Full wwPDB EM Validation Report

Mar 5, 2026 – 02:17 AM UTC

PDB ID	:	6VZ4 / pdb_00006vz4
EMDB ID	:	EMD-21484
Title	:	Cryo-EM structure of Sth1-Arp7-Arp9-Rtt102 bound to the nucleosome in ADP Beryllium Fluoride state
Authors	:	Leschziner, A.E.; Baker, R.W.
Deposited on	:	2020-02-27
Resolution	:	3.90 Å(reported)
Based on initial models	:	5TGC, 5Z3U, 4I6M

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 (i) 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 (1)) were used in the production of this report:

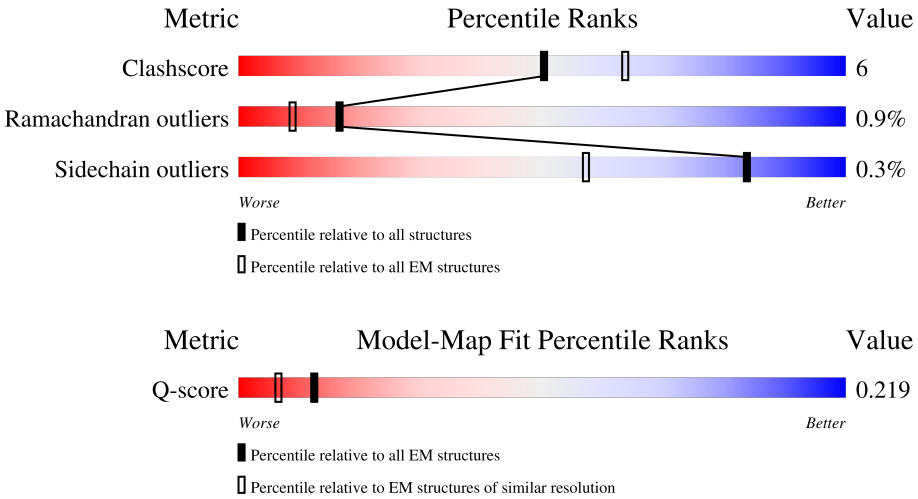
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 3.90 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8855 (3.40 - 4.40)

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	1-A	136	68% · · 28%
1	1-E	136	65% · 30%
1	10-A	136	68% · · 28%
1	10-E	136	65% · 30%

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Mol	Chain	Length	Quality of chain
1	2-A	136	68% 28%
1	2-E	136	64% 6% 30%
1	3-A	136	68% 28%
1	3-E	136	65% 5% 30%
1	4-A	136	67% 28%
1	4-E	136	65% 5% 30%
1	5-A	136	68% 28%
1	5-E	136	65% 5% 30%
1	6-A	136	68% 28%
1	6-E	136	65% 5% 30%
1	7-A	136	68% 28%
1	7-E	136	65% 5% 30%
1	8-A	136	68% 28%
1	8-E	136	65% 5% 30%
1	9-A	136	68% 28%
1	9-E	136	65% 5% 30%
2	1-B	103	83% 16%
2	1-F	103	74% 23%
2	10-B	103	83% 16%
2	10-F	103	73% 23%
2	2-B	103	83% 16%
2	2-F	103	75% 23%
2	3-B	103	83% 16%
2	3-F	103	75% 23%
2	4-B	103	83% 16%

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Mol	Chain	Length	Quality of chain
2	4-F	103	75% 23%
2	5-B	103	83% 16%
2	5-F	103	74% 23%
2	6-B	103	83% 16%
2	6-F	103	74% 23%
2	7-B	103	83% 16%
2	7-F	103	73% 23%
2	8-B	103	83% 16%
2	8-F	103	74% 23%
2	9-B	103	83% 16%
2	9-F	103	74% 23%
3	1-C	130	76% 5% 18%
3	1-G	130	73% 8% 18%
3	10-C	130	76% 5% 18%
3	10-G	130	73% 8% 18%
3	2-C	130	76% 5% 18%
3	2-G	130	73% 8% 18%
3	3-C	130	75% 7% 18%
3	3-G	130	73% 8% 18%
3	4-C	130	76% 5% 18%
3	4-G	130	73% 8% 18%
3	5-C	130	76% 5% 18%
3	5-G	130	73% 8% 18%
3	6-C	130	76% 5% 18%
3	6-G	130	73% 8% 18%

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Mol	Chain	Length	Quality of chain
3	7-C	130	76% 5% 18%
3	7-G	130	73% 8% 18%
3	8-C	130	76% 5% 18%
3	8-G	130	73% 8% 18%
3	9-C	130	76% 5% 18%
3	9-G	130	73% 8% 18%
4	1-D	125	73% 26%
4	1-H	125	70% 26%
4	10-D	125	73% 26%
4	10-H	125	70% 26%
4	2-D	125	73% 26%
4	2-H	125	71% 26%
4	3-D	125	72% 26%
4	3-H	125	71% 26%
4	4-D	125	73% 26%
4	4-H	125	70% 26%
4	5-D	125	73% 26%
4	5-H	125	70% 26%
4	6-D	125	73% 26%
4	6-H	125	71% 26%
4	7-D	125	73% 26%
4	7-H	125	71% 26%
4	8-D	125	73% 26%
4	8-H	125	70% 26%
4	9-D	125	73% 26%

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Mol	Chain	Length	Quality of chain
4	9-H	125	70% · 26%
5	1-I	185	67% 12% 21%
5	10-I	185	68% 11% 21%
5	2-I	185	66% 12% 21%
5	3-I	185	67% 12% 21%
5	4-I	185	67% 12% 21%
5	5-I	185	67% 12% 21%
5	6-I	185	67% 12% 21%
5	7-I	185	66% 12% 21%
5	8-I	185	67% 12% 21%
5	9-I	185	68% 11% 21%
6	1-J	185	69% 10% 21%
6	10-J	185	68% 11% 21%
6	2-J	185	69% 10% 21%
6	3-J	185	68% 11% 21%
6	4-J	185	68% 11% 21%
6	5-J	185	69% 10% 21%
6	6-J	185	68% 11% 21%
6	7-J	185	68% 11% 21%
6	8-J	185	68% 11% 21%
6	9-J	185	68% 11% 21%
7	1-K	813	66% 8% · 24%
7	10-K	813	65% 9% · 24%
7	2-K	813	66% 8% · 24%
7	3-K	813	67% 8% · 24%

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Mol	Chain	Length	Quality of chain
7	4-K	813	65% 9% 24%
7	5-K	813	65% 9% 24%
7	6-K	813	66% 8% 24%
7	7-K	813	66% 8% 24%
7	8-K	813	66% 9% 24%
7	9-K	813	66% 9% 24%
8	1-L	477	31% 75% 7% 18%
8	10-L	477	75% 7% 18%
8	2-L	477	75% 7% 18%
8	3-L	477	75% 7% 18%
8	4-L	477	75% 7% 18%
8	5-L	477	75% 7% 18%
8	6-L	477	75% 7% 18%
8	7-L	477	75% 7% 18%
8	8-L	477	75% 7% 18%
8	9-L	477	75% 7% 18%
9	1-M	467	19% 74% 9% 15%
9	10-M	467	74% 9% 15%
9	2-M	467	74% 9% 15%
9	3-M	467	74% 9% 15%
9	4-M	467	74% 9% 15%
9	5-M	467	74% 9% 15%
9	6-M	467	74% 9% 15%
9	7-M	467	74% 9% 15%
9	8-M	467	74% 10% 15%

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Mol	Chain	Length	Quality of chain
9	9-M	467	
10	1-N	157	
10	10-N	157	
10	2-N	157	
10	3-N	157	
10	4-N	157	
10	5-N	157	
10	6-N	157	
10	7-N	157	
10	8-N	157	
10	9-N	157	

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
13	BEF	3-K	1503	-	-	X	-
13	BEF	9-K	1503	-	-	X	-

2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 239500 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 Histone H3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1-A	98	Total	C	N	O	S	0	0
			809	510	157	139	3		
1	2-A	98	Total	C	N	O	S	0	0
			809	510	157	139	3		
1	3-A	98	Total	C	N	O	S	0	0
			809	510	157	139	3		
1	4-A	98	Total	C	N	O	S	0	0
			809	510	157	139	3		
1	5-A	98	Total	C	N	O	S	0	0
			809	510	157	139	3		
1	6-A	98	Total	C	N	O	S	0	0
			809	510	157	139	3		
1	7-A	98	Total	C	N	O	S	0	0
			809	510	157	139	3		
1	8-A	98	Total	C	N	O	S	0	0
			809	510	157	139	3		
1	9-A	98	Total	C	N	O	S	0	0
			809	510	157	139	3		
1	10-A	98	Total	C	N	O	S	0	0
			809	510	157	139	3		
1	1-E	95	Total	C	N	O	S	0	0
			783	493	151	136	3		
1	2-E	95	Total	C	N	O	S	0	0
			783	493	151	136	3		
1	3-E	95	Total	C	N	O	S	0	0
			783	493	151	136	3		
1	4-E	95	Total	C	N	O	S	0	0
			783	493	151	136	3		
1	5-E	95	Total	C	N	O	S	0	0
			783	493	151	136	3		
1	6-E	95	Total	C	N	O	S	0	0
			783	493	151	136	3		
1	7-E	95	Total	C	N	O	S	0	0
			783	493	151	136	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	8-E	95	Total	C	N	O	S	0	0
			783	493	151	136	3		
1	9-E	95	Total	C	N	O	S	0	0
			783	493	151	136	3		
1	10-E	95	Total	C	N	O	S	0	0
			783	493	151	136	3		

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1-B	87	Total	C	N	O	S	0	0
			703	443	142	117	1		
2	2-B	87	Total	C	N	O	S	0	0
			703	443	142	117	1		
2	3-B	87	Total	C	N	O	S	0	0
			703	443	142	117	1		
2	4-B	87	Total	C	N	O	S	0	0
			703	443	142	117	1		
2	5-B	87	Total	C	N	O	S	0	0
			703	443	142	117	1		
2	6-B	87	Total	C	N	O	S	0	0
			703	443	142	117	1		
2	7-B	87	Total	C	N	O	S	0	0
			703	443	142	117	1		
2	8-B	87	Total	C	N	O	S	0	0
			703	443	142	117	1		
2	9-B	87	Total	C	N	O	S	0	0
			703	443	142	117	1		
2	10-B	87	Total	C	N	O	S	0	0
			703	443	142	117	1		
2	1-F	79	Total	C	N	O	S	0	0
			627	395	121	110	1		
2	2-F	79	Total	C	N	O	S	0	0
			627	395	121	110	1		
2	3-F	79	Total	C	N	O	S	0	0
			627	395	121	110	1		
2	4-F	79	Total	C	N	O	S	0	0
			627	395	121	110	1		
2	5-F	79	Total	C	N	O	S	0	0
			627	395	121	110	1		
2	6-F	79	Total	C	N	O	S	0	0
			627	395	121	110	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	7-F	79	Total	C	N	O	S	0	0
			627	395	121	110	1		
2	8-F	79	Total	C	N	O	S	0	0
			627	395	121	110	1		
2	9-F	79	Total	C	N	O	S	0	0
			627	395	121	110	1		
2	10-F	79	Total	C	N	O	S	0	0
			627	395	121	110	1		

- Molecule 3 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	1-C	107	Total	C	N	O	0	0
			823	519	161	143		
3	2-C	107	Total	C	N	O	0	0
			823	519	161	143		
3	3-C	107	Total	C	N	O	0	0
			823	519	161	143		
3	4-C	107	Total	C	N	O	0	0
			823	519	161	143		
3	5-C	107	Total	C	N	O	0	0
			823	519	161	143		
3	6-C	107	Total	C	N	O	0	0
			823	519	161	143		
3	7-C	107	Total	C	N	O	0	0
			823	519	161	143		
3	8-C	107	Total	C	N	O	0	0
			823	519	161	143		
3	9-C	107	Total	C	N	O	0	0
			823	519	161	143		
3	10-C	107	Total	C	N	O	0	0
			823	519	161	143		
3	1-G	107	Total	C	N	O	0	0
			823	519	161	143		
3	2-G	107	Total	C	N	O	0	0
			823	519	161	143		
3	3-G	107	Total	C	N	O	0	0
			823	519	161	143		
3	4-G	107	Total	C	N	O	0	0
			823	519	161	143		
3	5-G	107	Total	C	N	O	0	0
			823	519	161	143		

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Mol	Chain	Residues	Atoms				AltConf	Trace
3	6-G	107	Total 823	C 519	N 161	O 143	0	0
3	7-G	107	Total 823	C 519	N 161	O 143	0	0
3	8-G	107	Total 823	C 519	N 161	O 143	0	0
3	9-G	107	Total 823	C 519	N 161	O 143	0	0
3	10-G	107	Total 823	C 519	N 161	O 143	0	0

- Molecule 4 is a protein called Histone H2B.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	1-D	92	Total 719	C 453	N 129	O 135	S 2	0	0
4	2-D	92	Total 719	C 453	N 129	O 135	S 2	0	0
4	3-D	92	Total 719	C 453	N 129	O 135	S 2	0	0
4	4-D	92	Total 719	C 453	N 129	O 135	S 2	0	0
4	5-D	92	Total 719	C 453	N 129	O 135	S 2	0	0
4	6-D	92	Total 719	C 453	N 129	O 135	S 2	0	0
4	7-D	92	Total 719	C 453	N 129	O 135	S 2	0	0
4	8-D	92	Total 719	C 453	N 129	O 135	S 2	0	0
4	9-D	92	Total 719	C 453	N 129	O 135	S 2	0	0
4	10-D	92	Total 719	C 453	N 129	O 135	S 2	0	0
4	1-H	92	Total 719	C 453	N 129	O 135	S 2	0	0
4	2-H	92	Total 719	C 453	N 129	O 135	S 2	0	0
4	3-H	92	Total 719	C 453	N 129	O 135	S 2	0	0
4	4-H	92	Total 719	C 453	N 129	O 135	S 2	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	5-H	92	Total	C	N	O	S	0	0
			719	453	129	135	2		
4	6-H	92	Total	C	N	O	S	0	0
			719	453	129	135	2		
4	7-H	92	Total	C	N	O	S	0	0
			719	453	129	135	2		
4	8-H	92	Total	C	N	O	S	0	0
			719	453	129	135	2		
4	9-H	92	Total	C	N	O	S	0	0
			719	453	129	135	2		
4	10-H	92	Total	C	N	O	S	0	0
			719	453	129	135	2		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	33	THR	SER	conflict	UNP Q92130
H	33	THR	SER	conflict	UNP Q92130

- Molecule 5 is a DNA chain called DNA (185-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	1-I	146	Total	C	N	O	P	0	0
			2975	1413	540	876	146		
5	2-I	146	Total	C	N	O	P	0	0
			2975	1413	540	876	146		
5	3-I	146	Total	C	N	O	P	0	0
			2975	1413	540	876	146		
5	4-I	146	Total	C	N	O	P	0	0
			2975	1413	540	876	146		
5	5-I	146	Total	C	N	O	P	0	0
			2975	1413	540	876	146		
5	6-I	146	Total	C	N	O	P	0	0
			2975	1413	540	876	146		
5	7-I	146	Total	C	N	O	P	0	0
			2975	1413	540	876	146		
5	8-I	146	Total	C	N	O	P	0	0
			2975	1413	540	876	146		
5	9-I	146	Total	C	N	O	P	0	0
			2975	1413	540	876	146		
5	10-I	146	Total	C	N	O	P	0	0
			2975	1413	540	876	146		

- Molecule 6 is a DNA chain called DNA (185-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	1-J	146	Total	C	N	O	P	0	0
			3011	1425	564	876	146		
6	2-J	146	Total	C	N	O	P	0	0
			3011	1425	564	876	146		
6	3-J	146	Total	C	N	O	P	0	0
			3011	1425	564	876	146		
6	4-J	146	Total	C	N	O	P	0	0
			3011	1425	564	876	146		
6	5-J	146	Total	C	N	O	P	0	0
			3011	1425	564	876	146		
6	6-J	146	Total	C	N	O	P	0	0
			3011	1425	564	876	146		
6	7-J	146	Total	C	N	O	P	0	0
			3011	1425	564	876	146		
6	8-J	146	Total	C	N	O	P	0	0
			3011	1425	564	876	146		
6	9-J	146	Total	C	N	O	P	0	0
			3011	1425	564	876	146		
6	10-J	146	Total	C	N	O	P	0	0
			3011	1425	564	876	146		

- Molecule 7 is a protein called Nuclear protein STH1/NPS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	1-K	616	Total	C	N	O	S	0	0
			5055	3201	900	934	20		
7	2-K	616	Total	C	N	O	S	0	0
			5055	3201	900	934	20		
7	3-K	616	Total	C	N	O	S	0	0
			5055	3201	900	934	20		
7	4-K	616	Total	C	N	O	S	0	0
			5055	3201	900	934	20		
7	5-K	616	Total	C	N	O	S	0	0
			5055	3201	900	934	20		
7	6-K	616	Total	C	N	O	S	0	0
			5055	3201	900	934	20		
7	7-K	616	Total	C	N	O	S	0	0
			5055	3201	900	934	20		
7	8-K	616	Total	C	N	O	S	0	0
			5055	3201	900	934	20		
7	9-K	616	Total	C	N	O	S	0	0
			5055	3201	900	934	20		

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Mol	Chain	Residues	Atoms					AltConf	Trace
7	10-K	616	Total	C	N	O	S	0	0
			5055	3201	900	934	20		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	285	MET	-	initiating methionine	UNP P32597
K	286	GLY	-	expression tag	UNP P32597
K	287	SER	-	expression tag	UNP P32597
K	288	SER	-	expression tag	UNP P32597
K	289	HIS	-	expression tag	UNP P32597
K	290	HIS	-	expression tag	UNP P32597
K	291	HIS	-	expression tag	UNP P32597
K	292	HIS	-	expression tag	UNP P32597
K	293	HIS	-	expression tag	UNP P32597
K	294	HIS	-	expression tag	UNP P32597
K	295	SER	-	expression tag	UNP P32597
K	296	GLN	-	expression tag	UNP P32597
K	297	ASP	-	expression tag	UNP P32597
K	298	PRO	-	expression tag	UNP P32597
K	299	ASN	-	expression tag	UNP P32597
K	300	SER	-	expression tag	UNP P32597

- Molecule 8 is a protein called Actin-related protein 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	1-L	393	Total	C	N	O	S	0	0
			3154	2035	514	590	15		
8	2-L	393	Total	C	N	O	S	0	0
			3154	2035	514	590	15		
8	3-L	393	Total	C	N	O	S	0	0
			3154	2035	514	590	15		
8	4-L	393	Total	C	N	O	S	0	0
			3154	2035	514	590	15		
8	5-L	393	Total	C	N	O	S	0	0
			3154	2035	514	590	15		
8	6-L	393	Total	C	N	O	S	0	0
			3154	2035	514	590	15		
8	7-L	393	Total	C	N	O	S	0	0
			3154	2035	514	590	15		
8	8-L	393	Total	C	N	O	S	0	0
			3154	2035	514	590	15		

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Mol	Chain	Residues	Atoms					AltConf	Trace
8	9-L	393	Total	C	N	O	S	0	0
			3154	2035	514	590	15		
8	10-L	393	Total	C	N	O	S	0	0
			3154	2035	514	590	15		

- Molecule 9 is a protein called Actin-like protein ARP9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	1-M	396	Total	C	N	O	S	0	0
			3192	2048	521	616	7		
9	2-M	396	Total	C	N	O	S	0	0
			3192	2048	521	616	7		
9	3-M	396	Total	C	N	O	S	0	0
			3192	2048	521	616	7		
9	4-M	396	Total	C	N	O	S	0	0
			3192	2048	521	616	7		
9	5-M	396	Total	C	N	O	S	0	0
			3192	2048	521	616	7		
9	6-M	396	Total	C	N	O	S	0	0
			3192	2048	521	616	7		
9	7-M	396	Total	C	N	O	S	0	0
			3192	2048	521	616	7		
9	8-M	396	Total	C	N	O	S	0	0
			3192	2048	521	616	7		
9	9-M	396	Total	C	N	O	S	0	0
			3192	2048	521	616	7		
9	10-M	396	Total	C	N	O	S	0	0
			3192	2048	521	616	7		

- Molecule 10 is a protein called Regulator of Ty1 transposition protein 102.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	1-N	55	Total	C	N	O	S	0	0
			494	315	85	92	2		
10	2-N	55	Total	C	N	O	S	0	0
			494	315	85	92	2		
10	3-N	55	Total	C	N	O	S	0	0
			494	315	85	92	2		
10	4-N	55	Total	C	N	O	S	0	0
			494	315	85	92	2		
10	5-N	55	Total	C	N	O	S	0	0
			494	315	85	92	2		

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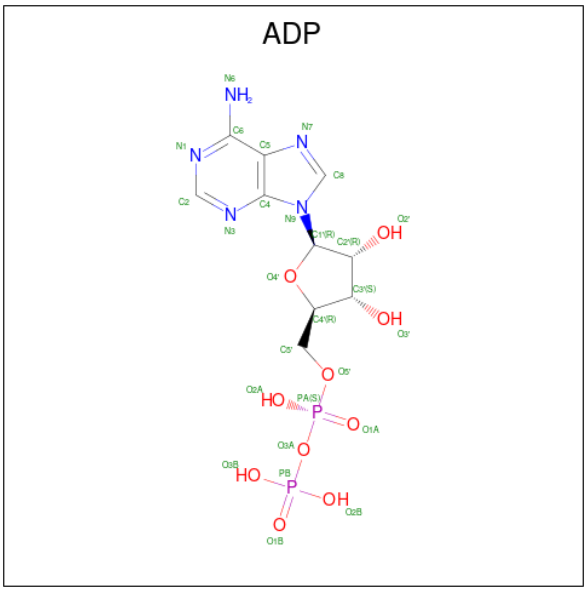
Mol	Chain	Residues	Atoms					AltConf	Trace
10	6-N	55	Total	C	N	O	S	0	0
			494	315	85	92	2		
10	7-N	55	Total	C	N	O	S	0	0
			494	315	85	92	2		
10	8-N	55	Total	C	N	O	S	0	0
			494	315	85	92	2		
10	9-N	55	Total	C	N	O	S	0	0
			494	315	85	92	2		
10	10-N	55	Total	C	N	O	S	0	0
			494	315	85	92	2		

- Molecule 11 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

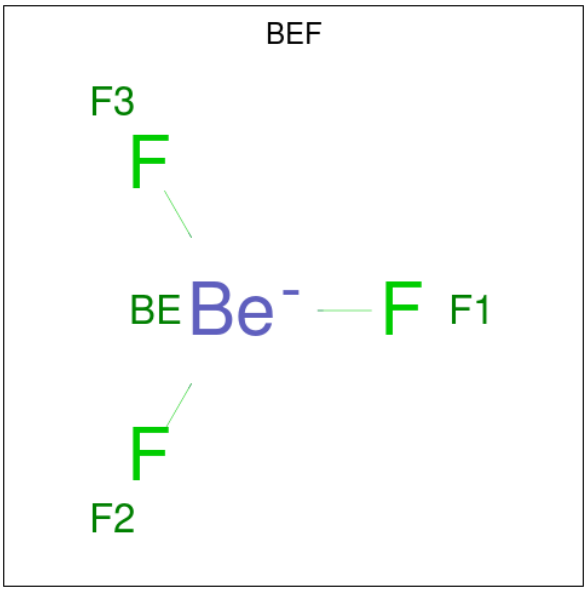
Mol	Chain	Residues	Atoms		AltConf
11	1-K	1	Total	Mg	0
			1	1	
11	2-K	1	Total	Mg	0
			1	1	
11	3-K	1	Total	Mg	0
			1	1	
11	4-K	1	Total	Mg	0
			1	1	
11	5-K	1	Total	Mg	0
			1	1	
11	6-K	1	Total	Mg	0
			1	1	
11	7-K	1	Total	Mg	0
			1	1	
11	8-K	1	Total	Mg	0
			1	1	
11	9-K	1	Total	Mg	0
			1	1	
11	10-K	1	Total	Mg	0
			1	1	

- Molecule 12 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



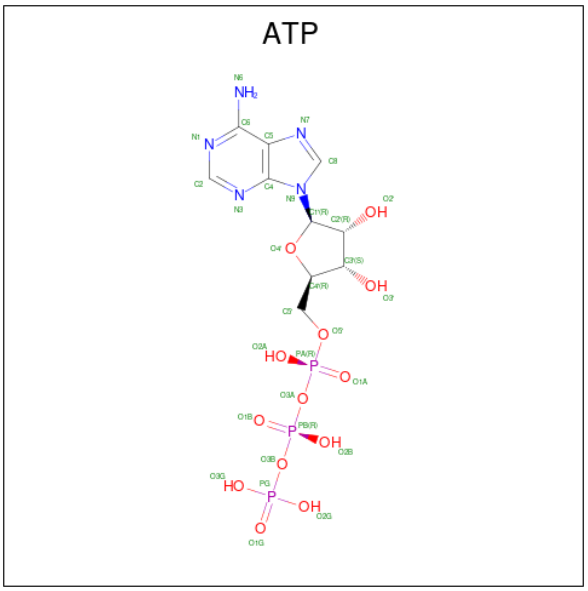
Mol	Chain	Residues	Atoms					AltConf
12	1-K	1	Total	C	N	O	P	0
			27	10	5	10	2	
12	2-K	1	Total	C	N	O	P	0
			27	10	5	10	2	
12	3-K	1	Total	C	N	O	P	0
			27	10	5	10	2	
12	4-K	1	Total	C	N	O	P	0
			27	10	5	10	2	
12	5-K	1	Total	C	N	O	P	0
			27	10	5	10	2	
12	6-K	1	Total	C	N	O	P	0
			27	10	5	10	2	
12	7-K	1	Total	C	N	O	P	0
			27	10	5	10	2	
12	8-K	1	Total	C	N	O	P	0
			27	10	5	10	2	
12	9-K	1	Total	C	N	O	P	0
			27	10	5	10	2	
12	10-K	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 13 is BERYLLIUM TRIFLUORIDE ION (CCD ID: BEF) (formula: BeF_3).



Mol	Chain	Residues	Atoms	AltConf
13	1-K	1	Total Be F 4 1 3	0
13	2-K	1	Total Be F 4 1 3	0
13	3-K	1	Total Be F 4 1 3	0
13	4-K	1	Total Be F 4 1 3	0
13	5-K	1	Total Be F 4 1 3	0
13	6-K	1	Total Be F 4 1 3	0
13	7-K	1	Total Be F 4 1 3	0
13	8-K	1	Total Be F 4 1 3	0
13	9-K	1	Total Be F 4 1 3	0
13	10-K	1	Total Be F 4 1 3	0

- Molecule 14 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



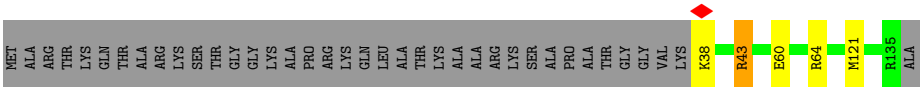
Mol	Chain	Residues	Atoms					AltConf
14	1-L	1	Total	C	N	O	P	0
			31	10	5	13	3	
14	2-L	1	Total	C	N	O	P	0
			31	10	5	13	3	
14	3-L	1	Total	C	N	O	P	0
			31	10	5	13	3	
14	4-L	1	Total	C	N	O	P	0
			31	10	5	13	3	
14	5-L	1	Total	C	N	O	P	0
			31	10	5	13	3	
14	6-L	1	Total	C	N	O	P	0
			31	10	5	13	3	
14	7-L	1	Total	C	N	O	P	0
			31	10	5	13	3	
14	8-L	1	Total	C	N	O	P	0
			31	10	5	13	3	
14	9-L	1	Total	C	N	O	P	0
			31	10	5	13	3	
14	10-L	1	Total	C	N	O	P	0
			31	10	5	13	3	

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.

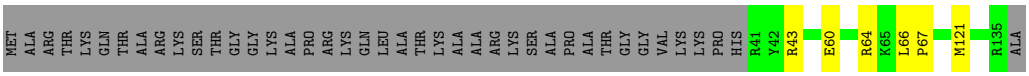
- Molecule 1: Histone H3

Chain 1-A:



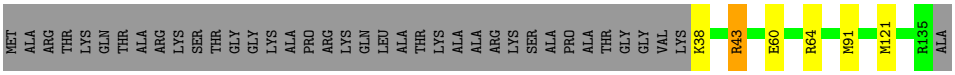
- Molecule 1: Histone H3

Chain 1-E:



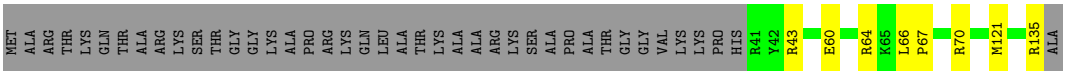
- Molecule 1: Histone H3

Chain 2-A:



- Molecule 1: Histone H3

Chain 2-E:

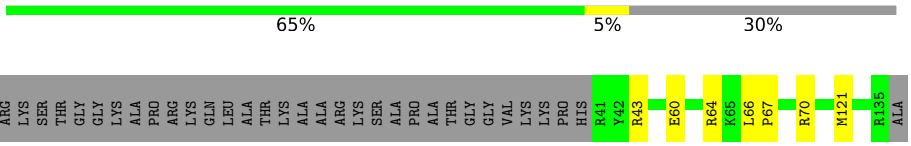


- Molecule 1: Histone H3

Chain 3-A:

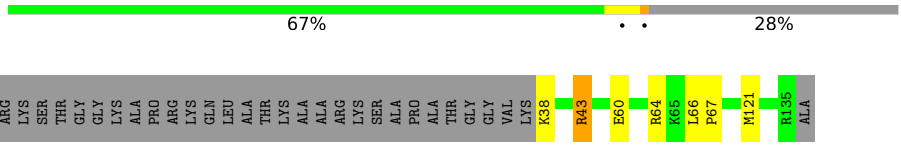
- Molecule 1: Histone H3

Chain 3-E:



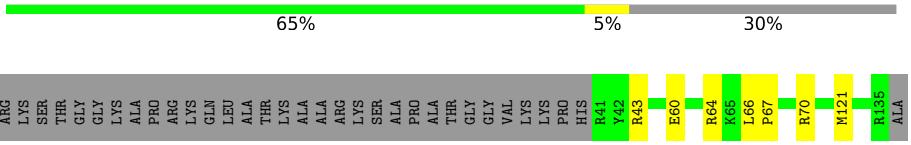
• Molecule 1: Histone H3

Chain 4-A:



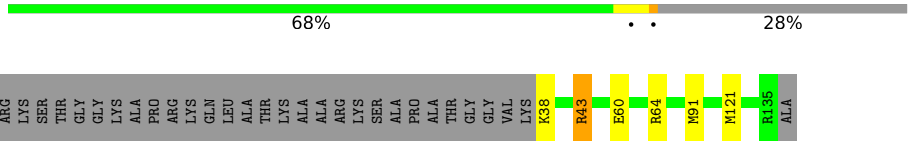
• Molecule 1: Histone H3

Chain 4-E:



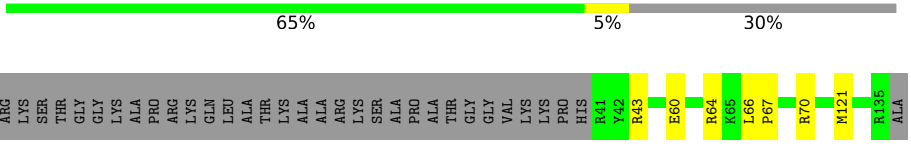
• Molecule 1: Histone H3

Chain 5-A:



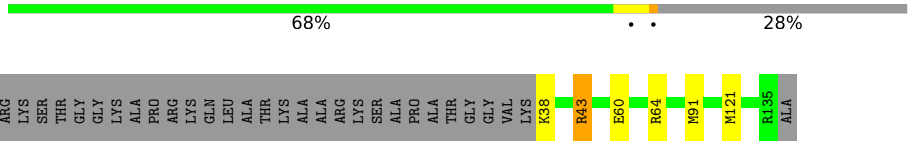
• Molecule 1: Histone H3

Chain 5-E:



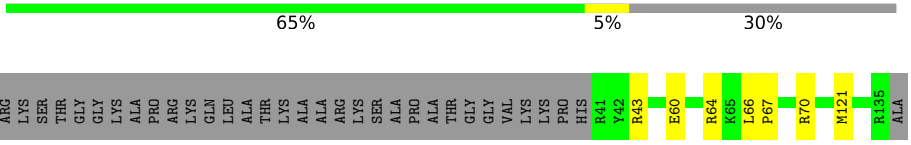
• Molecule 1: Histone H3

Chain 6-A:



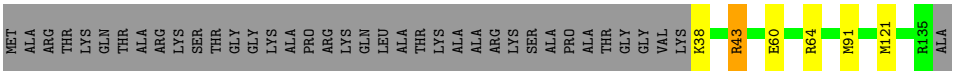
• Molecule 1: Histone H3

Chain 6-E:



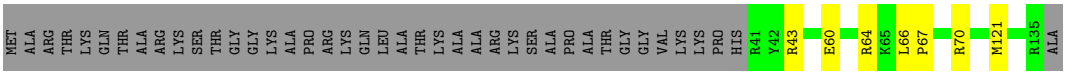
• Molecule 1: Histone H3

Chain 7-A:



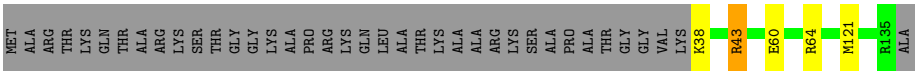
• Molecule 1: Histone H3

Chain 7-E:



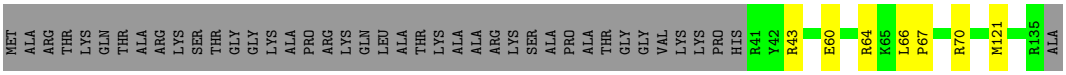
• Molecule 1: Histone H3

Chain 8-A:



• Molecule 1: Histone H3

Chain 8-E:

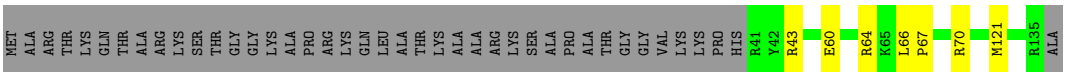


• Molecule 1: Histone H3

Chain 9-A:

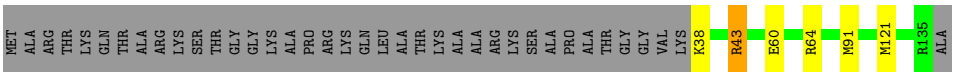
• Molecule 1: Histone H3

Chain 9-E:



• Molecule 1: Histone H3

Chain 10-A:

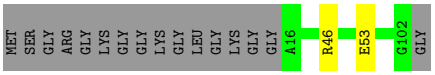


• Molecule 1: Histone H3

Chain 10-E:

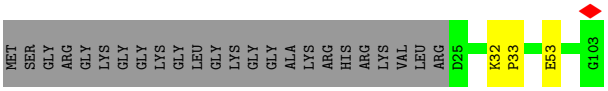
• Molecule 2: Histone H4

Chain 1-B:



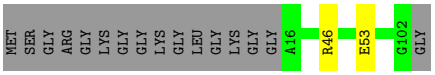
• Molecule 2: Histone H4

Chain 1-F:



• Molecule 2: Histone H4

Chain 2-B:

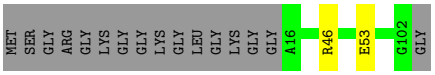


• Molecule 2: Histone H4

Chain 2-F:

• Molecule 2: Histone H4

Chain 3-B:

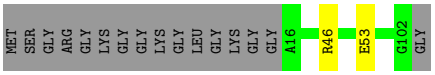


• Molecule 2: Histone H4

Chain 3-F:

• Molecule 2: Histone H4

Chain 4-B:

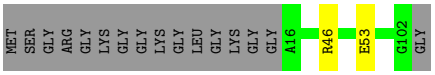


• Molecule 2: Histone H4

Chain 4-F:

• Molecule 2: Histone H4

Chain 5-B:

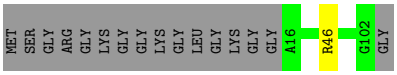


• Molecule 2: Histone H4

Chain 5-F:

• Molecule 2: Histone H4

Chain 6-B:

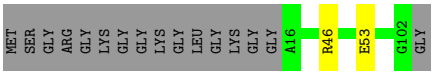


• Molecule 2: Histone H4

Chain 6-F:

• Molecule 2: Histone H4

Chain 7-B:

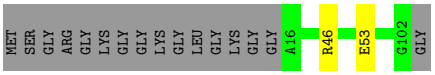


• Molecule 2: Histone H4

Chain 7-F:

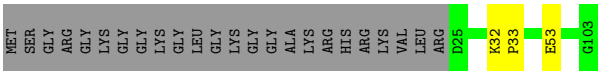
• Molecule 2: Histone H4

Chain 8-B:



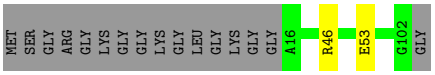
• Molecule 2: Histone H4

Chain 8-F:



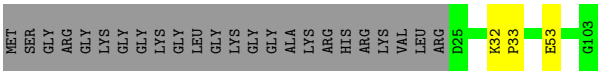
• Molecule 2: Histone H4

Chain 9-B:



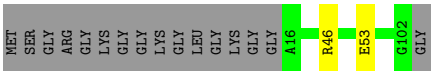
• Molecule 2: Histone H4

Chain 9-F:



• Molecule 2: Histone H4

Chain 10-B:

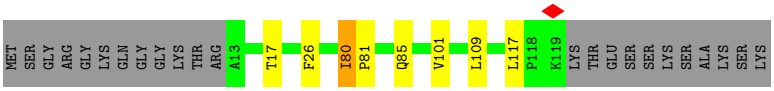


• Molecule 2: Histone H4

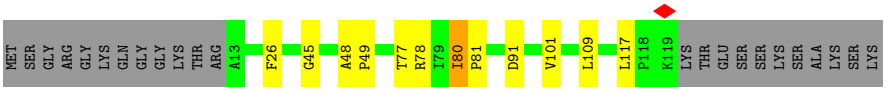
Chain 10-F:

• Molecule 3: Histone H2A

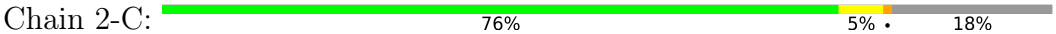
Chain 1-C:

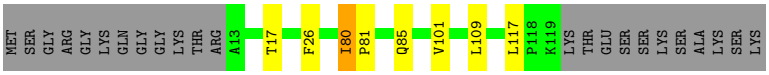


• Molecule 3: Histone H2A

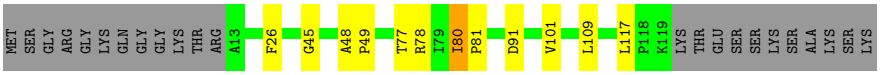


• Molecule 3: Histone H2A





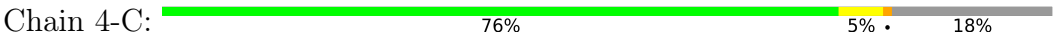
• Molecule 3: Histone H2A



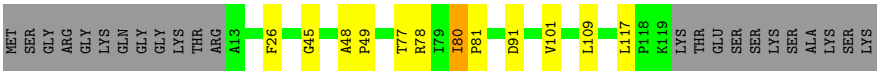
• Molecule 3: Histone H2A

• Molecule 3: Histone H2A

• Molecule 3: Histone H2A



• Molecule 3: Histone H2A



• Molecule 3: Histone H2A

Chain 5-C:

• Molecule 3: Histone H2A

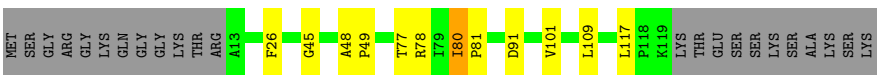
Chain 5-G:

• Molecule 3: Histone H2A

Chain 6-C:

• Molecule 3: Histone H2A

Chain 6-G:

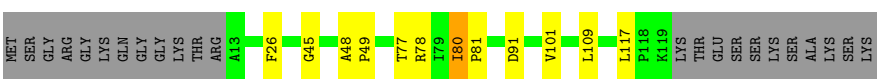


• Molecule 3: Histone H2A

Chain 7-C:

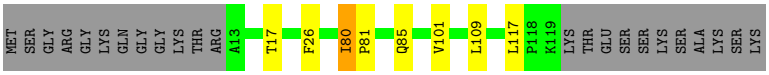
• Molecule 3: Histone H2A

Chain 7-G:



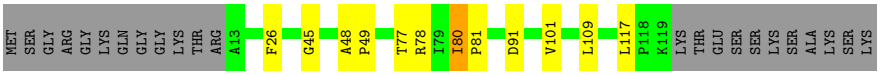
• Molecule 3: Histone H2A

Chain 8-C:



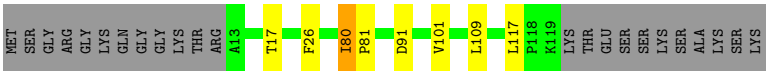
• Molecule 3: Histone H2A

Chain 8-G:



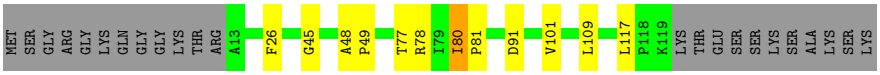
• Molecule 3: Histone H2A

Chain 9-C:



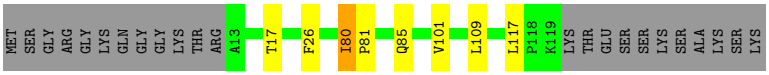
• Molecule 3: Histone H2A

Chain 9-G:



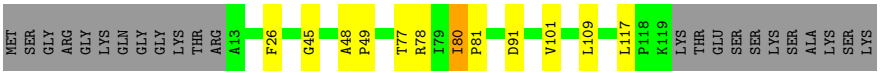
• Molecule 3: Histone H2A

Chain 10-C:



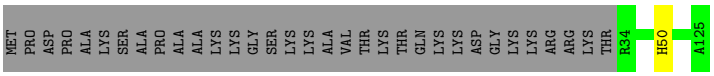
• Molecule 3: Histone H2A

Chain 10-G:



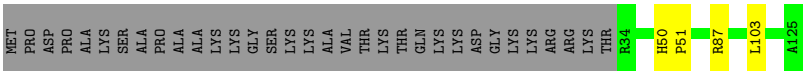
• Molecule 4: Histone H2B

Chain 1-D:



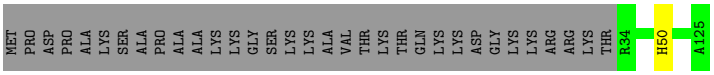
• Molecule 4: Histone H2B

Chain 1-H:



• Molecule 4: Histone H2B

Chain 2-D:

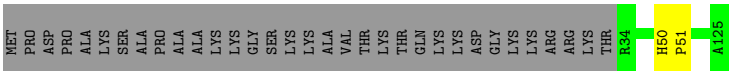


• Molecule 4: Histone H2B

Chain 2-H:

• Molecule 4: Histone H2B

Chain 3-D:

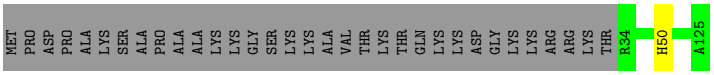


• Molecule 4: Histone H2B

Chain 3-H:

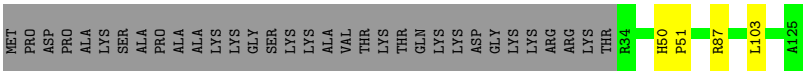
• Molecule 4: Histone H2B

Chain 4-D:



• Molecule 4: Histone H2B

Chain 4-H:

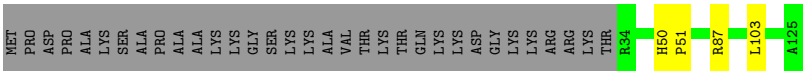


• Molecule 4: Histone H2B

Chain 5-D:

• Molecule 4: Histone H2B

Chain 5-H:



• Molecule 4: Histone H2B

Chain 6-D:

• Molecule 4: Histone H2B

Chain 6-H:

• Molecule 4: Histone H2B

Chain 7-D:

• Molecule 4: Histone H2B

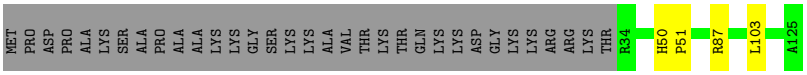
Chain 7-H:

• Molecule 4: Histone H2B

Chain 8-D:

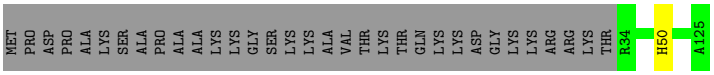
• Molecule 4: Histone H2B

Chain 8-H:



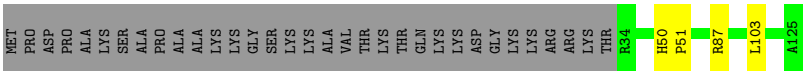
• Molecule 4: Histone H2B

Chain 9-D:



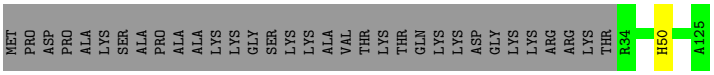
• Molecule 4: Histone H2B

Chain 9-H:



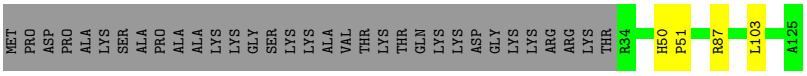
• Molecule 4: Histone H2B

Chain 10-D:



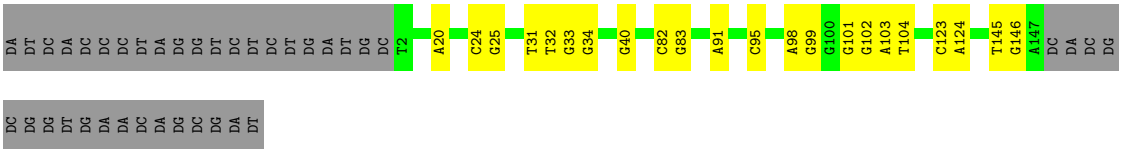
• Molecule 4: Histone H2B

Chain 10-H:



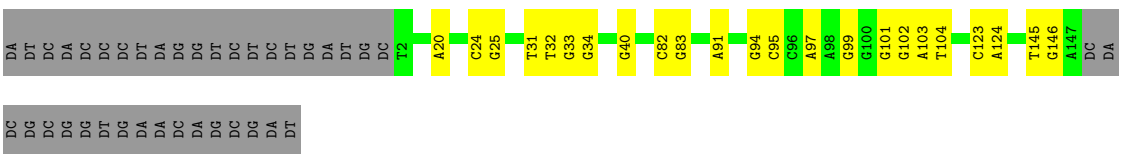
• Molecule 5: DNA (185-MER)

Chain 1-I:



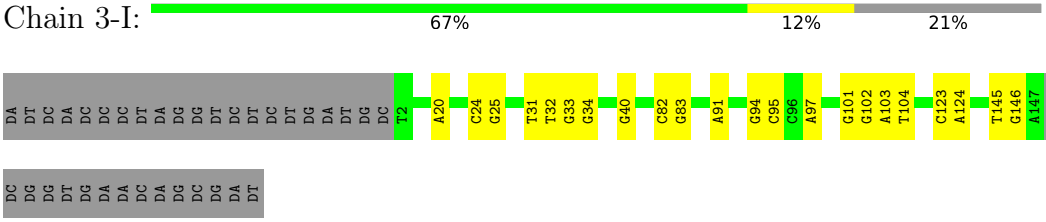
• Molecule 5: DNA (185-MER)

Chain 2-I:



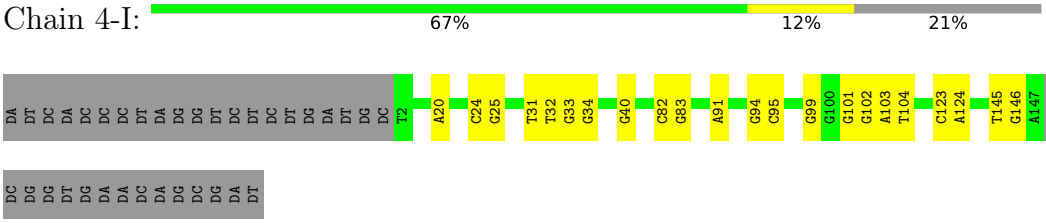
• Molecule 5: DNA (185-MER)

Chain 3-I:



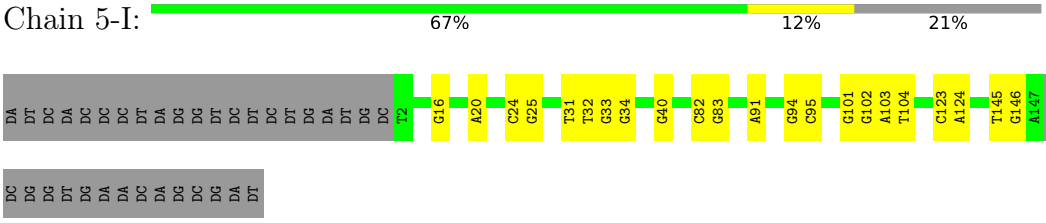
• Molecule 5: DNA (185-MER)

Chain 4-I:



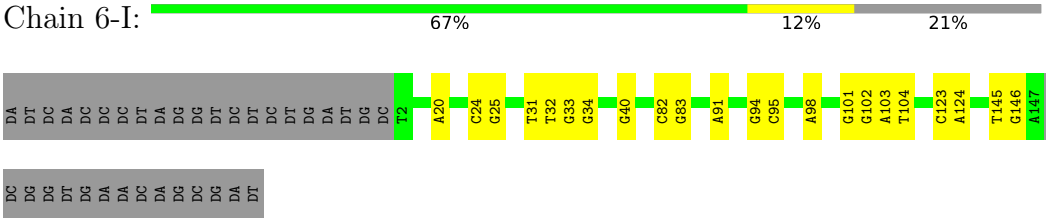
• Molecule 5: DNA (185-MER)

Chain 5-I:



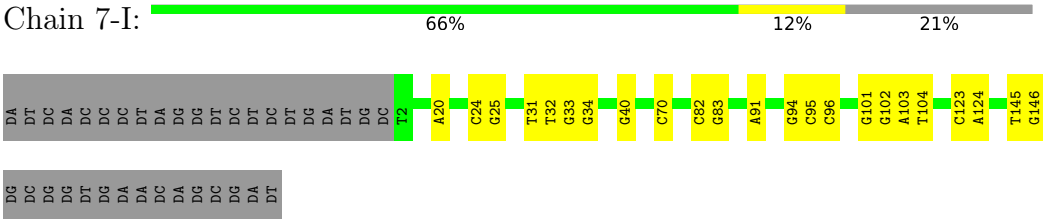
• Molecule 5: DNA (185-MER)

Chain 6-I:



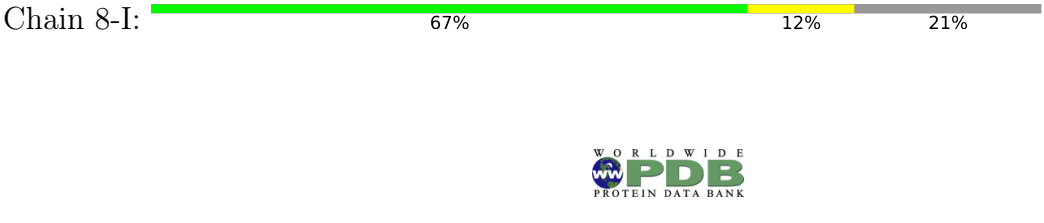
• Molecule 5: DNA (185-MER)

Chain 7-I:



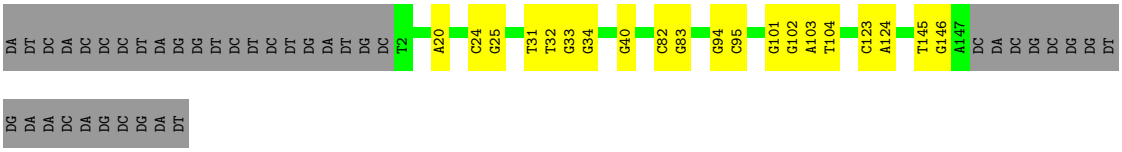
• Molecule 5: DNA (185-MER)

Chain 8-I:



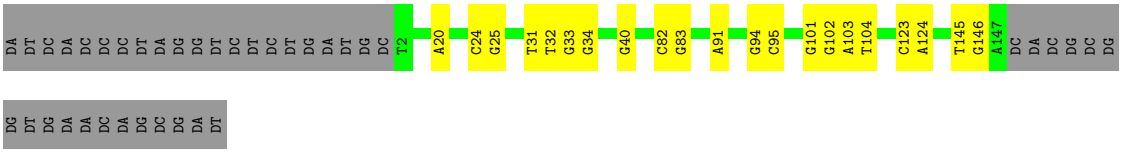
• Molecule 5: DNA (185-MER)

Chain 9-I:



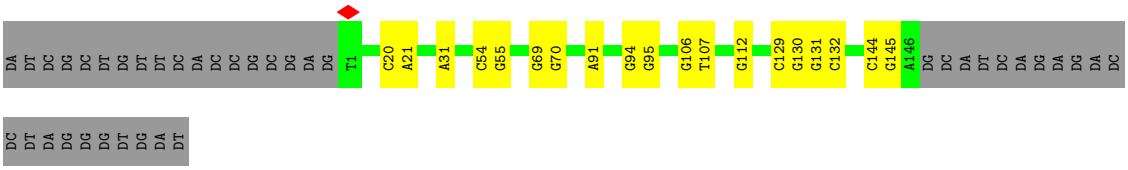
• Molecule 5: DNA (185-MER)

Chain 10-I:



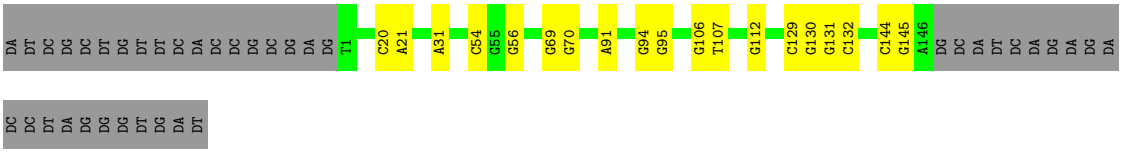
• Molecule 6: DNA (185-MER)

Chain 1-J:



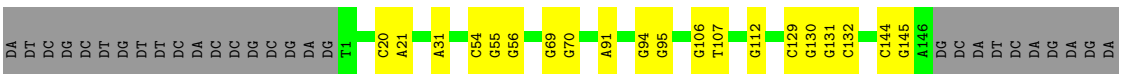
• Molecule 6: DNA (185-MER)

Chain 2-J:



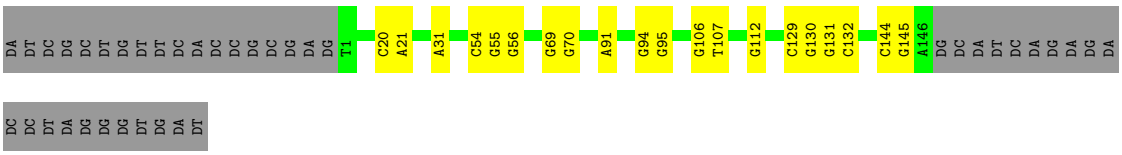
• Molecule 6: DNA (185-MER)

Chain 3-J:



• Molecule 6: DNA (185-MER)

Chain 4-J:

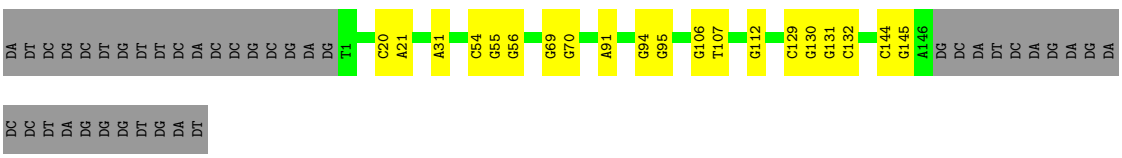


• Molecule 6: DNA (185-MER)

Chain 5-J:

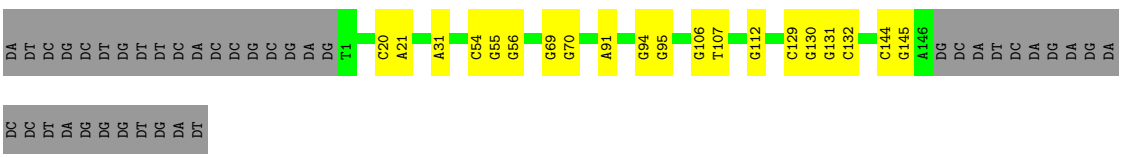
• Molecule 6: DNA (185-MER)

Chain 6-J:



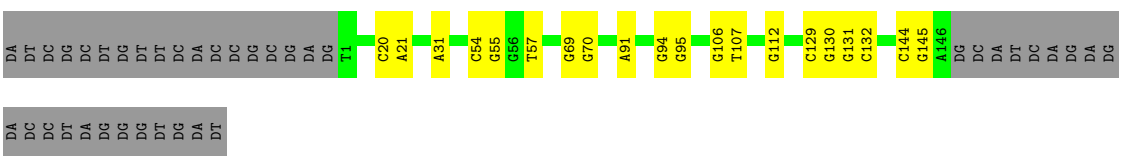
• Molecule 6: DNA (185-MER)

Chain 7-J:



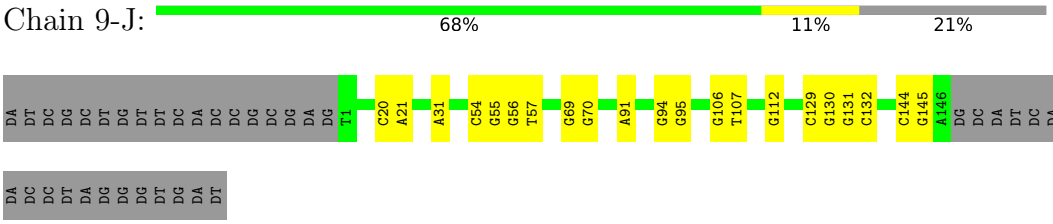
• Molecule 6: DNA (185-MER)

Chain 8-J:



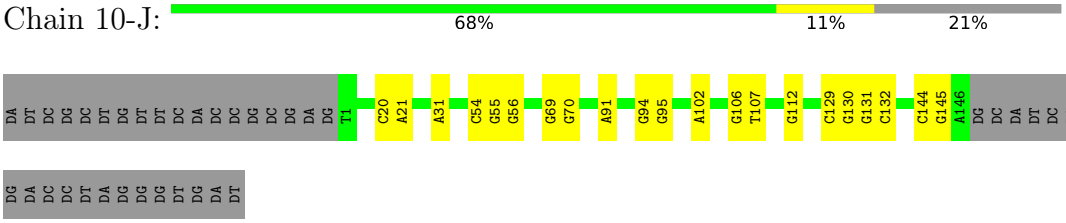
• Molecule 6: DNA (185-MER)

Chain 9-J:



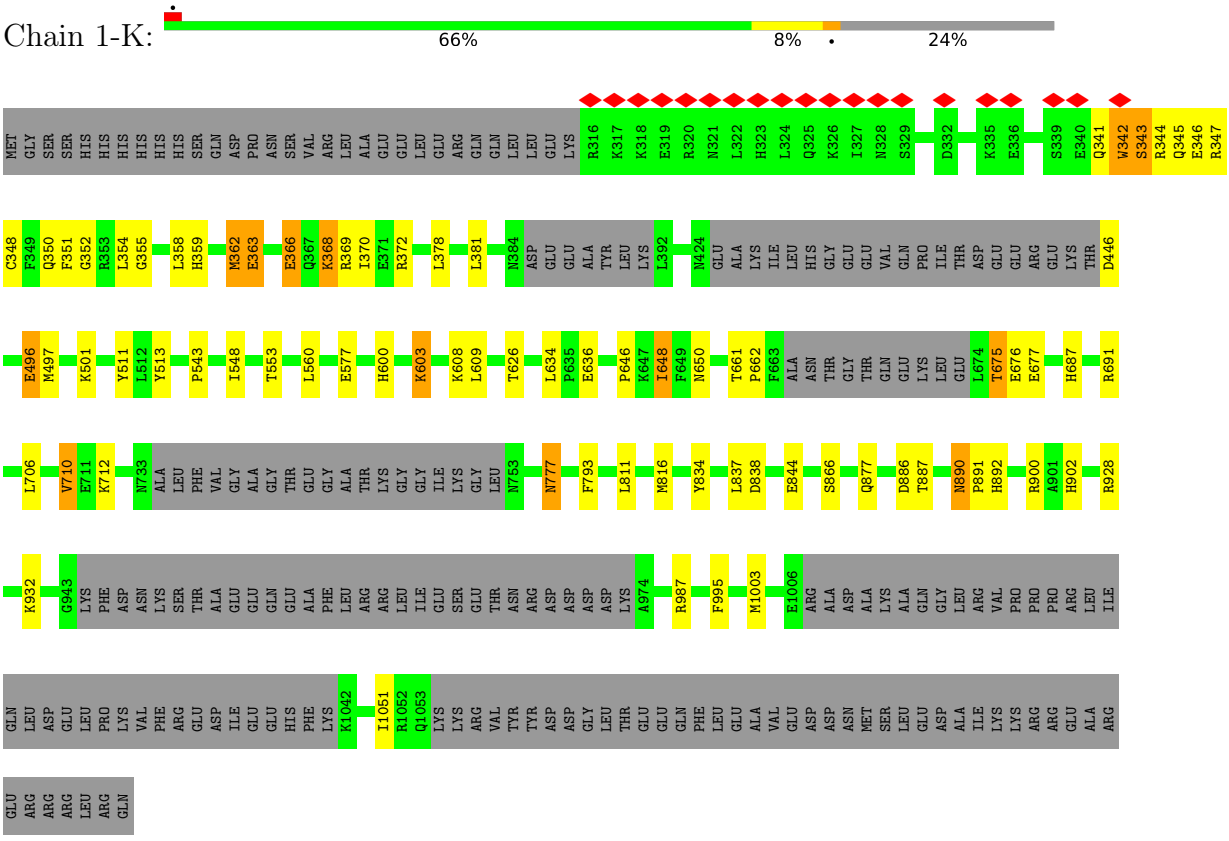
• Molecule 6: DNA (185-MER)

