29:LEU:H	1.72	0.55
2:B:126:ARG:HG2	2:B:188:PHE:CZ	2.42	0.55
2:E:63:HIS:HA	2:E:107:TYR:HB2	1.87	0.55
2:F:20:PRO:HD2	2:F:30:PRO:HB3	1.88	0.55
3:G:39:ARG:HH12	6:L:12:DG:H2'	1.72	0.55
3:G:77:TRP:HD1	3:G:80:ARG:NH2	2.04	0.55
5:K:3:U:H4'	5:K:4:G:N2	2.21	0.55
2:M:21:ASN:ND2	2:M:42:THR:OG1	2.40	0.55
2:A:148:THR:HG22	2:A:167:MET:SD	2.47	0.55
2:B:124:GLN:NE2	5:K:11:G:N3	2.55	0.55
2:D:113:GLY:HA2	2:D:125:VAL:HG12	1.88	0.55
2:C:36:THR:HG23	2:C:38:GLU:H	1.70	0.55
3:I:39:ARG:HG2	3:I:40:TYR:CD1	2.41	0.55
3:J:77:TRP:HD1	3:J:80:ARG:NH2	2.04	0.55
5:K:14:C:H5'	2:M:148:THR:O	2.07	0.55
2:M:161:THR:OG1	2:M:162:GLY:N	2.39	0.55
1:P:42:SER:OG	1:P:169:ASP:OD2	2.23	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:491:CYS:N	1:P:550:LEU:O	2.39	0.55
2:A:26:ALA:HB1	3:J:42:GLY:HA3	1.89	0.55
2:A:149:ARG:HH21	6:L:24:DG:N2	1.99	0.55
3:G:40:TYR:HD2	3:G:55:LEU:HD21	1.71	0.55
3:J:39:ARG:HG2	3:J:40:TYR:CD1	2.41	0.55
1:P:100:VAL:HA	1:P:108:GLY:HA3	1.87	0.55
2:A:27:GLY:HA2	3:J:40:TYR:HD1	1.68	0.55
2:A:42:THR:HG22	2:A:133:PHE:CE2	2.42	0.55
2:A:210:PHE:CD1	2:A:221:MET:HE3	2.42	0.55
2:E:148:THR:HA	2:E:167:MET:CB	2.37	0.55
2:F:9:PHE:HB3	2:F:228:VAL:HG12	1.89	0.55
5:K:7:A:H61	7:N:23:ARG:HH21	1.53	0.55
2:M:99:ARG:HE	2:M:125:VAL:HG22	1.71	0.55
1:P:276:THR:HG21	1:P:450:GLU:HG2	1.88	0.54
2:A:35:GLN:NE2	2:C:257:VAL:HG12	2.22	0.54
2:A:137:ILE:HG12	2:A:177:LEU:O	2.06	0.54
2:B:90:GLU:O	2:B:92:GLY:N	2.39	0.54
2:B:174:PRO:HB2	2:B:259:ARG:NH2	2.22	0.54
2:B:183:PHE:HZ	2:M:220:GLN:HG3	1.72	0.54
2:E:34:PRO:HB2	3:G:92:HIS:HB2	1.87	0.54
2:E:82:GLU:HA	2:E:86:VAL:HG22	1.88	0.54
4:H:134:ALA:H	4:H:137:LYS:NZ	2.05	0.54
4:H:247:MET:HA	4:H:250:TYR:CE1	2.42	0.54
4:H:426:GLU:OE2	4:H:433:ARG:NH1	2.40	0.54
2:M:62:HIS:HA	2:M:105:ARG:HA	1.89	0.54
7:N:6:GLU:HB2	7:N:152:LEU:HG	1.89	0.54
7:N:163:ASP:O	7:N:165:THR:HG23	2.06	0.54
2:D:36:THR:HG23	2:D:38:GLU:H	1.72	0.54
4:H:107:PHE:HE2	4:H:159:PHE:HE2	1.54	0.54
4:H:195:CYS:SG	4:H:202:ALA:HB3	2.47	0.54
1:P:90:PRO:HA	8:O:24:DA:H4'	1.88	0.54
2:C:23:ASP:HB3	2:C:26:ALA:HB3	1.90	0.54
2:E:144:GLU:OE1	3:G:57:ARG:HG2	2.07	0.54
2:F:137:ILE:HD11	2:F:179:ARG:HG3	1.88	0.54
4:H:84:HIS:HA	4:H:155:CYS:O	2.08	0.54
1:P:401:PHE:CE2	1:P:680:PHE:HA	2.40	0.54
2:A:44:VAL:HG12	5:K:25:A:OP2	2.07	0.54
2:E:237:ASP:HB2	2:E:277:LYS:HE3	1.89	0.54
2:F:220:GLN:NE2	2:F:222:ASN:OD1	2.32	0.54
2:M:110:ARG:HA	2:M:192:THR:HB	1.90	0.54
1:P:305:TYR:HD2	1:P:360:VAL:HG13	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:252:LYS:HG2	2:A:265:LEU:HG	1.90	0.54
2:A:258:VAL:HG11	2:A:264:TYR:CZ	2.42	0.54
2:D:20:PRO:HB3	2:D:221:MET:HE3	1.88	0.54
2:C:51:ARG:HH22	5:K:19:U:P	2.31	0.54
2:C:179:ARG:NH1	2:C:244:PHE:O	2.41	0.54
2:E:35:GLN:HA	3:G:91:ASN:HB3	1.90	0.54
3:G:32:LEU:HD11	6:L:12:DG:H5"	1.90	0.54
2:M:213:ASP:HB3	2:M:218:ARG:NH1	2.21	0.54
2:A:161:THR:HG22	2:E:91:LYS:HB2	1.89	0.54
2:D:113:GLY:HA3	5:K:30:G:H5"	1.90	0.54
2:C:69:GLU:HG3	2:C:70:LYS:H	1.70	0.54
2:C:150:MET:HE2	5:K:26:G:C4	2.42	0.54
2:C:203:TRP:HE1	2:C:280:ARG:HH11	1.54	0.54
2:E:55:GLN:HB2	2:E:65:ILE:HG13	1.88	0.54
3:I:21:LEU:HD13	3:I:55:LEU:HB3	1.90	0.54
4:H:80:LEU:HD11	4:H:114:LEU:HD12	1.88	0.54
4:H:331:SER:OG	4:H:340:ARG:NE	2.38	0.54
5:K:9:A:O2'	5:K:10:G:O5'	2.26	0.54
2:A:83:GLN:O	2:A:86:VAL:HG23	2.07	0.54
2:B:32:ILE:HG22	2:B:140:ILE:HD11	1.88	0.54
3:I:24:ILE:CD1	3:I:79:ILE:HD11	2.38	0.54
3:G:17:LEU:HD22	3:G:83:LEU:HD21	1.90	0.54
3:J:24:ILE:CD1	3:J:79:ILE:HD11	2.38	0.54
2:M:114:ALA:O	2:M:125:VAL:N	2.29	0.54
2:B:114:ALA:N	2:B:125:VAL:HG23	2.23	0.54
2:C:141:MET:HB3	3:J:92:HIS:CD2	2.43	0.54
3:G:25:GLN:HG3	3:G:62:HIS:NE2	2.23	0.54
3:G:37:ALA:HA	3:G:41:PHE:HB2	1.90	0.54
3:G:46:SER:HA	3:G:98:GLN:OE1	2.08	0.54
4:H:441:ILE:HD12	4:H:560:ILE:HD12	1.89	0.54
4:H:534:TRP:O	4:H:538:GLN:HG2	2.08	0.54
2:C:33:ASP:O	2:C:37:GLY:N	2.41	0.54
2:E:163:ASP:HA	2:F:69:GLU:HG3	1.88	0.54
3:I:17:LEU:HD22	3:I:83:LEU:HD21	1.90	0.54
3:I:25:GLN:HG3	3:I:62:HIS:NE2	2.23	0.54
3:I:46:SER:HA	3:I:98:GLN:OE1	2.08	0.54
3:G:24:ILE:CD1	3:G:79:ILE:HD11	2.38	0.54
3:G:119:LYS:HD2	9:Q:14:DA:H3'	1.89	0.54
4:H:563:TYR:HA	4:H:566:THR:HG22	1.90	0.54
3:J:37:ALA:HA	3:J:41:PHE:HB2	1.90	0.54
1:P:113:TYR:OH	1:P:125:TRP:HB2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:380:LYS:O	1:P:383:ASN:N	2.39	0.54
2:B:5:LYS:NZ	2:B:232:SER:O	2.23	0.54
2:E:56:MET:HG3	2:F:187:HIS:HB2	1.90	0.54
2:E:153:THR:HA	2:F:73:LEU:HB2	1.88	0.54
2:F:10:VAL:HG22	2:F:181:HIS:CD2	2.42	0.54
4:H:214:VAL:HG22	4:H:330:LEU:HD13	1.90	0.54
4:H:364:VAL:CG1	4:H:459:GLY:HA2	2.38	0.54
4:H:533:GLN:HA	4:H:536:ILE:HG22	1.90	0.54
3:J:25:GLN:HG3	3:J:62:HIS:NE2	2.23	0.54
8:O:11:DT:H2"	8:O:12:DT:H5"	1.90	0.54
1:P:410:ARG:HG3	1:P:446:PRO:HD3	1.89	0.53
2:B:253:ASP:OD1	2:B:254:GLY:N	2.41	0.53
2:C:42:THR:HB	2:C:44:VAL:HG22	1.90	0.53
4:H:64:PRO:HG3	4:H:179:VAL:HG21	1.90	0.53
3:J:46:SER:HA	3:J:98:GLN:OE1	2.08	0.53
2:M:160:GLU:HG3	2:M:161:THR:H	1.73	0.53
2:C:69:GLU:O	2:C:71:GLY:N	2.36	0.53
2:C:113:GLY:CA	5:K:18:U:H5"	2.37	0.53
2:M:63:HIS:HA	2:M:107:TYR:HB2	1.90	0.53
7:N:13:CYS:HG	7:N:15:THR:HG1	1.55	0.53
1:P:576:LEU:HD11	1:P:628:LEU:HD21	1.90	0.53
1:P:668:PRO:HB3	4:H:285:LEU:HD21	1.90	0.53
2:A:74:ASN:ND2	6:L:32:DC:OP1	2.41	0.53
2:B:41:VAL:HB	2:B:134:SER:OG	2.07	0.53
2:B:160:GLU:HG3	2:B:161:THR:H	1.73	0.53
2:F:280:ARG:HH22	2:F:282:LEU:HD21	1.73	0.53
4:H:344:GLU:OE1	7:N:166:GLN:NE2	2.40	0.53
4:H:478:LEU:HD23	4:H:516:LEU:HD13	1.90	0.53
5:K:9:A:OP1	2:M:21:ASN:ND2	2.39	0.53
1:P:320:PHE:HB3	1:P:328:VAL:HG21	1.91	0.53
2:E:213:ASP:HB3	2:E:218:ARG:NH1	2.24	0.53
2:E:252:LYS:HG2	2:E:253:ASP:H	1.71	0.53
3:G:21:LEU:HD13	3:G:55:LEU:HB3	1.90	0.53
7:N:101:ARG:HH22	7:N:157:ASP:N	2.06	0.53
1:P:50:LEU:HD23	1:P:159:PHE:HD1	1.73	0.53
1:P:174:TRP:CE3	1:P:178:ALA:HA	2.43	0.53
1:P:400:ASP:O	1:P:652:LYS:N	2.40	0.53
2:A:29:LEU:HD13	3:J:54:THR:CG2	2.38	0.53
2:B:50:VAL:O	2:B:54:ILE:HG12	2.07	0.53
2:D:150:MET:SD	2:E:48:ARG:HD3	2.49	0.53
2:E:53:PHE:CD2	2:E:205:ALA:HA	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:81:HIS:NE2	2:E:120:LYS:O	2.41	0.53
2:E:90:GLU:O	2:E:92:GLY:N	2.41	0.53
2:F:229:PHE:CG	2:F:243:LEU:HD12	2.44	0.53
3:I:33:ASN:ND2	6:L:20:DC:H3'	2.23	0.53
4:H:453:MET:HE3	4:H:557:LEU:HD11	1.91	0.53
6:L:8:DG:H2"	6:L:9:DG:H5"	1.91	0.53
2:M:133:PHE:CZ	7:N:67:ARG:HD3	2.44	0.53
2:M:149:ARG:NH2	2:M:166:THR:HG21	2.20	0.53
7:N:55:GLU:HB3	7:N:101:ARG:HG3	1.89	0.53
1:P:44:PHE:HE1	1:P:166:LEU:HD21	1.74	0.53
1:P:187:MET:HB2	1:P:673:PHE:CZ	2.43	0.53
2:D:21:ASN:OD1	2:D:42:THR:OG1	2.20	0.53
2:F:20:PRO:HB2	2:F:41:VAL:HG22	1.91	0.53
4:H:7:THR:HG23	4:H:249:GLU:OE1	2.09	0.53
4:H:51:LEU:HB3	4:H:56:LYS:HG2	1.89	0.53
4:H:291:GLY:N	4:H:292:GLY:HA2	2.24	0.53
7:N:34:ALA:HB1	7:N:102:ILE:HG12	1.90	0.53
8:O:5:DA:H2"	8:O:6:DT:C5	2.44	0.53
1:P:707:GLN:HE22	1:P:711:ALA:HA	1.73	0.53
2:A:259:ARG:NH2	2:D:33:ASP:OD2	2.34	0.53
2:B:174:PRO:HG3	2:C:35:GLN:HE22	1.74	0.53
2:D:104:SER:O	2:D:110:ARG:NH2	2.42	0.53
2:F:9:PHE:CZ	2:F:182:GLY:HA3	2.44	0.53
3:I:95:LEU:O	3:I:98:GLN:HB2	2.09	0.53
3:G:115:LYS:HA	9:Q:12:DT:H5"	1.89	0.53
4:H:196:LEU:HA	7:N:191:MET:SD	2.48	0.53
4:H:229:PHE:CD2	7:N:21:VAL:HG12	2.44	0.53
7:N:32:SER:HB3	7:N:174:ASP:HA	1.90	0.53
1:P:652:LYS:HG3	1:P:653:HIS:N	2.22	0.53
2:A:268:VAL:HG11	2:A:281:LYS:HE3	1.90	0.53
2:E:21:ASN:ND2	2:E:42:THR:OG1	2.41	0.53
2:E:147:ILE:O	2:E:167:MET:HB2	2.08	0.53
4:H:3:LEU:HD21	4:H:221:PHE:HE2	1.73	0.53
9:Q:-3:DA:H2"	9:Q:-2:DT:H5'	1.90	0.53
1:P:96:ALA:HB1	1:P:112:ALA:HB1	1.89	0.53
1:P:188:ARG:HG2	1:P:381:ILE:HD13	1.91	0.53
2:A:238:ALA:HB3	2:A:243:LEU:HD11	1.91	0.53
2:E:34:PRO:HG2	3:G:92:HIS:CD2	2.44	0.53
4:H:69:ARG:NH2	8:O:14:DA:OP2	2.40	0.53
3:J:95:LEU:O	3:J:98:GLN:HB2	2.09	0.53
5:K:6:A:O3'	2:M:51:ARG:NH2	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:36:PHE:HA	1:P:382:HIS:HE1	1.74	0.53
1:P:113:TYR:HA	1:P:131:LEU:HD11	1.91	0.53
2:A:142:THR:HG22	2:A:144:GLU:HG3	1.91	0.53
2:A:181:HIS:HB3	2:A:244:PHE:CE2	2.43	0.53
2:F:227:TYR:HB2	2:F:247:ILE:HD11	1.91	0.53
3:G:95:LEU:O	3:G:98:GLN:HB2	2.09	0.53
4:H:224:VAL:HG13	4:H:229:PHE:HB2	1.91	0.53
2:M:66:PHE:HD1	2:M:106:TYR:CZ	2.26	0.53
1:P:291:ALA:O	1:P:295:ALA:N	2.41	0.52
2:A:24:PRO:HG2	2:A:26:ALA:O	2.10	0.52
2:A:42:THR:HG21	2:C:147:ILE:HG22	1.90	0.52
2:B:56:MET:HE3	2:C:187:HIS:HB2	1.90	0.52
2:F:68:ARG:CD	2:F:69:GLU:H	2.19	0.52
1:P:495:VAL:HB	1:P:571:ARG:HG2	1.91	0.52
1:P:658:LEU:HD13	1:P:675:THR:HG22	1.90	0.52
2:A:23:ASP:HB3	2:A:29:LEU:O	2.09	0.52
2:A:218:ARG:HH11	2:A:221:MET:HE1	1.74	0.52
2:B:68:ARG:HG3	2:B:69:GLU:N	2.16	0.52
2:D:189:ALA:O	2:D:193:GLY:N	2.41	0.52
2:E:36:THR:HG23	2:E:38:GLU:H	1.73	0.52
2:E:246:ARG:HH12	2:E:272:ASN:HB3	1.73	0.52
3:G:16:ARG:NE	3:G:108:GLU:OE1	2.41	0.52
3:J:17:LEU:HD22	3:J:83:LEU:HD21	1.89	0.52
3:J:40:TYR:HD2	3:J:55:LEU:HD21	1.71	0.52
8:O:24:DA:H2"	11:O:101:PO4:O1	2.08	0.52
1:P:30:ALA:HB1	1:P:46:GLU:HB2	1.92	0.52
1:P:180:LEU:HD11	4:H:289:ILE:HD12	1.91	0.52
2:A:21:ASN:O	2:A:23:ASP:HA	2.09	0.52
2:A:31:ARG:HB3	2:A:40:LEU:O	2.09	0.52
2:B:128:PRO:HG3	2:B:189:ALA:HA	1.91	0.52
2:D:23:ASP:HB3	2:D:26:ALA:HB3	1.92	0.52
2:D:103:CYS:HB3	2:D:192:THR:O	2.09	0.52
2:C:49:LYS:HB2	2:C:209:MET:HE2	1.91	0.52
2:E:103:CYS:O	2:E:110:ARG:HG2	2.09	0.52
2:E:280:ARG:NH2	2:E:282:LEU:HD11	2.23	0.52
3:I:12:TYR:HE1	3:I:104:GLY:HA2	1.75	0.52
3:I:33:ASN:HD21	6:L:20:DC:C3'	2.19	0.52
3:I:48:PRO:HG2	3:I:93:LEU:HG	1.92	0.52
4:H:141:MET:HG3	4:H:146:TRP:CZ2	2.44	0.52
4:H:429:ILE:HD11	4:H:498:PHE:CZ	2.45	0.52
2:M:99:ARG:NH1	2:M:125:VAL:HG13	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:187:HIS:HB3	7:N:135:PHE:CE2	2.44	0.52
2:B:35:GLN:HB3	2:M:257:VAL:HG11	1.90	0.52
2:B:181:HIS:HB3	2:B:244:PHE:CE2	2.45	0.52
2:C:117:THR:HG21	6:L:38:DG:H21	1.73	0.52
2:M:143:LEU:HG	2:M:174:PRO:HG3	1.90	0.52
1:P:47:TYR:HE1	1:P:160:PRO:HG2	1.73	0.52
1:P:64:TYR:HB2	1:P:89:ILE:HD12	1.90	0.52
2:A:216:ALA:HB2	2:D:47:LYS:HZ2	1.74	0.52
2:B:147:ILE:HG22	2:C:42:THR:HG21	1.91	0.52
2:F:89:LYS:O	2:F:94:LYS:N	2.42	0.52
4:H:393:LEU:O	4:H:395:SER:N	2.42	0.52
3:J:16:ARG:NE	3:J:108:GLU:OE1	2.42	0.52
5:K:1:G:C2	7:N:43:TRP:HB3	2.44	0.52
2:M:203:TRP:CE3	2:M:226:LEU:HD21	2.44	0.52
1:P:47:TYR:CD2	1:P:166:LEU:HD12	2.44	0.52
1:P:106:PHE:CE1	1:P:669:LEU:HD12	2.44	0.52
1:P:368:GLU:OE1	1:P:681:HIS:HA	2.10	0.52
2:D:179:ARG:NH2	2:D:247:ILE:O	2.40	0.52
2:C:231:HIS:CE1	2:C:243:LEU:HD11	2.45	0.52
2:F:124:GLN:HB3	5:K:41:G:H1'	1.91	0.52
3:G:48:PRO:HG2	3:G:93:LEU:HG	1.92	0.52
4:H:85:TYR:CD2	4:H:155:CYS:HB3	2.43	0.52
4:H:101:ASP:O	4:H:105:ALA:N	2.42	0.52
4:H:108:THR:O	4:H:112:ASN:ND2	2.30	0.52
3:J:21:LEU:HD13	3:J:55:LEU:HB3	1.90	0.52
1:P:271:THR:O	1:P:419:THR:HA	2.08	0.52
2:E:48:ARG:HA	2:E:51:ARG:HD2	1.92	0.52
2:E:224:ARG:HD2	2:E:261:PHE:CD2	2.45	0.52
2:F:131:LEU:HD21	2:F:202:PHE:HZ	1.75	0.52
3:I:37:ALA:HA	3:I:41:PHE:HB2	1.90	0.52
4:H:530:VAL:HG13	9:Q:1:DT:C4	2.45	0.52
2:M:70:LYS:O	2:M:74:ASN:ND2	2.42	0.52
7:N:30:THR:HG23	7:N:172:LEU:O	2.09	0.52
1:P:517:HIS:CE1	1:P:770:ALA:HB2	2.45	0.52
1:P:639:GLU:OE1	1:P:642:ARG:NH1	2.25	0.52
1:P:658:LEU:HD21	1:P:679:ARG:NH2	2.25	0.52
2:C:106:TYR:HD2	2:C:109:ILE:HD12	1.75	0.52
2:C:268:VAL:HG11	2:C:281:LYS:HE2	1.90	0.52
2:E:54:ILE:HB	2:E:65:ILE:HD11	1.91	0.52
2:E:179:ARG:NH1	2:E:244:PHE:O	2.43	0.52
4:H:456:LEU:HD22	4:H:464:ARG:HH11	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:11:PHE:HB3	2:M:180:CYS:HB3	1.90	0.52
2:M:136:SER:HA	2:M:178:TYR:HA	1.91	0.52
7:N:51:VAL:HG13	7:N:102:ILE:HG23	1.91	0.52
1:P:236:TYR:HE2	1:P:263:PHE:HZ	1.56	0.52
1:P:391:LEU:HD11	1:P:420:PHE:HD2	1.75	0.52
2:B:156:LYS:H	2:B:159:SER:HB3	1.75	0.52
2:D:19:ASN:N	2:D:218:ARG:HA	2.24	0.52
3:I:7:ARG:HG2	3:I:12:TYR:CD2	2.34	0.52
4:H:225:ASN:ND2	6:L:49:DA:H8	2.08	0.52
3:J:12:TYR:HE1	3:J:104:GLY:HA2	1.75	0.52
3:J:22:GLU:OE1	3:J:37:ALA:HB2	2.10	0.52
1:P:252:ASN:HA	1:P:255:ARG:HB2	1.92	0.52
1:P:527:CYS:O	1:P:531:ILE:HD12	2.10	0.52
1:P:715:ASP:HA	1:P:718:ARG:HH11	1.75	0.52
2:A:32:ILE:CD1	3:I:95:LEU:HD21	2.40	0.52
2:A:149:ARG:NH2	2:A:153:THR:OG1	2.42	0.52
2:B:102:MET:HG3	2:B:106:TYR:CD1	2.44	0.52
2:C:29:LEU:HD22	4:H:511:THR:HG21	1.92	0.52
2:C:51:ARG:NH2	5:K:19:U:OP1	2.41	0.52
2:F:273:LEU:HD11	2:F:279:LEU:HB2	1.90	0.52
4:H:302:ASP:HA	4:H:305:LYS:HB2	1.93	0.52
7:N:68:ASN:HB3	7:N:87:ARG:NE	2.25	0.52
1:P:329:VAL:HG22	1:P:351:THR:HB	1.92	0.51
2:A:32:ILE:HD11	3:J:50:ALA:HB2	1.92	0.51
2:B:144:GLU:HG3	2:B:171:PHE:CE1	2.45	0.51
2:D:32:ILE:CD1	3:G:95:LEU:HD21	2.40	0.51
2:C:91:LYS:HD3	2:M:161:THR:HG22	1.91	0.51
2:E:34:PRO:HG3	3:G:47:THR:OG1	2.09	0.51
2:F:126:ARG:HG3	5:K:41:G:H5”	1.92	0.51
1:P:387:SER:O	1:P:418:VAL:HA	2.10	0.51
1:P:402:GLN:HG2	1:P:442:LEU:HD11	1.92	0.51
2:C:205:ALA:O	2:C:209:MET:CB	2.53	0.51
2:F:128:PRO:HD3	2:F:192:THR:HG21	1.92	0.51
4:H:263:ARG:NH1	8:O:18:DA:OP1	2.43	0.51
1:P:581:GLN:O	1:P:585:ARG:NH1	2.43	0.51
2:B:23:ASP:N	2:B:29:LEU:O	2.34	0.51
4:H:214:VAL:HG13	4:H:330:LEU:HD13	1.92	0.51
4:H:364:VAL:HG13	4:H:458:MET:O	2.11	0.51
2:M:55:GLN:HE21	2:M:73:LEU:HB3	1.75	0.51
7:N:39:MET:HG2	7:N:43:TRP:CD1	2.46	0.51
1:P:307:ILE:HG21	1:P:312:ILE:HB	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:429:GLU:HG2	1:P:642:ARG:HG3	1.91	0.51
1:P:646:GLY:O	4:H:59:ARG:NH1	2.44	0.51
2:A:21:ASN:ND2	2:A:42:THR:OG1	2.43	0.51
2:A:144:GLU:HG2	2:A:171:PHE:CD2	2.45	0.51
2:B:148:THR:HA	2:B:167:MET:HA	1.91	0.51
2:F:89:LYS:HB3	2:F:94:LYS:HA	1.92	0.51
3:I:106:TYR:HD1	3:J:80:ARG:HG2	1.75	0.51
3:G:12:TYR:HE1	3:G:104:GLY:HA2	1.75	0.51
4:H:212:LYS:HB2	4:H:218:PRO:HB3	1.92	0.51
1:P:40:TYR:OH	1:P:386:ASP:OD1	2.29	0.51
1:P:457:ALA:O	1:P:461:LYS:N	2.37	0.51
2:D:16:GLN:HB3	2:D:220:GLN:HB3	1.92	0.51
2:C:38:GLU:HA	2:C:139:PRO:HA	1.92	0.51
3:I:52:PHE:HA	3:I:55:LEU:HB2	1.93	0.51
4:H:328:LEU:HB2	4:H:342:TRP:HZ3	1.75	0.51
2:M:238:ALA:HB2	2:M:277:LYS:CE	2.40	0.51
1:P:48:ALA:HB2	1:P:111:LEU:CD1	2.39	0.51
1:P:366:LEU:O	1:P:370:LEU:N	2.30	0.51
1:P:455:LYS:HE3	1:P:634:PRO:HB2	1.93	0.51
2:C:2:THR:HG22	2:C:193:GLY:HA2	1.93	0.51
2:F:128:PRO:HG3	2:F:189:ALA:HA	1.93	0.51
2:F:187:HIS:O	2:F:191:GLN:NE2	2.43	0.51
2:F:253:ASP:N	2:F:253:ASP:OD1	2.42	0.51
3:I:29:ASN:HB3	3:I:65:LYS:HE3	1.93	0.51
3:I:71:ARG:HH22	3:I:118:LEU:HD23	1.76	0.51
3:G:29:ASN:HB3	3:G:65:LYS:HE3	1.93	0.51
4:H:537:ARG:NH2	3:J:110:GLN:OE1	2.40	0.51
3:J:71:ARG:HH22	3:J:118:LEU:HD23	1.76	0.51
1:P:178:ALA:N	4:H:288:MET:O	2.32	0.51
1:P:263:PHE:CD2	1:P:293:LYS:HD2	2.46	0.51
1:P:310:THR:HG21	1:P:334:SER:HB3	1.93	0.51
2:D:152:VAL:H	2:D:164:ASN:HB3	1.75	0.51
2:E:125:VAL:O	5:K:35:G:O2'	2.23	0.51
2:F:32:ILE:HG22	2:F:140:ILE:HD11	1.93	0.51
4:H:81:LEU:HD13	4:H:169:VAL:HG12	1.93	0.51
2:M:48:ARG:NH2	2:M:67:ILE:O	2.42	0.51
2:A:71:GLY:O	2:C:151:ALA:HB1	2.10	0.51
2:D:32:ILE:HD12	3:G:95:LEU:HD21	1.92	0.51
2:D:48:ARG:HA	2:D:51:ARG:HG2	1.92	0.51
2:D:188:PHE:O	2:D:192:THR:HG23	2.11	0.51
2:E:220:GLN:HG3	2:F:183:PHE:HZ	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:22:GLU:OE1	3:I:37:ALA:HB2	2.10	0.51
3:J:48:PRO:HG2	3:J:93:LEU:HG	1.92	0.51
5:K:27:G:N1	6:L:28:DC:N3	2.40	0.51
1:P:571:ARG:HH12	1:P:574:ALA:HB3	1.76	0.51
2:B:66:PHE:CD1	2:B:109:ILE:HD11	2.46	0.51
2:F:227:TYR:HB2	2:F:247:ILE:CD1	2.40	0.51
3:J:33:ASN:ND2	6:L:26:DC:H3'	2.18	0.51
6:L:52:DT:H3	8:O:8:DA:H61	1.59	0.51
7:N:5:LEU:HD11	7:N:41:ILE:HD12	1.93	0.51
7:N:66:ARG:HA	7:N:91:ALA:HA	1.93	0.51
7:N:83:ILE:HG13	7:N:84:GLU:N	2.25	0.51
1:P:229:ALA:HB1	1:P:296:LEU:HD11	1.92	0.51
2:B:71:GLY:O	2:M:151:ALA:HB1	2.11	0.51
3:J:29:ASN:HB3	3:J:65:LYS:HE3	1.93	0.51
1:P:7:ALA:HB2	1:P:22:LEU:HA	1.93	0.50
1:P:122:LEU:O	1:P:674:ARG:HG3	2.10	0.50
1:P:661:ALA:HA	1:P:671:ILE:HG12	1.92	0.50
2:A:144:GLU:HA	2:A:171:PHE:HA	1.94	0.50
2:B:35:GLN:HG2	2:M:141:MET:SD	2.50	0.50
2:B:145:HIS:HE1	2:C:40:LEU:HD13	1.76	0.50
2:D:177:LEU:HD23	2:D:249:VAL:HG11	1.93	0.50
3:G:52:PHE:HA	3:G:55:LEU:HB2	1.92	0.50
7:N:13:CYS:HB2	7:N:94:LEU:CD2	2.41	0.50
7:N:150:ARG:HE	7:N:152:LEU:HD21	1.76	0.50
1:P:147:SER:O	1:P:151:GLU:HB2	2.11	0.50
1:P:647:LYS:HZ1	4:H:160:ARG:CZ	2.24	0.50
2:A:14:ASP:OD2	2:A:224:ARG:NE	2.42	0.50
2:B:16:GLN:HB3	2:B:220:GLN:HB3	1.93	0.50
2:B:33:ASP:OD2	2:M:259:ARG:NE	2.36	0.50
2:B:196:GLU:O	2:B:200:GLU:HG2	2.10	0.50
2:D:89:LYS:HB3	2:D:94:LYS:HA	1.92	0.50
2:C:68:ARG:NE	2:C:69:GLU:H	2.01	0.50
2:F:65:ILE:HB	2:F:67:ILE:HG22	1.93	0.50
4:H:130:PHE:O	4:H:137:LYS:NZ	2.38	0.50
3:J:7:ARG:HG2	3:J:12:TYR:CD2	2.34	0.50
5:K:38:C:N4	5:K:40:C:HO2'	2.09	0.50
2:A:49:LYS:HB2	2:A:209:MET:SD	2.51	0.50
2:D:9:PHE:HB3	2:D:228:VAL:HG22	1.94	0.50
2:D:31:ARG:NE	2:D:42:THR:OG1	2.45	0.50
2:D:130:GLN:NE2	5:K:30:G:OP1	2.45	0.50
2:D:184:ILE:HD13	2:D:199:LEU:HD11	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:257:VAL:HG21	2:E:35:GLN:CB	2.34	0.50
2:F:188:PHE:HA	2:F:191:GLN:NE2	2.26	0.50
4:H:4:HIS:O	4:H:8:GLN:HB2	2.11	0.50
4:H:29:GLU:HG2	4:H:57:VAL:O	2.11	0.50
4:H:420:LEU:HD21	4:H:555:GLN:HB2	1.92	0.50
3:J:77:TRP:O	3:J:81:GLN:HG2	2.11	0.50
5:K:17:C:C2'	5:K:18:U:H5'	2.41	0.50
6:L:48:DA:H1'	6:L:49:DA:H5'	1.92	0.50
2:M:149:ARG:NH2	2:M:153:THR:HG23	2.26	0.50
2:M:188:PHE:HA	2:M:191:GLN:OE1	2.11	0.50
2:E:14:ASP:HA	2:E:176:GLY:O	2.12	0.50
4:H:152:VAL:HG23	4:H:155:CYS:HB2	1.93	0.50
4:H:324:LYS:HB3	4:H:344:GLU:O	2.12	0.50
4:H:397:LEU:HD13	4:H:401:ILE:HD11	1.93	0.50
4:H:467:ILE:HG13	4:H:547:PRO:HD3	1.93	0.50
3:J:52:PHE:HA	3:J:55:LEU:HB2	1.92	0.50
5:K:7:A:C5	7:N:69:GLU:OE1	2.65	0.50
5:K:21:C:H1'	5:K:22:C:O4'	2.12	0.50
2:M:54:ILE:HG21	2:M:107:TYR:CD2	2.46	0.50
8:O:22:DA:C8	8:O:23:DA:H2'	2.46	0.50
2:B:26:ALA:CB	4:H:417:GLN:HB3	2.42	0.50
2:D:7:TYR:HB2	2:D:184:ILE:HD12	1.94	0.50
4:H:554:GLN:HG3	4:H:557:LEU:HD12	1.93	0.50
2:M:58:GLN:HG3	2:M:63:HIS:HB3	1.94	0.50
7:N:18:GLU:HG2	7:N:19:LEU:H	1.75	0.50
7:N:194:GLN:HG3	7:N:201:VAL:CG2	2.40	0.50
2:A:130:GLN:NE2	2:C:215:SER:HA	2.26	0.50
2:B:145:HIS:CE1	2:C:40:LEU:HD13	2.47	0.50
2:D:13:PHE:HA	2:D:224:ARG:H	1.77	0.50
1:P:37:ALA:HB1	1:P:41:GLY:H	1.77	0.50
1:P:305:TYR:HD1	1:P:390:ILE:HB	1.77	0.50
1:P:556:GLN:HA	1:P:559:GLU:HG3	1.93	0.50
2:C:144:GLU:HA	2:C:171:PHE:HA	1.92	0.50
2:C:246:ARG:HD3	2:C:273:LEU:HD23	1.92	0.50
2:E:243:LEU:HA	2:E:246:ARG:HD2	1.94	0.50
2:M:186:THR:HG21	2:M:234:ASN:HA	1.92	0.50
7:N:56:ILE:H	7:N:56:ILE:HD12	1.76	0.50
7:N:68:ASN:HB3	7:N:87:ARG:CZ	2.40	0.50
7:N:98:VAL:HB	7:N:100:TYR:CE2	2.47	0.50
1:P:276:THR:HG22	1:P:427:GLN:OE1	2.12	0.50
1:P:515:LYS:HB3	1:P:551:TRP:HE1	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:65:ILE:O	2:A:66:PHE:HB2	2.12	0.50
2:B:42:THR:HG22	2:B:133:PHE:HE2	1.76	0.50
2:B:126:ARG:HD3	5:K:11:G:H5"	1.94	0.50
2:E:203:TRP:HB3	2:E:282:LEU:HD22	1.94	0.50
2:F:11:PHE:CD1	2:F:226:LEU:HD12	2.46	0.50
3:I:16:ARG:NE	3:I:108:GLU:OE1	2.42	0.50
4:H:28:LYS:HG2	4:H:82:TRP:CZ3	2.47	0.50
4:H:360:ASP:CG	4:H:446:ARG:HH22	2.15	0.50
2:M:64:ASP:O	2:M:107:TYR:N	2.43	0.50
1:P:44:PHE:HD1	1:P:166:LEU:HG	1.77	0.50
1:P:187:MET:HB2	1:P:673:PHE:HZ	1.76	0.50
1:P:354:TRP:CE2	1:P:380:LYS:HD2	2.46	0.50
1:P:402:GLN:HE22	1:P:645:ASN:HD22	1.60	0.50
2:B:231:HIS:CD2	2:B:277:LYS:NZ	2.80	0.50
2:D:91:LYS:HD2	2:D:92:GLY:N	2.26	0.50
2:F:13:PHE:HE1	2:F:134:SER:HG	1.60	0.50
3:I:77:TRP:O	3:I:81:GLN:HG2	2.11	0.50
4:H:196:LEU:CD2	7:N:18:GLU:HB3	2.42	0.50
4:H:210:ALA:HB1	4:H:218:PRO:HB2	1.92	0.50
5:K:8:C:H4'	2:M:45:CYS:HA	1.94	0.50
1:P:64:TYR:HE1	1:P:87:ARG:H	1.58	0.49
1:P:106:PHE:HB2	4:H:285:LEU:HD13	1.94	0.49
1:P:230:ARG:NH2	1:P:234:GLU:HG3	2.27	0.49
1:P:618:ILE:HG12	1:P:647:LYS:HE3	1.93	0.49
2:A:20:PRO:HG2	2:A:178:TYR:OH	2.12	0.49
2:A:23:ASP:O	2:A:31:ARG:NE	2.45	0.49
2:A:40:LEU:HD13	2:C:145:HIS:CE1	2.47	0.49
2:A:170:LYS:HZ2	2:D:44:VAL:HG13	1.77	0.49
2:A:246:ARG:HH22	2:A:273:LEU:H	1.60	0.49
2:D:8:ASP:O	2:D:229:PHE:HD1	1.95	0.49
2:C:137:ILE:HG12	2:C:177:LEU:O	2.11	0.49
2:E:41:VAL:HB	2:E:134:SER:HB2	1.94	0.49
3:I:58:LEU:HD11	6:L:17:DG:O3'	2.11	0.49
3:G:22:GLU:OE1	3:G:37:ALA:HB2	2.10	0.49
3:G:77:TRP:O	3:G:81:GLN:HG2	2.11	0.49
4:H:136:GLU:HA	4:H:139:LYS:HD3	1.94	0.49
1:P:107:PHE:HE1	1:P:170:PHE:CD2	2.30	0.49
2:C:22:GLY:O	2:C:24:PRO:HD3	2.13	0.49
2:C:228:VAL:HG21	2:C:282:LEU:HD12	1.94	0.49
2:E:44:VAL:HG12	5:K:37:C:OP2	2.13	0.49
2:E:45:CYS:SG	5:K:38:C:O2'	2.70	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:104:SER:O	2:F:110:ARG:NH2	2.45	0.49
2:F:117:THR:HB	2:F:121:ASN:HD22	1.77	0.49
4:H:69:ARG:HD2	4:H:87:TYR:OH	2.12	0.49
4:H:107:PHE:CE2	4:H:159:PHE:HE2	2.29	0.49
4:H:208:HIS:CE1	4:H:242:ILE:HD12	2.44	0.49
2:M:102:MET:CE	7:N:76:GLU:HA	2.41	0.49
2:M:278:LEU:HD13	2:M:280:ARG:NH1	2.26	0.49
7:N:42:LEU:HD23	7:N:125:PHE:HB2	1.94	0.49
1:P:288:LEU:HD21	1:P:292:LEU:HD12	1.94	0.49
1:P:428:PRO:HB2	1:P:430:LEU:HG	1.94	0.49
2:A:152:VAL:HG11	2:A:159:SER:HB3	1.94	0.49