Chain 10-J:



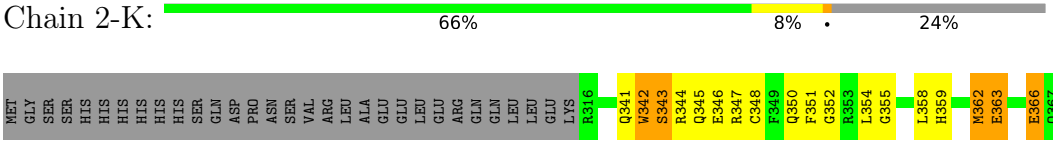
• Molecule 7: Nuclear protein STH1/NPS1

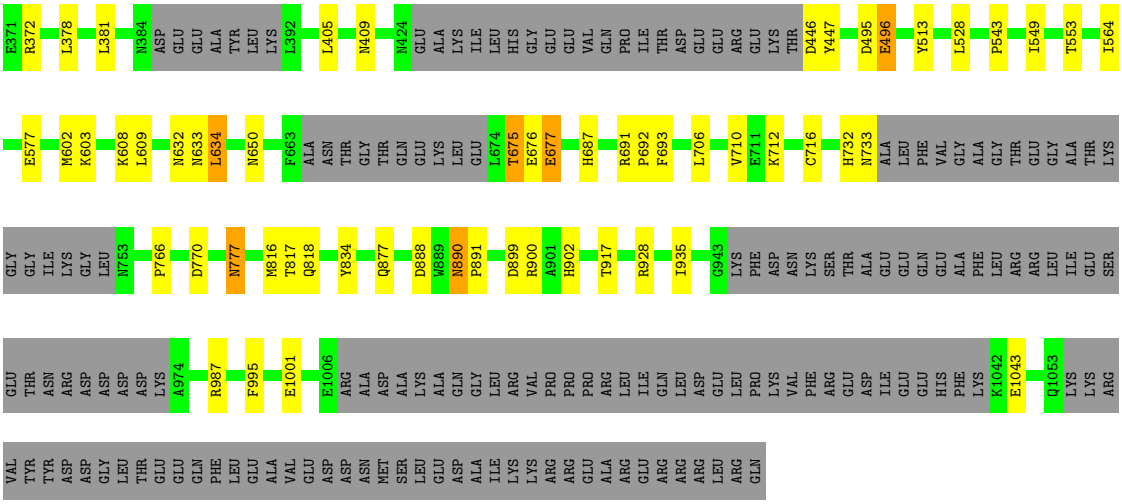
Chain 1-K:



• Molecule 7: Nuclear protein STH1/NPS1

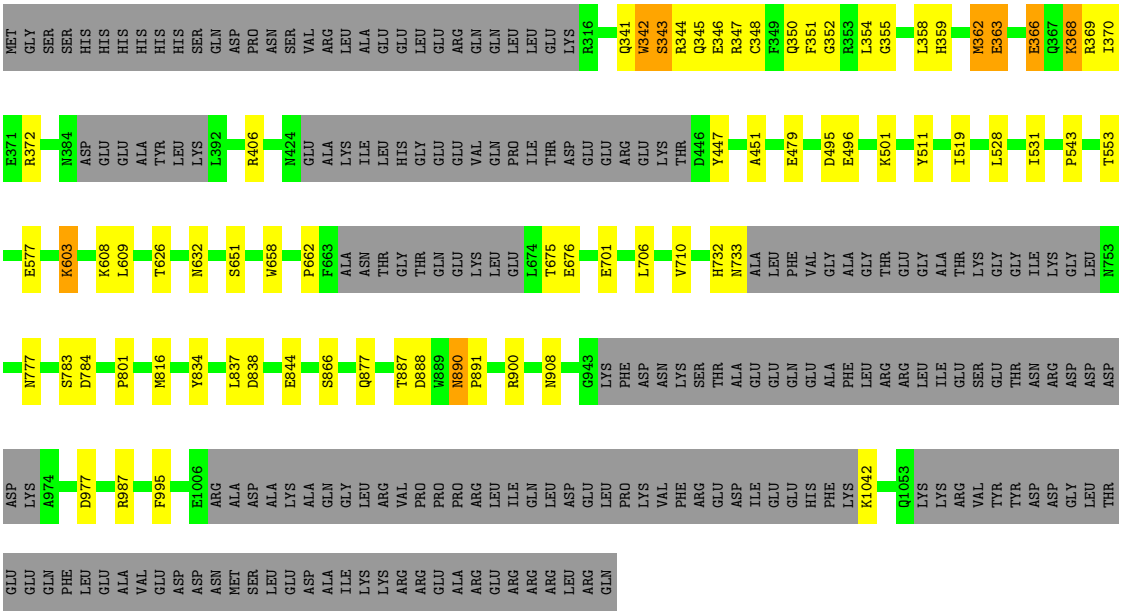
Chain 2-K:





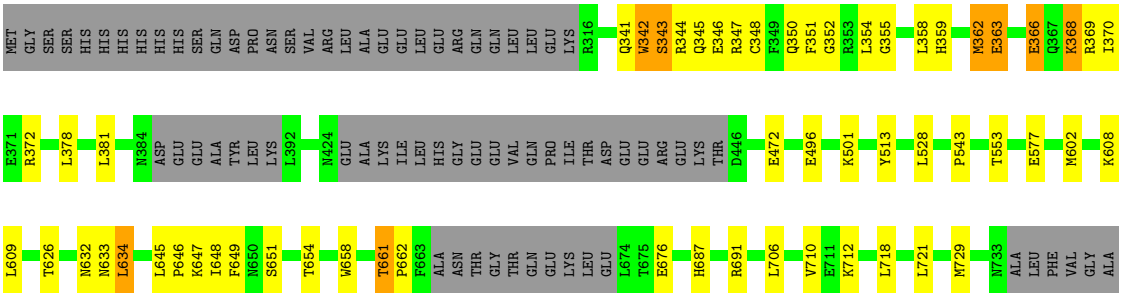
• Molecule 7: Nuclear protein STH1/NPS1

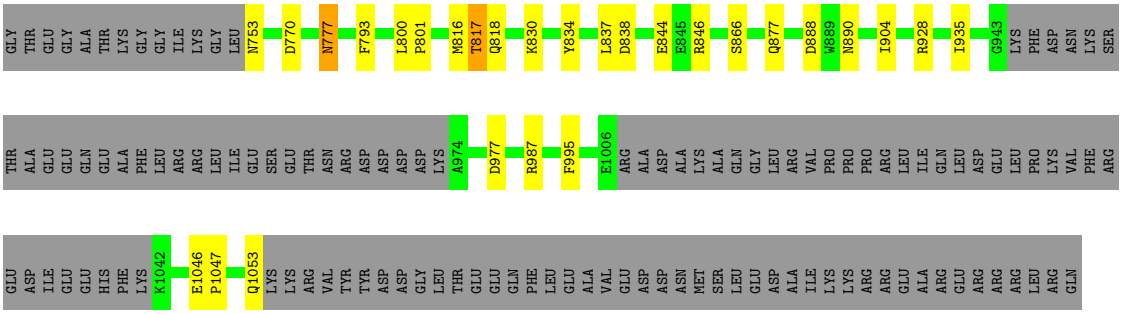
Chain 3-K:



• Molecule 7: Nuclear protein STH1/NPS1

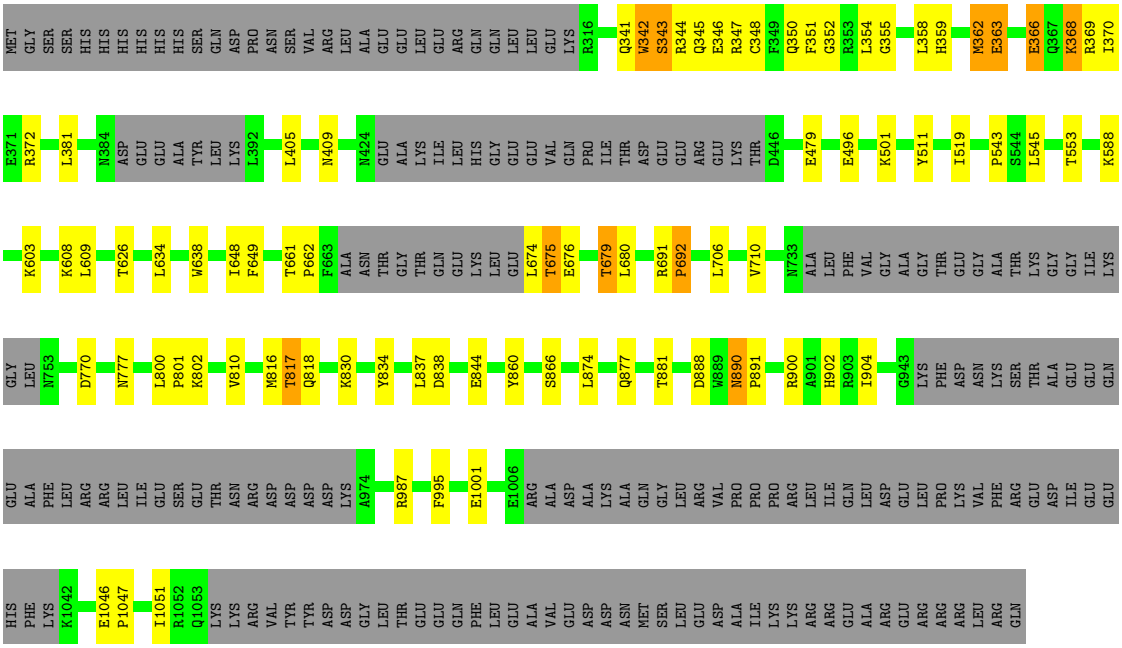
Chain 4-K:





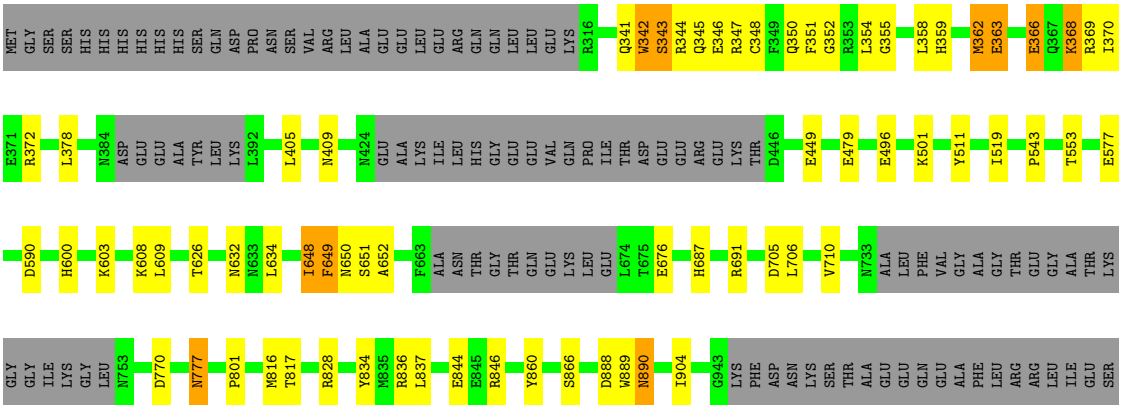
• Molecule 7: Nuclear protein STH1/NPS1

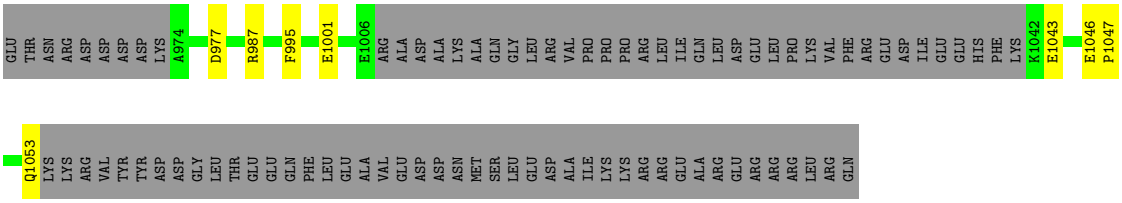
Chain 5-K:



• Molecule 7: Nuclear protein STH1/NPS1

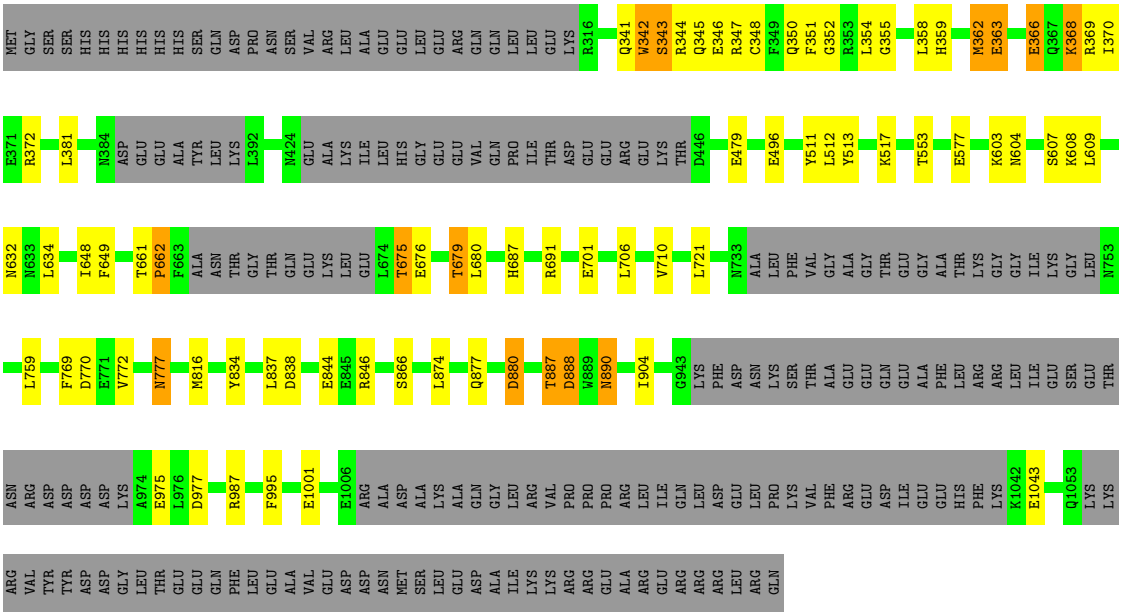
Chain 6-K:





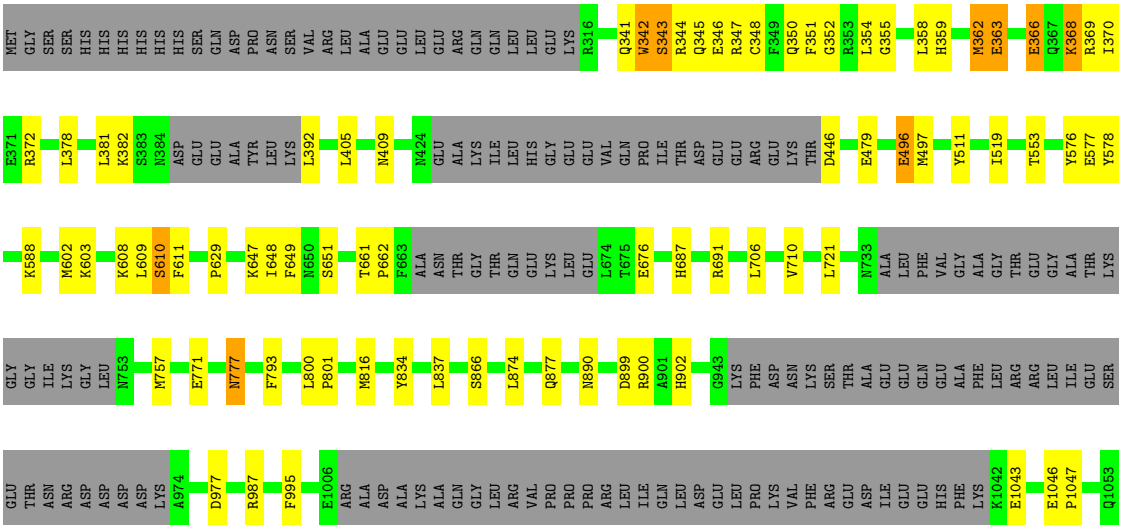
• Molecule 7: Nuclear protein STH1/NPS1

Chain 7-K:



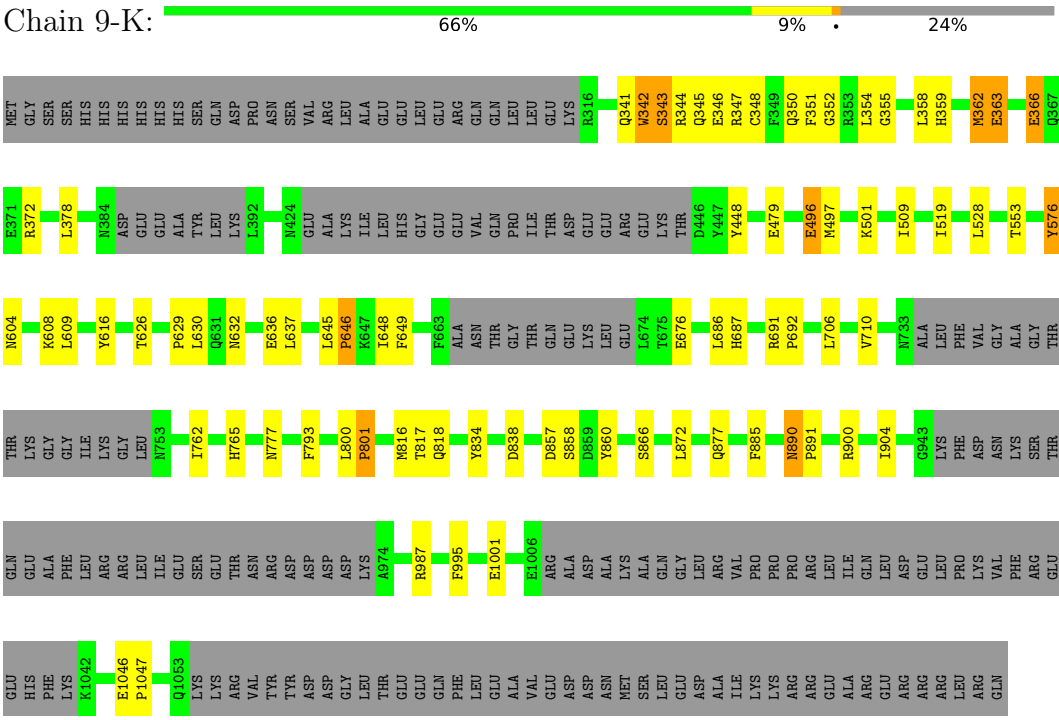
• Molecule 7: Nuclear protein STH1/NPS1

Chain 8-K:



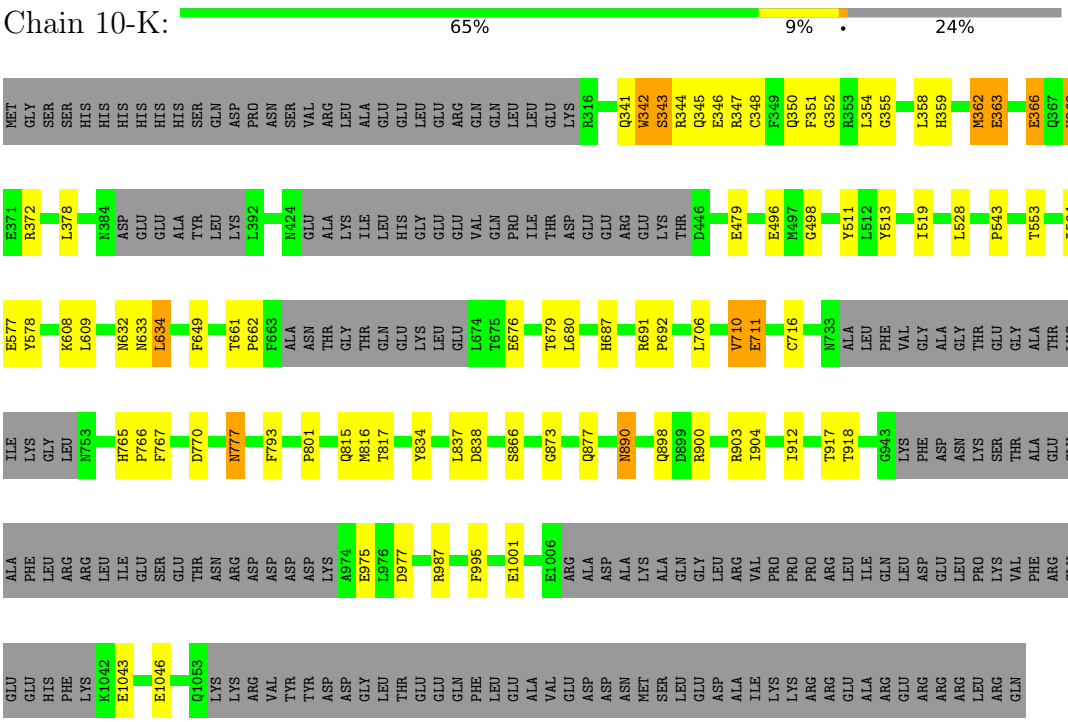
• Molecule 7: Nuclear protein STH1/NPS1

Chain 9-K:



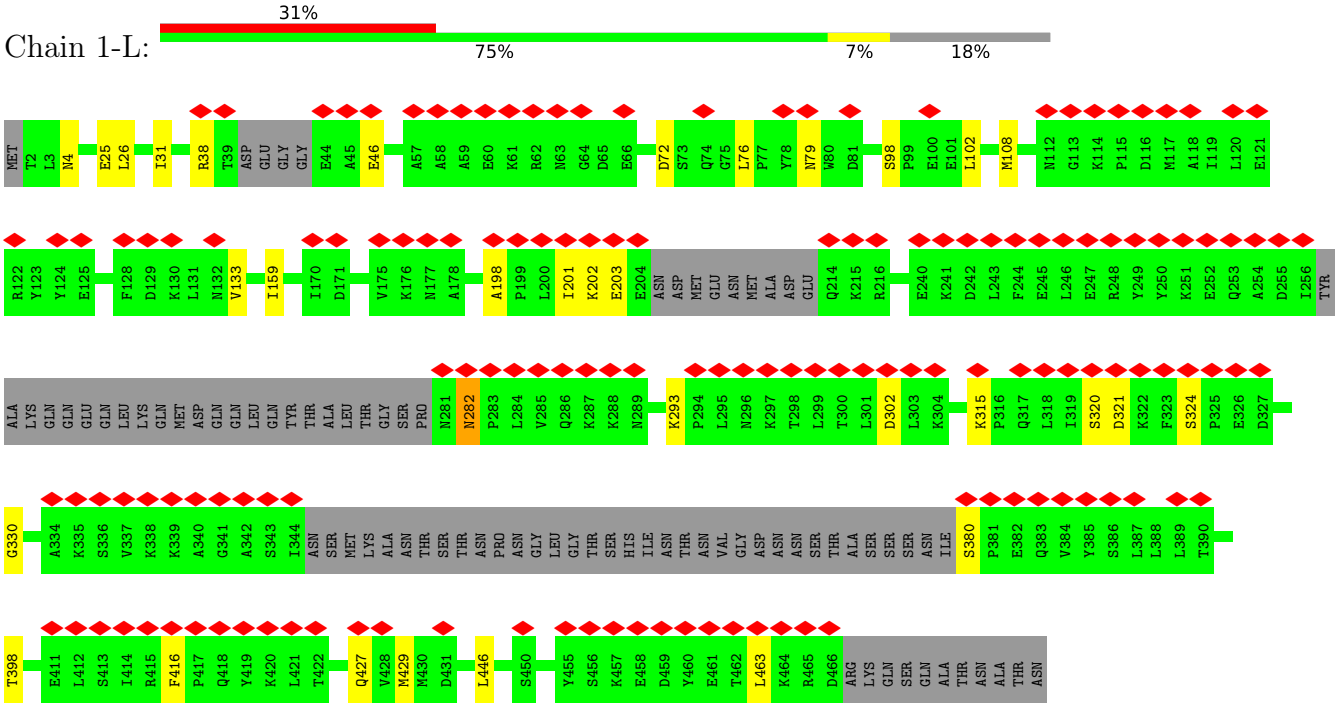
• Molecule 7: Nuclear protein STH1/NPS1

Chain 10-K:



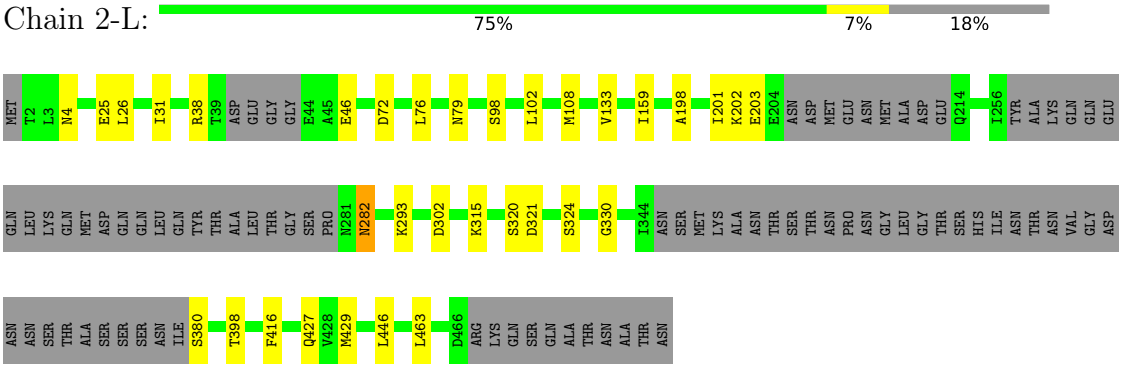
• Molecule 8: Actin-related protein 7

Chain 1-L:



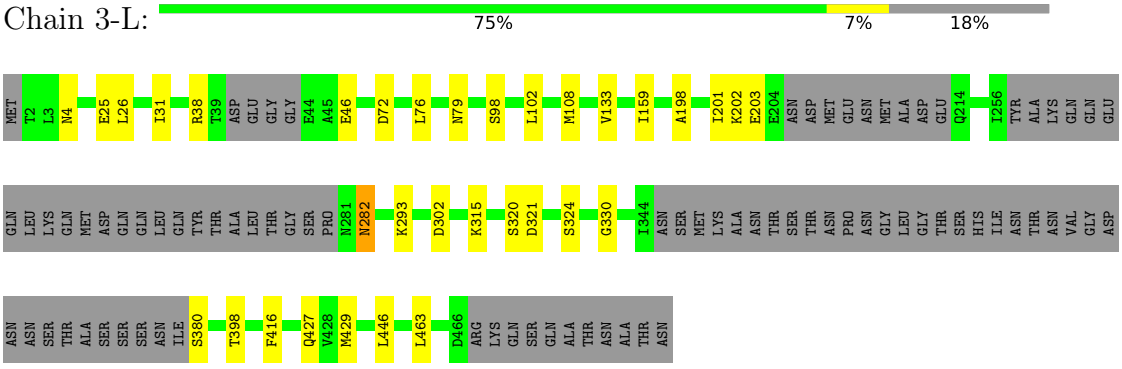
• Molecule 8: Actin-related protein 7

Chain 2-L:



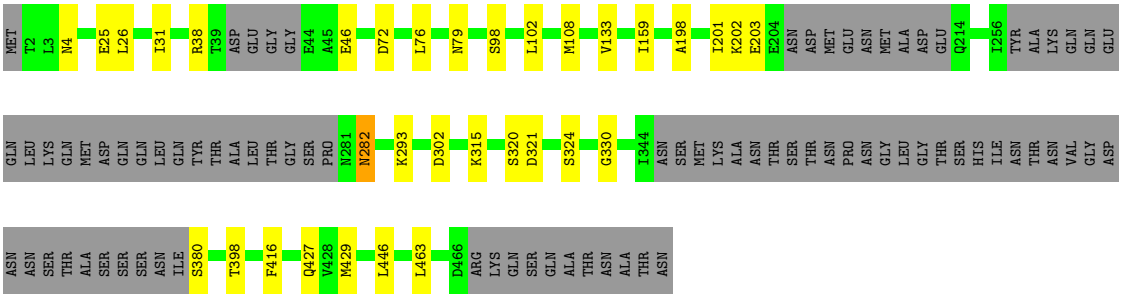
• Molecule 8: Actin-related protein 7

Chain 3-L:



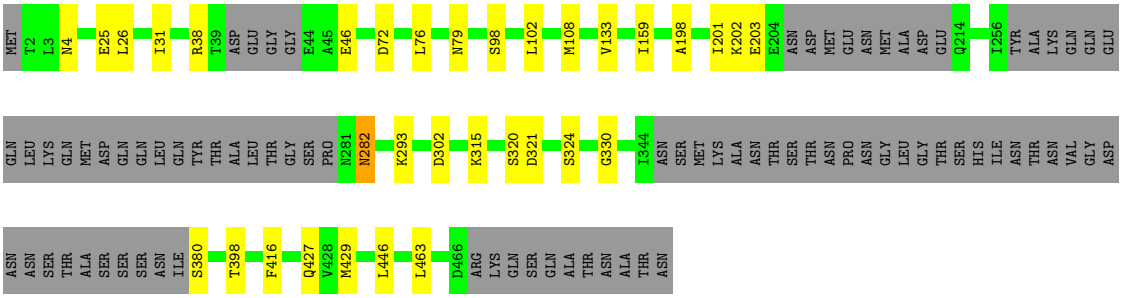
• Molecule 8: Actin-related protein 7

Chain 4-L:



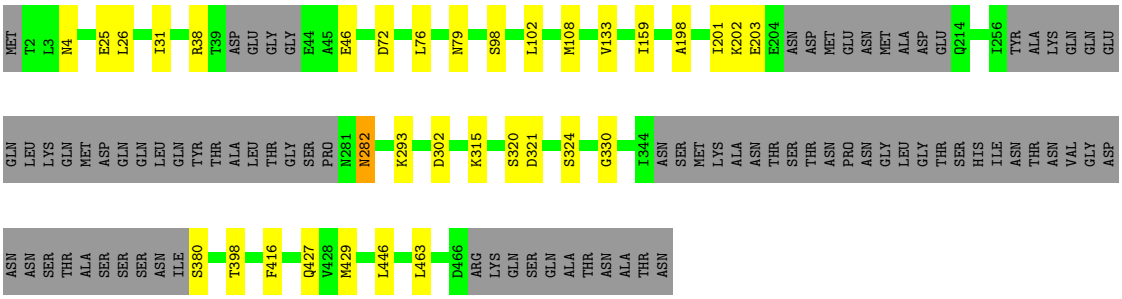
• Molecule 8: Actin-related protein 7

Chain 5-L:



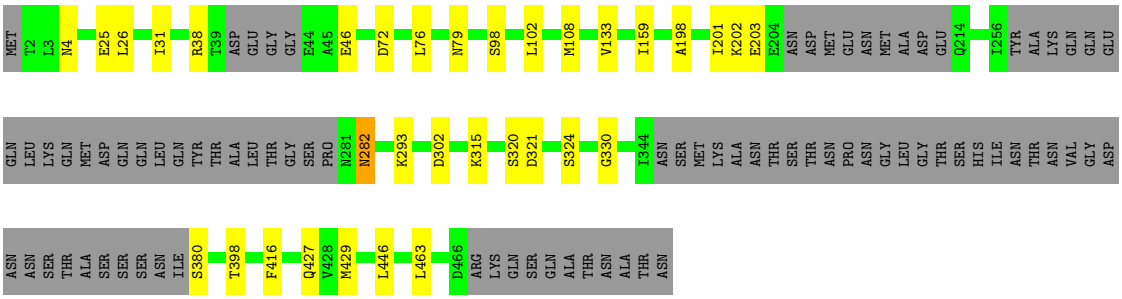
• Molecule 8: Actin-related protein 7

Chain 6-L:



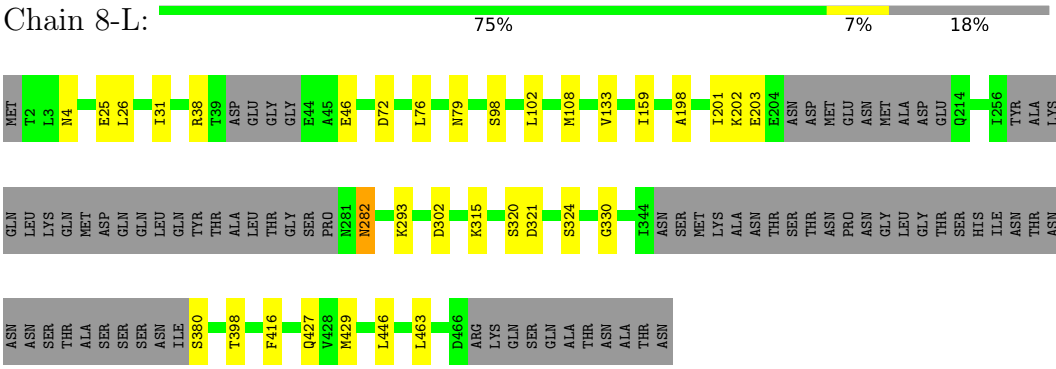
• Molecule 8: Actin-related protein 7

Chain 7-L:



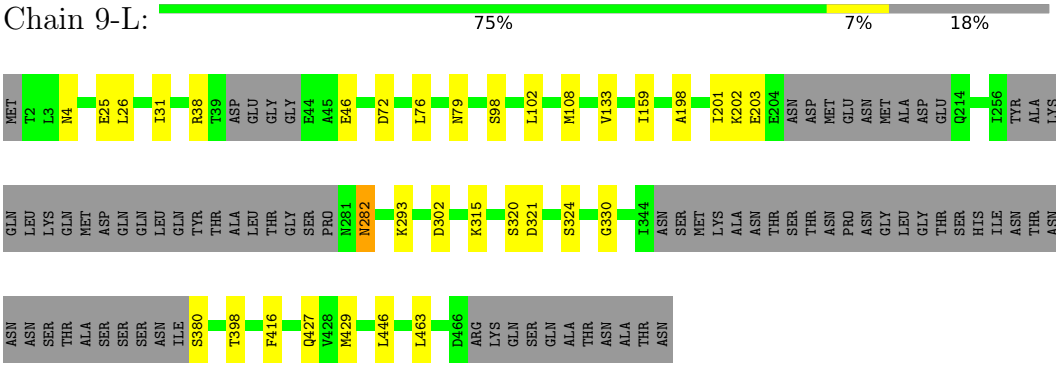
• Molecule 8: Actin-related protein 7

Chain 8-L:



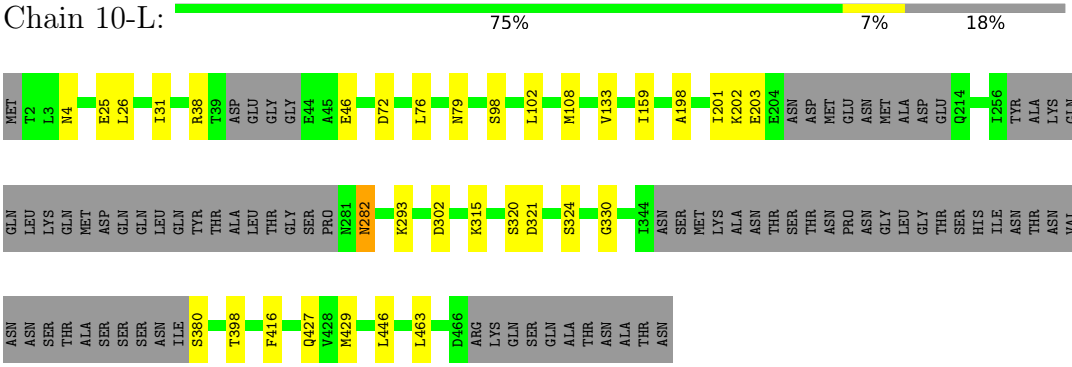
• Molecule 8: Actin-related protein 7

Chain 9-L:



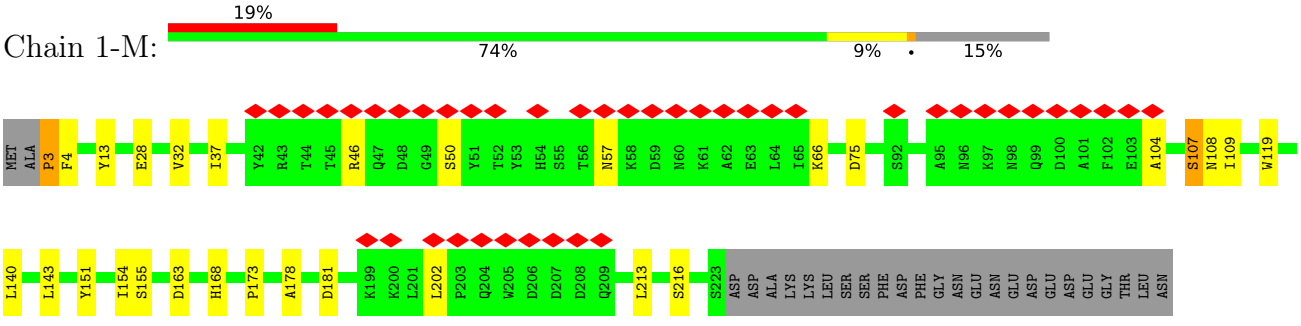
• Molecule 8: Actin-related protein 7

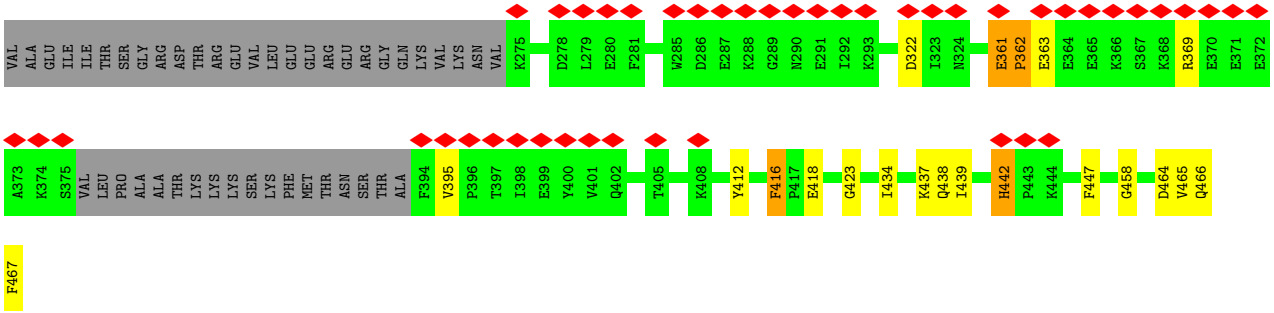
Chain 10-L:



• Molecule 9: Actin-like protein ARP9

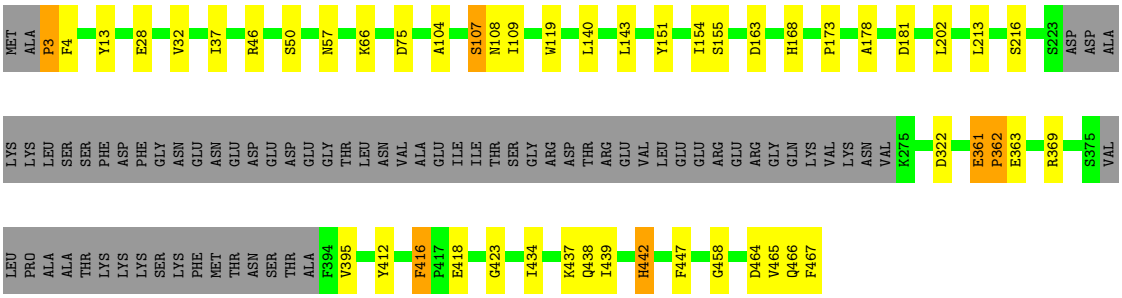
Chain 1-M:





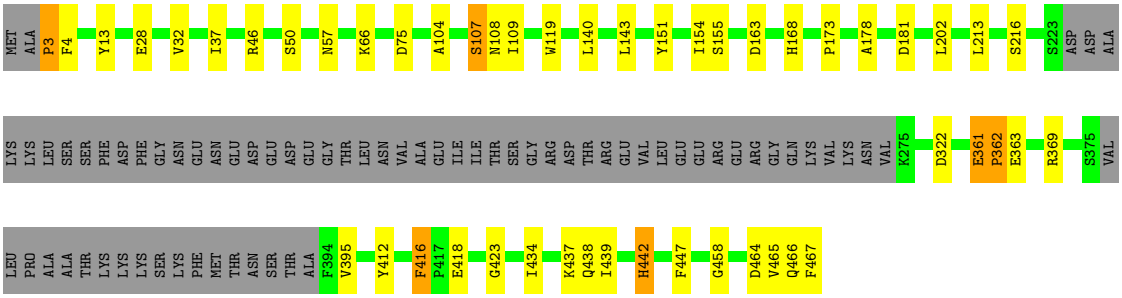
• Molecule 9: Actin-like protein ARP9

Chain 2-M:



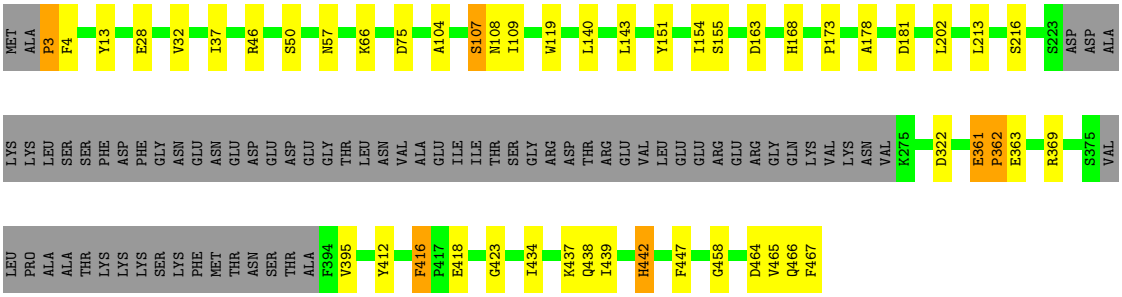
• Molecule 9: Actin-like protein ARP9

Chain 3-M:



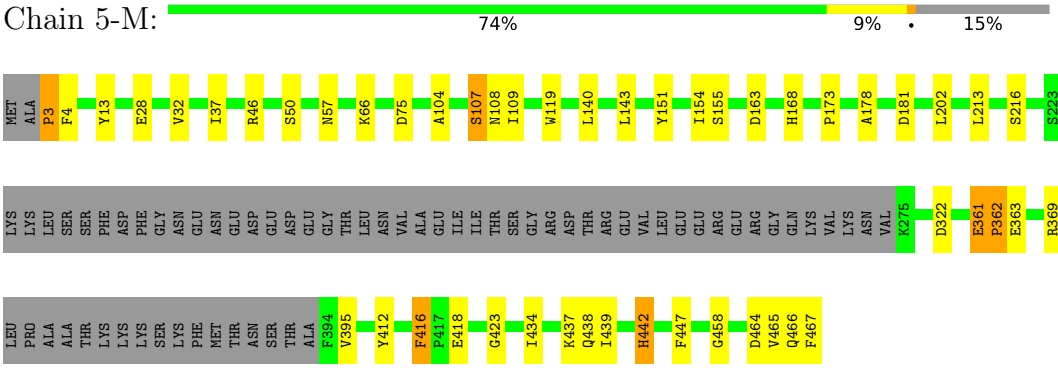
• Molecule 9: Actin-like protein ARP9

Chain 4-M:



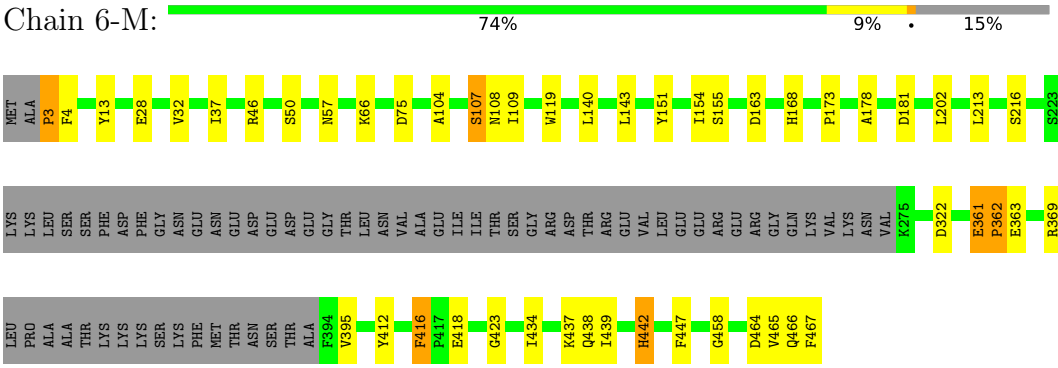
• Molecule 9: Actin-like protein ARP9

Chain 5-M:



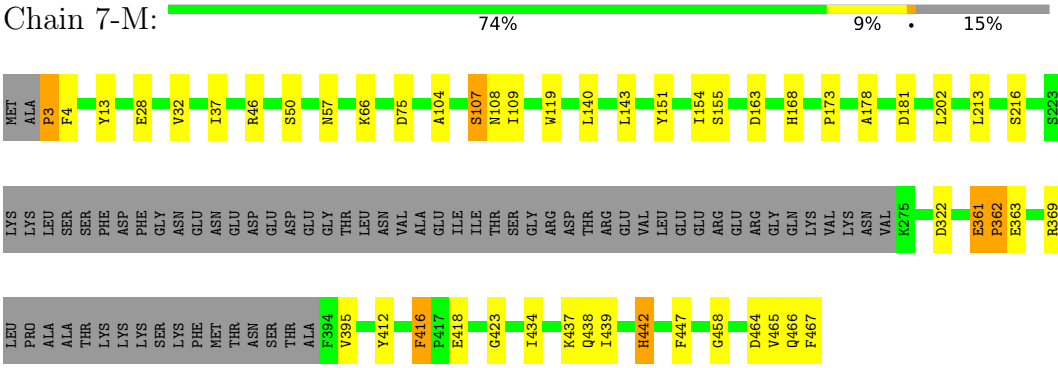
• Molecule 9: Actin-like protein ARP9

Chain 6-M:



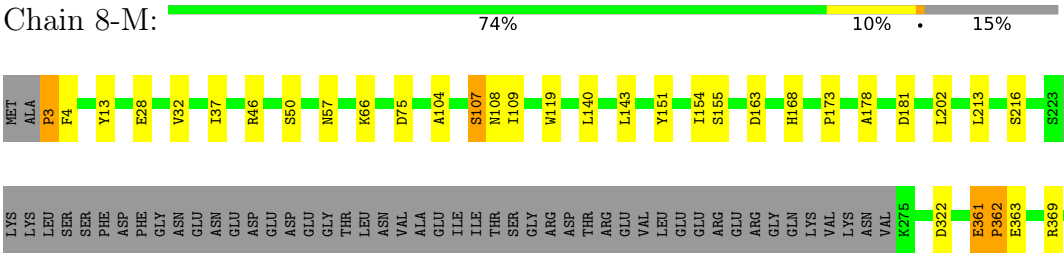
• Molecule 9: Actin-like protein ARP9

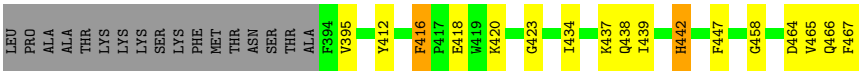
Chain 7-M:



• Molecule 9: Actin-like protein ARP9

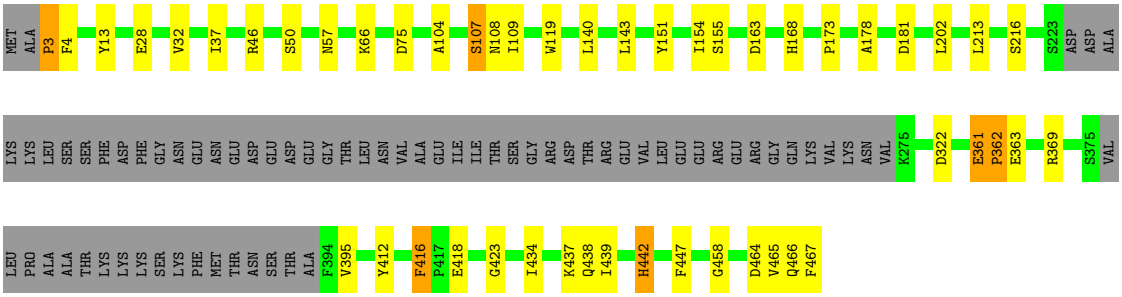
Chain 8-M:





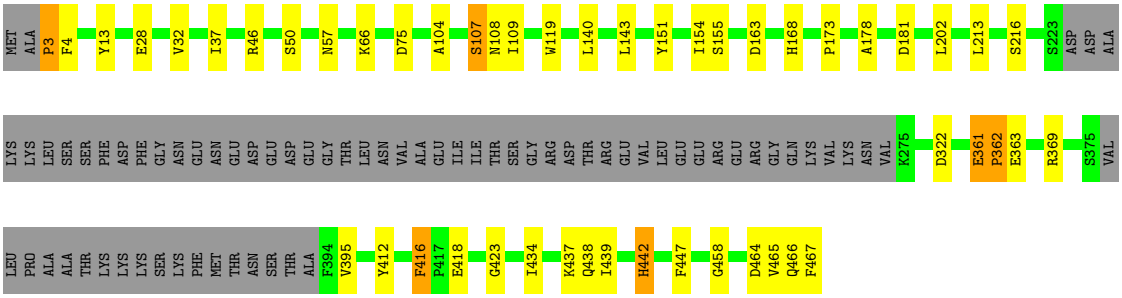
• Molecule 9: Actin-like protein ARP9

Chain 9-M:



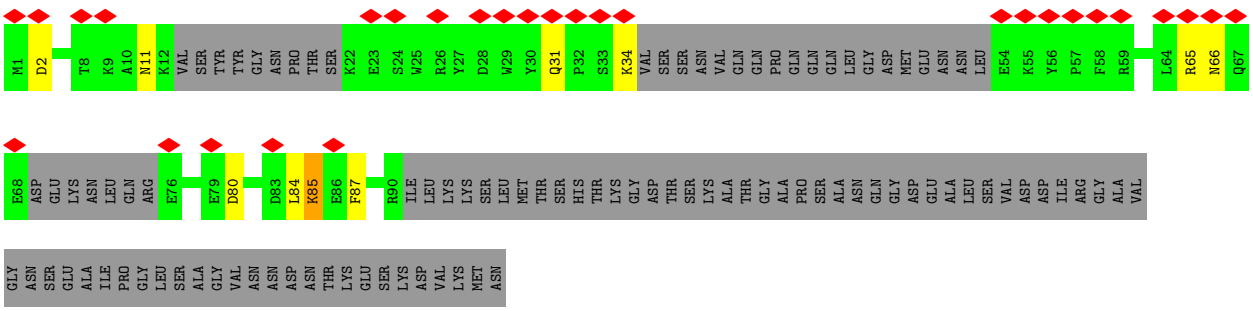
• Molecule 9: Actin-like protein ARP9

Chain 10-M:



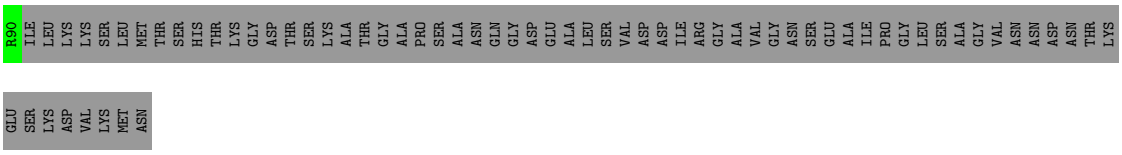
• Molecule 10: Regulator of Ty1 transposition protein 102

Chain 1-N:

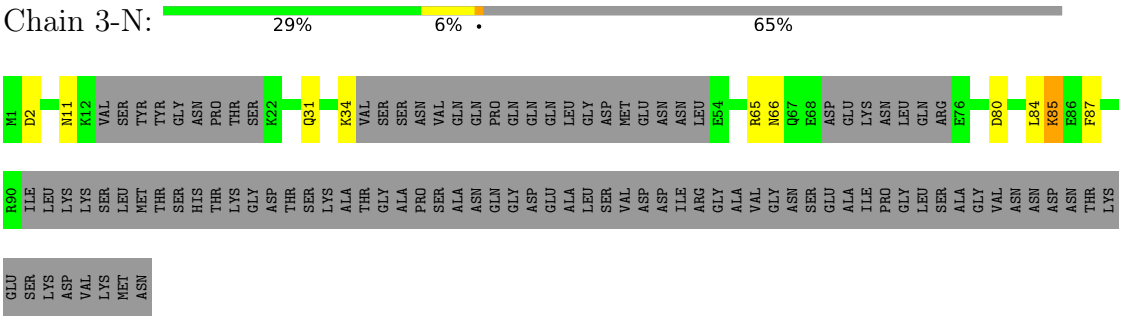


• Molecule 10: Regulator of Ty1 transposition protein 102

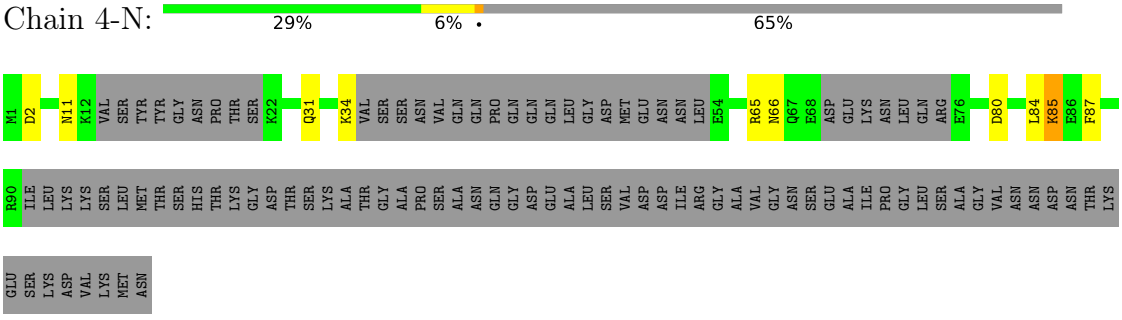
Chain 2-N:



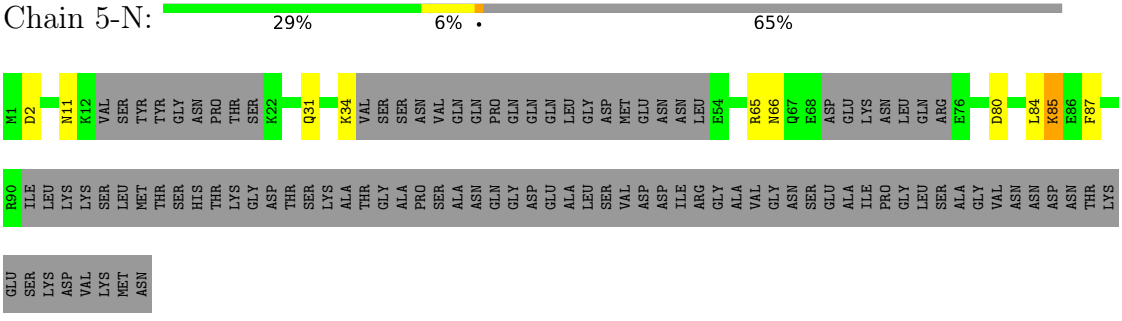
• Molecule 10: Regulator of Ty1 transposition protein 102



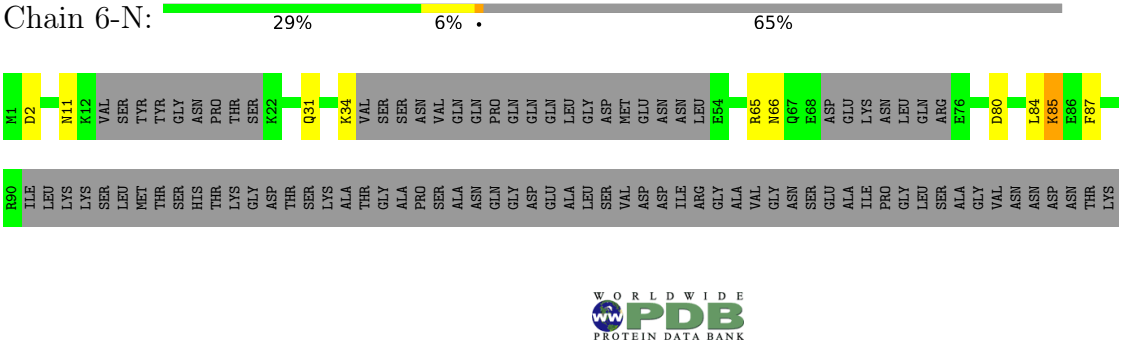
• Molecule 10: Regulator of Ty1 transposition protein 102



• Molecule 10: Regulator of Ty1 transposition protein 102

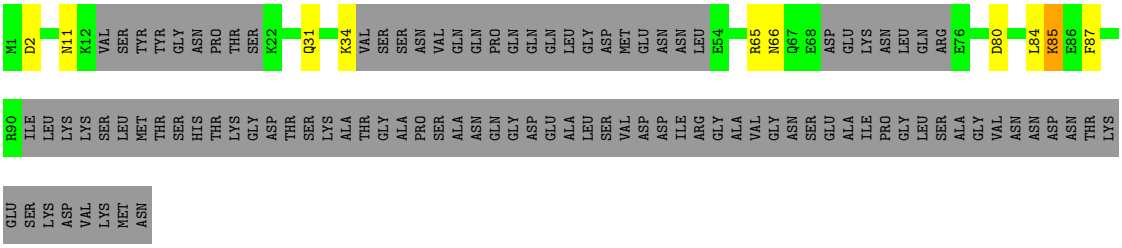


• Molecule 10: Regulator of Ty1 transposition protein 102



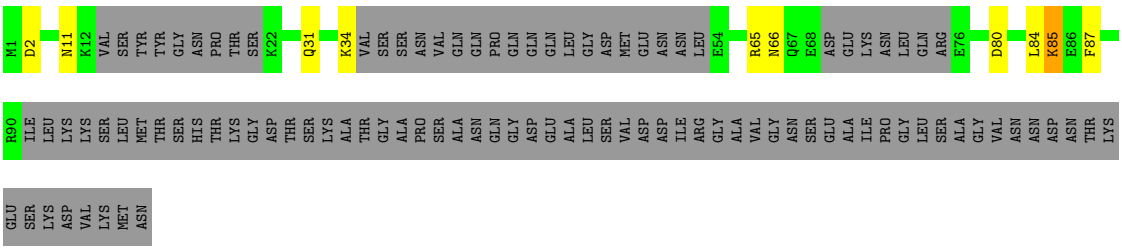
• Molecule 10: Regulator of Ty1 transposition protein 102

Chain 7-N:



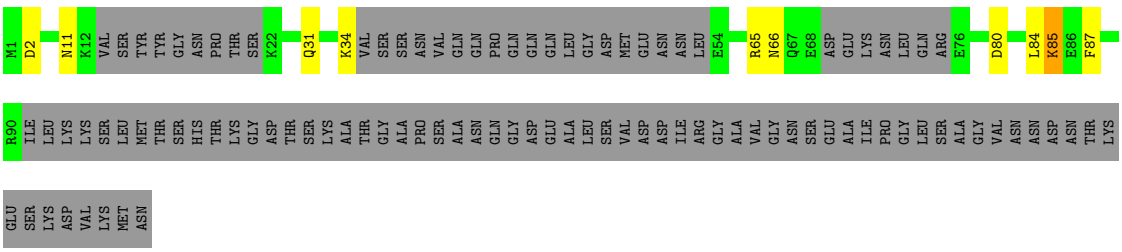
• Molecule 10: Regulator of Ty1 transposition protein 102

Chain 8-N:



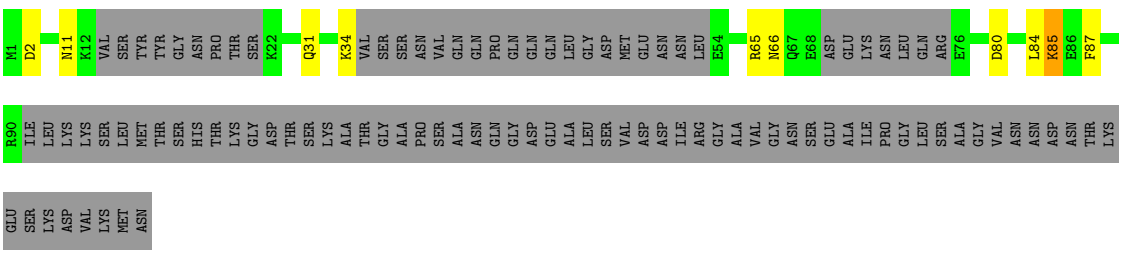
• Molecule 10: Regulator of Ty1 transposition protein 102

Chain 9-N:



• Molecule 10: Regulator of Ty1 transposition protein 102

Chain 10-N:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	293940	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 ($e^-/Å^2$)	53	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	36000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.055	Depositor
Minimum map value	-0.014	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	348.0, 348.0, 348.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.16, 1.16, 1.16	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ATP, BEF, ADP

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	1-A	0.91	0/821	0.94	6/1100 (0.5%)
1	1-E	0.92	0/793	0.91	4/1062 (0.4%)
1	2-A	0.91	0/821	0.94	6/1100 (0.5%)
1	2-E	0.92	0/793	0.91	4/1062 (0.4%)
1	3-A	0.91	0/821	0.94	6/1100 (0.5%)
1	3-E	0.92	0/793	0.91	4/1062 (0.4%)
1	4-A	0.91	0/821	0.94	6/1100 (0.5%)
1	4-E	0.92	0/793	0.91	4/1062 (0.4%)
1	5-A	0.91	0/821	0.94	6/1100 (0.5%)
1	5-E	0.92	0/793	0.91	4/1062 (0.4%)
1	6-A	0.91	0/821	0.94	6/1100 (0.5%)
1	6-E	0.92	0/793	0.91	4/1062 (0.4%)
1	7-A	0.91	0/821	0.94	6/1100 (0.5%)
1	7-E	0.92	0/793	0.91	4/1062 (0.4%)
1	8-A	0.91	0/821	0.94	6/1100 (0.5%)
1	8-E	0.92	0/793	0.91	4/1062 (0.4%)
1	9-A	0.91	0/821	0.94	6/1100 (0.5%)
1	9-E	0.92	0/793	0.91	4/1062 (0.4%)
1	10-A	0.91	0/821	0.94	6/1100 (0.5%)
1	10-E	0.92	0/793	0.91	4/1062 (0.4%)
2	1-B	0.87	0/711	0.73	0/950
2	1-F	0.88	0/634	0.77	0/848
2	2-B	0.87	0/711	0.73	0/950
2	2-F	0.88	0/634	0.77	0/848
2	3-B	0.87	0/711	0.73	0/950
2	3-F	0.88	0/634	0.77	0/848
2	4-B	0.87	0/711	0.73	0/950
2	4-F	0.88	0/634	0.77	0/848
2	5-B	0.87	0/711	0.73	0/950
2	5-F	0.88	0/634	0.77	0/848
2	6-B	0.87	0/711	0.73	0/950
2	6-F	0.88	0/634	0.77	0/848

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
2	7-B	0.87	0/711	0.73	0/950
2	7-F	0.88	0/634	0.77	0/848
2	8-B	0.87	0/711	0.73	0/950
2	8-F	0.88	0/634	0.77	0/848
2	9-B	0.87	0/711	0.73	0/950
2	9-F	0.88	0/634	0.77	0/848
2	10-B	0.87	0/711	0.73	0/950
2	10-F	0.88	0/634	0.77	0/848
3	1-C	0.87	0/833	0.92	9/1124 (0.8%)
3	1-G	0.88	0/833	0.97	9/1124 (0.8%)
3	2-C	0.87	0/833	0.92	9/1124 (0.8%)
3	2-G	0.88	0/833	0.97	9/1124 (0.8%)
3	3-C	0.87	0/833	0.92	9/1124 (0.8%)
3	3-G	0.88	0/833	0.97	9/1124 (0.8%)
3	4-C	0.87	0/833	0.92	9/1124 (0.8%)
3	4-G	0.88	0/833	0.97	9/1124 (0.8%)
3	5-C	0.87	0/833	0.92	9/1124 (0.8%)
3	5-G	0.88	0/833	0.97	9/1124 (0.8%)
3	6-C	0.87	0/833	0.92	9/1124 (0.8%)
3	6-G	0.88	0/833	0.97	9/1124 (0.8%)
3	7-C	0.87	0/833	0.92	9/1124 (0.8%)
3	7-G	0.88	0/833	0.97	9/1124 (0.8%)
3	8-C	0.87	0/833	0.92	9/1124 (0.8%)
3	8-G	0.88	0/833	0.97	9/1124 (0.8%)
3	9-C	0.87	0/833	0.92	9/1124 (0.8%)
3	9-G	0.88	0/833	0.97	9/1124 (0.8%)
3	10-C	0.87	0/833	0.92	9/1124 (0.8%)
3	10-G	0.88	0/833	0.97	9/1124 (0.8%)
4	1-D	0.93	0/730	0.78	2/983 (0.2%)
4	1-H	0.94	0/730	0.84	4/983 (0.4%)
4	2-D	0.93	0/730	0.78	2/983 (0.2%)
4	2-H	0.94	0/730	0.84	4/983 (0.4%)
4	3-D	0.93	0/730	0.78	2/983 (0.2%)
4	3-H	0.94	0/730	0.84	4/983 (0.4%)
4	4-D	0.93	0/730	0.78	2/983 (0.2%)
4	4-H	0.94	0/730	0.84	4/983 (0.4%)
4	5-D	0.93	0/730	0.78	2/983 (0.2%)
4	5-H	0.94	0/730	0.84	4/983 (0.4%)
4	6-D	0.93	0/730	0.78	2/983 (0.2%)
4	6-H	0.94	0/730	0.84	4/983 (0.4%)
4	7-D	0.93	0/730	0.78	2/983 (0.2%)
4	7-H	0.94	0/730	0.84	4/983 (0.4%)
4	8-D	0.93	0/730	0.78	2/983 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
4	8-H	0.94	0/730	0.84	4/983 (0.4%)
4	9-D	0.93	0/730	0.78	2/983 (0.2%)
4	9-H	0.94	0/730	0.84	4/983 (0.4%)
4	10-D	0.93	0/730	0.78	2/983 (0.2%)
4	10-H	0.94	0/730	0.84	4/983 (0.4%)
5	1-I	0.39	0/3333	0.50	0/5137
5	2-I	0.39	0/3333	0.50	0/5137
5	3-I	0.39	0/3333	0.50	0/5137
5	4-I	0.39	0/3333	0.50	0/5137
5	5-I	0.39	0/3333	0.50	0/5137
5	6-I	0.39	0/3333	0.50	0/5137
5	7-I	0.39	0/3333	0.50	0/5137
5	8-I	0.39	0/3333	0.50	0/5137
5	9-I	0.39	0/3333	0.50	0/5137
5	10-I	0.39	0/3333	0.50	0/5137
6	1-J	0.40	0/3381	0.49	0/5221
6	2-J	0.40	0/3381	0.49	0/5221
6	3-J	0.40	0/3381	0.49	0/5221
6	4-J	0.40	0/3381	0.49	0/5221
6	5-J	0.40	0/3381	0.49	0/5221
6	6-J	0.40	0/3381	0.49	0/5221
6	7-J	0.40	0/3381	0.49	0/5221
6	8-J	0.40	0/3381	0.49	0/5221
6	9-J	0.40	0/3381	0.49	0/5221
6	10-J	0.40	0/3381	0.49	0/5221
7	1-K	0.63	2/5138 (0.0%)	0.69	18/6910 (0.3%)
7	2-K	0.63	2/5138 (0.0%)	0.69	18/6910 (0.3%)
7	3-K	0.63	2/5138 (0.0%)	0.69	18/6910 (0.3%)
7	4-K	0.63	2/5138 (0.0%)	0.69	18/6910 (0.3%)
7	5-K	0.63	2/5138 (0.0%)	0.69	18/6910 (0.3%)
7	6-K	0.63	2/5138 (0.0%)	0.69	18/6910 (0.3%)
7	7-K	0.63	2/5138 (0.0%)	0.69	18/6910 (0.3%)
7	8-K	0.63	2/5138 (0.0%)	0.69	18/6910 (0.3%)
7	9-K	0.63	2/5138 (0.0%)	0.69	18/6910 (0.3%)
7	10-K	0.63	2/5138 (0.0%)	0.69	18/6910 (0.3%)
8	1-L	0.93	0/3220	1.12	32/4355 (0.7%)
8	2-L	0.93	0/3220	1.12	32/4355 (0.7%)
8	3-L	0.93	0/3220	1.12	32/4355 (0.7%)
8	4-L	0.93	0/3220	1.12	32/4355 (0.7%)
8	5-L	0.93	0/3220	1.12	32/4355 (0.7%)
8	6-L	0.93	0/3220	1.12	32/4355 (0.7%)
8	7-L	0.93	0/3220	1.12	32/4355 (0.7%)
8	8-L	0.93	0/3220	1.12	32/4355 (0.7%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
8	9-L	0.93	0/3220	1.12	32/4355 (0.7%)
8	10-L	0.93	0/3220	1.12	32/4355 (0.7%)
9	1-M	0.92	0/3259	1.11	32/4417 (0.7%)
9	2-M	0.92	0/3259	1.11	32/4417 (0.7%)
9	3-M	0.92	0/3259	1.11	32/4417 (0.7%)
9	4-M	0.92	0/3259	1.11	32/4417 (0.7%)
9	5-M	0.92	0/3259	1.11	32/4417 (0.7%)
9	6-M	0.92	0/3259	1.11	32/4417 (0.7%)
9	7-M	0.92	0/3259	1.11	32/4417 (0.7%)
9	8-M	0.92	0/3259	1.11	32/4417 (0.7%)
9	9-M	0.92	0/3259	1.11	32/4417 (0.7%)
9	10-M	0.92	0/3259	1.11	32/4417 (0.7%)
10	1-N	0.82	0/505	1.11	6/674 (0.9%)
10	2-N	0.82	0/505	1.11	6/674 (0.9%)
10	3-N	0.82	0/505	1.11	6/674 (0.9%)
10	4-N	0.82	0/505	1.11	6/674 (0.9%)
10	5-N	0.82	0/505	1.11	6/674 (0.9%)
10	6-N	0.82	0/505	1.11	6/674 (0.9%)
10	7-N	0.82	0/505	1.11	6/674 (0.9%)
10	8-N	0.82	0/505	1.11	6/674 (0.9%)
10	9-N	0.82	0/505	1.11	6/674 (0.9%)
10	10-N	0.82	0/505	1.11	6/674 (0.9%)
All	All	0.75	20/249210 (0.0%)	0.82	1220/348880 (0.3%)

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
7	6-K	0	2
9	1-M	0	2
9	2-M	0	2
9	3-M	0	2
9	4-M	0	2
9	5-M	0	2
9	6-M	0	2
9	7-M	0	2
9	8-M	0	2
9	9-M	0	2
9	10-M	0	2
All	All	0	22

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	1-K	342	TRP	C-N	14.11	1.53	1.33
7	2-K	342	TRP	C-N	14.11	1.53	1.33
7	3-K	342	TRP	C-N	14.11	1.53	1.33
7	4-K	342	TRP	C-N	14.11	1.53	1.33
7	5-K	342	TRP	C-N	14.11	1.53	1.33
7	6-K	342	TRP	C-N	14.11	1.53	1.33
7	7-K	342	TRP	C-N	14.11	1.53	1.33
7	8-K	342	TRP	C-N	14.11	1.53	1.33
7	9-K	342	TRP	C-N	14.11	1.53	1.33
7	10-K	342	TRP	C-N	14.11	1.53	1.33
7	1-K	342	TRP	N-CA	5.08	1.54	1.46
7	2-K	342	TRP	N-CA	5.08	1.54	1.46
7	3-K	342	TRP	N-CA	5.08	1.54	1.46
7	4-K	342	TRP	N-CA	5.08	1.54	1.46
7	5-K	342	TRP	N-CA	5.08	1.54	1.46
7	6-K	342	TRP	N-CA	5.08	1.54	1.46
7	7-K	342	TRP	N-CA	5.08	1.54	1.46
7	8-K	342	TRP	N-CA	5.08	1.54	1.46
7	9-K	342	TRP	N-CA	5.08	1.54	1.46
7	10-K	342	TRP	N-CA	5.08	1.54	1.46

All (1220) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	1-K	342	TRP	CA-C-N	17.78	155.50	121.54
7	1-K	342	TRP	C-N-CA	17.78	155.50	121.54
7	2-K	342	TRP	CA-C-N	17.78	155.50	121.54
7	2-K	342	TRP	C-N-CA	17.78	155.50	121.54
7	3-K	342	TRP	CA-C-N	17.78	155.50	121.54
7	3-K	342	TRP	C-N-CA	17.78	155.50	121.54
7	4-K	342	TRP	CA-C-N	17.78	155.50	121.54
7	4-K	342	TRP	C-N-CA	17.78	155.50	121.54
7	5-K	342	TRP	CA-C-N	17.78	155.50	121.54
7	5-K	342	TRP	C-N-CA	17.78	155.50	121.54
7	6-K	342	TRP	CA-C-N	17.78	155.50	121.54
7	6-K	342	TRP	C-N-CA	17.78	155.50	121.54
7	7-K	342	TRP	CA-C-N	17.78	155.50	121.54
7	7-K	342	TRP	C-N-CA	17.78	155.50	121.54
7	8-K	342	TRP	CA-C-N	17.78	155.50	121.54
7	8-K	342	TRP	C-N-CA	17.78	155.50	121.54
7	9-K	342	TRP	CA-C-N	17.78	155.50	121.54
7	9-K	342	TRP	C-N-CA	17.78	155.50	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	10-K	342	TRP	CA-C-N	17.78	155.50	121.54
7	10-K	342	TRP	C-N-CA	17.78	155.50	121.54
7	1-K	342	TRP	CA-C-O	-10.65	108.61	121.28
7	2-K	342	TRP	CA-C-O	-10.65	108.61	121.28
7	3-K	342	TRP	CA-C-O	-10.65	108.61	121.28
7	4-K	342	TRP	CA-C-O	-10.65	108.61	121.28
7	5-K	342	TRP	CA-C-O	-10.65	108.61	121.28
7	6-K	342	TRP	CA-C-O	-10.65	108.61	121.28
7	7-K	342	TRP	CA-C-O	-10.65	108.61	121.28
7	8-K	342	TRP	CA-C-O	-10.65	108.61	121.28
7	9-K	342	TRP	CA-C-O	-10.65	108.61	121.28
7	10-K	342	TRP	CA-C-O	-10.65	108.61	121.28
3	1-G	117	LEU	CA-C-N	8.65	128.79	120.31
3	1-G	117	LEU	C-N-CA	8.65	128.79	120.31
3	2-G	117	LEU	CA-C-N	8.65	128.79	120.31
3	2-G	117	LEU	C-N-CA	8.65	128.79	120.31
3	3-G	117	LEU	CA-C-N	8.65	128.79	120.31
3	3-G	117	LEU	C-N-CA	8.65	128.79	120.31
3	4-G	117	LEU	CA-C-N	8.65	128.79	120.31
3	4-G	117	LEU	C-N-CA	8.65	128.79	120.31
3	5-G	117	LEU	CA-C-N	8.65	128.79	120.31
3	5-G	117	LEU	C-N-CA	8.65	128.79	120.31
3	6-G	117	LEU	CA-C-N	8.65	128.79	120.31
3	6-G	117	LEU	C-N-CA	8.65	128.79	120.31
3	7-G	117	LEU	CA-C-N	8.65	128.79	120.31
3	7-G	117	LEU	C-N-CA	8.65	128.79	120.31
3	8-G	117	LEU	CA-C-N	8.65	128.79	120.31
3	8-G	117	LEU	C-N-CA	8.65	128.79	120.31
3	9-G	117	LEU	CA-C-N	8.65	128.79	120.31
3	9-G	117	LEU	C-N-CA	8.65	128.79	120.31
3	10-G	117	LEU	CA-C-N	8.65	128.79	120.31
3	10-G	117	LEU	C-N-CA	8.65	128.79	120.31
8	1-L	446	LEU	CA-C-N	8.54	128.26	119.64
8	1-L	446	LEU	C-N-CA	8.54	128.26	119.64
8	2-L	446	LEU	CA-C-N	8.54	128.26	119.64
8	2-L	446	LEU	C-N-CA	8.54	128.26	119.64
8	3-L	446	LEU	CA-C-N	8.54	128.26	119.64
8	3-L	446	LEU	C-N-CA	8.54	128.26	119.64
8	4-L	446	LEU	CA-C-N	8.54	128.26	119.64
8	4-L	446	LEU	C-N-CA	8.54	128.26	119.64
8	5-L	446	LEU	CA-C-N	8.54	128.26	119.64
8	5-L	446	LEU	C-N-CA	8.54	128.26	119.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	6-L	446	LEU	CA-C-N	8.54	128.26	119.64
8	6-L	446	LEU	C-N-CA	8.54	128.26	119.64
8	7-L	446	LEU	CA-C-N	8.54	128.26	119.64
8	7-L	446	LEU	C-N-CA	8.54	128.26	119.64
8	8-L	446	LEU	CA-C-N	8.54	128.26	119.64
8	8-L	446	LEU	C-N-CA	8.54	128.26	119.64
8	9-L	446	LEU	CA-C-N	8.54	128.26	119.64
8	9-L	446	LEU	C-N-CA	8.54	128.26	119.64
8	10-L	446	LEU	CA-C-N	8.54	128.26	119.64
8	10-L	446	LEU	C-N-CA	8.54	128.26	119.64
8	1-L	416	PHE	CA-C-N	8.50	128.15	119.56
8	1-L	416	PHE	C-N-CA	8.50	128.15	119.56
8	2-L	416	PHE	CA-C-N	8.50	128.15	119.56
8	2-L	416	PHE	C-N-CA	8.50	128.15	119.56
8	3-L	416	PHE	CA-C-N	8.50	128.15	119.56
8	3-L	416	PHE	C-N-CA	8.50	128.15	119.56
8	4-L	416	PHE	CA-C-N	8.50	128.15	119.56
8	4-L	416	PHE	C-N-CA	8.50	128.15	119.56
8	5-L	416	PHE	CA-C-N	8.50	128.15	119.56
8	5-L	416	PHE	C-N-CA	8.50	128.15	119.56
8	6-L	416	PHE	CA-C-N	8.50	128.15	119.56
8	6-L	416	PHE	C-N-CA	8.50	128.15	119.56
8	7-L	416	PHE	CA-C-N	8.50	128.15	119.56
8	7-L	416	PHE	C-N-CA	8.50	128.15	119.56
8	8-L	416	PHE	CA-C-N	8.50	128.15	119.56
8	8-L	416	PHE	C-N-CA	8.50	128.15	119.56
8	9-L	416	PHE	CA-C-N	8.50	128.15	119.56
8	9-L	416	PHE	C-N-CA	8.50	128.15	119.56
8	10-L	416	PHE	CA-C-N	8.50	128.15	119.56
8	10-L	416	PHE	C-N-CA	8.50	128.15	119.56
9	1-M	202	LEU	CA-C-N	8.24	127.90	119.82
9	1-M	202	LEU	C-N-CA	8.24	127.90	119.82
9	2-M	202	LEU	CA-C-N	8.24	127.90	119.82
9	2-M	202	LEU	C-N-CA	8.24	127.90	119.82
9	3-M	202	LEU	CA-C-N	8.24	127.90	119.82
9	3-M	202	LEU	C-N-CA	8.24	127.90	119.82
9	4-M	202	LEU	CA-C-N	8.24	127.90	119.82
9	4-M	202	LEU	C-N-CA	8.24	127.90	119.82
9	5-M	202	LEU	CA-C-N	8.24	127.90	119.82
9	5-M	202	LEU	C-N-CA	8.24	127.90	119.82
9	6-M	202	LEU	CA-C-N	8.24	127.90	119.82
9	6-M	202	LEU	C-N-CA	8.24	127.90	119.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	7-M	202	LEU	CA-C-N	8.24	127.90	119.82
9	7-M	202	LEU	C-N-CA	8.24	127.90	119.82
9	8-M	202	LEU	CA-C-N	8.24	127.90	119.82
9	8-M	202	LEU	C-N-CA	8.24	127.90	119.82
9	9-M	202	LEU	CA-C-N	8.24	127.90	119.82
9	9-M	202	LEU	C-N-CA	8.24	127.90	119.82
9	10-M	202	LEU	CA-C-N	8.24	127.90	119.82
9	10-M	202	LEU	C-N-CA	8.24	127.90	119.82
9	1-M	66	LYS	CA-C-N	7.89	128.63	119.47
9	1-M	66	LYS	C-N-CA	7.89	128.63	119.47
9	2-M	66	LYS	CA-C-N	7.89	128.63	119.47
9	2-M	66	LYS	C-N-CA	7.89	128.63	119.47
9	3-M	66	LYS	CA-C-N	7.89	128.63	119.47
9	3-M	66	LYS	C-N-CA	7.89	128.63	119.47
9	4-M	66	LYS	CA-C-N	7.89	128.63	119.47
9	4-M	66	LYS	C-N-CA	7.89	128.63	119.47
9	5-M	66	LYS	CA-C-N	7.89	128.63	119.47
9	5-M	66	LYS	C-N-CA	7.89	128.63	119.47
9	6-M	66	LYS	CA-C-N	7.89	128.63	119.47
9	6-M	66	LYS	C-N-CA	7.89	128.63	119.47
9	7-M	66	LYS	CA-C-N	7.89	128.63	119.47
9	7-M	66	LYS	C-N-CA	7.89	128.63	119.47
9	8-M	66	LYS	CA-C-N	7.89	128.63	119.47
9	8-M	66	LYS	C-N-CA	7.89	128.63	119.47
9	9-M	66	LYS	CA-C-N	7.89	128.63	119.47
9	9-M	66	LYS	C-N-CA	7.89	128.63	119.47
9	10-M	66	LYS	CA-C-N	7.89	128.63	119.47
9	10-M	66	LYS	C-N-CA	7.89	128.63	119.47
7	1-K	777	ASN	CA-C-N	7.82	128.54	119.47
7	1-K	777	ASN	C-N-CA	7.82	128.54	119.47
7	2-K	777	ASN	CA-C-N	7.82	128.54	119.47
7	2-K	777	ASN	C-N-CA	7.82	128.54	119.47
7	3-K	777	ASN	CA-C-N	7.82	128.54	119.47
7	3-K	777	ASN	C-N-CA	7.82	128.54	119.47
7	4-K	777	ASN	CA-C-N	7.82	128.54	119.47
7	4-K	777	ASN	C-N-CA	7.82	128.54	119.47
7	5-K	777	ASN	CA-C-N	7.82	128.54	119.47
7	5-K	777	ASN	C-N-CA	7.82	128.54	119.47
7	6-K	777	ASN	CA-C-N	7.82	128.54	119.47
7	6-K	777	ASN	C-N-CA	7.82	128.54	119.47
7	7-K	777	ASN	CA-C-N	7.82	128.54	119.47
7	7-K	777	ASN	C-N-CA	7.82	128.54	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	8-K	777	ASN	CA-C-N	7.82	128.54	119.47
7	8-K	777	ASN	C-N-CA	7.82	128.54	119.47
7	9-K	777	ASN	CA-C-N	7.82	128.54	119.47
7	9-K	777	ASN	C-N-CA	7.82	128.54	119.47
7	10-K	777	ASN	CA-C-N	7.82	128.54	119.47
7	10-K	777	ASN	C-N-CA	7.82	128.54	119.47
1	1-A	38	LYS	CA-C-N	7.79	127.74	120.03
1	1-A	38	LYS	C-N-CA	7.79	127.74	120.03
1	2-A	38	LYS	CA-C-N	7.79	127.74	120.03
1	2-A	38	LYS	C-N-CA	7.79	127.74	120.03
1	3-A	38	LYS	CA-C-N	7.79	127.74	120.03
1	3-A	38	LYS	C-N-CA	7.79	127.74	120.03
1	4-A	38	LYS	CA-C-N	7.79	127.74	120.03
1	4-A	38	LYS	C-N-CA	7.79	127.74	120.03
1	5-A	38	LYS	CA-C-N	7.79	127.74	120.03
1	5-A	38	LYS	C-N-CA	7.79	127.74	120.03
1	6-A	38	LYS	CA-C-N	7.79	127.74	120.03
1	6-A	38	LYS	C-N-CA	7.79	127.74	120.03
1	7-A	38	LYS	CA-C-N	7.79	127.74	120.03
1	7-A	38	LYS	C-N-CA	7.79	127.74	120.03
1	8-A	38	LYS	CA-C-N	7.79	127.74	120.03
1	8-A	38	LYS	C-N-CA	7.79	127.74	120.03
1	9-A	38	LYS	CA-C-N	7.79	127.74	120.03
1	9-A	38	LYS	C-N-CA	7.79	127.74	120.03
1	10-A	38	LYS	CA-C-N	7.79	127.74	120.03
1	10-A	38	LYS	C-N-CA	7.79	127.74	120.03
8	1-L	102	LEU	CA-C-N	7.72	127.65	119.85
8	1-L	102	LEU	C-N-CA	7.72	127.65	119.85
8	2-L	102	LEU	CA-C-N	7.72	127.65	119.85
8	2-L	102	LEU	C-N-CA	7.72	127.65	119.85
8	3-L	102	LEU	CA-C-N	7.72	127.65	119.85
8	3-L	102	LEU	C-N-CA	7.72	127.65	119.85
8	4-L	102	LEU	CA-C-N	7.72	127.65	119.85
8	4-L	102	LEU	C-N-CA	7.72	127.65	119.85
8	5-L	102	LEU	CA-C-N	7.72	127.65	119.85
8	5-L	102	LEU	C-N-CA	7.72	127.65	119.85
8	6-L	102	LEU	CA-C-N	7.72	127.65	119.85
8	6-L	102	LEU	C-N-CA	7.72	127.65	119.85
8	7-L	102	LEU	CA-C-N	7.72	127.65	119.85
8	7-L	102	LEU	C-N-CA	7.72	127.65	119.85
8	8-L	102	LEU	CA-C-N	7.72	127.65	119.85
8	8-L	102	LEU	C-N-CA	7.72	127.65	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	9-L	102	LEU	CA-C-N	7.72	127.65	119.85
8	9-L	102	LEU	C-N-CA	7.72	127.65	119.85
8	10-L	102	LEU	CA-C-N	7.72	127.65	119.85
8	10-L	102	LEU	C-N-CA	7.72	127.65	119.85
9	1-M	458	GLY	CA-C-N	7.71	128.41	119.47
9	1-M	458	GLY	C-N-CA	7.71	128.41	119.47
9	2-M	458	GLY	CA-C-N	7.71	128.41	119.47
9	2-M	458	GLY	C-N-CA	7.71	128.41	119.47
9	3-M	458	GLY	CA-C-N	7.71	128.41	119.47
9	3-M	458	GLY	C-N-CA	7.71	128.41	119.47
9	4-M	458	GLY	CA-C-N	7.71	128.41	119.47
9	4-M	458	GLY	C-N-CA	7.71	128.41	119.47
9	5-M	458	GLY	CA-C-N	7.71	128.41	119.47
9	5-M	458	GLY	C-N-CA	7.71	128.41	119.47
9	6-M	458	GLY	CA-C-N	7.71	128.41	119.47
9	6-M	458	GLY	C-N-CA	7.71	128.41	119.47
9	7-M	458	GLY	CA-C-N	7.71	128.41	119.47
9	7-M	458	GLY	C-N-CA	7.71	128.41	119.47
9	8-M	458	GLY	CA-C-N	7.71	128.41	119.47
9	8-M	458	GLY	C-N-CA	7.71	128.41	119.47
9	9-M	458	GLY	CA-C-N	7.71	128.41	119.47
9	9-M	458	GLY	C-N-CA	7.71	128.41	119.47
9	10-M	458	GLY	CA-C-N	7.71	128.41	119.47
9	10-M	458	GLY	C-N-CA	7.71	128.41	119.47
9	1-M	216	SER	CA-C-N	7.68	127.86	119.87
9	1-M	216	SER	C-N-CA	7.68	127.86	119.87
9	2-M	216	SER	CA-C-N	7.68	127.86	119.87
9	2-M	216	SER	C-N-CA	7.68	127.86	119.87
9	3-M	216	SER	CA-C-N	7.68	127.86	119.87
9	3-M	216	SER	C-N-CA	7.68	127.86	119.87
9	4-M	216	SER	CA-C-N	7.68	127.86	119.87
9	4-M	216	SER	C-N-CA	7.68	127.86	119.87
9	5-M	216	SER	CA-C-N	7.68	127.86	119.87
9	5-M	216	SER	C-N-CA	7.68	127.86	119.87
9	6-M	216	SER	CA-C-N	7.68	127.86	119.87
9	6-M	216	SER	C-N-CA	7.68	127.86	119.87
9	7-M	216	SER	CA-C-N	7.68	127.86	119.87
9	7-M	216	SER	C-N-CA	7.68	127.86	119.87
9	8-M	216	SER	CA-C-N	7.68	127.86	119.87
9	8-M	216	SER	C-N-CA	7.68	127.86	119.87
9	9-M	216	SER	CA-C-N	7.68	127.86	119.87
9	9-M	216	SER	C-N-CA	7.68	127.86	119.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	10-M	216	SER	CA-C-N	7.68	127.86	119.87
9	10-M	216	SER	C-N-CA	7.68	127.86	119.87
8	1-L	98	SER	CA-C-N	7.65	127.36	119.56
8	1-L	98	SER	C-N-CA	7.65	127.36	119.56
8	2-L	98	SER	CA-C-N	7.65	127.36	119.56
8	2-L	98	SER	C-N-CA	7.65	127.36	119.56
8	3-L	98	SER	CA-C-N	7.65	127.36	119.56
8	3-L	98	SER	C-N-CA	7.65	127.36	119.56
8	4-L	98	SER	CA-C-N	7.65	127.36	119.56
8	4-L	98	SER	C-N-CA	7.65	127.36	119.56
8	5-L	98	SER	CA-C-N	7.65	127.36	119.56
8	5-L	98	SER	C-N-CA	7.65	127.36	119.56
8	6-L	98	SER	CA-C-N	7.65	127.36	119.56
8	6-L	98	SER	C-N-CA	7.65	127.36	119.56
8	7-L	98	SER	CA-C-N	7.65	127.36	119.56
8	7-L	98	SER	C-N-CA	7.65	127.36	119.56
8	8-L	98	SER	CA-C-N	7.65	127.36	119.56
8	8-L	98	SER	C-N-CA	7.65	127.36	119.56
8	9-L	98	SER	CA-C-N	7.65	127.36	119.56
8	9-L	98	SER	C-N-CA	7.65	127.36	119.56
8	10-L	98	SER	CA-C-N	7.65	127.36	119.56
8	10-L	98	SER	C-N-CA	7.65	127.36	119.56
10	1-N	31	GLN	CA-C-N	7.61	127.61	119.78
10	1-N	31	GLN	C-N-CA	7.61	127.61	119.78
10	2-N	31	GLN	CA-C-N	7.61	127.61	119.78
10	2-N	31	GLN	C-N-CA	7.61	127.61	119.78
10	3-N	31	GLN	CA-C-N	7.61	127.61	119.78
10	3-N	31	GLN	C-N-CA	7.61	127.61	119.78
10	4-N	31	GLN	CA-C-N	7.61	127.61	119.78
10	4-N	31	GLN	C-N-CA	7.61	127.61	119.78
10	5-N	31	GLN	CA-C-N	7.61	127.61	119.78
10	5-N	31	GLN	C-N-CA	7.61	127.61	119.78
10	6-N	31	GLN	CA-C-N	7.61	127.61	119.78
10	6-N	31	GLN	C-N-CA	7.61	127.61	119.78
10	7-N	31	GLN	CA-C-N	7.61	127.61	119.78
10	7-N	31	GLN	C-N-CA	7.61	127.61	119.78
10	8-N	31	GLN	CA-C-N	7.61	127.61	119.78
10	8-N	31	GLN	C-N-CA	7.61	127.61	119.78
10	9-N	31	GLN	CA-C-N	7.61	127.61	119.78
10	9-N	31	GLN	C-N-CA	7.61	127.61	119.78
10	10-N	31	GLN	CA-C-N	7.61	127.61	119.78
10	10-N	31	GLN	C-N-CA	7.61	127.61	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	1-C	117	LEU	CA-C-N	7.55	127.47	119.85
3	1-C	117	LEU	C-N-CA	7.55	127.47	119.85
3	2-C	117	LEU	CA-C-N	7.55	127.47	119.85
3	2-C	117	LEU	C-N-CA	7.55	127.47	119.85
3	3-C	117	LEU	CA-C-N	7.55	127.47	119.85
3	3-C	117	LEU	C-N-CA	7.55	127.47	119.85
3	4-C	117	LEU	CA-C-N	7.55	127.47	119.85
3	4-C	117	LEU	C-N-CA	7.55	127.47	119.85
3	5-C	117	LEU	CA-C-N	7.55	127.47	119.85
3	5-C	117	LEU	C-N-CA	7.55	127.47	119.85
3	6-C	117	LEU	CA-C-N	7.55	127.47	119.85
3	6-C	117	LEU	C-N-CA	7.55	127.47	119.85
3	7-C	117	LEU	CA-C-N	7.55	127.47	119.85
3	7-C	117	LEU	C-N-CA	7.55	127.47	119.85
3	8-C	117	LEU	CA-C-N	7.55	127.47	119.85
3	8-C	117	LEU	C-N-CA	7.55	127.47	119.85
3	9-C	117	LEU	CA-C-N	7.55	127.47	119.85
3	9-C	117	LEU	C-N-CA	7.55	127.47	119.85
3	10-C	117	LEU	CA-C-N	7.55	127.47	119.85
3	10-C	117	LEU	C-N-CA	7.55	127.47	119.85
8	1-L	380	SER	CA-C-N	7.51	129.23	119.84
8	1-L	380	SER	C-N-CA	7.51	129.23	119.84
8	2-L	380	SER	CA-C-N	7.51	129.23	119.84
8	2-L	380	SER	C-N-CA	7.51	129.23	119.84
8	3-L	380	SER	CA-C-N	7.51	129.23	119.84
8	3-L	380	SER	C-N-CA	7.51	129.23	119.84
8	4-L	380	SER	CA-C-N	7.51	129.23	119.84
8	4-L	380	SER	C-N-CA	7.51	129.23	119.84
8	5-L	380	SER	CA-C-N	7.51	129.23	119.84
8	5-L	380	SER	C-N-CA	7.51	129.23	119.84
8	6-L	380	SER	CA-C-N	7.51	129.23	119.84
8	6-L	380	SER	C-N-CA	7.51	129.23	119.84
8	7-L	380	SER	CA-C-N	7.51	129.23	119.84
8	7-L	380	SER	C-N-CA	7.51	129.23	119.84
8	8-L	380	SER	CA-C-N	7.51	129.23	119.84
8	8-L	380	SER	C-N-CA	7.51	129.23	119.84
8	9-L	380	SER	CA-C-N	7.51	129.23	119.84
8	9-L	380	SER	C-N-CA	7.51	129.23	119.84
8	10-L	380	SER	CA-C-N	7.51	129.23	119.84
8	10-L	380	SER	C-N-CA	7.51	129.23	119.84
9	1-M	395	VAL	CA-C-N	7.47	127.46	119.76
9	1-M	395	VAL	C-N-CA	7.47	127.46	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	2-M	395	VAL	CA-C-N	7.47	127.46	119.76
9	2-M	395	VAL	C-N-CA	7.47	127.46	119.76
9	3-M	395	VAL	CA-C-N	7.47	127.46	119.76
9	3-M	395	VAL	C-N-CA	7.47	127.46	119.76
9	4-M	395	VAL	CA-C-N	7.47	127.46	119.76
9	4-M	395	VAL	C-N-CA	7.47	127.46	119.76
9	5-M	395	VAL	CA-C-N	7.47	127.46	119.76
9	5-M	395	VAL	C-N-CA	7.47	127.46	119.76
9	6-M	395	VAL	CA-C-N	7.47	127.46	119.76
9	6-M	395	VAL	C-N-CA	7.47	127.46	119.76
9	7-M	395	VAL	CA-C-N	7.47	127.46	119.76
9	7-M	395	VAL	C-N-CA	7.47	127.46	119.76
9	8-M	395	VAL	CA-C-N	7.47	127.46	119.76
9	8-M	395	VAL	C-N-CA	7.47	127.46	119.76
9	9-M	395	VAL	CA-C-N	7.47	127.46	119.76
9	9-M	395	VAL	C-N-CA	7.47	127.46	119.76
9	10-M	395	VAL	CA-C-N	7.47	127.46	119.76
9	10-M	395	VAL	C-N-CA	7.47	127.46	119.76
7	1-K	342	TRP	N-CA-C	7.41	121.74	111.74
7	2-K	342	TRP	N-CA-C	7.41	121.74	111.74
7	3-K	342	TRP	N-CA-C	7.41	121.74	111.74
7	4-K	342	TRP	N-CA-C	7.41	121.74	111.74
7	5-K	342	TRP	N-CA-C	7.41	121.74	111.74
7	6-K	342	TRP	N-CA-C	7.41	121.74	111.74
7	7-K	342	TRP	N-CA-C	7.41	121.74	111.74
7	8-K	342	TRP	N-CA-C	7.41	121.74	111.74
7	9-K	342	TRP	N-CA-C	7.41	121.74	111.74
7	10-K	342	TRP	N-CA-C	7.41	121.74	111.74
8	1-L	315	LYS	CA-C-N	7.35	126.98	119.56
8	1-L	315	LYS	C-N-CA	7.35	126.98	119.56
8	2-L	315	LYS	CA-C-N	7.35	126.98	119.56
8	2-L	315	LYS	C-N-CA	7.35	126.98	119.56
8	3-L	315	LYS	CA-C-N	7.35	126.98	119.56
8	3-L	315	LYS	C-N-CA	7.35	126.98	119.56
8	4-L	315	LYS	CA-C-N	7.35	126.98	119.56
8	4-L	315	LYS	C-N-CA	7.35	126.98	119.56
8	5-L	315	LYS	CA-C-N	7.35	126.98	119.56
8	5-L	315	LYS	C-N-CA	7.35	126.98	119.56
8	6-L	315	LYS	CA-C-N	7.35	126.98	119.56
8	6-L	315	LYS	C-N-CA	7.35	126.98	119.56
8	7-L	315	LYS	CA-C-N	7.35	126.98	119.56
8	7-L	315	LYS	C-N-CA	7.35	126.98	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	8-L	315	LYS	CA-C-N	7.35	126.98	119.56
8	8-L	315	LYS	C-N-CA	7.35	126.98	119.56
8	9-L	315	LYS	CA-C-N	7.35	126.98	119.56
8	9-L	315	LYS	C-N-CA	7.35	126.98	119.56
8	10-L	315	LYS	CA-C-N	7.35	126.98	119.56
8	10-L	315	LYS	C-N-CA	7.35	126.98	119.56
3	1-G	80	ILE	CA-C-N	7.23	127.56	119.32
3	1-G	80	ILE	C-N-CA	7.23	127.56	119.32
3	2-G	80	ILE	CA-C-N	7.23	127.56	119.32
3	2-G	80	ILE	C-N-CA	7.23	127.56	119.32
3	3-G	80	ILE	CA-C-N	7.23	127.56	119.32
3	3-G	80	ILE	C-N-CA	7.23	127.56	119.32
3	4-G	80	ILE	CA-C-N	7.23	127.56	119.32
3	4-G	80	ILE	C-N-CA	7.23	127.56	119.32
3	5-G	80	ILE	CA-C-N	7.23	127.56	119.32
3	5-G	80	ILE	C-N-CA	7.23	127.56	119.32
3	6-G	80	ILE	CA-C-N	7.23	127.56	119.32
3	6-G	80	ILE	C-N-CA	7.23	127.56	119.32
3	7-G	80	ILE	CA-C-N	7.23	127.56	119.32
3	7-G	80	ILE	C-N-CA	7.23	127.56	119.32
3	8-G	80	ILE	CA-C-N	7.23	127.56	119.32
3	8-G	80	ILE	C-N-CA	7.23	127.56	119.32
3	9-G	80	ILE	CA-C-N	7.23	127.56	119.32
3	9-G	80	ILE	C-N-CA	7.23	127.56	119.32
3	10-G	80	ILE	CA-C-N	7.23	127.56	119.32
3	10-G	80	ILE	C-N-CA	7.23	127.56	119.32
8	1-L	282	ASN	CA-C-N	7.23	127.39	119.87
8	1-L	282	ASN	C-N-CA	7.23	127.39	119.87
8	2-L	282	ASN	CA-C-N	7.23	127.39	119.87
8	2-L	282	ASN	C-N-CA	7.23	127.39	119.87
8	3-L	282	ASN	CA-C-N	7.23	127.39	119.87
8	3-L	282	ASN	C-N-CA	7.23	127.39	119.87
8	4-L	282	ASN	CA-C-N	7.23	127.39	119.87
8	4-L	282	ASN	C-N-CA	7.23	127.39	119.87
8	5-L	282	ASN	CA-C-N	7.23	127.39	119.87
8	5-L	282	ASN	C-N-CA	7.23	127.39	119.87
8	6-L	282	ASN	CA-C-N	7.23	127.39	119.87
8	6-L	282	ASN	C-N-CA	7.23	127.39	119.87
8	7-L	282	ASN	CA-C-N	7.23	127.39	119.87
8	7-L	282	ASN	C-N-CA	7.23	127.39	119.87
8	8-L	282	ASN	CA-C-N	7.23	127.39	119.87
8	8-L	282	ASN	C-N-CA	7.23	127.39	119.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	9-L	282	ASN	CA-C-N	7.23	127.39	119.87
8	9-L	282	ASN	C-N-CA	7.23	127.39	119.87
8	10-L	282	ASN	CA-C-N	7.23	127.39	119.87
8	10-L	282	ASN	C-N-CA	7.23	127.39	119.87
3	1-C	80	ILE	CA-C-N	7.10	127.42	119.32
3	1-C	80	ILE	C-N-CA	7.10	127.42	119.32
3	2-C	80	ILE	CA-C-N	7.10	127.42	119.32
3	2-C	80	ILE	C-N-CA	7.10	127.42	119.32
3	3-C	80	ILE	CA-C-N	7.10	127.42	119.32
3	3-C	80	ILE	C-N-CA	7.10	127.42	119.32
3	4-C	80	ILE	CA-C-N	7.10	127.42	119.32
3	4-C	80	ILE	C-N-CA	7.10	127.42	119.32
3	5-C	80	ILE	CA-C-N	7.10	127.42	119.32
3	5-C	80	ILE	C-N-CA	7.10	127.42	119.32
3	6-C	80	ILE	CA-C-N	7.10	127.42	119.32
3	6-C	80	ILE	C-N-CA	7.10	127.42	119.32
3	7-C	80	ILE	CA-C-N	7.10	127.42	119.32
3	7-C	80	ILE	C-N-CA	7.10	127.42	119.32
3	8-C	80	ILE	CA-C-N	7.10	127.42	119.32
3	8-C	80	ILE	C-N-CA	7.10	127.42	119.32
3	9-C	80	ILE	CA-C-N	7.10	127.42	119.32
3	9-C	80	ILE	C-N-CA	7.10	127.42	119.32
3	10-C	80	ILE	CA-C-N	7.10	127.42	119.32
3	10-C	80	ILE	C-N-CA	7.10	127.42	119.32
9	1-M	416	PHE	CA-C-N	6.97	128.55	119.84
9	1-M	416	PHE	C-N-CA	6.97	128.55	119.84
9	2-M	416	PHE	CA-C-N	6.97	128.55	119.84
9	2-M	416	PHE	C-N-CA	6.97	128.55	119.84
9	3-M	416	PHE	CA-C-N	6.97	128.55	119.84
9	3-M	416	PHE	C-N-CA	6.97	128.55	119.84
9	4-M	416	PHE	CA-C-N	6.97	128.55	119.84
9	4-M	416	PHE	C-N-CA	6.97	128.55	119.84
9	5-M	416	PHE	CA-C-N	6.97	128.55	119.84
9	5-M	416	PHE	C-N-CA	6.97	128.55	119.84
9	6-M	416	PHE	CA-C-N	6.97	128.55	119.84
9	6-M	416	PHE	C-N-CA	6.97	128.55	119.84
9	7-M	416	PHE	CA-C-N	6.97	128.55	119.84
9	7-M	416	PHE	C-N-CA	6.97	128.55	119.84
9	8-M	416	PHE	CA-C-N	6.97	128.55	119.84
9	8-M	416	PHE	C-N-CA	6.97	128.55	119.84
9	9-M	416	PHE	CA-C-N	6.97	128.55	119.84
9	9-M	416	PHE	C-N-CA	6.97	128.55	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	10-M	416	PHE	CA-C-N	6.97	128.55	119.84
9	10-M	416	PHE	C-N-CA	6.97	128.55	119.84
7	1-K	553	THR	CA-C-N	6.88	126.50	119.56
7	1-K	553	THR	C-N-CA	6.88	126.50	119.56
7	2-K	553	THR	CA-C-N	6.88	126.50	119.56
7	2-K	553	THR	C-N-CA	6.88	126.50	119.56
7	3-K	553	THR	CA-C-N	6.88	126.50	119.56
7	3-K	553	THR	C-N-CA	6.88	126.50	119.56
7	4-K	553	THR	CA-C-N	6.88	126.50	119.56
7	4-K	553	THR	C-N-CA	6.88	126.50	119.56
7	5-K	553	THR	CA-C-N	6.88	126.50	119.56
7	5-K	553	THR	C-N-CA	6.88	126.50	119.56
7	6-K	553	THR	CA-C-N	6.88	126.50	119.56
7	6-K	553	THR	C-N-CA	6.88	126.50	119.56
7	7-K	553	THR	CA-C-N	6.88	126.50	119.56
7	7-K	553	THR	C-N-CA	6.88	126.50	119.56
7	8-K	553	THR	CA-C-N	6.88	126.50	119.56
7	8-K	553	THR	C-N-CA	6.88	126.50	119.56
7	9-K	553	THR	CA-C-N	6.88	126.50	119.56
7	9-K	553	THR	C-N-CA	6.88	126.50	119.56
7	10-K	553	THR	CA-C-N	6.88	126.50	119.56
7	10-K	553	THR	C-N-CA	6.88	126.50	119.56
1	1-E	121	MET	CA-C-N	6.82	127.10	119.32
1	1-E	121	MET	C-N-CA	6.82	127.10	119.32
1	2-E	121	MET	CA-C-N	6.82	127.10	119.32
1	2-E	121	MET	C-N-CA	6.82	127.10	119.32
1	3-E	121	MET	CA-C-N	6.82	127.10	119.32
1	3-E	121	MET	C-N-CA	6.82	127.10	119.32
1	4-E	121	MET	CA-C-N	6.82	127.10	119.32
1	4-E	121	MET	C-N-CA	6.82	127.10	119.32
1	5-E	121	MET	CA-C-N	6.82	127.10	119.32
1	5-E	121	MET	C-N-CA	6.82	127.10	119.32
1	6-E	121	MET	CA-C-N	6.82	127.10	119.32
1	6-E	121	MET	C-N-CA	6.82	127.10	119.32
1	7-E	121	MET	CA-C-N	6.82	127.10	119.32
1	7-E	121	MET	C-N-CA	6.82	127.10	119.32
1	8-E	121	MET	CA-C-N	6.82	127.10	119.32
1	8-E	121	MET	C-N-CA	6.82	127.10	119.32
1	9-E	121	MET	CA-C-N	6.82	127.10	119.32
1	9-E	121	MET	C-N-CA	6.82	127.10	119.32
1	10-E	121	MET	CA-C-N	6.82	127.10	119.32
1	10-E	121	MET	C-N-CA	6.82	127.10	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	1-L	108	MET	CA-C-N	6.81	126.78	120.03
8	1-L	108	MET	C-N-CA	6.81	126.78	120.03
8	2-L	108	MET	CA-C-N	6.81	126.78	120.03
8	2-L	108	MET	C-N-CA	6.81	126.78	120.03
8	3-L	108	MET	CA-C-N	6.81	126.78	120.03
8	3-L	108	MET	C-N-CA	6.81	126.78	120.03
8	4-L	108	MET	CA-C-N	6.81	126.78	120.03
8	4-L	108	MET	C-N-CA	6.81	126.78	120.03
8	5-L	108	MET	CA-C-N	6.81	126.78	120.03
8	5-L	108	MET	C-N-CA	6.81	126.78	120.03
8	6-L	108	MET	CA-C-N	6.81	126.78	120.03
8	6-L	108	MET	C-N-CA	6.81	126.78	120.03
8	7-L	108	MET	CA-C-N	6.81	126.78	120.03
8	7-L	108	MET	C-N-CA	6.81	126.78	120.03
8	8-L	108	MET	CA-C-N	6.81	126.78	120.03
8	8-L	108	MET	C-N-CA	6.81	126.78	120.03
8	9-L	108	MET	CA-C-N	6.81	126.78	120.03
8	9-L	108	MET	C-N-CA	6.81	126.78	120.03
8	10-L	108	MET	CA-C-N	6.81	126.78	120.03
8	10-L	108	MET	C-N-CA	6.81	126.78	120.03
1	1-A	121	MET	CA-C-N	6.80	127.36	119.47
1	1-A	121	MET	C-N-CA	6.80	127.36	119.47
1	2-A	121	MET	CA-C-N	6.80	127.36	119.47
1	2-A	121	MET	C-N-CA	6.80	127.36	119.47
1	3-A	121	MET	CA-C-N	6.80	127.36	119.47
1	3-A	121	MET	C-N-CA	6.80	127.36	119.47
1	4-A	121	MET	CA-C-N	6.80	127.36	119.47
1	4-A	121	MET	C-N-CA	6.80	127.36	119.47
1	5-A	121	MET	CA-C-N	6.80	127.36	119.47
1	5-A	121	MET	C-N-CA	6.80	127.36	119.47
1	6-A	121	MET	CA-C-N	6.80	127.36	119.47
1	6-A	121	MET	C-N-CA	6.80	127.36	119.47
1	7-A	121	MET	CA-C-N	6.80	127.36	119.47
1	7-A	121	MET	C-N-CA	6.80	127.36	119.47
1	8-A	121	MET	CA-C-N	6.80	127.36	119.47
1	8-A	121	MET	C-N-CA	6.80	127.36	119.47
1	9-A	121	MET	CA-C-N	6.80	127.36	119.47
1	9-A	121	MET	C-N-CA	6.80	127.36	119.47
1	10-A	121	MET	CA-C-N	6.80	127.36	119.47
1	10-A	121	MET	C-N-CA	6.80	127.36	119.47
9	1-M	442	HIS	CA-C-N	6.75	126.38	119.56
9	1-M	442	HIS	C-N-CA	6.75	126.38	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	2-M	442	HIS	CA-C-N	6.75	126.38	119.56
9	2-M	442	HIS	C-N-CA	6.75	126.38	119.56
9	3-M	442	HIS	CA-C-N	6.75	126.38	119.56
9	3-M	442	HIS	C-N-CA	6.75	126.38	119.56
9	4-M	442	HIS	CA-C-N	6.75	126.38	119.56
9	4-M	442	HIS	C-N-CA	6.75	126.38	119.56
9	5-M	442	HIS	CA-C-N	6.75	126.38	119.56
9	5-M	442	HIS	C-N-CA	6.75	126.38	119.56
9	6-M	442	HIS	CA-C-N	6.75	126.38	119.56
9	6-M	442	HIS	C-N-CA	6.75	126.38	119.56
9	7-M	442	HIS	CA-C-N	6.75	126.38	119.56
9	7-M	442	HIS	C-N-CA	6.75	126.38	119.56
9	8-M	442	HIS	CA-C-N	6.75	126.38	119.56
9	8-M	442	HIS	C-N-CA	6.75	126.38	119.56
9	9-M	442	HIS	CA-C-N	6.75	126.38	119.56
9	9-M	442	HIS	C-N-CA	6.75	126.38	119.56
9	10-M	442	HIS	CA-C-N	6.75	126.38	119.56
9	10-M	442	HIS	C-N-CA	6.75	126.38	119.56
9	1-M	412	TYR	CA-C-N	6.72	126.48	119.76
9	1-M	412	TYR	C-N-CA	6.72	126.48	119.76
9	2-M	412	TYR	CA-C-N	6.72	126.48	119.76
9	2-M	412	TYR	C-N-CA	6.72	126.48	119.76
9	3-M	412	TYR	CA-C-N	6.72	126.48	119.76
9	3-M	412	TYR	C-N-CA	6.72	126.48	119.76
9	4-M	412	TYR	CA-C-N	6.72	126.48	119.76
9	4-M	412	TYR	C-N-CA	6.72	126.48	119.76
9	5-M	412	TYR	CA-C-N	6.72	126.48	119.76
9	5-M	412	TYR	C-N-CA	6.72	126.48	119.76
9	6-M	412	TYR	CA-C-N	6.72	126.48	119.76
9	6-M	412	TYR	C-N-CA	6.72	126.48	119.76
9	7-M	412	TYR	CA-C-N	6.72	126.48	119.76
9	7-M	412	TYR	C-N-CA	6.72	126.48	119.76
9	8-M	412	TYR	CA-C-N	6.72	126.48	119.76
9	8-M	412	TYR	C-N-CA	6.72	126.48	119.76
9	9-M	412	TYR	CA-C-N	6.72	126.48	119.76
9	9-M	412	TYR	C-N-CA	6.72	126.48	119.76
9	10-M	412	TYR	CA-C-N	6.72	126.48	119.76
9	10-M	412	TYR	C-N-CA	6.72	126.48	119.76
8	1-L	26	LEU	CA-C-N	6.68	126.60	119.85
8	1-L	26	LEU	C-N-CA	6.68	126.60	119.85
8	2-L	26	LEU	CA-C-N	6.68	126.60	119.85
8	2-L	26	LEU	C-N-CA	6.68	126.60	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	3-L	26	LEU	CA-C-N	6.68	126.60	119.85
8	3-L	26	LEU	C-N-CA	6.68	126.60	119.85
8	4-L	26	LEU	CA-C-N	6.68	126.60	119.85
8	4-L	26	LEU	C-N-CA	6.68	126.60	119.85
8	5-L	26	LEU	CA-C-N	6.68	126.60	119.85
8	5-L	26	LEU	C-N-CA	6.68	126.60	119.85
8	6-L	26	LEU	CA-C-N	6.68	126.60	119.85
8	6-L	26	LEU	C-N-CA	6.68	126.60	119.85
8	7-L	26	LEU	CA-C-N	6.68	126.60	119.85
8	7-L	26	LEU	C-N-CA	6.68	126.60	119.85
8	8-L	26	LEU	CA-C-N	6.68	126.60	119.85
8	8-L	26	LEU	C-N-CA	6.68	126.60	119.85
8	9-L	26	LEU	CA-C-N	6.68	126.60	119.85
8	9-L	26	LEU	C-N-CA	6.68	126.60	119.85
8	10-L	26	LEU	CA-C-N	6.68	126.60	119.85
8	10-L	26	LEU	C-N-CA	6.68	126.60	119.85
7	1-K	706	LEU	CA-C-N	6.66	126.91	119.32
7	1-K	706	LEU	C-N-CA	6.66	126.91	119.32
7	2-K	706	LEU	CA-C-N	6.66	126.91	119.32
7	2-K	706	LEU	C-N-CA	6.66	126.91	119.32
7	3-K	706	LEU	CA-C-N	6.66	126.91	119.32
7	3-K	706	LEU	C-N-CA	6.66	126.91	119.32
7	4-K	706	LEU	CA-C-N	6.66	126.91	119.32
7	4-K	706	LEU	C-N-CA	6.66	126.91	119.32
7	5-K	706	LEU	CA-C-N	6.66	126.91	119.32
7	5-K	706	LEU	C-N-CA	6.66	126.91	119.32
7	6-K	706	LEU	CA-C-N	6.66	126.91	119.32
7	6-K	706	LEU	C-N-CA	6.66	126.91	119.32
7	7-K	706	LEU	CA-C-N	6.66	126.91	119.32
7	7-K	706	LEU	C-N-CA	6.66	126.91	119.32
7	8-K	706	LEU	CA-C-N	6.66	126.91	119.32
7	8-K	706	LEU	C-N-CA	6.66	126.91	119.32
7	9-K	706	LEU	CA-C-N	6.66	126.91	119.32
7	9-K	706	LEU	C-N-CA	6.66	126.91	119.32
7	10-K	706	LEU	CA-C-N	6.66	126.91	119.32
7	10-K	706	LEU	C-N-CA	6.66	126.91	119.32
10	1-N	2	ASP	CA-C-N	6.48	126.41	119.28
10	1-N	2	ASP	C-N-CA	6.48	126.41	119.28
10	2-N	2	ASP	CA-C-N	6.48	126.41	119.28
10	2-N	2	ASP	C-N-CA	6.48	126.41	119.28
10	3-N	2	ASP	CA-C-N	6.48	126.41	119.28
10	3-N	2	ASP	C-N-CA	6.48	126.41	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	4-N	2	ASP	CA-C-N	6.48	126.41	119.28
10	4-N	2	ASP	C-N-CA	6.48	126.41	119.28
10	5-N	2	ASP	CA-C-N	6.48	126.41	119.28
10	5-N	2	ASP	C-N-CA	6.48	126.41	119.28
10	6-N	2	ASP	CA-C-N	6.48	126.41	119.28
10	6-N	2	ASP	C-N-CA	6.48	126.41	119.28
10	7-N	2	ASP	CA-C-N	6.48	126.41	119.28
10	7-N	2	ASP	C-N-CA	6.48	126.41	119.28
10	8-N	2	ASP	CA-C-N	6.48	126.41	119.28
10	8-N	2	ASP	C-N-CA	6.48	126.41	119.28
10	9-N	2	ASP	CA-C-N	6.48	126.41	119.28
10	9-N	2	ASP	C-N-CA	6.48	126.41	119.28
10	10-N	2	ASP	CA-C-N	6.48	126.41	119.28
10	10-N	2	ASP	C-N-CA	6.48	126.41	119.28
3	1-G	109	LEU	CA-C-N	6.48	126.83	119.83
3	1-G	109	LEU	C-N-CA	6.48	126.83	119.83
3	2-G	109	LEU	CA-C-N	6.48	126.83	119.83
3	2-G	109	LEU	C-N-CA	6.48	126.83	119.83
3	3-G	109	LEU	CA-C-N	6.48	126.83	119.83
3	3-G	109	LEU	C-N-CA	6.48	126.83	119.83
3	4-G	109	LEU	CA-C-N	6.48	126.83	119.83
3	4-G	109	LEU	C-N-CA	6.48	126.83	119.83
3	5-G	109	LEU	CA-C-N	6.48	126.83	119.83
3	5-G	109	LEU	C-N-CA	6.48	126.83	119.83
3	6-G	109	LEU	CA-C-N	6.48	126.83	119.83
3	6-G	109	LEU	C-N-CA	6.48	126.83	119.83
3	7-G	109	LEU	CA-C-N	6.48	126.83	119.83
3	7-G	109	LEU	C-N-CA	6.48	126.83	119.83
3	8-G	109	LEU	CA-C-N	6.48	126.83	119.83
3	8-G	109	LEU	C-N-CA	6.48	126.83	119.83
3	9-G	109	LEU	CA-C-N	6.48	126.83	119.83
3	9-G	109	LEU	C-N-CA	6.48	126.83	119.83
3	10-G	109	LEU	CA-C-N	6.48	126.83	119.83
3	10-G	109	LEU	C-N-CA	6.48	126.83	119.83
9	1-M	423	GLY	N-CA-C	-6.45	105.06	112.29
9	2-M	423	GLY	N-CA-C	-6.45	105.06	112.29
9	3-M	423	GLY	N-CA-C	-6.45	105.06	112.29
9	4-M	423	GLY	N-CA-C	-6.45	105.06	112.29
9	5-M	423	GLY	N-CA-C	-6.45	105.06	112.29
9	6-M	423	GLY	N-CA-C	-6.45	105.06	112.29
9	7-M	423	GLY	N-CA-C	-6.45	105.06	112.29
9	8-M	423	GLY	N-CA-C	-6.45	105.06	112.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	9-M	423	GLY	N-CA-C	-6.45	105.06	112.29
9	10-M	423	GLY	N-CA-C	-6.45	105.06	112.29
9	1-M	361	GLU	CA-C-N	6.43	127.88	119.84
9	1-M	361	GLU	C-N-CA	6.43	127.88	119.84
9	2-M	361	GLU	CA-C-N	6.43	127.88	119.84
9	2-M	361	GLU	C-N-CA	6.43	127.88	119.84
9	3-M	361	GLU	CA-C-N	6.43	127.88	119.84
9	3-M	361	GLU	C-N-CA	6.43	127.88	119.84
9	4-M	361	GLU	CA-C-N	6.43	127.88	119.84
9	4-M	361	GLU	C-N-CA	6.43	127.88	119.84
9	5-M	361	GLU	CA-C-N	6.43	127.88	119.84
9	5-M	361	GLU	C-N-CA	6.43	127.88	119.84
9	6-M	361	GLU	CA-C-N	6.43	127.88	119.84
9	6-M	361	GLU	C-N-CA	6.43	127.88	119.84
9	7-M	361	GLU	CA-C-N	6.43	127.88	119.84
9	7-M	361	GLU	C-N-CA	6.43	127.88	119.84
9	8-M	361	GLU	CA-C-N	6.43	127.88	119.84
9	8-M	361	GLU	C-N-CA	6.43	127.88	119.84
9	9-M	361	GLU	CA-C-N	6.43	127.88	119.84
9	9-M	361	GLU	C-N-CA	6.43	127.88	119.84
9	10-M	361	GLU	CA-C-N	6.43	127.88	119.84
9	10-M	361	GLU	C-N-CA	6.43	127.88	119.84
9	1-M	37	ILE	CA-C-N	6.42	126.76	119.83
9	1-M	37	ILE	C-N-CA	6.42	126.76	119.83
9	2-M	37	ILE	CA-C-N	6.42	126.76	119.83
9	2-M	37	ILE	C-N-CA	6.42	126.76	119.83
9	3-M	37	ILE	CA-C-N	6.42	126.76	119.83
9	3-M	37	ILE	C-N-CA	6.42	126.76	119.83
9	4-M	37	ILE	CA-C-N	6.42	126.76	119.83
9	4-M	37	ILE	C-N-CA	6.42	126.76	119.83
9	5-M	37	ILE	CA-C-N	6.42	126.76	119.83
9	5-M	37	ILE	C-N-CA	6.42	126.76	119.83
9	6-M	37	ILE	CA-C-N	6.42	126.76	119.83
9	6-M	37	ILE	C-N-CA	6.42	126.76	119.83
9	7-M	37	ILE	CA-C-N	6.42	126.76	119.83
9	7-M	37	ILE	C-N-CA	6.42	126.76	119.83
9	8-M	37	ILE	CA-C-N	6.42	126.76	119.83
9	8-M	37	ILE	C-N-CA	6.42	126.76	119.83
9	9-M	37	ILE	CA-C-N	6.42	126.76	119.83
9	9-M	37	ILE	C-N-CA	6.42	126.76	119.83
9	10-M	37	ILE	CA-C-N	6.42	126.76	119.83
9	10-M	37	ILE	C-N-CA	6.42	126.76	119.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	1-M	32	VAL	CA-C-N	6.39	127.82	119.84
9	1-M	32	VAL	C-N-CA	6.39	127.82	119.84
9	2-M	32	VAL	CA-C-N	6.39	127.82	119.84
9	2-M	32	VAL	C-N-CA	6.39	127.82	119.84
9	3-M	32	VAL	CA-C-N	6.39	127.82	119.84
9	3-M	32	VAL	C-N-CA	6.39	127.82	119.84
9	4-M	32	VAL	CA-C-N	6.39	127.82	119.84
9	4-M	32	VAL	C-N-CA	6.39	127.82	119.84
9	5-M	32	VAL	CA-C-N	6.39	127.82	119.84
9	5-M	32	VAL	C-N-CA	6.39	127.82	119.84
9	6-M	32	VAL	CA-C-N	6.39	127.82	119.84
9	6-M	32	VAL	C-N-CA	6.39	127.82	119.84
9	7-M	32	VAL	CA-C-N	6.39	127.82	119.84
9	7-M	32	VAL	C-N-CA	6.39	127.82	119.84
9	8-M	32	VAL	CA-C-N	6.39	127.82	119.84
9	8-M	32	VAL	C-N-CA	6.39	127.82	119.84
9	9-M	32	VAL	CA-C-N	6.39	127.82	119.84
9	9-M	32	VAL	C-N-CA	6.39	127.82	119.84
9	10-M	32	VAL	CA-C-N	6.39	127.82	119.84
9	10-M	32	VAL	C-N-CA	6.39	127.82	119.84
7	1-K	987	ARG	N-CA-C	-6.33	105.69	113.41
7	2-K	987	ARG	N-CA-C	-6.33	105.69	113.41
7	3-K	987	ARG	N-CA-C	-6.33	105.69	113.41
7	4-K	987	ARG	N-CA-C	-6.33	105.69	113.41
7	5-K	987	ARG	N-CA-C	-6.33	105.69	113.41
7	6-K	987	ARG	N-CA-C	-6.33	105.69	113.41
7	7-K	987	ARG	N-CA-C	-6.33	105.69	113.41
7	8-K	987	ARG	N-CA-C	-6.33	105.69	113.41
7	9-K	987	ARG	N-CA-C	-6.33	105.69	113.41
7	10-K	987	ARG	N-CA-C	-6.33	105.69	113.41
8	1-L	133	VAL	CA-C-N	6.29	126.20	119.28
8	1-L	133	VAL	C-N-CA	6.29	126.20	119.28
8	2-L	133	VAL	CA-C-N	6.29	126.20	119.28
8	2-L	133	VAL	C-N-CA	6.29	126.20	119.28
8	3-L	133	VAL	CA-C-N	6.29	126.20	119.28
8	3-L	133	VAL	C-N-CA	6.29	126.20	119.28
8	4-L	133	VAL	CA-C-N	6.29	126.20	119.28
8	4-L	133	VAL	C-N-CA	6.29	126.20	119.28
8	5-L	133	VAL	CA-C-N	6.29	126.20	119.28
8	5-L	133	VAL	C-N-CA	6.29	126.20	119.28
8	6-L	133	VAL	CA-C-N	6.29	126.20	119.28
8	6-L	133	VAL	C-N-CA	6.29	126.20	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	7-L	133	VAL	CA-C-N	6.29	126.20	119.28
8	7-L	133	VAL	C-N-CA	6.29	126.20	119.28
8	8-L	133	VAL	CA-C-N	6.29	126.20	119.28
8	8-L	133	VAL	C-N-CA	6.29	126.20	119.28
8	9-L	133	VAL	CA-C-N	6.29	126.20	119.28
8	9-L	133	VAL	C-N-CA	6.29	126.20	119.28
8	10-L	133	VAL	CA-C-N	6.29	126.20	119.28
8	10-L	133	VAL	C-N-CA	6.29	126.20	119.28
3	1-G	26	PHE	CA-C-N	6.25	127.65	119.84
3	1-G	26	PHE	C-N-CA	6.25	127.65	119.84
3	2-G	26	PHE	CA-C-N	6.25	127.65	119.84
3	2-G	26	PHE	C-N-CA	6.25	127.65	119.84
3	3-G	26	PHE	CA-C-N	6.25	127.65	119.84
3	3-G	26	PHE	C-N-CA	6.25	127.65	119.84
3	4-G	26	PHE	CA-C-N	6.25	127.65	119.84
3	4-G	26	PHE	C-N-CA	6.25	127.65	119.84
3	5-G	26	PHE	CA-C-N	6.25	127.65	119.84
3	5-G	26	PHE	C-N-CA	6.25	127.65	119.84
3	6-G	26	PHE	CA-C-N	6.25	127.65	119.84
3	6-G	26	PHE	C-N-CA	6.25	127.65	119.84
3	7-G	26	PHE	CA-C-N	6.25	127.65	119.84
3	7-G	26	PHE	C-N-CA	6.25	127.65	119.84
3	8-G	26	PHE	CA-C-N	6.25	127.65	119.84
3	8-G	26	PHE	C-N-CA	6.25	127.65	119.84
3	9-G	26	PHE	CA-C-N	6.25	127.65	119.84
3	9-G	26	PHE	C-N-CA	6.25	127.65	119.84
3	10-G	26	PHE	CA-C-N	6.25	127.65	119.84
3	10-G	26	PHE	C-N-CA	6.25	127.65	119.84
8	1-L	324	SER	CA-C-N	6.22	126.69	119.47
8	1-L	324	SER	C-N-CA	6.22	126.69	119.47
8	2-L	324	SER	CA-C-N	6.22	126.69	119.47
8	2-L	324	SER	C-N-CA	6.22	126.69	119.47
8	3-L	324	SER	CA-C-N	6.22	126.69	119.47
8	3-L	324	SER	C-N-CA	6.22	126.69	119.47
8	4-L	324	SER	CA-C-N	6.22	126.69	119.47
8	4-L	324	SER	C-N-CA	6.22	126.69	119.47
8	5-L	324	SER	CA-C-N	6.22	126.69	119.47
8	5-L	324	SER	C-N-CA	6.22	126.69	119.47
8	6-L	324	SER	CA-C-N	6.22	126.69	119.47
8	6-L	324	SER	C-N-CA	6.22	126.69	119.47
8	7-L	324	SER	CA-C-N	6.22	126.69	119.47
8	7-L	324	SER	C-N-CA	6.22	126.69	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	8-L	324	SER	CA-C-N	6.22	126.69	119.47
8	8-L	324	SER	C-N-CA	6.22	126.69	119.47
8	9-L	324	SER	CA-C-N	6.22	126.69	119.47
8	9-L	324	SER	C-N-CA	6.22	126.69	119.47
8	10-L	324	SER	CA-C-N	6.22	126.69	119.47
8	10-L	324	SER	C-N-CA	6.22	126.69	119.47
4	1-H	103	LEU	CA-C-N	6.22	126.73	120.14
4	1-H	103	LEU	C-N-CA	6.22	126.73	120.14
4	2-H	103	LEU	CA-C-N	6.22	126.73	120.14
4	2-H	103	LEU	C-N-CA	6.22	126.73	120.14
4	3-H	103	LEU	CA-C-N	6.22	126.73	120.14
4	3-H	103	LEU	C-N-CA	6.22	126.73	120.14
4	4-H	103	LEU	CA-C-N	6.22	126.73	120.14
4	4-H	103	LEU	C-N-CA	6.22	126.73	120.14
4	5-H	103	LEU	CA-C-N	6.22	126.73	120.14
4	5-H	103	LEU	C-N-CA	6.22	126.73	120.14
4	6-H	103	LEU	CA-C-N	6.22	126.73	120.14
4	6-H	103	LEU	C-N-CA	6.22	126.73	120.14
4	7-H	103	LEU	CA-C-N	6.22	126.73	120.14
4	7-H	103	LEU	C-N-CA	6.22	126.73	120.14
4	8-H	103	LEU	CA-C-N	6.22	126.73	120.14
4	8-H	103	LEU	C-N-CA	6.22	126.73	120.14
4	9-H	103	LEU	CA-C-N	6.22	126.73	120.14
4	9-H	103	LEU	C-N-CA	6.22	126.73	120.14
4	10-H	103	LEU	CA-C-N	6.22	126.73	120.14
4	10-H	103	LEU	C-N-CA	6.22	126.73	120.14
4	1-H	50	HIS	CA-C-N	6.22	127.61	119.84
4	1-H	50	HIS	C-N-CA	6.22	127.61	119.84
4	2-H	50	HIS	CA-C-N	6.22	127.61	119.84
4	2-H	50	HIS	C-N-CA	6.22	127.61	119.84
4	3-H	50	HIS	CA-C-N	6.22	127.61	119.84
4	3-H	50	HIS	C-N-CA	6.22	127.61	119.84
4	4-H	50	HIS	CA-C-N	6.22	127.61	119.84
4	4-H	50	HIS	C-N-CA	6.22	127.61	119.84
4	5-H	50	HIS	CA-C-N	6.22	127.61	119.84
4	5-H	50	HIS	C-N-CA	6.22	127.61	119.84
4	6-H	50	HIS	CA-C-N	6.22	127.61	119.84
4	6-H	50	HIS	C-N-CA	6.22	127.61	119.84
4	7-H	50	HIS	CA-C-N	6.22	127.61	119.84
4	7-H	50	HIS	C-N-CA	6.22	127.61	119.84
4	8-H	50	HIS	CA-C-N	6.22	127.61	119.84
4	8-H	50	HIS	C-N-CA	6.22	127.61	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	9-H	50	HIS	CA-C-N	6.22	127.61	119.84
4	9-H	50	HIS	C-N-CA	6.22	127.61	119.84
4	10-H	50	HIS	CA-C-N	6.22	127.61	119.84
4	10-H	50	HIS	C-N-CA	6.22	127.61	119.84
9	1-M	109	ILE	N-CA-C	6.21	114.25	107.60
9	2-M	109	ILE	N-CA-C	6.21	114.25	107.60
9	3-M	109	ILE	N-CA-C	6.21	114.25	107.60
9	4-M	109	ILE	N-CA-C	6.21	114.25	107.60
9	5-M	109	ILE	N-CA-C	6.21	114.25	107.60
9	6-M	109	ILE	N-CA-C	6.21	114.25	107.60
9	7-M	109	ILE	N-CA-C	6.21	114.25	107.60
9	8-M	109	ILE	N-CA-C	6.21	114.25	107.60
9	9-M	109	ILE	N-CA-C	6.21	114.25	107.60
9	10-M	109	ILE	N-CA-C	6.21	114.25	107.60
8	1-L	31	ILE	CA-C-N	6.19	126.14	119.76
8	1-L	31	ILE	C-N-CA	6.19	126.14	119.76
8	2-L	31	ILE	CA-C-N	6.19	126.14	119.76
8	2-L	31	ILE	C-N-CA	6.19	126.14	119.76
8	3-L	31	ILE	CA-C-N	6.19	126.14	119.76
8	3-L	31	ILE	C-N-CA	6.19	126.14	119.76
8	4-L	31	ILE	CA-C-N	6.19	126.14	119.76
8	4-L	31	ILE	C-N-CA	6.19	126.14	119.76
8	5-L	31	ILE	CA-C-N	6.19	126.14	119.76
8	5-L	31	ILE	C-N-CA	6.19	126.14	119.76
8	6-L	31	ILE	CA-C-N	6.19	126.14	119.76
8	6-L	31	ILE	C-N-CA	6.19	126.14	119.76
8	7-L	31	ILE	CA-C-N	6.19	126.14	119.76
8	7-L	31	ILE	C-N-CA	6.19	126.14	119.76
8	8-L	31	ILE	CA-C-N	6.19	126.14	119.76
8	8-L	31	ILE	C-N-CA	6.19	126.14	119.76
8	9-L	31	ILE	CA-C-N	6.19	126.14	119.76
8	9-L	31	ILE	C-N-CA	6.19	126.14	119.76
8	10-L	31	ILE	CA-C-N	6.19	126.14	119.76
8	10-L	31	ILE	C-N-CA	6.19	126.14	119.76
3	1-C	26	PHE	CA-C-N	6.15	127.53	119.84
3	1-C	26	PHE	C-N-CA	6.15	127.53	119.84
3	2-C	26	PHE	CA-C-N	6.15	127.53	119.84
3	2-C	26	PHE	C-N-CA	6.15	127.53	119.84
3	3-C	26	PHE	CA-C-N	6.15	127.53	119.84
3	3-C	26	PHE	C-N-CA	6.15	127.53	119.84
3	4-C	26	PHE	CA-C-N	6.15	127.53	119.84
3	4-C	26	PHE	C-N-CA	6.15	127.53	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	5-C	26	PHE	CA-C-N	6.15	127.53	119.84
3	5-C	26	PHE	C-N-CA	6.15	127.53	119.84
3	6-C	26	PHE	CA-C-N	6.15	127.53	119.84
3	6-C	26	PHE	C-N-CA	6.15	127.53	119.84
3	7-C	26	PHE	CA-C-N	6.15	127.53	119.84
3	7-C	26	PHE	C-N-CA	6.15	127.53	119.84
3	8-C	26	PHE	CA-C-N	6.15	127.53	119.84
3	8-C	26	PHE	C-N-CA	6.15	127.53	119.84
3	9-C	26	PHE	CA-C-N	6.15	127.53	119.84
3	9-C	26	PHE	C-N-CA	6.15	127.53	119.84
3	10-C	26	PHE	CA-C-N	6.15	127.53	119.84
3	10-C	26	PHE	C-N-CA	6.15	127.53	119.84
7	1-K	890	ASN	CA-C-N	6.14	127.51	119.84
7	1-K	890	ASN	C-N-CA	6.14	127.51	119.84
7	2-K	890	ASN	CA-C-N	6.14	127.51	119.84
7	2-K	890	ASN	C-N-CA	6.14	127.51	119.84
7	3-K	890	ASN	CA-C-N	6.14	127.51	119.84
7	3-K	890	ASN	C-N-CA	6.14	127.51	119.84
7	4-K	890	ASN	CA-C-N	6.14	127.51	119.84
7	4-K	890	ASN	C-N-CA	6.14	127.51	119.84
7	5-K	890	ASN	CA-C-N	6.14	127.51	119.84
7	5-K	890	ASN	C-N-CA	6.14	127.51	119.84
7	6-K	890	ASN	CA-C-N	6.14	127.51	119.84
7	6-K	890	ASN	C-N-CA	6.14	127.51	119.84
7	7-K	890	ASN	CA-C-N	6.14	127.51	119.84
7	7-K	890	ASN	C-N-CA	6.14	127.51	119.84
7	8-K	890	ASN	CA-C-N	6.14	127.51	119.84
7	8-K	890	ASN	C-N-CA	6.14	127.51	119.84
7	9-K	890	ASN	CA-C-N	6.14	127.51	119.84
7	9-K	890	ASN	C-N-CA	6.14	127.51	119.84
7	10-K	890	ASN	CA-C-N	6.14	127.51	119.84
7	10-K	890	ASN	C-N-CA	6.14	127.51	119.84
8	1-L	76	LEU	CA-C-N	6.12	126.06	119.76
8	1-L	76	LEU	C-N-CA	6.12	126.06	119.76
8	2-L	76	LEU	CA-C-N	6.12	126.06	119.76
8	2-L	76	LEU	C-N-CA	6.12	126.06	119.76
8	3-L	76	LEU	CA-C-N	6.12	126.06	119.76
8	3-L	76	LEU	C-N-CA	6.12	126.06	119.76
8	4-L	76	LEU	CA-C-N	6.12	126.06	119.76
8	4-L	76	LEU	C-N-CA	6.12	126.06	119.76
8	5-L	76	LEU	CA-C-N	6.12	126.06	119.76
8	5-L	76	LEU	C-N-CA	6.12	126.06	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	6-L	76	LEU	CA-C-N	6.12	126.06	119.76
8	6-L	76	LEU	C-N-CA	6.12	126.06	119.76
8	7-L	76	LEU	CA-C-N	6.12	126.06	119.76
8	7-L	76	LEU	C-N-CA	6.12	126.06	119.76
8	8-L	76	LEU	CA-C-N	6.12	126.06	119.76
8	8-L	76	LEU	C-N-CA	6.12	126.06	119.76
8	9-L	76	LEU	CA-C-N	6.12	126.06	119.76
8	9-L	76	LEU	C-N-CA	6.12	126.06	119.76
8	10-L	76	LEU	CA-C-N	6.12	126.06	119.76
8	10-L	76	LEU	C-N-CA	6.12	126.06	119.76
9	1-M	13	TYR	CA-C-N	6.09	126.28	120.31
9	1-M	13	TYR	C-N-CA	6.09	126.28	120.31
9	2-M	13	TYR	CA-C-N	6.09	126.28	120.31
9	2-M	13	TYR	C-N-CA	6.09	126.28	120.31
9	3-M	13	TYR	CA-C-N	6.09	126.28	120.31
9	3-M	13	TYR	C-N-CA	6.09	126.28	120.31
9	4-M	13	TYR	CA-C-N	6.09	126.28	120.31
9	4-M	13	TYR	C-N-CA	6.09	126.28	120.31
9	5-M	13	TYR	CA-C-N	6.09	126.28	120.31
9	5-M	13	TYR	C-N-CA	6.09	126.28	120.31
9	6-M	13	TYR	CA-C-N	6.09	126.28	120.31
9	6-M	13	TYR	C-N-CA	6.09	126.28	120.31
9	7-M	13	TYR	CA-C-N	6.09	126.28	120.31
9	7-M	13	TYR	C-N-CA	6.09	126.28	120.31
9	8-M	13	TYR	CA-C-N	6.09	126.28	120.31
9	8-M	13	TYR	C-N-CA	6.09	126.28	120.31
9	9-M	13	TYR	CA-C-N	6.09	126.28	120.31
9	9-M	13	TYR	C-N-CA	6.09	126.28	120.31
9	10-M	13	TYR	CA-C-N	6.09	126.28	120.31
9	10-M	13	TYR	C-N-CA	6.09	126.28	120.31
8	1-L	330	GLY	CA-C-N	5.98	125.53	119.19
8	1-L	330	GLY	C-N-CA	5.98	125.53	119.19
8	2-L	330	GLY	CA-C-N	5.98	125.53	119.19
8	2-L	330	GLY	C-N-CA	5.98	125.53	119.19
8	3-L	330	GLY	CA-C-N	5.98	125.53	119.19
8	3-L	330	GLY	C-N-CA	5.98	125.53	119.19
8	4-L	330	GLY	CA-C-N	5.98	125.53	119.19
8	4-L	330	GLY	C-N-CA	5.98	125.53	119.19
8	5-L	330	GLY	CA-C-N	5.98	125.53	119.19
8	5-L	330	GLY	C-N-CA	5.98	125.53	119.19
8	6-L	330	GLY	CA-C-N	5.98	125.53	119.19
8	6-L	330	GLY	C-N-CA	5.98	125.53	119.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	7-L	330	GLY	CA-C-N	5.98	125.53	119.19
8	7-L	330	GLY	C-N-CA	5.98	125.53	119.19
8	8-L	330	GLY	CA-C-N	5.98	125.53	119.19
8	8-L	330	GLY	C-N-CA	5.98	125.53	119.19
8	9-L	330	GLY	CA-C-N	5.98	125.53	119.19
8	9-L	330	GLY	C-N-CA	5.98	125.53	119.19
8	10-L	330	GLY	CA-C-N	5.98	125.53	119.19
8	10-L	330	GLY	C-N-CA	5.98	125.53	119.19
9	1-M	140	LEU	N-CA-C	5.86	118.45	108.90
9	2-M	140	LEU	N-CA-C	5.86	118.45	108.90
9	3-M	140	LEU	N-CA-C	5.86	118.45	108.90
9	4-M	140	LEU	N-CA-C	5.86	118.45	108.90
9	5-M	140	LEU	N-CA-C	5.86	118.45	108.90
9	6-M	140	LEU	N-CA-C	5.86	118.45	108.90
9	7-M	140	LEU	N-CA-C	5.86	118.45	108.90
9	8-M	140	LEU	N-CA-C	5.86	118.45	108.90
9	9-M	140	LEU	N-CA-C	5.86	118.45	108.90
9	10-M	140	LEU	N-CA-C	5.86	118.45	108.90
1	1-A	43	ARG	CA-C-N	5.84	127.14	119.84
1	1-A	43	ARG	C-N-CA	5.84	127.14	119.84
1	2-A	43	ARG	CA-C-N	5.84	127.14	119.84
1	2-A	43	ARG	C-N-CA	5.84	127.14	119.84
1	3-A	43	ARG	CA-C-N	5.84	127.14	119.84
1	3-A	43	ARG	C-N-CA	5.84	127.14	119.84
1	4-A	43	ARG	CA-C-N	5.84	127.14	119.84
1	4-A	43	ARG	C-N-CA	5.84	127.14	119.84
1	5-A	43	ARG	CA-C-N	5.84	127.14	119.84
1	5-A	43	ARG	C-N-CA	5.84	127.14	119.84
1	6-A	43	ARG	CA-C-N	5.84	127.14	119.84
1	6-A	43	ARG	C-N-CA	5.84	127.14	119.84
1	7-A	43	ARG	CA-C-N	5.84	127.14	119.84
1	7-A	43	ARG	C-N-CA	5.84	127.14	119.84
1	8-A	43	ARG	CA-C-N	5.84	127.14	119.84
1	8-A	43	ARG	C-N-CA	5.84	127.14	119.84
1	9-A	43	ARG	CA-C-N	5.84	127.14	119.84
1	9-A	43	ARG	C-N-CA	5.84	127.14	119.84
1	10-A	43	ARG	CA-C-N	5.84	127.14	119.84
1	10-A	43	ARG	C-N-CA	5.84	127.14	119.84
7	1-K	341	GLN	CA-C-N	-5.81	114.00	122.19
7	1-K	341	GLN	C-N-CA	-5.81	114.00	122.19
7	2-K	341	GLN	CA-C-N	-5.81	114.00	122.19
7	2-K	341	GLN	C-N-CA	-5.81	114.00	122.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	3-K	341	GLN	CA-C-N	-5.81	114.00	122.19
7	3-K	341	GLN	C-N-CA	-5.81	114.00	122.19
7	4-K	341	GLN	CA-C-N	-5.81	114.00	122.19
7	4-K	341	GLN	C-N-CA	-5.81	114.00	122.19
7	5-K	341	GLN	CA-C-N	-5.81	114.00	122.19
7	5-K	341	GLN	C-N-CA	-5.81	114.00	122.19
7	6-K	341	GLN	CA-C-N	-5.81	114.00	122.19
7	6-K	341	GLN	C-N-CA	-5.81	114.00	122.19
7	7-K	341	GLN	CA-C-N	-5.81	114.00	122.19
7	7-K	341	GLN	C-N-CA	-5.81	114.00	122.19
7	8-K	341	GLN	CA-C-N	-5.81	114.00	122.19
7	8-K	341	GLN	C-N-CA	-5.81	114.00	122.19
7	9-K	341	GLN	CA-C-N	-5.81	114.00	122.19
7	9-K	341	GLN	C-N-CA	-5.81	114.00	122.19
7	10-K	341	GLN	CA-C-N	-5.81	114.00	122.19
7	10-K	341	GLN	C-N-CA	-5.81	114.00	122.19
7	1-K	342	TRP	O-C-N	-5.79	114.66	122.41
7	2-K	342	TRP	O-C-N	-5.79	114.66	122.41
7	3-K	342	TRP	O-C-N	-5.79	114.66	122.41
7	4-K	342	TRP	O-C-N	-5.79	114.66	122.41
7	5-K	342	TRP	O-C-N	-5.79	114.66	122.41
7	6-K	342	TRP	O-C-N	-5.79	114.66	122.41
7	7-K	342	TRP	O-C-N	-5.79	114.66	122.41
7	8-K	342	TRP	O-C-N	-5.79	114.66	122.41
7	9-K	342	TRP	O-C-N	-5.79	114.66	122.41
7	10-K	342	TRP	O-C-N	-5.79	114.66	122.41
8	1-L	198	ALA	CA-C-N	5.76	125.44	119.56
8	1-L	198	ALA	C-N-CA	5.76	125.44	119.56
8	2-L	198	ALA	CA-C-N	5.76	125.44	119.56
8	2-L	198	ALA	C-N-CA	5.76	125.44	119.56
8	3-L	198	ALA	CA-C-N	5.76	125.44	119.56
8	3-L	198	ALA	C-N-CA	5.76	125.44	119.56
8	4-L	198	ALA	CA-C-N	5.76	125.44	119.56
8	4-L	198	ALA	C-N-CA	5.76	125.44	119.56
8	5-L	198	ALA	CA-C-N	5.76	125.44	119.56
8	5-L	198	ALA	C-N-CA	5.76	125.44	119.56
8	6-L	198	ALA	CA-C-N	5.76	125.44	119.56
8	6-L	198	ALA	C-N-CA	5.76	125.44	119.56
8	7-L	198	ALA	CA-C-N	5.76	125.44	119.56
8	7-L	198	ALA	C-N-CA	5.76	125.44	119.56
8	8-L	198	ALA	CA-C-N	5.76	125.44	119.56
8	8-L	198	ALA	C-N-CA	5.76	125.44	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	9-L	198	ALA	CA-C-N	5.76	125.44	119.56
8	9-L	198	ALA	C-N-CA	5.76	125.44	119.56
8	10-L	198	ALA	CA-C-N	5.76	125.44	119.56
8	10-L	198	ALA	C-N-CA	5.76	125.44	119.56
9	1-M	143	LEU	CA-C-N	5.71	126.00	119.83
9	1-M	143	LEU	C-N-CA	5.71	126.00	119.83
9	2-M	143	LEU	CA-C-N	5.71	126.00	119.83
9	2-M	143	LEU	C-N-CA	5.71	126.00	119.83
9	3-M	143	LEU	CA-C-N	5.71	126.00	119.83
9	3-M	143	LEU	C-N-CA	5.71	126.00	119.83
9	4-M	143	LEU	CA-C-N	5.71	126.00	119.83
9	4-M	143	LEU	C-N-CA	5.71	126.00	119.83
9	5-M	143	LEU	CA-C-N	5.71	126.00	119.83
9	5-M	143	LEU	C-N-CA	5.71	126.00	119.83
9	6-M	143	LEU	CA-C-N	5.71	126.00	119.83
9	6-M	143	LEU	C-N-CA	5.71	126.00	119.83
9	7-M	143	LEU	CA-C-N	5.71	126.00	119.83
9	7-M	143	LEU	C-N-CA	5.71	126.00	119.83
9	8-M	143	LEU	CA-C-N	5.71	126.00	119.83
9	8-M	143	LEU	C-N-CA	5.71	126.00	119.83
9	9-M	143	LEU	CA-C-N	5.71	126.00	119.83
9	9-M	143	LEU	C-N-CA	5.71	126.00	119.83
9	10-M	143	LEU	CA-C-N	5.71	126.00	119.83
9	10-M	143	LEU	C-N-CA	5.71	126.00	119.83
1	1-E	43	ARG	CA-C-N	5.70	126.96	119.84
1	1-E	43	ARG	C-N-CA	5.70	126.96	119.84
1	2-E	43	ARG	CA-C-N	5.70	126.96	119.84
1	2-E	43	ARG	C-N-CA	5.70	126.96	119.84
1	3-E	43	ARG	CA-C-N	5.70	126.96	119.84
1	3-E	43	ARG	C-N-CA	5.70	126.96	119.84
1	4-E	43	ARG	CA-C-N	5.70	126.96	119.84
1	4-E	43	ARG	C-N-CA	5.70	126.96	119.84
1	5-E	43	ARG	CA-C-N	5.70	126.96	119.84
1	5-E	43	ARG	C-N-CA	5.70	126.96	119.84
1	6-E	43	ARG	CA-C-N	5.70	126.96	119.84
1	6-E	43	ARG	C-N-CA	5.70	126.96	119.84
1	7-E	43	ARG	CA-C-N	5.70	126.96	119.84
1	7-E	43	ARG	C-N-CA	5.70	126.96	119.84
1	8-E	43	ARG	CA-C-N	5.70	126.96	119.84
1	8-E	43	ARG	C-N-CA	5.70	126.96	119.84
1	9-E	43	ARG	CA-C-N	5.70	126.96	119.84
1	9-E	43	ARG	C-N-CA	5.70	126.96	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	10-E	43	ARG	CA-C-N	5.70	126.96	119.84
1	10-E	43	ARG	C-N-CA	5.70	126.96	119.84
4	1-D	50	HIS	CA-C-N	5.65	126.91	119.84
4	1-D	50	HIS	C-N-CA	5.65	126.91	119.84
4	2-D	50	HIS	CA-C-N	5.65	126.91	119.84
4	2-D	50	HIS	C-N-CA	5.65	126.91	119.84
4	3-D	50	HIS	CA-C-N	5.65	126.91	119.84
4	3-D	50	HIS	C-N-CA	5.65	126.91	119.84
4	4-D	50	HIS	CA-C-N	5.65	126.91	119.84
4	4-D	50	HIS	C-N-CA	5.65	126.91	119.84
4	5-D	50	HIS	CA-C-N	5.65	126.91	119.84
4	5-D	50	HIS	C-N-CA	5.65	126.91	119.84
4	6-D	50	HIS	CA-C-N	5.65	126.91	119.84
4	6-D	50	HIS	C-N-CA	5.65	126.91	119.84
4	7-D	50	HIS	CA-C-N	5.65	126.91	119.84
4	7-D	50	HIS	C-N-CA	5.65	126.91	119.84
4	8-D	50	HIS	CA-C-N	5.65	126.91	119.84
4	8-D	50	HIS	C-N-CA	5.65	126.91	119.84
4	9-D	50	HIS	CA-C-N	5.65	126.91	119.84
4	9-D	50	HIS	C-N-CA	5.65	126.91	119.84
4	10-D	50	HIS	CA-C-N	5.65	126.91	119.84
4	10-D	50	HIS	C-N-CA	5.65	126.91	119.84
9	1-M	109	ILE	CA-C-N	5.53	125.70	119.90
9	1-M	109	ILE	C-N-CA	5.53	125.70	119.90
9	2-M	109	ILE	CA-C-N	5.53	125.70	119.90
9	2-M	109	ILE	C-N-CA	5.53	125.70	119.90
9	3-M	109	ILE	CA-C-N	5.53	125.70	119.90
9	3-M	109	ILE	C-N-CA	5.53	125.70	119.90
9	4-M	109	ILE	CA-C-N	5.53	125.70	119.90
9	4-M	109	ILE	C-N-CA	5.53	125.70	119.90
9	5-M	109	ILE	CA-C-N	5.53	125.70	119.90
9	5-M	109	ILE	C-N-CA	5.53	125.70	119.90
9	6-M	109	ILE	CA-C-N	5.53	125.70	119.90
9	6-M	109	ILE	C-N-CA	5.53	125.70	119.90
9	7-M	109	ILE	CA-C-N	5.53	125.70	119.90
9	7-M	109	ILE	C-N-CA	5.53	125.70	119.90
9	8-M	109	ILE	CA-C-N	5.53	125.70	119.90
9	8-M	109	ILE	C-N-CA	5.53	125.70	119.90
9	9-M	109	ILE	CA-C-N	5.53	125.70	119.90
9	9-M	109	ILE	C-N-CA	5.53	125.70	119.90
9	10-M	109	ILE	CA-C-N	5.53	125.70	119.90
9	10-M	109	ILE	C-N-CA	5.53	125.70	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	1-C	109	LEU	CA-C-N	5.46	126.31	119.98
3	1-C	109	LEU	C-N-CA	5.46	126.31	119.98
10	1-N	65	ARG	N-CA-C	-5.46	101.97	110.10
3	2-C	109	LEU	CA-C-N	5.46	126.31	119.98
3	2-C	109	LEU	C-N-CA	5.46	126.31	119.98
10	2-N	65	ARG	N-CA-C	-5.46	101.97	110.10
3	3-C	109	LEU	CA-C-N	5.46	126.31	119.98
3	3-C	109	LEU	C-N-CA	5.46	126.31	119.98
10	3-N	65	ARG	N-CA-C	-5.46	101.97	110.10
3	4-C	109	LEU	CA-C-N	5.46	126.31	119.98
3	4-C	109	LEU	C-N-CA	5.46	126.31	119.98
10	4-N	65	ARG	N-CA-C	-5.46	101.97	110.10
3	5-C	109	LEU	CA-C-N	5.46	126.31	119.98
3	5-C	109	LEU	C-N-CA	5.46	126.31	119.98
10	5-N	65	ARG	N-CA-C	-5.46	101.97	110.10
3	6-C	109	LEU	CA-C-N	5.46	126.31	119.98
3	6-C	109	LEU	C-N-CA	5.46	126.31	119.98
10	6-N	65	ARG	N-CA-C	-5.46	101.97	110.10
3	7-C	109	LEU	CA-C-N	5.46	126.31	119.98
3	7-C	109	LEU	C-N-CA	5.46	126.31	119.98
10	7-N	65	ARG	N-CA-C	-5.46	101.97	110.10
3	8-C	109	LEU	CA-C-N	5.46	126.31	119.98
3	8-C	109	LEU	C-N-CA	5.46	126.31	119.98
10	8-N	65	ARG	N-CA-C	-5.46	101.97	110.10
3	9-C	109	LEU	CA-C-N	5.46	126.31	119.98
3	9-C	109	LEU	C-N-CA	5.46	126.31	119.98
10	9-N	65	ARG	N-CA-C	-5.46	101.97	110.10
3	10-C	109	LEU	CA-C-N	5.46	126.31	119.98
3	10-C	109	LEU	C-N-CA	5.46	126.31	119.98
10	10-N	65	ARG	N-CA-C	-5.46	101.97	110.10
9	1-M	168	HIS	CA-CB-CG	-5.32	108.48	113.80
9	2-M	168	HIS	CA-CB-CG	-5.32	108.48	113.80
9	3-M	168	HIS	CA-CB-CG	-5.32	108.48	113.80
9	4-M	168	HIS	CA-CB-CG	-5.32	108.48	113.80
9	5-M	168	HIS	CA-CB-CG	-5.32	108.48	113.80
9	6-M	168	HIS	CA-CB-CG	-5.32	108.48	113.80
9	7-M	168	HIS	CA-CB-CG	-5.32	108.48	113.80
9	8-M	168	HIS	CA-CB-CG	-5.32	108.48	113.80
9	9-M	168	HIS	CA-CB-CG	-5.32	108.48	113.80
9	10-M	168	HIS	CA-CB-CG	-5.32	108.48	113.80
3	1-C	101	VAL	N-CA-C	5.31	115.60	108.17
3	2-C	101	VAL	N-CA-C	5.31	115.60	108.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	3-C	101	VAL	N-CA-C	5.31	115.60	108.17
3	4-C	101	VAL	N-CA-C	5.31	115.60	108.17
3	5-C	101	VAL	N-CA-C	5.31	115.60	108.17
3	6-C	101	VAL	N-CA-C	5.31	115.60	108.17
3	7-C	101	VAL	N-CA-C	5.31	115.60	108.17
3	8-C	101	VAL	N-CA-C	5.31	115.60	108.17
3	9-C	101	VAL	N-CA-C	5.31	115.60	108.17
3	10-C	101	VAL	N-CA-C	5.31	115.60	108.17
7	1-K	995	PHE	CA-CB-CG	-5.30	108.50	113.80
7	2-K	995	PHE	CA-CB-CG	-5.30	108.50	113.80
7	3-K	995	PHE	CA-CB-CG	-5.30	108.50	113.80
7	4-K	995	PHE	CA-CB-CG	-5.30	108.50	113.80
7	5-K	995	PHE	CA-CB-CG	-5.30	108.50	113.80
7	6-K	995	PHE	CA-CB-CG	-5.30	108.50	113.80
7	7-K	995	PHE	CA-CB-CG	-5.30	108.50	113.80
7	8-K	995	PHE	CA-CB-CG	-5.30	108.50	113.80
7	9-K	995	PHE	CA-CB-CG	-5.30	108.50	113.80
7	10-K	995	PHE	CA-CB-CG	-5.30	108.50	113.80
8	1-L	293	LYS	CA-C-N	5.15	124.81	119.56
8	1-L	293	LYS	C-N-CA	5.15	124.81	119.56
8	2-L	293	LYS	CA-C-N	5.15	124.81	119.56
8	2-L	293	LYS	C-N-CA	5.15	124.81	119.56
8	3-L	293	LYS	CA-C-N	5.15	124.81	119.56
8	3-L	293	LYS	C-N-CA	5.15	124.81	119.56
8	4-L	293	LYS	CA-C-N	5.15	124.81	119.56
8	4-L	293	LYS	C-N-CA	5.15	124.81	119.56
8	5-L	293	LYS	CA-C-N	5.15	124.81	119.56
8	5-L	293	LYS	C-N-CA	5.15	124.81	119.56
8	6-L	293	LYS	CA-C-N	5.15	124.81	119.56
8	6-L	293	LYS	C-N-CA	5.15	124.81	119.56
8	7-L	293	LYS	CA-C-N	5.15	124.81	119.56
8	7-L	293	LYS	C-N-CA	5.15	124.81	119.56
8	8-L	293	LYS	CA-C-N	5.15	124.81	119.56
8	8-L	293	LYS	C-N-CA	5.15	124.81	119.56
8	9-L	293	LYS	CA-C-N	5.15	124.81	119.56
8	9-L	293	LYS	C-N-CA	5.15	124.81	119.56
8	10-L	293	LYS	CA-C-N	5.15	124.81	119.56
8	10-L	293	LYS	C-N-CA	5.15	124.81	119.56
10	1-N	87	PHE	CA-CB-CG	-5.13	108.67	113.80
10	2-N	87	PHE	CA-CB-CG	-5.13	108.67	113.80
10	3-N	87	PHE	CA-CB-CG	-5.13	108.67	113.80
10	4-N	87	PHE	CA-CB-CG	-5.13	108.67	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	5-N	87	PHE	CA-CB-CG	-5.13	108.67	113.80
10	6-N	87	PHE	CA-CB-CG	-5.13	108.67	113.80
10	7-N	87	PHE	CA-CB-CG	-5.13	108.67	113.80
10	8-N	87	PHE	CA-CB-CG	-5.13	108.67	113.80
10	9-N	87	PHE	CA-CB-CG	-5.13	108.67	113.80
10	10-N	87	PHE	CA-CB-CG	-5.13	108.67	113.80
7	1-K	341	GLN	N-CA-C	5.13	117.27	111.02
7	2-K	341	GLN	N-CA-C	5.13	117.27	111.02
7	3-K	341	GLN	N-CA-C	5.13	117.27	111.02
7	4-K	341	GLN	N-CA-C	5.13	117.27	111.02
7	5-K	341	GLN	N-CA-C	5.13	117.27	111.02
7	6-K	341	GLN	N-CA-C	5.13	117.27	111.02
7	7-K	341	GLN	N-CA-C	5.13	117.27	111.02
7	8-K	341	GLN	N-CA-C	5.13	117.27	111.02
7	9-K	341	GLN	N-CA-C	5.13	117.27	111.02
7	10-K	341	GLN	N-CA-C	5.13	117.27	111.02
3	1-G	101	VAL	N-CA-C	5.02	115.54	108.36
3	2-G	101	VAL	N-CA-C	5.02	115.54	108.36
3	3-G	101	VAL	N-CA-C	5.02	115.54	108.36
3	4-G	101	VAL	N-CA-C	5.02	115.54	108.36
3	5-G	101	VAL	N-CA-C	5.02	115.54	108.36
3	6-G	101	VAL	N-CA-C	5.02	115.54	108.36
3	7-G	101	VAL	N-CA-C	5.02	115.54	108.36
3	8-G	101	VAL	N-CA-C	5.02	115.54	108.36
3	9-G	101	VAL	N-CA-C	5.02	115.54	108.36
3	10-G	101	VAL	N-CA-C	5.02	115.54	108.36