2:A:170:LYS:NZ	2:A:216:ALA:HB1	2.28	0.49
2:B:151:ALA:HB2	2:C:67:ILE:O	2.12	0.49
2:D:280:ARG:NH2	2:D:282:LEU:HD11	2.26	0.49
2:C:232:SER:HB3	2:C:276:THR:O	2.12	0.49
2:C:249:VAL:HG13	2:C:266:VAL:HG22	1.94	0.49
2:E:69:GLU:HG2	2:E:70:LYS:HE2	1.94	0.49
2:E:130:GLN:O	2:E:182:GLY:HA2	2.12	0.49
2:E:179:ARG:NH2	2:E:247:ILE:O	2.46	0.49
2:E:249:VAL:HG22	2:E:266:VAL:HG22	1.92	0.49
4:H:265:ARG:HG2	4:H:270:THR:HG22	1.94	0.49
4:H:265:ARG:NH2	8:O:17:DA:H1'	2.27	0.49
7:N:18:GLU:HG2	7:N:19:LEU:N	2.28	0.49
7:N:29:ILE:HG23	7:N:54:ILE:HG12	1.93	0.49
1:P:154:LEU:HD12	1:P:158:PHE:CD2	2.48	0.49
1:P:434:ILE:O	1:P:441:ILE:HB	2.12	0.49
1:P:594:GLN:HG2	1:P:595:LEU:N	2.27	0.49
2:A:160:GLU:CG	2:A:161:THR:H	2.25	0.49
2:C:102:MET:HB3	2:C:109:ILE:HD13	1.94	0.49
2:C:131:LEU:HD11	2:C:202:PHE:CZ	2.46	0.49
2:F:167:MET:HB2	2:F:169:ARG:HH22	1.78	0.49
5:K:5:A:H1'	2:M:124:GLN:CB	2.42	0.49
6:L:9:DG:H2'	6:L:10:DA:C4	2.48	0.49
2:M:65:ILE:O	2:M:108:ASP:HB3	2.12	0.49
1:P:104:ASN:HB2	1:P:163:ASP:OD2	2.12	0.49
1:P:364:VAL:O	1:P:368:GLU:HB2	2.12	0.49
1:P:571:ARG:HD2	1:P:579:ILE:HD13	1.94	0.49
2:D:62:HIS:O	2:D:110:ARG:NH1	2.46	0.49
2:D:211:ASP:OD2	2:E:239:PRO:HA	2.12	0.49
2:C:128:PRO:HG2	2:C:194:PHE:CB	2.43	0.49
2:C:215:SER:HB2	2:C:218:ARG:H	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:229:PHE:HB3	2:C:277:LYS:CE	2.42	0.49
2:E:229:PHE:HZ	2:E:247:ILE:HG12	1.78	0.49
4:H:467:ILE:HD11	4:H:545:ARG:O	2.13	0.49
7:N:48:ARG:HB2	7:N:109:THR:HG22	1.95	0.49
2:A:69:GLU:O	2:C:164:ASN:HB2	2.12	0.49
2:A:170:LYS:HZ3	2:A:216:ALA:HB1	1.78	0.49
2:B:24:PRO:HG3	5:K:15:A:H2'	1.95	0.49
2:D:56:MET:SD	2:D:212:HIS:HB3	2.52	0.49
2:E:13:PHE:O	2:E:177:LEU:HD12	2.12	0.49
3:G:71:ARG:HH22	3:G:118:LEU:HD23	1.76	0.49
4:H:48:THR:HG21	4:H:61:PHE:CZ	2.47	0.49
4:H:164:GLU:HB3	4:H:167:ASP:HB2	1.95	0.49
1:P:44:PHE:HE2	1:P:110:LEU:HD22	1.76	0.49
1:P:47:TYR:CE1	1:P:160:PRO:HG2	2.48	0.49
2:D:152:VAL:HG12	2:D:166:THR:HG23	1.94	0.49
2:D:153:THR:HA	2:E:73:LEU:HB2	1.93	0.49
2:F:126:ARG:HA	5:K:41:G:O3'	2.13	0.49
1:P:69:SER:HG	11:P:803:PO4:P	2.27	0.49
1:P:708:ILE:HG23	1:P:709:VAL:HG13	1.95	0.49
2:A:42:THR:HG22	2:A:133:PHE:CZ	2.48	0.49
2:A:68:ARG:HG3	2:C:150:MET:SD	2.53	0.49
2:A:145:HIS:CE1	2:D:40:LEU:HD13	2.48	0.49
2:D:149:ARG:NH2	2:D:166:THR:OG1	2.41	0.49
2:E:231:HIS:HD1	2:E:236:GLY:HA2	1.78	0.49
3:I:95:LEU:HA	3:I:98:GLN:HB2	1.95	0.49
3:I:110:GLN:O	3:I:114:THR:HG23	2.13	0.49
4:H:83:ASP:HB3	4:H:87:TYR:CB	2.42	0.49
5:K:3:U:C5	7:N:184:ASP:HB3	2.47	0.49
2:M:48:ARG:NH2	2:M:67:ILE:HG22	2.28	0.49
2:M:246:ARG:HD3	2:M:269:ASP:O	2.12	0.49
1:P:581:GLN:NE2	1:P:585:ARG:HH22	2.11	0.49
1:P:745:PRO:C	1:P:748:PRO:HD3	2.33	0.49
2:A:6:ARG:NH1	2:A:8:ASP:OD2	2.46	0.49
2:C:17:ASP:O	2:C:219:GLY:HA3	2.12	0.49
2:E:27:GLY:HA3	3:G:40:TYR:HE1	1.78	0.49
2:F:126:ARG:HD3	2:F:188:PHE:CE1	2.47	0.49
4:H:396:ASP:HB2	2:M:169:ARG:NH1	2.27	0.49
5:K:1:G:N2	7:N:39:MET:O	2.41	0.49
5:K:14:C:O2'	5:K:16:G:OP1	2.30	0.49
1:P:28:LYS:NZ	1:P:210:ALA:O	2.40	0.49
1:P:32:LEU:HD23	1:P:197:ALA:HA	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:36:THR:HG23	2:C:259:ARG:HG3	1.95	0.49
2:A:74:ASN:HB2	2:C:154:ASN:HA	1.94	0.49
2:B:114:ALA:H	2:B:125:VAL:HG23	1.77	0.49
2:E:51:ARG:HH22	5:K:37:C:P	2.35	0.49
2:F:30:PRO:O	2:F:32:ILE:HG23	2.13	0.49
3:I:98:GLN:NE2	3:J:57:ARG:NH2	2.60	0.49
6:L:43:DC:H3'	6:L:44:DC:H5"	1.94	0.49
2:M:11:PHE:CG	2:M:206:LEU:HD23	2.47	0.49
1:P:98:TYR:OH	1:P:102:ARG:NH2	2.40	0.48
2:D:138:ASP:OD2	2:D:251:LYS:HG3	2.12	0.48
2:E:220:GLN:OE1	2:F:181:HIS:ND1	2.41	0.48
4:H:32:PHE:CG	4:H:149:CYS:HB3	2.48	0.48
4:H:168:LEU:H	4:H:171:GLN:HG3	1.78	0.48
4:H:224:VAL:O	4:H:236:GLN:HA	2.13	0.48
4:H:227:SER:HB2	7:N:72:THR:HA	1.94	0.48
4:H:422:ARG:NH2	4:H:426:GLU:OE1	2.44	0.48
5:K:6:A:H5"	2:M:112:PHE:O	2.13	0.48
5:K:12:G:H21	2:M:149:ARG:NH1	2.11	0.48
2:M:54:ILE:HG13	2:M:107:TYR:CE2	2.48	0.48
2:M:228:VAL:HG21	2:M:282:LEU:HD12	1.95	0.48
1:P:518:LEU:HD11	1:P:527:CYS:SG	2.52	0.48
2:A:174:PRO:HB2	2:A:259:ARG:NH1	2.28	0.48
2:B:26:ALA:HB2	4:H:417:GLN:HB3	1.95	0.48
2:B:54:ILE:HG13	2:B:107:TYR:CE2	2.48	0.48
2:C:154:ASN:N	2:C:154:ASN:OD1	2.45	0.48
2:F:250:VAL:O	2:F:265:LEU:HD23	2.13	0.48
3:I:19:ALA:HB3	3:I:108:GLU:HB3	1.95	0.48
3:I:110:GLN:HA	3:J:80:ARG:NH1	2.27	0.48
3:G:94:ASN:HB3	3:G:97:GLN:HG2	1.95	0.48
4:H:245:GLN:O	4:H:249:GLU:HG3	2.13	0.48
4:H:445:ILE:HD11	4:H:453:MET:HB2	1.94	0.48
4:H:514:ARG:CG	3:J:42:GLY:HA2	2.43	0.48
3:J:110:GLN:O	3:J:114:THR:HG23	2.13	0.48
6:L:9:DG:H2'	6:L:10:DA:C5	2.47	0.48
2:M:134:SER:OG	2:M:180:CYS:HB2	2.13	0.48
1:P:181:GLU:HA	1:P:660:THR:HA	1.93	0.48
1:P:254:GLU:HA	1:P:257:ALA:HB3	1.96	0.48
1:P:558:ILE:HG22	1:P:585:ARG:HG3	1.95	0.48
2:B:107:TYR:HD1	2:B:110:ARG:HH11	1.60	0.48
2:B:134:SER:HB3	2:B:180:CYS:HB2	1.95	0.48
2:D:165:ARG:HB2	6:L:16:DA:H1'	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:68:ARG:HG3	2:C:69:GLU:H	1.78	0.48
2:E:13:PHE:HA	2:E:224:ARG:H	1.79	0.48
2:E:115:VAL:HG22	5:K:35:G:C4	2.48	0.48
2:E:268:VAL:HG21	2:E:281:LYS:HE3	1.94	0.48
2:F:134:SER:HB2	2:F:180:CYS:HB2	1.95	0.48
3:G:71:ARG:NH2	3:G:118:LEU:HD23	2.29	0.48
4:H:34:ILE:O	4:H:160:ARG:N	2.33	0.48
4:H:474:LEU:HD12	4:H:536:ILE:HG13	1.95	0.48
2:M:25:ASP:OD1	7:N:66:ARG:HG3	2.13	0.48
2:M:203:TRP:HE3	2:M:226:LEU:HD21	1.78	0.48
7:N:4:ILE:HG22	7:N:4:ILE:O	2.14	0.48
7:N:16:ARG:HG2	7:N:26:TYR:CD1	2.49	0.48
1:P:126:TYR:CD2	4:H:302:ASP:HB2	2.49	0.48
1:P:329:VAL:HG23	1:P:347:THR:HG22	1.94	0.48
1:P:678:GLU:O	1:P:681:HIS:NE2	2.46	0.48
2:D:48:ARG:HG2	5:K:32:A:O4'	2.14	0.48
2:C:44:VAL:HG12	5:K:19:U:OP2	2.13	0.48
2:F:10:VAL:HG22	2:F:181:HIS:HD2	1.78	0.48
2:F:99:ARG:NH2	2:F:191:GLN:O	2.37	0.48
2:F:129:VAL:HG22	2:F:184:ILE:CG1	2.43	0.48
2:F:169:ARG:HB3	2:F:171:PHE:CE1	2.49	0.48
4:H:3:LEU:HD21	4:H:221:PHE:CE2	2.47	0.48
1:P:231:ARG:HH12	1:P:292:LEU:HD13	1.78	0.48
1:P:564:LEU:HD13	1:P:566:PHE:HE1	1.78	0.48
1:P:613:LYS:HE3	4:H:47:ASP:OD2	2.13	0.48
1:P:643:ARG:HB3	1:P:647:LYS:HE3	1.95	0.48
2:B:54:ILE:HG13	2:B:107:TYR:CD2	2.48	0.48
2:D:13:PHE:CZ	2:D:46:LEU:HD21	2.49	0.48
2:C:76:LEU:HD23	2:C:106:TYR:CZ	2.48	0.48
2:E:13:PHE:CE1	2:E:46:LEU:HD11	2.48	0.48
2:F:43:ASP:HB3	2:F:132:THR:C	2.34	0.48
2:F:51:ARG:NH2	5:K:43:C:H5"	2.29	0.48
2:F:62:HIS:HA	2:F:104:SER:O	2.14	0.48
3:G:25:GLN:OE1	3:G:36:ILE:N	2.42	0.48
4:H:273:CYS:SG	4:H:301:ILE:HB	2.54	0.48
4:H:301:ILE:HG13	4:H:305:LYS:HD3	1.96	0.48
4:H:482:GLN:HG3	4:H:519:HIS:CE1	2.48	0.48
2:M:149:ARG:HE	2:M:166:THR:CG2	2.24	0.48
1:P:125:TRP:NE1	1:P:667:ASN:OD1	2.31	0.48
1:P:669:LEU:O	1:P:669:LEU:HD23	2.14	0.48
2:A:68:ARG:HG2	2:A:69:GLU:H	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:195:SER:H	2:A:198:ASP:HB2	1.79	0.48
2:B:51:ARG:HE	2:B:108:ASP:CG	2.17	0.48
2:E:3:ILE:HD12	2:E:196:GLU:HG3	1.95	0.48
3:G:7:ARG:HG2	3:G:12:TYR:CD2	2.34	0.48
4:H:287:SER:OG	4:H:288:MET:SD	2.71	0.48
3:J:95:LEU:HA	3:J:98:GLN:HB2	1.95	0.48
7:N:35:ARG:NH1	7:N:174:ASP:OD1	2.43	0.48
7:N:171:MET:HG3	7:N:194:GLN:NE2	2.26	0.48
8:O:16:DA:H1'	8:O:17:DA:H5'	1.95	0.48
1:P:96:ALA:O	1:P:100:VAL:HG13	2.13	0.48
2:B:56:MET:SD	2:B:212:HIS:HB3	2.54	0.48
2:B:246:ARG:HD3	2:B:273:LEU:HD23	1.96	0.48
2:D:77:ILE:HA	2:D:102:MET:CE	2.43	0.48
2:D:273:LEU:HB2	2:D:277:LYS:HE2	1.95	0.48
2:E:69:GLU:O	2:E:71:GLY:N	2.43	0.48
3:G:110:GLN:O	3:G:114:THR:HG23	2.13	0.48
7:N:128:ARG:HG2	7:N:133:GLN:HB2	1.96	0.48
1:P:189:PHE:HD2	1:P:190:LEU:HD12	1.79	0.48
1:P:424:THR:HG21	1:P:428:PRO:HD3	1.95	0.48
1:P:651:ASP:OD2	1:P:656:THR:HG22	2.14	0.48
2:A:134:SER:HB3	2:A:178:TYR:HB3	1.95	0.48
2:B:47:LYS:HD3	5:K:13:U:OP1	2.14	0.48
2:B:109:ILE:HD13	2:B:116:MET:CE	2.43	0.48
2:D:68:ARG:NH2	2:D:69:GLU:HB2	2.28	0.48
2:D:116:MET:C	2:D:118:THR:H	2.17	0.48
2:D:270:ASP:OD1	2:D:270:ASP:N	2.38	0.48
2:F:13:PHE:CZ	2:F:46:LEU:HD21	2.48	0.48
2:F:270:ASP:HA	2:F:273:LEU:HD21	1.96	0.48
4:H:3:LEU:HA	4:H:6:LEU:HD12	1.95	0.48
4:H:85:TYR:HE1	4:H:93:GLY:H	1.62	0.48
4:H:471:LEU:HD23	4:H:505:PRO:HB3	1.95	0.48
2:M:102:MET:HG3	2:M:116:MET:SD	2.53	0.48
2:M:128:PRO:HG2	2:M:194:PHE:CD2	2.49	0.48
1:P:576:LEU:HA	1:P:579:ILE:HB	1.96	0.48
2:B:18:GLY:O	2:B:20:PRO:HD3	2.14	0.48
2:B:146:SER:HB2	2:B:169:ARG:NH2	2.29	0.48
2:E:144:GLU:HG2	2:E:171:PHE:HE1	1.78	0.48
2:E:156:LYS:HZ2	2:E:158:ALA:HB3	1.79	0.48
2:F:243:LEU:HD11	2:F:277:LYS:CD	2.43	0.48
3:G:49:ILE:HD13	3:G:91:ASN:OD1	2.14	0.48
4:H:40:GLY:HA2	4:H:130:PHE:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:127:VAL:HA	4:H:130:PHE:HB3	1.96	0.48
4:H:392:ASN:HB3	4:H:398:ILE:HG23	1.96	0.48
4:H:482:GLN:HG3	4:H:519:HIS:NE2	2.29	0.48
5:K:13:U:C4	2:M:147:ILE:HD11	2.49	0.48
6:L:39:DC:H2"	6:L:40:DT:H5'	1.95	0.48
2:M:20:PRO:HD2	2:M:30:PRO:HB3	1.95	0.48
2:M:96:GLU:OE2	2:M:99:ARG:NH2	2.47	0.48
2:M:140:ILE:HB	2:M:173:VAL:HG13	1.95	0.48
7:N:7:ILE:HD11	7:N:37:ILE:HG21	1.95	0.48
9:Q:-1:DA:OP2	9:Q:-1:DA:H8	1.96	0.48
1:P:21:PRO:HG2	1:P:24:LYS:NZ	2.29	0.48
1:P:30:ALA:CB	1:P:50:LEU:HD12	2.44	0.48
1:P:170:PHE:HZ	1:P:178:ALA:HB2	1.77	0.48
1:P:184:HIS:CG	1:P:659:LEU:HB3	2.49	0.48
2:B:89:LYS:O	2:B:94:LYS:N	2.47	0.48
2:F:83:GLN:O	2:F:86:VAL:N	2.46	0.48
2:F:215:SER:HB3	2:F:218:ARG:HB2	1.95	0.48
3:G:95:LEU:HA	3:G:98:GLN:HB2	1.95	0.48
4:H:42:PHE:HB2	4:H:130:PHE:HE1	1.79	0.48
4:H:240:PHE:HB3	7:N:17:SER:C	2.34	0.48
3:J:71:ARG:NH2	3:J:118:LEU:HD23	2.29	0.48
1:P:506:PHE:CD1	1:P:517:HIS:HB2	2.49	0.47
2:A:91:LYS:HD2	2:A:92:GLY:N	2.29	0.47
2:B:51:ARG:CZ	2:B:108:ASP:OD1	2.62	0.47
2:D:31:ARG:HB2	2:D:40:LEU:O	2.14	0.47
3:I:71:ARG:NH2	3:I:118:LEU:HD23	2.28	0.47
6:L:23:DT:H5'	6:L:23:DT:O2	2.14	0.47
2:M:13:PHE:O	2:M:177:LEU:HD12	2.14	0.47
7:N:8:SER:HA	7:N:99:ALA:HA	1.96	0.47
1:P:487:ALA:HA	1:P:551:TRP:CZ3	2.49	0.47
2:A:21:ASN:HD22	2:A:42:THR:N	2.04	0.47
2:B:77:ILE:HG23	2:B:122:ALA:CB	2.44	0.47
2:B:102:MET:CE	2:B:122:ALA:HB1	2.44	0.47
2:B:152:VAL:HB	2:B:164:ASN:HB3	1.96	0.47
2:D:137:ILE:HG12	2:D:177:LEU:O	2.14	0.47
2:E:143:LEU:HG	2:E:145:HIS:CE1	2.49	0.47
2:F:45:CYS:O	2:F:49:LYS:HG2	2.13	0.47
1:P:354:TRP:CD2	1:P:359:ILE:HG12	2.50	0.47
1:P:518:LEU:HA	1:P:522:MET:SD	2.54	0.47
1:P:580:ALA:HB2	1:P:637:PHE:CZ	2.49	0.47
2:A:34:PRO:HB3	3:J:47:THR:HG23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:199:LEU:HD21	2:A:203:TRP:HE1	1.79	0.47
2:C:115:VAL:HG22	5:K:17:C:C2	2.50	0.47
2:E:246:ARG:NE	2:E:273:LEU:HD23	2.18	0.47
2:F:40:LEU:HD21	2:F:135:ARG:NH1	2.29	0.47
3:I:7:ARG:CG	3:I:12:TYR:HD2	2.22	0.47
3:J:44:ALA:HB2	3:J:51:VAL:HG21	1.96	0.47
5:K:7:A:OP1	2:M:47:LYS:HD3	2.15	0.47
2:M:233:ASN:OD1	2:M:237:ASP:HB3	2.14	0.47
7:N:168:PHE:HB2	7:N:194:GLN:NE2	2.30	0.47
8:O:19:DA:H1'	8:O:20:DA:C4	2.49	0.47
1:P:69:SER:OG	11:P:803:PO4:P	2.71	0.47
1:P:123:ALA:HB1	1:P:129:GLY:O	2.14	0.47
2:A:129:VAL:HG11	2:A:202:PHE:CZ	2.49	0.47
3:I:25:GLN:OE1	3:I:36:ILE:N	2.42	0.47
3:I:49:ILE:HD13	3:I:91:ASN:OD1	2.14	0.47
3:G:19:ALA:HB3	3:G:108:GLU:HB3	1.95	0.47
1:P:381:ILE:H	1:P:381:ILE:HD12	1.78	0.47
1:P:518:LEU:HD23	1:P:558:ILE:HG12	1.96	0.47
2:C:81:HIS:NE2	2:C:120:LYS:O	2.47	0.47
2:E:65:ILE:HB	2:E:67:ILE:HG22	1.96	0.47
2:E:79:GLU:HA	2:E:82:GLU:HG2	1.96	0.47
2:F:42:THR:HG23	2:F:133:PHE:CE2	2.50	0.47
4:H:361:LEU:HD11	4:H:380:LEU:HD21	1.96	0.47
4:H:431:TYR:HB2	4:H:563:TYR:OH	2.15	0.47
4:H:490:ASN:HD21	6:L:32:DC:H3'	1.78	0.47
6:L:23:DT:O2	6:L:23:DT:H2'	2.14	0.47
2:M:6:ARG:HD3	2:M:236:GLY:HA3	1.96	0.47
2:M:42:THR:HG21	7:N:67:ARG:HG2	1.96	0.47
1:P:186:TRP:HD1	1:P:416:TYR:HH	1.61	0.47
2:A:174:PRO:HB2	2:A:259:ARG:HH12	1.79	0.47
2:D:91:LYS:HA	2:D:94:LYS:HB3	1.96	0.47
2:D:112:PHE:HE1	2:D:131:LEU:HD13	1.80	0.47
2:D:121:ASN:ND2	2:C:163:ASP:OD2	2.46	0.47
2:C:11:PHE:HE1	2:C:223:ALA:HB1	1.80	0.47
2:C:32:ILE:HD11	4:H:507:ALA:HA	1.97	0.47
2:C:68:ARG:HG3	2:C:69:GLU:N	2.30	0.47
2:C:258:VAL:HG11	2:C:264:TYR:CZ	2.49	0.47
3:I:44:ALA:HB2	3:I:51:VAL:HG21	1.96	0.47
4:H:31:PRO:HB2	4:H:32:PHE:CD2	2.50	0.47
4:H:37:ASP:HA	4:H:162:VAL:HG12	1.96	0.47
4:H:535:GLU:OE2	4:H:569:LEU:HD21	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:19:ALA:HB3	3:J:108:GLU:HB3	1.95	0.47
5:K:3:U:O2	7:N:35:ARG:NH1	2.42	0.47
2:M:6:ARG:NH2	2:M:236:GLY:HA3	2.30	0.47
2:M:103:CYS:SG	2:M:125:VAL:HG11	2.54	0.47
2:M:133:PHE:HZ	7:N:67:ARG:HD3	1.79	0.47
1:P:55:GLY:O	1:P:58:GLN:HB2	2.14	0.47
1:P:345:ALA:H	1:P:348:ARG:HB3	1.80	0.47
1:P:399:ARG:NH2	1:P:614:GLN:OE1	2.33	0.47
2:A:135:ARG:NE	2:C:17:ASP:OD2	2.36	0.47
2:A:143:LEU:HD21	2:D:34:PRO:HG2	1.97	0.47
2:A:147:ILE:HD11	5:K:31:C:C4	2.50	0.47
2:A:218:ARG:HD3	2:A:221:MET:HE2	1.96	0.47
2:B:17:ASP:CG	2:C:135:ARG:HH22	2.18	0.47
2:D:22:GLY:HA3	2:D:28:ASN:OD1	2.15	0.47
2:D:102:MET:HG3	2:D:116:MET:SD	2.55	0.47
2:D:246:ARG:NE	2:D:269:ASP:O	2.36	0.47
2:C:33:ASP:N	2:C:38:GLU:O	2.38	0.47
2:C:142:THR:HG22	2:C:144:GLU:HG3	1.97	0.47
3:G:7:ARG:CG	3:G:12:TYR:HD2	2.22	0.47
3:G:48:PRO:CG	3:G:93:LEU:HG	2.45	0.47
4:H:24:GLY:HA2	4:H:183:ASN:HD22	1.78	0.47
4:H:127:VAL:O	4:H:131:LEU:N	2.45	0.47
4:H:437:LEU:C	4:H:560:ILE:HD11	2.35	0.47
4:H:474:LEU:HD23	4:H:509:PHE:CD1	2.50	0.47
3:J:88:ARG:NH2	3:J:90:PRO:HA	2.30	0.47
5:K:5:A:H1'	2:M:124:GLN:HB3	1.97	0.47
2:A:109:ILE:HD13	2:A:116:MET:SD	2.54	0.47
2:D:243:LEU:HD23	2:D:246:ARG:HD2	1.97	0.47
2:E:40:LEU:HD23	2:E:133:PHE:CD2	2.47	0.47
2:F:58:GLN:HE21	2:F:63:HIS:CD2	2.32	0.47
4:H:42:PHE:HB2	4:H:130:PHE:CE1	2.50	0.47
3:J:48:PRO:CG	3:J:93:LEU:HG	2.45	0.47
3:J:49:ILE:HD13	3:J:91:ASN:OD1	2.14	0.47
2:M:48:ARG:HH22	2:M:67:ILE:HG22	1.79	0.47
2:M:120:LYS:HE3	7:N:183:ARG:HB2	1.97	0.47
1:P:224:ALA:HB3	1:P:350:ALA:HB2	1.97	0.47
2:A:144:GLU:OE1	3:J:54:THR:HG22	2.15	0.47
2:B:126:ARG:CD	5:K:11:G:H5"	2.45	0.47
2:B:149:ARG:NH2	2:B:153:THR:HG1	2.12	0.47
2:D:126:ARG:HG3	5:K:29:G:H5"	1.96	0.47
2:D:129:VAL:HG13	2:D:184:ILE:HG12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:149:ARG:HG2	2:C:151:ALA:H	1.80	0.47
2:E:229:PHE:CE2	2:E:279:LEU:HD11	2.49	0.47
3:G:88:ARG:NH2	3:G:90:PRO:HA	2.30	0.47
4:H:328:LEU:HB2	4:H:342:TRP:CZ3	2.49	0.47
5:K:17:C:H2'	5:K:18:U:H5'	1.97	0.47
2:M:40:LEU:HD12	2:M:133:PHE:HB3	1.97	0.47
7:N:7:ILE:HD13	7:N:149:PHE:HB3	1.96	0.47
7:N:198:VAL:HG23	7:N:199:ASN:N	2.28	0.47
2:D:91:LYS:HD3	2:C:160:GLU:O	2.15	0.47
3:I:48:PRO:CG	3:I:93:LEU:HG	2.45	0.47
3:G:33:ASN:N	6:L:13:DG:OP2	2.43	0.47
4:H:461:ASP:O	4:H:463:ASN:N	2.43	0.47
3:J:94:ASN:HB3	3:J:97:GLN:HG2	1.95	0.47
5:K:3:U:C6	7:N:184:ASP:HB3	2.50	0.47
1:P:30:ALA:HB1	1:P:50:LEU:HD12	1.97	0.46
1:P:32:LEU:HD13	1:P:213:ASP:HB3	1.98	0.46
1:P:256:HIS:O	1:P:260:GLN:HB2	2.15	0.46
1:P:306:ALA:HA	1:P:361:THR:O	2.15	0.46
1:P:492:VAL:HG22	1:P:568:CYS:SG	2.54	0.46
2:A:69:GLU:O	2:A:71:GLY:N	2.47	0.46
2:A:215:SER:HB3	2:A:218:ARG:HG2	1.98	0.46
2:B:47:LYS:O	2:B:51:ARG:HG3	2.14	0.46
2:B:143:LEU:HA	2:B:143:LEU:HD23	1.66	0.46
2:B:148:THR:O	5:K:20:G:H5"	2.15	0.46
2:D:131:LEU:HD11	2:D:202:PHE:HZ	1.79	0.46
2:E:246:ARG:HB3	2:E:269:ASP:HB2	1.97	0.46
3:I:94:ASN:HB3	3:I:97:GLN:HG2	1.96	0.46
3:G:44:ALA:HB2	3:G:51:VAL:HG21	1.96	0.46
4:H:393:LEU:HB2	4:H:397:LEU:HD23	1.97	0.46
4:H:395:SER:OG	2:M:169:ARG:NH1	2.47	0.46
4:H:411:LEU:HD23	4:H:415:LEU:CD1	2.45	0.46
4:H:420:LEU:O	4:H:424:LYS:HG2	2.15	0.46
7:N:36:ASN:ND2	7:N:139:TYR:OH	2.38	0.46
1:P:20:HIS:HB2	1:P:205:PHE:CD2	2.51	0.46
1:P:103:LEU:CD2	1:P:166:LEU:HD13	2.46	0.46
1:P:104:ASN:OD1	1:P:105:PRO:HD2	2.15	0.46
1:P:199:PHE:CE1	1:P:203:GLU:HG3	2.50	0.46
1:P:270:ARG:HB2	1:P:273:PHE:CZ	2.51	0.46
2:A:23:ASP:HB2	2:A:28:ASN:HA	1.97	0.46
2:A:252:LYS:HE2	2:A:262:ASP:O	2.14	0.46
2:B:5:LYS:HD3	2:B:231:HIS:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:183:PHE:CZ	2:M:220:GLN:HG3	2.49	0.46
2:E:229:PHE:CZ	2:E:279:LEU:HD11	2.50	0.46
2:F:129:VAL:HG22	2:F:184:ILE:HG12	1.97	0.46
3:I:112:LEU:HD23	3:I:112:LEU:HA	1.66	0.46
3:G:21:LEU:HD21	3:G:59:LEU:HD22	1.98	0.46
4:H:173:LYS:HD2	4:H:173:LYS:O	2.15	0.46
4:H:226:LEU:HD23	4:H:226:LEU:HA	1.84	0.46
5:K:8:C:O2'	7:N:68:ASN:OD1	2.33	0.46
6:L:20:DC:H2"	6:L:21:DG:C8	2.50	0.46
7:N:180:SER:HB3	7:N:184:ASP:HA	1.96	0.46
1:P:9:ALA:HB1	1:P:71:PHE:HB2	1.97	0.46
1:P:36:PHE:CD1	1:P:382:HIS:CE1	3.04	0.46
1:P:536:ARG:HG2	1:P:721:LEU:HD11	1.97	0.46
2:A:269:ASP:OD1	2:A:269:ASP:N	2.46	0.46
2:B:35:GLN:HG3	2:M:257:VAL:HG21	1.98	0.46
2:B:72:ILE:H	2:B:72:ILE:HD12	1.81	0.46
2:B:126:ARG:HG2	2:B:188:PHE:CE1	2.50	0.46
2:B:218:ARG:NH2	5:K:16:G:H5'	2.30	0.46
2:D:259:ARG:NH1	2:E:35:GLN:HB2	2.31	0.46
2:C:179:ARG:NH1	2:C:181:HIS:HE1	2.14	0.46
2:E:149:ARG:HB2	5:K:43:C:H1'	1.96	0.46
2:E:153:THR:HB	6:L:13:DG:H4'	1.98	0.46
4:H:224:VAL:HG22	7:N:21:VAL:HG13	1.96	0.46
4:H:269:VAL:O	4:H:269:VAL:HG13	2.16	0.46
5:K:14:C:C2'	5:K:15:A:H4'	2.46	0.46
5:K:26:G:H2'	5:K:27:G:H4'	1.97	0.46
2:M:48:ARG:O	2:M:48:ARG:HD3	2.15	0.46
7:N:62:TRP:CE3	7:N:93:MET:HG2	2.50	0.46
1:P:133:ARG:NH1	4:H:316:TYR:O	2.49	0.46
2:A:149:ARG:NH2	6:L:24:DG:H21	2.04	0.46
2:A:246:ARG:HH12	2:A:273:LEU:N	2.12	0.46
2:B:249:VAL:HG13	2:B:266:VAL:HG22	1.97	0.46
2:D:81:HIS:NE2	2:D:120:LYS:O	2.49	0.46
2:C:82:GLU:HA	2:C:86:VAL:HG12	1.96	0.46
2:F:39:GLY:N	2:F:136:SER:OG	2.46	0.46
3:I:108:GLU:O	3:I:112:LEU:HG	2.16	0.46
4:H:83:ASP:HB2	4:H:107:PHE:CE1	2.50	0.46
5:K:8:C:O2'	7:N:68:ASN:HB2	2.15	0.46
2:M:275:GLU:OE2	2:M:277:LYS:NZ	2.26	0.46
7:N:26:TYR:O	7:N:95:LEU:HD11	2.15	0.46
1:P:44:PHE:HD2	1:P:190:LEU:CD2	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:441:ILE:H	1:P:441:ILE:HD12	1.80	0.46
2:A:95:THR:HG21	2:B:162:GLY:HA2	1.97	0.46
2:B:99:ARG:HB2	2:B:123:GLY:HA3	1.98	0.46
2:B:232:SER:N	2:B:237:ASP:OD2	2.35	0.46
2:D:54:ILE:HG13	2:D:107:TYR:CE2	2.51	0.46
2:D:148:THR:O	5:K:38:C:H5"	2.15	0.46
2:E:21:ASN:ND2	2:E:42:THR:H	2.14	0.46
2:F:19:ASN:HB3	2:F:22:GLY:H	1.80	0.46
3:I:88:ARG:NH2	3:I:90:PRO:HA	2.30	0.46
4:H:30:ILE:HG23	4:H:156:ASN:O	2.14	0.46
4:H:490:ASN:ND2	6:L:32:DC:H3'	2.31	0.46
4:H:540:LEU:HA	4:H:540:LEU:HD12	1.71	0.46
3:J:108:GLU:O	3:J:112:LEU:HG	2.16	0.46
7:N:57:LEU:HB2	7:N:99:ALA:HB3	1.97	0.46
1:P:331:GLU:N	1:P:361:THR:HG22	2.29	0.46
1:P:611:SER:HB2	1:P:644:PHE:HZ	1.80	0.46
2:B:128:PRO:O	2:B:184:ILE:HA	2.15	0.46
2:B:136:SER:HA	2:B:178:TYR:HA	1.98	0.46
2:E:62:HIS:HA	2:E:104:SER:O	2.16	0.46
2:E:102:MET:O	2:E:106:TYR:HB2	2.15	0.46
2:E:127:GLY:O	2:E:130:GLN:NE2	2.37	0.46
3:I:106:TYR:CD1	3:J:80:ARG:HG2	2.51	0.46
4:H:481:ILE:HG22	4:H:519:HIS:HB3	1.97	0.46
3:J:21:LEU:HD21	3:J:59:LEU:HD22	1.98	0.46
2:M:12:LEU:HD21	2:M:249:VAL:CG2	2.46	0.46
7:N:57:LEU:HD11	7:N:101:ARG:HB3	1.96	0.46
1:P:126:TYR:O	1:P:130:SER:HB3	2.15	0.46
1:P:203:GLU:HA	1:P:206:MET:HB2	1.96	0.46
1:P:307:ILE:CD1	1:P:392:ASP:HB3	2.46	0.46
2:A:151:ALA:HB2	2:D:67:ILE:O	2.16	0.46
2:B:20:PRO:HD2	2:B:30:PRO:HB3	1.98	0.46
2:B:44:VAL:HG12	5:K:13:U:OP2	2.16	0.46
2:B:110:ARG:NE	2:B:198:ASP:OD2	2.49	0.46
2:D:44:VAL:HG12	5:K:31:C:OP2	2.16	0.46
2:D:109:ILE:HG12	2:D:114:ALA:HB2	1.97	0.46
2:D:243:LEU:HD21	2:D:277:LYS:CE	2.42	0.46
2:C:61:GLU:CD	2:C:62:HIS:HD1	2.19	0.46
2:C:63:HIS:HA	2:C:107:TYR:HB2	1.96	0.46
2:C:89:LYS:HA	2:C:89:LYS:HD2	1.73	0.46
2:E:99:ARG:NH1	2:E:100:GLN:OE1	2.48	0.46
2:E:144:GLU:HA	2:E:171:PHE:HD1	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:113:GLY:HA3	5:K:42:U:H5”	1.98	0.46
4:H:407:ASN:HB2	4:H:409:ARG:HG2	1.98	0.46
4:H:482:GLN:CD	4:H:493:ILE:HG23	2.36	0.46
2:A:45:CYS:O	2:A:49:LYS:HG2	2.15	0.46
2:D:144:GLU:HA	2:D:171:PHE:CD1	2.49	0.46
2:D:154:ASN:OD1	2:E:74:ASN:ND2	2.44	0.46
2:C:68:ARG:HH22	5:K:20:G:H1	1.63	0.46
2:C:99:ARG:CG	2:C:123:GLY:HA3	2.46	0.46
3:I:57:ARG:NH2	3:G:46:SER:HB3	2.30	0.46
4:H:376:PRO:O	4:H:380:LEU:N	2.45	0.46
3:J:93:LEU:HA	3:J:93:LEU:HD23	1.79	0.46
2:M:238:ALA:HB2	2:M:277:LYS:HE3	1.97	0.46
1:P:44:PHE:CE1	1:P:166:LEU:HD21	2.50	0.46
2:F:38:GLU:OE1	2:F:135:ARG:NH2	2.48	0.46
1:P:320:PHE:CD2	1:P:358:LEU:HD21	2.50	0.46
1:P:464:ARG:HD3	1:P:587:ASN:ND2	2.31	0.46
1:P:499:ARG:HH11	1:P:521:ASN:HA	1.80	0.46
1:P:580:ALA:HB2	1:P:637:PHE:CE1	2.51	0.46
1:P:592:LEU:HG	1:P:593:PRO:HD2	1.98	0.46
2:A:39:GLY:O	2:A:135:ARG:HA	2.16	0.46
2:A:106:TYR:HB2	2:A:109:ILE:HD12	1.98	0.46
2:A:161:THR:O	2:D:70:LYS:NZ	2.35	0.46
2:B:20:PRO:HB2	2:B:41:VAL:HG22	1.98	0.46
2:D:39:GLY:N	2:D:136:SER:OG	2.48	0.46
2:E:110:ARG:HD3	2:E:198:ASP:OD2	2.16	0.46
2:E:118:THR:HA	6:L:20:DC:H5”	1.97	0.46
2:E:280:ARG:HH12	2:E:282:LEU:HD21	1.81	0.46
4:H:39:GLN:HG2	4:H:41:ASN:ND2	2.30	0.46
4:H:219:ALA:HB1	4:H:335:ALA:O	2.16	0.46
6:L:7:DA:H2”	6:L:8:DG:H5’	1.96	0.46
1:P:412:LEU:C	1:P:418:VAL:HG22	2.37	0.45
1:P:519:SER:HA	1:P:555:THR:OG1	2.15	0.45
2:A:89:LYS:HA	2:A:89:LYS:HD2	1.74	0.45
2:D:164:ASN:HB2	2:E:69:GLU:O	2.16	0.45
2:C:6:ARG:HH12	2:C:240:ALA:HB2	1.81	0.45
3:I:61:HIS:HB3	6:L:17:DG:C5	2.51	0.45
4:H:54:LYS:HD2	8:O:17:DA:OP2	2.16	0.45
4:H:539:ILE:HD11	4:H:565:GLU:CD	2.37	0.45
5:K:36:C:O2’	5:K:37:C:OP2	2.29	0.45