There are no chirality outliers.

All (22) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	1-M	3	PRO	Mainchain,Peptide
9	10-M	3	PRO	Mainchain,Peptide
9	2-M	3	PRO	Mainchain,Peptide
9	3-M	3	PRO	Mainchain,Peptide
9	4-M	3	PRO	Mainchain,Peptide
9	5-M	3	PRO	Mainchain,Peptide
7	6-K	650	ASN	Mainchain,Peptide
9	6-M	3	PRO	Mainchain,Peptide
9	7-M	3	PRO	Mainchain,Peptide
9	8-M	3	PRO	Mainchain,Peptide
9	9-M	3	PRO	Mainchain,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	1-A	809	0	849	3	0
1	1-E	783	0	822	3	0
1	2-A	809	0	849	4	0
1	2-E	783	0	822	5	0
1	3-A	809	0	849	3	0
1	3-E	783	0	822	4	0
1	4-A	809	0	849	4	0
1	4-E	783	0	822	4	0
1	5-A	809	0	849	4	0
1	5-E	783	0	822	4	0
1	6-A	809	0	849	4	0
1	6-E	783	0	822	4	0
1	7-A	809	0	849	5	0
1	7-E	783	0	822	4	0
1	8-A	809	0	849	3	0
1	8-E	783	0	822	4	0
1	9-A	809	0	849	3	0
1	9-E	783	0	822	4	0
1	10-A	809	0	849	4	0
1	10-E	783	0	822	3	0
2	1-B	703	0	757	3	0
2	1-F	627	0	663	2	0
2	2-B	703	0	757	2	0
2	2-F	627	0	663	1	0
2	3-B	703	0	757	2	0
2	3-F	627	0	663	1	0
2	4-B	703	0	757	3	0
2	4-F	627	0	663	1	0
2	5-B	703	0	757	3	0
2	5-F	627	0	663	2	0
2	6-B	703	0	757	2	0
2	6-F	627	0	663	2	0
2	7-B	703	0	757	3	0
2	7-F	627	0	663	3	0
2	8-B	703	0	757	2	0
2	8-F	627	0	663	2	0
2	9-B	703	0	757	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	9-F	627	0	663	2	0
2	10-B	703	0	757	2	0
2	10-F	627	0	663	3	0
3	1-C	823	0	882	3	0
3	1-G	823	0	882	8	0
3	2-C	823	0	882	3	0
3	2-G	823	0	882	8	0
3	3-C	823	0	882	4	0
3	3-G	823	0	882	8	0
3	4-C	823	0	882	3	0
3	4-G	823	0	882	8	0
3	5-C	823	0	882	3	0
3	5-G	823	0	882	8	0
3	6-C	823	0	882	3	0
3	6-G	823	0	882	8	0
3	7-C	823	0	882	3	0
3	7-G	823	0	882	8	0
3	8-C	823	0	882	3	0
3	8-G	823	0	882	8	0
3	9-C	823	0	882	3	0
3	9-G	823	0	882	8	0
3	10-C	823	0	882	3	0
3	10-G	823	0	882	8	0
4	1-D	719	0	740	0	0
4	1-H	719	0	740	2	0
4	2-D	719	0	740	0	0
4	2-H	719	0	740	2	0
4	3-D	719	0	740	0	0
4	3-H	719	0	740	2	0
4	4-D	719	0	740	0	0
4	4-H	719	0	740	2	0
4	5-D	719	0	740	0	0
4	5-H	719	0	740	2	0
4	6-D	719	0	740	0	0
4	6-H	719	0	740	2	0
4	7-D	719	0	740	0	0
4	7-H	719	0	740	2	0
4	8-D	719	0	740	0	0
4	8-H	719	0	740	2	0
4	9-D	719	0	740	0	0
4	9-H	719	0	740	2	0
4	10-D	719	0	740	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	10-H	719	0	740	2	0
5	1-I	2975	0	1639	20	0
5	2-I	2975	0	1639	18	0
5	3-I	2975	0	1639	28	0
5	4-I	2975	0	1639	23	0
5	5-I	2975	0	1639	22	0
5	6-I	2975	0	1639	26	0
5	7-I	2975	0	1639	29	0
5	8-I	2975	0	1639	34	0
5	9-I	2975	0	1639	22	0
5	10-I	2975	0	1639	30	0
6	1-J	3011	0	1639	17	0
6	2-J	3011	0	1639	18	0
6	3-J	3011	0	1639	18	0
6	4-J	3011	0	1639	27	0
6	5-J	3011	0	1639	19	0
6	6-J	3011	0	1639	20	0
6	7-J	3011	0	1639	21	0
6	8-J	3011	0	1639	20	0
6	9-J	3011	0	1639	23	0
6	10-J	3011	0	1639	20	0
7	1-K	5055	0	5102	173	0
7	2-K	5055	0	5102	173	0
7	3-K	5055	0	5102	170	0
7	4-K	5055	0	5102	187	0
7	5-K	5055	0	5102	177	0
7	6-K	5055	0	5102	187	0
7	7-K	5055	0	5102	185	0
7	8-K	5055	0	5102	201	0
7	9-K	5055	0	5102	187	0
7	10-K	5055	0	5102	186	0
8	1-L	3154	0	3173	13	0
8	2-L	3154	0	3173	13	0
8	3-L	3154	0	3173	13	0
8	4-L	3154	0	3173	13	0
8	5-L	3154	0	3173	13	0
8	6-L	3154	0	3173	13	0
8	7-L	3154	0	3173	13	0
8	8-L	3154	0	3173	13	0
8	9-L	3154	0	3173	13	0
8	10-L	3154	0	3173	13	0
9	1-M	3192	0	3180	126	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	2-M	3192	0	3180	126	0
9	3-M	3192	0	3180	126	0
9	4-M	3192	0	3180	126	0
9	5-M	3192	0	3180	126	0
9	6-M	3192	0	3180	126	0
9	7-M	3192	0	3180	126	0
9	8-M	3192	0	3180	134	0
9	9-M	3192	0	3180	126	0
9	10-M	3192	0	3180	126	0
10	1-N	494	0	473	6	0
10	2-N	494	0	473	6	0
10	3-N	494	0	473	6	0
10	4-N	494	0	473	6	0
10	5-N	494	0	473	6	0
10	6-N	494	0	473	6	0
10	7-N	494	0	473	6	0
10	8-N	494	0	473	6	0
10	9-N	494	0	473	6	0
10	10-N	494	0	473	6	0
11	1-K	1	0	0	0	0
11	2-K	1	0	0	0	0
11	3-K	1	0	0	0	0
11	4-K	1	0	0	0	0
11	5-K	1	0	0	0	0
11	6-K	1	0	0	0	0
11	7-K	1	0	0	0	0
11	8-K	1	0	0	0	0
11	9-K	1	0	0	0	0
11	10-K	1	0	0	0	0
12	1-K	27	0	12	3	0
12	2-K	27	0	12	1	0
12	3-K	27	0	12	5	0
12	4-K	27	0	12	3	0
12	5-K	27	0	12	2	0
12	6-K	27	0	12	2	0
12	7-K	27	0	12	1	0
12	8-K	27	0	12	2	0
12	9-K	27	0	12	3	0
12	10-K	27	0	12	4	0
13	1-K	4	0	0	0	0
13	2-K	4	0	0	0	0
13	3-K	4	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	4-K	4	0	0	0	0
13	5-K	4	0	0	0	0
13	6-K	4	0	0	1	0
13	7-K	4	0	0	0	0
13	8-K	4	0	0	0	0
13	9-K	4	0	0	2	0
13	10-K	4	0	0	0	0
14	1-L	31	0	12	1	0
14	2-L	31	0	12	1	0
14	3-L	31	0	12	1	0
14	4-L	31	0	12	1	0
14	5-L	31	0	12	1	0
14	6-L	31	0	12	1	0
14	7-L	31	0	12	1	0
14	8-L	31	0	12	1	0
14	9-L	31	0	12	1	0
14	10-L	31	0	12	1	0
All	All	239500	0	215650	2562	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 6.

All (2562) 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)
7:K:351:PHE:CE1	9:M:467:PHE:CE2	1.78	1.70
7:K:351:PHE:CE1	9:M:467:PHE:CE2	1.78	1.70
7:K:351:PHE:CE1	9:M:467:PHE:CE2	1.78	1.70
7:K:351:PHE:CE1	9:M:467:PHE:CE2	1.78	1.70
7:K:351:PHE:CE1	9:M:467:PHE:CE2	1.78	1.70
7:K:351:PHE:CE1	9:M:467:PHE:CE2	1.78	1.70
7:K:351:PHE:CE1	9:M:467:PHE:CE2	1.78	1.70
7:K:351:PHE:CE1	9:M:467:PHE:CE2	1.78	1.70
7:K:351:PHE:CE1	9:M:467:PHE:CE2	1.78	1.70
7:K:351:PHE:CE1	9:M:467:PHE:CE2	1.78	1.70
7:K:351:PHE:CE1	9:M:467:PHE:HE2	1.12	1.61
7:K:351:PHE:CE1	9:M:467:PHE:HE2	1.12	1.61
7:K:351:PHE:CE1	9:M:467:PHE:HE2	1.12	1.61
7:K:351:PHE:CE1	9:M:467:PHE:HE2	1.12	1.61
7:K:351:PHE:CE1	9:M:467:PHE:HE2	1.12	1.61
7:K:351:PHE:CE1	9:M:467:PHE:HE2	1.12	1.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:351:PHE:CE1	9:M:467:PHE:HE2	1.12	1.61
7:K:351:PHE:CE1	9:M:467:PHE:HE2	1.12	1.61
7:K:351:PHE:CE1	9:M:467:PHE:HE2	1.12	1.61
7:K:351:PHE:CE1	9:M:467:PHE:HE2	1.12	1.61
7:K:359:HIS:CE1	9:M:434:ILE:HG21	1.04	1.54
7:K:359:HIS:CE1	9:M:434:ILE:HG21	1.04	1.54
7:K:359:HIS:CE1	9:M:434:ILE:HG21	1.04	1.54
7:K:359:HIS:CE1	9:M:434:ILE:HG21	1.04	1.54
7:K:359:HIS:CE1	9:M:434:ILE:HG21	1.04	1.54
7:K:359:HIS:CE1	9:M:434:ILE:HG21	1.04	1.54
7:K:359:HIS:CE1	9:M:434:ILE:HG21	1.04	1.54
7:K:359:HIS:CE1	9:M:434:ILE:HG21	1.04	1.54
7:K:359:HIS:CE1	9:M:434:ILE:HG21	1.04	1.54
7:K:359:HIS:CE1	9:M:434:ILE:HG21	1.04	1.54
7:K:359:HIS:CE1	9:M:434:ILE:HG21	1.04	1.54
7:K:359:HIS:CE1	9:M:434:ILE:CG2	1.86	1.53
7:K:359:HIS:CE1	9:M:434:ILE:CG2	1.86	1.53
7:K:359:HIS:CE1	9:M:434:ILE:CG2	1.86	1.53
7:K:359:HIS:CE1	9:M:434:ILE:CG2	1.86	1.53
7:K:359:HIS:CE1	9:M:434:ILE:CG2	1.86	1.53
7:K:359:HIS:CE1	9:M:434:ILE:CG2	1.86	1.53
7:K:359:HIS:CE1	9:M:434:ILE:CG2	1.86	1.53
7:K:359:HIS:CE1	9:M:434:ILE:CG2	1.86	1.53
7:K:359:HIS:CE1	9:M:434:ILE:CG2	1.86	1.53
7:K:359:HIS:CE1	9:M:434:ILE:CG2	1.86	1.53
7:K:381:LEU:CB	7:K:676:GLU:CD	1.81	1.50
7:K:362:MET:CB	9:M:437:LYS:NZ	1.77	1.46
7:K:362:MET:CB	9:M:437:LYS:NZ	1.77	1.46
7:K:362:MET:CB	9:M:437:LYS:NZ	1.77	1.46
7:K:362:MET:CB	9:M:437:LYS:NZ	1.77	1.46
7:K:362:MET:CB	9:M:437:LYS:NZ	1.77	1.46
7:K:362:MET:CB	9:M:437:LYS:NZ	1.77	1.46
7:K:362:MET:CB	9:M:437:LYS:NZ	1.77	1.46
7:K:362:MET:CB	9:M:437:LYS:NZ	1.77	1.46
7:K:362:MET:CB	9:M:437:LYS:NZ	1.77	1.46
7:K:362:MET:CB	9:M:437:LYS:NZ	1.77	1.46
7:K:381:LEU:CB	7:K:676:GLU:OE2	1.69	1.36
7:K:381:LEU:CB	7:K:676:GLU:OE1	1.74	1.34
5:I:95:DC:P	7:K:608:LYS:H	1.49	1.34
7:K:362:MET:CG	9:M:437:LYS:HZ1	1.41	1.34
7:K:362:MET:CG	9:M:437:LYS:HZ1	1.41	1.34
7:K:362:MET:CG	9:M:437:LYS:HZ1	1.41	1.34

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:362:MET:CG	9:M:437:LYS:HZ1	1.41	1.34
7:K:362:MET:CG	9:M:437:LYS:HZ1	1.41	1.34
7:K:362:MET:CG	9:M:437:LYS:HZ1	1.41	1.34
7:K:362:MET:CG	9:M:437:LYS:HZ1	1.41	1.34
7:K:362:MET:CG	9:M:437:LYS:HZ1	1.41	1.34
7:K:362:MET:CG	9:M:437:LYS:HZ1	1.41	1.34
7:K:362:MET:CG	9:M:437:LYS:HZ1	1.41	1.34
7:K:378:LEU:HA	7:K:676:GLU:CD	1.53	1.32
6:J:54:DC:H5"	7:K:816:MET:CG	1.63	1.29
7:K:359:HIS:HE1	9:M:434:ILE:CG2	1.29	1.29
7:K:359:HIS:HE1	9:M:434:ILE:CG2	1.29	1.29
7:K:359:HIS:HE1	9:M:434:ILE:CG2	1.29	1.29
7:K:359:HIS:HE1	9:M:434:ILE:CG2	1.29	1.29
7:K:359:HIS:HE1	9:M:434:ILE:CG2	1.29	1.29
7:K:359:HIS:HE1	9:M:434:ILE:CG2	1.29	1.29
7:K:359:HIS:HE1	9:M:434:ILE:CG2	1.29	1.29
7:K:359:HIS:HE1	9:M:434:ILE:CG2	1.29	1.29
7:K:359:HIS:HE1	9:M:434:ILE:CG2	1.29	1.29
7:K:359:HIS:HE1	9:M:434:ILE:CG2	1.29	1.29
7:K:359:HIS:HE1	9:M:434:ILE:CG2	1.29	1.29
7:K:358:LEU:HD22	9:M:438:GLN:CA	1.61	1.29
7:K:358:LEU:HD22	9:M:438:GLN:CA	1.61	1.29
7:K:358:LEU:HD22	9:M:438:GLN:CA	1.61	1.29
7:K:358:LEU:HD22	9:M:438:GLN:CA	1.61	1.29
7:K:358:LEU:HD22	9:M:438:GLN:CA	1.61	1.29
7:K:358:LEU:HD22	9:M:438:GLN:CA	1.61	1.29
7:K:358:LEU:HD22	9:M:438:GLN:CA	1.61	1.29
7:K:358:LEU:HD22	9:M:438:GLN:CA	1.61	1.29
7:K:358:LEU:HD22	9:M:438:GLN:CA	1.61	1.29
7:K:358:LEU:HD22	9:M:438:GLN:CA	1.61	1.29
7:K:362:MET:HB2	9:M:437:LYS:NZ	0.97	1.28
7:K:362:MET:HB2	9:M:437:LYS:NZ	0.97	1.28
7:K:362:MET:HB2	9:M:437:LYS:NZ	0.97	1.28
7:K:362:MET:HB2	9:M:437:LYS:NZ	0.97	1.28
7:K:362:MET:HB2	9:M:437:LYS:NZ	0.97	1.28
7:K:362:MET:HB2	9:M:437:LYS:NZ	0.97	1.28
7:K:362:MET:HB2	9:M:437:LYS:NZ	0.97	1.28
7:K:362:MET:HB2	9:M:437:LYS:NZ	0.97	1.28
7:K:362:MET:HB2	9:M:437:LYS:NZ	0.97	1.28
7:K:362:MET:HB2	9:M:437:LYS:NZ	0.97	1.28
7:K:358:LEU:HB2	9:M:438:GLN:OE1	1.16	1.27
7:K:358:LEU:HB2	9:M:438:GLN:OE1	1.16	1.27

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:358:LEU:HB2	9:M:438:GLN:OE1	1.16	1.27
7:K:358:LEU:HB2	9:M:438:GLN:OE1	1.16	1.27
7:K:358:LEU:HB2	9:M:438:GLN:OE1	1.16	1.27
6:J:54:DC:OP1	7:K:816:MET:HB2	1.15	1.27
7:K:358:LEU:HB2	9:M:438:GLN:OE1	1.16	1.27
7:K:358:LEU:HB2	9:M:438:GLN:OE1	1.16	1.27
7:K:358:LEU:HB2	9:M:438:GLN:OE1	1.16	1.27
7:K:358:LEU:HB2	9:M:438:GLN:OE1	1.16	1.27
7:K:358:LEU:HB2	9:M:438:GLN:OE1	1.16	1.27
6:J:54:DC:OP1	7:K:816:MET:CB	1.81	1.25
5:I:95:DC:P	7:K:608:LYS:HB3	1.75	1.25
6:J:54:DC:C5'	7:K:816:MET:HG2	1.66	1.23
7:K:378:LEU:HA	7:K:676:GLU:OE1	1.37	1.22
7:K:381:LEU:CB	7:K:676:GLU:OE1	1.82	1.21
7:K:378:LEU:CA	7:K:676:GLU:OE1	1.88	1.21
7:K:351:PHE:CZ	9:M:467:PHE:HE2	1.61	1.19
7:K:351:PHE:CZ	9:M:467:PHE:HE2	1.61	1.19
7:K:351:PHE:CZ	9:M:467:PHE:HE2	1.61	1.19
7:K:351:PHE:CZ	9:M:467:PHE:HE2	1.61	1.19
7:K:351:PHE:CZ	9:M:467:PHE:HE2	1.61	1.19
7:K:351:PHE:CZ	9:M:467:PHE:HE2	1.61	1.19
7:K:351:PHE:CZ	9:M:467:PHE:HE2	1.61	1.19
7:K:351:PHE:CZ	9:M:467:PHE:HE2	1.61	1.19
7:K:351:PHE:CZ	9:M:467:PHE:HE2	1.61	1.19
7:K:351:PHE:CZ	9:M:467:PHE:HE2	1.61	1.19
7:K:362:MET:CB	9:M:437:LYS:HZ2	1.40	1.19
7:K:362:MET:CB	9:M:437:LYS:HZ2	1.40	1.19
7:K:362:MET:CB	9:M:437:LYS:HZ2	1.40	1.19
7:K:362:MET:CB	9:M:437:LYS:HZ2	1.40	1.19
7:K:362:MET:CB	9:M:437:LYS:HZ2	1.40	1.19
7:K:362:MET:CB	9:M:437:LYS:HZ2	1.40	1.19
7:K:362:MET:CB	9:M:437:LYS:HZ2	1.40	1.19
7:K:362:MET:CB	9:M:437:LYS:HZ2	1.40	1.19
7:K:362:MET:CB	9:M:437:LYS:HZ2	1.40	1.19
7:K:362:MET:CB	9:M:437:LYS:HZ2	1.40	1.19
7:K:358:LEU:HD22	9:M:438:GLN:N	1.55	1.19
7:K:358:LEU:HD22	9:M:438:GLN:N	1.55	1.19
7:K:358:LEU:HD22	9:M:438:GLN:N	1.55	1.19
7:K:358:LEU:HD22	9:M:438:GLN:N	1.55	1.19
7:K:358:LEU:HD22	9:M:438:GLN:N	1.55	1.19
7:K:358:LEU:HD22	9:M:438:GLN:N	1.55	1.19

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:358:LEU:HD22	9:M:438:GLN:N	1.55	1.19
7:K:358:LEU:HD22	9:M:438:GLN:N	1.55	1.19
7:K:358:LEU:HD22	9:M:438:GLN:N	1.55	1.19
7:K:358:LEU:HD22	9:M:438:GLN:N	1.55	1.19
6:J:54:DC:OP1	7:K:816:MET:HB2	1.42	1.18
7:K:358:LEU:CB	9:M:438:GLN:OE1	1.92	1.17
7:K:358:LEU:CB	9:M:438:GLN:OE1	1.92	1.17
7:K:358:LEU:CB	9:M:438:GLN:OE1	1.92	1.17
7:K:358:LEU:CB	9:M:438:GLN:OE1	1.92	1.17
7:K:358:LEU:CB	9:M:438:GLN:OE1	1.92	1.17
7:K:358:LEU:CB	9:M:438:GLN:OE1	1.92	1.17
7:K:378:LEU:HA	7:K:676:GLU:OE1	1.40	1.17
7:K:358:LEU:CB	9:M:438:GLN:OE1	1.92	1.17
7:K:358:LEU:CB	9:M:438:GLN:OE1	1.92	1.17
7:K:358:LEU:CB	9:M:438:GLN:OE1	1.92	1.17
7:K:358:LEU:CB	9:M:438:GLN:OE1	1.92	1.17
7:K:362:MET:HG3	9:M:437:LYS:HZ1	1.06	1.16
7:K:362:MET:HG3	9:M:437:LYS:HZ1	1.06	1.16
7:K:362:MET:HG3	9:M:437:LYS:HZ1	1.06	1.16
7:K:362:MET:HG3	9:M:437:LYS:HZ1	1.06	1.16
7:K:362:MET:HG3	9:M:437:LYS:HZ1	1.06	1.16
7:K:362:MET:HG3	9:M:437:LYS:HZ1	1.06	1.16
7:K:362:MET:HG3	9:M:437:LYS:HZ1	1.06	1.16
7:K:362:MET:HG3	9:M:437:LYS:HZ1	1.06	1.16
6:J:54:DC:OP1	7:K:816:MET:HB2	1.43	1.16
7:K:362:MET:HG3	9:M:437:LYS:HZ1	1.06	1.16
7:K:362:MET:HG3	9:M:437:LYS:HZ1	1.06	1.16
5:I:95:DC:OP1	7:K:608:LYS:N	1.79	1.16
7:K:378:LEU:CA	7:K:676:GLU:OE1	1.95	1.13
1:A:43:ARG:NH1	6:J:69:DG:OP1	1.81	1.13
1:A:43:ARG:NH1	6:J:69:DG:OP1	1.82	1.12
7:K:358:LEU:HD22	9:M:438:GLN:CB	1.81	1.11
7:K:358:LEU:HD22	9:M:438:GLN:CB	1.81	1.11
7:K:358:LEU:HD22	9:M:438:GLN:CB	1.81	1.11
7:K:358:LEU:HD22	9:M:438:GLN:CB	1.81	1.11
7:K:358:LEU:HD22	9:M:438:GLN:CB	1.81	1.11
7:K:358:LEU:HD22	9:M:438:GLN:CB	1.81	1.11
7:K:358:LEU:HD22	9:M:438:GLN:CB	1.81	1.11
1:A:43:ARG:NH1	6:J:69:DG:OP1	1.83	1.11
7:K:358:LEU:HD22	9:M:438:GLN:CB	1.81	1.11
7:K:358:LEU:HD22	9:M:438:GLN:CB	1.81	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:358:LEU:HD22	9:M:438:GLN:CB	1.81	1.11
6:J:54:DC:OP1	7:K:816:MET:CB	1.99	1.10
1:A:43:ARG:NH1	6:J:69:DG:OP1	1.84	1.10
1:A:43:ARG:NH1	6:J:69:DG:OP1	1.85	1.09
1:A:43:ARG:NH1	6:J:69:DG:OP1	1.85	1.09
1:A:43:ARG:NH1	6:J:69:DG:OP1	1.85	1.09
1:A:43:ARG:NH1	6:J:69:DG:OP1	1.86	1.08
1:A:43:ARG:NH1	6:J:69:DG:OP1	1.86	1.08
7:K:378:LEU:CA	7:K:676:GLU:CD	2.25	1.08
5:I:95:DC:P	7:K:608:LYS:HB3	1.94	1.07
5:I:95:DC:P	7:K:608:LYS:CB	2.43	1.07
6:J:54:DC:OP1	7:K:816:MET:HB2	1.55	1.06
1:A:43:ARG:NH1	6:J:69:DG:OP1	1.88	1.06
5:I:95:DC:P	7:K:608:LYS:CB	2.43	1.06
5:I:95:DC:P	7:K:608:LYS:N	2.28	1.05
7:K:358:LEU:HD21	9:M:437:LYS:CG	1.87	1.05
7:K:362:MET:HE1	9:M:416:PHE:HZ	1.21	1.05
7:K:358:LEU:HD21	9:M:437:LYS:CG	1.87	1.05
7:K:362:MET:HE1	9:M:416:PHE:HZ	1.21	1.05
7:K:358:LEU:HD21	9:M:437:LYS:CG	1.87	1.05
7:K:362:MET:HE1	9:M:416:PHE:HZ	1.21	1.05
7:K:358:LEU:HD21	9:M:437:LYS:CG	1.87	1.05
7:K:362:MET:HE1	9:M:416:PHE:HZ	1.21	1.05
7:K:358:LEU:HD21	9:M:437:LYS:CG	1.87	1.05
7:K:362:MET:HE1	9:M:416:PHE:HZ	1.21	1.05
7:K:358:LEU:HD21	9:M:437:LYS:CG	1.87	1.05
7:K:362:MET:HE1	9:M:416:PHE:HZ	1.21	1.05
7:K:358:LEU:HD21	9:M:437:LYS:CG	1.87	1.05
7:K:362:MET:HE1	9:M:416:PHE:HZ	1.21	1.05
7:K:358:LEU:HD21	9:M:437:LYS:CG	1.87	1.05
7:K:362:MET:HE1	9:M:416:PHE:HZ	1.21	1.05
7:K:358:LEU:HD21	9:M:437:LYS:CG	1.87	1.05
7:K:362:MET:HE1	9:M:416:PHE:HZ	1.21	1.05
7:K:358:LEU:HD21	9:M:437:LYS:CG	1.87	1.05
7:K:362:MET:HE1	9:M:416:PHE:HZ	1.21	1.05
7:K:381:LEU:CB	7:K:676:GLU:OE2	2.02	1.05
7:K:378:LEU:CB	7:K:676:GLU:OE1	2.04	1.04
7:K:358:LEU:CD2	9:M:438:GLN:HB2	1.89	1.03
7:K:358:LEU:CD2	9:M:438:GLN:HB2	1.89	1.03
7:K:358:LEU:CD2	9:M:438:GLN:HB2	1.89	1.03
7:K:358:LEU:CD2	9:M:438:GLN:HB2	1.89	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:358:LEU:CD2	9:M:438:GLN:HB2	1.89	1.03
7:K:358:LEU:CD2	9:M:438:GLN:HB2	1.89	1.03
7:K:358:LEU:CD2	9:M:438:GLN:HB2	1.89	1.03
7:K:358:LEU:CD2	9:M:438:GLN:HB2	1.89	1.03
7:K:358:LEU:CD2	9:M:438:GLN:HB2	1.89	1.03
7:K:358:LEU:CD2	9:M:438:GLN:HB2	1.89	1.03
7:K:358:LEU:HD21	9:M:437:LYS:HG3	1.38	1.03
7:K:358:LEU:HD21	9:M:437:LYS:HG3	1.38	1.03
7:K:358:LEU:HD21	9:M:437:LYS:HG3	1.38	1.03
7:K:358:LEU:HD21	9:M:437:LYS:HG3	1.38	1.03
7:K:358:LEU:HD21	9:M:437:LYS:HG3	1.38	1.03
7:K:358:LEU:HD21	9:M:437:LYS:HG3	1.38	1.03
7:K:358:LEU:HD21	9:M:437:LYS:HG3	1.38	1.03
7:K:358:LEU:HD21	9:M:437:LYS:HG3	1.38	1.03
7:K:358:LEU:HD21	9:M:437:LYS:HG3	1.38	1.03
7:K:358:LEU:HD21	9:M:437:LYS:HG3	1.38	1.03
7:K:358:LEU:HD21	9:M:437:LYS:HG3	1.38	1.03
7:K:344:ARG:NH1	9:M:181:ASP:OD2	1.90	1.03
7:K:378:LEU:O	7:K:676:GLU:OE2	1.75	1.03
7:K:344:ARG:NH1	9:M:181:ASP:OD2	1.90	1.03
7:K:344:ARG:NH1	9:M:181:ASP:OD2	1.90	1.03
7:K:344:ARG:NH1	9:M:181:ASP:OD2	1.90	1.03
7:K:344:ARG:NH1	9:M:181:ASP:OD2	1.90	1.03
7:K:344:ARG:NH1	9:M:181:ASP:OD2	1.90	1.03
7:K:344:ARG:NH1	9:M:181:ASP:OD2	1.90	1.03
7:K:344:ARG:NH1	9:M:181:ASP:OD2	1.90	1.03
7:K:344:ARG:NH1	9:M:181:ASP:OD2	1.90	1.03
7:K:344:ARG:NH1	9:M:181:ASP:OD2	1.90	1.03
7:K:358:LEU:CD2	9:M:438:GLN:N	2.21	1.02
7:K:358:LEU:CD2	9:M:438:GLN:N	2.21	1.02
7:K:358:LEU:CD2	9:M:438:GLN:N	2.21	1.02
7:K:358:LEU:CD2	9:M:438:GLN:N	2.21	1.02
7:K:358:LEU:CD2	9:M:438:GLN:N	2.21	1.02
7:K:358:LEU:CD2	9:M:438:GLN:N	2.21	1.02
7:K:358:LEU:CD2	9:M:438:GLN:N	2.21	1.02
7:K:358:LEU:CD2	9:M:438:GLN:N	2.21	1.02
7:K:358:LEU:CD2	9:M:438:GLN:N	2.21	1.02
7:K:358:LEU:CD2	9:M:438:GLN:N	2.21	1.02
7:K:362:MET:HB2	9:M:437:LYS:CE	1.90	1.02
7:K:362:MET:HB2	9:M:437:LYS:CE	1.90	1.02
7:K:362:MET:HB2	9:M:437:LYS:CE	1.90	1.02
7:K:362:MET:HB2	9:M:437:LYS:CE	1.90	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:362:MET:HB2	9:M:437:LYS:CE	1.90	1.02
7:K:362:MET:HB2	9:M:437:LYS:CE	1.90	1.02
7:K:362:MET:HB2	9:M:437:LYS:CE	1.90	1.02
7:K:362:MET:HB2	9:M:437:LYS:CE	1.90	1.02
7:K:362:MET:HB2	9:M:437:LYS:CE	1.90	1.02
7:K:362:MET:HB2	9:M:437:LYS:CE	1.90	1.02
7:K:378:LEU:HA	7:K:676:GLU:OE1	1.55	1.02
7:K:351:PHE:CE2	9:M:439:ILE:HD11	1.96	1.00
7:K:351:PHE:CE2	9:M:439:ILE:HD11	1.96	1.00
7:K:351:PHE:CE2	9:M:439:ILE:HD11	1.96	1.00
7:K:351:PHE:CE2	9:M:439:ILE:HD11	1.96	1.00
7:K:351:PHE:CE2	9:M:439:ILE:HD11	1.96	1.00
7:K:351:PHE:CE2	9:M:439:ILE:HD11	1.96	1.00
7:K:378:LEU:CA	7:K:676:GLU:OE2	2.10	1.00
7:K:351:PHE:CE2	9:M:439:ILE:HD11	1.96	1.00
7:K:351:PHE:CE2	9:M:439:ILE:HD11	1.96	1.00
7:K:351:PHE:CE2	9:M:439:ILE:HD11	1.96	1.00
7:K:351:PHE:CE2	9:M:439:ILE:HD11	1.96	1.00
7:K:362:MET:HE1	9:M:416:PHE:CZ	1.97	0.98
7:K:362:MET:HE1	9:M:416:PHE:CZ	1.97	0.98
7:K:362:MET:HE1	9:M:416:PHE:CZ	1.97	0.98
7:K:362:MET:HE1	9:M:416:PHE:CZ	1.97	0.98
7:K:362:MET:HE1	9:M:416:PHE:CZ	1.97	0.98
7:K:362:MET:HE1	9:M:416:PHE:CZ	1.97	0.98
7:K:362:MET:HE1	9:M:416:PHE:CZ	1.97	0.98
7:K:362:MET:HE1	9:M:416:PHE:CZ	1.97	0.98
7:K:362:MET:HE1	9:M:416:PHE:CZ	1.97	0.98
5:I:95:DC:P	7:K:608:LYS:H	1.86	0.98
7:K:362:MET:HE1	9:M:416:PHE:CZ	1.97	0.98
7:K:369:ARG:HG2	9:M:28:GLU:OE2	1.61	0.98
7:K:369:ARG:HG2	9:M:28:GLU:OE2	1.61	0.98
7:K:369:ARG:HG2	9:M:28:GLU:OE2	1.61	0.98
7:K:369:ARG:HG2	9:M:28:GLU:OE2	1.61	0.98
7:K:369:ARG:HG2	9:M:28:GLU:OE2	1.61	0.98
7:K:369:ARG:HG2	9:M:28:GLU:OE2	1.61	0.98
7:K:369:ARG:HG2	9:M:28:GLU:OE2	1.61	0.98
7:K:369:ARG:HG2	9:M:28:GLU:OE2	1.61	0.98
7:K:369:ARG:HG2	9:M:28:GLU:OE2	1.61	0.98
7:K:369:ARG:HG2	9:M:28:GLU:OE2	1.61	0.98
7:K:369:ARG:HG2	9:M:28:GLU:OE2	1.61	0.98
5:I:95:DC:P	7:K:608:LYS:HB3	2.02	0.98
7:K:362:MET:CE	9:M:416:PHE:CZ	2.47	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:362:MET:CE	9:M:416:PHE:CZ	2.47	0.97
7:K:362:MET:CE	9:M:416:PHE:CZ	2.47	0.97
7:K:362:MET:CE	9:M:416:PHE:CZ	2.47	0.97
7:K:362:MET:CE	9:M:416:PHE:CZ	2.47	0.97
7:K:362:MET:CE	9:M:416:PHE:CZ	2.47	0.97
7:K:362:MET:CE	9:M:416:PHE:CZ	2.47	0.97
7:K:362:MET:CE	9:M:416:PHE:CZ	2.47	0.97
7:K:362:MET:CE	9:M:416:PHE:CZ	2.47	0.97
7:K:362:MET:CE	9:M:416:PHE:CZ	2.47	0.97
7:K:378:LEU:HA	7:K:676:GLU:OE2	1.62	0.97
5:I:95:DC:P	7:K:608:LYS:CB	2.53	0.96
7:K:351:PHE:CE1	9:M:467:PHE:CD2	2.51	0.96
7:K:351:PHE:CE1	9:M:467:PHE:CD2	2.51	0.96
7:K:351:PHE:CE1	9:M:467:PHE:CD2	2.51	0.96
7:K:351:PHE:CE1	9:M:467:PHE:CD2	2.51	0.96
7:K:351:PHE:CE1	9:M:467:PHE:CD2	2.51	0.96
7:K:351:PHE:CE1	9:M:467:PHE:CD2	2.51	0.96
7:K:351:PHE:CE1	9:M:467:PHE:CD2	2.51	0.96
7:K:351:PHE:CE1	9:M:467:PHE:CD2	2.51	0.96
7:K:351:PHE:CE1	9:M:467:PHE:CD2	2.51	0.96
7:K:351:PHE:CE1	9:M:467:PHE:CD2	2.51	0.96
7:K:378:LEU:CB	7:K:676:GLU:CD	2.38	0.96
7:K:362:MET:CB	9:M:437:LYS:HZ1	1.57	0.95
7:K:362:MET:CB	9:M:437:LYS:HZ1	1.57	0.95
7:K:362:MET:CB	9:M:437:LYS:HZ1	1.57	0.95
7:K:362:MET:CB	9:M:437:LYS:HZ1	1.57	0.95
7:K:362:MET:CB	9:M:437:LYS:HZ1	1.57	0.95
7:K:362:MET:CB	9:M:437:LYS:HZ1	1.57	0.95
7:K:362:MET:CB	9:M:437:LYS:HZ1	1.57	0.95
7:K:362:MET:CB	9:M:437:LYS:HZ1	1.57	0.95
7:K:362:MET:CB	9:M:437:LYS:HZ1	1.57	0.95
7:K:362:MET:CB	9:M:437:LYS:HZ1	1.57	0.95
5:I:95:DC:P	7:K:608:LYS:HB3	2.06	0.94
7:K:358:LEU:HD22	9:M:438:GLN:HB2	1.45	0.94
7:K:358:LEU:HD22	9:M:438:GLN:HB2	1.45	0.94
7:K:358:LEU:HD22	9:M:438:GLN:HB2	1.45	0.94
7:K:358:LEU:HD22	9:M:438:GLN:HB2	1.45	0.94
7:K:358:LEU:HD22	9:M:438:GLN:HB2	1.45	0.94
7:K:358:LEU:HD22	9:M:438:GLN:HB2	1.45	0.94
7:K:358:LEU:HD22	9:M:438:GLN:HB2	1.45	0.94
7:K:358:LEU:HD22	9:M:438:GLN:HB2	1.45	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:358:LEU:HD22	9:M:438:GLN:HB2	1.45	0.94
7:K:358:LEU:HD22	9:M:438:GLN:HB2	1.45	0.94
6:J:55:DG:OP1	7:K:866:SER:OG	1.86	0.93
12:K:1502:ADP:O2A	12:K:1502:ADP:O4'	1.86	0.93
12:K:1502:ADP:O2A	12:K:1502:ADP:C4'	2.17	0.93
6:J:54:DC:OP1	7:K:816:MET:HB2	1.68	0.93
7:K:649:PHE:CD2	7:K:649:PHE:O	2.21	0.93
7:K:354:LEU:HG	9:M:438:GLN:CG	2.00	0.92
7:K:354:LEU:HG	9:M:438:GLN:CG	2.00	0.92
7:K:354:LEU:HG	9:M:438:GLN:CG	2.00	0.92
7:K:354:LEU:HG	9:M:438:GLN:CG	2.00	0.92
7:K:354:LEU:HG	9:M:438:GLN:CG	2.00	0.92
7:K:354:LEU:HG	9:M:438:GLN:CG	2.00	0.92
7:K:354:LEU:HG	9:M:438:GLN:CG	2.00	0.92
7:K:354:LEU:HG	9:M:438:GLN:CG	2.00	0.92
7:K:354:LEU:HG	9:M:438:GLN:CG	2.00	0.92
7:K:354:LEU:HG	9:M:438:GLN:CG	2.00	0.92
7:K:354:LEU:HG	9:M:438:GLN:CG	2.00	0.92
5:I:95:DC:P	7:K:608:LYS:HB3	2.10	0.92
7:K:347:ARG:HD3	9:M:466:GLN:O	1.69	0.92
7:K:347:ARG:HD3	9:M:466:GLN:O	1.69	0.92
7:K:347:ARG:HD3	9:M:466:GLN:O	1.69	0.92
7:K:347:ARG:HD3	9:M:466:GLN:O	1.69	0.92
7:K:347:ARG:HD3	9:M:466:GLN:O	1.69	0.92
7:K:347:ARG:HD3	9:M:466:GLN:O	1.69	0.92
7:K:347:ARG:HD3	9:M:466:GLN:O	1.69	0.92
7:K:347:ARG:HD3	9:M:466:GLN:O	1.69	0.92
7:K:347:ARG:HD3	9:M:466:GLN:O	1.69	0.92
7:K:347:ARG:HD3	9:M:466:GLN:O	1.69	0.92
6:J:54:DC:OP1	7:K:816:MET:HB2	1.69	0.92
7:K:358:LEU:HB2	9:M:438:GLN:CD	1.94	0.92
7:K:358:LEU:HB2	9:M:438:GLN:CD	1.94	0.92
7:K:358:LEU:HB2	9:M:438:GLN:CD	1.94	0.92
7:K:358:LEU:HB2	9:M:438:GLN:CD	1.94	0.92
7:K:358:LEU:HB2	9:M:438:GLN:CD	1.94	0.92
7:K:358:LEU:HB2	9:M:438:GLN:CD	1.94	0.92
7:K:358:LEU:HB2	9:M:438:GLN:CD	1.94	0.92
7:K:358:LEU:HB2	9:M:438:GLN:CD	1.94	0.92
7:K:358:LEU:HB2	9:M:438:GLN:CD	1.94	0.92
7:K:358:LEU:HB2	9:M:438:GLN:CD	1.94	0.92
7:K:358:LEU:HB2	9:M:438:GLN:CD	1.94	0.92
7:K:392:LEU:HD11	9:M:420:LYS:NZ	1.86	0.91
7:K:378:LEU:HA	7:K:676:GLU:CD	1.93	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:378:LEU:O	7:K:676:GLU:OE2	1.87	0.91
7:K:351:PHE:HB3	9:M:151:TYR:OH	1.69	0.91
7:K:351:PHE:HB3	9:M:151:TYR:OH	1.69	0.91
7:K:351:PHE:HB3	9:M:151:TYR:OH	1.69	0.91
7:K:351:PHE:HB3	9:M:151:TYR:OH	1.69	0.91
7:K:351:PHE:HB3	9:M:151:TYR:OH	1.69	0.91
7:K:351:PHE:HB3	9:M:151:TYR:OH	1.69	0.91
7:K:351:PHE:HB3	9:M:151:TYR:OH	1.69	0.91
7:K:351:PHE:HB3	9:M:151:TYR:OH	1.69	0.91
7:K:351:PHE:HB3	9:M:151:TYR:OH	1.69	0.91
7:K:351:PHE:HB3	9:M:151:TYR:OH	1.69	0.91
7:K:351:PHE:HB3	9:M:151:TYR:OH	1.69	0.91
12:K:1502:ADP:O2A	12:K:1502:ADP:C4'	2.18	0.90
5:I:94:DG:OP1	7:K:608:LYS:NZ	2.03	0.90
12:K:1502:ADP:O2A	12:K:1502:ADP:O4'	1.89	0.89
7:K:347:ARG:NH1	9:M:466:GLN:N	2.20	0.89
7:K:347:ARG:NH1	9:M:466:GLN:N	2.20	0.89
7:K:347:ARG:NH1	9:M:466:GLN:N	2.20	0.89
7:K:347:ARG:NH1	9:M:466:GLN:N	2.20	0.89
7:K:347:ARG:NH1	9:M:466:GLN:N	2.20	0.89
7:K:347:ARG:NH1	9:M:466:GLN:N	2.20	0.89
7:K:347:ARG:NH1	9:M:466:GLN:N	2.20	0.89
7:K:347:ARG:NH1	9:M:466:GLN:N	2.20	0.89
7:K:347:ARG:NH1	9:M:466:GLN:N	2.20	0.89
7:K:347:ARG:NH1	9:M:466:GLN:N	2.20	0.89
6:J:54:DC:OP1	7:K:816:MET:HB2	1.72	0.89
7:K:354:LEU:HG	9:M:438:GLN:HG3	1.51	0.89
7:K:354:LEU:HG	9:M:438:GLN:HG3	1.51	0.89
7:K:354:LEU:HG	9:M:438:GLN:HG3	1.51	0.89
7:K:354:LEU:HG	9:M:438:GLN:HG3	1.51	0.89
7:K:354:LEU:HG	9:M:438:GLN:HG3	1.51	0.89
7:K:354:LEU:HG	9:M:438:GLN:HG3	1.51	0.89
6:J:55:DG:OP1	7:K:866:SER:OG	1.90	0.89
7:K:354:LEU:HG	9:M:438:GLN:HG3	1.51	0.89
7:K:354:LEU:HG	9:M:438:GLN:HG3	1.51	0.89
7:K:354:LEU:HG	9:M:438:GLN:HG3	1.51	0.89
7:K:354:LEU:HG	9:M:438:GLN:HG3	1.51	0.89
6:J:54:DC:H3'	7:K:816:MET:HG3	1.53	0.87
9:M:154:ILE:HG22	9:M:154:ILE:O	1.74	0.87
9:M:154:ILE:HG22	9:M:154:ILE:O	1.74	0.87
9:M:154:ILE:HG22	9:M:154:ILE:O	1.74	0.87
9:M:154:ILE:HG22	9:M:154:ILE:O	1.74	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:54:DC:OP1	7:K:816:MET:HB2	1.75	0.87
9:M:154:ILE:HG22	9:M:154:ILE:O	1.74	0.87
9:M:154:ILE:HG22	9:M:154:ILE:O	1.74	0.87
9:M:154:ILE:HG22	9:M:154:ILE:O	1.74	0.87
9:M:154:ILE:HG22	9:M:154:ILE:O	1.74	0.87
9:M:154:ILE:HG22	9:M:154:ILE:O	1.74	0.87
9:M:154:ILE:HG22	9:M:154:ILE:O	1.74	0.87
7:K:351:PHE:HE1	9:M:467:PHE:CE2	1.43	0.87
7:K:351:PHE:HE1	9:M:467:PHE:CE2	1.43	0.87
7:K:351:PHE:HE1	9:M:467:PHE:CE2	1.43	0.87
7:K:351:PHE:HE1	9:M:467:PHE:CE2	1.43	0.87
7:K:351:PHE:HE1	9:M:467:PHE:CE2	1.43	0.87
7:K:351:PHE:HE1	9:M:467:PHE:CE2	1.43	0.87
7:K:649:PHE:O	7:K:649:PHE:CD1	2.28	0.87
7:K:351:PHE:HE1	9:M:467:PHE:CE2	1.43	0.87
7:K:351:PHE:HE1	9:M:467:PHE:CE2	1.43	0.87
7:K:351:PHE:HE1	9:M:467:PHE:CE2	1.43	0.87
7:K:351:PHE:HE1	9:M:467:PHE:CE2	1.43	0.87
5:I:95:DC:P	7:K:608:LYS:HB3	2.15	0.86
7:K:369:ARG:CG	9:M:28:GLU:OE2	2.23	0.86
7:K:369:ARG:CG	9:M:28:GLU:OE2	2.23	0.86
7:K:369:ARG:CG	9:M:28:GLU:OE2	2.23	0.86
7:K:369:ARG:CG	9:M:28:GLU:OE2	2.23	0.86
7:K:369:ARG:CG	9:M:28:GLU:OE2	2.23	0.86
7:K:369:ARG:CG	9:M:28:GLU:OE2	2.23	0.86
7:K:369:ARG:CG	9:M:28:GLU:OE2	2.23	0.86
7:K:369:ARG:CG	9:M:28:GLU:OE2	2.23	0.86
7:K:369:ARG:CG	9:M:28:GLU:OE2	2.23	0.86
7:K:369:ARG:CG	9:M:28:GLU:OE2	2.23	0.86
7:K:369:ARG:CG	9:M:28:GLU:OE2	2.23	0.86
5:I:95:DC:P	7:K:608:LYS:H	1.98	0.86
5:I:94:DG:O3'	7:K:608:LYS:HB3	1.76	0.85
5:I:16:DG:OP1	7:K:588:LYS:NZ	2.09	0.85
7:K:362:MET:CG	9:M:437:LYS:NZ	2.22	0.85
7:K:362:MET:CG	9:M:437:LYS:NZ	2.22	0.85
5:I:95:DC:OP1	7:K:608:LYS:HB3	1.76	0.85
7:K:362:MET:CG	9:M:437:LYS:NZ	2.22	0.85
7:K:362:MET:CG	9:M:437:LYS:NZ	2.22	0.85
7:K:362:MET:CG	9:M:437:LYS:NZ	2.22	0.85
7:K:362:MET:CG	9:M:437:LYS:NZ	2.22	0.85
7:K:362:MET:CG	9:M:437:LYS:NZ	2.22	0.85
7:K:362:MET:CG	9:M:437:LYS:NZ	2.22	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:362:MET:CG	9:M:437:LYS:NZ	2.22	0.85
7:K:362:MET:CG	9:M:437:LYS:NZ	2.22	0.85
5:I:95:DC:OP1	7:K:608:LYS:CA	2.26	0.84
12:K:1502:ADP:O1A	12:K:1502:ADP:O3B	1.94	0.84
7:K:649:PHE:O	7:K:649:PHE:CD1	2.31	0.84
7:K:369:ARG:NE	9:M:28:GLU:OE2	2.10	0.83
7:K:369:ARG:NE	9:M:28:GLU:OE2	2.10	0.83
7:K:369:ARG:NE	9:M:28:GLU:OE2	2.10	0.83
7:K:369:ARG:NE	9:M:28:GLU:OE2	2.10	0.83
7:K:369:ARG:NE	9:M:28:GLU:OE2	2.10	0.83
7:K:369:ARG:NE	9:M:28:GLU:OE2	2.10	0.83
7:K:369:ARG:NE	9:M:28:GLU:OE2	2.10	0.83
7:K:369:ARG:NE	9:M:28:GLU:OE2	2.10	0.83
7:K:369:ARG:NE	9:M:28:GLU:OE2	2.10	0.83
7:K:369:ARG:NE	9:M:28:GLU:OE2	2.10	0.83
7:K:369:ARG:NE	9:M:28:GLU:OE2	2.10	0.83
7:K:369:ARG:CD	9:M:28:GLU:OE2	2.26	0.83
7:K:369:ARG:CD	9:M:28:GLU:OE2	2.26	0.83
7:K:369:ARG:CD	9:M:28:GLU:OE2	2.26	0.83
7:K:369:ARG:CD	9:M:28:GLU:OE2	2.26	0.83
7:K:369:ARG:CD	9:M:28:GLU:OE2	2.26	0.83
7:K:369:ARG:CD	9:M:28:GLU:OE2	2.26	0.83
7:K:369:ARG:CD	9:M:28:GLU:OE2	2.26	0.83
7:K:369:ARG:CD	9:M:28:GLU:OE2	2.26	0.83
7:K:369:ARG:CD	9:M:28:GLU:OE2	2.26	0.83
7:K:369:ARG:CD	9:M:28:GLU:OE2	2.26	0.83
7:K:369:ARG:CD	9:M:28:GLU:OE2	2.26	0.83
5:I:95:DC:OP1	7:K:609:LEU:N	2.12	0.83
7:K:351:PHE:CD1	9:M:467:PHE:CE2	2.65	0.82
7:K:351:PHE:CD1	9:M:467:PHE:CE2	2.65	0.82
7:K:351:PHE:CD1	9:M:467:PHE:CE2	2.65	0.82
7:K:351:PHE:CD1	9:M:467:PHE:CE2	2.65	0.82
7:K:351:PHE:CD1	9:M:467:PHE:CE2	2.65	0.82
7:K:351:PHE:CD1	9:M:467:PHE:CE2	2.65	0.82
7:K:351:PHE:CD1	9:M:467:PHE:CE2	2.65	0.82
7:K:351:PHE:CD1	9:M:467:PHE:CE2	2.65	0.82
7:K:351:PHE:CD1	9:M:467:PHE:CE2	2.65	0.82
7:K:351:PHE:CD1	9:M:467:PHE:CE2	2.65	0.82
12:K:1502:ADP:O2A	12:K:1502:ADP:H4'	1.77	0.82
5:I:95:DC:OP1	7:K:608:LYS:N	2.13	0.82
7:K:358:LEU:CD2	9:M:437:LYS:HG3	2.09	0.82
7:K:358:LEU:CD2	9:M:437:LYS:HG3	2.09	0.82
7:K:358:LEU:CD2	9:M:437:LYS:HG3	2.09	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:358:LEU:CD2	9:M:437:LYS:HG3	2.09	0.82
7:K:358:LEU:CD2	9:M:437:LYS:HG3	2.09	0.82
7:K:358:LEU:CD2	9:M:437:LYS:HG3	2.09	0.82
7:K:358:LEU:CD2	9:M:437:LYS:HG3	2.09	0.82
7:K:358:LEU:CD2	9:M:437:LYS:HG3	2.09	0.82
7:K:358:LEU:CD2	9:M:437:LYS:HG3	2.09	0.82
7:K:358:LEU:CD2	9:M:437:LYS:HG3	2.09	0.82
5:I:95:DC:OP2	7:K:608:LYS:HB2	1.79	0.82
6:J:54:DC:H3'	7:K:816:MET:HG3	1.61	0.81
7:K:616:TYR:O	7:K:616:TYR:CD2	2.33	0.81
7:K:351:PHE:CZ	9:M:467:PHE:CE2	2.48	0.80
7:K:351:PHE:CZ	9:M:467:PHE:CE2	2.48	0.80
7:K:351:PHE:CZ	9:M:467:PHE:CE2	2.48	0.80
7:K:351:PHE:CZ	9:M:467:PHE:CE2	2.48	0.80
7:K:351:PHE:CZ	9:M:467:PHE:CE2	2.48	0.80
7:K:351:PHE:CZ	9:M:467:PHE:CE2	2.48	0.80
7:K:351:PHE:CZ	9:M:467:PHE:CE2	2.48	0.80
7:K:351:PHE:CZ	9:M:467:PHE:CE2	2.48	0.80
7:K:351:PHE:CZ	9:M:467:PHE:CE2	2.48	0.80
7:K:351:PHE:CZ	9:M:467:PHE:CE2	2.48	0.80
7:K:351:PHE:CZ	9:M:467:PHE:CE2	2.48	0.80
3:G:78:ARG:HE	5:I:20:DA:H4'	1.43	0.80
5:I:95:DC:P	7:K:608:LYS:H	2.04	0.80
6:J:55:DG:OP1	7:K:866:SER:OG	1.98	0.80
7:K:358:LEU:HD11	9:M:437:LYS:HG3	1.64	0.80
7:K:358:LEU:HD11	9:M:437:LYS:HG3	1.64	0.80
7:K:358:LEU:HD11	9:M:437:LYS:HG3	1.64	0.80
7:K:358:LEU:HD11	9:M:437:LYS:HG3	1.64	0.80
7:K:358:LEU:HD11	9:M:437:LYS:HG3	1.64	0.80
7:K:358:LEU:HD11	9:M:437:LYS:HG3	1.64	0.80
7:K:358:LEU:HD11	9:M:437:LYS:HG3	1.64	0.80
7:K:358:LEU:HD11	9:M:437:LYS:HG3	1.64	0.80
7:K:358:LEU:HD11	9:M:437:LYS:HG3	1.64	0.80
7:K:358:LEU:HD11	9:M:437:LYS:HG3	1.64	0.80
7:K:358:LEU:HD11	9:M:437:LYS:HG3	1.64	0.80
7:K:392:LEU:CD1	9:M:420:LYS:NZ	2.44	0.80
7:K:378:LEU:O	7:K:676:GLU:CD	2.24	0.80
7:K:887:THR:O	7:K:887:THR:HG22	1.81	0.79
12:K:1502:ADP:O1A	12:K:1502:ADP:O3B	1.97	0.79
7:K:359:HIS:CE1	9:M:434:ILE:HG23	2.14	0.79
7:K:359:HIS:CE1	9:M:434:ILE:HG23	2.14	0.79
7:K:359:HIS:CE1	9:M:434:ILE:HG23	2.14	0.79
7:K:359:HIS:CE1	9:M:434:ILE:HG23	2.14	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:359:HIS:CE1	9:M:434:ILE:HG23	2.14	0.79
7:K:359:HIS:CE1	9:M:434:ILE:HG23	2.14	0.79
7:K:359:HIS:CE1	9:M:434:ILE:HG23	2.14	0.79
7:K:359:HIS:CE1	9:M:434:ILE:HG23	2.14	0.79
7:K:359:HIS:CE1	9:M:434:ILE:HG23	2.14	0.79
7:K:359:HIS:CE1	9:M:434:ILE:HG23	2.14	0.79
7:K:358:LEU:CD2	9:M:438:GLN:H	1.94	0.79
7:K:358:LEU:CD2	9:M:438:GLN:H	1.94	0.79
7:K:358:LEU:CD2	9:M:438:GLN:H	1.94	0.79
7:K:358:LEU:CD2	9:M:438:GLN:H	1.94	0.79
7:K:358:LEU:CD2	9:M:438:GLN:H	1.94	0.79
7:K:358:LEU:CD2	9:M:438:GLN:H	1.94	0.79
7:K:358:LEU:CD2	9:M:438:GLN:H	1.94	0.79
7:K:358:LEU:CD2	9:M:438:GLN:H	1.94	0.79
7:K:358:LEU:CD2	9:M:438:GLN:H	1.94	0.79
7:K:358:LEU:CD2	9:M:438:GLN:H	1.94	0.79
7:K:358:LEU:CD2	9:M:438:GLN:H	1.94	0.79
5:I:16:DG:OP1	7:K:588:LYS:NZ	2.15	0.79
7:K:347:ARG:HH12	9:M:466:GLN:N	1.79	0.79
7:K:347:ARG:HH12	9:M:466:GLN:N	1.79	0.79
7:K:347:ARG:HH12	9:M:466:GLN:N	1.79	0.79
7:K:347:ARG:HH12	9:M:466:GLN:N	1.79	0.79
7:K:347:ARG:HH12	9:M:466:GLN:N	1.79	0.79
7:K:347:ARG:HH12	9:M:466:GLN:N	1.79	0.79
7:K:347:ARG:HH12	9:M:466:GLN:N	1.79	0.79
7:K:347:ARG:HH12	9:M:466:GLN:N	1.79	0.79
7:K:347:ARG:HH12	9:M:466:GLN:N	1.79	0.79
7:K:347:ARG:HH12	9:M:466:GLN:N	1.79	0.79
7:K:347:ARG:HH12	9:M:466:GLN:N	1.79	0.79
7:K:344:ARG:HH12	9:M:181:ASP:CG	1.90	0.79
7:K:344:ARG:HH12	9:M:181:ASP:CG	1.90	0.79
7:K:344:ARG:HH12	9:M:181:ASP:CG	1.90	0.79
7:K:344:ARG:HH12	9:M:181:ASP:CG	1.90	0.79
7:K:344:ARG:HH12	9:M:181:ASP:CG	1.90	0.79
7:K:344:ARG:HH12	9:M:181:ASP:CG	1.90	0.79
7:K:344:ARG:HH12	9:M:181:ASP:CG	1.90	0.79
7:K:344:ARG:HH12	9:M:181:ASP:CG	1.90	0.79
7:K:344:ARG:HH12	9:M:181:ASP:CG	1.90	0.79
7:K:344:ARG:HH12	9:M:181:ASP:CG	1.90	0.79
3:G:78:ARG:HE	5:I:20:DA:H4'	1.45	0.79
7:K:362:MET:HE3	9:M:416:PHE:CE2	2.19	0.78
7:K:362:MET:HE3	9:M:416:PHE:CE2	2.19	0.78
7:K:362:MET:HE3	9:M:416:PHE:CE2	2.19	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:362:MET:HE3	9:M:416:PHE:CE2	2.19	0.78
7:K:362:MET:HE3	9:M:416:PHE:CE2	2.19	0.78
7:K:362:MET:HE3	9:M:416:PHE:CE2	2.19	0.78
7:K:362:MET:HE3	9:M:416:PHE:CE2	2.19	0.78
7:K:362:MET:HE3	9:M:416:PHE:CE2	2.19	0.78
7:K:362:MET:HE3	9:M:416:PHE:CE2	2.19	0.78
7:K:362:MET:HE3	9:M:416:PHE:CE2	2.19	0.78
12:K:1502:ADP:O1A	13:K:1503:BEF:F2	1.91	0.78
6:J:54:DC:OP1	7:K:816:MET:HB3	1.83	0.78
12:K:1502:ADP:O2A	12:K:1502:ADP:H4'	1.82	0.78
7:K:362:MET:HE3	9:M:416:PHE:CZ	2.19	0.78
7:K:362:MET:HE3	9:M:416:PHE:CZ	2.19	0.78
7:K:362:MET:HE3	9:M:416:PHE:CZ	2.19	0.78
7:K:362:MET:HE3	9:M:416:PHE:CZ	2.19	0.78
7:K:362:MET:HE3	9:M:416:PHE:CZ	2.19	0.78
7:K:362:MET:HE3	9:M:416:PHE:CZ	2.19	0.78
7:K:378:LEU:CB	7:K:676:GLU:OE2	2.31	0.78
7:K:362:MET:HE3	9:M:416:PHE:CZ	2.19	0.78
7:K:362:MET:HE3	9:M:416:PHE:CZ	2.19	0.78
12:K:1502:ADP:O1A	12:K:1502:ADP:O3B	1.98	0.78
7:K:362:MET:HE3	9:M:416:PHE:CZ	2.19	0.78
7:K:362:MET:HE3	9:M:416:PHE:CZ	2.19	0.78
5:I:95:DC:OP2	7:K:608:LYS:CB	2.32	0.78
7:K:362:MET:HG3	9:M:437:LYS:NZ	1.92	0.78
7:K:362:MET:HG3	9:M:437:LYS:NZ	1.92	0.78
7:K:362:MET:HG3	9:M:437:LYS:NZ	1.92	0.78
7:K:362:MET:HG3	9:M:437:LYS:NZ	1.92	0.78
5:I:95:DC:P	7:K:608:LYS:H	2.06	0.78
7:K:362:MET:HG3	9:M:437:LYS:NZ	1.92	0.78
7:K:362:MET:HG3	9:M:437:LYS:NZ	1.92	0.78
7:K:362:MET:HG3	9:M:437:LYS:NZ	1.92	0.78
7:K:362:MET:HG3	9:M:437:LYS:NZ	1.92	0.78
7:K:362:MET:HG3	9:M:437:LYS:NZ	1.92	0.78
7:K:362:MET:HG3	9:M:437:LYS:NZ	1.92	0.78
7:K:351:PHE:CE2	9:M:439:ILE:CD1	2.67	0.78
7:K:351:PHE:CE2	9:M:439:ILE:CD1	2.67	0.78
5:I:95:DC:OP1	7:K:609:LEU:N	2.16	0.78
7:K:351:PHE:CE2	9:M:439:ILE:CD1	2.67	0.78
7:K:351:PHE:CE2	9:M:439:ILE:CD1	2.67	0.78
7:K:351:PHE:CE2	9:M:439:ILE:CD1	2.67	0.78
7:K:351:PHE:CE2	9:M:439:ILE:CD1	2.67	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:351:PHE:CE2	9:M:439:ILE:CD1	2.67	0.78
7:K:351:PHE:CE2	9:M:439:ILE:CD1	2.67	0.78
7:K:351:PHE:CE2	9:M:439:ILE:CD1	2.67	0.78
7:K:351:PHE:CE2	9:M:439:ILE:CD1	2.67	0.78
6:J:55:DG:OP1	7:K:866:SER:OG	2.02	0.77
5:I:95:DC:P	7:K:608:LYS:CB	2.71	0.77
7:K:351:PHE:CD1	9:M:467:PHE:CD2	2.73	0.77
7:K:351:PHE:CD1	9:M:467:PHE:CD2	2.73	0.77
7:K:351:PHE:CD1	9:M:467:PHE:CD2	2.73	0.77
7:K:351:PHE:CD1	9:M:467:PHE:CD2	2.73	0.77
7:K:351:PHE:CD1	9:M:467:PHE:CD2	2.73	0.77
7:K:351:PHE:CD1	9:M:467:PHE:CD2	2.73	0.77
7:K:351:PHE:CD1	9:M:467:PHE:CD2	2.73	0.77
7:K:351:PHE:CD1	9:M:467:PHE:CD2	2.73	0.77
7:K:351:PHE:CD1	9:M:467:PHE:CD2	2.73	0.77
7:K:351:PHE:CD1	9:M:467:PHE:CD2	2.73	0.77
7:K:351:PHE:CD1	9:M:467:PHE:CD2	2.73	0.77
7:K:359:HIS:HB3	7:K:363:GLU:OE2	1.83	0.77
7:K:359:HIS:HB3	7:K:363:GLU:OE2	1.83	0.77
7:K:359:HIS:HB3	7:K:363:GLU:OE2	1.83	0.77
7:K:359:HIS:HB3	7:K:363:GLU:OE2	1.83	0.77
7:K:359:HIS:HB3	7:K:363:GLU:OE2	1.83	0.77
7:K:359:HIS:HB3	7:K:363:GLU:OE2	1.83	0.77
7:K:359:HIS:HB3	7:K:363:GLU:OE2	1.83	0.77
7:K:359:HIS:HB3	7:K:363:GLU:OE2	1.83	0.77
7:K:359:HIS:HB3	7:K:363:GLU:OE2	1.83	0.77
7:K:359:HIS:HB3	7:K:363:GLU:OE2	1.83	0.77
7:K:359:HIS:HB3	7:K:363:GLU:OE2	1.83	0.77
3:G:78:ARG:HE	5:I:20:DA:H4'	1.47	0.77
5:I:94:DG:O3'	7:K:608:LYS:HB3	1.84	0.77
6:J:54:DC:OP1	7:K:816:MET:HB3	1.80	0.77
7:K:358:LEU:HD21	9:M:437:LYS:HG2	1.65	0.77
7:K:358:LEU:HD21	9:M:437:LYS:HG2	1.65	0.77
7:K:358:LEU:HD21	9:M:437:LYS:HG2	1.65	0.77
7:K:358:LEU:HD21	9:M:437:LYS:HG2	1.65	0.77
5:I:95:DC:P	7:K:608:LYS:HB3	2.25	0.77
7:K:358:LEU:HD21	9:M:437:LYS:HG2	1.65	0.77
7:K:358:LEU:HD21	9:M:437:LYS:HG2	1.65	0.77
7:K:358:LEU:HD21	9:M:437:LYS:HG2	1.65	0.77
7:K:358:LEU:HD21	9:M:437:LYS:HG2	1.65	0.77
7:K:358:LEU:HD21	9:M:437:LYS:HG2	1.65	0.77
7:K:358:LEU:HD21	9:M:437:LYS:HG2	1.65	0.77
12:K:1502:ADP:O1A	12:K:1502:ADP:O3B	2.01	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:54:DC:OP1	7:K:817:THR:HG23	1.85	0.76
12:K:1502:ADP:O1A	12:K:1502:ADP:O3B	2.01	0.76
5:I:95:DC:P	7:K:608:LYS:HB2	2.24	0.76
5:I:95:DC:P	7:K:608:LYS:CB	2.73	0.76
6:J:54:DC:H3'	7:K:816:MET:HG3	1.67	0.76
6:J:55:DG:OP1	7:K:866:SER:OG	2.04	0.75
7:K:844:GLU:N	7:K:844:GLU:OE1	2.18	0.75
5:I:94:DG:O3'	7:K:608:LYS:HB3	1.86	0.75
3:G:78:ARG:NE	5:I:20:DA:H4'	2.02	0.75
5:I:95:DC:OP1	7:K:608:LYS:HB3	1.86	0.74
7:K:358:LEU:HD23	9:M:434:ILE:O	1.87	0.74
3:G:78:ARG:HE	5:I:20:DA:H4'	1.50	0.74
7:K:358:LEU:HD23	9:M:434:ILE:O	1.87	0.74
7:K:358:LEU:HD23	9:M:434:ILE:O	1.87	0.74
7:K:358:LEU:HD23	9:M:434:ILE:O	1.87	0.74
7:K:358:LEU:HD23	9:M:434:ILE:O	1.87	0.74
7:K:358:LEU:HD23	9:M:434:ILE:O	1.87	0.74
7:K:358:LEU:HD23	9:M:434:ILE:O	1.87	0.74
7:K:358:LEU:HD23	9:M:434:ILE:O	1.87	0.74
7:K:358:LEU:HD23	9:M:434:ILE:O	1.87	0.74
5:I:95:DC:P	7:K:608:LYS:N	2.60	0.74
7:K:358:LEU:HD23	9:M:434:ILE:O	1.87	0.74
7:K:351:PHE:HE2	9:M:439:ILE:HD11	1.49	0.74
5:I:97:DA:OP2	7:K:603:LYS:NZ	2.18	0.74
7:K:351:PHE:HE2	9:M:439:ILE:HD11	1.49	0.74
7:K:351:PHE:HE2	9:M:439:ILE:HD11	1.49	0.74
7:K:351:PHE:HE2	9:M:439:ILE:HD11	1.49	0.74
7:K:351:PHE:HE2	9:M:439:ILE:HD11	1.49	0.74
7:K:351:PHE:HE2	9:M:439:ILE:HD11	1.49	0.74
5:I:96:DC:OP1	7:K:603:LYS:HG3	1.87	0.74
7:K:351:PHE:HE2	9:M:439:ILE:HD11	1.49	0.74
7:K:351:PHE:HE2	9:M:439:ILE:HD11	1.49	0.74
7:K:351:PHE:HE2	9:M:439:ILE:HD11	1.49	0.74
7:K:351:PHE:HE2	9:M:439:ILE:HD11	1.49	0.74
7:K:844:GLU:N	7:K:844:GLU:OE1	2.20	0.74
5:I:95:DC:OP1	7:K:608:LYS:N	2.19	0.74
7:K:351:PHE:HE2	9:M:439:ILE:CD1	1.99	0.73
7:K:358:LEU:CD2	9:M:438:GLN:CB	2.55	0.73
7:K:351:PHE:HE2	9:M:439:ILE:CD1	1.99	0.73
7:K:358:LEU:CD2	9:M:438:GLN:CB	2.55	0.73
7:K:351:PHE:HE2	9:M:439:ILE:CD1	1.99	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:358:LEU:CD2	9:M:438:GLN:CB	2.55	0.73
7:K:351:PHE:HE2	9:M:439:ILE:CD1	1.99	0.73
7:K:358:LEU:CD2	9:M:438:GLN:CB	2.55	0.73
7:K:351:PHE:HE2	9:M:439:ILE:CD1	1.99	0.73
7:K:358:LEU:CD2	9:M:438:GLN:CB	2.55	0.73
7:K:351:PHE:HE2	9:M:439:ILE:CD1	1.99	0.73
7:K:358:LEU:CD2	9:M:438:GLN:CB	2.55	0.73
7:K:351:PHE:HE2	9:M:439:ILE:CD1	1.99	0.73
7:K:358:LEU:CD2	9:M:438:GLN:CB	2.55	0.73
7:K:351:PHE:HE2	9:M:439:ILE:CD1	1.99	0.73
7:K:358:LEU:CD2	9:M:438:GLN:CB	2.55	0.73
7:K:351:PHE:HE2	9:M:439:ILE:CD1	1.99	0.73
7:K:358:LEU:CD2	9:M:438:GLN:CB	2.55	0.73
7:K:351:PHE:HE2	9:M:439:ILE:CD1	1.99	0.73
7:K:358:LEU:CD2	9:M:438:GLN:CB	2.55	0.73
7:K:351:PHE:HE2	9:M:439:ILE:CD1	1.99	0.73
7:K:358:LEU:CD2	9:M:438:GLN:CB	2.55	0.73
7:K:378:LEU:HA	7:K:676:GLU:OE1	1.89	0.73
5:I:95:DC:OP2	7:K:608:LYS:N	2.19	0.73
7:K:1001:GLU:OE1	7:K:1001:GLU:HA	1.89	0.73
5:I:95:DC:P	7:K:608:LYS:H	2.11	0.73
7:K:381:LEU:CB	7:K:676:GLU:OE1	2.36	0.73
6:J:56:DG:H5"	7:K:528:LEU:HD12	1.70	0.73
6:J:55:DG:OP1	7:K:866:SER:OG	2.06	0.73
3:G:78:ARG:NE	5:I:20:DA:H4'	2.04	0.73
5:I:95:DC:OP1	7:K:608:LYS:HB3	1.87	0.73
7:K:358:LEU:CD2	9:M:434:ILE:O	2.37	0.73
7:K:358:LEU:CD2	9:M:434:ILE:O	2.37	0.73
7:K:358:LEU:CD2	9:M:434:ILE:O	2.37	0.73
7:K:358:LEU:CD2	9:M:434:ILE:O	2.37	0.73
7:K:358:LEU:CD2	9:M:434:ILE:O	2.37	0.73
7:K:358:LEU:CD2	9:M:434:ILE:O	2.37	0.73
7:K:358:LEU:CD2	9:M:434:ILE:O	2.37	0.73
7:K:358:LEU:CD2	9:M:434:ILE:O	2.37	0.73
7:K:358:LEU:CD2	9:M:434:ILE:O	2.37	0.73
7:K:358:LEU:CD2	9:M:434:ILE:O	2.37	0.73
7:K:358:LEU:CD2	9:M:434:ILE:O	2.37	0.73
7:K:649:PHE:O	7:K:649:PHE:CG	2.42	0.72
7:K:844:GLU:OE1	7:K:844:GLU:N	2.23	0.72
12:K:1502:ADP:O2A	12:K:1502:ADP:H4'	1.87	0.72
3:G:78:ARG:NE	5:I:20:DA:H4'	2.05	0.72
7:K:358:LEU:CA	9:M:438:GLN:OE1	2.37	0.72
7:K:358:LEU:CA	9:M:438:GLN:OE1	2.37	0.72
7:K:358:LEU:CA	9:M:438:GLN:OE1	2.37	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:358:LEU:CA	9:M:438:GLN:OE1	2.37	0.72
7:K:358:LEU:CA	9:M:438:GLN:OE1	2.37	0.72
7:K:358:LEU:CA	9:M:438:GLN:OE1	2.37	0.72
5:I:95:DC:P	7:K:608:LYS:H	2.13	0.72
7:K:358:LEU:CA	9:M:438:GLN:OE1	2.37	0.72
7:K:358:LEU:CA	9:M:438:GLN:OE1	2.37	0.72
7:K:358:LEU:CA	9:M:438:GLN:OE1	2.37	0.72
7:K:358:LEU:CA	9:M:438:GLN:OE1	2.37	0.72
5:I:95:DC:P	7:K:608:LYS:CB	2.77	0.72
7:K:354:LEU:HD11	9:M:438:GLN:HE21	1.52	0.71
7:K:354:LEU:HD11	9:M:438:GLN:HE21	1.52	0.71
7:K:354:LEU:HD11	9:M:438:GLN:HE21	1.52	0.71
3:G:78:ARG:HE	5:I:20:DA:H4'	1.53	0.71
7:K:354:LEU:HD11	9:M:438:GLN:HE21	1.52	0.71
7:K:354:LEU:HD11	9:M:438:GLN:HE21	1.52	0.71
7:K:354:LEU:HD11	9:M:438:GLN:HE21	1.52	0.71
7:K:354:LEU:HD11	9:M:438:GLN:HE21	1.52	0.71
7:K:354:LEU:HD11	9:M:438:GLN:HE21	1.52	0.71
7:K:381:LEU:CB	7:K:676:GLU:CD	2.63	0.71
7:K:354:LEU:HD11	9:M:438:GLN:HE21	1.52	0.71
7:K:354:LEU:HD11	9:M:438:GLN:HE21	1.52	0.71
7:K:877:GLN:N	7:K:877:GLN:OE1	2.24	0.71
7:K:378:LEU:CB	7:K:676:GLU:OE2	2.39	0.71
7:K:378:LEU:C	7:K:676:GLU:OE1	2.33	0.71
12:K:1502:ADP:O2A	12:K:1502:ADP:C4'	2.38	0.71
7:K:362:MET:CE	9:M:416:PHE:HZ	1.91	0.71
7:K:362:MET:CE	9:M:416:PHE:HZ	1.91	0.71
7:K:362:MET:CE	9:M:416:PHE:HZ	1.91	0.71
7:K:362:MET:CE	9:M:416:PHE:HZ	1.91	0.71
7:K:362:MET:CE	9:M:416:PHE:HZ	1.91	0.71
7:K:362:MET:CE	9:M:416:PHE:HZ	1.91	0.71
7:K:362:MET:CE	9:M:416:PHE:HZ	1.91	0.71
7:K:362:MET:CE	9:M:416:PHE:HZ	1.91	0.71
7:K:362:MET:CE	9:M:416:PHE:HZ	1.91	0.71
7:K:362:MET:CE	9:M:416:PHE:HZ	1.91	0.71
7:K:362:MET:CE	9:M:416:PHE:HZ	1.91	0.71
5:I:95:DC:P	7:K:608:LYS:HB3	2.30	0.70
7:K:815:GLN:O	7:K:815:GLN:HG2	1.91	0.70
3:G:78:ARG:NE	5:I:20:DA:H4'	2.07	0.70
7:K:351:PHE:HE2	9:M:439:ILE:CG1	2.05	0.70
1:E:70:ARG:NH2	6:J:91:DA:OP1	2.24	0.70
7:K:351:PHE:HE2	9:M:439:ILE:CG1	2.05	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:351:PHE:HE2	9:M:439:ILE:CG1	2.05	0.70
7:K:351:PHE:HE2	9:M:439:ILE:CG1	2.05	0.70
1:E:70:ARG:NH2	6:J:91:DA:OP1	2.24	0.70
7:K:351:PHE:HE2	9:M:439:ILE:CG1	2.05	0.70
7:K:351:PHE:HE2	9:M:439:ILE:CG1	2.05	0.70
7:K:351:PHE:HE2	9:M:439:ILE:CG1	2.05	0.70
7:K:351:PHE:HE2	9:M:439:ILE:CG1	2.05	0.70
7:K:351:PHE:HE2	9:M:439:ILE:CG1	2.05	0.70
7:K:351:PHE:HE2	9:M:439:ILE:CG1	2.05	0.70
7:K:362:MET:CB	9:M:437:LYS:CE	2.59	0.69
7:K:362:MET:CB	9:M:437:LYS:CE	2.59	0.69
7:K:362:MET:CB	9:M:437:LYS:CE	2.59	0.69
7:K:362:MET:CB	9:M:437:LYS:CE	2.59	0.69
7:K:362:MET:CB	9:M:437:LYS:CE	2.59	0.69
7:K:362:MET:CB	9:M:437:LYS:CE	2.59	0.69
3:C:17:THR:HA	6:J:31:DA:H5"	1.75	0.69
7:K:362:MET:CB	9:M:437:LYS:CE	2.59	0.69
7:K:362:MET:CB	9:M:437:LYS:CE	2.59	0.69
7:K:362:MET:CB	9:M:437:LYS:CE	2.59	0.69
7:K:362:MET:CB	9:M:437:LYS:CE	2.59	0.69
1:A:64:ARG:HD3	5:I:91:DA:H4'	1.73	0.69
5:I:95:DC:OP1	7:K:608:LYS:HB3	1.92	0.69
7:K:392:LEU:CD1	9:M:420:LYS:HZ1	2.05	0.69
5:I:95:DC:P	7:K:608:LYS:H	2.15	0.69
1:E:70:ARG:NH2	6:J:91:DA:OP1	2.24	0.69
1:E:70:ARG:NH2	6:J:91:DA:OP1	2.24	0.69
1:E:70:ARG:NH2	6:J:91:DA:OP1	2.24	0.69
5:I:94:DG:O3'	7:K:608:LYS:CB	2.39	0.69
5:I:95:DC:OP1	7:K:608:LYS:N	2.26	0.69
5:I:95:DC:OP1	7:K:608:LYS:HB3	1.92	0.69
6:J:56:DG:H5"	7:K:528:LEU:HD12	1.74	0.69
3:G:78:ARG:NE	5:I:20:DA:H4'	2.08	0.69
5:I:95:DC:OP1	7:K:608:LYS:N	2.26	0.68
5:I:95:DC:OP1	7:K:609:LEU:N	2.25	0.68
7:K:347:ARG:NH2	9:M:464:ASP:O	2.27	0.68
7:K:347:ARG:NH2	9:M:464:ASP:O	2.27	0.68
7:K:347:ARG:NH2	9:M:464:ASP:O	2.27	0.68
7:K:347:ARG:NH2	9:M:464:ASP:O	2.27	0.68
7:K:381:LEU:CB	7:K:676:GLU:OE2	2.42	0.68
7:K:347:ARG:NH2	9:M:464:ASP:O	2.27	0.68
7:K:347:ARG:NH2	9:M:464:ASP:O	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:347:ARG:NH2	9:M:464:ASP:O	2.27	0.68
7:K:347:ARG:NH2	9:M:464:ASP:O	2.27	0.68
7:K:347:ARG:NH2	9:M:464:ASP:O	2.27	0.68
7:K:347:ARG:NH2	9:M:464:ASP:O	2.27	0.68
7:K:358:LEU:HD22	9:M:438:GLN:HA	1.72	0.68
7:K:358:LEU:HD22	9:M:438:GLN:HA	1.72	0.68
7:K:358:LEU:HD22	9:M:438:GLN:HA	1.72	0.68
7:K:358:LEU:HD22	9:M:438:GLN:HA	1.72	0.68
7:K:358:LEU:HD22	9:M:438:GLN:HA	1.72	0.68
7:K:358:LEU:HD22	9:M:438:GLN:HA	1.72	0.68
7:K:358:LEU:HD22	9:M:438:GLN:HA	1.72	0.68
7:K:358:LEU:HD22	9:M:438:GLN:HA	1.72	0.68
7:K:358:LEU:HD22	9:M:438:GLN:HA	1.72	0.68
7:K:358:LEU:HD22	9:M:438:GLN:HA	1.72	0.68
7:K:358:LEU:HD22	9:M:438:GLN:HA	1.72	0.68
7:K:354:LEU:CD1	9:M:438:GLN:NE2	2.57	0.67
7:K:354:LEU:CD1	9:M:438:GLN:NE2	2.57	0.67
7:K:354:LEU:CD1	9:M:438:GLN:NE2	2.57	0.67
7:K:354:LEU:CD1	9:M:438:GLN:NE2	2.57	0.67
7:K:354:LEU:CD1	9:M:438:GLN:NE2	2.57	0.67
7:K:354:LEU:CD1	9:M:438:GLN:NE2	2.57	0.67
7:K:354:LEU:CD1	9:M:438:GLN:NE2	2.57	0.67
7:K:354:LEU:CD1	9:M:438:GLN:NE2	2.57	0.67
7:K:354:LEU:CD1	9:M:438:GLN:NE2	2.57	0.67
7:K:354:LEU:CD1	9:M:438:GLN:NE2	2.57	0.67
5:I:99:DG:P	7:K:928:ARG:HH12	2.17	0.67
3:C:17:THR:HA	6:J:31:DA:H5"	1.77	0.67
7:K:378:LEU:HA	7:K:676:GLU:OE1	1.93	0.67
3:C:17:THR:HA	6:J:31:DA:H5"	1.77	0.67
3:C:17:THR:HA	6:J:31:DA:H5"	1.77	0.67
5:I:95:DC:OP1	7:K:608:LYS:CB	2.38	0.67
7:K:649:PHE:O	7:K:649:PHE:CD1	2.48	0.67
5:I:95:DC:P	7:K:608:LYS:HB3	2.33	0.67
5:I:95:DC:OP1	7:K:608:LYS:N	2.27	0.67
5:I:95:DC:OP1	7:K:608:LYS:HB3	1.94	0.67
7:K:649:PHE:O	7:K:649:PHE:CG	2.42	0.66
7:K:358:LEU:HD23	9:M:438:GLN:HB2	1.76	0.66
7:K:358:LEU:HD23	9:M:438:GLN:HB2	1.76	0.66
7:K:358:LEU:HD23	9:M:438:GLN:HB2	1.76	0.66
7:K:358:LEU:HD23	9:M:438:GLN:HB2	1.76	0.66
7:K:358:LEU:HD23	9:M:438:GLN:HB2	1.76	0.66
7:K:358:LEU:HD23	9:M:438:GLN:HB2	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:358:LEU:HD23	9:M:438:GLN:HB2	1.76	0.66
7:K:358:LEU:HD23	9:M:438:GLN:HB2	1.76	0.66
7:K:358:LEU:HD23	9:M:438:GLN:HB2	1.76	0.66
7:K:358:LEU:HD23	9:M:438:GLN:HB2	1.76	0.66
5:I:94:DG:H3'	7:K:608:LYS:HB2	1.77	0.66
5:I:95:DC:OP2	7:K:608:LYS:HB2	1.96	0.66
7:K:354:LEU:CD1	9:M:438:GLN:HE21	2.08	0.66
7:K:354:LEU:CD1	9:M:438:GLN:HE21	2.08	0.66
7:K:354:LEU:CD1	9:M:438:GLN:HE21	2.08	0.66
7:K:354:LEU:CD1	9:M:438:GLN:HE21	2.08	0.66
5:I:95:DC:OP1	7:K:609:LEU:N	2.29	0.66
7:K:354:LEU:CD1	9:M:438:GLN:HE21	2.08	0.66
7:K:354:LEU:CD1	9:M:438:GLN:HE21	2.08	0.66
7:K:354:LEU:CD1	9:M:438:GLN:HE21	2.08	0.66
5:I:95:DC:P	7:K:608:LYS:CA	2.83	0.66
7:K:354:LEU:CD1	9:M:438:GLN:HE21	2.08	0.66
7:K:354:LEU:CD1	9:M:438:GLN:HE21	2.08	0.66
7:K:354:LEU:CD1	9:M:438:GLN:HE21	2.08	0.66
7:K:351:PHE:CZ	9:M:447:PHE:CB	2.79	0.66
7:K:351:PHE:CZ	9:M:447:PHE:CB	2.79	0.66
7:K:351:PHE:CZ	9:M:447:PHE:CB	2.79	0.66
7:K:351:PHE:CZ	9:M:447:PHE:CB	2.79	0.66
7:K:351:PHE:CZ	9:M:447:PHE:CB	2.79	0.66
7:K:351:PHE:CZ	9:M:447:PHE:CB	2.79	0.66
7:K:351:PHE:CZ	9:M:447:PHE:CB	2.79	0.66
7:K:351:PHE:CZ	9:M:447:PHE:CB	2.79	0.66
7:K:351:PHE:CZ	9:M:447:PHE:CB	2.79	0.66
7:K:351:PHE:CZ	9:M:447:PHE:CB	2.79	0.66
7:K:351:PHE:CZ	9:M:447:PHE:CB	2.79	0.66
7:K:392:LEU:HD11	9:M:420:LYS:HZ1	1.60	0.66
12:K:1502:ADP:O1A	12:K:1502:ADP:O3B	2.10	0.65
7:K:701:GLU:N	7:K:701:GLU:OE1	2.27	0.65
7:K:899:ASP:OD1	7:K:899:ASP:C	2.40	0.65
1:A:64:ARG:HD3	5:I:91:DA:H4'	1.79	0.65
1:E:70:ARG:NH2	6:J:91:DA:OP1	2.26	0.65
1:E:70:ARG:NH2	6:J:91:DA:OP1	2.26	0.65
7:K:378:LEU:O	7:K:676:GLU:OE1	2.13	0.65
7:K:347:ARG:CD	9:M:466:GLN:O	2.45	0.65
7:K:347:ARG:CD	9:M:466:GLN:O	2.45	0.65
7:K:347:ARG:CD	9:M:466:GLN:O	2.45	0.65
7:K:347:ARG:CD	9:M:466:GLN:O	2.45	0.65
7:K:347:ARG:CD	9:M:466:GLN:O	2.45	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:347:ARG:CD	9:M:466:GLN:O	2.45	0.65
7:K:347:ARG:CD	9:M:466:GLN:O	2.45	0.65
7:K:347:ARG:CD	9:M:466:GLN:O	2.45	0.65
7:K:347:ARG:CD	9:M:466:GLN:O	2.45	0.65
7:K:347:ARG:CD	9:M:466:GLN:O	2.45	0.65
7:K:358:LEU:CD1	9:M:437:LYS:HG3	2.27	0.64
7:K:358:LEU:CD1	9:M:437:LYS:HG3	2.27	0.64
7:K:358:LEU:CD1	9:M:437:LYS:HG3	2.27	0.64
7:K:358:LEU:CD1	9:M:437:LYS:HG3	2.27	0.64
7:K:358:LEU:CD1	9:M:437:LYS:HG3	2.27	0.64
7:K:358:LEU:CD1	9:M:437:LYS:HG3	2.27	0.64
7:K:358:LEU:CD1	9:M:437:LYS:HG3	2.27	0.64
7:K:358:LEU:CD1	9:M:437:LYS:HG3	2.27	0.64
7:K:358:LEU:CD1	9:M:437:LYS:HG3	2.27	0.64
1:E:70:ARG:NH2	6:J:91:DA:OP1	2.26	0.64
7:K:358:LEU:CD1	9:M:437:LYS:HG3	2.27	0.64
7:K:358:LEU:CD1	9:M:437:LYS:HG3	2.27	0.64
7:K:446:ASP:C	7:K:446:ASP:OD1	2.39	0.64
1:A:64:ARG:HD3	5:I:91:DA:H4'	1.80	0.64
5:I:95:DC:OP2	7:K:608:LYS:HB2	1.97	0.64
7:K:564:ILE:HD12	7:K:564:ILE:C	2.22	0.64
12:K:1502:ADP:O3B	13:K:1503:BEF:F2	2.04	0.64
1:A:64:ARG:HD3	5:I:91:DA:H4'	1.80	0.64
5:I:95:DC:OP1	7:K:608:LYS:N	2.30	0.64
7:K:392:LEU:CD1	9:M:420:LYS:HZ3	2.10	0.64
7:K:1046:GLU:N	7:K:1046:GLU:OE1	2.31	0.64
12:K:1502:ADP:O2A	12:K:1502:ADP:H4'	1.97	0.63
7:K:872:LEU:HD12	7:K:872:LEU:C	2.22	0.63
7:K:351:PHE:CE1	9:M:447:PHE:HB3	2.32	0.63
5:I:99:DG:P	7:K:928:ARG:HH12	2.21	0.63
7:K:351:PHE:CE1	9:M:447:PHE:HB3	2.32	0.63
7:K:351:PHE:CE1	9:M:447:PHE:HB3	2.32	0.63
7:K:351:PHE:CE1	9:M:447:PHE:HB3	2.32	0.63
7:K:351:PHE:CE1	9:M:447:PHE:HB3	2.32	0.63
7:K:351:PHE:CE1	9:M:447:PHE:HB3	2.32	0.63
7:K:351:PHE:CE1	9:M:447:PHE:HB3	2.32	0.63
7:K:351:PHE:CE1	9:M:447:PHE:HB3	2.32	0.63
7:K:351:PHE:CE1	9:M:447:PHE:HB3	2.32	0.63
7:K:351:PHE:CE1	9:M:447:PHE:HB3	2.32	0.63
7:K:351:PHE:CE1	9:M:447:PHE:HB3	2.32	0.63
7:K:677:GLU:H	7:K:677:GLU:CD	2.06	0.63
5:I:95:DC:P	7:K:608:LYS:N	2.72	0.63
1:A:64:ARG:HD3	5:I:91:DA:H4'	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:56:DG:OP2	7:K:846:ARG:NH2	2.28	0.63
7:K:648:ILE:O	7:K:648:ILE:HG23	1.99	0.63
7:K:648:ILE:HG13	7:K:648:ILE:O	1.99	0.62
6:J:54:DC:H3'	7:K:816:MET:HG3	1.81	0.62
5:I:95:DC:OP1	7:K:608:LYS:CA	2.48	0.62
5:I:95:DC:P	7:K:608:LYS:CB	2.88	0.62
5:I:95:DC:OP1	7:K:608:LYS:N	2.33	0.62
5:I:98:DA:OP1	7:K:932:LYS:NZ	2.26	0.62
7:K:649:PHE:O	7:K:649:PHE:CG	2.51	0.62
7:K:366:GLU:OE1	7:K:366:GLU:HA	1.99	0.62
7:K:366:GLU:OE1	7:K:366:GLU:HA	1.99	0.62
7:K:366:GLU:OE1	7:K:366:GLU:HA	1.99	0.62
7:K:366:GLU:OE1	7:K:366:GLU:HA	1.99	0.62
7:K:366:GLU:OE1	7:K:366:GLU:HA	1.99	0.62
7:K:366:GLU:OE1	7:K:366:GLU:HA	1.99	0.62
7:K:366:GLU:OE1	7:K:366:GLU:HA	1.99	0.62
7:K:366:GLU:OE1	7:K:366:GLU:HA	1.99	0.62
7:K:366:GLU:OE1	7:K:366:GLU:HA	1.99	0.62
7:K:378:LEU:CB	7:K:676:GLU:OE1	2.46	0.62
7:K:366:GLU:OE1	7:K:366:GLU:HA	1.99	0.62
7:K:366:GLU:OE1	7:K:366:GLU:HA	1.99	0.62
7:K:358:LEU:N	9:M:438:GLN:OE1	2.33	0.62
7:K:358:LEU:N	9:M:438:GLN:OE1	2.33	0.62
7:K:381:LEU:CB	7:K:676:GLU:CD	2.73	0.62
7:K:358:LEU:N	9:M:438:GLN:OE1	2.33	0.62
7:K:358:LEU:N	9:M:438:GLN:OE1	2.33	0.62
7:K:358:LEU:N	9:M:438:GLN:OE1	2.33	0.62
7:K:358:LEU:N	9:M:438:GLN:OE1	2.33	0.62
7:K:358:LEU:N	9:M:438:GLN:OE1	2.33	0.62
7:K:358:LEU:N	9:M:438:GLN:OE1	2.33	0.62
7:K:358:LEU:N	9:M:438:GLN:OE1	2.33	0.62
7:K:358:LEU:N	9:M:438:GLN:OE1	2.33	0.62
7:K:902:HIS:ND1	7:K:902:HIS:C	2.58	0.61
7:K:783:SER:OG	7:K:784:ASP:N	2.32	0.61
7:K:844:GLU:N	7:K:844:GLU:OE1	2.31	0.61
8:L:302:ASP:C	8:L:302:ASP:OD1	2.42	0.61
5:I:95:DC:OP1	7:K:609:LEU:N	2.33	0.61
8:L:302:ASP:C	8:L:302:ASP:OD1	2.42	0.61
4:H:87:ARG:HH12	5:I:40:DG:H3'	1.65	0.61
8:L:302:ASP:C	8:L:302:ASP:OD1	2.42	0.61
8:L:302:ASP:C	8:L:302:ASP:OD1	2.42	0.61
8:L:302:ASP:C	8:L:302:ASP:OD1	2.42	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L:302:ASP:C	8:L:302:ASP:OD1	2.42	0.61
8:L:302:ASP:C	8:L:302:ASP:OD1	2.42	0.61
8:L:302:ASP:C	8:L:302:ASP:OD1	2.42	0.61
8:L:302:ASP:C	8:L:302:ASP:OD1	2.42	0.61
8:L:302:ASP:C	8:L:302:ASP:OD1	2.42	0.61
7:K:519:ILE:HG23	7:K:519:ILE:O	2.00	0.61
7:K:577:GLU:H	7:K:577:GLU:CD	2.08	0.61
7:K:378:LEU:O	7:K:676:GLU:OE2	2.19	0.61
12:K:1502:ADP:O2A	12:K:1502:ADP:H4'	2.00	0.61
5:I:95:DC:OP2	7:K:608:LYS:HB2	2.01	0.61
3:G:77:THR:OG1	6:J:131:DG:O3'	2.18	0.60
5:I:95:DC:OP1	7:K:608:LYS:CA	2.49	0.60
7:K:710:VAL:O	7:K:710:VAL:HG23	1.99	0.60
3:G:77:THR:OG1	6:J:131:DG:O3'	2.19	0.60
1:E:64:ARG:HD3	6:J:91:DA:H4'	1.82	0.60
1:A:60:GLU:OE1	1:A:60:GLU:N	2.31	0.60
7:K:900:ARG:NE	7:K:900:ARG:HA	2.16	0.60
6:J:54:DC:OP1	7:K:816:MET:HB2	2.01	0.60
6:J:54:DC:OP1	7:K:816:MET:HB2	2.02	0.60
12:K:1502:ADP:O3B	13:K:1503:BEF:F2	2.10	0.60
12:K:1502:ADP:O2A	12:K:1502:ADP:H4'	2.00	0.60
10:N:34:LYS:O	10:N:34:LYS:HG2	2.01	0.59
10:N:34:LYS:O	10:N:34:LYS:HG2	2.01	0.59
10:N:34:LYS:O	10:N:34:LYS:HG2	2.01	0.59
10:N:34:LYS:O	10:N:34:LYS:HG2	2.01	0.59
1:E:64:ARG:HD3	6:J:91:DA:H4'	1.83	0.59
10:N:34:LYS:O	10:N:34:LYS:HG2	2.01	0.59
10:N:34:LYS:O	10:N:34:LYS:HG2	2.01	0.59
10:N:34:LYS:O	10:N:34:LYS:HG2	2.01	0.59
10:N:34:LYS:O	10:N:34:LYS:HG2	2.01	0.59
12:K:1502:ADP:O3B	13:K:1503:BEF:F2	2.10	0.59
10:N:34:LYS:O	10:N:34:LYS:HG2	2.01	0.59
10:N:34:LYS:O	10:N:34:LYS:HG2	2.01	0.59
5:I:95:DC:P	7:K:608:LYS:CB	2.89	0.59
7:K:351:PHE:HE2	9:M:439:ILE:HG12	1.67	0.59
1:E:64:ARG:HD3	6:J:91:DA:H4'	1.83	0.59
7:K:351:PHE:HE2	9:M:439:ILE:HG12	1.67	0.59
7:K:351:PHE:HE2	9:M:439:ILE:HG12	1.67	0.59
7:K:351:PHE:HE2	9:M:439:ILE:HG12	1.67	0.59
7:K:351:PHE:HE2	9:M:439:ILE:HG12	1.67	0.59
7:K:351:PHE:HE2	9:M:439:ILE:HG12	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:351:PHE:HE2	9:M:439:ILE:HG12	1.67	0.59
7:K:351:PHE:HE2	9:M:439:ILE:HG12	1.67	0.59
7:K:351:PHE:HE2	9:M:439:ILE:HG12	1.67	0.59
7:K:351:PHE:HE2	9:M:439:ILE:HG12	1.67	0.59
6:J:56:DG:H5"	7:K:528:LEU:HD12	1.83	0.59
1:E:64:ARG:HD3	6:J:91:DA:H4'	1.84	0.59
6:J:55:DG:OP1	7:K:866:SER:OG	2.14	0.59
7:K:378:LEU:CA	7:K:676:GLU:OE1	2.50	0.59
3:G:77:THR:OG1	6:J:131:DG:O3'	2.19	0.59
1:E:64:ARG:HD3	6:J:91:DA:H4'	1.84	0.59
6:J:54:DC:H3'	7:K:816:MET:HG3	1.83	0.59
6:J:56:DG:H5"	7:K:528:LEU:HD12	1.83	0.59
3:G:77:THR:OG1	6:J:131:DG:O3'	2.19	0.59
7:K:351:PHE:CZ	9:M:447:PHE:HB3	2.37	0.59
7:K:351:PHE:CZ	9:M:447:PHE:HB3	2.37	0.59
7:K:351:PHE:CZ	9:M:447:PHE:HB3	2.37	0.59
7:K:351:PHE:CZ	9:M:447:PHE:HB3	2.37	0.59
7:K:351:PHE:CZ	9:M:447:PHE:HB3	2.37	0.59
7:K:710:VAL:O	7:K:710:VAL:HG23	2.01	0.59
7:K:351:PHE:CZ	9:M:447:PHE:HB3	2.37	0.59
7:K:351:PHE:CZ	9:M:447:PHE:HB3	2.37	0.59
7:K:351:PHE:CZ	9:M:447:PHE:HB3	2.37	0.59
7:K:351:PHE:CZ	9:M:447:PHE:HB3	2.37	0.59
7:K:351:PHE:CZ	9:M:447:PHE:HB3	2.37	0.59
7:K:710:VAL:O	7:K:710:VAL:HG23	2.03	0.59
7:K:616:TYR:O	7:K:616:TYR:CG	2.55	0.59
7:K:648:ILE:HG22	7:K:648:ILE:O	2.03	0.59
1:E:60:GLU:OE1	1:E:60:GLU:N	2.31	0.58
7:K:677:GLU:H	7:K:677:GLU:CD	2.11	0.58
3:G:77:THR:OG1	6:J:131:DG:O3'	2.20	0.58
1:E:60:GLU:OE1	1:E:60:GLU:N	2.31	0.58
6:J:54:DC:H3'	7:K:816:MET:HG3	1.84	0.58
1:E:60:GLU:OE1	1:E:60:GLU:N	2.31	0.58
7:K:378:LEU:CB	7:K:676:GLU:OE1	2.52	0.58
7:K:710:VAL:O	7:K:710:VAL:HG23	2.03	0.58
1:E:60:GLU:OE1	1:E:60:GLU:N	2.31	0.58
7:K:378:LEU:CB	7:K:676:GLU:OE2	2.51	0.58
7:K:576:TYR:O	7:K:578:TYR:N	2.36	0.58
1:A:64:ARG:HD3	5:I:91:DA:H4'	1.86	0.58
8:L:427:GLN:OE1	8:L:427:GLN:N	2.32	0.58
8:L:427:GLN:OE1	8:L:427:GLN:N	2.32	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:60:GLU:OE1	1:E:60:GLU:N	2.32	0.58
8:L:427:GLN:OE1	8:L:427:GLN:N	2.32	0.58
8:L:427:GLN:OE1	8:L:427:GLN:N	2.32	0.58
8:L:427:GLN:OE1	8:L:427:GLN:N	2.32	0.58
8:L:427:GLN:OE1	8:L:427:GLN:N	2.32	0.58
8:L:427:GLN:OE1	8:L:427:GLN:N	2.32	0.58
8:L:427:GLN:OE1	8:L:427:GLN:N	2.32	0.58
8:L:427:GLN:OE1	8:L:427:GLN:N	2.32	0.58
8:L:427:GLN:OE1	8:L:427:GLN:N	2.32	0.58
3:G:77:THR:OG1	6:J:131:DG:O3'	2.21	0.58
1:E:60:GLU:OE1	1:E:60:GLU:N	2.32	0.58
1:E:60:GLU:OE1	1:E:60:GLU:N	2.32	0.58
7:K:378:LEU:CA	7:K:676:GLU:CD	2.70	0.58
1:E:60:GLU:OE1	1:E:60:GLU:N	2.32	0.58
1:E:60:GLU:OE1	1:E:60:GLU:N	2.32	0.58
1:E:60:GLU:OE1	1:E:60:GLU:N	2.32	0.58
5:I:95:DC:OP1	7:K:609:LEU:N	2.37	0.58
5:I:95:DC:OP2	7:K:608:LYS:N	2.37	0.58
7:K:576:TYR:O	7:K:578:TYR:N	2.37	0.58
3:G:78:ARG:NE	5:I:20:DA:H4'	2.19	0.57
3:G:78:ARG:NE	5:I:20:DA:H4'	2.19	0.57
1:E:64:ARG:HD3	6:J:91:DA:H4'	1.85	0.57
1:E:64:ARG:HD3	6:J:91:DA:H4'	1.86	0.57
7:K:347:ARG:HH11	9:M:466:GLN:C	2.10	0.57
7:K:347:ARG:HH11	9:M:466:GLN:C	2.10	0.57
7:K:347:ARG:HH11	9:M:466:GLN:C	2.10	0.57
7:K:347:ARG:HH11	9:M:466:GLN:C	2.10	0.57
7:K:347:ARG:HH11	9:M:466:GLN:C	2.10	0.57
7:K:830:LYS:HE2	7:K:830:LYS:HA	1.86	0.57
7:K:347:ARG:HH11	9:M:466:GLN:C	2.10	0.57
7:K:1001:GLU:OE1	7:K:1001:GLU:HA	2.03	0.57
7:K:347:ARG:HH11	9:M:466:GLN:C	2.10	0.57
7:K:701:GLU:OE1	7:K:701:GLU:N	2.31	0.57
1:E:64:ARG:HD3	6:J:91:DA:H4'	1.86	0.57
7:K:347:ARG:HH11	9:M:466:GLN:C	2.10	0.57
7:K:347:ARG:HH11	9:M:466:GLN:C	2.10	0.57
7:K:347:ARG:HH11	9:M:466:GLN:C	2.10	0.57
7:K:834:TYR:CD1	7:K:834:TYR:C	2.82	0.57
3:G:78:ARG:NE	5:I:20:DA:H4'	2.20	0.57
5:I:95:DC:OP1	7:K:609:LEU:N	2.37	0.57
7:K:757:MET:SD	7:K:757:MET:C	2.88	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:95:DC:OP2	7:K:608:LYS:CB	2.52	0.57
7:K:577:GLU:OE1	7:K:577:GLU:N	2.34	0.57
5:I:95:DC:OP1	7:K:609:LEU:N	2.37	0.57
1:E:64:ARG:HD3	6:J:91:DA:H4'	1.87	0.56
3:G:78:ARG:NE	5:I:20:DA:H4'	2.20	0.56
7:K:710:VAL:O	7:K:710:VAL:HG23	2.05	0.56
7:K:816:MET:SD	7:K:816:MET:N	2.78	0.56
7:K:649:PHE:O	7:K:649:PHE:CD1	2.58	0.56
5:I:99:DG:P	7:K:928:ARG:HH12	2.28	0.56
7:K:347:ARG:NH1	9:M:465:VAL:C	2.64	0.56
7:K:347:ARG:NH1	9:M:465:VAL:C	2.64	0.56
7:K:347:ARG:NH1	9:M:465:VAL:C	2.64	0.56
7:K:347:ARG:NH1	9:M:465:VAL:C	2.64	0.56
7:K:347:ARG:NH1	9:M:465:VAL:C	2.64	0.56
7:K:347:ARG:NH1	9:M:465:VAL:C	2.64	0.56
7:K:347:ARG:NH1	9:M:465:VAL:C	2.64	0.56
3:G:77:THR:OG1	6:J:131:DG:O3'	2.22	0.56
7:K:347:ARG:NH1	9:M:465:VAL:C	2.64	0.56
7:K:347:ARG:NH1	9:M:465:VAL:C	2.64	0.56
4:H:87:ARG:HH12	5:I:40:DG:H3'	1.70	0.56
7:K:347:ARG:NH1	9:M:465:VAL:C	2.64	0.56
7:K:564:ILE:HD12	7:K:564:ILE:C	2.30	0.56
3:C:17:THR:HA	6:J:31:DA:H5"	1.86	0.56
6:J:54:DC:C3'	7:K:816:MET:HG3	2.35	0.56
5:I:95:DC:OP1	7:K:608:LYS:CB	2.44	0.56
1:A:60:GLU:OE1	1:A:60:GLU:N	2.34	0.56
3:C:17:THR:HA	6:J:31:DA:H5"	1.86	0.56
7:K:710:VAL:O	7:K:710:VAL:HG23	2.06	0.56
7:K:1001:GLU:OE1	7:K:1001:GLU:HA	2.05	0.56
7:K:382:LYS:N	7:K:676:GLU:OE2	2.39	0.56
3:C:17:THR:HA	6:J:31:DA:H5"	1.87	0.56
1:E:64:ARG:HD3	6:J:91:DA:H4'	1.87	0.56
3:G:78:ARG:NE	5:I:20:DA:H4'	2.21	0.55
7:K:777:ASN:C	7:K:777:ASN:OD1	2.47	0.55
4:H:87:ARG:HH12	5:I:40:DG:H3'	1.71	0.55
5:I:95:DC:OP1	7:K:608:LYS:CB	2.49	0.55
1:A:60:GLU:OE1	1:A:60:GLU:N	2.34	0.55
3:C:17:THR:HA	6:J:31:DA:H5"	1.87	0.55
5:I:95:DC:P	7:K:608:LYS:N	2.76	0.55
1:A:64:ARG:HD3	5:I:91:DA:H4'	1.89	0.55
7:K:777:ASN:C	7:K:777:ASN:OD1	2.47	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:838:ASP:OD1	7:K:838:ASP:C	2.49	0.55
5:I:95:DC:P	7:K:608:LYS:H	2.29	0.55
7:K:900:ARG:HA	7:K:900:ARG:HE	1.72	0.55
7:K:793:PHE:CD1	7:K:793:PHE:N	2.75	0.55
5:I:95:DC:OP2	7:K:608:LYS:HB2	2.07	0.55
8:L:72:ASP:C	8:L:72:ASP:OD1	2.50	0.55
8:L:72:ASP:C	8:L:72:ASP:OD1	2.50	0.55
8:L:72:ASP:C	8:L:72:ASP:OD1	2.50	0.55
4:H:87:ARG:HH12	5:I:40:DG:H3'	1.71	0.55
8:L:72:ASP:C	8:L:72:ASP:OD1	2.50	0.55
8:L:72:ASP:C	8:L:72:ASP:OD1	2.50	0.55
8:L:72:ASP:C	8:L:72:ASP:OD1	2.50	0.55
8:L:72:ASP:C	8:L:72:ASP:OD1	2.50	0.55
8:L:72:ASP:C	8:L:72:ASP:OD1	2.50	0.55
8:L:72:ASP:C	8:L:72:ASP:OD1	2.50	0.55
8:L:72:ASP:C	8:L:72:ASP:OD1	2.50	0.55
3:G:91:ASP:C	3:G:91:ASP:OD1	2.49	0.54
3:G:91:ASP:C	3:G:91:ASP:OD1	2.49	0.54
3:G:77:THR:OG1	6:J:131:DG:O3'	2.24	0.54
7:K:358:LEU:HD21	9:M:438:GLN:N	2.15	0.54
7:K:890:ASN:OD1	7:K:890:ASN:C	2.48	0.54
7:K:358:LEU:HD21	9:M:438:GLN:N	2.15	0.54
7:K:1001:GLU:OE1	7:K:1001:GLU:HA	2.06	0.54
3:G:77:THR:OG1	6:J:132:DC:P	2.66	0.54
7:K:358:LEU:HD21	9:M:438:GLN:N	2.15	0.54
7:K:358:LEU:HD21	9:M:438:GLN:N	2.15	0.54
4:H:87:ARG:HH12	5:I:40:DG:H3'	1.72	0.54
5:I:95:DC:P	7:K:608:LYS:N	2.80	0.54
7:K:358:LEU:HD21	9:M:438:GLN:N	2.15	0.54
7:K:358:LEU:HD21	9:M:438:GLN:N	2.15	0.54
7:K:358:LEU:HD21	9:M:438:GLN:N	2.15	0.54
7:K:358:LEU:HD21	9:M:438:GLN:N	2.15	0.54
4:H:87:ARG:HH12	5:I:40:DG:H3'	1.72	0.54
7:K:358:LEU:HD21	9:M:438:GLN:N	2.15	0.54
3:G:91:ASP:C	3:G:91:ASP:OD1	2.49	0.54
7:K:358:LEU:HD21	9:M:438:GLN:N	2.15	0.54
4:H:87:ARG:HH12	5:I:40:DG:H3'	1.72	0.54
3:G:91:ASP:C	3:G:91:ASP:OD1	2.49	0.54
3:C:17:THR:HA	6:J:31:DA:H5"	1.88	0.54
3:G:91:ASP:C	3:G:91:ASP:OD1	2.49	0.54
3:G:91:ASP:C	3:G:91:ASP:OD1	2.50	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:710:VAL:O	7:K:710:VAL:HG23	2.08	0.54
7:K:759:LEU:HD13	7:K:759:LEU:C	2.32	0.54
7:K:636:GLU:OE1	7:K:636:GLU:N	2.33	0.54
7:K:817:THR:OG1	7:K:818:GLN:N	2.40	0.54
9:M:154:ILE:O	9:M:154:ILE:CG2	2.47	0.54
3:G:77:THR:OG1	6:J:131:DG:O3'	2.25	0.54
9:M:154:ILE:O	9:M:154:ILE:CG2	2.47	0.54
9:M:154:ILE:O	9:M:154:ILE:CG2	2.47	0.54
9:M:154:ILE:O	9:M:154:ILE:CG2	2.47	0.54
3:G:77:THR:OG1	6:J:132:DC:P	2.66	0.54
9:M:154:ILE:O	9:M:154:ILE:CG2	2.47	0.54
9:M:154:ILE:O	9:M:154:ILE:CG2	2.47	0.54
9:M:154:ILE:O	9:M:154:ILE:CG2	2.47	0.54
9:M:154:ILE:O	9:M:154:ILE:CG2	2.47	0.54
7:K:860:TYR:CD2	7:K:860:TYR:N	2.74	0.54
9:M:154:ILE:O	9:M:154:ILE:CG2	2.47	0.54
7:K:900:ARG:NE	7:K:900:ARG:HA	2.23	0.54
9:M:154:ILE:O	9:M:154:ILE:CG2	2.47	0.54
7:K:381:LEU:CB	7:K:676:GLU:CD	2.81	0.53
7:K:777:ASN:C	7:K:777:ASN:OD1	2.50	0.53
2:F:80:LYS:N	6:J:102:DA:OP1	2.34	0.53
7:K:649:PHE:CD1	7:K:649:PHE:C	2.85	0.53
3:C:17:THR:HA	6:J:31:DA:H5"	1.89	0.53
7:K:359:HIS:HB3	7:K:363:GLU:CD	2.32	0.53
7:K:359:HIS:HB3	7:K:363:GLU:CD	2.32	0.53
7:K:359:HIS:HB3	7:K:363:GLU:CD	2.32	0.53
2:B:53:GLU:OE1	2:B:53:GLU:HA	2.07	0.53
7:K:359:HIS:HB3	7:K:363:GLU:CD	2.32	0.53
7:K:359:HIS:HB3	7:K:363:GLU:CD	2.32	0.53
7:K:359:HIS:HB3	7:K:363:GLU:CD	2.32	0.53
7:K:359:HIS:HB3	7:K:363:GLU:CD	2.32	0.53
7:K:359:HIS:HB3	7:K:363:GLU:CD	2.32	0.53
7:K:721:LEU:C	7:K:721:LEU:HD23	2.33	0.53
7:K:359:HIS:HB3	7:K:363:GLU:CD	2.32	0.53
7:K:359:HIS:HB3	7:K:363:GLU:CD	2.32	0.53
4:H:87:ARG:HH12	5:I:40:DG:H3'	1.72	0.53
7:K:777:ASN:C	7:K:777:ASN:OD1	2.51	0.53
7:K:834:TYR:CD1	7:K:834:TYR:C	2.87	0.53
2:B:53:GLU:OE1	2:B:53:GLU:HA	2.07	0.53
7:K:347:ARG:HH12	9:M:466:GLN:H	1.56	0.53
7:K:347:ARG:HH12	9:M:466:GLN:H	1.56	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:347:ARG:HH12	9:M:466:GLN:H	1.56	0.53
7:K:347:ARG:HH12	9:M:466:GLN:H	1.56	0.53
7:K:347:ARG:HH12	9:M:466:GLN:H	1.56	0.53
7:K:519:ILE:HG23	7:K:519:ILE:O	2.08	0.53
4:H:87:ARG:HH12	5:I:40:DG:H3'	1.74	0.53
7:K:347:ARG:HH12	9:M:466:GLN:H	1.56	0.53
7:K:705:ASP:C	7:K:705:ASP:OD1	2.50	0.53
7:K:347:ARG:HH12	9:M:466:GLN:H	1.56	0.53
7:K:347:ARG:HH12	9:M:466:GLN:H	1.56	0.53
7:K:347:ARG:HH12	9:M:466:GLN:H	1.56	0.53
5:I:95:DC:P	7:K:608:LYS:HB2	2.45	0.53
7:K:347:ARG:HH12	9:M:466:GLN:H	1.56	0.53
6:J:55:DG:OP1	7:K:866:SER:OG	2.11	0.53
7:K:838:ASP:OD1	7:K:838:ASP:C	2.52	0.53
7:K:342:TRP:CD1	7:K:342:TRP:O	2.62	0.53
7:K:342:TRP:CD1	7:K:342:TRP:O	2.62	0.53
7:K:342:TRP:CD1	7:K:342:TRP:O	2.62	0.53
7:K:577:GLU:OE1	7:K:577:GLU:N	2.36	0.53
7:K:342:TRP:CD1	7:K:342:TRP:O	2.62	0.53
7:K:342:TRP:CD1	7:K:342:TRP:O	2.62	0.53
7:K:342:TRP:CD1	7:K:342:TRP:O	2.62	0.53
7:K:342:TRP:CD1	7:K:342:TRP:O	2.62	0.53
7:K:342:TRP:CD1	7:K:342:TRP:O	2.62	0.53
7:K:342:TRP:CD1	7:K:342:TRP:O	2.62	0.53
7:K:342:TRP:CD1	7:K:342:TRP:O	2.62	0.53
7:K:342:TRP:CD1	7:K:342:TRP:O	2.62	0.53
7:K:877:GLN:OE1	7:K:877:GLN:N	2.32	0.53
7:K:902:HIS:O	7:K:902:HIS:ND1	2.42	0.53
7:K:545:LEU:C	7:K:545:LEU:HD12	2.34	0.53
3:G:77:THR:OG1	6:J:132:DC:P	2.67	0.53
7:K:604:ASN:OD1	7:K:604:ASN:C	2.52	0.53
8:L:79:ASN:C	8:L:79:ASN:OD1	2.52	0.52
8:L:79:ASN:C	8:L:79:ASN:OD1	2.52	0.52
8:L:79:ASN:C	8:L:79:ASN:OD1	2.52	0.52
8:L:79:ASN:C	8:L:79:ASN:OD1	2.52	0.52
8:L:79:ASN:C	8:L:79:ASN:OD1	2.52	0.52
8:L:79:ASN:C	8:L:79:ASN:OD1	2.52	0.52
8:L:79:ASN:C	8:L:79:ASN:OD1	2.52	0.52
2:B:53:GLU:OE1	2:B:53:GLU:HA	2.07	0.52
8:L:79:ASN:C	8:L:79:ASN:OD1	2.52	0.52
8:L:79:ASN:C	8:L:79:ASN:OD1	2.52	0.52
8:L:79:ASN:C	8:L:79:ASN:OD1	2.52	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:354:LEU:HD11	9:M:438:GLN:NE2	2.20	0.52
7:K:354:LEU:HD11	9:M:438:GLN:NE2	2.20	0.52
7:K:354:LEU:HD11	9:M:438:GLN:NE2	2.20	0.52
6:J:54:DC:H5"	7:K:816:MET:HG2	0.73	0.52
7:K:354:LEU:HD11	9:M:438:GLN:NE2	2.20	0.52
7:K:354:LEU:HD11	9:M:438:GLN:NE2	2.20	0.52
5:I:94:DG:O3'	7:K:608:LYS:HB3	2.09	0.52
7:K:354:LEU:HD11	9:M:438:GLN:NE2	2.20	0.52
7:K:354:LEU:HD11	9:M:438:GLN:NE2	2.20	0.52
7:K:354:LEU:HD11	9:M:438:GLN:NE2	2.20	0.52
7:K:354:LEU:HD11	9:M:438:GLN:NE2	2.20	0.52
7:K:354:LEU:HD11	9:M:438:GLN:NE2	2.20	0.52
7:K:590:ASP:C	7:K:590:ASP:OD1	2.51	0.52
6:J:56:DG:OP2	7:K:846:ARG:NH2	2.29	0.52
5:I:94:DG:C3'	7:K:608:LYS:HB2	2.38	0.52
7:K:838:ASP:OD1	7:K:838:ASP:C	2.51	0.52
7:K:890:ASN:OD1	7:K:890:ASN:C	2.51	0.52
7:K:347:ARG:NH1	9:M:466:GLN:CA	2.72	0.52
7:K:347:ARG:NH1	9:M:466:GLN:CA	2.72	0.52
7:K:347:ARG:NH1	9:M:466:GLN:CA	2.72	0.52
7:K:347:ARG:NH1	9:M:466:GLN:CA	2.72	0.52
7:K:838:ASP:OD1	7:K:838:ASP:C	2.52	0.52
7:K:347:ARG:NH1	9:M:466:GLN:CA	2.72	0.52
7:K:347:ARG:NH1	9:M:466:GLN:CA	2.72	0.52
3:G:77:THR:OG1	6:J:132:DC:P	2.68	0.52
7:K:347:ARG:NH1	9:M:466:GLN:CA	2.72	0.52
7:K:347:ARG:NH1	9:M:466:GLN:CA	2.72	0.52
5:I:95:DC:OP1	7:K:609:LEU:N	2.43	0.52
7:K:347:ARG:NH1	9:M:466:GLN:CA	2.72	0.52
7:K:347:ARG:NH1	9:M:466:GLN:CA	2.72	0.52
7:K:362:MET:CE	9:M:416:PHE:CE2	2.85	0.52
7:K:362:MET:CE	9:M:416:PHE:CE2	2.85	0.52
7:K:362:MET:CE	9:M:416:PHE:CE2	2.85	0.52
7:K:362:MET:CE	9:M:416:PHE:CE2	2.85	0.52
7:K:362:MET:CE	9:M:416:PHE:CE2	2.85	0.52
7:K:362:MET:CE	9:M:416:PHE:CE2	2.85	0.52
7:K:362:MET:CE	9:M:416:PHE:CE2	2.85	0.52
4:H:87:ARG:HH12	5:I:40:DG:H3'	1.75	0.52
7:K:362:MET:CE	9:M:416:PHE:CE2	2.85	0.52
7:K:362:MET:CE	9:M:416:PHE:CE2	2.85	0.52
7:K:362:MET:CE	9:M:416:PHE:CE2	2.85	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L:463:LEU:C	8:L:463:LEU:HD23	2.34	0.52
6:J:54:DC:H3'	7:K:816:MET:HG3	1.90	0.52
7:K:890:ASN:OD1	7:K:890:ASN:C	2.51	0.52
8:L:463:LEU:C	8:L:463:LEU:HD23	2.34	0.52
8:L:463:LEU:C	8:L:463:LEU:HD23	2.34	0.52
8:L:463:LEU:C	8:L:463:LEU:HD23	2.34	0.52
8:L:463:LEU:C	8:L:463:LEU:HD23	2.34	0.52
8:L:463:LEU:C	8:L:463:LEU:HD23	2.34	0.52
2:B:53:GLU:OE1	2:B:53:GLU:HA	2.08	0.52
8:L:463:LEU:C	8:L:463:LEU:HD23	2.34	0.52
8:L:463:LEU:C	8:L:463:LEU:HD23	2.34	0.52
8:L:463:LEU:C	8:L:463:LEU:HD23	2.34	0.52
3:G:77:THR:OG1	6:J:131:DG:O3'	2.26	0.52
8:L:463:LEU:C	8:L:463:LEU:HD23	2.34	0.52
2:B:53:GLU:OE1	2:B:53:GLU:HA	2.08	0.52
5:I:95:DC:OP1	7:K:609:LEU:N	2.42	0.52
3:G:77:THR:OG1	6:J:132:DC:P	2.68	0.52
3:G:78:ARG:HE	5:I:20:DA:H4'	1.75	0.52
3:G:77:THR:OG1	6:J:132:DC:P	2.68	0.52
7:K:392:LEU:HD11	9:M:420:LYS:HZ3	1.66	0.52
7:K:392:LEU:HD11	9:M:420:LYS:CE	2.40	0.52
10:N:85:LYS:HB2	10:N:85:LYS:NZ	2.25	0.51
10:N:85:LYS:HB2	10:N:85:LYS:NZ	2.25	0.51
10:N:85:LYS:HB2	10:N:85:LYS:NZ	2.25	0.51
10:N:85:LYS:HB2	10:N:85:LYS:NZ	2.25	0.51
10:N:85:LYS:HB2	10:N:85:LYS:NZ	2.25	0.51
10:N:85:LYS:HB2	10:N:85:LYS:NZ	2.25	0.51
10:N:85:LYS:HB2	10:N:85:LYS:NZ	2.25	0.51
10:N:85:LYS:HB2	10:N:85:LYS:NZ	2.25	0.51
10:N:85:LYS:HB2	10:N:85:LYS:NZ	2.25	0.51
10:N:85:LYS:HB2	10:N:85:LYS:NZ	2.25	0.51
7:K:777:ASN:C	7:K:777:ASN:OD1	2.50	0.51
7:K:817:THR:OG1	7:K:818:GLN:N	2.40	0.51
5:I:95:DC:OP2	7:K:608:LYS:N	2.43	0.51
7:K:793:PHE:CD1	7:K:793:PHE:N	2.77	0.51
2:B:53:GLU:OE1	2:B:53:GLU:HA	2.09	0.51
7:K:777:ASN:C	7:K:777:ASN:OD1	2.49	0.51
2:B:53:GLU:OE1	2:B:53:GLU:HA	2.09	0.51
3:G:78:ARG:HE	5:I:20:DA:H4'	1.76	0.51
7:K:392:LEU:HD12	9:M:420:LYS:NZ	2.25	0.51
3:G:77:THR:OG1	6:J:132:DC:P	2.69	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:1053:GLN:HG2	7:K:1053:GLN:O	2.11	0.51
12:K:1502:ADP:N3	12:K:1502:ADP:H2'	2.25	0.51
3:C:91:ASP:OD1	3:C:91:ASP:C	2.53	0.51
7:K:648:ILE:HG22	7:K:648:ILE:O	2.10	0.51
3:C:91:ASP:OD1	3:C:91:ASP:C	2.53	0.51
6:J:55:DG:OP1	7:K:866:SER:OG	2.17	0.51
7:K:687:HIS:O	7:K:691:ARG:N	2.44	0.51
7:K:890:ASN:OD1	7:K:890:ASN:C	2.53	0.51
5:I:95:DC:OP1	7:K:608:LYS:CB	2.58	0.51
7:K:358:LEU:CB	9:M:438:GLN:HB2	2.41	0.51
1:A:64:ARG:HD3	5:I:91:DA:H4'	1.93	0.51
7:K:358:LEU:CB	9:M:438:GLN:HB2	2.41	0.51
7:K:358:LEU:CB	9:M:438:GLN:HB2	2.41	0.51
7:K:358:LEU:CB	9:M:438:GLN:HB2	2.41	0.51
7:K:1046:GLU:HB3	7:K:1047:PRO:HD3	1.93	0.51
7:K:358:LEU:CB	9:M:438:GLN:HB2	2.41	0.51
3:C:91:ASP:OD1	3:C:91:ASP:C	2.53	0.51
7:K:358:LEU:CB	9:M:438:GLN:HB2	2.41	0.51
7:K:358:LEU:CB	9:M:438:GLN:HB2	2.41	0.51
7:K:358:LEU:CB	9:M:438:GLN:HB2	2.41	0.51
3:C:91:ASP:OD1	3:C:91:ASP:C	2.54	0.51
7:K:358:LEU:CB	9:M:438:GLN:HB2	2.41	0.51
7:K:358:LEU:CB	9:M:438:GLN:HB2	2.41	0.51
7:K:359:HIS:CE1	9:M:434:ILE:HG22	2.27	0.51
7:K:359:HIS:CE1	9:M:434:ILE:HG22	2.27	0.51
7:K:359:HIS:CE1	9:M:434:ILE:HG22	2.27	0.51
7:K:359:HIS:CE1	9:M:434:ILE:HG22	2.27	0.51
7:K:513:TYR:CD1	7:K:513:TYR:N	2.77	0.51
7:K:359:HIS:CE1	9:M:434:ILE:HG22	2.27	0.51
7:K:359:HIS:CE1	9:M:434:ILE:HG22	2.27	0.51