2:M:105:ARG:HG3	2:M:106:TYR:CD2	2.51	0.45
1:P:489:ARG:HG3	1:P:492:VAL:CG2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:16:GLN:N	2:A:220:GLN:O	2.46	0.45
2:A:89:LYS:O	2:A:93:GLU:HG2	2.15	0.45
2:B:89:LYS:O	2:B:93:GLU:HG2	2.16	0.45
2:B:105:ARG:HD3	2:B:106:TYR:CE1	2.50	0.45
2:B:243:LEU:O	2:B:246:ARG:HB3	2.16	0.45
2:D:53:PHE:CD2	2:D:205:ALA:HA	2.51	0.45
2:D:101:TYR:OH	2:D:105:ARG:HD2	2.16	0.45
2:C:109:ILE:CG2	2:C:116:MET:HE1	2.46	0.45
2:C:243:LEU:CD1	2:C:277:LYS:HE3	2.46	0.45
2:E:33:ASP:HB2	2:E:40:LEU:HD11	1.99	0.45
2:F:273:LEU:HB2	2:F:277:LYS:HD2	1.97	0.45
4:H:168:LEU:HB2	4:H:171:GLN:CG	2.43	0.45
6:L:44:DC:H2"	6:L:45:DC:H5'	1.98	0.45
2:M:129:VAL:HG11	2:M:202:PHE:CE1	2.50	0.45
1:P:48:ALA:CB	1:P:194:LEU:HD21	2.41	0.45
1:P:206:MET:HE2	11:P:803:PO4:O2	2.13	0.45
1:P:275:LEU:HB2	1:P:451:ILE:HD11	1.99	0.45
1:P:275:LEU:HG	1:P:277:VAL:HG12	1.98	0.45
1:P:381:ILE:HA	1:P:384:ILE:HD13	1.99	0.45
1:P:415:ASP:N	1:P:415:ASP:OD1	2.48	0.45
1:P:571:ARG:NH1	1:P:574:ALA:HB3	2.31	0.45
2:A:6:ARG:NH1	2:A:231:HIS:HE1	2.14	0.45
2:D:229:PHE:CD2	2:D:243:LEU:HD22	2.52	0.45
2:D:280:ARG:HH21	2:D:282:LEU:HD11	1.81	0.45
2:C:31:ARG:HB2	2:C:40:LEU:O	2.16	0.45
2:C:47:LYS:HD3	5:K:19:U:OP1	2.15	0.45
2:C:101:TYR:O	2:C:104:SER:N	2.50	0.45
2:E:2:THR:HG22	2:E:193:GLY:HA2	1.98	0.45
2:E:34:PRO:HG2	3:G:92:HIS:HD2	1.81	0.45
2:E:50:VAL:O	2:E:54:ILE:HG12	2.16	0.45
2:F:258:VAL:HG11	2:F:264:TYR:CE2	2.51	0.45
3:G:61:HIS:CD2	6:L:11:DG:C2	3.04	0.45
4:H:31:PRO:HG2	4:H:155:CYS:SG	2.56	0.45
4:H:69:ARG:HG2	4:H:77:VAL:CB	2.45	0.45
3:J:120:ASN:O	3:J:123:ASN:N	2.48	0.45
2:M:15:VAL:CG1	2:M:20:PRO:HG3	2.46	0.45
2:M:47:LYS:HB3	2:M:51:ARG:HH12	1.82	0.45
2:M:70:LYS:N	7:N:84:GLU:OE2	2.49	0.45
2:M:131:LEU:HD12	2:M:131:LEU:HA	1.85	0.45
1:P:140:ASP:OD1	1:P:141:GLU:N	2.49	0.45
1:P:412:LEU:HB3	1:P:418:VAL:HG21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:523:CYS:O	1:P:527:CYS:N	2.36	0.45
2:A:34:PRO:HA	3:J:49:ILE:HD11	1.98	0.45
2:B:17:ASP:CB	2:C:133:PHE:HB2	2.46	0.45
2:B:247:ILE:HD12	2:B:268:VAL:HG12	1.97	0.45
2:D:224:ARG:HD3	2:D:224:ARG:HA	1.71	0.45
2:C:42:THR:OG1	5:K:21:C:OP1	2.16	0.45
2:C:138:ASP:HB2	2:C:264:TYR:OH	2.17	0.45
2:C:149:ARG:NH2	2:C:166:THR:OG1	2.46	0.45
2:E:72:ILE:H	2:E:72:ILE:HD12	1.80	0.45
2:E:247:ILE:HD12	2:E:268:VAL:HG12	1.97	0.45
3:G:108:GLU:O	3:G:112:LEU:HG	2.16	0.45
4:H:1:MET:HE1	7:N:27:PRO:HG3	1.98	0.45
4:H:196:LEU:N	4:H:241:PRO:O	2.46	0.45
4:H:207:LEU:HA	4:H:207:LEU:HD13	1.77	0.45
4:H:363:MET:HE2	4:H:434:ALA:HB1	1.99	0.45
4:H:478:LEU:HD13	4:H:512:LEU:HB3	1.98	0.45
4:H:517:PRO:HB3	3:J:37:ALA:HB1	1.99	0.45
5:K:9:A:OP1	2:M:42:THR:OG1	2.33	0.45
2:M:7:TYR:O	2:M:184:ILE:N	2.49	0.45
2:M:116:MET:O	2:M:123:GLY:HA2	2.16	0.45
1:P:46:GLU:O	1:P:50:LEU:N	2.35	0.45
1:P:403:LYS:HA	1:P:442:LEU:HD12	1.99	0.45
2:A:131:LEU:HD23	2:A:180:CYS:SG	2.57	0.45
2:C:117:THR:O	2:C:121:ASN:ND2	2.50	0.45
2:C:125:VAL:O	5:K:17:C:O2'	2.33	0.45
2:E:24:PRO:HD3	5:K:39:U:H5'	1.99	0.45
2:F:6:ARG:HH11	2:F:236:GLY:HA3	1.81	0.45
4:H:32:PHE:CD1	4:H:47:ASP:HB3	2.52	0.45
4:H:66:GLY:HA2	4:H:79:ASN:ND2	2.31	0.45
4:H:514:ARG:O	4:H:517:PRO:HD2	2.16	0.45
2:M:156:LYS:HB3	2:M:159:SER:HB3	1.97	0.45
1:P:11:GLN:HE21	1:P:15:ASN:HA	1.81	0.45
2:B:154:ASN:HD22	6:L:38:DG:P	2.40	0.45
2:D:163:ASP:HA	2:E:69:GLU:HG3	1.99	0.45
2:E:9:PHE:HB3	2:E:228:VAL:HG22	1.98	0.45
2:F:12:LEU:HA	2:F:178:TYR:O	2.17	0.45
3:I:120:ASN:O	3:I:123:ASN:N	2.48	0.45
5:K:7:A:C4	7:N:69:GLU:OE1	2.69	0.45
5:K:9:A:H1'	5:K:10:G:O4'	2.17	0.45
7:N:36:ASN:HB2	7:N:139:TYR:CE1	2.52	0.45
1:P:329:VAL:HG11	1:P:356:ALA:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:658:LEU:HD22	1:P:672:LYS:HE3	1.98	0.45
2:A:17:ASP:O	2:A:219:GLY:HA3	2.17	0.45
2:A:50:VAL:O	2:A:54:ILE:HG12	2.16	0.45
2:C:181:HIS:HB3	2:C:244:PHE:CE2	2.52	0.45
2:E:8:ASP:O	2:E:229:PHE:HD1	1.99	0.45
2:F:15:VAL:O	2:F:175:TYR:HA	2.17	0.45
3:I:58:LEU:HD11	6:L:18:DG:P	2.56	0.45
4:H:429:ILE:CD1	4:H:559:ALA:HA	2.46	0.45
4:H:466:ASP:O	4:H:470:VAL:HG22	2.16	0.45
5:K:6:A:C4	2:M:115:VAL:HG11	2.52	0.45
2:M:213:ASP:O	2:M:218:ARG:NH1	2.50	0.45
1:P:532:ALA:HB1	1:P:712:GLU:HA	1.98	0.45
2:B:231:HIS:CD2	2:B:277:LYS:HZ2	2.35	0.45
2:D:247:ILE:HD12	2:D:268:VAL:HG12	1.99	0.45
2:E:42:THR:HG22	2:E:133:PHE:CZ	2.51	0.45
2:F:109:ILE:O	2:F:125:VAL:HG11	2.17	0.45
3:I:21:LEU:HD21	3:I:59:LEU:HD22	1.98	0.45
3:I:29:ASN:ND2	3:I:32:LEU:HD13	2.32	0.45
3:J:29:ASN:ND2	3:J:32:LEU:HD13	2.32	0.45
1:P:7:ALA:O	1:P:56:LYS:HD3	2.17	0.45
2:A:54:ILE:HG13	2:A:107:TYR:CE2	2.51	0.45
2:A:70:LYS:NZ	2:D:96:GLU:HB2	2.32	0.45
2:A:126:ARG:NH2	2:C:213:ASP:OD1	2.50	0.45
2:A:130:GLN:OE1	2:A:130:GLN:HA	2.17	0.45
2:A:208:ASN:O	2:A:212:HIS:ND1	2.47	0.45
2:A:256:GLU:HG3	2:A:257:VAL:HG22	1.99	0.45
2:B:46:LEU:HB3	2:B:209:MET:HE1	1.99	0.45
2:D:126:ARG:HH21	5:K:26:G:H21	1.65	0.45
2:C:3:ILE:HG22	2:C:196:GLU:HG3	1.99	0.45
2:C:31:ARG:NE	2:C:42:THR:HG23	2.32	0.45
2:E:68:ARG:HD3	2:E:69:GLU:HB3	1.97	0.45
2:E:211:ASP:OD2	2:F:239:PRO:HA	2.17	0.45
4:H:45:LEU:O	4:H:145:ASN:ND2	2.46	0.45
2:M:3:ILE:O	2:M:186:THR:OG1	2.33	0.45
2:M:259:ARG:HA	2:M:259:ARG:HD3	1.69	0.45
7:N:24:VAL:HA	7:N:93:MET:HB3	1.98	0.45
7:N:55:GLU:HB3	7:N:101:ARG:CG	2.46	0.45
7:N:161:LEU:HB3	7:N:165:THR:OG1	2.17	0.45
7:N:180:SER:CB	7:N:184:ASP:HA	2.47	0.45
1:P:5:TYR:HD2	1:P:62:GLN:HG3	1.82	0.45
1:P:277:VAL:HG11	1:P:283:LYS:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:9:PHE:CZ	2:A:182:GLY:HA3	2.52	0.45
2:A:95:THR:HG22	2:A:121:ASN:O	2.17	0.45
2:A:109:ILE:HG12	2:A:114:ALA:HB2	1.99	0.45
2:A:163:ASP:HA	2:D:69:GLU:HG3	1.99	0.45
2:D:215:SER:HB3	2:D:218:ARG:HG2	1.99	0.45
2:C:47:LYS:HG2	2:C:112:PHE:CE1	2.52	0.45
2:F:144:GLU:HA	2:F:171:PHE:CD1	2.52	0.45
2:F:258:VAL:HG11	2:F:264:TYR:CD2	2.52	0.45
3:I:98:GLN:HE21	3:J:57:ARG:NH1	2.15	0.45
4:H:535:GLU:HB3	4:H:575:LEU:HD11	1.99	0.45
5:K:9:A:C2	6:L:46:DT:H72	2.53	0.45
2:M:21:ASN:O	2:M:31:ARG:HG3	2.16	0.45
2:M:102:MET:HE2	7:N:76:GLU:OE1	2.17	0.45
1:P:354:TRP:CG	1:P:359:ILE:HG12	2.52	0.44
1:P:620:GLU:O	1:P:624:LYS:HG3	2.17	0.44
2:B:95:THR:HG23	2:B:123:GLY:H	1.82	0.44
2:D:99:ARG:HD3	2:D:125:VAL:HG22	1.98	0.44
2:E:54:ILE:HG13	2:E:107:TYR:CE2	2.51	0.44
2:E:259:ARG:NH1	2:F:35:GLN:HB2	2.32	0.44
4:H:141:MET:HG3	4:H:146:TRP:CE2	2.52	0.44
4:H:290:ASN:C	4:H:292:GLY:HA2	2.36	0.44
4:H:429:ILE:HD11	4:H:498:PHE:CE2	2.52	0.44
4:H:479:GLU:OE1	4:H:562:TYR:OH	2.09	0.44
2:M:114:ALA:HB3	2:M:125:VAL:HB	1.98	0.44
1:P:56:LYS:HG3	1:P:61:PHE:HE2	1.80	0.44
1:P:102:ARG:NH1	1:P:160:PRO:O	2.51	0.44
1:P:601:PHE:CE1	1:P:603:ALA:HB2	2.52	0.44
1:P:707:GLN:NE2	1:P:711:ALA:HA	2.33	0.44
2:B:110:ARG:O	2:B:128:PRO:HD2	2.17	0.44
2:D:53:PHE:CZ	2:D:57:THR:HG21	2.52	0.44
3:I:55:LEU:HA	3:I:55:LEU:HD23	1.72	0.44
3:G:120:ASN:O	3:G:123:ASN:N	2.48	0.44
4:H:281:LEU:HD22	4:H:293:GLY:HA3	1.98	0.44
4:H:375:MET:HE3	4:H:379:ARG:NH2	2.32	0.44
2:M:68:ARG:HD2	7:N:82:TYR:CE1	2.52	0.44
7:N:129:ALA:HB1	7:N:151:LEU:HB2	1.98	0.44
7:N:129:ALA:CB	7:N:151:LEU:HB2	2.47	0.44
7:N:177:PHE:CD1	7:N:184:ASP:HB2	2.51	0.44
1:P:275:LEU:HA	1:P:451:ILE:HG12	1.98	0.44
1:P:275:LEU:HD13	1:P:451:ILE:HD11	1.98	0.44
1:P:618:ILE:O	1:P:621:GLU:HG2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:8:ASP:O	2:A:229:PHE:HD2	2.01	0.44
2:A:51:ARG:HH21	2:A:112:PHE:HB2	1.82	0.44
2:A:62:HIS:HA	2:A:105:ARG:HA	1.98	0.44
2:A:167:MET:HG2	6:L:23:DT:C6	2.53	0.44
2:C:13:PHE:CE1	2:C:46:LEU:HD11	2.52	0.44
2:C:64:ASP:OD2	2:C:105:ARG:NH1	2.51	0.44
2:C:91:LYS:HD2	2:C:92:GLY:N	2.32	0.44
2:C:148:THR:O	5:K:25:A:O2'	2.27	0.44
2:F:113:GLY:HA2	2:F:125:VAL:HG12	1.99	0.44
2:F:203:TRP:HB3	2:F:282:LEU:HD22	1.98	0.44
4:H:32:PHE:HD2	4:H:155:CYS:SG	2.41	0.44
4:H:481:ILE:HG12	4:H:532:LEU:HD13	2.00	0.44
5:K:7:A:N1	7:N:90:ARG:NH1	2.65	0.44
6:L:48:DA:C6	6:L:49:DA:C6	3.06	0.44
2:M:47:LYS:HG2	2:M:112:PHE:CE1	2.52	0.44
7:N:23:ARG:O	7:N:93:MET:N	2.48	0.44
7:N:40:ALA:HB1	7:N:136:HIS:O	2.17	0.44
1:P:109:HIS:CD2	1:P:668:PRO:HG2	2.52	0.44
1:P:169:ASP:HA	1:P:172:ALA:HB3	1.98	0.44
1:P:562:VAL:HG23	1:P:564:LEU:HG	1.98	0.44
2:A:229:PHE:CE1	2:A:279:LEU:HD13	2.53	0.44
2:B:19:ASN:N	2:B:218:ARG:HA	2.33	0.44
2:B:150:MET:SD	2:C:48:ARG:HD3	2.57	0.44
2:B:205:ALA:O	2:B:209:MET:CB	2.57	0.44
2:D:72:ILE:H	2:D:72:ILE:HD12	1.81	0.44
2:E:20:PRO:HB2	2:E:41:VAL:HG22	1.98	0.44
2:E:128:PRO:HG2	2:E:194:PHE:CB	2.47	0.44
3:I:109:THR:O	3:I:113:PHE:HD2	2.01	0.44
3:G:58:LEU:HD12	6:L:11:DG:H2"	1.99	0.44
4:H:420:LEU:CD2	4:H:555:GLN:HB2	2.47	0.44
3:J:109:THR:O	3:J:113:PHE:HD2	2.01	0.44
5:K:7:A:N3	7:N:69:GLU:HB3	2.33	0.44
2:M:9:PHE:CZ	2:M:182:GLY:HA3	2.53	0.44
2:M:187:HIS:CD2	7:N:135:PHE:HA	2.52	0.44
2:A:41:VAL:N	2:A:134:SER:O	2.47	0.44
2:A:105:ARG:HD3	2:A:106:TYR:CE1	2.52	0.44
2:A:160:GLU:HG3	2:A:161:THR:N	2.25	0.44
2:B:280:ARG:NH2	2:B:282:LEU:HD11	2.32	0.44
2:D:186:THR:O	2:D:190:LYS:HG2	2.17	0.44
2:C:103:CYS:O	2:C:110:ARG:HB2	2.17	0.44
2:E:9:PHE:CE1	2:E:182:GLY:HA3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:220:GLN:HE21	2:E:222:ASN:HD21	1.65	0.44
3:I:18:PHE:HZ	3:I:36:ILE:O	2.00	0.44
4:H:208:HIS:HE1	4:H:242:ILE:HB	1.78	0.44
4:H:385:VAL:CG1	4:H:392:ASN:HB2	2.43	0.44
4:H:450:LEU:HD11	4:H:553:GLU:HB3	1.99	0.44
4:H:450:LEU:HG	4:H:453:MET:SD	2.57	0.44
5:K:2:U:H2'	7:N:43:TRP:CH2	2.52	0.44
1:P:51:LEU:HD11	1:P:161:LEU:HD11	2.00	0.44
1:P:304:ILE:HG12	1:P:359:ILE:CG2	2.47	0.44
1:P:516:LEU:O	1:P:553:VAL:N	2.50	0.44
1:P:749:ASP:OD1	1:P:751:PRO:HD3	2.17	0.44
2:A:23:ASP:CG	2:A:30:PRO:HA	2.38	0.44
2:B:114:ALA:O	2:B:116:MET:HG3	2.18	0.44
2:B:131:LEU:HD11	2:B:202:PHE:HZ	1.82	0.44
2:D:13:PHE:O	2:D:177:LEU:HD12	2.18	0.44
2:C:18:GLY:HA3	2:C:218:ARG:O	2.18	0.44
2:E:137:ILE:HD11	2:E:179:ARG:HB2	2.00	0.44
2:E:145:HIS:CD2	2:F:31:ARG:HD3	2.52	0.44
3:G:109:THR:O	3:G:113:PHE:HD2	2.01	0.44
4:H:121:ASP:HB3	4:H:124:VAL:HG22	1.99	0.44
4:H:362:GLN:O	4:H:438:LYS:HD2	2.18	0.44
5:K:3:U:H2'	7:N:39:MET:HE1	2.00	0.44
2:M:31:ARG:NH2	7:N:66:ARG:O	2.33	0.44
8:O:23:DA:H8	8:O:24:DA:C2	2.36	0.44
1:P:40:TYR:HD2	1:P:189:PHE:CZ	2.36	0.44
1:P:363:ASN:HA	1:P:366:LEU:HB3	1.99	0.44
1:P:691:ILE:HA	1:P:748:PRO:HA	1.99	0.44
2:D:129:VAL:HG22	2:D:184:ILE:HG12	1.99	0.44
2:E:113:GLY:HA3	5:K:36:C:H5"	1.98	0.44
3:G:18:PHE:HZ	3:G:36:ILE:O	2.00	0.44
4:H:396:ASP:C	4:H:397:LEU:HD22	2.38	0.44
4:H:543:CYS:O	3:J:107:HIS:NE2	2.49	0.44
5:K:8:C:H6	2:M:48:ARG:HG2	1.83	0.44
2:M:6:ARG:NH1	2:M:231:HIS:HE1	2.16	0.44
7:N:15:THR:HG21	7:N:23:ARG:HG2	1.99	0.44
7:N:83:ILE:HD12	7:N:87:ARG:HH12	1.79	0.44
1:P:185:ILE:HG23	1:P:408:MET:HE2	1.99	0.44
2:A:81:HIS:ND1	2:A:94:LYS:HE2	2.32	0.44
2:B:6:ARG:NH1	2:B:231:HIS:HE1	2.15	0.44
2:D:140:ILE:O	2:D:140:ILE:HG13	2.18	0.44
2:C:259:ARG:HD3	2:C:259:ARG:HA	1.79	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:211:ASP:O	2:F:6:ARG:NH2	2.50	0.44
2:E:218:ARG:NH2	5:K:38:C:H6	2.15	0.44
2:F:252:LYS:HA	2:F:265:LEU:HD22	1.99	0.44
3:I:99:GLY:HA3	3:J:89:PHE:HD2	1.82	0.44
3:G:93:LEU:HD23	3:G:93:LEU:HA	1.79	0.44
4:H:10:TYR:CD1	4:H:249:GLU:HG2	2.53	0.44
4:H:360:ASP:O	4:H:438:LYS:HD3	2.17	0.44
4:H:461:ASP:OD1	4:H:463:ASN:HB2	2.17	0.44
3:J:55:LEU:HA	3:J:55:LEU:HD23	1.72	0.44
2:M:5:LYS:O	2:M:186:THR:HB	2.18	0.44
2:M:183:PHE:CD2	7:N:137:GLN:HG2	2.52	0.44
1:P:281:GLY:HA3	1:P:462:LEU:HD21	1.99	0.44
1:P:442:LEU:HD22	1:P:650:VAL:HG21	2.00	0.44
2:A:210:PHE:CE1	2:A:221:MET:HE3	2.53	0.44
2:B:52:ASN:O	2:B:56:MET:HG3	2.17	0.44
2:B:129:VAL:HG11	2:B:202:PHE:CZ	2.53	0.44
2:B:214:HIS:O	2:C:126:ARG:NH1	2.51	0.44
2:B:227:TYR:OH	2:B:266:VAL:HG11	2.18	0.44
2:D:3:ILE:HG22	2:D:196:GLU:HA	1.99	0.44
2:D:12:LEU:HD12	2:D:227:TYR:HE1	1.82	0.44
2:D:124:GLN:HG3	5:K:29:G:H1'	1.98	0.44
4:H:97:GLN:C	4:H:99:GLN:H	2.21	0.44
4:H:262:ASN:HA	4:H:301:ILE:HD12	1.99	0.44
3:J:4:ASP:HB3	3:J:7:ARG:HB2	1.99	0.44
3:J:28:ALA:HB1	3:J:65:LYS:HB3	2.00	0.44
2:M:197:ASN:O	2:M:201:LEU:HD23	2.17	0.44
1:P:55:GLY:C	1:P:91:HIS:HB2	2.38	0.43
1:P:308:PRO:HD2	1:P:393:GLU:HB3	2.00	0.43
1:P:766:ALA:HA	1:P:771:ALA:HA	1.99	0.43
2:A:47:LYS:HD3	5:K:25:A:OP1	2.18	0.43
2:D:115:VAL:HG22	5:K:29:G:C4	2.53	0.43
2:C:239:PRO:HG2	2:C:242:SER:HB3	1.99	0.43
2:E:68:ARG:CD	2:E:69:GLU:H	2.25	0.43
2:F:42:THR:CG2	2:F:44:VAL:HG22	2.47	0.43
4:H:357:TRP:HA	4:H:443:ARG:NH1	2.33	0.43
4:H:481:ILE:HD13	4:H:520:LEU:HD21	1.99	0.43
4:H:550:LEU:HA	4:H:550:LEU:HD23	1.65	0.43
5:K:32:A:O2'	5:K:33:U:OP1	2.36	0.43
2:M:241:ASP:OD2	7:N:148:ASP:HB3	2.18	0.43
7:N:29:ILE:HD13	7:N:102:ILE:HD11	2.00	0.43
7:N:108:MET:HE2	7:N:118:TYR:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:35:ARG:HH12	1:P:213:ASP:CB	2.31	0.43
1:P:568:CYS:HA	1:P:597:GLU:O	2.18	0.43
2:A:21:ASN:HB2	2:A:41:VAL:HG22	2.00	0.43
2:A:273:LEU:HB2	2:A:277:LYS:HB2	2.00	0.43
2:B:124:GLN:HG3	5:K:11:G:H1'	1.99	0.43
2:B:151:ALA:HB1	2:C:71:GLY:O	2.18	0.43
2:C:129:VAL:HG11	2:C:202:PHE:CZ	2.53	0.43
2:E:23:ASP:N	2:E:29:LEU:O	2.44	0.43
2:E:102:MET:HB3	2:E:109:ILE:HD12	2.01	0.43
2:E:124:GLN:HG3	5:K:35:G:H1'	2.00	0.43
2:F:90:GLU:O	2:F:92:GLY:N	2.51	0.43
3:I:28:ALA:HB1	3:I:65:LYS:HB3	2.00	0.43
3:I:83:LEU:HD23	3:I:83:LEU:HA	1.76	0.43
4:H:357:TRP:O	4:H:361:LEU:HB2	2.17	0.43
4:H:404:ALA:HA	4:H:409:ARG:HB2	2.00	0.43
4:H:512:LEU:HA	4:H:512:LEU:HD23	1.78	0.43
3:J:18:PHE:HZ	3:J:36:ILE:O	2.00	0.43
1:P:6:ILE:HD12	1:P:19:SER:OG	2.18	0.43
1:P:465:VAL:HG22	1:P:596:GLY:HA3	2.00	0.43
2:A:110:ARG:NH2	2:A:198:ASP:OD2	2.51	0.43
2:A:258:VAL:O	2:A:259:ARG:NE	2.46	0.43
2:D:23:ASP:N	2:D:29:LEU:O	2.47	0.43
2:E:27:GLY:O	5:K:39:U:H5	2.01	0.43
2:F:229:PHE:CE1	2:F:279:LEU:HD22	2.48	0.43
3:G:29:ASN:ND2	3:G:32:LEU:HD13	2.32	0.43
4:H:82:TRP:O	4:H:82:TRP:CG	2.72	0.43
4:H:571:THR:HG22	4:H:572:LYS:H	1.84	0.43
2:M:39:GLY:H	2:M:136:SER:HB3	1.83	0.43
1:P:251:LEU:O	1:P:252:ASN:HB3	2.19	0.43
1:P:570:TYR:HA	1:P:599:VAL:O	2.18	0.43
2:A:144:GLU:CD	3:J:54:THR:HG22	2.39	0.43
2:B:107:TYR:HD1	2:B:110:ARG:NH1	2.16	0.43
2:B:115:VAL:HG22	5:K:11:G:C4	2.53	0.43
2:D:7:TYR:HE2	2:D:280:ARG:HH11	1.61	0.43
2:D:156:LYS:HZ2	6:L:17:DG:P	2.39	0.43
2:E:144:GLU:HG2	2:E:171:PHE:CE1	2.53	0.43
2:E:273:LEU:C	2:E:275:GLU:H	2.22	0.43
2:F:167:MET:HG3	2:F:168:GLY:N	2.33	0.43
3:G:28:ALA:HB1	3:G:65:LYS:HB3	2.00	0.43
3:G:41:PHE:HE2	3:G:105:TYR:CG	2.36	0.43
3:G:119:LYS:HD3	9:Q:14:DA:OP1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:206:ARG:HG3	4:H:236:GLN:O	2.19	0.43
4:H:221:PHE:CE2	7:N:19:LEU:HD21	2.54	0.43
4:H:396:ASP:OD2	4:H:414:SER:OG	2.26	0.43
2:M:9:PHE:HE1	2:M:11:PHE:HB2	1.83	0.43
7:N:168:PHE:HB2	7:N:194:GLN:HE21	1.83	0.43
1:P:125:TRP:HE1	1:P:667:ASN:CG	2.19	0.43
1:P:144:ALA:O	1:P:147:SER:OG	2.37	0.43
1:P:288:LEU:HD12	1:P:320:PHE:CE2	2.53	0.43
1:P:479:TRP:NE1	1:P:604:GLU:HB2	2.33	0.43
2:A:140:ILE:O	2:A:140:ILE:HG13	2.18	0.43
2:A:227:TYR:HB3	2:A:279:LEU:HD11	2.00	0.43
2:B:132:THR:HG23	2:B:181:HIS:O	2.18	0.43
2:B:239:PRO:HG2	2:B:242:SER:HB3	2.00	0.43
2:D:15:VAL:O	2:D:175:TYR:HA	2.18	0.43
2:D:128:PRO:HG3	2:D:189:ALA:HA	2.00	0.43
2:C:134:SER:HB3	2:C:178:TYR:HB3	2.01	0.43
2:E:205:ALA:O	2:E:209:MET:CB	2.54	0.43
3:I:21:LEU:HD23	3:I:59:LEU:HD13	2.01	0.43
3:G:39:ARG:HH12	6:L:12:DG:C2'	2.31	0.43
4:H:9:TYR:HB2	4:H:297:PRO:HB3	2.00	0.43
4:H:64:PRO:HD3	4:H:170:CYS:HB2	2.01	0.43
4:H:466:ASP:HB2	4:H:469:TYR:HB3	2.00	0.43
3:J:112:LEU:HD23	3:J:112:LEU:HA	1.66	0.43
2:M:21:ASN:HD22	2:M:42:THR:N	2.16	0.43
1:P:569:VAL:O	1:P:598:VAL:HA	2.18	0.43
2:A:54:ILE:HG23	2:A:58:GLN:HG2	2.01	0.43
2:C:109:ILE:HG12	2:C:114:ALA:CB	2.48	0.43
2:E:164:ASN:ND2	2:F:69:GLU:O	2.35	0.43
2:F:18:GLY:HA3	2:F:219:GLY:HA3	1.99	0.43
2:F:126:ARG:HD3	2:F:188:PHE:CZ	2.53	0.43
3:G:76:GLN:O	3:G:80:ARG:HG3	2.18	0.43
3:G:97:GLN:OE1	3:G:97:GLN:HA	2.19	0.43
4:H:6:LEU:HA	4:H:9:TYR:CE1	2.54	0.43
4:H:133:SER:H	4:H:137:LYS:HZ1	1.66	0.43
4:H:266:ILE:HG13	4:H:341:PHE:CE2	2.54	0.43
4:H:440:TYR:CD2	4:H:440:TYR:C	2.91	0.43
2:M:184:ILE:HG21	2:M:199:LEU:HD12	2.01	0.43
1:P:92:SER:HB2	1:P:116:ALA:HA	2.00	0.43
1:P:224:ALA:H	1:P:346:LYS:HE2	1.84	0.43
1:P:332:HIS:C	1:P:334:SER:H	2.22	0.43
1:P:554:SER:OG	1:P:555:THR:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:6:ARG:NH2	2:C:211:ASP:O	2.51	0.43
2:B:63:HIS:HA	2:B:107:TYR:HB2	1.99	0.43
2:E:112:PHE:HE1	2:E:131:LEU:HD13	1.84	0.43
2:E:130:GLN:NE2	5:K:36:C:OP1	2.51	0.43
2:F:39:GLY:O	2:F:135:ARG:HA	2.19	0.43
2:F:227:TYR:HB3	2:F:279:LEU:HD11	2.00	0.43
2:F:269:ASP:OD1	2:F:269:ASP:N	2.45	0.43
3:I:97:GLN:OE1	3:I:97:GLN:HA	2.19	0.43
3:G:7:ARG:NE	3:G:9:ASP:OD2	2.52	0.43
3:G:39:ARG:NH1	6:L:12:DG:H2'	2.33	0.43
3:G:68:PHE:CD1	9:Q:14:DA:N7	2.87	0.43
2:M:243:LEU:O	2:M:246:ARG:HB2	2.18	0.43
7:N:38:LEU:O	7:N:49:TRP:NE1	2.52	0.43
7:N:45:PRO:O	7:N:111:GLU:HG2	2.17	0.43
8:O:12:DT:H2'	8:O:13:DC:O4'	2.18	0.43
1:P:8:HIS:CD2	1:P:20:HIS:HD1	2.34	0.43
1:P:38:GLY:O	1:P:42:SER:HB3	2.19	0.43
1:P:424:THR:CG2	1:P:428:PRO:HD3	2.49	0.43
1:P:505:LEU:HD12	1:P:505:LEU:HA	1.89	0.43
2:B:42:THR:HA	2:B:133:PHE:CD2	2.54	0.43
2:B:118:THR:HG21	2:M:153:THR:HG21	2.01	0.43
2:D:47:LYS:HG2	2:D:112:PHE:CD1	2.54	0.43
2:C:61:GLU:O	2:C:62:HIS:HB2	2.19	0.43
2:C:90:GLU:HB3	2:C:93:GLU:OE2	2.17	0.43
2:C:106:TYR:CD2	2:C:109:ILE:HD12	2.52	0.43
2:C:128:PRO:HG3	2:C:189:ALA:HA	2.01	0.43
2:E:224:ARG:HD3	2:E:224:ARG:HA	1.72	0.43
2:F:7:TYR:HA	2:F:229:PHE:O	2.18	0.43
2:F:21:ASN:O	2:F:23:ASP:N	2.47	0.43
2:F:103:CYS:O	2:F:110:ARG:NH2	2.51	0.43
2:F:110:ARG:HE	2:F:198:ASP:CG	2.21	0.43
4:H:208:HIS:HD1	4:H:250:TYR:HH	0.55	0.43
3:J:76:GLN:O	3:J:80:ARG:HG3	2.18	0.43
7:N:142:CYS:HB2	7:N:145:PHE:CD2	2.54	0.43
1:P:306:ALA:HB2	1:P:366:LEU:HD13	2.00	0.43
1:P:455:LYS:HG2	1:P:634:PRO:HG2	2.01	0.43
2:A:26:ALA:HB1	3:J:42:GLY:CA	2.49	0.43
2:B:238:ALA:HB3	2:B:243:LEU:HD21	2.01	0.43
2:D:47:LYS:HD3	5:K:31:C:OP1	2.19	0.43
2:C:149:ARG:HB2	5:K:25:A:H1'	2.01	0.43
2:E:53:PHE:O	2:E:57:THR:HG23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:229:PHE:CD1	2:F:243:LEU:HD12	2.54	0.43
3:I:7:ARG:NE	3:I:9:ASP:OD2	2.52	0.43
4:H:108:THR:HG22	4:H:131:LEU:HG	2.01	0.43
4:H:225:ASN:O	4:H:226:LEU:HG	2.19	0.43
4:H:281:LEU:CD2	4:H:293:GLY:HA3	2.48	0.43
4:H:557:LEU:O	4:H:561:GLY:N	2.27	0.43
2:M:15:VAL:HG12	2:M:178:TYR:HE1	1.84	0.43
2:A:130:GLN:HE22	5:K:24:U:P	2.41	0.43
2:B:35:GLN:HB3	2:M:257:VAL:HG21	2.01	0.43
2:C:140:ILE:HB	2:C:173:VAL:HG13	2.00	0.43
2:C:248:GLN:HG2	2:C:267:SER:HB2	2.00	0.43
2:F:14:ASP:OD2	2:F:224:ARG:NE	2.50	0.43
3:I:4:ASP:HB3	3:I:7:ARG:HB2	1.99	0.43
3:I:41:PHE:HE2	3:I:105:TYR:CG	2.36	0.43
3:G:4:ASP:HB3	3:G:7:ARG:HB2	1.99	0.43
3:G:14:LEU:HD11	3:G:90:PRO:CD	2.42	0.43
4:H:226:LEU:HB2	4:H:229:PHE:CD2	2.53	0.43
4:H:335:ALA:HB3	6:L:47:DG:H1'	2.00	0.43
5:K:7:A:C2	7:N:69:GLU:HB3	2.53	0.43
6:L:35:DC:H2"	6:L:36:DA:OP2	2.19	0.43
2:M:55:GLN:HB2	2:M:65:ILE:HG13	2.01	0.43
2:M:66:PHE:HE2	7:N:74:MET:HB3	1.81	0.43
7:N:117:ASN:HB3	7:N:120:LYS:HB2	2.01	0.43
1:P:104:ASN:HB3	1:P:107:PHE:HB2	2.01	0.42
1:P:274:SER:HA	1:P:422:LEU:H	1.82	0.42
1:P:486:ILE:HD11	1:P:509:LEU:HD11	2.01	0.42
1:P:576:LEU:HB2	1:P:640:TYR:CG	2.54	0.42
1:P:699:HIS:CE1	1:P:707:GLN:HG3	2.54	0.42
1:P:715:ASP:O	1:P:719:ARG:HG2	2.19	0.42
2:A:116:MET:HB2	2:A:123:GLY:O	2.19	0.42
2:B:152:VAL:HG11	2:B:159:SER:HB2	2.01	0.42
2:B:273:LEU:C	2:B:275:GLU:H	2.22	0.42
2:D:203:TRP:CE3	2:D:226:LEU:HD21	2.54	0.42
2:E:117:THR:HA	2:E:121:ASN:OD1	2.19	0.42
3:I:9:ASP:O	3:I:13:VAL:HG13	2.19	0.42
3:G:83:LEU:HD23	3:G:83:LEU:HA	1.76	0.42
4:H:32:PHE:CD2	4:H:155:CYS:SG	3.12	0.42
4:H:69:ARG:HB3	4:H:74:SER:OG	2.19	0.42
4:H:460:LEU:HA	4:H:564:HIS:HB3	2.01	0.42
3:J:41:PHE:HE2	3:J:105:TYR:CG	2.36	0.42
5:K:5:A:C8	5:K:6:A:N7	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:N:29:ILE:HD11	7:N:37:ILE:HD12	2.01	0.42
7:N:32:SER:N	7:N:173:TYR:O	2.52	0.42
1:P:367:PHE:O	1:P:371:PHE:N	2.50	0.42
1:P:665:ASN:OD1	4:H:282:GLU:N	2.51	0.42
2:A:48:ARG:HA	2:A:48:ARG:HD2	1.80	0.42
2:A:133:PHE:HB2	2:C:17:ASP:HB3	2.00	0.42
2:B:126:ARG:HG2	2:B:188:PHE:CE2	2.54	0.42
2:D:49:LYS:HA	2:D:213:ASP:OD2	2.19	0.42
2:D:116:MET:HB3	2:D:122:ALA:HB3	2.01	0.42
2:D:150:MET:HE3	2:E:68:ARG:HG2	2.01	0.42
2:C:140:ILE:O	2:C:140:ILE:HG13	2.19	0.42
2:F:53:PHE:CD2	2:F:205:ALA:HA	2.54	0.42
3:I:33:ASN:HB3	6:L:19:DG:OP2	2.18	0.42
4:H:6:LEU:HD13	4:H:254:LEU:CD2	2.49	0.42
4:H:131:LEU:HD11	4:H:159:PHE:CZ	2.55	0.42
4:H:160:ARG:HB2	4:H:168:LEU:HD13	2.00	0.42
4:H:208:HIS:ND1	4:H:250:TYR:OH	2.10	0.42
4:H:357:TRP:HZ3	4:H:411:LEU:HD11	1.84	0.42
4:H:474:LEU:HD13	4:H:540:LEU:HD13	2.00	0.42
3:J:7:ARG:CG	3:J:12:TYR:HD2	2.22	0.42
9:Q:-3:DA:H5'	9:Q:-3:DA:C8	2.55	0.42
1:P:149:PHE:CE1	1:P:154:LEU:HB3	2.54	0.42
1:P:509:LEU:HD13	1:P:551:TRP:CD1	2.55	0.42
2:A:19:ASN:OD1	2:A:23:ASP:OD1	2.37	0.42
2:B:34:PRO:HG2	4:H:413:VAL:HG21	2.01	0.42
2:B:160:GLU:CG	2:B:161:THR:H	2.32	0.42
2:D:130:GLN:O	2:D:182:GLY:HA2	2.19	0.42