7:K:359:HIS:CE1	9:M:434:ILE:HG22	2.27	0.51
7:K:359:HIS:CE1	9:M:434:ILE:HG22	2.27	0.51
7:K:1043:GLU:OE1	7:K:1043:GLU:N	2.29	0.51
7:K:359:HIS:CE1	9:M:434:ILE:HG22	2.27	0.51
2:B:53:GLU:OE1	2:B:53:GLU:HA	2.09	0.51
7:K:359:HIS:CE1	9:M:434:ILE:HG22	2.27	0.51
7:K:358:LEU:HD11	9:M:437:LYS:CG	2.38	0.51
7:K:358:LEU:HD11	9:M:437:LYS:CG	2.38	0.51
7:K:358:LEU:HD11	9:M:437:LYS:CG	2.38	0.51
7:K:358:LEU:HD11	9:M:437:LYS:CG	2.38	0.51
7:K:358:LEU:HD11	9:M:437:LYS:CG	2.38	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:358:LEU:HD11	9:M:437:LYS:CG	2.38	0.51
7:K:710:VAL:O	7:K:710:VAL:HG23	2.11	0.51
5:I:95:DC:OP2	7:K:608:LYS:CB	2.59	0.51
7:K:358:LEU:HD11	9:M:437:LYS:CG	2.38	0.51
7:K:358:LEU:HD11	9:M:437:LYS:CG	2.38	0.51
7:K:358:LEU:HD11	9:M:437:LYS:CG	2.38	0.51
7:K:358:LEU:HD11	9:M:437:LYS:CG	2.38	0.51
2:B:53:GLU:OE1	2:B:53:GLU:HA	2.09	0.50
7:K:378:LEU:C	7:K:676:GLU:OE1	2.52	0.50
5:I:95:DC:OP1	7:K:608:LYS:HB3	2.11	0.50
5:I:95:DC:OP2	7:K:608:LYS:HB2	2.12	0.50
6:J:54:DC:P	7:K:816:MET:HB2	2.47	0.50
7:K:354:LEU:O	9:M:438:GLN:CD	2.54	0.50
7:K:354:LEU:O	9:M:438:GLN:CD	2.54	0.50
7:K:354:LEU:O	9:M:438:GLN:CD	2.54	0.50
7:K:354:LEU:O	9:M:438:GLN:CD	2.54	0.50
7:K:354:LEU:O	9:M:438:GLN:CD	2.54	0.50
7:K:354:LEU:O	9:M:438:GLN:CD	2.54	0.50
7:K:354:LEU:O	9:M:438:GLN:CD	2.54	0.50
7:K:354:LEU:O	9:M:438:GLN:CD	2.54	0.50
7:K:354:LEU:O	9:M:438:GLN:CD	2.54	0.50
7:K:610:SER:OG	7:K:611:PHE:N	2.41	0.50
7:K:354:LEU:O	9:M:438:GLN:CD	2.54	0.50
7:K:354:LEU:O	9:M:438:GLN:CD	2.54	0.50
7:K:358:LEU:HD21	9:M:434:ILE:O	2.11	0.50
7:K:358:LEU:HD21	9:M:434:ILE:O	2.11	0.50
4:H:87:ARG:NH1	5:I:40:DG:H3'	2.25	0.50
7:K:358:LEU:HD21	9:M:434:ILE:O	2.11	0.50
12:K:1502:ADP:PB	13:K:1503:BEF:F2	2.60	0.50
7:K:358:LEU:HD21	9:M:434:ILE:O	2.11	0.50
7:K:358:LEU:HD21	9:M:434:ILE:O	2.11	0.50
7:K:358:LEU:HD21	9:M:434:ILE:O	2.11	0.50
7:K:358:LEU:HD21	9:M:434:ILE:O	2.11	0.50
7:K:358:LEU:HD21	9:M:434:ILE:O	2.11	0.50
7:K:358:LEU:HD21	9:M:434:ILE:O	2.11	0.50
7:K:358:LEU:HD21	9:M:434:ILE:O	2.11	0.50
7:K:577:GLU:OE1	7:K:577:GLU:N	2.30	0.50
7:K:342:TRP:HZ2	7:K:350:GLN:HG3	1.77	0.50
7:K:342:TRP:HZ2	7:K:350:GLN:HG3	1.77	0.50
7:K:342:TRP:HZ2	7:K:350:GLN:HG3	1.77	0.50
7:K:342:TRP:HZ2	7:K:350:GLN:HG3	1.77	0.50
3:C:91:ASP:OD1	3:C:91:ASP:C	2.53	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:342:TRP:HZ2	7:K:350:GLN:HG3	1.77	0.50
7:K:342:TRP:HZ2	7:K:350:GLN:HG3	1.77	0.50
7:K:651:SER:OG	7:K:652:ALA:N	2.44	0.50
7:K:342:TRP:HZ2	7:K:350:GLN:HG3	1.77	0.50
7:K:342:TRP:HZ2	7:K:350:GLN:HG3	1.77	0.50
7:K:342:TRP:HZ2	7:K:350:GLN:HG3	1.77	0.50
7:K:342:TRP:HZ2	7:K:350:GLN:HG3	1.77	0.50
9:M:119:TRP:CD1	9:M:119:TRP:N	2.77	0.49
9:M:119:TRP:CD1	9:M:119:TRP:N	2.77	0.49
9:M:119:TRP:CD1	9:M:119:TRP:N	2.77	0.49
9:M:119:TRP:CD1	9:M:119:TRP:N	2.77	0.49
3:G:78:ARG:HE	5:I:20:DA:H4'	1.77	0.49
9:M:119:TRP:CD1	9:M:119:TRP:N	2.77	0.49
9:M:119:TRP:CD1	9:M:119:TRP:N	2.77	0.49
9:M:119:TRP:CD1	9:M:119:TRP:N	2.77	0.49
9:M:119:TRP:CD1	9:M:119:TRP:N	2.77	0.49
9:M:119:TRP:CD1	9:M:119:TRP:N	2.77	0.49
7:K:834:TYR:CD1	7:K:834:TYR:C	2.89	0.49
9:M:119:TRP:CD1	9:M:119:TRP:N	2.77	0.49
7:K:1043:GLU:OE1	7:K:1043:GLU:N	2.38	0.49
7:K:874:LEU:C	7:K:874:LEU:HD12	2.37	0.49
7:K:342:TRP:O	7:K:342:TRP:CG	2.61	0.49
7:K:900:ARG:NE	7:K:900:ARG:HA	2.27	0.49
7:K:342:TRP:O	7:K:342:TRP:CG	2.61	0.49
7:K:447:TYR:HD1	7:K:447:TYR:H	1.58	0.49
7:K:577:GLU:OE1	7:K:577:GLU:N	2.40	0.49
7:K:342:TRP:O	7:K:342:TRP:CG	2.61	0.49
7:K:710:VAL:O	7:K:710:VAL:HG23	2.11	0.49
7:K:342:TRP:O	7:K:342:TRP:CG	2.61	0.49
7:K:342:TRP:O	7:K:342:TRP:CG	2.61	0.49
7:K:342:TRP:O	7:K:342:TRP:CG	2.61	0.49
7:K:342:TRP:O	7:K:342:TRP:CG	2.61	0.49
7:K:342:TRP:O	7:K:342:TRP:CG	2.61	0.49
7:K:342:TRP:O	7:K:342:TRP:CG	2.61	0.49
7:K:342:TRP:O	7:K:342:TRP:CG	2.61	0.49
7:K:479:GLU:OE1	7:K:479:GLU:HA	2.12	0.49
7:K:604:ASN:OD1	7:K:604:ASN:C	2.55	0.49
7:K:721:LEU:C	7:K:721:LEU:HD23	2.37	0.49
7:K:732:HIS:O	7:K:733:ASN:CB	2.59	0.49
7:K:675:THR:OG1	7:K:676:GLU:N	2.45	0.49
3:G:78:ARG:HE	5:I:20:DA:H4'	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:95:DC:P	7:K:608:LYS:N	2.84	0.49
7:K:577:GLU:CD	7:K:577:GLU:N	2.70	0.49
6:J:54:DC:P	7:K:816:MET:HB2	2.52	0.49
7:K:381:LEU:CA	7:K:676:GLU:OE2	2.60	0.49
7:K:358:LEU:O	7:K:362:MET:HB3	2.12	0.49
7:K:358:LEU:O	7:K:362:MET:HB3	2.12	0.49
7:K:358:LEU:O	7:K:362:MET:HB3	2.12	0.49
7:K:358:LEU:O	7:K:362:MET:HB3	2.12	0.49
3:G:91:ASP:C	3:G:91:ASP:OD1	2.53	0.49
7:K:358:LEU:O	7:K:362:MET:HB3	2.12	0.49
7:K:358:LEU:O	7:K:362:MET:HB3	2.12	0.49
7:K:904:ILE:HG23	7:K:904:ILE:O	2.13	0.49
7:K:358:LEU:O	7:K:362:MET:HB3	2.12	0.49
7:K:358:LEU:O	7:K:362:MET:HB3	2.12	0.49
7:K:358:LEU:O	7:K:362:MET:HB3	2.12	0.49
7:K:358:LEU:O	7:K:362:MET:HB3	2.12	0.49
7:K:687:HIS:O	7:K:691:ARG:N	2.45	0.49
7:K:710:VAL:O	7:K:710:VAL:HG23	2.13	0.49
9:M:418:GLU:OE1	9:M:418:GLU:N	2.36	0.49
3:G:77:THR:OG1	6:J:132:DC:P	2.71	0.49
9:M:418:GLU:OE1	9:M:418:GLU:N	2.36	0.49
9:M:418:GLU:OE1	9:M:418:GLU:N	2.36	0.49
9:M:418:GLU:OE1	9:M:418:GLU:N	2.36	0.49
9:M:418:GLU:OE1	9:M:418:GLU:N	2.36	0.49
9:M:418:GLU:OE1	9:M:418:GLU:N	2.36	0.49
9:M:418:GLU:OE1	9:M:418:GLU:N	2.36	0.49
3:G:91:ASP:C	3:G:91:ASP:OD1	2.54	0.49
7:K:609:LEU:O	7:K:610:SER:C	2.56	0.49
9:M:418:GLU:OE1	9:M:418:GLU:N	2.36	0.49
9:M:418:GLU:OE1	9:M:418:GLU:N	2.36	0.49
9:M:418:GLU:OE1	9:M:418:GLU:N	2.36	0.49
3:G:77:THR:OG1	6:J:132:DC:P	2.71	0.48
7:K:513:TYR:CD1	7:K:513:TYR:N	2.78	0.48
7:K:406:ARG:NE	7:K:406:ARG:HA	2.28	0.48
7:K:887:THR:O	7:K:887:THR:CG2	2.53	0.48
2:B:46:ARG:NH1	6:J:70:DG:H4'	2.28	0.48
10:N:66:ASN:OD1	10:N:66:ASN:C	2.55	0.48
7:K:381:LEU:CB	7:K:676:GLU:OE1	2.61	0.48
10:N:66:ASN:OD1	10:N:66:ASN:C	2.55	0.48
3:G:91:ASP:C	3:G:91:ASP:OD1	2.54	0.48
7:K:834:TYR:CD1	7:K:834:TYR:C	2.91	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:N:66:ASN:OD1	10:N:66:ASN:C	2.55	0.48
7:K:753:ASN:OD1	7:K:753:ASN:C	2.56	0.48
10:N:66:ASN:OD1	10:N:66:ASN:C	2.55	0.48
7:K:649:PHE:O	7:K:649:PHE:HD1	1.96	0.48
10:N:66:ASN:OD1	10:N:66:ASN:C	2.55	0.48
10:N:66:ASN:OD1	10:N:66:ASN:C	2.55	0.48
2:B:46:ARG:NH1	6:J:70:DG:H4'	2.28	0.48
7:K:679:THR:OG1	7:K:680:LEU:N	2.42	0.48
10:N:66:ASN:OD1	10:N:66:ASN:C	2.55	0.48
10:N:66:ASN:OD1	10:N:66:ASN:C	2.55	0.48
10:N:66:ASN:OD1	10:N:66:ASN:C	2.55	0.48
10:N:66:ASN:OD1	10:N:66:ASN:C	2.55	0.48
7:K:351:PHE:CE1	9:M:447:PHE:CB	2.96	0.48
7:K:351:PHE:CE1	9:M:447:PHE:CB	2.96	0.48
7:K:351:PHE:CE1	9:M:447:PHE:CB	2.96	0.48
7:K:351:PHE:CE1	9:M:447:PHE:CB	2.96	0.48
7:K:351:PHE:CE1	9:M:447:PHE:CB	2.96	0.48
2:B:46:ARG:NH1	6:J:70:DG:H4'	2.28	0.48
7:K:351:PHE:CE1	9:M:447:PHE:CB	2.96	0.48
7:K:351:PHE:CE1	9:M:447:PHE:CB	2.96	0.48
7:K:351:PHE:CE1	9:M:447:PHE:CB	2.96	0.48
7:K:351:PHE:CE1	9:M:447:PHE:CB	2.96	0.48
7:K:351:PHE:CE1	9:M:447:PHE:CB	2.96	0.48
7:K:354:LEU:HD11	9:M:442:HIS:HD2	1.78	0.48
7:K:354:LEU:HD11	9:M:442:HIS:HD2	1.78	0.48
7:K:354:LEU:HD11	9:M:442:HIS:HD2	1.78	0.48
7:K:354:LEU:HD11	9:M:442:HIS:HD2	1.78	0.48
7:K:354:LEU:HD11	9:M:442:HIS:HD2	1.78	0.48
7:K:354:LEU:HD11	9:M:442:HIS:HD2	1.78	0.48
7:K:354:LEU:HD11	9:M:442:HIS:HD2	1.78	0.48
7:K:354:LEU:HD11	9:M:442:HIS:HD2	1.78	0.48
7:K:354:LEU:HD11	9:M:442:HIS:HD2	1.78	0.48
14:L:501:ATP:O2B	14:L:501:ATP:O1A	2.27	0.48
14:L:501:ATP:O2B	14:L:501:ATP:O1A	2.27	0.48
14:L:501:ATP:O2B	14:L:501:ATP:O1A	2.27	0.48
6:J:56:DG:OP2	7:K:846:ARG:NH2	2.39	0.48
14:L:501:ATP:O2B	14:L:501:ATP:O1A	2.27	0.48
14:L:501:ATP:O2B	14:L:501:ATP:O1A	2.27	0.48
3:G:91:ASP:C	3:G:91:ASP:OD1	2.54	0.48
14:L:501:ATP:O2B	14:L:501:ATP:O1A	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:L:501:ATP:O2B	14:L:501:ATP:O1A	2.27	0.48
14:L:501:ATP:O2B	14:L:501:ATP:O1A	2.27	0.48
14:L:501:ATP:O2B	14:L:501:ATP:O1A	2.27	0.48
14:L:501:ATP:O2B	14:L:501:ATP:O1A	2.27	0.48
6:J:56:DG:H5"	7:K:528:LEU:HD12	1.96	0.48
3:G:45:GLY:HA2	6:J:112:DG:H5"	1.96	0.48
3:G:45:GLY:HA2	6:J:112:DG:H5"	1.96	0.48
5:I:95:DC:OP2	7:K:608:LYS:CB	2.62	0.48
7:K:577:GLU:H	7:K:577:GLU:CD	2.21	0.48
7:K:902:HIS:CD2	7:K:902:HIS:C	2.90	0.48
7:K:816:MET:HE2	7:K:816:MET:HA	1.95	0.48
7:K:1043:GLU:OE1	7:K:1043:GLU:N	2.40	0.48
7:K:342:TRP:CZ3	7:K:346:GLU:OE1	2.67	0.48
7:K:687:HIS:O	7:K:691:ARG:N	2.47	0.48
7:K:342:TRP:CZ3	7:K:346:GLU:OE1	2.67	0.48
7:K:342:TRP:CZ3	7:K:346:GLU:OE1	2.67	0.48
7:K:977:ASP:OD1	7:K:977:ASP:C	2.57	0.48
7:K:342:TRP:CZ3	7:K:346:GLU:OE1	2.67	0.48
7:K:1053:GLN:HG2	7:K:1053:GLN:O	2.14	0.48
7:K:342:TRP:CZ3	7:K:346:GLU:OE1	2.67	0.48
7:K:342:TRP:CZ3	7:K:346:GLU:OE1	2.67	0.48
7:K:479:GLU:OE1	7:K:479:GLU:HA	2.13	0.48
7:K:342:TRP:CZ3	7:K:346:GLU:OE1	2.67	0.48
5:I:95:DC:OP2	7:K:608:LYS:CB	2.58	0.48
7:K:342:TRP:CZ3	7:K:346:GLU:OE1	2.67	0.48
6:J:54:DC:H5"	7:K:816:MET:CG	2.44	0.48
7:K:342:TRP:CZ3	7:K:346:GLU:OE1	2.67	0.48
7:K:501:LYS:NZ	7:K:626:THR:O	2.47	0.48
7:K:342:TRP:CZ3	7:K:346:GLU:OE1	2.67	0.48
7:K:975:GLU:OE1	7:K:975:GLU:N	2.33	0.48
5:I:95:DC:OP1	7:K:608:LYS:CA	2.62	0.47
2:B:46:ARG:NH1	6:J:70:DG:H4'	2.29	0.47
7:K:358:LEU:CD1	9:M:437:LYS:HE3	2.43	0.47
7:K:358:LEU:CD1	9:M:437:LYS:HE3	2.43	0.47
7:K:358:LEU:CD1	9:M:437:LYS:HE3	2.43	0.47
7:K:479:GLU:OE1	7:K:479:GLU:HA	2.14	0.47
7:K:358:LEU:CD1	9:M:437:LYS:HE3	2.43	0.47
7:K:358:LEU:CD1	9:M:437:LYS:HE3	2.43	0.47
7:K:358:LEU:CD1	9:M:437:LYS:HE3	2.43	0.47
7:K:358:LEU:CD1	9:M:437:LYS:HE3	2.43	0.47
7:K:358:LEU:CD1	9:M:437:LYS:HE3	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:358:LEU:CD1	9:M:437:LYS:HE3	2.43	0.47
7:K:872:LEU:HD12	7:K:872:LEU:O	2.13	0.47
3:G:77:THR:OG1	6:J:132:DC:P	2.72	0.47
7:K:358:LEU:CD1	9:M:437:LYS:HE3	2.43	0.47
2:B:46:ARG:NH1	6:J:70:DG:H4'	2.29	0.47
3:G:45:GLY:HA2	6:J:112:DG:H5"	1.96	0.47
5:I:95:DC:OP1	7:K:608:LYS:CB	2.60	0.47
3:G:45:GLY:HA2	6:J:112:DG:H5"	1.96	0.47
5:I:33:DG:H2"	5:I:34:DG:H5"	1.96	0.47
7:K:355:GLY:HA2	9:M:438:GLN:HG2	1.96	0.47
5:I:33:DG:H2"	5:I:34:DG:H5"	1.96	0.47
7:K:355:GLY:HA2	9:M:438:GLN:HG2	1.96	0.47
5:I:33:DG:H2"	5:I:34:DG:H5"	1.96	0.47
7:K:355:GLY:HA2	9:M:438:GLN:HG2	1.96	0.47
5:I:33:DG:H2"	5:I:34:DG:H5"	1.96	0.47
7:K:355:GLY:HA2	9:M:438:GLN:HG2	1.96	0.47
5:I:33:DG:H2"	5:I:34:DG:H5"	1.96	0.47
7:K:355:GLY:HA2	9:M:438:GLN:HG2	1.96	0.47
5:I:33:DG:H2"	5:I:34:DG:H5"	1.96	0.47
7:K:355:GLY:HA2	9:M:438:GLN:HG2	1.96	0.47
5:I:33:DG:H2"	5:I:34:DG:H5"	1.96	0.47
6:J:54:DC:OP1	7:K:816:MET:CB	2.52	0.47
7:K:355:GLY:HA2	9:M:438:GLN:HG2	1.96	0.47
7:K:513:TYR:N	7:K:513:TYR:HD1	2.11	0.47
5:I:33:DG:H2"	5:I:34:DG:H5"	1.96	0.47
7:K:355:GLY:HA2	9:M:438:GLN:HG2	1.96	0.47
5:I:33:DG:H2"	5:I:34:DG:H5"	1.96	0.47
7:K:355:GLY:HA2	9:M:438:GLN:HG2	1.96	0.47
5:I:33:DG:H2"	5:I:34:DG:H5"	1.96	0.47
7:K:355:GLY:HA2	9:M:438:GLN:HG2	1.96	0.47
7:K:368:LYS:O	7:K:372:ARG:HG3	2.14	0.47
7:K:368:LYS:O	7:K:372:ARG:HG3	2.14	0.47
7:K:368:LYS:O	7:K:372:ARG:HG3	2.14	0.47
7:K:368:LYS:O	7:K:372:ARG:HG3	2.14	0.47
7:K:368:LYS:O	7:K:372:ARG:HG3	2.14	0.47
7:K:368:LYS:O	7:K:372:ARG:HG3	2.14	0.47
7:K:368:LYS:O	7:K:372:ARG:HG3	2.14	0.47
7:K:368:LYS:O	7:K:372:ARG:HG3	2.14	0.47
7:K:368:LYS:O	7:K:372:ARG:HG3	2.14	0.47
7:K:838:ASP:OD1	7:K:838:ASP:C	2.56	0.47
3:G:78:ARG:HE	5:I:20:DA:H4'	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:368:LYS:O	7:K:372:ARG:HG3	2.14	0.47
7:K:1001:GLU:OE1	7:K:1001:GLU:HA	2.14	0.47
7:K:765:HIS:O	7:K:767:PHE:N	2.48	0.47
7:K:354:LEU:HD11	9:M:442:HIS:CD2	2.49	0.47
7:K:354:LEU:HD11	9:M:442:HIS:CD2	2.49	0.47
7:K:354:LEU:HD11	9:M:442:HIS:CD2	2.49	0.47
7:K:354:LEU:HD11	9:M:442:HIS:CD2	2.49	0.47
7:K:354:LEU:HD11	9:M:442:HIS:CD2	2.49	0.47
7:K:354:LEU:HD11	9:M:442:HIS:CD2	2.49	0.47
7:K:354:LEU:HD11	9:M:442:HIS:CD2	2.49	0.47
7:K:513:TYR:N	7:K:513:TYR:CD1	2.80	0.47
7:K:977:ASP:OD1	7:K:977:ASP:C	2.58	0.47
7:K:354:LEU:HD11	9:M:442:HIS:CD2	2.49	0.47
7:K:354:LEU:HD11	9:M:442:HIS:CD2	2.49	0.47
7:K:354:LEU:HD11	9:M:442:HIS:CD2	2.49	0.47
7:K:977:ASP:OD2	7:K:977:ASP:C	2.56	0.47
3:G:45:GLY:HA2	6:J:112:DG:H5”	1.97	0.47
7:K:686:LEU:C	7:K:686:LEU:HD23	2.40	0.47
7:K:358:LEU:HG	9:M:437:LYS:HE3	1.96	0.47
7:K:358:LEU:HG	9:M:437:LYS:HE3	1.96	0.47
7:K:358:LEU:HG	9:M:437:LYS:HE3	1.96	0.47
7:K:358:LEU:HG	9:M:437:LYS:HE3	1.96	0.47
7:K:358:LEU:HG	9:M:437:LYS:HE3	1.96	0.47
5:I:95:DC:OP1	7:K:608:LYS:CB	2.60	0.47
7:K:358:LEU:HG	9:M:437:LYS:HE3	1.96	0.47
7:K:358:LEU:HG	9:M:437:LYS:HE3	1.96	0.47
7:K:358:LEU:HG	9:M:437:LYS:HE3	1.96	0.47
7:K:358:LEU:HG	9:M:437:LYS:HE3	1.96	0.47
7:K:636:GLU:CD	7:K:636:GLU:H	2.22	0.47
7:K:358:LEU:HG	9:M:437:LYS:HE3	1.96	0.47
12:K:1502:ADP:O3B	12:K:1502:ADP:O5’	2.33	0.47
7:K:351:PHE:CE1	9:M:447:PHE:CG	3.03	0.46
7:K:351:PHE:CD1	9:M:467:PHE:HD2	2.27	0.46
9:M:213:LEU:C	9:M:213:LEU:HD23	2.40	0.46
7:K:351:PHE:CE1	9:M:447:PHE:CG	3.03	0.46
7:K:351:PHE:CD1	9:M:467:PHE:HD2	2.27	0.46
9:M:213:LEU:C	9:M:213:LEU:HD23	2.40	0.46
7:K:351:PHE:CE1	9:M:447:PHE:CG	3.03	0.46
7:K:351:PHE:CD1	9:M:467:PHE:HD2	2.27	0.46
9:M:213:LEU:C	9:M:213:LEU:HD23	2.40	0.46
7:K:351:PHE:CE1	9:M:447:PHE:CG	3.03	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:351:PHE:CD1	9:M:467:PHE:HD2	2.27	0.46
9:M:213:LEU:C	9:M:213:LEU:HD23	2.40	0.46
7:K:351:PHE:CE1	9:M:447:PHE:CG	3.03	0.46
7:K:351:PHE:CD1	9:M:467:PHE:HD2	2.27	0.46
9:M:213:LEU:C	9:M:213:LEU:HD23	2.40	0.46
7:K:351:PHE:CE1	9:M:447:PHE:CG	3.03	0.46
7:K:351:PHE:CD1	9:M:467:PHE:HD2	2.27	0.46
9:M:213:LEU:C	9:M:213:LEU:HD23	2.40	0.46
7:K:351:PHE:CE1	9:M:447:PHE:CG	3.03	0.46
7:K:351:PHE:CD1	9:M:467:PHE:HD2	2.27	0.46
9:M:213:LEU:C	9:M:213:LEU:HD23	2.40	0.46
7:K:351:PHE:CE1	9:M:447:PHE:CG	3.03	0.46
7:K:351:PHE:CD1	9:M:467:PHE:HD2	2.27	0.46
9:M:213:LEU:C	9:M:213:LEU:HD23	2.40	0.46
7:K:351:PHE:CE1	9:M:447:PHE:CG	3.03	0.46
7:K:351:PHE:CD1	9:M:467:PHE:HD2	2.27	0.46
9:M:213:LEU:C	9:M:213:LEU:HD23	2.40	0.46
7:K:351:PHE:CE1	9:M:447:PHE:CG	3.03	0.46
7:K:351:PHE:CD1	9:M:467:PHE:HD2	2.27	0.46
7:K:904:ILE:HG23	7:K:904:ILE:O	2.14	0.46
9:M:213:LEU:C	9:M:213:LEU:HD23	2.40	0.46
9:M:57:ASN:C	9:M:57:ASN:OD1	2.57	0.46
9:M:57:ASN:C	9:M:57:ASN:OD1	2.57	0.46
9:M:57:ASN:C	9:M:57:ASN:OD1	2.57	0.46
7:K:834:TYR:CD1	7:K:834:TYR:C	2.94	0.46
9:M:57:ASN:C	9:M:57:ASN:OD1	2.57	0.46
9:M:57:ASN:C	9:M:57:ASN:OD1	2.57	0.46
9:M:57:ASN:C	9:M:57:ASN:OD1	2.57	0.46
9:M:57:ASN:C	9:M:57:ASN:OD1	2.57	0.46
7:K:977:ASP:OD1	7:K:977:ASP:C	2.58	0.46
9:M:57:ASN:C	9:M:57:ASN:OD1	2.57	0.46
3:G:45:GLY:HA2	6:J:112:DG:H5"	1.97	0.46
9:M:57:ASN:C	9:M:57:ASN:OD1	2.57	0.46
9:M:57:ASN:C	9:M:57:ASN:OD1	2.57	0.46
10:N:80:ASP:OD1	10:N:80:ASP:C	2.57	0.46
7:K:1043:GLU:OE1	7:K:1043:GLU:N	2.37	0.46
10:N:80:ASP:OD1	10:N:80:ASP:C	2.57	0.46
10:N:80:ASP:OD1	10:N:80:ASP:C	2.57	0.46
7:K:721:LEU:C	7:K:721:LEU:HD23	2.40	0.46
7:K:977:ASP:OD1	7:K:977:ASP:C	2.57	0.46
10:N:80:ASP:OD1	10:N:80:ASP:C	2.57	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:N:80:ASP:OD1	10:N:80:ASP:C	2.57	0.46
7:K:816:MET:SD	7:K:816:MET:C	2.98	0.46
10:N:80:ASP:OD1	10:N:80:ASP:C	2.57	0.46
7:K:877:GLN:OE1	7:K:877:GLN:N	2.42	0.46
10:N:80:ASP:OD1	10:N:80:ASP:C	2.57	0.46
10:N:80:ASP:OD1	10:N:80:ASP:C	2.57	0.46
5:I:95:DC:OP1	7:K:608:LYS:CA	2.63	0.46
7:K:479:GLU:OE1	7:K:479:GLU:HA	2.14	0.46
7:K:649:PHE:O	7:K:649:PHE:HD2	1.92	0.46
10:N:80:ASP:OD1	10:N:80:ASP:C	2.57	0.46
10:N:80:ASP:OD1	10:N:80:ASP:C	2.57	0.46
2:B:46:ARG:NH1	6:J:70:DG:H4'	2.30	0.46
7:K:732:HIS:O	7:K:733:ASN:CB	2.63	0.46
7:K:810:VAL:HG12	7:K:881:THR:HB	1.96	0.46
2:B:46:ARG:NH1	6:J:70:DG:H4'	2.31	0.46
9:M:107:SER:OG	9:M:108:ASN:N	2.41	0.46
9:M:107:SER:OG	9:M:108:ASN:N	2.41	0.46
9:M:107:SER:OG	9:M:108:ASN:N	2.41	0.46
7:K:830:LYS:HE2	7:K:830:LYS:HA	1.96	0.46
9:M:107:SER:OG	9:M:108:ASN:N	2.41	0.46
9:M:107:SER:OG	9:M:108:ASN:N	2.41	0.46
9:M:107:SER:OG	9:M:108:ASN:N	2.41	0.46
7:K:675:THR:OG1	7:K:676:GLU:N	2.47	0.46
9:M:107:SER:OG	9:M:108:ASN:N	2.41	0.46
9:M:107:SER:OG	9:M:108:ASN:N	2.41	0.46
9:M:107:SER:OG	9:M:108:ASN:N	2.41	0.46
9:M:107:SER:OG	9:M:108:ASN:N	2.41	0.46
6:J:54:DC:H5"	7:K:816:MET:CB	2.42	0.46
6:J:56:DG:C5'	7:K:528:LEU:HD12	2.43	0.46
7:K:771:GLU:OE1	7:K:771:GLU:N	2.33	0.46
7:K:877:GLN:OE1	7:K:877:GLN:N	2.36	0.46
7:K:342:TRP:CE2	7:K:346:GLU:HB3	2.50	0.46
7:K:342:TRP:CE2	7:K:346:GLU:HB3	2.50	0.46
7:K:342:TRP:CE2	7:K:346:GLU:HB3	2.50	0.46
7:K:342:TRP:CE2	7:K:346:GLU:HB3	2.50	0.46
7:K:777:ASN:C	7:K:777:ASN:OD1	2.57	0.46
1:A:60:GLU:OE1	1:A:60:GLU:N	2.35	0.46
7:K:342:TRP:CE2	7:K:346:GLU:HB3	2.50	0.46
7:K:342:TRP:CE2	7:K:346:GLU:HB3	2.50	0.46
7:K:342:TRP:CE2	7:K:346:GLU:HB3	2.50	0.46
7:K:342:TRP:CE2	7:K:346:GLU:HB3	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:342:TRP:CE2	7:K:346:GLU:HB3	2.50	0.46
7:K:342:TRP:CE2	7:K:346:GLU:HB3	2.50	0.46
7:K:877:GLN:OE1	7:K:877:GLN:N	2.38	0.46
7:K:381:LEU:CB	7:K:676:GLU:CD	2.74	0.46
1:A:60:GLU:OE1	1:A:60:GLU:N	2.36	0.46
6:J:54:DC:P	7:K:816:MET:HB2	2.55	0.46
7:K:405:LEU:O	7:K:409:ASN:N	2.48	0.46
7:K:347:ARG:H	7:K:347:ARG:HD2	1.81	0.46
7:K:347:ARG:H	7:K:347:ARG:HD2	1.81	0.46
7:K:347:ARG:H	7:K:347:ARG:HD2	1.81	0.46
7:K:347:ARG:H	7:K:347:ARG:HD2	1.81	0.46
7:K:347:ARG:H	7:K:347:ARG:HD2	1.81	0.46
7:K:347:ARG:H	7:K:347:ARG:HD2	1.81	0.46
7:K:347:ARG:H	7:K:347:ARG:HD2	1.81	0.46
1:A:60:GLU:OE1	1:A:60:GLU:N	2.36	0.46
7:K:347:ARG:H	7:K:347:ARG:HD2	1.81	0.46
7:K:347:ARG:H	7:K:347:ARG:HD2	1.81	0.46
7:K:347:ARG:H	7:K:347:ARG:HD2	1.81	0.46
1:A:60:GLU:OE1	1:A:60:GLU:N	2.36	0.45
7:K:495:ASP:O	7:K:496:GLU:C	2.59	0.45
1:A:60:GLU:OE1	1:A:60:GLU:N	2.36	0.45
6:J:56:DG:H4’	7:K:577:GLU:HG3	1.98	0.45
7:K:645:LEU:O	7:K:647:LYS:N	2.48	0.45
7:K:1001:GLU:OE1	7:K:1001:GLU:HA	2.16	0.45
7:K:834:TYR:CD1	7:K:834:TYR:C	2.94	0.45
7:K:479:GLU:OE1	7:K:479:GLU:HA	2.16	0.45
7:K:837:LEU:C	7:K:837:LEU:HD23	2.41	0.45
7:K:877:GLN:OE1	7:K:877:GLN:N	2.33	0.45
7:K:904:ILE:HG23	7:K:904:ILE:O	2.15	0.45
7:K:519:ILE:O	7:K:519:ILE:HG22	2.15	0.45
1:A:60:GLU:OE1	1:A:60:GLU:N	2.36	0.45
3:C:85:GLN:HA	3:C:85:GLN:OE1	2.16	0.45
5:I:31:DT:H2’	5:I:32:DT:C6	2.51	0.45
2:B:46:ARG:NH1	6:J:70:DG:H4’	2.31	0.45
5:I:31:DT:H2’	5:I:32:DT:C6	2.51	0.45
7:K:513:TYR:CD1	7:K:513:TYR:N	2.82	0.45
1:A:60:GLU:OE1	1:A:60:GLU:N	2.36	0.45
5:I:31:DT:H2’	5:I:32:DT:C6	2.51	0.45
7:K:908:ASN:OD1	7:K:908:ASN:C	2.56	0.45
5:I:31:DT:H2’	5:I:32:DT:C6	2.51	0.45
5:I:31:DT:H2’	5:I:32:DT:C6	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:860:TYR:N	7:K:860:TYR:CD2	2.81	0.45
5:I:31:DT:H2'	5:I:32:DT:C6	2.51	0.45
5:I:31:DT:H2'	5:I:32:DT:C6	2.51	0.45
5:I:31:DT:H2'	5:I:32:DT:C6	2.51	0.45
5:I:31:DT:H2'	5:I:32:DT:C6	2.51	0.45
2:B:46:ARG:NH1	6:J:70:DG:H4'	2.31	0.45
5:I:31:DT:H2'	5:I:32:DT:C6	2.51	0.45
7:K:633:ASN:O	7:K:634:LEU:HB2	2.15	0.45
7:K:679:THR:OG1	7:K:680:LEU:N	2.49	0.45
7:K:800:LEU:N	7:K:801:PRO:CD	2.79	0.45
7:K:511:TYR:C	7:K:511:TYR:CD2	2.94	0.45
7:K:578:TYR:N	7:K:578:TYR:CD1	2.84	0.45
7:K:834:TYR:CD1	7:K:834:TYR:C	2.93	0.45
7:K:687:HIS:O	7:K:691:ARG:N	2.49	0.45
5:I:94:DG:C3'	7:K:608:LYS:CB	2.94	0.45
12:K:1502:ADP:PB	13:K:1503:BEF:F2	2.65	0.45
4:H:87:ARG:NH1	5:I:40:DG:H3'	2.30	0.45
5:I:95:DC:P	7:K:608:LYS:CA	3.05	0.45
7:K:815:GLN:O	7:K:815:GLN:CG	2.61	0.45
7:K:1046:GLU:HB3	7:K:1047:PRO:HD3	1.98	0.45
7:K:347:ARG:HH11	9:M:466:GLN:N	2.10	0.45
7:K:347:ARG:HH11	9:M:466:GLN:N	2.10	0.45
7:K:347:ARG:HH11	9:M:466:GLN:N	2.10	0.45
7:K:347:ARG:HH11	9:M:466:GLN:N	2.10	0.45
7:K:347:ARG:HH11	9:M:466:GLN:N	2.10	0.45
7:K:347:ARG:HH11	9:M:466:GLN:N	2.10	0.45
7:K:405:LEU:O	7:K:409:ASN:N	2.48	0.45
7:K:347:ARG:HH11	9:M:466:GLN:N	2.10	0.45
7:K:347:ARG:HH11	9:M:466:GLN:N	2.10	0.45
7:K:347:ARG:HH11	9:M:466:GLN:N	2.10	0.45
7:K:347:ARG:HH11	9:M:466:GLN:N	2.10	0.45
7:K:358:LEU:CG	9:M:437:LYS:HG3	2.46	0.45
7:K:834:TYR:CD1	7:K:834:TYR:C	2.95	0.45
7:K:358:LEU:CG	9:M:437:LYS:HG3	2.46	0.45
7:K:677:GLU:CD	7:K:677:GLU:N	2.73	0.45
7:K:358:LEU:CG	9:M:437:LYS:HG3	2.46	0.45
7:K:358:LEU:CG	9:M:437:LYS:HG3	2.46	0.45
7:K:358:LEU:CG	9:M:437:LYS:HG3	2.46	0.45
7:K:358:LEU:CG	9:M:437:LYS:HG3	2.46	0.45
7:K:519:ILE:O	7:K:519:ILE:CG2	2.65	0.45
7:K:890:ASN:OD1	7:K:890:ASN:C	2.60	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:358:LEU:CG	9:M:437:LYS:HG3	2.46	0.45
7:K:887:THR:O	7:K:888:ASP:CB	2.64	0.45
7:K:358:LEU:CG	9:M:437:LYS:HG3	2.46	0.45
7:K:358:LEU:CG	9:M:437:LYS:HG3	2.46	0.45
7:K:834:TYR:CD1	7:K:834:TYR:C	2.95	0.45
7:K:358:LEU:CG	9:M:437:LYS:HG3	2.46	0.45
6:J:144:DC:H2'	6:J:145:DG:C8	2.52	0.45
6:J:144:DC:H2'	6:J:145:DG:C8	2.52	0.45
5:I:95:DC:P	7:K:608:LYS:CA	3.04	0.45
6:J:144:DC:H2'	6:J:145:DG:C8	2.52	0.45
6:J:144:DC:H2'	6:J:145:DG:C8	2.52	0.45
6:J:144:DC:H2'	6:J:145:DG:C8	2.52	0.45
6:J:144:DC:H2'	6:J:145:DG:C8	2.52	0.45
6:J:144:DC:H2'	6:J:145:DG:C8	2.52	0.45
7:K:880:ASP:OD1	7:K:880:ASP:C	2.60	0.45
6:J:144:DC:H2'	6:J:145:DG:C8	2.52	0.45
7:K:446:ASP:C	7:K:446:ASP:OD1	2.56	0.45
6:J:144:DC:H2'	6:J:145:DG:C8	2.52	0.45
6:J:144:DC:H2'	6:J:145:DG:C8	2.52	0.45
9:M:46:ARG:NH2	9:M:50:SER:OG	2.49	0.45
7:K:900:ARG:HA	7:K:900:ARG:HD3	1.65	0.45
9:M:46:ARG:NH2	9:M:50:SER:OG	2.49	0.45
9:M:46:ARG:NH2	9:M:50:SER:OG	2.49	0.45
9:M:46:ARG:NH2	9:M:50:SER:OG	2.49	0.45
5:I:95:DC:OP1	7:K:608:LYS:HB3	2.16	0.45
9:M:46:ARG:NH2	9:M:50:SER:OG	2.49	0.45
9:M:46:ARG:NH2	9:M:50:SER:OG	2.49	0.45
9:M:46:ARG:NH2	9:M:50:SER:OG	2.49	0.45
9:M:46:ARG:NH2	9:M:50:SER:OG	2.49	0.45
9:M:46:ARG:NH2	9:M:50:SER:OG	2.49	0.45
9:M:46:ARG:NH2	9:M:50:SER:OG	2.49	0.45
7:K:718:LEU:HD12	7:K:718:LEU:N	2.31	0.44
5:I:94:DG:H5"	7:K:608:LYS:HG2	1.99	0.44
12:K:1502:ADP:O2A	12:K:1502:ADP:H4'	2.17	0.44
7:K:405:LEU:O	7:K:409:ASN:N	2.48	0.44
7:K:647:LYS:O	7:K:649:PHE:N	2.51	0.44
7:K:564:ILE:C	7:K:564:ILE:CD1	2.88	0.44
6:J:106:DG:H2"	6:J:107:DT:H5"	2.00	0.44
6:J:106:DG:H2"	6:J:107:DT:H5"	2.00	0.44
6:J:106:DG:H2"	6:J:107:DT:H5"	2.00	0.44
6:J:106:DG:H2"	6:J:107:DT:H5"	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:106:DG:H2”	6:J:107:DT:H5”	2.00	0.44
7:K:405:LEU:O	7:K:409:ASN:N	2.48	0.44
7:K:648:ILE:O	7:K:648:ILE:HG22	2.16	0.44
6:J:106:DG:H2”	6:J:107:DT:H5”	2.00	0.44
6:J:106:DG:H2”	6:J:107:DT:H5”	2.00	0.44
6:J:106:DG:H2”	6:J:107:DT:H5”	2.00	0.44
6:J:106:DG:H2”	6:J:107:DT:H5”	2.00	0.44
6:J:106:DG:H2”	6:J:107:DT:H5”	2.00	0.44
7:K:479:GLU:OE1	7:K:479:GLU:HA	2.18	0.44
7:K:675:THR:OG1	7:K:676:GLU:N	2.50	0.44
7:K:837:LEU:C	7:K:837:LEU:HD23	2.42	0.44
7:K:378:LEU:N	7:K:676:GLU:OE2	2.49	0.44
7:K:498:GLY:HA3	7:K:903:ARG:HD3	2.00	0.44
9:M:369:ARG:NE	9:M:369:ARG:HA	2.32	0.44
7:K:447:TYR:CD1	7:K:447:TYR:N	2.85	0.44
9:M:369:ARG:NE	9:M:369:ARG:HA	2.32	0.44
9:M:369:ARG:NE	9:M:369:ARG:HA	2.32	0.44
9:M:369:ARG:NE	9:M:369:ARG:HA	2.32	0.44
3:G:80:ILE:HB	3:G:81:PRO:HD2	2.00	0.44
9:M:369:ARG:NE	9:M:369:ARG:HA	2.32	0.44
9:M:369:ARG:NE	9:M:369:ARG:HA	2.32	0.44
7:K:837:LEU:C	7:K:837:LEU:HD23	2.42	0.44
9:M:369:ARG:NE	9:M:369:ARG:HA	2.32	0.44
3:G:80:ILE:HB	3:G:81:PRO:HD2	2.00	0.44
9:M:369:ARG:NE	9:M:369:ARG:HA	2.32	0.44
9:M:369:ARG:NE	9:M:369:ARG:HA	2.32	0.44
9:M:369:ARG:NE	9:M:369:ARG:HA	2.32	0.44
3:G:45:GLY:HA2	6:J:112:DG:H5”	1.99	0.44
3:G:80:ILE:HB	3:G:81:PRO:HD2	2.00	0.44
3:G:80:ILE:HB	3:G:81:PRO:HD2	2.00	0.44
3:G:80:ILE:HB	3:G:81:PRO:HD2	2.00	0.44
3:G:80:ILE:HB	3:G:81:PRO:HD2	2.00	0.44
3:G:80:ILE:HB	3:G:81:PRO:HD2	2.00	0.44
7:K:837:LEU:C	7:K:837:LEU:HD23	2.42	0.44
4:H:87:ARG:NH1	5:I:40:DG:H3’	2.32	0.44
7:K:604:ASN:OD1	7:K:604:ASN:O	2.36	0.44
3:G:80:ILE:HB	3:G:81:PRO:HD2	2.00	0.44
7:K:902:HIS:O	7:K:902:HIS:CG	2.71	0.44
7:K:837:LEU:C	7:K:837:LEU:HD23	2.42	0.44
3:G:80:ILE:HB	3:G:81:PRO:HD2	2.00	0.44
7:K:687:HIS:O	7:K:691:ARG:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:57:DT:OP1	7:K:578:TYR:OH	2.14	0.44
7:K:352:GLY:HA2	9:M:151:TYR:HE2	1.83	0.44
7:K:352:GLY:HA2	9:M:151:TYR:HE2	1.83	0.44
7:K:352:GLY:HA2	9:M:151:TYR:HE2	1.83	0.44
1:A:64:ARG:HD3	5:I:91:DA:H4'	2.00	0.44
7:K:352:GLY:HA2	9:M:151:TYR:HE2	1.83	0.44
7:K:352:GLY:HA2	9:M:151:TYR:HE2	1.83	0.44
7:K:834:TYR:CD1	7:K:834:TYR:C	2.96	0.44
7:K:890:ASN:OD1	7:K:890:ASN:C	2.59	0.44
7:K:352:GLY:HA2	9:M:151:TYR:HE2	1.83	0.44
7:K:860:TYR:CD2	7:K:860:TYR:N	2.76	0.44
7:K:352:GLY:HA2	9:M:151:TYR:HE2	1.83	0.44
7:K:352:GLY:HA2	9:M:151:TYR:HE2	1.83	0.44
7:K:352:GLY:HA2	9:M:151:TYR:HE2	1.83	0.44
7:K:352:GLY:HA2	9:M:151:TYR:HE2	1.83	0.44
7:K:347:ARG:HH11	9:M:466:GLN:CA	2.30	0.43
3:G:48:ALA:N	3:G:49:PRO:HD2	2.33	0.43
7:K:347:ARG:HH11	9:M:466:GLN:CA	2.30	0.43
7:K:602:MET:O	7:K:602:MET:HG2	2.17	0.43
7:K:347:ARG:HH11	9:M:466:GLN:CA	2.30	0.43
7:K:347:ARG:HH11	9:M:466:GLN:CA	2.30	0.43
7:K:1046:GLU:HB3	7:K:1047:PRO:CD	2.48	0.43
7:K:347:ARG:HH11	9:M:466:GLN:CA	2.30	0.43
7:K:347:ARG:HH11	9:M:466:GLN:CA	2.30	0.43
7:K:347:ARG:HH11	9:M:466:GLN:CA	2.30	0.43
7:K:347:ARG:HH11	9:M:466:GLN:CA	2.30	0.43
3:G:80:ILE:HB	3:G:81:PRO:HD2	2.00	0.43
7:K:347:ARG:HH11	9:M:466:GLN:CA	2.30	0.43
7:K:347:ARG:HH11	9:M:466:GLN:CA	2.30	0.43
5:I:103:DA:H2'	5:I:104:DT:C6	2.52	0.43
5:I:103:DA:H2'	5:I:104:DT:C6	2.52	0.43
7:K:692:PRO:O	7:K:693:PHE:HB2	2.19	0.43
5:I:103:DA:H2'	5:I:104:DT:C6	2.52	0.43
5:I:103:DA:H2'	5:I:104:DT:C6	2.52	0.43
7:K:513:TYR:N	7:K:513:TYR:HD1	2.16	0.43
5:I:103:DA:H2'	5:I:104:DT:C6	2.52	0.43
7:K:501:LYS:NZ	7:K:626:THR:O	2.51	0.43
5:I:103:DA:H2'	5:I:104:DT:C6	2.52	0.43
5:I:95:DC:OP1	7:K:607:SER:OG	2.36	0.43
5:I:103:DA:H2'	5:I:104:DT:C6	2.52	0.43
7:K:479:GLU:OE1	7:K:479:GLU:HA	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:103:DA:H2'	5:I:104:DT:C6	2.52	0.43
5:I:103:DA:H2'	5:I:104:DT:C6	2.52	0.43
5:I:103:DA:H2'	5:I:104:DT:C6	2.52	0.43
5:I:95:DC:P	7:K:608:LYS:HB3	2.58	0.43
7:K:902:HIS:C	7:K:902:HIS:CD2	2.95	0.43
4:H:87:ARG:NH1	5:I:40:DG:H3'	2.32	0.43
7:K:661:THR:N	7:K:662:PRO:CD	2.81	0.43
7:K:648:ILE:O	7:K:648:ILE:CG2	2.66	0.43
7:K:977:ASP:OD1	7:K:977:ASP:C	2.61	0.43
7:K:496:GLU:O	7:K:497:MET:HB3	2.18	0.43
7:K:359:HIS:CE1	9:M:434:ILE:HD13	2.53	0.43
7:K:359:HIS:CE1	9:M:434:ILE:HD13	2.53	0.43
7:K:359:HIS:CE1	9:M:434:ILE:HD13	2.53	0.43
4:H:87:ARG:NH1	5:I:40:DG:H3'	2.32	0.43
7:K:359:HIS:CE1	9:M:434:ILE:HD13	2.53	0.43
7:K:359:HIS:CE1	9:M:434:ILE:HD13	2.53	0.43
7:K:359:HIS:CE1	9:M:434:ILE:HD13	2.53	0.43
7:K:828:ARG:NH1	7:K:834:TYR:OH	2.51	0.43
7:K:359:HIS:CE1	9:M:434:ILE:HD13	2.53	0.43
6:J:54:DC:C3'	7:K:816:MET:HG3	2.36	0.43
7:K:359:HIS:CE1	9:M:434:ILE:HD13	2.53	0.43
7:K:359:HIS:CE1	9:M:434:ILE:HD13	2.53	0.43
7:K:765:HIS:ND1	7:K:765:HIS:C	2.76	0.43
7:K:359:HIS:CE1	9:M:434:ILE:HD13	2.53	0.43
4:H:87:ARG:NH1	5:I:40:DG:H3'	2.32	0.43
6:J:129:DC:H2"	6:J:130:DG:N7	2.34	0.43
7:K:511:TYR:CD2	7:K:511:TYR:C	2.96	0.43
7:K:811:LEU:N	7:K:811:LEU:HD12	2.34	0.43
3:G:45:GLY:HA2	6:J:112:DG:H5"	2.00	0.43
6:J:129:DC:H2"	6:J:130:DG:N7	2.34	0.43
6:J:129:DC:H2"	6:J:130:DG:N7	2.34	0.43
7:K:658:TRP:CE3	7:K:658:TRP:HA	2.52	0.43
6:J:129:DC:H2"	6:J:130:DG:N7	2.34	0.43
7:K:661:THR:HB	7:K:662:PRO:CD	2.48	0.43
6:J:129:DC:H2"	6:J:130:DG:N7	2.34	0.43
6:J:129:DC:H2"	6:J:130:DG:N7	2.34	0.43
6:J:129:DC:H2"	6:J:130:DG:N7	2.34	0.43
7:K:769:PHE:O	7:K:772:VAL:N	2.51	0.43
6:J:129:DC:H2"	6:J:130:DG:N7	2.34	0.43
6:J:129:DC:H2"	6:J:130:DG:N7	2.34	0.43
6:J:54:DC:OP1	7:K:817:THR:CG2	2.60	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:129:DC:H2”	6:J:130:DG:N7	2.34	0.43
7:K:513:TYR:CD1	7:K:513:TYR:N	2.83	0.43
7:K:348:CYS:HB3	9:M:467:PHE:O	2.19	0.43
7:K:348:CYS:HB3	9:M:467:PHE:O	2.19	0.43
7:K:633:ASN:O	7:K:634:LEU:HB2	2.18	0.43
7:K:348:CYS:HB3	9:M:467:PHE:O	2.19	0.43
7:K:447:TYR:O	7:K:451:ALA:N	2.52	0.43
7:K:900:ARG:NE	7:K:900:ARG:HA	2.34	0.43
7:K:348:CYS:HB3	9:M:467:PHE:O	2.19	0.43
7:K:348:CYS:HB3	9:M:467:PHE:O	2.19	0.43
7:K:511:TYR:CD2	7:K:511:TYR:C	2.96	0.43
7:K:348:CYS:HB3	9:M:467:PHE:O	2.19	0.43
7:K:348:CYS:HB3	9:M:467:PHE:O	2.19	0.43
7:K:348:CYS:HB3	9:M:467:PHE:O	2.19	0.43
7:K:348:CYS:HB3	9:M:467:PHE:O	2.19	0.43
7:K:348:CYS:HB3	9:M:467:PHE:O	2.19	0.43
6:J:20:DC:H2”	6:J:21:DA:C8	2.54	0.43
7:K:342:TRP:CZ2	7:K:350:GLN:HG3	2.54	0.43
7:K:345:GLN:HG2	9:M:178:ALA:HB2	2.00	0.43
7:K:368:LYS:HD3	7:K:368:LYS:HA	1.37	0.43
6:J:20:DC:H2”	6:J:21:DA:C8	2.54	0.43
7:K:342:TRP:CZ2	7:K:350:GLN:HG3	2.54	0.43
7:K:345:GLN:HG2	9:M:178:ALA:HB2	2.00	0.43
7:K:368:LYS:HD3	7:K:368:LYS:HA	1.37	0.43
7:K:675:THR:OG1	7:K:676:GLU:N	2.45	0.43
6:J:20:DC:H2”	6:J:21:DA:C8	2.54	0.43
7:K:342:TRP:CZ2	7:K:350:GLN:HG3	2.54	0.43
7:K:345:GLN:HG2	9:M:178:ALA:HB2	2.00	0.43
7:K:368:LYS:HD3	7:K:368:LYS:HA	1.37	0.43
6:J:20:DC:H2”	6:J:21:DA:C8	2.54	0.43
7:K:342:TRP:CZ2	7:K:350:GLN:HG3	2.54	0.43
7:K:345:GLN:HG2	9:M:178:ALA:HB2	2.00	0.43
7:K:368:LYS:HD3	7:K:368:LYS:HA	1.37	0.43
6:J:20:DC:H2”	6:J:21:DA:C8	2.54	0.43
7:K:342:TRP:CZ2	7:K:350:GLN:HG3	2.54	0.43
7:K:345:GLN:HG2	9:M:178:ALA:HB2	2.00	0.43
7:K:368:LYS:HD3	7:K:368:LYS:HA	1.37	0.43
6:J:20:DC:H2”	6:J:21:DA:C8	2.54	0.43
7:K:342:TRP:CZ2	7:K:350:GLN:HG3	2.54	0.43
7:K:345:GLN:HG2	9:M:178:ALA:HB2	2.00	0.43
7:K:368:LYS:HD3	7:K:368:LYS:HA	1.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:501:LYS:NZ	7:K:626:THR:O	2.51	0.43
7:K:1043:GLU:OE1	7:K:1043:GLU:N	2.31	0.43
5:I:94:DG:O3'	7:K:608:LYS:HB3	2.18	0.43
6:J:20:DC:H2"	6:J:21:DA:C8	2.54	0.43
7:K:342:TRP:CZ2	7:K:350:GLN:HG3	2.54	0.43
7:K:345:GLN:HG2	9:M:178:ALA:HB2	2.00	0.43
7:K:368:LYS:HD3	7:K:368:LYS:HA	1.37	0.43
6:J:20:DC:H2"	6:J:21:DA:C8	2.54	0.43
7:K:342:TRP:CZ2	7:K:350:GLN:HG3	2.54	0.43
7:K:345:GLN:HG2	9:M:178:ALA:HB2	2.00	0.43
7:K:368:LYS:HD3	7:K:368:LYS:HA	1.37	0.43
4:H:87:ARG:NH1	5:I:40:DG:H3'	2.32	0.43
6:J:20:DC:H2"	6:J:21:DA:C8	2.54	0.43
7:K:342:TRP:CZ2	7:K:350:GLN:HG3	2.54	0.43
7:K:345:GLN:HG2	9:M:178:ALA:HB2	2.00	0.43
7:K:368:LYS:HD3	7:K:368:LYS:HA	1.37	0.43
6:J:20:DC:H2"	6:J:21:DA:C8	2.54	0.43
7:K:342:TRP:CZ2	7:K:350:GLN:HG3	2.54	0.43
7:K:345:GLN:HG2	9:M:178:ALA:HB2	2.00	0.43
7:K:368:LYS:HD3	7:K:368:LYS:HA	1.37	0.43
7:K:501:LYS:NZ	7:K:626:THR:O	2.52	0.43
7:K:654:THR:O	7:K:658:TRP:N	2.51	0.43
7:K:844:GLU:OE1	7:K:844:GLU:N	2.42	0.43
2:B:46:ARG:NH1	6:J:70:DG:H4'	2.34	0.43
7:K:793:PHE:HD1	7:K:793:PHE:HA	1.74	0.43
3:G:48:ALA:N	3:G:49:PRO:HD2	2.34	0.43
7:K:899:ASP:HA	7:K:902:HIS:HB3	2.01	0.43
7:K:874:LEU:HB2	7:K:900:ARG:HD2	2.01	0.43
5:I:96:DC:OP1	7:K:603:LYS:CG	2.63	0.43
7:K:519:ILE:O	7:K:519:ILE:HG22	2.19	0.43
7:K:899:ASP:O	7:K:900:ARG:C	2.62	0.43
3:G:48:ALA:N	3:G:49:PRO:HD2	2.34	0.43
3:C:80:ILE:HB	3:C:81:PRO:HD2	2.01	0.43
8:L:38:ARG:HB2	8:L:46:GLU:HB3	2.01	0.43
8:L:320:SER:OG	8:L:321:ASP:N	2.51	0.43
3:C:85:GLN:HA	3:C:85:GLN:OE1	2.19	0.43
8:L:38:ARG:HB2	8:L:46:GLU:HB3	2.01	0.43
8:L:320:SER:OG	8:L:321:ASP:N	2.51	0.43
8:L:38:ARG:HB2	8:L:46:GLU:HB3	2.01	0.43
8:L:320:SER:OG	8:L:321:ASP:N	2.51	0.43
3:G:48:ALA:N	3:G:49:PRO:HD2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L:38:ARG:HB2	8:L:46:GLU:HB3	2.01	0.43
8:L:320:SER:OG	8:L:321:ASP:N	2.51	0.43
3:G:48:ALA:N	3:G:49:PRO:HD2	2.34	0.43
8:L:38:ARG:HB2	8:L:46:GLU:HB3	2.01	0.43
8:L:320:SER:OG	8:L:321:ASP:N	2.51	0.43
5:I:95:DC:P	7:K:608:LYS:N	2.85	0.43
8:L:38:ARG:HB2	8:L:46:GLU:HB3	2.01	0.43
8:L:320:SER:OG	8:L:321:ASP:N	2.51	0.43
7:K:904:ILE:HG23	7:K:904:ILE:O	2.19	0.43
8:L:38:ARG:HB2	8:L:46:GLU:HB3	2.01	0.43
8:L:320:SER:OG	8:L:321:ASP:N	2.51	0.43
8:L:38:ARG:HB2	8:L:46:GLU:HB3	2.01	0.43
8:L:320:SER:OG	8:L:321:ASP:N	2.51	0.43
7:K:687:HIS:O	7:K:691:ARG:N	2.51	0.43
7:K:1046:GLU:HB3	7:K:1047:PRO:HD3	2.01	0.43
8:L:38:ARG:HB2	8:L:46:GLU:HB3	2.01	0.43
8:L:320:SER:OG	8:L:321:ASP:N	2.51	0.43
8:L:38:ARG:HB2	8:L:46:GLU:HB3	2.01	0.43
8:L:320:SER:OG	8:L:321:ASP:N	2.51	0.43
7:K:904:ILE:HG23	7:K:904:ILE:O	2.19	0.42
7:K:674:LEU:O	7:K:675:THR:C	2.62	0.42
7:K:1046:GLU:HB3	7:K:1047:PRO:CD	2.49	0.42
7:K:687:HIS:O	7:K:691:ARG:N	2.52	0.42
3:G:48:ALA:N	3:G:49:PRO:HD2	2.34	0.42
6:J:54:DC:H5”	7:K:816:MET:HG3	2.00	0.42
7:K:347:ARG:CZ	9:M:464:ASP:O	2.68	0.42
8:L:159:ILE:HG22	8:L:398:THR:HB	2.01	0.42
7:K:347:ARG:CZ	9:M:464:ASP:O	2.68	0.42
8:L:159:ILE:HG22	8:L:398:THR:HB	2.01	0.42
7:K:347:ARG:CZ	9:M:464:ASP:O	2.68	0.42
8:L:159:ILE:HG22	8:L:398:THR:HB	2.01	0.42
3:C:85:GLN:HA	3:C:85:GLN:OE1	2.19	0.42
7:K:347:ARG:CZ	9:M:464:ASP:O	2.68	0.42
8:L:159:ILE:HG22	8:L:398:THR:HB	2.01	0.42
7:K:347:ARG:CZ	9:M:464:ASP:O	2.68	0.42
8:L:159:ILE:HG22	8:L:398:THR:HB	2.01	0.42
5:I:98:DA:H5”	7:K:889:TRP:CZ3	2.54	0.42
7:K:347:ARG:CZ	9:M:464:ASP:O	2.68	0.42
8:L:159:ILE:HG22	8:L:398:THR:HB	2.01	0.42
7:K:347:ARG:CZ	9:M:464:ASP:O	2.68	0.42
7:K:649:PHE:CD1	7:K:649:PHE:C	2.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L:159:ILE:HG22	8:L:398:THR:HB	2.01	0.42
7:K:347:ARG:CZ	9:M:464:ASP:O	2.68	0.42
8:L:159:ILE:HG22	8:L:398:THR:HB	2.01	0.42
7:K:347:ARG:CZ	9:M:464:ASP:O	2.68	0.42
8:L:159:ILE:HG22	8:L:398:THR:HB	2.01	0.42
3:C:85:GLN:HA	3:C:85:GLN:OE1	2.19	0.42
3:G:45:GLY:HA2	6:J:112:DG:H5"	2.00	0.42
7:K:347:ARG:CZ	9:M:464:ASP:O	2.68	0.42
8:L:159:ILE:HG22	8:L:398:THR:HB	2.01	0.42
7:K:837:LEU:C	7:K:837:LEU:HD23	2.45	0.42
7:K:890:ASN:O	7:K:892:HIS:N	2.52	0.42
7:K:513:TYR:N	7:K:513:TYR:HD1	2.18	0.42
7:K:602:MET:HG3	7:K:602:MET:O	2.18	0.42
3:G:48:ALA:N	3:G:49:PRO:HD2	2.34	0.42
7:K:511:TYR:CD2	7:K:511:TYR:C	2.96	0.42
6:J:57:DT:OP1	7:K:578:TYR:OH	2.34	0.42
7:K:900:ARG:HA	7:K:900:ARG:HE	1.84	0.42
7:K:1003:MET:SD	7:K:1003:MET:C	3.02	0.42
7:K:1051:ILE:O	7:K:1051:ILE:HG13	2.18	0.42
3:C:85:GLN:HA	3:C:85:GLN:OE1	2.19	0.42
7:K:509:ILE:HD12	7:K:509:ILE:HA	1.85	0.42
9:M:163:ASP:OD1	9:M:163:ASP:C	2.62	0.42
9:M:163:ASP:OD1	9:M:163:ASP:C	2.62	0.42
9:M:163:ASP:OD1	9:M:163:ASP:C	2.62	0.42
7:K:729:MET:SD	7:K:729:MET:C	3.02	0.42
9:M:163:ASP:OD1	9:M:163:ASP:C	2.62	0.42
9:M:163:ASP:OD1	9:M:163:ASP:C	2.62	0.42
3:G:48:ALA:N	3:G:49:PRO:HD2	2.34	0.42
4:H:87:ARG:NH1	5:I:40:DG:H3'	2.33	0.42
5:I:95:DC:OP1	7:K:608:LYS:CA	2.67	0.42
9:M:163:ASP:OD1	9:M:163:ASP:C	2.62	0.42
9:M:163:ASP:OD1	9:M:163:ASP:C	2.62	0.42
9:M:163:ASP:OD1	9:M:163:ASP:C	2.62	0.42
9:M:163:ASP:OD1	9:M:163:ASP:C	2.62	0.42
9:M:163:ASP:OD1	9:M:163:ASP:C	2.62	0.42
5:I:95:DC:OP1	7:K:608:LYS:N	2.53	0.42
3:G:48:ALA:N	3:G:49:PRO:HD2	2.35	0.42
7:K:633:ASN:O	7:K:634:LEU:HB2	2.19	0.42
3:G:48:ALA:N	3:G:49:PRO:HD2	2.35	0.42
7:K:343:SER:HB2	8:L:25:GLU:HB2	2.02	0.42
9:M:3:PRO:HA	9:M:4:PHE:HA	1.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:87:ARG:NH1	5:I:40:DG:H3'	2.33	0.42
7:K:343:SER:HB2	8:L:25:GLU:HB2	2.02	0.42
7:K:877:GLN:OE1	7:K:877:GLN:N	2.32	0.42
9:M:3:PRO:HA	9:M:4:PHE:HA	1.81	0.42
7:K:343:SER:HB2	8:L:25:GLU:HB2	2.02	0.42
9:M:3:PRO:HA	9:M:4:PHE:HA	1.81	0.42
3:G:45:GLY:HA2	6:J:112:DG:H5"	2.01	0.42
7:K:343:SER:HB2	8:L:25:GLU:HB2	2.02	0.42
9:M:3:PRO:HA	9:M:4:PHE:HA	1.81	0.42
7:K:343:SER:HB2	8:L:25:GLU:HB2	2.02	0.42
9:M:3:PRO:HA	9:M:4:PHE:HA	1.81	0.42
7:K:343:SER:HB2	8:L:25:GLU:HB2	2.02	0.42
9:M:3:PRO:HA	9:M:4:PHE:HA	1.81	0.42
7:K:343:SER:HB2	8:L:25:GLU:HB2	2.02	0.42
7:K:975:GLU:OE1	7:K:975:GLU:N	2.40	0.42
9:M:3:PRO:HA	9:M:4:PHE:HA	1.81	0.42
7:K:343:SER:HB2	8:L:25:GLU:HB2	2.02	0.42
9:M:3:PRO:HA	9:M:4:PHE:HA	1.81	0.42
7:K:343:SER:HB2	8:L:25:GLU:HB2	2.02	0.42
9:M:3:PRO:HA	9:M:4:PHE:HA	1.81	0.42
7:K:343:SER:HB2	8:L:25:GLU:HB2	2.02	0.42
7:K:716:CYS:SG	7:K:917:THR:HA	2.60	0.42
9:M:3:PRO:HA	9:M:4:PHE:HA	1.81	0.42
7:K:358:LEU:HD11	9:M:437:LYS:HE3	2.01	0.42
8:L:429:MET:SD	9:M:322:ASP:HA	2.60	0.42
7:K:358:LEU:HD11	9:M:437:LYS:HE3	2.01	0.42
8:L:429:MET:SD	9:M:322:ASP:HA	2.60	0.42
7:K:358:LEU:HD11	9:M:437:LYS:HE3	2.01	0.42
8:L:429:MET:SD	9:M:322:ASP:HA	2.60	0.42
7:K:358:LEU:HD11	9:M:437:LYS:HE3	2.01	0.42
8:L:429:MET:SD	9:M:322:ASP:HA	2.60	0.42
7:K:358:LEU:HD11	9:M:437:LYS:HE3	2.01	0.42
8:L:429:MET:SD	9:M:322:ASP:HA	2.60	0.42
7:K:358:LEU:HD11	9:M:437:LYS:HE3	2.01	0.42
8:L:429:MET:SD	9:M:322:ASP:HA	2.60	0.42
7:K:358:LEU:HD11	9:M:437:LYS:HE3	2.01	0.42
7:K:661:THR:HB	7:K:662:PRO:HD3	2.02	0.42
7:K:874:LEU:C	7:K:874:LEU:HD12	2.45	0.42
8:L:429:MET:SD	9:M:322:ASP:HA	2.60	0.42
4:H:87:ARG:NH1	5:I:40:DG:H3'	2.34	0.42
7:K:358:LEU:HD11	9:M:437:LYS:HE3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L:429:MET:SD	9:M:322:ASP:HA	2.60	0.42
7:K:358:LEU:HD11	9:M:437:LYS:HE3	2.01	0.42
8:L:429:MET:SD	9:M:322:ASP:HA	2.60	0.42
7:K:358:LEU:HD11	9:M:437:LYS:HE3	2.01	0.42
8:L:429:MET:SD	9:M:322:ASP:HA	2.60	0.42
6:J:94:DG:H2'	6:J:95:DG:C8	2.54	0.42
6:J:94:DG:H2'	6:J:95:DG:C8	2.54	0.42
6:J:94:DG:H2'	6:J:95:DG:C8	2.54	0.42
6:J:94:DG:H2'	6:J:95:DG:C8	2.54	0.42
7:K:888:ASP:CG	7:K:888:ASP:O	2.61	0.42
6:J:94:DG:H2'	6:J:95:DG:C8	2.54	0.42
6:J:94:DG:H2'	6:J:95:DG:C8	2.54	0.42
6:J:54:DC:H3'	7:K:816:MET:HG3	2.02	0.42
6:J:94:DG:H2'	6:J:95:DG:C8	2.54	0.42
6:J:94:DG:H2'	6:J:95:DG:C8	2.54	0.42
7:K:661:THR:HB	7:K:662:PRO:CD	2.50	0.42
5:I:94:DG:O3'	7:K:608:LYS:HB3	2.19	0.42
6:J:94:DG:H2'	6:J:95:DG:C8	2.54	0.42
7:K:885:PHE:CD1	7:K:885:PHE:N	2.87	0.42
6:J:94:DG:H2'	6:J:95:DG:C8	2.54	0.42
7:K:898:GLN:HG3	7:K:912:ILE:HD13	2.02	0.42
7:K:446:ASP:C	7:K:446:ASP:OD1	2.61	0.42
1:E:66:LEU:HB2	1:E:67:PRO:HD3	2.02	0.42
5:I:94:DG:O3'	7:K:608:LYS:CB	2.62	0.42
2:B:46:ARG:HH11	6:J:70:DG:H4'	1.85	0.41
7:K:513:TYR:N	7:K:513:TYR:HD1	2.18	0.41
7:K:886:ASP:O	7:K:887:THR:OG1	2.25	0.41
7:K:691:ARG:HB3	7:K:692:PRO:CD	2.50	0.41
1:E:66:LEU:HB2	1:E:67:PRO:HD3	2.02	0.41
7:K:638:TRP:CE3	7:K:638:TRP:C	2.98	0.41
7:K:661:THR:N	7:K:662:PRO:HD2	2.35	0.41
3:C:80:ILE:HB	3:C:81:PRO:HD2	2.01	0.41
7:K:1046:GLU:HB2	7:K:1047:PRO:HD3	2.01	0.41
7:K:511:TYR:CD2	7:K:511:TYR:C	2.97	0.41
7:K:661:THR:N	7:K:662:PRO:HD2	2.35	0.41
7:K:837:LEU:C	7:K:837:LEU:HD23	2.45	0.41
5:I:24:DC:H2"	5:I:25:DG:C8	2.54	0.41
8:L:4:ASN:OD1	8:L:4:ASN:C	2.62	0.41
1:E:135:ARG:O	1:E:135:ARG:HG2	2.19	0.41
5:I:24:DC:H2"	5:I:25:DG:C8	2.54	0.41
7:K:816:MET:HE2	7:K:816:MET:HA	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L:4:ASN:OD1	8:L:4:ASN:C	2.62	0.41
5:I:24:DC:H2"	5:I:25:DG:C8	2.54	0.41
8:L:4:ASN:OD1	8:L:4:ASN:C	2.62	0.41
5:I:24:DC:H2"	5:I:25:DG:C8	2.54	0.41
5:I:94:DG:O3'	7:K:608:LYS:HB3	2.19	0.41
8:L:4:ASN:OD1	8:L:4:ASN:C	2.62	0.41
5:I:24:DC:H2"	5:I:25:DG:C8	2.54	0.41
8:L:4:ASN:OD1	8:L:4:ASN:C	2.62	0.41
5:I:24:DC:H2"	5:I:25:DG:C8	2.54	0.41
8:L:4:ASN:OD1	8:L:4:ASN:C	2.62	0.41
5:I:24:DC:H2"	5:I:25:DG:C8	2.54	0.41
7:K:381:LEU:CA	7:K:676:GLU:OE2	2.59	0.41
7:K:844:GLU:OE1	7:K:844:GLU:N	2.43	0.41
8:L:4:ASN:OD1	8:L:4:ASN:C	2.62	0.41
5:I:24:DC:H2"	5:I:25:DG:C8	2.54	0.41
8:L:4:ASN:OD1	8:L:4:ASN:C	2.62	0.41
5:I:24:DC:H2"	5:I:25:DG:C8	2.54	0.41
7:K:448:TYR:CD1	7:K:448:TYR:C	2.98	0.41
7:K:857:ASP:O	7:K:858:SER:C	2.63	0.41
8:L:4:ASN:OD1	8:L:4:ASN:C	2.62	0.41
5:I:24:DC:H2"	5:I:25:DG:C8	2.54	0.41
8:L:4:ASN:OD1	8:L:4:ASN:C	2.62	0.41
7:K:362:MET:CA	9:M:437:LYS:HZ2	2.20	0.41
7:K:362:MET:CA	9:M:437:LYS:HZ2	2.20	0.41
7:K:935:ILE:HD12	7:K:935:ILE:HA	1.87	0.41
1:E:66:LEU:HB2	1:E:67:PRO:HD3	2.03	0.41
7:K:362:MET:CA	9:M:437:LYS:HZ2	2.20	0.41
7:K:362:MET:CA	9:M:437:LYS:HZ2	2.20	0.41
7:K:362:MET:CA	9:M:437:LYS:HZ2	2.20	0.41
7:K:675:THR:OG1	7:K:676:GLU:N	2.54	0.41
7:K:817:THR:OG1	7:K:818:GLN:N	2.52	0.41
7:K:362:MET:CA	9:M:437:LYS:HZ2	2.20	0.41
2:F:46:ARG:NH1	5:I:70:DC:H4'	2.35	0.41
7:K:362:MET:CA	9:M:437:LYS:HZ2	2.20	0.41
1:E:66:LEU:HB2	1:E:67:PRO:HD3	2.03	0.41
7:K:362:MET:CA	9:M:437:LYS:HZ2	2.20	0.41
7:K:362:MET:CA	9:M:437:LYS:HZ2	2.20	0.41
7:K:362:MET:CA	9:M:437:LYS:HZ2	2.20	0.41
1:E:66:LEU:HB2	1:E:67:PRO:HD3	2.03	0.41
7:K:1042:LYS:N	7:K:1042:LYS:HD2	2.35	0.41
7:K:935:ILE:HD12	7:K:935:ILE:HA	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:ARG:HA	1:A:64:ARG:NE	2.35	0.41
1:E:66:LEU:HB2	1:E:67:PRO:HD3	2.03	0.41
7:K:513:TYR:N	7:K:513:TYR:HD1	2.17	0.41
7:K:890:ASN:OD1	7:K:890:ASN:C	2.63	0.41
1:E:66:LEU:HB2	1:E:67:PRO:HD3	2.03	0.41
2:F:32:LYS:HB3	2:F:33:PRO:CD	2.51	0.41
5:I:123:DC:H2"	5:I:124:DA:C8	2.55	0.41
3:C:80:ILE:HB	3:C:81:PRO:HD2	2.01	0.41
5:I:123:DC:H2"	5:I:124:DA:C8	2.55	0.41
5:I:123:DC:H2"	5:I:124:DA:C8	2.55	0.41
5:I:123:DC:H2"	5:I:124:DA:C8	2.55	0.41
1:E:66:LEU:HB2	1:E:67:PRO:HD3	2.03	0.41
5:I:123:DC:H2"	5:I:124:DA:C8	2.55	0.41
7:K:679:THR:O	7:K:680:LEU:C	2.63	0.41
5:I:123:DC:H2"	5:I:124:DA:C8	2.55	0.41
7:K:577:GLU:OE1	7:K:577:GLU:N	2.46	0.41
1:E:66:LEU:HB2	1:E:67:PRO:HD3	2.03	0.41
5:I:123:DC:H2"	5:I:124:DA:C8	2.55	0.41
5:I:123:DC:H2"	5:I:124:DA:C8	2.55	0.41
7:K:800:LEU:N	7:K:801:PRO:CD	2.83	0.41
5:I:123:DC:H2"	5:I:124:DA:C8	2.55	0.41
5:I:123:DC:H2"	5:I:124:DA:C8	2.55	0.41
7:K:496:GLU:O	7:K:497:MET:HG3	2.20	0.41
7:K:817:THR:OG1	7:K:818:GLN:N	2.54	0.41
3:C:80:ILE:HB	3:C:81:PRO:HD2	2.01	0.41
1:E:66:LEU:HB2	1:E:67:PRO:HD3	2.03	0.41
7:K:578:TYR:H	7:K:578:TYR:HD1	1.65	0.41
3:C:80:ILE:HB	3:C:81:PRO:HD2	2.01	0.41
6:J:94:DG:H2'	6:J:95:DG:H8	1.86	0.41
7:K:1051:ILE:O	7:K:1051:ILE:HG13	2.21	0.41
8:L:201:ILE:O	8:L:203:GLU:N	2.54	0.41
9:M:75:ASP:OD1	9:M:75:ASP:C	2.64	0.41
6:J:94:DG:H2'	6:J:95:DG:H8	1.86	0.41
8:L:201:ILE:O	8:L:203:GLU:N	2.54	0.41
9:M:75:ASP:OD1	9:M:75:ASP:C	2.64	0.41
6:J:94:DG:H2'	6:J:95:DG:H8	1.86	0.41
8:L:201:ILE:O	8:L:203:GLU:N	2.54	0.41
9:M:75:ASP:OD1	9:M:75:ASP:C	2.64	0.41
6:J:94:DG:H2'	6:J:95:DG:H8	1.86	0.41
8:L:201:ILE:O	8:L:203:GLU:N	2.54	0.41
9:M:75:ASP:OD1	9:M:75:ASP:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:80:ILE:HB	3:C:81:PRO:HD2	2.01	0.41
6:J:94:DG:H2'	6:J:95:DG:H8	1.86	0.41
7:K:904:ILE:O	7:K:904:ILE:HG23	2.21	0.41
8:L:201:ILE:O	8:L:203:GLU:N	2.54	0.41
9:M:75:ASP:OD1	9:M:75:ASP:C	2.64	0.41
6:J:94:DG:H2'	6:J:95:DG:H8	1.86	0.41
8:L:201:ILE:O	8:L:203:GLU:N	2.54	0.41
9:M:75:ASP:OD1	9:M:75:ASP:C	2.64	0.41
6:J:94:DG:H2'	6:J:95:DG:H8	1.86	0.41
8:L:201:ILE:O	8:L:203:GLU:N	2.54	0.41
9:M:75:ASP:OD1	9:M:75:ASP:C	2.64	0.41
3:C:80:ILE:HB	3:C:81:PRO:HD2	2.01	0.41
6:J:94:DG:H2'	6:J:95:DG:H8	1.86	0.41
8:L:201:ILE:O	8:L:203:GLU:N	2.54	0.41
9:M:75:ASP:OD1	9:M:75:ASP:C	2.64	0.41
6:J:94:DG:H2'	6:J:95:DG:H8	1.86	0.41
7:K:762:ILE:HD12	7:K:762:ILE:HA	1.92	0.41
8:L:201:ILE:O	8:L:203:GLU:N	2.54	0.41
9:M:75:ASP:OD1	9:M:75:ASP:C	2.64	0.41
6:J:94:DG:H2'	6:J:95:DG:H8	1.86	0.41
8:L:201:ILE:O	8:L:203:GLU:N	2.54	0.41
9:M:75:ASP:OD1	9:M:75:ASP:C	2.64	0.41
3:C:80:ILE:HB	3:C:81:PRO:HD2	2.01	0.41
2:B:46:ARG:HH11	6:J:70:DG:H4'	1.85	0.41
5:I:94:DG:O3'	7:K:608:LYS:HB3	2.21	0.41
7:K:838:ASP:OD1	7:K:838:ASP:C	2.63	0.41
7:K:496:GLU:O	7:K:497:MET:HB2	2.20	0.41
2:F:53:GLU:OE1	2:F:53:GLU:HA	2.21	0.41
5:I:145:DT:H2"	5:I:146:DG:C8	2.55	0.41
7:K:347:ARG:NH1	9:M:466:GLN:O	2.35	0.41
7:K:378:LEU:O	7:K:676:GLU:CD	2.56	0.41
7:K:501:LYS:NZ	7:K:626:THR:O	2.53	0.41
2:F:32:LYS:HB3	2:F:33:PRO:CD	2.51	0.41
5:I:145:DT:H2"	5:I:146:DG:C8	2.55	0.41
7:K:347:ARG:NH1	9:M:466:GLN:O	2.35	0.41
7:K:549:ILE:O	7:K:549:ILE:HG13	2.20	0.41
7:K:716:CYS:HB2	7:K:917:THR:HA	2.03	0.41
5:I:145:DT:H2"	5:I:146:DG:C8	2.55	0.41
7:K:347:ARG:NH1	9:M:466:GLN:O	2.35	0.41
1:A:66:LEU:HB2	1:A:67:PRO:HD3	2.02	0.41
3:C:80:ILE:HB	3:C:81:PRO:HD2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:32:LYS:HB3	2:F:33:PRO:CD	2.51	0.41
5:I:145:DT:H2"	5:I:146:DG:C8	2.55	0.41
7:K:347:ARG:NH1	9:M:466:GLN:O	2.35	0.41
5:I:145:DT:H2"	5:I:146:DG:C8	2.55	0.41
6:J:54:DC:P	7:K:816:MET:HB2	2.59	0.41
7:K:347:ARG:NH1	9:M:466:GLN:O	2.35	0.41
2:F:32:LYS:HB3	2:F:33:PRO:CD	2.51	0.41
5:I:145:DT:H2"	5:I:146:DG:C8	2.55	0.41
7:K:347:ARG:NH1	9:M:466:GLN:O	2.35	0.41
7:K:1046:GLU:HB3	7:K:1047:PRO:HD3	2.02	0.41
5:I:145:DT:H2"	5:I:146:DG:C8	2.55	0.41
7:K:347:ARG:NH1	9:M:466:GLN:O	2.35	0.41
7:K:890:ASN:OD1	7:K:890:ASN:C	2.64	0.41
5:I:145:DT:H2"	5:I:146:DG:C8	2.55	0.41
7:K:347:ARG:NH1	9:M:466:GLN:O	2.35	0.41
7:K:511:TYR:CD2	7:K:511:TYR:C	2.98	0.41
5:I:145:DT:H2"	5:I:146:DG:C8	2.55	0.41
7:K:347:ARG:NH1	9:M:466:GLN:O	2.35	0.41
7:K:872:LEU:C	7:K:872:LEU:CD1	2.93	0.41
2:F:32:LYS:HB3	2:F:33:PRO:CD	2.51	0.41
5:I:145:DT:H2"	5:I:146:DG:C8	2.55	0.41
7:K:347:ARG:NH1	9:M:466:GLN:O	2.35	0.41
7:K:661:THR:HB	7:K:662:PRO:HD3	2.04	0.41
8:L:282:ASN:OD1	8:L:282:ASN:C	2.64	0.41
8:L:282:ASN:OD1	8:L:282:ASN:C	2.64	0.41
2:F:32:LYS:HB3	2:F:33:PRO:CD	2.51	0.41
8:L:282:ASN:OD1	8:L:282:ASN:C	2.64	0.41
8:L:282:ASN:OD1	8:L:282:ASN:C	2.64	0.41
2:F:32:LYS:HB3	2:F:33:PRO:CD	2.51	0.41
8:L:282:ASN:OD1	8:L:282:ASN:C	2.64	0.41
1:A:91:MET:HE2	1:A:91:MET:HA	2.03	0.41
8:L:282:ASN:OD1	8:L:282:ASN:C	2.64	0.41
2:B:46:ARG:HH11	6:J:70:DG:H4'	1.86	0.41
3:C:80:ILE:HB	3:C:81:PRO:HD2	2.02	0.41
2:F:32:LYS:HB3	2:F:33:PRO:CD	2.51	0.41
8:L:282:ASN:OD1	8:L:282:ASN:C	2.64	0.41
2:F:32:LYS:HB3	2:F:33:PRO:CD	2.51	0.41
8:L:282:ASN:OD1	8:L:282:ASN:C	2.64	0.41
2:F:32:LYS:HB3	2:F:33:PRO:CD	2.51	0.41
8:L:282:ASN:OD1	8:L:282:ASN:C	2.64	0.41
7:K:687:HIS:O	7:K:691:ARG:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:710:VAL:O	7:K:711:GLU:HB2	2.21	0.41
8:L:282:ASN:OD1	8:L:282:ASN:C	2.64	0.41
7:K:351:PHE:CZ	9:M:447:PHE:HB2	2.55	0.40
7:K:600:HIS:O	7:K:603:LYS:HG3	2.21	0.40
7:K:351:PHE:CZ	9:M:447:PHE:HB2	2.55	0.40
7:K:351:PHE:CZ	9:M:447:PHE:HB2	2.55	0.40
7:K:577:GLU:N	7:K:577:GLU:CD	2.79	0.40
7:K:351:PHE:CZ	9:M:447:PHE:HB2	2.55	0.40
7:K:837:LEU:HD23	7:K:837:LEU:C	2.46	0.40
7:K:351:PHE:CZ	9:M:447:PHE:HB2	2.55	0.40
7:K:691:ARG:HB3	7:K:692:PRO:HD3	2.02	0.40
7:K:802:LYS:HB3	7:K:802:LYS:HE2	1.84	0.40
7:K:877:GLN:OE1	7:K:877:GLN:N	2.30	0.40
7:K:351:PHE:CZ	9:M:447:PHE:HB2	2.55	0.40
7:K:351:PHE:CZ	9:M:447:PHE:HB2	2.55	0.40
7:K:351:PHE:CZ	9:M:447:PHE:HB2	2.55	0.40
2:F:53:GLU:OE1	2:F:53:GLU:HA	2.21	0.40
7:K:351:PHE:CZ	9:M:447:PHE:HB2	2.55	0.40
7:K:351:PHE:CZ	9:M:447:PHE:HB2	2.55	0.40
7:K:691:ARG:HB3	7:K:692:PRO:HD3	2.04	0.40
2:F:53:GLU:OE1	2:F:53:GLU:HA	2.21	0.40
5:I:97:DA:OP1	7:K:603:LYS:NZ	2.52	0.40
2:F:53:GLU:OE1	2:F:53:GLU:HA	2.21	0.40
2:F:53:GLU:OE1	2:F:53:GLU:HA	2.21	0.40
2:F:53:GLU:OE1	2:F:53:GLU:HA	2.21	0.40
2:F:53:GLU:OE1	2:F:53:GLU:HA	2.21	0.40
7:K:645:LEU:HA	7:K:646:PRO:HD2	1.89	0.40
7:K:800:LEU:N	7:K:801:PRO:CD	2.84	0.40
5:I:94:DG:H3'	7:K:608:LYS:HB2	2.02	0.40
7:K:838:ASP:OD1	7:K:838:ASP:C	2.64	0.40
6:J:54:DC:OP1	7:K:816:MET:CB	2.46	0.40
7:K:511:TYR:CD2	7:K:511:TYR:C	2.99	0.40
2:B:46:ARG:HH11	6:J:70:DG:H4'	1.86	0.40
7:K:793:PHE:N	7:K:793:PHE:CD1	2.90	0.40
7:K:800:LEU:N	7:K:801:PRO:CD	2.84	0.40
7:K:877:GLN:OE1	7:K:877:GLN:N	2.43	0.40
7:K:602:MET:HE2	7:K:602:MET:HB2	1.96	0.40
7:K:630:LEU:HD12	7:K:637:LEU:HA	2.03	0.40
5:I:82:DC:H2"	5:I:83:DG:C8	2.56	0.40
5:I:95:DC:P	7:K:608:LYS:CB	3.06	0.40
7:K:354:LEU:HG	9:M:438:GLN:HG2	1.97	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:354:LEU:HD12	9:M:438:GLN:NE2	2.34	0.40
7:K:548:ILE:HG23	7:K:560:LEU:HD11	2.03	0.40
9:M:107:SER:O	10:N:11:ASN:HA	2.22	0.40
10:N:84:LEU:O	10:N:85:LYS:HB2	2.20	0.40
5:I:82:DC:H2"	5:I:83:DG:C8	2.56	0.40
7:K:354:LEU:HG	9:M:438:GLN:HG2	1.97	0.40
7:K:354:LEU:HD12	9:M:438:GLN:NE2	2.34	0.40
9:M:107:SER:O	10:N:11:ASN:HA	2.22	0.40
10:N:84:LEU:O	10:N:85:LYS:HB2	2.20	0.40
3:C:48:ALA:N	3:C:49:PRO:HD2	2.36	0.40
5:I:82:DC:H2"	5:I:83:DG:C8	2.56	0.40
7:K:354:LEU:HG	9:M:438:GLN:HG2	1.97	0.40
7:K:354:LEU:HD12	9:M:438:GLN:NE2	2.34	0.40
7:K:519:ILE:O	7:K:519:ILE:HG22	2.21	0.40
9:M:107:SER:O	10:N:11:ASN:HA	2.22	0.40
10:N:84:LEU:O	10:N:85:LYS:HB2	2.20	0.40
5:I:82:DC:H2"	5:I:83:DG:C8	2.56	0.40
5:I:95:DC:OP1	7:K:608:LYS:CA	2.69	0.40
7:K:354:LEU:HG	9:M:438:GLN:HG2	1.97	0.40
7:K:354:LEU:HD12	9:M:438:GLN:NE2	2.34	0.40
9:M:107:SER:O	10:N:11:ASN:HA	2.22	0.40
10:N:84:LEU:O	10:N:85:LYS:HB2	2.20	0.40
5:I:82:DC:H2"	5:I:83:DG:C8	2.56	0.40
7:K:354:LEU:HG	9:M:438:GLN:HG2	1.97	0.40
7:K:354:LEU:HD12	9:M:438:GLN:NE2	2.34	0.40
9:M:107:SER:O	10:N:11:ASN:HA	2.22	0.40
10:N:84:LEU:O	10:N:85:LYS:HB2	2.20	0.40
2:B:46:ARG:HH11	6:J:70:DG:H4'	1.86	0.40
5:I:82:DC:H2"	5:I:83:DG:C8	2.56	0.40
7:K:354:LEU:HG	9:M:438:GLN:HG2	1.97	0.40
7:K:354:LEU:HD12	9:M:438:GLN:NE2	2.34	0.40
7:K:816:MET:SD	7:K:816:MET:O	2.79	0.40
7:K:836:ARG:HD3	7:K:836:ARG:C	2.47	0.40
9:M:107:SER:O	10:N:11:ASN:HA	2.22	0.40
10:N:84:LEU:O	10:N:85:LYS:HB2	2.20	0.40
1:A:91:MET:HA	1:A:91:MET:HE2	2.03	0.40
5:I:82:DC:H2"	5:I:83:DG:C8	2.56	0.40
7:K:354:LEU:HG	9:M:438:GLN:HG2	1.97	0.40
7:K:354:LEU:HD12	9:M:438:GLN:NE2	2.34	0.40
9:M:107:SER:O	10:N:11:ASN:HA	2.22	0.40
10:N:84:LEU:O	10:N:85:LYS:HB2	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:82:DC:H2"	5:I:83:DG:C8	2.56	0.40
7:K:354:LEU:HG	9:M:438:GLN:HG2	1.97	0.40
7:K:354:LEU:HD12	9:M:438:GLN:NE2	2.34	0.40
9:M:107:SER:O	10:N:11:ASN:HA	2.22	0.40
10:N:84:LEU:O	10:N:85:LYS:HB2	2.20	0.40
5:I:82:DC:H2"	5:I:83:DG:C8	2.56	0.40
7:K:354:LEU:HG	9:M:438:GLN:HG2	1.97	0.40
7:K:354:LEU:HD12	9:M:438:GLN:NE2	2.34	0.40
9:M:107:SER:O	10:N:11:ASN:HA	2.22	0.40
10:N:84:LEU:O	10:N:85:LYS:HB2	2.20	0.40
5:I:82:DC:H2"	5:I:83:DG:C8	2.56	0.40
7:K:354:LEU:HG	9:M:438:GLN:HG2	1.97	0.40
7:K:354:LEU:HD12	9:M:438:GLN:NE2	2.34	0.40
7:K:918:THR:O	7:K:918:THR:HG23	2.21	0.40
9:M:107:SER:O	10:N:11:ASN:HA	2.22	0.40
10:N:84:LEU:O	10:N:85:LYS:HB2	2.20	0.40
5:I:101:DG:H2"	5:I:102:DG:C8	2.56	0.40
9:M:361:GLU:HA	9:M:362:PRO:HD3	1.90	0.40
1:A:91:MET:HA	1:A:91:MET:HE2	2.04	0.40
5:I:101:DG:H2"	5:I:102:DG:C8	2.56	0.40
9:M:361:GLU:HA	9:M:362:PRO:HD3	1.90	0.40
5:I:101:DG:H2"	5:I:102:DG:C8	2.56	0.40
9:M:361:GLU:HA	9:M:362:PRO:HD3	1.90	0.40
5:I:101:DG:H2"	5:I:102:DG:C8	2.56	0.40
7:K:501:LYS:NZ	7:K:626:THR:O	2.55	0.40
9:M:361:GLU:HA	9:M:362:PRO:HD3	1.90	0.40
1:A:91:MET:HA	1:A:91:MET:HE2	2.04	0.40
5:I:101:DG:H2"	5:I:102:DG:C8	2.56	0.40
9:M:361:GLU:HA	9:M:362:PRO:HD3	1.90	0.40
5:I:101:DG:H2"	5:I:102:DG:C8	2.56	0.40
7:K:600:HIS:O	7:K:603:LYS:HG3	2.21	0.40
9:M:361:GLU:HA	9:M:362:PRO:HD3	1.90	0.40
5:I:101:DG:H2"	5:I:102:DG:C8	2.56	0.40
7:K:512:LEU:O	7:K:517:LYS:N	2.54	0.40
9:M:361:GLU:HA	9:M:362:PRO:HD3	1.90	0.40
5:I:101:DG:H2"	5:I:102:DG:C8	2.56	0.40
9:M:361:GLU:HA	9:M:362:PRO:HD3	1.90	0.40
1:A:66:LEU:HB2	1:A:67:PRO:HD3	2.03	0.40
5:I:101:DG:H2"	5:I:102:DG:C8	2.56	0.40
7:K:691:ARG:N	7:K:692:PRO:HD2	2.35	0.40
7:K:793:PHE:CD1	7:K:793:PHE:N	2.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:M:361:GLU:HA	9:M:362:PRO:HD3	1.90	0.40
1:A:91:MET:HA	1:A:91:MET:HE2	2.04	0.40
5:I:101:DG:H2"	5:I:102:DG:C8	2.56	0.40
9:M:361:GLU:HA	9:M:362:PRO:HD3	1.90	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	1-A	96/136 (71%)	95 (99%)	1 (1%)	0	100	100
1	1-E	93/136 (68%)	92 (99%)	1 (1%)	0	100	100
1	2-A	96/136 (71%)	95 (99%)	1 (1%)	0	100	100
1	2-E	93/136 (68%)	92 (99%)	1 (1%)	0	100	100
1	3-A	96/136 (71%)	95 (99%)	1 (1%)	0	100	100
1	3-E	93/136 (68%)	92 (99%)	1 (1%)	0	100	100
1	4-A	96/136 (71%)	95 (99%)	1 (1%)	0	100	100
1	4-E	93/136 (68%)	92 (99%)	1 (1%)	0	100	100
1	5-A	96/136 (71%)	95 (99%)	1 (1%)	0	100	100
1	5-E	93/136 (68%)	92 (99%)	1 (1%)	0	100	100
1	6-A	96/136 (71%)	95 (99%)	1 (1%)	0	100	100
1	6-E	93/136 (68%)	93 (100%)	0	0	100	100
1	7-A	96/136 (71%)	95 (99%)	1 (1%)	0	100	100
1	7-E	93/136 (68%)	92 (99%)	1 (1%)	0	100	100
1	8-A	96/136 (71%)	95 (99%)	1 (1%)	0	100	100
1	8-E	93/136 (68%)	91 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	9-A	96/136 (71%)	95 (99%)	1 (1%)	0	100	100
1	9-E	93/136 (68%)	92 (99%)	1 (1%)	0	100	100
1	10-A	96/136 (71%)	95 (99%)	1 (1%)	0	100	100
1	10-E	93/136 (68%)	92 (99%)	1 (1%)	0	100	100
2	1-B	85/103 (82%)	83 (98%)	2 (2%)	0	100	100
2	1-F	77/103 (75%)	76 (99%)	1 (1%)	0	100	100
2	2-B	85/103 (82%)	83 (98%)	2 (2%)	0	100	100
2	2-F	77/103 (75%)	76 (99%)	1 (1%)	0	100	100
2	3-B	85/103 (82%)	83 (98%)	2 (2%)	0	100	100
2	3-F	77/103 (75%)	76 (99%)	1 (1%)	0	100	100
2	4-B	85/103 (82%)	83 (98%)	2 (2%)	0	100	100
2	4-F	77/103 (75%)	76 (99%)	1 (1%)	0	100	100
2	5-B	85/103 (82%)	83 (98%)	2 (2%)	0	100	100
2	5-F	77/103 (75%)	76 (99%)	1 (1%)	0	100	100
2	6-B	85/103 (82%)	82 (96%)	3 (4%)	0	100	100
2	6-F	77/103 (75%)	76 (99%)	1 (1%)	0	100	100
2	7-B	85/103 (82%)	82 (96%)	3 (4%)	0	100	100
2	7-F	77/103 (75%)	76 (99%)	1 (1%)	0	100	100
2	8-B	85/103 (82%)	83 (98%)	2 (2%)	0	100	100
2	8-F	77/103 (75%)	76 (99%)	1 (1%)	0	100	100
2	9-B	85/103 (82%)	83 (98%)	2 (2%)	0	100	100
2	9-F	77/103 (75%)	76 (99%)	1 (1%)	0	100	100
2	10-B	85/103 (82%)	83 (98%)	2 (2%)	0	100	100
2	10-F	77/103 (75%)	75 (97%)	2 (3%)	0	100	100
3	1-C	105/130 (81%)	102 (97%)	3 (3%)	0	100	100
3	1-G	105/130 (81%)	102 (97%)	3 (3%)	0	100	100
3	2-C	105/130 (81%)	102 (97%)	3 (3%)	0	100	100
3	2-G	105/130 (81%)	102 (97%)	3 (3%)	0	100	100
3	3-C	105/130 (81%)	103 (98%)	2 (2%)	0	100	100
3	3-G	105/130 (81%)	102 (97%)	3 (3%)	0	100	100
3	4-C	105/130 (81%)	102 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	4-G	105/130 (81%)	102 (97%)	3 (3%)	0	100	100
3	5-C	105/130 (81%)	102 (97%)	3 (3%)	0	100	100
3	5-G	105/130 (81%)	102 (97%)	3 (3%)	0	100	100
3	6-C	105/130 (81%)	103 (98%)	2 (2%)	0	100	100
3	6-G	105/130 (81%)	102 (97%)	3 (3%)	0	100	100
3	7-C	105/130 (81%)	102 (97%)	3 (3%)	0	100	100
3	7-G	105/130 (81%)	102 (97%)	3 (3%)	0	100	100
3	8-C	105/130 (81%)	102 (97%)	3 (3%)	0	100	100
3	8-G	105/130 (81%)	102 (97%)	3 (3%)	0	100	100
3	9-C	105/130 (81%)	103 (98%)	2 (2%)	0	100	100
3	9-G	105/130 (81%)	102 (97%)	3 (3%)	0	100	100
3	10-C	105/130 (81%)	102 (97%)	3 (3%)	0	100	100
3	10-G	105/130 (81%)	102 (97%)	3 (3%)	0	100	100
4	1-D	90/125 (72%)	85 (94%)	5 (6%)	0	100	100
4	1-H	90/125 (72%)	88 (98%)	1 (1%)	1 (1%)	11	43
4	2-D	90/125 (72%)	86 (96%)	4 (4%)	0	100	100
4	2-H	90/125 (72%)	89 (99%)	1 (1%)	0	100	100
4	3-D	90/125 (72%)	86 (96%)	3 (3%)	1 (1%)	11	43
4	3-H	90/125 (72%)	88 (98%)	2 (2%)	0	100	100
4	4-D	90/125 (72%)	85 (94%)	5 (6%)	0	100	100
4	4-H	90/125 (72%)	89 (99%)	0	1 (1%)	11	43
4	5-D	90/125 (72%)	85 (94%)	5 (6%)	0	100	100
4	5-H	90/125 (72%)	88 (98%)	1 (1%)	1 (1%)	11	43
4	6-D	90/125 (72%)	86 (96%)	4 (4%)	0	100	100
4	6-H	90/125 (72%)	89 (99%)	1 (1%)	0	100	100
4	7-D	90/125 (72%)	85 (94%)	5 (6%)	0	100	100
4	7-H	90/125 (72%)	89 (99%)	1 (1%)	0	100	100
4	8-D	90/125 (72%)	85 (94%)	5 (6%)	0	100	100
4	8-H	90/125 (72%)	89 (99%)	0	1 (1%)	11	43
4	9-D	90/125 (72%)	87 (97%)	3 (3%)	0	100	100
4	9-H	90/125 (72%)	89 (99%)	0	1 (1%)	11	43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	10-D	90/125 (72%)	85 (94%)	5 (6%)	0	100	100
4	10-H	90/125 (72%)	88 (98%)	1 (1%)	1 (1%)	11	43
7	1-K	602/813 (74%)	566 (94%)	24 (4%)	12 (2%)	6	32
7	2-K	602/813 (74%)	564 (94%)	25 (4%)	13 (2%)	5	31
7	3-K	602/813 (74%)	560 (93%)	30 (5%)	12 (2%)	6	32
7	4-K	602/813 (74%)	566 (94%)	24 (4%)	12 (2%)	6	32
7	5-K	602/813 (74%)	560 (93%)	30 (5%)	12 (2%)	6	32
7	6-K	602/813 (74%)	558 (93%)	32 (5%)	12 (2%)	6	32
7	7-K	602/813 (74%)	560 (93%)	31 (5%)	11 (2%)	6	34
7	8-K	602/813 (74%)	558 (93%)	36 (6%)	8 (1%)	9	40
7	9-K	602/813 (74%)	559 (93%)	32 (5%)	11 (2%)	6	34
7	10-K	602/813 (74%)	561 (93%)	29 (5%)	12 (2%)	6	32
8	1-L	383/477 (80%)	371 (97%)	11 (3%)	1 (0%)	36	69
8	2-L	383/477 (80%)	371 (97%)	11 (3%)	1 (0%)	36	69
8	3-L	383/477 (80%)	371 (97%)	11 (3%)	1 (0%)	36	69
8	4-L	383/477 (80%)	371 (97%)	11 (3%)	1 (0%)	36	69
8	5-L	383/477 (80%)	371 (97%)	11 (3%)	1 (0%)	36	69
8	6-L	383/477 (80%)	371 (97%)	11 (3%)	1 (0%)	36	69
8	7-L	383/477 (80%)	371 (97%)	11 (3%)	1 (0%)	36	69
8	8-L	383/477 (80%)	371 (97%)	11 (3%)	1 (0%)	36	69
8	9-L	383/477 (80%)	371 (97%)	11 (3%)	1 (0%)	36	69
8	10-L	383/477 (80%)	371 (97%)	11 (3%)	1 (0%)	36	69
9	1-M	390/467 (84%)	371 (95%)	13 (3%)	6 (2%)	8	37
9	2-M	390/467 (84%)	371 (95%)	13 (3%)	6 (2%)	8	37
9	3-M	390/467 (84%)	371 (95%)	13 (3%)	6 (2%)	8	37
9	4-M	390/467 (84%)	371 (95%)	13 (3%)	6 (2%)	8	37
9	5-M	390/467 (84%)	371 (95%)	13 (3%)	6 (2%)	8	37
9	6-M	390/467 (84%)	371 (95%)	13 (3%)	6 (2%)	8	37
9	7-M	390/467 (84%)	371 (95%)	13 (3%)	6 (2%)	8	37
9	8-M	390/467 (84%)	371 (95%)	13 (3%)	6 (2%)	8	37
9	9-M	390/467 (84%)	371 (95%)	13 (3%)	6 (2%)	8	37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
9	10-M	390/467 (84%)	371 (95%)	13 (3%)	6 (2%)	8 37
10	1-N	47/157 (30%)	44 (94%)	2 (4%)	1 (2%)	5 31
10	2-N	47/157 (30%)	44 (94%)	2 (4%)	1 (2%)	5 31
10	3-N	47/157 (30%)	44 (94%)	2 (4%)	1 (2%)	5 31
10	4-N	47/157 (30%)	44 (94%)	2 (4%)	1 (2%)	5 31
10	5-N	47/157 (30%)	44 (94%)	2 (4%)	1 (2%)	5 31
10	6-N	47/157 (30%)	44 (94%)	2 (4%)	1 (2%)	5 31
10	7-N	47/157 (30%)	44 (94%)	2 (4%)	1 (2%)	5 31
10	8-N	47/157 (30%)	44 (94%)	2 (4%)	1 (2%)	5 31
10	9-N	47/157 (30%)	44 (94%)	2 (4%)	1 (2%)	5 31
10	10-N	47/157 (30%)	44 (94%)	2 (4%)	1 (2%)	5 31
All	All	21630/29020 (74%)	20713 (96%)	715 (3%)	202 (1%)	16 47