2:D:168:GLY:HA3	6:L:18:DG:C5	2.53	0.42
2:C:68:ARG:CG	2:C:69:GLU:H	2.32	0.42
2:C:95:THR:O	2:C:99:ARG:HG3	2.19	0.42
2:C:111:THR:HG23	2:C:129:VAL:HG21	2.00	0.42
2:F:215:SER:HB3	2:F:218:ARG:HD3	2.01	0.42
4:H:133:SER:H	4:H:137:LYS:NZ	2.16	0.42
4:H:262:ASN:HD21	4:H:298:ASP:HB3	1.84	0.42
4:H:396:ASP:O	4:H:397:LEU:HD22	2.19	0.42
2:M:38:GLU:HA	2:M:139:PRO:HA	2.01	0.42
2:M:68:ARG:HD2	7:N:82:TYR:CZ	2.53	0.42
2:M:99:ARG:HH11	2:M:125:VAL:HG13	1.84	0.42
7:N:83:ILE:O	7:N:87:ARG:N	2.52	0.42
7:N:101:ARG:HG3	7:N:101:ARG:O	2.19	0.42
1:P:594:GLN:OE1	1:P:594:GLN:N	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:203:TRP:HB3	2:A:282:LEU:HD22	2.01	0.42
2:D:44:VAL:CG1	5:K:31:C:H2'	2.48	0.42
2:D:152:VAL:HA	2:D:166:THR:HG23	2.01	0.42
2:C:174:PRO:HB2	2:C:259:ARG:CZ	2.49	0.42
2:E:2:THR:HG21	2:E:190:LYS:HA	2.01	0.42
2:E:19:ASN:N	2:E:217:ALA:O	2.33	0.42
3:I:52:PHE:HB3	3:I:89:PHE:CE2	2.54	0.42
3:I:58:LEU:HD12	6:L:17:DG:H2"	2.00	0.42
4:H:69:ARG:NH2	8:O:14:DA:P	2.92	0.42
3:J:25:GLN:OE1	3:J:36:ILE:N	2.42	0.42
3:J:97:GLN:OE1	3:J:97:GLN:HA	2.19	0.42
7:N:108:MET:CE	7:N:118:TYR:HA	2.50	0.42
1:P:29:VAL:HG11	1:P:52:HIS:ND1	2.34	0.42
1:P:40:TYR:HD2	1:P:189:PHE:CE2	2.36	0.42
1:P:336:LEU:HA	1:P:336:LEU:HD23	1.87	0.42
1:P:437:PHE:CE1	4:H:62:LEU:HD22	2.54	0.42
1:P:696:PRO:O	1:P:697:LEU:HG	2.20	0.42
2:A:24:PRO:HD2	2:A:27:GLY:O	2.18	0.42
2:A:66:PHE:CE2	2:A:109:ILE:HD11	2.54	0.42
2:D:149:ARG:HH22	2:D:153:THR:HG1	1.57	0.42
2:D:273:LEU:HD11	2:D:279:LEU:H	1.84	0.42
2:C:6:ARG:O	2:C:231:HIS:HD2	2.03	0.42
2:E:26:ALA:O	2:E:29:LEU:N	2.42	0.42
4:H:52:LYS:NZ	8:O:18:DA:H3'	2.34	0.42
4:H:146:TRP:CD1	4:H:149:CYS:SG	3.13	0.42
4:H:182:ALA:O	4:H:186:GLN:HG2	2.19	0.42
4:H:217:LYS:HE2	8:O:14:DA:O4'	2.19	0.42
3:J:7:ARG:NE	3:J:9:ASP:OD2	2.52	0.42
5:K:4:G:H3'	7:N:139:TYR:CE2	2.53	0.42
2:M:151:ALA:O	2:M:166:THR:HG22	2.20	0.42
1:P:513:GLY:HA2	1:P:549:PRO:HD2	2.00	0.42
1:P:559:GLU:OE1	1:P:578:SER:HB3	2.19	0.42
2:A:83:GLN:O	2:A:86:VAL:N	2.52	0.42
2:B:5:LYS:HG3	2:B:230:GLU:OE2	2.20	0.42
2:B:11:PHE:CZ	2:B:210:PHE:HE2	2.38	0.42
2:B:153:THR:HB	6:L:37:DA:H4'	2.02	0.42
2:D:34:PRO:HB3	3:I:91:ASN:O	2.20	0.42
2:D:233:ASN:HB2	2:D:235:LEU:O	2.19	0.42
2:C:12:LEU:CD2	2:C:249:VAL:HG21	2.49	0.42
2:C:232:SER:N	2:C:237:ASP:OD2	2.33	0.42
2:E:39:GLY:C	2:E:178:TYR:HE1	2.23	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:43:ASP:HB3	2:E:47:LYS:HE3	2.01	0.42
2:E:65:ILE:HD13	2:E:65:ILE:HA	1.74	0.42
2:E:77:ILE:HG23	2:E:122:ALA:CB	2.49	0.42
2:E:168:GLY:HA3	6:L:12:DG:C6	2.54	0.42
2:F:7:TYR:CE2	2:F:230:GLU:HG2	2.55	0.42
3:I:76:GLN:O	3:I:80:ARG:HG3	2.18	0.42
4:H:32:PHE:HD2	4:H:155:CYS:HG	1.59	0.42
4:H:471:LEU:HD21	4:H:546:PHE:HD1	1.84	0.42
3:J:9:ASP:O	3:J:13:VAL:HG13	2.19	0.42
2:M:152:VAL:HG13	2:M:164:ASN:HB3	2.02	0.42
2:M:166:THR:HG23	2:M:166:THR:O	2.19	0.42
1:P:478:SER:HB3	1:P:481:LYS:HB2	2.00	0.42
1:P:491:CYS:HA	1:P:550:LEU:HD22	2.01	0.42
1:P:570:TYR:CE1	1:P:599:VAL:HB	2.55	0.42
2:B:203:TRP:HA	2:B:203:TRP:CE3	2.55	0.42
2:D:44:VAL:HA	2:D:47:LYS:HB2	2.00	0.42
2:D:51:ARG:HH11	2:D:51:ARG:HG3	1.85	0.42
2:C:238:ALA:HB3	2:C:243:LEU:HD21	2.01	0.42
2:F:19:ASN:HB3	2:F:22:GLY:CA	2.48	0.42
2:F:188:PHE:HA	2:F:191:GLN:HE21	1.82	0.42
3:G:9:ASP:O	3:G:13:VAL:HG13	2.19	0.42
3:G:21:LEU:HD23	3:G:59:LEU:HD13	2.01	0.42
4:H:127:VAL:HG21	4:H:159:PHE:CD2	2.55	0.42
3:J:74:GLN:HG3	9:Q:4:DT:H5”	2.02	0.42
5:K:7:A:P	2:M:51:ARG:HH22	2.42	0.42
7:N:176:ASP:HB2	7:N:190:PRO:HD3	2.00	0.42
1:P:46:GLU:O	1:P:49:GLY:N	2.53	0.42
1:P:122:LEU:O	1:P:373:ALA:HB1	2.20	0.42
1:P:496:VAL:HA	1:P:572:ALA:HB2	2.01	0.42
1:P:624:LYS:HB2	4:H:43:ILE:HG23	2.02	0.42
2:A:131:LEU:HD11	2:A:202:PHE:CZ	2.55	0.42
2:D:126:ARG:HA	5:K:29:G:O3’	2.19	0.42
2:C:43:ASP:OD1	2:C:44:VAL:N	2.53	0.42
2:C:48:ARG:NH1	5:K:20:G:OP1	2.43	0.42
2:C:229:PHE:HB3	2:C:277:LYS:HE2	2.01	0.42
2:F:231:HIS:HE2	2:F:243:LEU:HG	1.85	0.42
3:I:25:GLN:CD	3:I:36:ILE:HG23	2.40	0.42
3:G:52:PHE:HB3	3:G:89:PHE:CE2	2.55	0.42
3:G:62:HIS:O	3:G:66:LEU:HG	2.20	0.42
4:H:84:HIS:CD2	4:H:154:GLY:HA2	2.54	0.42
4:H:196:LEU:HD21	7:N:18:GLU:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:234:LYS:HD3	4:H:234:LYS:HA	1.80	0.42
4:H:431:TYR:HB2	4:H:563:TYR:CZ	2.54	0.42
4:H:454:LYS:O	4:H:464:ARG:NH1	2.53	0.42
4:H:469:TYR:HB2	4:H:557:LEU:HD13	2.01	0.42
4:H:570:PHE:HB3	9:Q:-4:DT:C2	2.54	0.42
3:J:45:SER:C	3:J:98:GLN:HE22	2.23	0.42
3:J:78:GLU:OE1	3:J:112:LEU:HD21	2.20	0.42
7:N:69:GLU:CG	7:N:90:ARG:HB2	2.48	0.42
7:N:83:ILE:HG13	7:N:84:GLU:H	1.84	0.42
1:P:449:ARG:NE	1:P:449:ARG:HA	2.35	0.42
2:A:161:THR:OG1	2:A:162:GLY:N	2.53	0.42
2:A:165:ARG:HH21	2:E:124:GLN:HE22	1.66	0.42
2:B:55:GLN:HG3	2:B:65:ILE:HG13	2.02	0.42
2:D:24:PRO:CG	5:K:33:U:H5"	2.49	0.42
2:D:156:LYS:NZ	6:L:17:DG:OP1	2.38	0.42
2:D:243:LEU:HD23	2:D:243:LEU:HA	1.77	0.42
2:E:181:HIS:HB3	2:E:244:PHE:CE2	2.55	0.42
2:F:243:LEU:HA	2:F:246:ARG:HG3	2.01	0.42
3:G:78:GLU:OE1	3:G:112:LEU:HD21	2.20	0.42
4:H:118:LEU:HD12	4:H:178:TYR:HB2	2.01	0.42
4:H:308:TYR:HD1	4:H:406:LEU:HD22	1.85	0.42
4:H:334:SER:HB3	6:L:47:DG:H5'	2.01	0.42
5:K:6:A:C5	2:M:115:VAL:HG11	2.54	0.42
6:L:40:DT:H6	6:L:40:DT:H2'	1.60	0.42
2:M:9:PHE:CE1	2:M:11:PHE:HB2	2.55	0.42
2:M:54:ILE:HG21	2:M:107:TYR:CG	2.55	0.42
7:N:19:LEU:O	7:N:23:ARG:HA	2.20	0.42
7:N:23:ARG:O	7:N:92:SER:HA	2.19	0.42
7:N:43:TRP:HA	7:N:47:ILE:HG21	2.02	0.42
1:P:263:PHE:HD2	1:P:293:LYS:HD2	1.83	0.42
1:P:305:TYR:CD1	1:P:390:ILE:HB	2.54	0.42
1:P:365:GLN:HG2	1:P:365:GLN:O	2.20	0.42
2:B:74:ASN:HA	2:B:77:ILE:HB	2.01	0.42
2:B:145:HIS:CD2	2:C:133:PHE:CE2	3.08	0.42
2:D:102:MET:HB3	2:D:109:ILE:HD12	2.02	0.42
3:G:25:GLN:CD	3:G:36:ILE:HG23	2.40	0.42
4:H:537:ARG:HD2	3:J:109:THR:CG2	2.50	0.42
5:K:8:C:OP1	7:N:87:ARG:NH1	2.51	0.42
2:M:13:PHE:CZ	2:M:46:LEU:HD21	2.55	0.42
2:M:42:THR:HG22	2:M:133:PHE:CE2	2.55	0.42
2:M:147:ILE:HD13	2:M:170:LYS:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:N:44:LYS:C	7:N:46:ALA:H	2.23	0.42
7:N:48:ARG:HB2	7:N:109:THR:CG2	2.50	0.42
1:P:44:PHE:CZ	1:P:110:LEU:HD22	2.54	0.41
1:P:251:LEU:HD21	1:P:464:ARG:HH22	1.85	0.41
2:B:68:ARG:NH2	2:B:69:GLU:HB2	2.35	0.41
2:B:277:LYS:HE2	2:B:277:LYS:HB2	1.83	0.41
2:D:128:PRO:HG2	2:D:194:PHE:CB	2.50	0.41
2:C:8:ASP:HB3	2:C:244:PHE:CZ	2.55	0.41
2:E:31:ARG:HB2	2:E:40:LEU:O	2.20	0.41
2:E:259:ARG:HG3	2:F:36:THR:HG21	2.02	0.41
2:F:69:GLU:C	2:F:71:GLY:H	2.23	0.41
2:F:116:MET:HB2	2:F:123:GLY:O	2.20	0.41
2:F:145:HIS:HB2	2:F:170:LYS:O	2.20	0.41
4:H:12:ARG:HB2	4:H:297:PRO:HG3	2.02	0.41
4:H:345:THR:HB	4:H:349:ALA:HB3	2.02	0.41
4:H:427:GLN:HB3	4:H:495:ASP:HA	2.01	0.41
4:H:465:GLN:HA	4:H:542:HIS:HB3	2.02	0.41
4:H:523:LEU:HB2	4:H:529:ALA:HB2	2.01	0.41
3:J:21:LEU:HD23	3:J:59:LEU:HD13	2.01	0.41
3:J:52:PHE:HB3	3:J:89:PHE:CE2	2.55	0.41
7:N:175:MET:HA	7:N:190:PRO:HD2	2.02	0.41
1:P:29:VAL:HG21	1:P:52:HIS:CE1	2.54	0.41
1:P:56:LYS:HG3	1:P:61:PHE:CD2	2.55	0.41
1:P:126:TYR:CE1	4:H:303:ALA:HB2	2.55	0.41
1:P:352:GLU:CD	1:P:379:ARG:HH22	2.23	0.41
2:B:102:MET:HE1	2:B:122:ALA:HB1	2.02	0.41
2:C:12:LEU:HD21	2:C:249:VAL:HG21	2.01	0.41
2:C:76:LEU:HD23	2:C:106:TYR:CE2	2.55	0.41
2:C:118:THR:HA	6:L:38:DG:H5”	2.01	0.41
2:C:181:HIS:CE1	2:C:244:PHE:HB3	2.55	0.41
2:E:12:LEU:HA	2:E:178:TYR:O	2.20	0.41
2:E:21:ASN:OD1	2:E:31:ARG:NE	2.51	0.41
2:F:280:ARG:NH2	2:F:282:LEU:HD11	2.36	0.41
3:I:78:GLU:OE1	3:I:112:LEU:HD21	2.20	0.41
4:H:13:LYS:HB2	4:H:297:PRO:HG2	2.01	0.41
4:H:95:LYS:CE	8:O:15:DA:H61	2.33	0.41
4:H:131:LEU:HD11	4:H:159:PHE:HZ	1.84	0.41
4:H:480:LYS:NZ	4:H:528:ARG:HH11	2.18	0.41
3:J:51:VAL:HG23	3:J:52:PHE:N	2.35	0.41
3:J:62:HIS:O	3:J:66:LEU:HG	2.20	0.41
5:K:10:G:C5	5:K:11:G:C6	3.09	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:42:U:H3	6:L:13:DG:H1	1.68	0.41
2:M:47:LYS:HE3	2:M:131:LEU:HB2	2.02	0.41
1:P:102:ARG:HE	1:P:102:ARG:HB3	1.55	0.41
1:P:116:ALA:O	1:P:134:ARG:NH2	2.44	0.41
1:P:349:LEU:HD23	1:P:349:LEU:HA	1.89	0.41
2:A:131:LEU:HD11	2:A:202:PHE:HZ	1.85	0.41
2:A:148:THR:HA	2:A:167:MET:HA	2.02	0.41
2:B:276:THR:HG22	2:B:276:THR:O	2.20	0.41
2:D:17:ASP:OD2	2:E:135:ARG:HD3	2.21	0.41
2:D:21:ASN:ND2	2:D:45:CYS:HB2	2.35	0.41
2:C:21:ASN:OD1	2:C:31:ARG:NE	2.42	0.41
2:C:256:GLU:HG3	2:C:257:VAL:H	1.85	0.41
4:H:24:GLY:HA2	4:H:183:ASN:ND2	2.35	0.41
4:H:84:HIS:HB3	4:H:87:TYR:HB2	2.02	0.41
4:H:196:LEU:HD21	7:N:18:GLU:OE1	2.20	0.41
4:H:540:LEU:HD11	3:J:103:ILE:CD1	2.50	0.41
5:K:26:G:O2'	5:K:28:U:OP1	2.17	0.41
5:K:33:U:H1'	5:K:34:C:O4'	2.20	0.41
1:P:202:THR:HG23	1:P:203:GLU:HG2	2.03	0.41
1:P:433:ASN:OD1	1:P:443:GLU:HG2	2.20	0.41
1:P:499:ARG:NH2	1:P:750:ASN:O	2.53	0.41
1:P:695:ILE:O	1:P:695:ILE:HG13	2.20	0.41
2:A:15:VAL:O	2:A:15:VAL:HG13	2.20	0.41
2:A:28:ASN:O	2:A:171:PHE:CD1	2.73	0.41
2:A:34:PRO:HG3	3:J:47:THR:HG23	2.02	0.41
2:A:113:GLY:N	2:A:127:GLY:HA3	2.35	0.41
2:A:181:HIS:CE1	2:A:244:PHE:HB3	2.56	0.41
2:A:241:ASP:OD2	2:A:245:LYS:HE3	2.20	0.41
2:B:15:VAL:CG1	2:B:20:PRO:HG3	2.50	0.41
2:B:103:CYS:HB3	2:B:192:THR:O	2.19	0.41
2:D:62:HIS:O	2:D:110:ARG:NH2	2.53	0.41
2:D:203:TRP:CE3	2:D:203:TRP:HA	2.55	0.41
2:E:186:THR:OG1	2:E:234:ASN:HB3	2.20	0.41
2:E:229:PHE:CD2	2:E:279:LEU:HD21	2.55	0.41
2:F:4:GLU:OE1	2:F:4:GLU:N	2.53	0.41
3:I:12:TYR:HH	3:I:107:HIS:CG	2.31	0.41
4:H:31:PRO:HA	4:H:58:GLY:CA	2.50	0.41
4:H:569:LEU:HA	4:H:569:LEU:HD23	1.55	0.41
3:J:25:GLN:CD	3:J:36:ILE:HG23	2.40	0.41
5:K:8:C:C5'	2:M:48:ARG:HB2	2.49	0.41
5:K:14:C:O2	5:K:14:C:H2'	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:11:DG:H5'	6:L:12:DG:H5'	2.02	0.41
2:M:22:GLY:HA3	2:M:28:ASN:OD1	2.20	0.41
2:M:47:LYS:HG2	2:M:112:PHE:CD1	2.55	0.41
1:P:259:LEU:HA	1:P:262:CYS:HB2	2.02	0.41
1:P:344:THR:C	1:P:346:LYS:H	2.23	0.41
1:P:412:LEU:O	1:P:418:VAL:HG22	2.21	0.41
1:P:435:ASP:OD1	1:P:435:ASP:N	2.39	0.41
1:P:470:PRO:HD3	1:P:600:VAL:HB	2.01	0.41
1:P:516:LEU:O	1:P:552:LEU:HD12	2.20	0.41
1:P:566:PHE:O	1:P:586:CYS:HA	2.21	0.41
1:P:707:GLN:NE2	1:P:710:GLU:O	2.53	0.41
2:A:47:LYS:HD3	5:K:25:A:P	2.60	0.41
2:A:153:THR:HB	6:L:25:DC:H4'	2.02	0.41
2:B:65:ILE:O	2:B:65:ILE:HG22	2.19	0.41
2:D:41:VAL:HG23	2:D:178:TYR:CE2	2.55	0.41
2:D:145:HIS:HB2	2:D:170:LYS:O	2.21	0.41
2:D:183:PHE:CE1	2:D:244:PHE:CE2	3.08	0.41
2:E:147:ILE:O	2:E:147:ILE:HG13	2.19	0.41
3:I:51:VAL:HG23	3:I:52:PHE:N	2.35	0.41
4:H:78:SER:HA	4:H:87:TYR:CE2	2.56	0.41
4:H:217:LYS:HE3	8:O:13:DC:C2	2.55	0.41
2:M:160:GLU:CG	2:M:161:THR:H	2.33	0.41
1:P:60:SER:HB3	1:P:89:ILE:HD13	2.03	0.41
1:P:270:ARG:O	1:P:272:LEU:N	2.53	0.41
2:A:115:VAL:HG13	5:K:23:G:C2	2.55	0.41
2:B:21:ASN:HB2	2:B:41:VAL:HG13	2.02	0.41
2:B:203:TRP:CE3	2:B:226:LEU:HD21	2.55	0.41
2:D:56:MET:HE2	2:E:187:HIS:HB2	2.03	0.41
2:D:163:ASP:OD1	2:E:69:GLU:HB2	2.21	0.41
2:D:208:ASN:O	2:D:212:HIS:ND1	2.54	0.41
2:D:280:ARG:HH22	2:D:282:LEU:HD21	1.86	0.41
2:C:7:TYR:HB2	2:C:184:ILE:CG1	2.51	0.41
2:C:46:LEU:HB2	2:C:131:LEU:HD22	2.02	0.41
2:C:50:VAL:HG13	2:C:205:ALA:HB1	2.03	0.41
2:C:137:ILE:HB	2:C:264:TYR:CE1	2.55	0.41
2:C:206:LEU:O	2:C:209:MET:HG2	2.20	0.41
2:C:258:VAL:HG21	2:C:264:TYR:CE2	2.55	0.41
2:E:259:ARG:HH11	2:F:35:GLN:HB2	1.84	0.41
3:I:113:PHE:HB2	3:J:80:ARG:NH1	2.16	0.41
4:H:206:ARG:HG2	4:H:207:LEU:CD2	2.46	0.41
6:L:9:DG:C8	6:L:10:DA:N6	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:39:GLY:N	2:M:136:SER:HB3	2.36	0.41
2:M:137:ILE:HG12	2:M:177:LEU:O	2.20	0.41
1:P:93:THR:HG22	1:P:134:ARG:NH2	2.34	0.41
1:P:195:VAL:HG12	1:P:379:ARG:CG	2.50	0.41
2:A:23:ASP:CB	2:A:24:PRO:HD3	2.51	0.41
2:A:186:THR:O	2:A:190:LYS:HG3	2.20	0.41
2:B:36:THR:HG21	2:M:259:ARG:HG3	2.02	0.41
2:B:73:LEU:N	2:M:152:VAL:O	2.44	0.41
2:B:138:ASP:OD2	2:B:251:LYS:HB3	2.20	0.41
2:D:113:GLY:CA	5:K:30:G:H5”	2.50	0.41
2:D:258:VAL:HG11	2:D:264:TYR:CE2	2.55	0.41
2:C:143:LEU:HD23	2:C:143:LEU:HA	1.61	0.41
2:E:54:ILE:HG21	2:E:107:TYR:CD2	2.55	0.41
2:E:259:ARG:HD3	2:E:259:ARG:HA	1.86	0.41
3:I:22:GLU:N	3:I:36:ILE:HD11	2.36	0.41
4:H:248:PHE:CE1	4:H:252:THR:HG21	2.55	0.41
4:H:384:LEU:HD21	4:H:436:LEU:HD23	2.02	0.41
4:H:441:ILE:HG23	4:H:450:LEU:CD2	2.51	0.41
2:M:29:LEU:HB3	2:M:171:PHE:CE2	2.55	0.41
2:M:166:THR:O	2:M:167:MET:C	2.59	0.41
1:P:182:GLU:OE1	1:P:411:VAL:HG11	2.20	0.41
1:P:329:VAL:HG13	1:P:359:ILE:CD1	2.50	0.41
1:P:333:HIS:HD1	1:P:362:THR:HG1	1.66	0.41
1:P:573:MET:HE1	1:P:619:THR:HG22	2.02	0.41
1:P:616:GLN:O	1:P:620:GLU:HG3	2.21	0.41
1:P:628:LEU:HD23	1:P:636:ALA:HB1	2.03	0.41
1:P:647:LYS:HD3	4:H:46:GLU:OE2	2.21	0.41
2:A:34:PRO:HG3	3:J:47:THR:CG2	2.50	0.41
2:A:134:SER:HA	2:A:179:ARG:O	2.20	0.41
2:B:147:ILE:HD11	5:K:19:U:C4	2.56	0.41
2:B:243:LEU:HD21	2:B:277:LYS:HE3	2.02	0.41
2:D:109:ILE:HD13	2:D:116:MET:SD	2.61	0.41
2:C:11:PHE:CZ	2:C:210:PHE:HE2	2.38	0.41
2:C:43:ASP:OD1	2:C:44:VAL:HG13	2.20	0.41
2:C:66:PHE:N	2:C:67:ILE:HG23	2.36	0.41
2:E:44:VAL:HG11	5:K:37:C:H2’	2.02	0.41
2:E:51:ARG:HH12	5:K:37:C:P	2.44	0.41
2:F:51:ARG:NH2	2:F:108:ASP:OD2	2.54	0.41
2:F:89:LYS:HD3	2:F:89:LYS:HA	1.93	0.41
3:I:93:LEU:HA	3:I:93:LEU:HD23	1.79	0.41
3:G:51:VAL:HG23	3:G:52:PHE:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:478:LEU:HD21	4:H:516:LEU:HD22	2.02	0.41
3:J:49:ILE:HG13	3:J:50:ALA:N	2.36	0.41
1:P:47:TYR:HD2	1:P:166:LEU:HD12	1.84	0.41
1:P:93:THR:HG22	1:P:134:ARG:HE	1.86	0.41
1:P:272:LEU:HD21	1:P:445:LEU:HB3	2.03	0.41
1:P:274:SER:OG	1:P:422:LEU:HB2	2.21	0.41
1:P:471:PRO:HA	1:P:472:PRO:HD3	1.96	0.41
1:P:493:LEU:HD13	1:P:552:LEU:HD23	2.03	0.41
2:A:134:SER:OG	2:A:180:CYS:HB2	2.21	0.41
2:A:166:THR:O	2:A:167:MET:C	2.59	0.41
2:B:18:GLY:HA3	2:B:218:ARG:C	2.41	0.41
2:B:48:ARG:HD2	5:K:14:C:P	2.61	0.41
2:B:137:ILE:HD11	2:B:179:ARG:HB2	2.02	0.41
2:B:144:GLU:HG3	2:B:171:PHE:HD1	1.81	0.41
2:B:149:ARG:NE	2:B:166:THR:OG1	2.51	0.41
2:D:27:GLY:CA	3:I:40:TYR:HE1	2.29	0.41
2:D:128:PRO:HG2	2:D:194:PHE:CD2	2.55	0.41
2:D:129:VAL:HG22	2:D:184:ILE:HG23	2.02	0.41
2:D:252:LYS:HG2	2:D:253:ASP:H	1.86	0.41
2:C:78:ASP:O	2:C:82:GLU:HG2	2.20	0.41
2:C:109:ILE:HG12	2:C:114:ALA:HB3	2.02	0.41
2:E:203:TRP:CE3	2:E:226:LEU:HD21	2.55	0.41
2:E:218:ARG:NH1	2:F:126:ARG:HH22	2.18	0.41
2:F:66:PHE:CD1	2:F:109:ILE:HD11	2.56	0.41
3:I:49:ILE:HG13	3:I:50:ALA:N	2.36	0.41
3:I:62:HIS:O	3:I:66:LEU:HG	2.20	0.41
3:G:76:GLN:HA	3:G:79:ILE:HD12	2.03	0.41
4:H:112:ASN:O	4:H:116:GLN:HG2	2.20	0.41
4:H:214:VAL:CG2	4:H:330:LEU:HD13	2.50	0.41
4:H:269:VAL:HG23	4:H:331:SER:HB3	2.02	0.41
4:H:424:LYS:O	4:H:427:GLN:NE2	2.54	0.41
4:H:441:ILE:HD12	4:H:560:ILE:CD1	2.50	0.41
4:H:482:GLN:HG2	4:H:489:LEU:HD11	2.02	0.41
4:H:537:ARG:HD2	3:J:109:THR:HG22	2.03	0.41
4:H:554:GLN:HA	4:H:557:LEU:HB2	2.03	0.41
3:J:14:LEU:HD11	3:J:90:PRO:CD	2.42	0.41
3:J:40:TYR:HD2	3:J:55:LEU:CD2	2.34	0.41
5:K:39:U:C2	5:K:40:C:C2	3.08	0.41
2:M:32:ILE:HG22	2:M:140:ILE:HD11	2.03	0.41
2:M:69:GLU:OE2	7:N:83:ILE:HD11	2.21	0.41
2:M:127:GLY:HA2	2:M:192:THR:HG21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:N:40:ALA:HB1	7:N:136:HIS:HB3	2.02	0.41
7:N:65:ILE:HG13	7:N:94:LEU:HD12	2.03	0.41
9:Q:11:DT:H6	9:Q:11:DT:H2'	1.72	0.41
1:P:106:PHE:HB2	4:H:285:LEU:CD1	2.51	0.41
1:P:186:TRP:HD1	1:P:416:TYR:OH	2.03	0.41
1:P:192:SER:CB	1:P:382:HIS:H	2.33	0.41
1:P:395:GLN:N	1:P:428:PRO:HG3	2.36	0.41
1:P:464:ARG:HD3	1:P:587:ASN:HD22	1.86	0.41
1:P:632:LEU:HA	1:P:637:PHE:CE2	2.56	0.41
2:A:51:ARG:NH2	2:A:112:PHE:HB2	2.36	0.41
2:A:137:ILE:HD11	2:A:179:ARG:HB2	2.03	0.41
2:B:50:VAL:HG21	2:B:202:PHE:CE1	2.56	0.41
2:C:102:MET:HG3	2:C:116:MET:SD	2.61	0.41
2:C:107:TYR:OH	2:C:202:PHE:HB2	2.21	0.41
2:E:40:LEU:HA	2:E:134:SER:O	2.21	0.41
4:H:263:ARG:NH2	8:O:17:DA:H4'	2.36	0.41
5:K:2:U:H6	7:N:43:TRP:CH2	2.39	0.41
6:L:26:DC:H2'	6:L:27:DA:C8	2.56	0.41
2:M:67:ILE:HG23	2:M:67:ILE:HD12	1.60	0.41
2:M:141:MET:O	2:M:174:PRO:HD3	2.21	0.41
2:M:236:GLY:O	7:N:133:GLN:HG2	2.20	0.41
7:N:36:ASN:HA	7:N:39:MET:HE2	2.03	0.41
1:P:202:THR:O	1:P:206:MET:N	2.49	0.40
1:P:231:ARG:HG3	1:P:235:GLN:NE2	2.36	0.40
2:A:143:LEU:HD21	2:D:34:PRO:CG	2.51	0.40
2:A:218:ARG:HD3	2:A:221:MET:CE	2.52	0.40
2:D:128:PRO:HG2	2:D:194:PHE:CG	2.57	0.40
2:D:214:HIS:O	2:E:126:ARG:NH1	2.46	0.40
2:C:14:ASP:CG	2:C:224:ARG:HE	2.23	0.40
2:C:54:ILE:HG13	2:C:107:TYR:CE1	2.57	0.40
2:C:203:TRP:CE3	2:C:226:LEU:HD21	2.57	0.40
2:E:137:ILE:HG13	2:E:249:VAL:CG1	2.51	0.40
2:E:177:LEU:HD12	2:E:177:LEU:HA	1.83	0.40
2:F:9:PHE:CB	2:F:228:VAL:HG12	2.50	0.40
2:F:20:PRO:HB2	2:F:41:VAL:CG2	2.51	0.40
2:F:143:LEU:HB2	2:F:172:THR:HG23	2.03	0.40
3:I:14:LEU:HD11	3:I:90:PRO:CD	2.42	0.40
3:G:40:TYR:HD2	3:G:55:LEU:CD2	2.34	0.40
4:H:33:ILE:HD13	4:H:160:ARG:NH2	2.35	0.40
4:H:234:LYS:HB3	4:H:239:ALA:N	2.35	0.40
4:H:398:ILE:HG13	4:H:399:ALA:N	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:14:ASP:OD2	2:M:224:ARG:NE	2.44	0.40
1:P:129:GLY:HA3	1:P:674:ARG:NH2	2.36	0.40
1:P:213:ASP:OD1	1:P:214:ALA:N	2.53	0.40
1:P:302:ARG:CD	1:P:383:ASN:HB3	2.47	0.40
1:P:303:ILE:CD1	1:P:388:VAL:HB	2.52	0.40
1:P:515:LYS:HA	1:P:551:TRP:CD1	2.56	0.40
2:B:44:VAL:HG21	2:M:147:ILE:HB	2.02	0.40
2:B:258:VAL:HG21	2:B:264:TYR:OH	2.21	0.40
2:D:31:ARG:HH21	5:K:33:U:P	2.43	0.40
2:D:113:GLY:N	2:D:127:GLY:HA3	2.37	0.40
2:D:129:VAL:HG11	2:D:202:PHE:CE2	2.56	0.40
2:C:105:ARG:HB3	2:C:106:TYR:CD1	2.56	0.40
3:I:12:TYR:HB2	3:I:100:LEU:HD22	2.03	0.40
3:G:12:TYR:HB2	3:G:100:LEU:HD22	2.03	0.40
4:H:39:GLN:HG2	4:H:41:ASN:HD21	1.86	0.40
4:H:51:LEU:HD12	4:H:51:LEU:HA	1.75	0.40
4:H:234:LYS:O	4:H:238:PHE:HB2	2.21	0.40
4:H:313:ASN:OD1	8:O:20:DA:H4'	2.21	0.40
4:H:475:PHE:CE1	4:H:512:LEU:HD11	2.57	0.40
5:K:13:U:C5	2:M:147:ILE:HD11	2.57	0.40
7:N:47:ILE:HG13	7:N:106:PHE:CG	2.57	0.40
1:P:63:LYS:HB3	1:P:63:LYS:HE2	1.93	0.40
1:P:106:PHE:CE2	1:P:110:LEU:HD12	2.57	0.40
1:P:244:ASP:HA	1:P:252:ASN:ND2	2.32	0.40
1:P:332:HIS:HB2	1:P:336:LEU:H	1.87	0.40
2:A:22:GLY:HA3	5:K:27:G:C2'	2.51	0.40
2:A:25:ASP:HB3	2:C:167:MET:HE1	2.03	0.40
2:D:127:GLY:HA2	2:D:128:PRO:HD3	1.87	0.40
2:D:147:ILE:HA	2:E:31:ARG:HH22	1.85	0.40
2:C:56:MET:CE	2:C:212:HIS:HB3	2.51	0.40
2:E:113:GLY:CA	5:K:36:C:H5"	2.51	0.40
2:E:213:ASP:HB3	2:E:218:ARG:HH12	1.86	0.40
2:F:19:ASN:HB3	2:F:22:GLY:N	2.36	0.40
4:H:12:ARG:O	4:H:16:SER:N	2.53	0.40
4:H:257:LEU:HB3	4:H:272:VAL:HB	2.02	0.40
4:H:274:TRP:HA	4:H:301:ILE:HG22	2.02	0.40
4:H:514:ARG:HH21	3:J:45:SER:HB3	1.87	0.40
2:M:282:LEU:HA	2:M:282:LEU:HD23	1.90	0.40
7:N:16:ARG:HG3	7:N:24:VAL:O	2.20	0.40
9:Q:2:DA:H2'	9:Q:3:DA:C8	2.56	0.40
1:P:125:TRP:CE3	1:P:131:LEU:HB2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:300:LYS:HD2	1:P:387:SER:O	2.21	0.40
1:P:331:GLU:HB3	1:P:365:GLN:HE22	1.86	0.40
1:P:395:GLN:HA	1:P:428:PRO:HG3	2.03	0.40
1:P:426:THR:HB	1:P:637:PHE:CG	2.57	0.40
1:P:486:ILE:HG22	1:P:570:TYR:HD2	1.84	0.40
2:B:67:ILE:HB	2:B:68:ARG:H	1.66	0.40
2:B:87:LYS:HE3	2:B:87:LYS:HB3	1.93	0.40
2:B:144:GLU:OE1	4:H:424:LYS:HD2	2.22	0.40
2:B:149:ARG:HB2	5:K:19:U:H1'	2.04	0.40
2:D:54:ILE:HG13	2:D:107:TYR:CD2	2.57	0.40
2:D:259:ARG:HD3	2:D:259:ARG:HA	1.71	0.40
2:C:76:LEU:HD12	2:C:76:LEU:H	1.86	0.40
2:E:113:GLY:C	5:K:36:C:H5"	2.41	0.40
2:E:126:ARG:HD2	2:E:188:PHE:CG	2.56	0.40
4:H:465:GLN:OE1	4:H:542:HIS:ND1	2.54	0.40
3:J:12:TYR:HB2	3:J:100:LEU:HD22	2.03	0.40
5:K:3:U:O2	7:N:39:MET:HE1	2.22	0.40
6:L:19:DG:OP2	6:L:19:DG:H2'	2.21	0.40
2:M:115:VAL:HA	2:M:124:GLN:HA	2.03	0.40
1:P:65:ILE:CD1	11:P:803:PO4:P	3.09	0.40
1:P:412:LEU:HA	1:P:416:TYR:HB2	2.04	0.40
2:A:38:GLU:HA	2:A:139:PRO:HA	2.03	0.40
2:A:128:PRO:HG3	2:A:189:ALA:CA	2.50	0.40
2:B:15:VAL:O	2:B:175:TYR:HA	2.21	0.40
2:B:259:ARG:NH2	2:C:33:ASP:OD1	2.54	0.40
2:C:40:LEU:HA	2:C:134:SER:O	2.22	0.40
2:C:109:ILE:HG21	2:C:116:MET:HE1	2.04	0.40
2:E:273:LEU:C	2:E:275:GLU:N	2.75	0.40
3:I:73:VAL:HG13	9:Q:11:DT:C4	2.57	0.40
3:G:96:GLU:HG3	3:G:100:LEU:HD12	2.04	0.40
4:H:333:ASN:HB2	4:H:338:VAL:HG23	2.04	0.40
4:H:508:VAL:CG1	4:H:512:LEU:HG	2.51	0.40
4:H:516:LEU:CD2	4:H:536:ILE:HD13	2.51	0.40
5:K:17:C:N4	5:K:18:U:O4	2.54	0.40
5:K:18:U:O2'	5:K:19:U:OP2	2.30	0.40
2:M:6:ARG:HH11	2:M:231:HIS:HE1	1.69	0.40
2:M:238:ALA:HB2	2:M:277:LYS:HE2	2.03	0.40
7:N:57:LEU:HA	7:N:159:LEU:HA	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	P	752/771 (98%)	627 (83%)	123 (16%)	2 (0%)	41 76
2	A	281/283 (99%)	223 (79%)	55 (20%)	3 (1%)	14 50
2	B	281/283 (99%)	223 (79%)	56 (20%)	2 (1%)	22 60
2	C	281/283 (99%)	233 (83%)	47 (17%)	1 (0%)	34 72
2	D	281/283 (99%)	229 (82%)	51 (18%)	1 (0%)	34 72
2	E	281/283 (99%)	231 (82%)	49 (17%)	1 (0%)	34 72
2	F	267/283 (94%)	218 (82%)	48 (18%)	1 (0%)	34 72
2	M	260/283 (92%)	214 (82%)	46 (18%)	0	100 100
3	G	122/124 (98%)	114 (93%)	8 (7%)	0	100 100
3	I	122/124 (98%)	114 (93%)	8 (7%)	0	100 100
3	J	122/124 (98%)	114 (93%)	8 (7%)	0	100 100
4	H	580/582 (100%)	477 (82%)	102 (18%)	1 (0%)	47 82
7	N	203/205 (99%)	163 (80%)	39 (19%)	1 (0%)	29 68
All	All	3833/3911 (98%)	3180 (83%)	640 (17%)	13 (0%)	44 76

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	P	745	PRO
2	A	91	LYS
2	D	91	LYS
2	C	91	LYS
2	E	91	LYS
2	B	91	LYS
2	F	91	LYS
4	H	398	ILE
2	A	68	ARG
7	N	194	GLN

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Mol	Chain	Res	Type
2	A	23	ASP
2	B	68	ARG
1	P	744	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	P	588/601 (98%)	587 (100%)	1 (0%)	93 98
2	A	245/245 (100%)	244 (100%)	1 (0%)	91 97
2	B	245/245 (100%)	245 (100%)	0	100 100
2	C	245/245 (100%)	243 (99%)	2 (1%)	81 93
2	D	245/245 (100%)	243 (99%)	2 (1%)	81 93
2	E	245/245 (100%)	244 (100%)	1 (0%)	91 97
2	F	235/245 (96%)	235 (100%)	0	100 100
2	M	229/245 (94%)	229 (100%)	0	100 100
3	G	104/104 (100%)	98 (94%)	6 (6%)	20 55
3	I	104/104 (100%)	99 (95%)	5 (5%)	25 62
3	J	104/104 (100%)	99 (95%)	5 (5%)	25 62
4	H	475/475 (100%)	475 (100%)	0	100 100
7	N	182/182 (100%)	182 (100%)	0	100 100
All	All	3246/3285 (99%)	3223 (99%)	23 (1%)	84 94