All (202) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	1-K	343	SER
7	1-K	496	GLU
7	1-K	634	LEU
8	1-L	202	LYS
9	1-M	155	SER
9	1-M	363	GLU
7	2-K	343	SER
7	2-K	496	GLU
7	2-K	634	LEU
8	2-L	202	LYS
9	2-M	155	SER
9	2-M	363	GLU
7	3-K	343	SER
7	3-K	632	ASN
7	3-K	888	ASP
8	3-L	202	LYS
9	3-M	155	SER
9	3-M	363	GLU
7	4-K	343	SER
7	4-K	496	GLU
7	4-K	634	LEU
7	4-K	770	ASP

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Mol	Chain	Res	Type
7	4-K	817	THR
8	4-L	202	LYS
9	4-M	155	SER
9	4-M	363	GLU
7	5-K	343	SER
7	5-K	496	GLU
7	5-K	543	PRO
7	5-K	603	LYS
7	5-K	634	LEU
8	5-L	202	LYS
9	5-M	155	SER
9	5-M	363	GLU
7	6-K	343	SER
7	6-K	496	GLU
7	6-K	543	PRO
7	6-K	649	PHE
7	6-K	770	ASP
7	6-K	817	THR
7	6-K	888	ASP
8	6-L	202	LYS
9	6-M	155	SER
9	6-M	363	GLU
7	7-K	343	SER
7	7-K	634	LEU
8	7-L	202	LYS
9	7-M	155	SER
9	7-M	363	GLU
7	8-K	343	SER
7	8-K	496	GLU
7	8-K	603	LYS
7	8-K	610	SER
8	8-L	202	LYS
9	8-M	155	SER
9	8-M	363	GLU
7	9-K	343	SER
7	9-K	496	GLU
7	9-K	577	GLU
8	9-L	202	LYS
9	9-M	155	SER
9	9-M	363	GLU
7	10-K	343	SER
7	10-K	496	GLU