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	439	ARG
2	A	91	LYS
2	D	68	ARG
2	D	91	LYS
2	C	91	LYS

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Mol	Chain	Res	Type
2	C	156	LYS
2	E	271	LYS
3	I	6	ASN
3	I	13	VAL
3	I	39	ARG
3	I	97	GLN
3	I	100	LEU
3	G	6	ASN
3	G	13	VAL
3	G	33	ASN
3	G	39	ARG
3	G	97	GLN
3	G	100	LEU
3	J	6	ASN
3	J	13	VAL
3	J	39	ARG
3	J	97	GLN
3	J	100	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	P	8	HIS
1	P	184	HIS
1	P	252	ASN
1	P	382	HIS
1	P	402	GLN
1	P	427	GLN
1	P	501	HIS
1	P	517	HIS
1	P	587	ASN
1	P	707	GLN
2	A	21	ASN
2	A	130	GLN
2	B	74	ASN
2	B	124	GLN
2	B	181	HIS
2	B	231	HIS
2	D	181	HIS
2	D	222	ASN
2	C	145	HIS
2	C	181	HIS

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Mol	Chain	Res	Type
2	E	181	HIS
2	E	222	ASN
2	F	21	ASN
2	F	58	GLN
3	I	33	ASN
3	I	85	HIS
3	G	85	HIS
4	H	79	ASN
4	H	225	ASN
4	H	236	GLN
4	H	490	ASN
4	H	544	GLN
3	J	33	ASN
3	J	85	HIS
2	M	21	ASN
2	M	220	GLN
7	N	68	ASN
7	N	89	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
5	K	42/43 (97%)	33 (78%)	3 (7%)

All (33) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	K	2	U
5	K	3	U
5	K	4	G
5	K	5	A
5	K	6	A
5	K	8	C
5	K	9	A
5	K	10	G
5	K	11	G
5	K	13	U
5	K	15	A
5	K	16	G
5	K	17	C
5	K	18	U

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Mol	Chain	Res	Type
5	K	19	U
5	K	20	G
5	K	21	C
5	K	22	C
5	K	23	G
5	K	24	U
5	K	25	A
5	K	27	G
5	K	29	G
5	K	31	C
5	K	33	U
5	K	34	C
5	K	35	G
5	K	36	C
5	K	37	C
5	K	38	C
5	K	39	U
5	K	41	G
5	K	43	C

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	K	4	G
5	K	9	A
5	K	14	C

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
11	PO4	P	804	10	4,4,4	1.21	0	6,6,6	0.29	0
11	PO4	P	803	-	4,4,4	0.91	0	6,6,6	0.41	0
11	PO4	O	101	-	4,4,4	0.84	0	6,6,6	0.43	0
11	PO4	Q	101	-	4,4,4	0.70	0	6,6,6	0.43	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

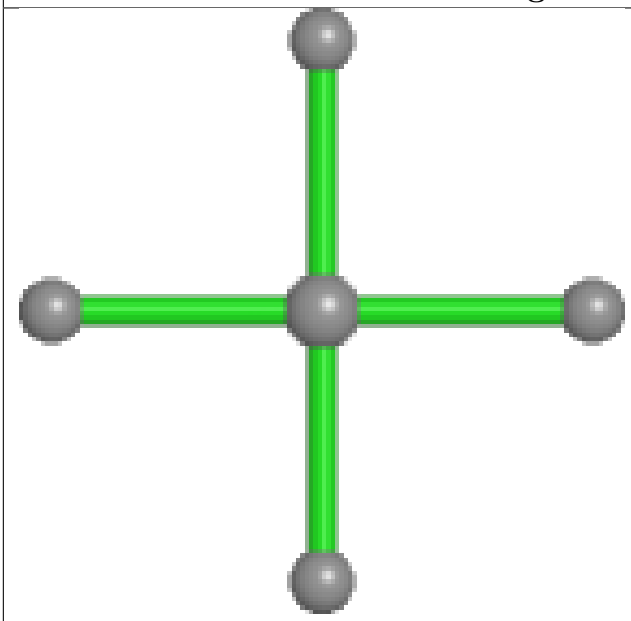
There are no ring outliers.

4 monomers are involved in 17 short contacts:

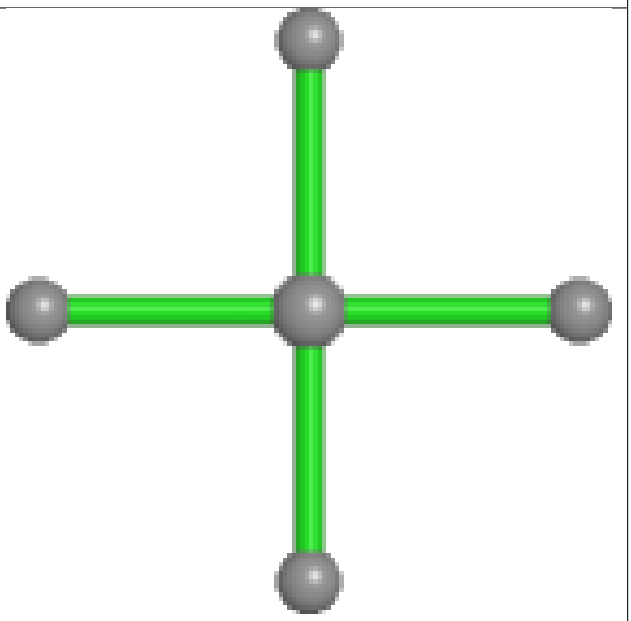
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	P	804	PO4	4	0
11	P	803	PO4	10	0
11	O	101	PO4	1	0
11	Q	101	PO4	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

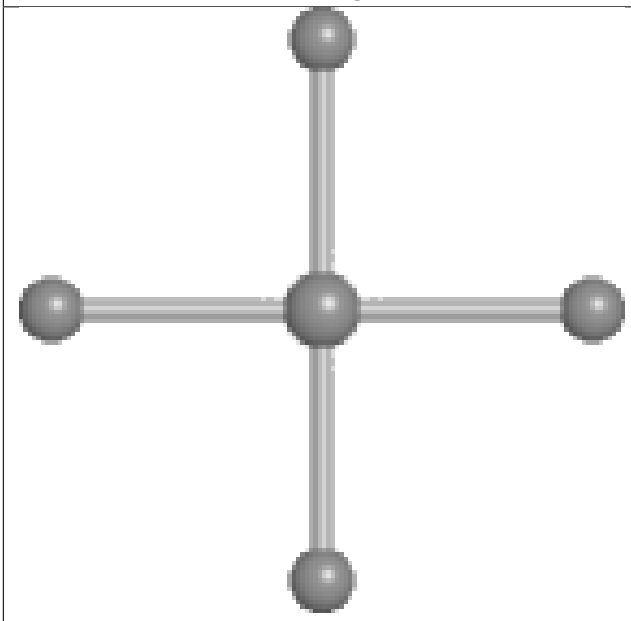
Ligand PO4 P 804



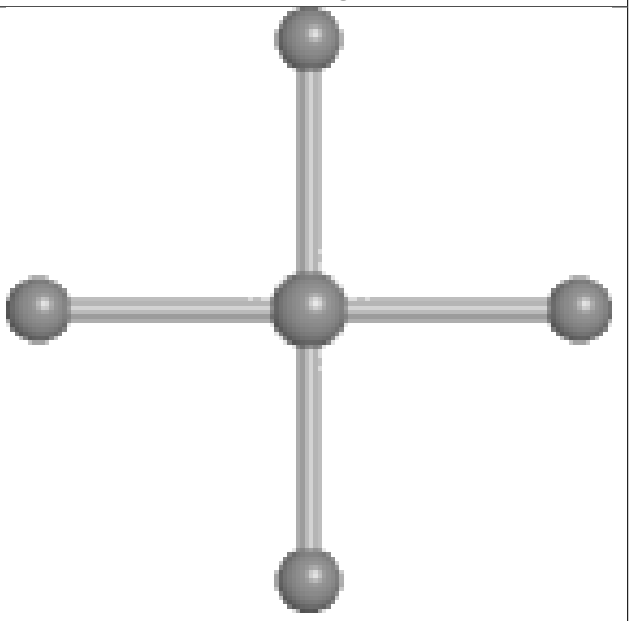
Bond lengths



Bond angles

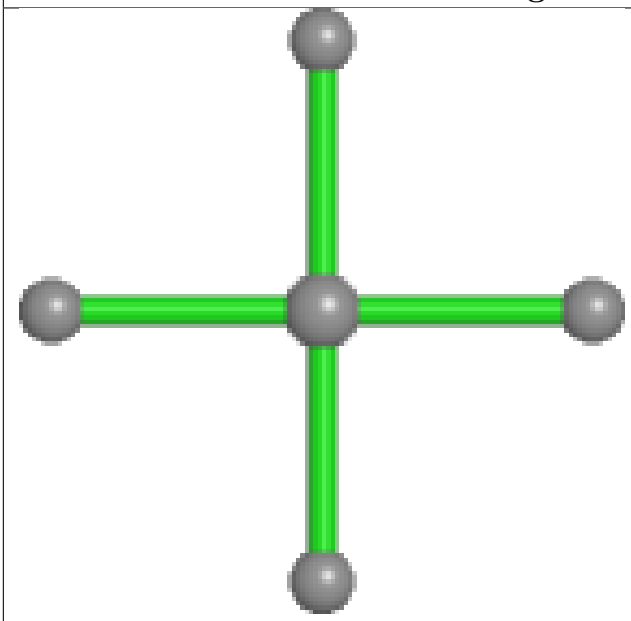


Torsions

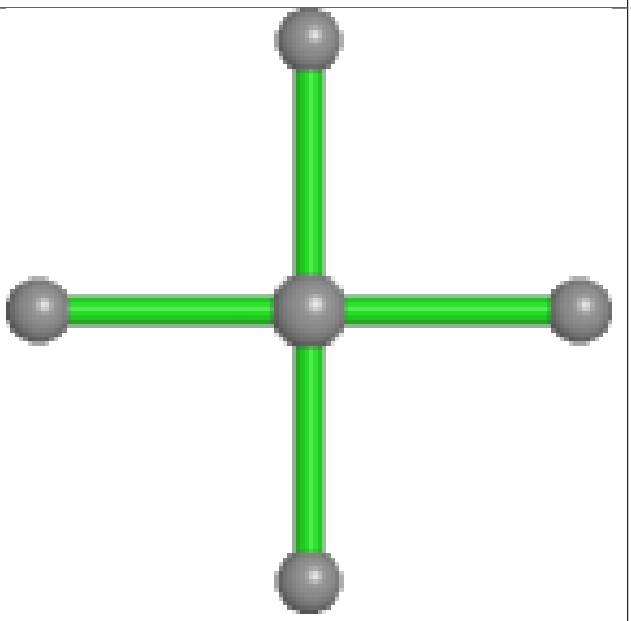


Rings

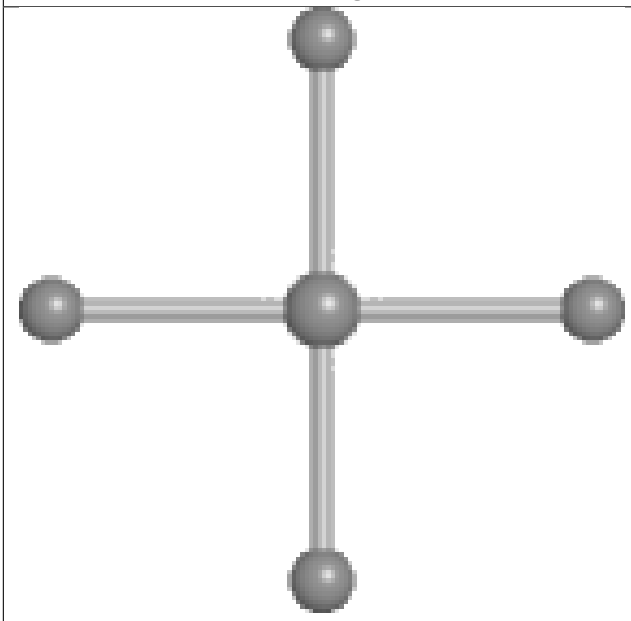
Ligand PO4 P 803



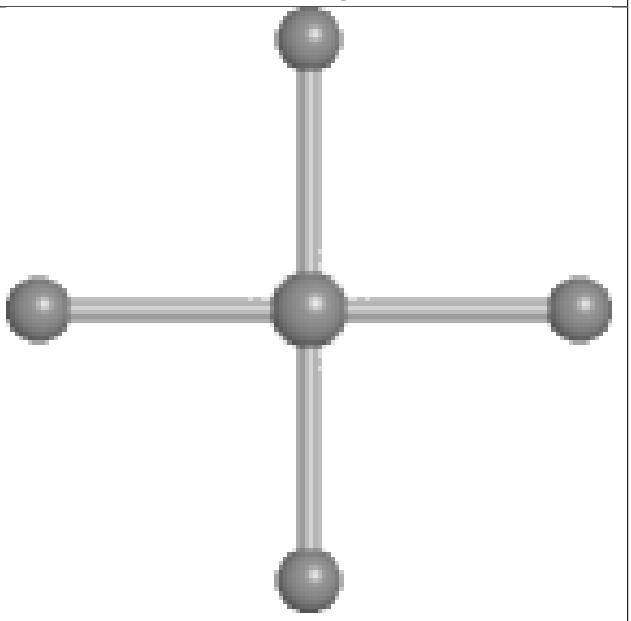
Bond lengths



Bond angles

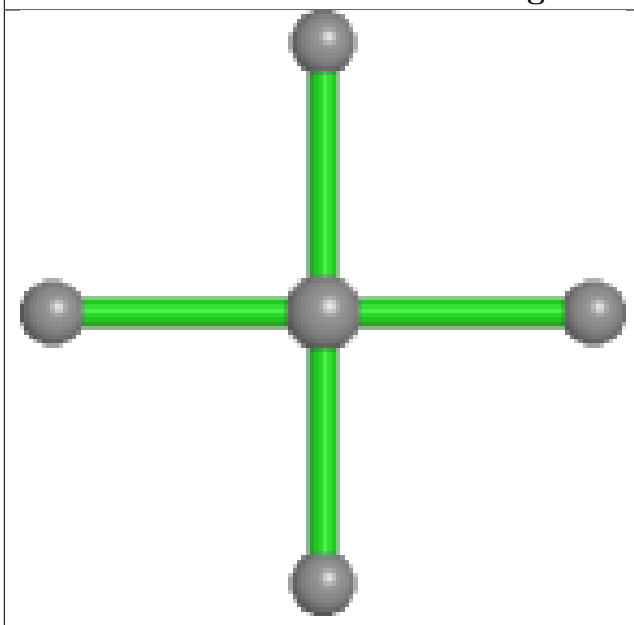


Torsions

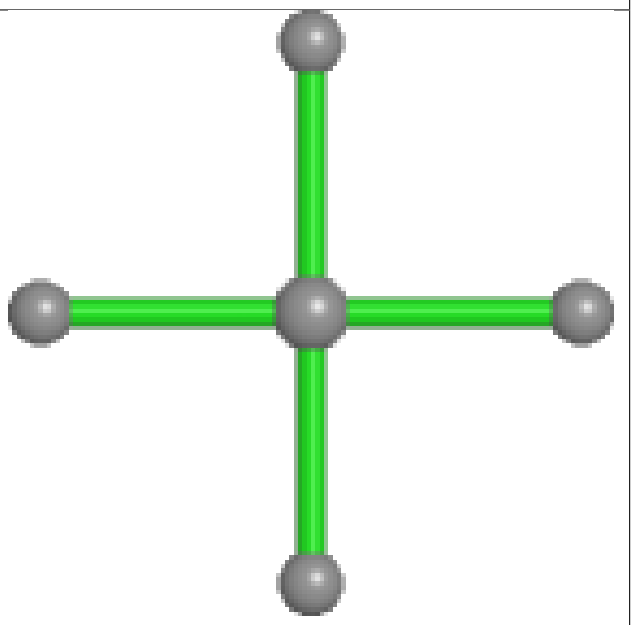


Rings

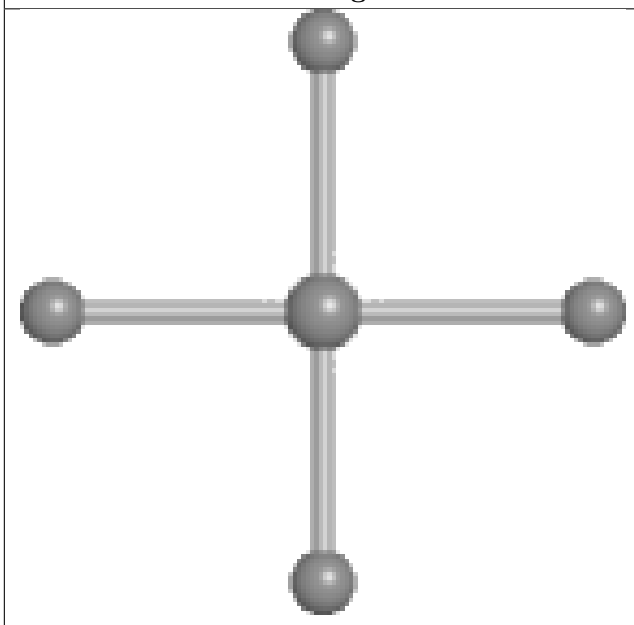
Ligand PO4 O 101



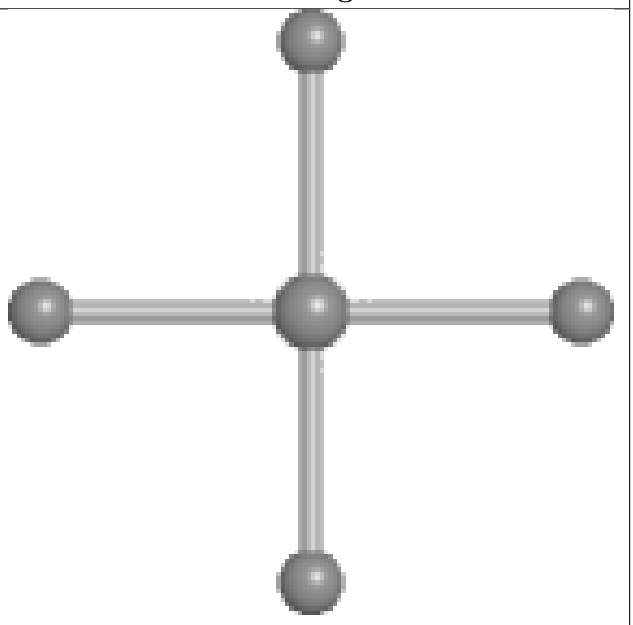
Bond lengths



Bond angles

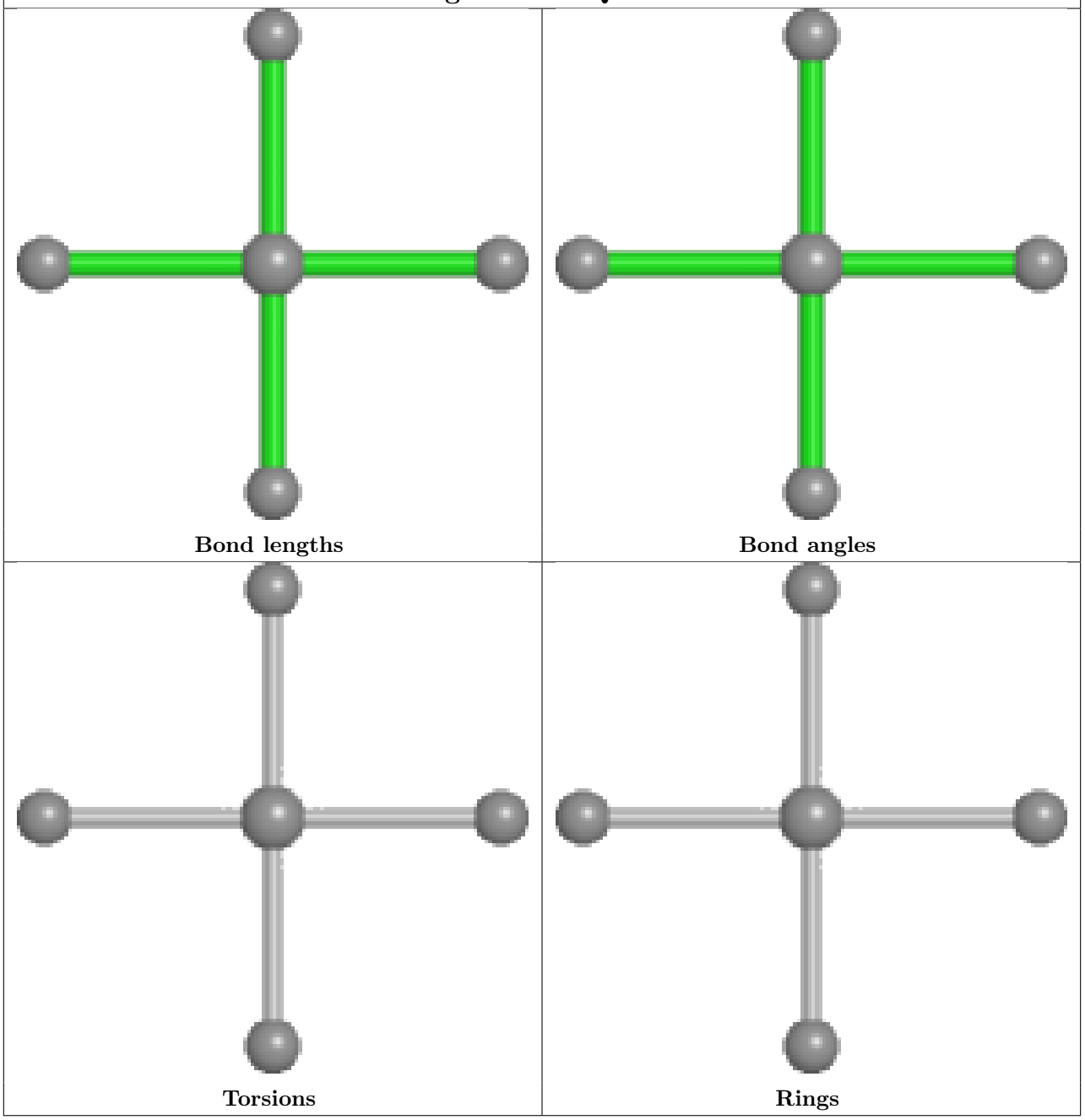


Torsions



Rings

Ligand PO4 Q 101



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
1	P	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	P	759:LEU	C	760:ALA	N	6.63

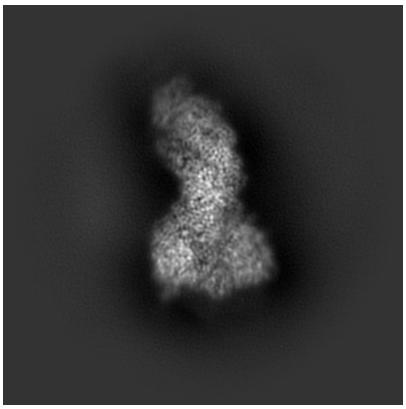
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-29879. These allow visual inspection of the internal detail of the map and identification of artifacts.

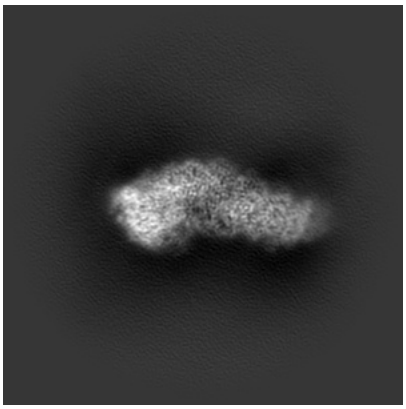
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

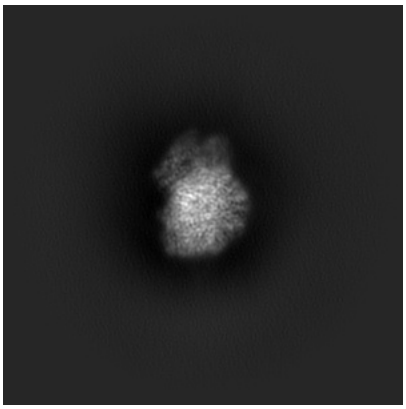
6.1.1 Primary map



X

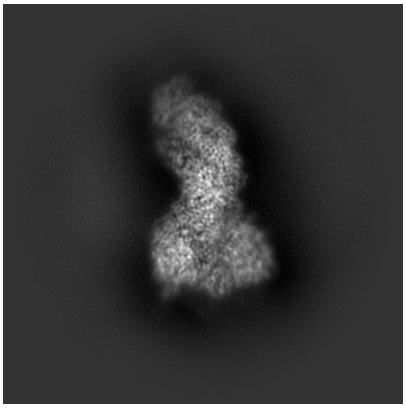


Y

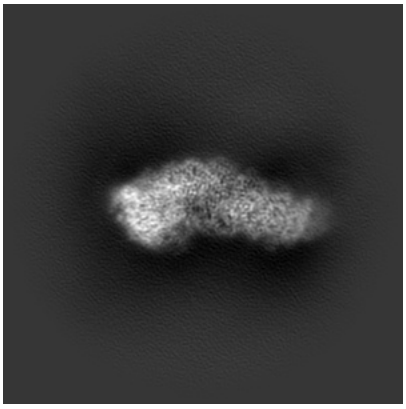


Z

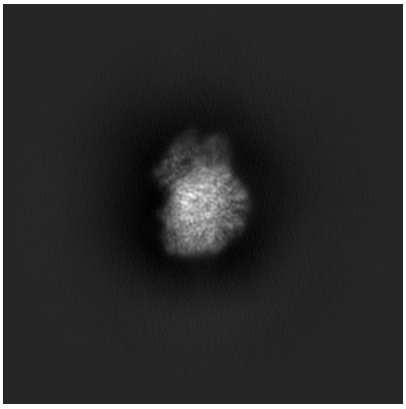
6.1.2 Raw map



X



Y

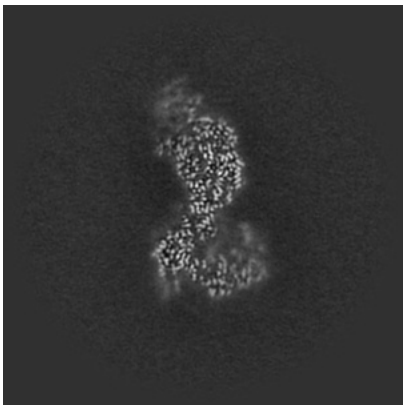


Z

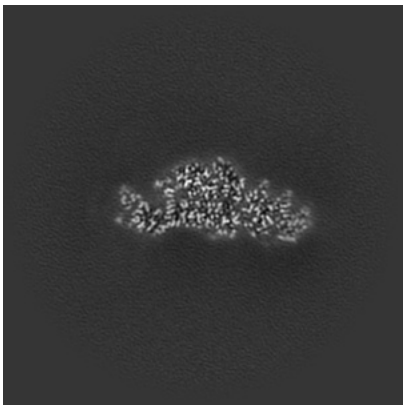
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

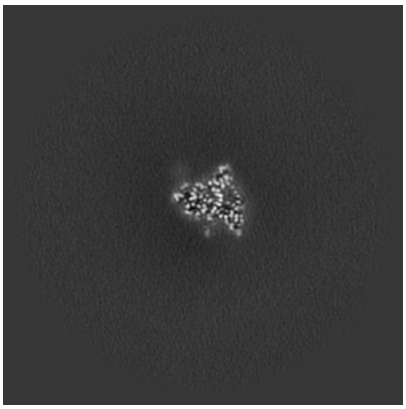
6.2.1 Primary map



X Index: 150

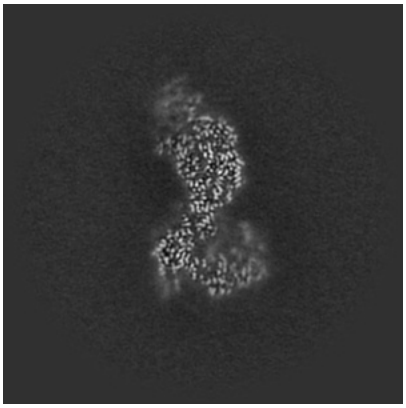


Y Index: 150

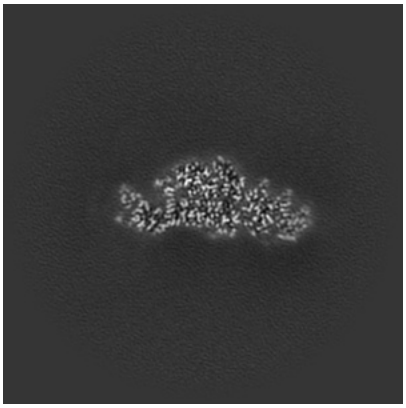


Z Index: 150

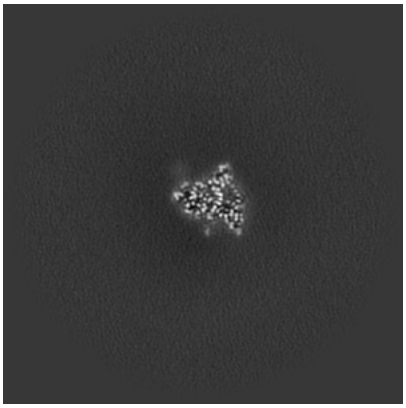
6.2.2 Raw map



X Index: 150



Y Index: 150

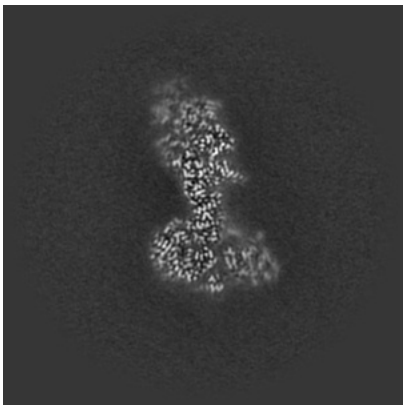


Z Index: 150

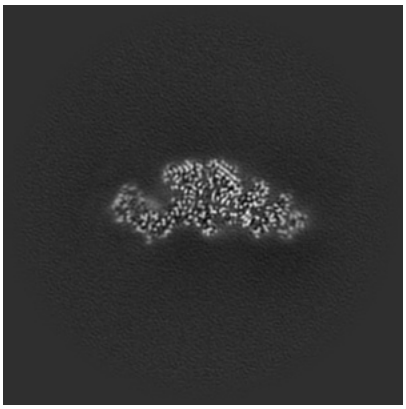
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

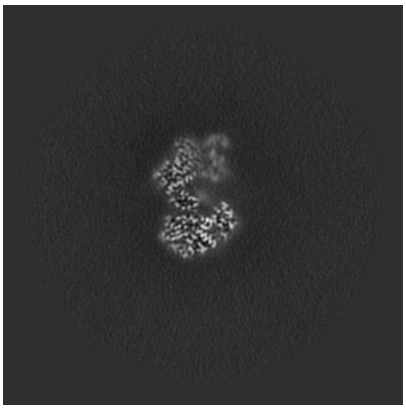
6.3.1 Primary map



X Index: 141

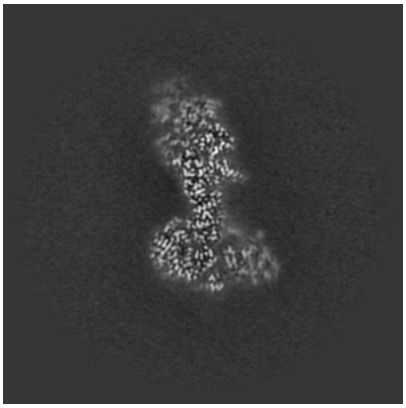


Y Index: 155

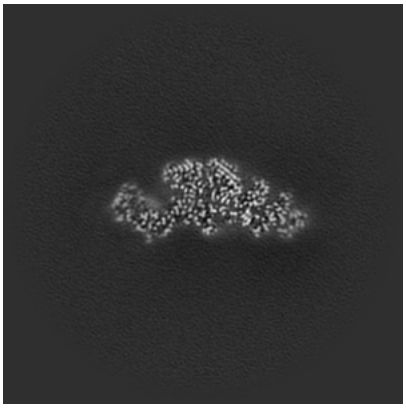


Z Index: 115

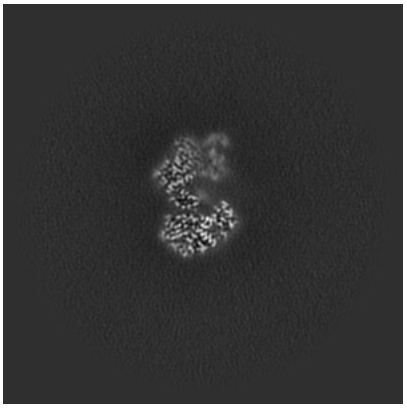
6.3.2 Raw map



X Index: 141



Y Index: 155

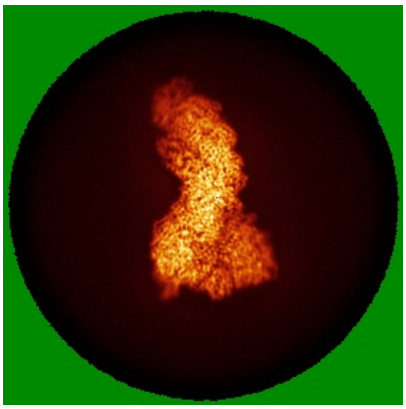


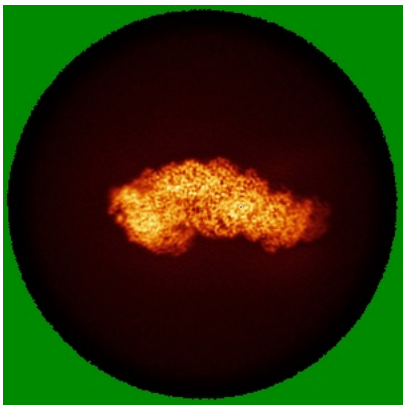
Z Index: 115

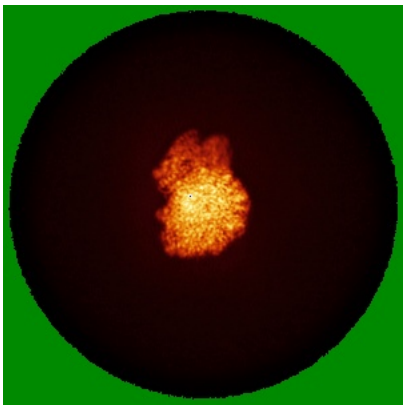
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

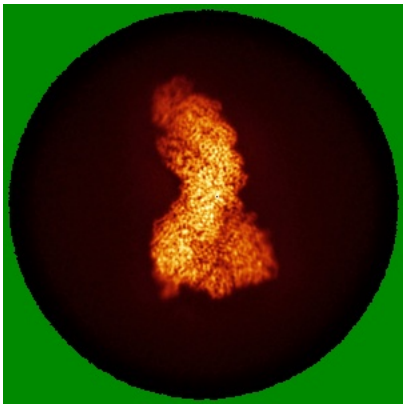
6.4.1 Primary map

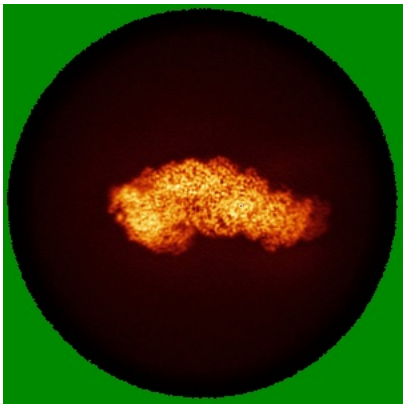

X

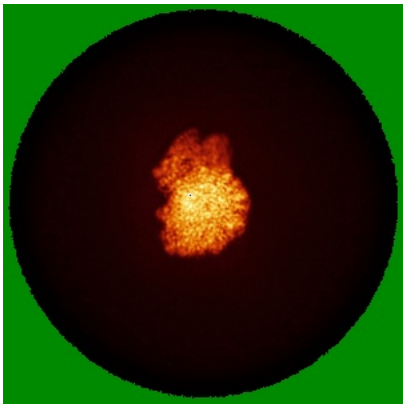

Y


Z

6.4.2 Raw 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

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.111. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

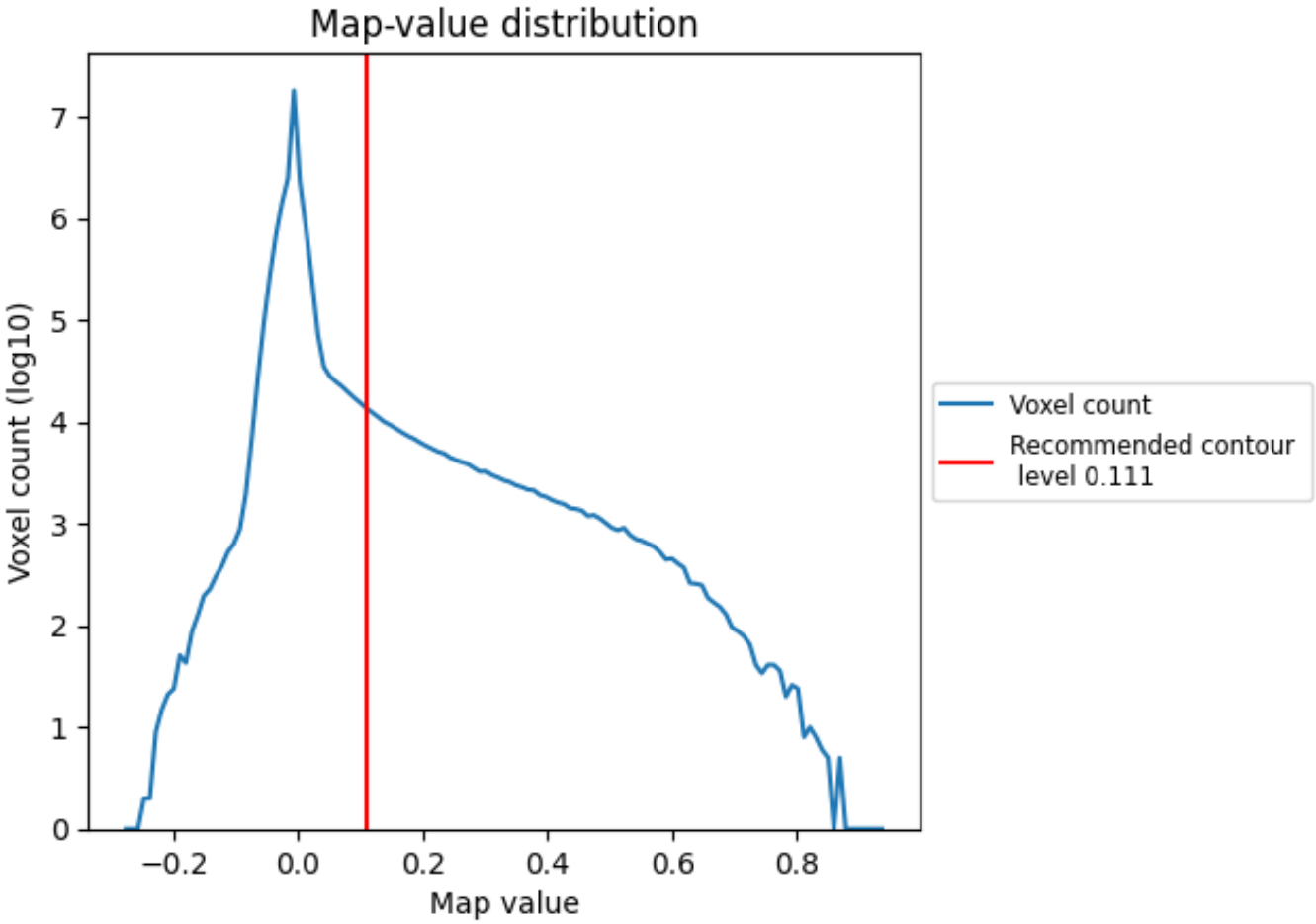
6.6 Mask visualisation (i)

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

7 Map analysis

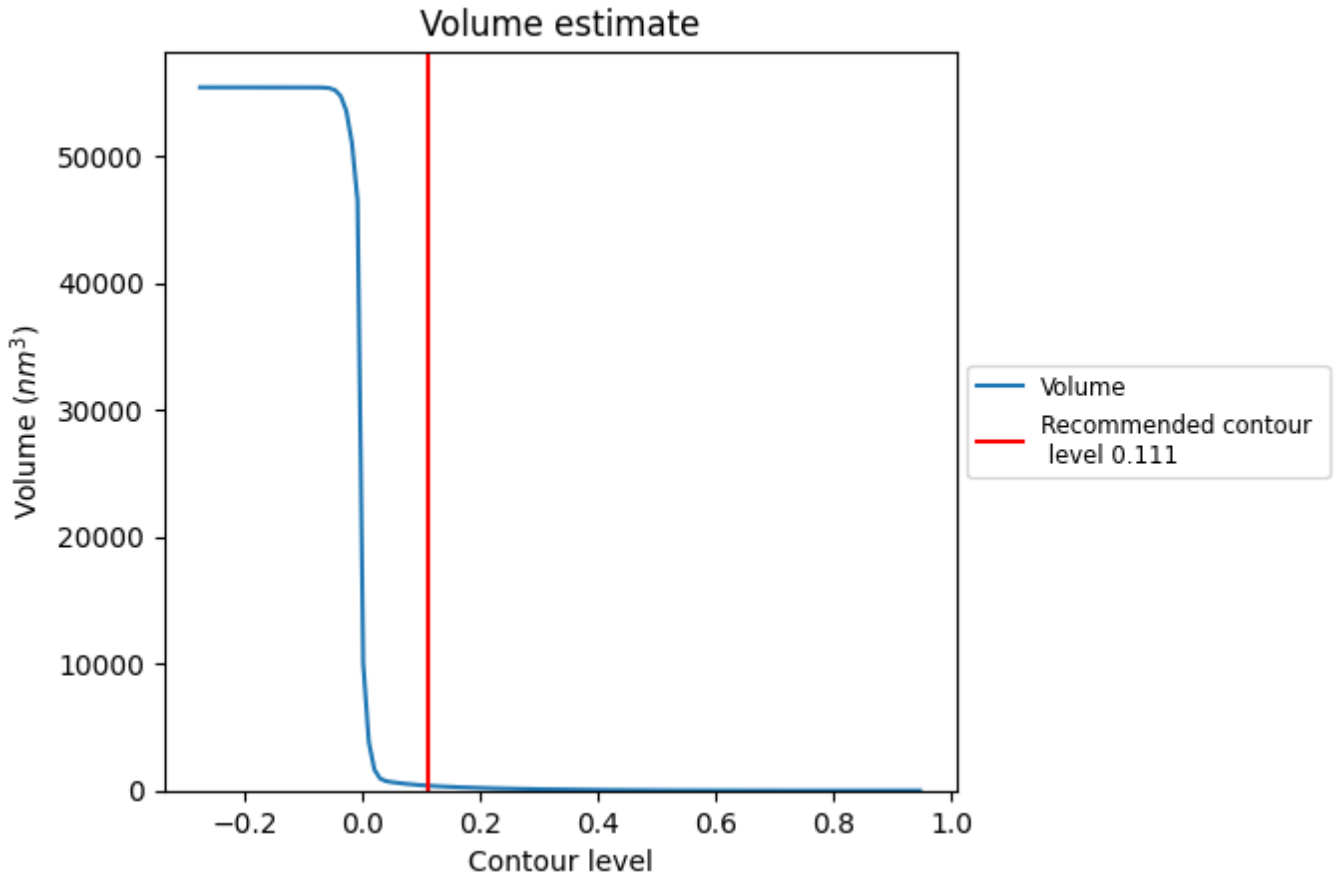
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

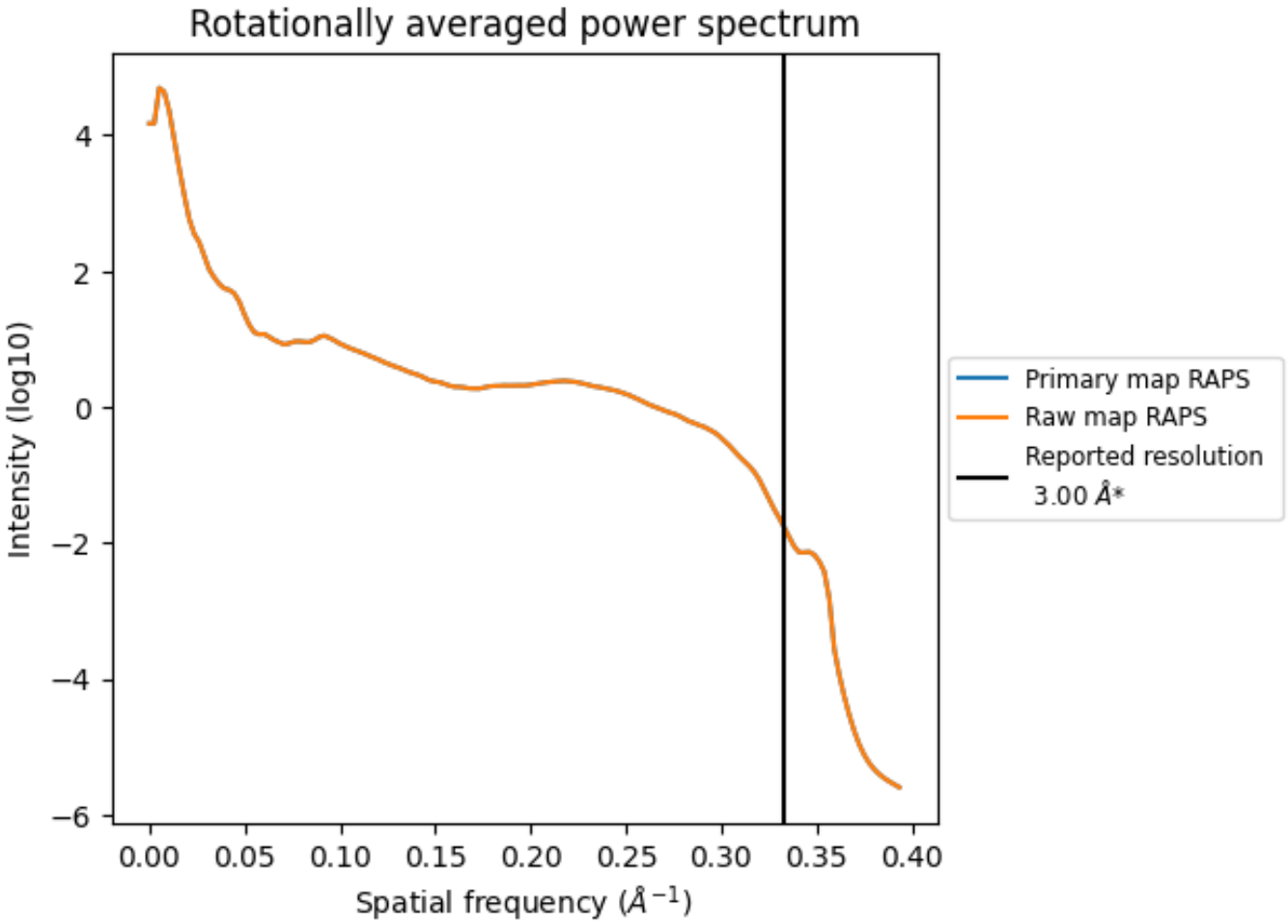
7.2 Volume estimate



The volume at the recommended contour level is 384 nm^3; this corresponds to an approximate mass of 347 kDa.

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

7.3 Rotationally averaged power spectrum (i)

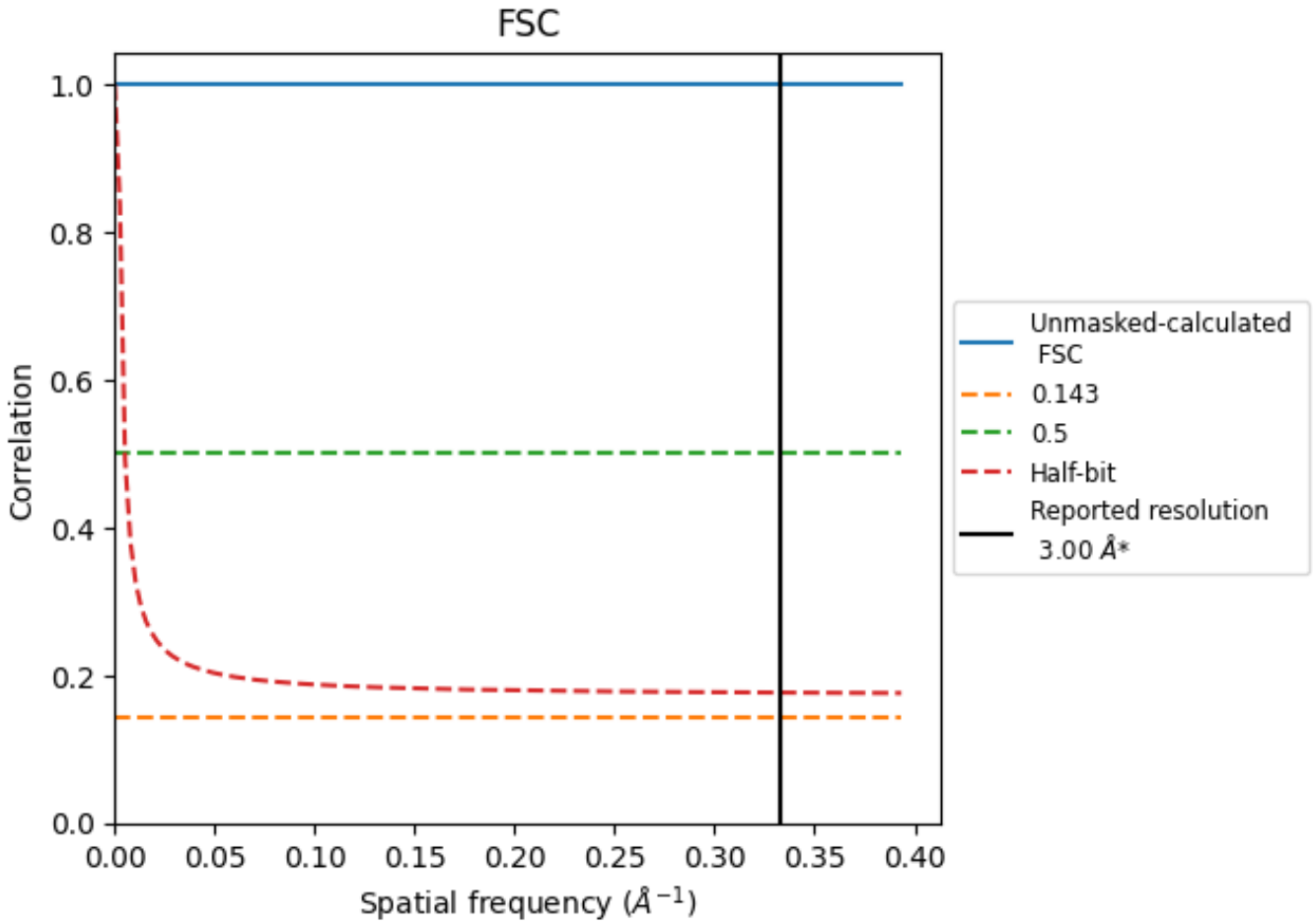


*Reported resolution corresponds to spatial frequency of 0.333 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.333 Å^{-1}

8.2 Resolution estimates (i)

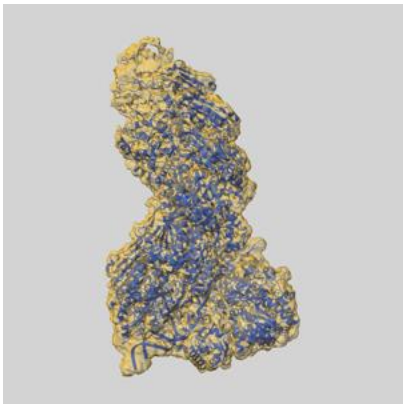
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	-	-	-

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

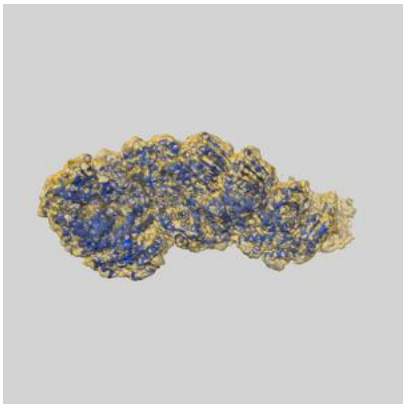
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-29879 and PDB model 8G9U. Per-residue inclusion information can be found in section 3 on page 8.

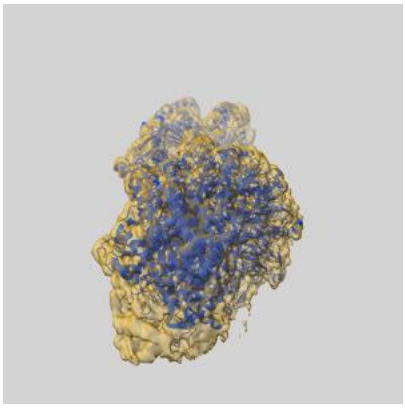
9.1 Map-model overlay



X



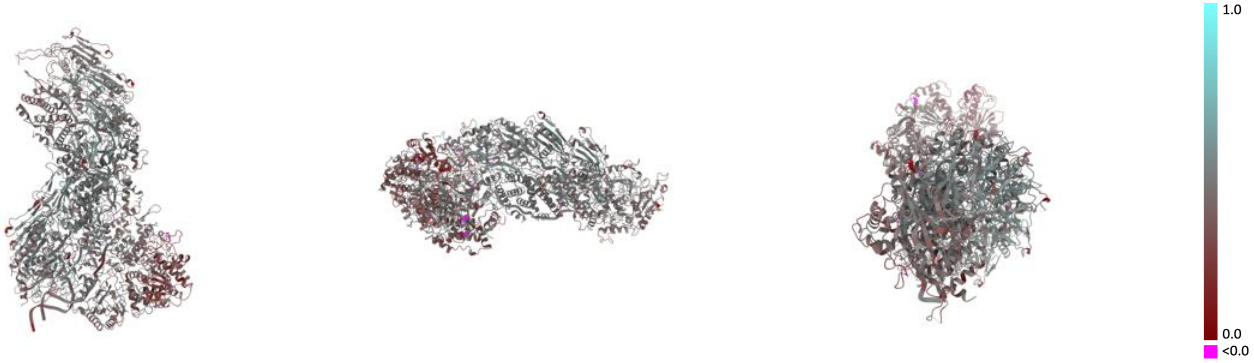
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.111 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

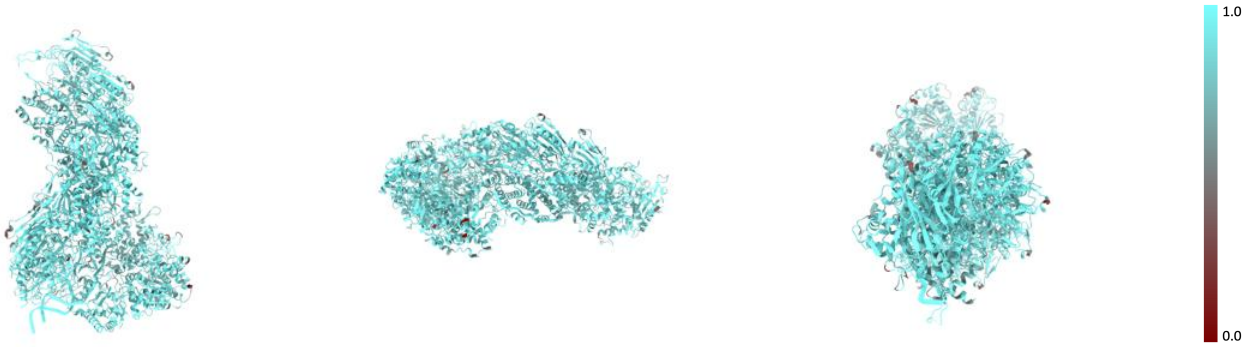
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

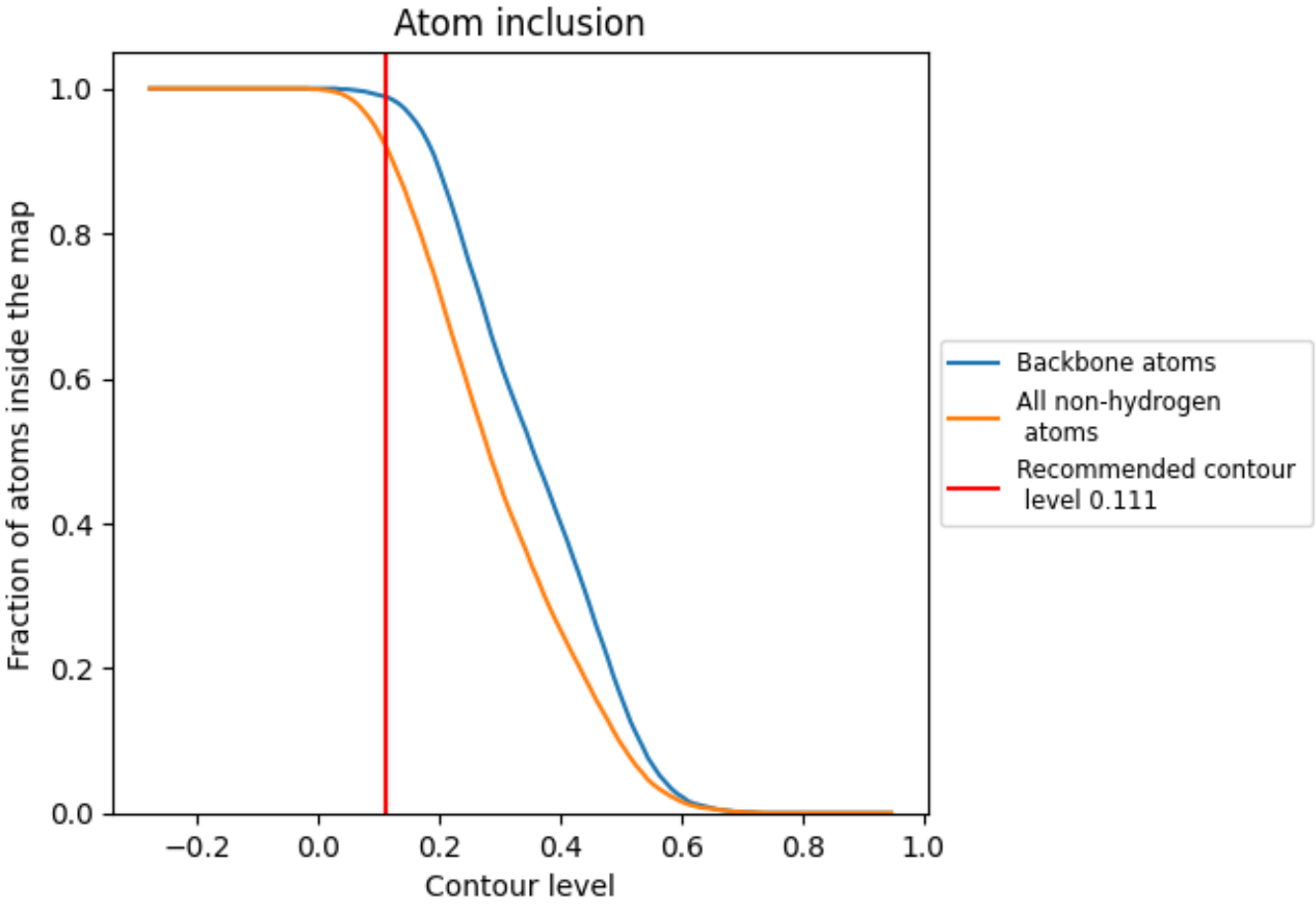
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.111).

9.4 Atom inclusion (i)



At the recommended contour level, 99% of all backbone atoms, 92% 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 (0.111) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9230	0.4400
A	0.9470	0.4750
B	0.9280	0.4660
C	0.9490	0.4800
D	0.9320	0.4710
E	0.9180	0.4500
F	0.9050	0.4000
G	0.8340	0.4130
H	0.9250	0.4580
I	0.9340	0.4510
J	0.9500	0.4620
K	0.9960	0.4920
L	0.9950	0.4760
M	0.9210	0.4580
N	0.9220	0.4530
O	0.9760	0.3930
P	0.8840	0.3630
Q	0.9400	0.4630