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Mol	Chain	Res	Type
7	10-K	577	GLU
7	10-K	634	LEU
7	10-K	766	PRO
7	10-K	770	ASP
8	10-L	202	LYS
9	10-M	155	SER
9	10-M	363	GLU
7	1-K	603	LYS
7	1-K	650	ASN
7	1-K	891	PRO
10	1-N	85	LYS
7	2-K	543	PRO
7	2-K	632	ASN
7	2-K	650	ASN
7	2-K	675	THR
7	2-K	770	ASP
7	2-K	891	PRO
10	2-N	85	LYS
7	3-K	496	GLU
7	3-K	531	ILE
7	3-K	603	LYS
10	3-N	85	LYS
7	4-K	472	GLU
7	4-K	543	PRO
7	4-K	632	ASN
10	4-N	85	LYS
7	5-K	770	ASP
7	5-K	891	PRO
10	5-N	85	LYS
7	6-K	449	GLU
7	6-K	632	ASN
10	6-N	85	LYS
7	7-K	496	GLU
7	7-K	632	ASN
7	7-K	675	THR
7	7-K	679	THR
7	7-K	770	ASP
7	7-K	888	ASP
10	7-N	85	LYS
7	8-K	648	ILE
10	8-N	85	LYS
7	9-K	629	PRO

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Mol	Chain	Res	Type
7	9-K	632	ASN
7	9-K	646	PRO
7	9-K	648	ILE
10	9-N	85	LYS
7	10-K	632	ASN
7	10-K	710	VAL
7	10-K	873	GLY
10	10-N	85	LYS
4	1-H	51	PRO
7	1-K	675	THR
7	1-K	712	LYS
9	1-M	104	ALA
9	1-M	107	SER
9	1-M	362	PRO
7	2-K	712	LYS
9	2-M	104	ALA
9	2-M	107	SER
9	2-M	362	PRO
4	3-D	51	PRO
7	3-K	651	SER
7	3-K	662	PRO
7	3-K	891	PRO
9	3-M	104	ALA
9	3-M	107	SER
9	3-M	362	PRO
4	4-H	51	PRO
7	4-K	651	SER
7	4-K	712	LYS
9	4-M	104	ALA
9	4-M	107	SER
9	4-M	362	PRO
4	5-H	51	PRO
7	5-K	675	THR
7	5-K	692	PRO
7	5-K	817	THR
9	5-M	104	ALA
9	5-M	107	SER
9	5-M	362	PRO
9	6-M	104	ALA
9	6-M	107	SER
9	6-M	362	PRO
7	7-K	662	PRO

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Mol	Chain	Res	Type
9	7-M	104	ALA
9	7-M	107	SER
9	7-M	362	PRO
4	8-H	51	PRO
7	8-K	651	SER
9	8-M	104	ALA
9	8-M	107	SER
9	8-M	362	PRO
4	9-H	51	PRO
7	9-K	576	TYR
7	9-K	891	PRO
9	9-M	104	ALA
9	9-M	107	SER
9	9-M	362	PRO
4	10-H	51	PRO
7	10-K	711	GLU
9	10-M	104	ALA
9	10-M	107	SER
9	10-M	362	PRO
9	1-M	173	PRO
7	2-K	888	ASP
9	2-M	173	PRO
7	3-K	495	ASP
9	3-M	173	PRO
7	4-K	661	THR
9	4-M	173	PRO
7	5-K	679	THR
9	5-M	173	PRO
7	6-K	634	LEU
7	6-K	648	ILE
9	6-M	173	PRO
9	7-M	173	PRO
7	8-K	576	TYR
9	8-M	173	PRO
7	9-K	801	PRO
9	9-M	173	PRO
9	10-M	173	PRO
7	1-K	648	ILE
7	2-K	677	GLU
7	2-K	766	PRO
7	5-K	888	ASP
7	6-K	801	PRO

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Mol	Chain	Res	Type
7	7-K	880	ASP
7	9-K	519	ILE
7	10-K	801	PRO
7	7-K	887	THR
7	3-K	543	PRO
7	10-K	543	PRO
7	4-K	646	PRO
7	8-K	629	PRO
7	1-K	543	PRO
7	1-K	646	PRO
7	1-K	710	VAL
7	3-K	801	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	1-A	86/111 (78%)	86 (100%)	0	100	100
1	1-E	83/111 (75%)	83 (100%)	0	100	100
1	2-A	86/111 (78%)	86 (100%)	0	100	100
1	2-E	83/111 (75%)	83 (100%)	0	100	100
1	3-A	86/111 (78%)	86 (100%)	0	100	100
1	3-E	83/111 (75%)	83 (100%)	0	100	100
1	4-A	86/111 (78%)	86 (100%)	0	100	100
1	4-E	83/111 (75%)	83 (100%)	0	100	100
1	5-A	86/111 (78%)	86 (100%)	0	100	100
1	5-E	83/111 (75%)	83 (100%)	0	100	100
1	6-A	86/111 (78%)	86 (100%)	0	100	100
1	6-E	83/111 (75%)	83 (100%)	0	100	100
1	7-A	86/111 (78%)	86 (100%)	0	100	100
1	7-E	83/111 (75%)	83 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	8-A	86/111 (78%)	86 (100%)	0	100	100
1	8-E	83/111 (75%)	83 (100%)	0	100	100
1	9-A	86/111 (78%)	86 (100%)	0	100	100
1	9-E	83/111 (75%)	83 (100%)	0	100	100
1	10-A	86/111 (78%)	86 (100%)	0	100	100
1	10-E	83/111 (75%)	83 (100%)	0	100	100
2	1-B	72/79 (91%)	72 (100%)	0	100	100
2	1-F	64/79 (81%)	64 (100%)	0	100	100
2	2-B	72/79 (91%)	72 (100%)	0	100	100
2	2-F	64/79 (81%)	64 (100%)	0	100	100
2	3-B	72/79 (91%)	72 (100%)	0	100	100
2	3-F	64/79 (81%)	64 (100%)	0	100	100
2	4-B	72/79 (91%)	72 (100%)	0	100	100
2	4-F	64/79 (81%)	64 (100%)	0	100	100
2	5-B	72/79 (91%)	72 (100%)	0	100	100
2	5-F	64/79 (81%)	64 (100%)	0	100	100
2	6-B	72/79 (91%)	72 (100%)	0	100	100
2	6-F	64/79 (81%)	64 (100%)	0	100	100
2	7-B	72/79 (91%)	72 (100%)	0	100	100
2	7-F	64/79 (81%)	64 (100%)	0	100	100
2	8-B	72/79 (91%)	72 (100%)	0	100	100
2	8-F	64/79 (81%)	64 (100%)	0	100	100
2	9-B	72/79 (91%)	72 (100%)	0	100	100
2	9-F	64/79 (81%)	64 (100%)	0	100	100
2	10-B	72/79 (91%)	72 (100%)	0	100	100
2	10-F	64/79 (81%)	64 (100%)	0	100	100
3	1-C	84/102 (82%)	84 (100%)	0	100	100
3	1-G	84/102 (82%)	84 (100%)	0	100	100
3	2-C	84/102 (82%)	84 (100%)	0	100	100
3	2-G	84/102 (82%)	84 (100%)	0	100	100
3	3-C	84/102 (82%)	84 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	3-G	84/102 (82%)	84 (100%)	0	100	100
3	4-C	84/102 (82%)	84 (100%)	0	100	100
3	4-G	84/102 (82%)	84 (100%)	0	100	100
3	5-C	84/102 (82%)	84 (100%)	0	100	100
3	5-G	84/102 (82%)	84 (100%)	0	100	100
3	6-C	84/102 (82%)	84 (100%)	0	100	100
3	6-G	84/102 (82%)	84 (100%)	0	100	100
3	7-C	84/102 (82%)	84 (100%)	0	100	100
3	7-G	84/102 (82%)	84 (100%)	0	100	100
3	8-C	84/102 (82%)	84 (100%)	0	100	100
3	8-G	84/102 (82%)	84 (100%)	0	100	100
3	9-C	84/102 (82%)	84 (100%)	0	100	100
3	9-G	84/102 (82%)	84 (100%)	0	100	100
3	10-C	84/102 (82%)	84 (100%)	0	100	100
3	10-G	84/102 (82%)	84 (100%)	0	100	100
4	1-D	78/104 (75%)	78 (100%)	0	100	100
4	1-H	78/104 (75%)	78 (100%)	0	100	100
4	2-D	78/104 (75%)	78 (100%)	0	100	100
4	2-H	78/104 (75%)	78 (100%)	0	100	100
4	3-D	78/104 (75%)	78 (100%)	0	100	100
4	3-H	78/104 (75%)	78 (100%)	0	100	100
4	4-D	78/104 (75%)	78 (100%)	0	100	100
4	4-H	78/104 (75%)	78 (100%)	0	100	100
4	5-D	78/104 (75%)	78 (100%)	0	100	100
4	5-H	78/104 (75%)	78 (100%)	0	100	100
4	6-D	78/104 (75%)	78 (100%)	0	100	100
4	6-H	78/104 (75%)	78 (100%)	0	100	100
4	7-D	78/104 (75%)	78 (100%)	0	100	100
4	7-H	78/104 (75%)	78 (100%)	0	100	100
4	8-D	78/104 (75%)	78 (100%)	0	100	100
4	8-H	78/104 (75%)	78 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	9-D	78/104 (75%)	78 (100%)	0	100	100
4	9-H	78/104 (75%)	78 (100%)	0	100	100
4	10-D	78/104 (75%)	78 (100%)	0	100	100
4	10-H	78/104 (75%)	78 (100%)	0	100	100
7	1-K	558/735 (76%)	553 (99%)	5 (1%)	70	75
7	2-K	558/735 (76%)	553 (99%)	5 (1%)	70	75
7	3-K	558/735 (76%)	553 (99%)	5 (1%)	70	75
7	4-K	558/735 (76%)	553 (99%)	5 (1%)	70	75
7	5-K	558/735 (76%)	553 (99%)	5 (1%)	70	75
7	6-K	558/735 (76%)	553 (99%)	5 (1%)	70	75
7	7-K	558/735 (76%)	553 (99%)	5 (1%)	70	75
7	8-K	558/735 (76%)	553 (99%)	5 (1%)	70	75
7	9-K	558/735 (76%)	553 (99%)	5 (1%)	70	75
7	10-K	558/735 (76%)	553 (99%)	5 (1%)	70	75
8	1-L	349/420 (83%)	349 (100%)	0	100	100
8	2-L	349/420 (83%)	349 (100%)	0	100	100
8	3-L	349/420 (83%)	349 (100%)	0	100	100
8	4-L	349/420 (83%)	349 (100%)	0	100	100
8	5-L	349/420 (83%)	349 (100%)	0	100	100
8	6-L	349/420 (83%)	349 (100%)	0	100	100
8	7-L	349/420 (83%)	349 (100%)	0	100	100
8	8-L	349/420 (83%)	349 (100%)	0	100	100
8	9-L	349/420 (83%)	349 (100%)	0	100	100
8	10-L	349/420 (83%)	349 (100%)	0	100	100
9	1-M	362/423 (86%)	362 (100%)	0	100	100
9	2-M	362/423 (86%)	362 (100%)	0	100	100
9	3-M	362/423 (86%)	362 (100%)	0	100	100
9	4-M	362/423 (86%)	362 (100%)	0	100	100
9	5-M	362/423 (86%)	362 (100%)	0	100	100
9	6-M	362/423 (86%)	362 (100%)	0	100	100
9	7-M	362/423 (86%)	362 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	8-M	362/423 (86%)	362 (100%)	0	100	100
9	9-M	362/423 (86%)	362 (100%)	0	100	100
9	10-M	362/423 (86%)	362 (100%)	0	100	100
10	1-N	54/140 (39%)	54 (100%)	0	100	100
10	2-N	54/140 (39%)	54 (100%)	0	100	100
10	3-N	54/140 (39%)	54 (100%)	0	100	100
10	4-N	54/140 (39%)	54 (100%)	0	100	100
10	5-N	54/140 (39%)	54 (100%)	0	100	100
10	6-N	54/140 (39%)	54 (100%)	0	100	100
10	7-N	54/140 (39%)	54 (100%)	0	100	100
10	8-N	54/140 (39%)	54 (100%)	0	100	100
10	9-N	54/140 (39%)	54 (100%)	0	100	100
10	10-N	54/140 (39%)	54 (100%)	0	100	100
All	All	19520/25100 (78%)	19470 (100%)	50 (0%)	84	85

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	1-K	362	MET
7	1-K	363	GLU
7	1-K	366	GLU
7	1-K	368	LYS
7	1-K	370	ILE
7	2-K	362	MET
7	2-K	363	GLU
7	2-K	366	GLU
7	2-K	368	LYS
7	2-K	370	ILE
7	3-K	362	MET
7	3-K	363	GLU
7	3-K	366	GLU
7	3-K	368	LYS
7	3-K	370	ILE
7	4-K	362	MET
7	4-K	363	GLU
7	4-K	366	GLU
7	4-K	368	LYS

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Mol	Chain	Res	Type
7	4-K	370	ILE
7	5-K	362	MET
7	5-K	363	GLU
7	5-K	366	GLU
7	5-K	368	LYS
7	5-K	370	ILE
7	6-K	362	MET
7	6-K	363	GLU
7	6-K	366	GLU
7	6-K	368	LYS
7	6-K	370	ILE
7	7-K	362	MET
7	7-K	363	GLU
7	7-K	366	GLU
7	7-K	368	LYS
7	7-K	370	ILE
7	8-K	362	MET
7	8-K	363	GLU
7	8-K	366	GLU
7	8-K	368	LYS
7	8-K	370	ILE
7	9-K	362	MET
7	9-K	363	GLU
7	9-K	366	GLU
7	9-K	368	LYS
7	9-K	370	ILE
7	10-K	362	MET
7	10-K	363	GLU
7	10-K	366	GLU
7	10-K	368	LYS
7	10-K	370	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (100) such sidechains are listed below:

Mol	Chain	Res	Type
7	1-K	359	HIS
7	1-K	361	GLN
7	1-K	593	HIS
7	1-K	642	ASN
7	1-K	818	GLN
8	1-L	74	GLN
8	1-L	194	HIS

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Mol	Chain	Res	Type
8	1-L	214	GLN
9	1-M	17	GLN
2	2-B	19	HIS
3	2-C	25	GLN
7	2-K	359	HIS
7	2-K	361	GLN
8	2-L	74	GLN
8	2-L	194	HIS
8	2-L	214	GLN
9	2-M	17	GLN
3	3-C	25	GLN
1	3-E	77	GLN
3	3-G	25	GLN
7	3-K	359	HIS
7	3-K	361	GLN
7	3-K	395	GLN
7	3-K	724	GLN
7	3-K	728	GLN
8	3-L	74	GLN
8	3-L	194	HIS
8	3-L	214	GLN
9	3-M	17	GLN
3	4-C	25	GLN
3	4-G	25	GLN
7	4-K	359	HIS
7	4-K	361	GLN
8	4-L	74	GLN
8	4-L	194	HIS
8	4-L	214	GLN
9	4-M	17	GLN
3	5-C	25	GLN
3	5-G	25	GLN
7	5-K	359	HIS
7	5-K	361	GLN
7	5-K	423	GLN
7	5-K	589	HIS
7	5-K	631	GLN
7	5-K	724	GLN
7	5-K	815	GLN
8	5-L	74	GLN
8	5-L	194	HIS
8	5-L	214	GLN

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Mol	Chain	Res	Type
9	5-M	17	GLN
3	6-G	25	GLN
7	6-K	359	HIS
7	6-K	361	GLN
7	6-K	642	ASN
7	6-K	650	ASN
7	6-K	898	GLN
8	6-L	74	GLN
8	6-L	194	HIS
8	6-L	214	GLN
9	6-M	17	GLN
3	7-C	25	GLN
3	7-G	25	GLN
7	7-K	359	HIS
7	7-K	361	GLN
7	7-K	395	GLN
8	7-L	74	GLN
8	7-L	194	HIS
8	7-L	214	GLN
9	7-M	17	GLN
3	8-G	25	GLN
7	8-K	359	HIS
7	8-K	361	GLN
7	8-K	395	GLN
7	8-K	727	GLN
8	8-L	74	GLN
8	8-L	194	HIS
8	8-L	214	GLN
9	8-M	17	GLN
3	9-C	25	GLN
3	9-G	25	GLN
7	9-K	359	HIS
7	9-K	361	GLN
8	9-L	74	GLN
8	9-L	194	HIS
8	9-L	214	GLN
9	9-M	17	GLN
3	10-C	25	GLN
3	10-G	25	GLN
7	10-K	359	HIS
7	10-K	361	GLN
7	10-K	561	GLN

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Mol	Chain	Res	Type
7	10-K	562	HIS
7	10-K	642	ASN
7	10-K	724	GLN
7	10-K	728	GLN
7	10-K	733	ASN
8	10-L	74	GLN
8	10-L	194	HIS
8	10-L	214	GLN
9	10-M	17	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 40 ligands modelled in this entry, 10 are monoatomic - leaving 30 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	$\#\|Z\| > 2$
12	ADP	5-K	1502	13	28,29,29	1.46	6 (21%)	43,45,45	1.96	11 (25%)
13	BEF	6-K	1503	12	0,3,3	-	-	-		
14	ATP	3-L	501	-	32,33,33	1.49	8 (25%)	48,52,52	1.85	10 (20%)
12	ADP	9-K	1502	13	28,29,29	1.36	5 (17%)	43,45,45	1.92	9 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	BEF	8-K	1503	12	0,3,3	-	-	-		
13	BEF	9-K	1503	12	0,3,3	-	-	-		
14	ATP	10-L	501	-	32,33,33	1.49	8 (25%)	48,52,52	1.85	10 (20%)
13	BEF	7-K	1503	12	0,3,3	-	-	-		
13	BEF	4-K	1503	12	0,3,3	-	-	-		
12	ADP	1-K	1502	13	28,29,29	1.40	5 (17%)	43,45,45	2.02	10 (23%)
12	ADP	7-K	1502	13	28,29,29	1.36	5 (17%)	43,45,45	1.99	9 (20%)
14	ATP	7-L	501	-	32,33,33	1.49	8 (25%)	48,52,52	1.85	10 (20%)
12	ADP	6-K	1502	13	28,29,29	1.37	4 (14%)	43,45,45	1.91	10 (23%)
14	ATP	2-L	501	-	32,33,33	1.49	8 (25%)	48,52,52	1.85	10 (20%)
13	BEF	1-K	1503	12	0,3,3	-	-	-		
14	ATP	8-L	501	-	32,33,33	1.49	8 (25%)	48,52,52	1.85	10 (20%)
14	ATP	5-L	501	-	32,33,33	1.49	8 (25%)	48,52,52	1.85	10 (20%)
13	BEF	3-K	1503	12	0,3,3	-	-	-		
13	BEF	2-K	1503	12	0,3,3	-	-	-		
14	ATP	9-L	501	-	32,33,33	1.49	8 (25%)	48,52,52	1.85	10 (20%)
12	ADP	2-K	1502	13	28,29,29	1.45	6 (21%)	43,45,45	1.94	11 (25%)
14	ATP	1-L	501	-	32,33,33	1.49	8 (25%)	48,52,52	1.85	10 (20%)
12	ADP	8-K	1502	13	28,29,29	1.47	6 (21%)	43,45,45	1.96	10 (23%)
12	ADP	10-K	1502	13	28,29,29	1.47	6 (21%)	43,45,45	1.89	12 (27%)
14	ATP	4-L	501	-	32,33,33	1.49	8 (25%)	48,52,52	1.85	10 (20%)
12	ADP	4-K	1502	13	28,29,29	1.39	5 (17%)	43,45,45	1.91	11 (25%)
14	ATP	6-L	501	-	32,33,33	1.49	8 (25%)	48,52,52	1.85	10 (20%)
12	ADP	3-K	1502	13	28,29,29	1.39	5 (17%)	43,45,45	1.89	9 (20%)
13	BEF	5-K	1503	12	0,3,3	-	-	-		
13	BEF	10-K	1503	12	0,3,3	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	ADP	5-K	1502	13	-	4/16/32/32	0/3/3/3
14	ATP	3-L	501	-	-	2/22/38/38	0/3/3/3
12	ADP	9-K	1502	13	-	4/16/32/32	0/3/3/3
14	ATP	10-L	501	-	-	2/22/38/38	0/3/3/3
12	ADP	1-K	1502	13	-	3/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	ATP	7-L	501	-	-	2/22/38/38	0/3/3/3
12	ADP	7-K	1502	13	-	4/16/32/32	0/3/3/3
12	ADP	6-K	1502	13	-	4/16/32/32	0/3/3/3
14	ATP	2-L	501	-	-	2/22/38/38	0/3/3/3
14	ATP	5-L	501	-	-	2/22/38/38	0/3/3/3
14	ATP	9-L	501	-	-	2/22/38/38	0/3/3/3
12	ADP	2-K	1502	13	-	2/16/32/32	0/3/3/3
14	ATP	1-L	501	-	-	2/22/38/38	0/3/3/3
12	ADP	8-K	1502	13	-	4/16/32/32	0/3/3/3
12	ADP	10-K	1502	13	-	5/16/32/32	0/3/3/3
14	ATP	4-L	501	-	-	2/22/38/38	0/3/3/3
12	ADP	4-K	1502	13	-	3/16/32/32	0/3/3/3
14	ATP	6-L	501	-	-	2/22/38/38	0/3/3/3
12	ADP	3-K	1502	13	-	7/16/32/32	0/3/3/3
14	ATP	8-L	501	-	-	2/22/38/38	0/3/3/3

All (133) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	10-K	1502	ADP	C5-C4	4.39	1.46	1.39
12	5-K	1502	ADP	C5-C4	4.37	1.46	1.39
12	6-K	1502	ADP	C5-C4	4.27	1.46	1.39
12	1-K	1502	ADP	C5-C4	4.21	1.46	1.39
12	3-K	1502	ADP	C5-C4	4.18	1.46	1.39
12	9-K	1502	ADP	C5-C4	4.10	1.46	1.39
12	7-K	1502	ADP	C5-C4	4.07	1.46	1.39
12	2-K	1502	ADP	C5-C4	4.04	1.46	1.39
12	4-K	1502	ADP	C5-C4	3.99	1.46	1.39
14	1-L	501	ATP	C5-C4	3.98	1.46	1.39
14	2-L	501	ATP	C5-C4	3.98	1.46	1.39
14	3-L	501	ATP	C5-C4	3.98	1.46	1.39
14	4-L	501	ATP	C5-C4	3.98	1.46	1.39
14	5-L	501	ATP	C5-C4	3.98	1.46	1.39
14	6-L	501	ATP	C5-C4	3.98	1.46	1.39
14	7-L	501	ATP	C5-C4	3.98	1.46	1.39
14	8-L	501	ATP	C5-C4	3.98	1.46	1.39
14	9-L	501	ATP	C5-C4	3.98	1.46	1.39
14	10-L	501	ATP	C5-C4	3.98	1.46	1.39
12	8-K	1502	ADP	C5-C4	3.94	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	1-L	501	ATP	C5-N7	-2.99	1.33	1.39
14	2-L	501	ATP	C5-N7	-2.99	1.33	1.39
14	3-L	501	ATP	C5-N7	-2.99	1.33	1.39
14	4-L	501	ATP	C5-N7	-2.99	1.33	1.39
14	5-L	501	ATP	C5-N7	-2.99	1.33	1.39
14	6-L	501	ATP	C5-N7	-2.99	1.33	1.39
14	7-L	501	ATP	C5-N7	-2.99	1.33	1.39
14	8-L	501	ATP	C5-N7	-2.99	1.33	1.39
14	9-L	501	ATP	C5-N7	-2.99	1.33	1.39
14	10-L	501	ATP	C5-N7	-2.99	1.33	1.39
12	6-K	1502	ADP	C5-N7	-2.87	1.33	1.39
12	9-K	1502	ADP	C5-N7	-2.86	1.33	1.39
12	3-K	1502	ADP	C5-N7	-2.78	1.34	1.39
12	4-K	1502	ADP	C5-N7	-2.76	1.34	1.39
12	5-K	1502	ADP	C5-C6	2.72	1.48	1.41
12	8-K	1502	ADP	C5-N7	-2.70	1.34	1.39
12	1-K	1502	ADP	C5-N7	-2.66	1.34	1.39
14	1-L	501	ATP	PB-O3B	-2.66	1.56	1.59
14	2-L	501	ATP	PB-O3B	-2.66	1.56	1.59
14	3-L	501	ATP	PB-O3B	-2.66	1.56	1.59
14	4-L	501	ATP	PB-O3B	-2.66	1.56	1.59
14	5-L	501	ATP	PB-O3B	-2.66	1.56	1.59
14	6-L	501	ATP	PB-O3B	-2.66	1.56	1.59
14	7-L	501	ATP	PB-O3B	-2.66	1.56	1.59
14	8-L	501	ATP	PB-O3B	-2.66	1.56	1.59
14	9-L	501	ATP	PB-O3B	-2.66	1.56	1.59
14	10-L	501	ATP	PB-O3B	-2.66	1.56	1.59
12	10-K	1502	ADP	C5-C6	2.64	1.48	1.41
12	10-K	1502	ADP	C5-N7	-2.63	1.34	1.39
12	4-K	1502	ADP	C4-N9	-2.63	1.32	1.37
12	2-K	1502	ADP	C4-N9	-2.61	1.32	1.37
12	1-K	1502	ADP	C5-C6	2.56	1.48	1.41
12	7-K	1502	ADP	C5-N7	-2.56	1.34	1.39
12	8-K	1502	ADP	C4-N9	-2.52	1.32	1.37
12	2-K	1502	ADP	C5-C6	2.51	1.48	1.41
12	2-K	1502	ADP	C5-N7	-2.50	1.34	1.39
12	5-K	1502	ADP	C8-N9	-2.44	1.33	1.37
12	6-K	1502	ADP	C5-C6	2.43	1.47	1.41
12	5-K	1502	ADP	C5-N7	-2.42	1.34	1.39
12	7-K	1502	ADP	C8-N9	-2.42	1.33	1.37
14	1-L	501	ATP	C8-N9	-2.41	1.33	1.37
14	2-L	501	ATP	C8-N9	-2.41	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	3-L	501	ATP	C8-N9	-2.41	1.33	1.37
14	4-L	501	ATP	C8-N9	-2.41	1.33	1.37
14	5-L	501	ATP	C8-N9	-2.41	1.33	1.37
14	6-L	501	ATP	C8-N9	-2.41	1.33	1.37
14	7-L	501	ATP	C8-N9	-2.41	1.33	1.37
14	8-L	501	ATP	C8-N9	-2.41	1.33	1.37
14	9-L	501	ATP	C8-N9	-2.41	1.33	1.37
14	10-L	501	ATP	C8-N9	-2.41	1.33	1.37
12	7-K	1502	ADP	C5-C6	2.40	1.47	1.41
12	8-K	1502	ADP	C5-C6	2.38	1.47	1.41
12	10-K	1502	ADP	C8-N9	-2.34	1.33	1.37
12	3-K	1502	ADP	C5-C6	2.34	1.47	1.41
12	8-K	1502	ADP	C8-N9	-2.33	1.33	1.37
12	2-K	1502	ADP	C8-N9	-2.31	1.33	1.37
12	3-K	1502	ADP	C8-N9	-2.31	1.33	1.37
12	9-K	1502	ADP	C8-N9	-2.30	1.33	1.37
12	9-K	1502	ADP	C4-N9	-2.28	1.32	1.37
14	1-L	501	ATP	C4-N9	-2.28	1.33	1.37
14	2-L	501	ATP	C4-N9	-2.28	1.33	1.37
14	3-L	501	ATP	C4-N9	-2.28	1.33	1.37
14	4-L	501	ATP	C4-N9	-2.28	1.33	1.37
14	5-L	501	ATP	C4-N9	-2.28	1.33	1.37
14	6-L	501	ATP	C4-N9	-2.28	1.33	1.37
14	7-L	501	ATP	C4-N9	-2.28	1.33	1.37
14	8-L	501	ATP	C4-N9	-2.28	1.33	1.37
14	9-L	501	ATP	C4-N9	-2.28	1.33	1.37
14	10-L	501	ATP	C4-N9	-2.28	1.33	1.37
12	3-K	1502	ADP	C4-N9	-2.26	1.33	1.37
12	10-K	1502	ADP	C4-N9	-2.25	1.33	1.37
12	9-K	1502	ADP	C5-C6	2.24	1.47	1.41
12	4-K	1502	ADP	C5-C6	2.24	1.47	1.41
12	1-K	1502	ADP	C8-N9	-2.22	1.33	1.37
12	6-K	1502	ADP	C8-N9	-2.20	1.33	1.37
12	8-K	1502	ADP	PA-O3A	-2.17	1.57	1.59
12	4-K	1502	ADP	C8-N9	-2.16	1.33	1.37
12	5-K	1502	ADP	C8-N7	2.14	1.35	1.31
12	2-K	1502	ADP	C8-N7	2.12	1.35	1.31
12	1-K	1502	ADP	C8-N7	2.10	1.35	1.31
14	1-L	501	ATP	C5-C6	2.08	1.46	1.41
14	2-L	501	ATP	C5-C6	2.08	1.46	1.41
14	3-L	501	ATP	C5-C6	2.08	1.46	1.41
14	4-L	501	ATP	C5-C6	2.08	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	5-L	501	ATP	C5-C6	2.08	1.46	1.41
14	6-L	501	ATP	C5-C6	2.08	1.46	1.41
14	7-L	501	ATP	C5-C6	2.08	1.46	1.41
14	8-L	501	ATP	C5-C6	2.08	1.46	1.41
14	9-L	501	ATP	C5-C6	2.08	1.46	1.41
14	10-L	501	ATP	C5-C6	2.08	1.46	1.41
14	1-L	501	ATP	PB-O3A	-2.07	1.57	1.59
14	2-L	501	ATP	PB-O3A	-2.07	1.57	1.59
14	3-L	501	ATP	PB-O3A	-2.07	1.57	1.59
14	4-L	501	ATP	PB-O3A	-2.07	1.57	1.59
14	5-L	501	ATP	PB-O3A	-2.07	1.57	1.59
14	6-L	501	ATP	PB-O3A	-2.07	1.57	1.59
14	7-L	501	ATP	PB-O3A	-2.07	1.57	1.59
14	8-L	501	ATP	PB-O3A	-2.07	1.57	1.59
14	9-L	501	ATP	PB-O3A	-2.07	1.57	1.59
14	10-L	501	ATP	PB-O3A	-2.07	1.57	1.59
12	5-K	1502	ADP	C4-N9	-2.07	1.33	1.37
14	1-L	501	ATP	PA-O3A	-2.03	1.57	1.59
14	2-L	501	ATP	PA-O3A	-2.03	1.57	1.59
14	3-L	501	ATP	PA-O3A	-2.03	1.57	1.59
14	4-L	501	ATP	PA-O3A	-2.03	1.57	1.59
14	5-L	501	ATP	PA-O3A	-2.03	1.57	1.59
14	6-L	501	ATP	PA-O3A	-2.03	1.57	1.59
14	7-L	501	ATP	PA-O3A	-2.03	1.57	1.59
14	8-L	501	ATP	PA-O3A	-2.03	1.57	1.59
14	9-L	501	ATP	PA-O3A	-2.03	1.57	1.59
14	10-L	501	ATP	PA-O3A	-2.03	1.57	1.59
12	10-K	1502	ADP	C8-N7	2.03	1.35	1.31
12	7-K	1502	ADP	C4-N9	-2.00	1.33	1.37

All (202) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	1-L	501	ATP	C5-C4-N3	-6.24	118.13	126.72
14	2-L	501	ATP	C5-C4-N3	-6.24	118.13	126.72
14	3-L	501	ATP	C5-C4-N3	-6.24	118.13	126.72
14	4-L	501	ATP	C5-C4-N3	-6.24	118.13	126.72
14	5-L	501	ATP	C5-C4-N3	-6.24	118.13	126.72
14	6-L	501	ATP	C5-C4-N3	-6.24	118.13	126.72
14	7-L	501	ATP	C5-C4-N3	-6.24	118.13	126.72
14	8-L	501	ATP	C5-C4-N3	-6.24	118.13	126.72
14	9-L	501	ATP	C5-C4-N3	-6.24	118.13	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	10-L	501	ATP	C5-C4-N3	-6.24	118.13	126.72
12	7-K	1502	ADP	C5-C4-N3	-6.21	118.17	126.72
12	1-K	1502	ADP	C5-C4-N3	-6.13	118.28	126.72
12	6-K	1502	ADP	C5-C4-N3	-6.05	118.39	126.72
12	9-K	1502	ADP	C5-C4-N3	-5.87	118.64	126.72
12	5-K	1502	ADP	C5-C4-N3	-5.83	118.69	126.72
12	3-K	1502	ADP	C5-C4-N3	-5.81	118.72	126.72
12	10-K	1502	ADP	C5-C4-N3	-5.76	118.79	126.72
12	4-K	1502	ADP	C5-C4-N3	-5.62	118.98	126.72
12	8-K	1502	ADP	C5-C4-N3	-5.52	119.12	126.72
12	2-K	1502	ADP	C5-C4-N3	-5.48	119.17	126.72
12	7-K	1502	ADP	N3-C4-N9	5.35	136.26	127.17
12	6-K	1502	ADP	N3-C4-N9	5.14	135.91	127.17
14	1-L	501	ATP	N3-C4-N9	5.01	135.68	127.17
14	2-L	501	ATP	N3-C4-N9	5.01	135.68	127.17
14	3-L	501	ATP	N3-C4-N9	5.01	135.68	127.17
14	4-L	501	ATP	N3-C4-N9	5.01	135.68	127.17
14	5-L	501	ATP	N3-C4-N9	5.01	135.68	127.17
14	6-L	501	ATP	N3-C4-N9	5.01	135.68	127.17
14	7-L	501	ATP	N3-C4-N9	5.01	135.68	127.17
14	8-L	501	ATP	N3-C4-N9	5.01	135.68	127.17
14	9-L	501	ATP	N3-C4-N9	5.01	135.68	127.17
14	10-L	501	ATP	N3-C4-N9	5.01	135.68	127.17
12	1-K	1502	ADP	N3-C4-N9	4.96	135.60	127.17
12	9-K	1502	ADP	N3-C4-N9	4.89	135.48	127.17
12	3-K	1502	ADP	N3-C4-N9	4.84	135.41	127.17
12	5-K	1502	ADP	N3-C4-N9	4.77	135.29	127.17
12	10-K	1502	ADP	N3-C4-N9	4.66	135.10	127.17
12	4-K	1502	ADP	N3-C4-N9	4.62	135.02	127.17
12	8-K	1502	ADP	N3-C4-N9	4.47	134.77	127.17
12	2-K	1502	ADP	N3-C4-N9	4.37	134.60	127.17
12	7-K	1502	ADP	C2-N3-C4	3.85	121.24	111.83
12	5-K	1502	ADP	C4-C5-N7	-3.79	106.25	110.58
14	1-L	501	ATP	C2-N3-C4	3.79	121.08	111.83
14	2-L	501	ATP	C2-N3-C4	3.79	121.08	111.83
14	3-L	501	ATP	C2-N3-C4	3.79	121.08	111.83
14	4-L	501	ATP	C2-N3-C4	3.79	121.08	111.83
14	5-L	501	ATP	C2-N3-C4	3.79	121.08	111.83
14	6-L	501	ATP	C2-N3-C4	3.79	121.08	111.83
14	7-L	501	ATP	C2-N3-C4	3.79	121.08	111.83
14	8-L	501	ATP	C2-N3-C4	3.79	121.08	111.83
14	9-L	501	ATP	C2-N3-C4	3.79	121.08	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	10-L	501	ATP	C2-N3-C4	3.79	121.08	111.83
12	1-K	1502	ADP	C2-N3-C4	3.78	121.07	111.83
12	10-K	1502	ADP	C4-C5-N7	-3.75	106.30	110.58
12	4-K	1502	ADP	C2-N3-C4	3.70	120.86	111.83
12	5-K	1502	ADP	C2-N3-C4	3.68	120.82	111.83
12	6-K	1502	ADP	C2-N3-C4	3.67	120.79	111.83
12	2-K	1502	ADP	C2-N3-C4	3.67	120.79	111.83
12	10-K	1502	ADP	C2-N3-C4	3.64	120.72	111.83
12	9-K	1502	ADP	C2-N3-C4	3.64	120.72	111.83
12	8-K	1502	ADP	C2-N3-C4	3.61	120.64	111.83
12	2-K	1502	ADP	C4-C5-N7	-3.60	106.47	110.58
12	3-K	1502	ADP	C2-N3-C4	3.59	120.61	111.83
12	8-K	1502	ADP	C4-C5-N7	-3.55	106.53	110.58
12	1-K	1502	ADP	C4-C5-N7	-3.54	106.54	110.58
12	7-K	1502	ADP	C4-N9-C8	3.50	109.42	105.74
12	3-K	1502	ADP	C4-C5-N7	-3.50	106.58	110.58
12	7-K	1502	ADP	C4-C5-N7	-3.45	106.64	110.58
12	4-K	1502	ADP	N3-C2-N1	-3.43	123.39	128.58
12	2-K	1502	ADP	C4-N9-C8	3.41	109.32	105.74
12	9-K	1502	ADP	C4-C5-N7	-3.41	106.68	110.58
12	5-K	1502	ADP	C4-N9-C8	3.38	109.29	105.74
12	8-K	1502	ADP	C4-N9-C8	3.35	109.26	105.74
12	2-K	1502	ADP	N3-C2-N1	-3.35	123.51	128.58
12	1-K	1502	ADP	N3-C2-N1	-3.32	123.56	128.58
12	6-K	1502	ADP	C4-C5-N7	-3.29	106.81	110.58
12	9-K	1502	ADP	N3-C2-N1	-3.29	123.61	128.58
12	8-K	1502	ADP	N3-C2-N1	-3.28	123.62	128.58
12	1-K	1502	ADP	C2'-C1'-N9	-3.26	105.22	113.30
12	5-K	1502	ADP	C2'-C1'-N9	-3.24	105.26	113.30
12	3-K	1502	ADP	C4-N9-C8	3.23	109.12	105.74
12	4-K	1502	ADP	C4-C5-N7	-3.22	106.90	110.58
12	4-K	1502	ADP	C4-N9-C8	3.22	109.11	105.74
14	1-L	501	ATP	C4-C5-N7	-3.21	106.91	110.58
14	2-L	501	ATP	C4-C5-N7	-3.21	106.91	110.58
14	3-L	501	ATP	C4-C5-N7	-3.21	106.91	110.58
14	4-L	501	ATP	C4-C5-N7	-3.21	106.91	110.58
14	5-L	501	ATP	C4-C5-N7	-3.21	106.91	110.58
14	6-L	501	ATP	C4-C5-N7	-3.21	106.91	110.58
14	7-L	501	ATP	C4-C5-N7	-3.21	106.91	110.58
14	8-L	501	ATP	C4-C5-N7	-3.21	106.91	110.58
14	9-L	501	ATP	C4-C5-N7	-3.21	106.91	110.58
14	10-L	501	ATP	C4-C5-N7	-3.21	106.91	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	3-K	1502	ADP	N3-C2-N1	-3.20	123.74	128.58
12	10-K	1502	ADP	N3-C2-N1	-3.17	123.78	128.58
12	10-K	1502	ADP	C4-N9-C8	3.17	109.06	105.74
12	5-K	1502	ADP	N3-C2-N1	-3.16	123.79	128.58
12	4-K	1502	ADP	C2'-C1'-N9	-3.15	105.48	113.30
12	9-K	1502	ADP	C4-N9-C8	3.13	109.02	105.74
12	7-K	1502	ADP	N3-C2-N1	-3.13	123.84	128.58
12	8-K	1502	ADP	C2'-C1'-N9	-3.11	105.59	113.30
14	1-L	501	ATP	N3-C2-N1	-3.08	123.91	128.58
14	2-L	501	ATP	N3-C2-N1	-3.08	123.91	128.58
14	3-L	501	ATP	N3-C2-N1	-3.08	123.91	128.58
14	4-L	501	ATP	N3-C2-N1	-3.08	123.91	128.58
14	5-L	501	ATP	N3-C2-N1	-3.08	123.91	128.58
14	6-L	501	ATP	N3-C2-N1	-3.08	123.91	128.58
14	7-L	501	ATP	N3-C2-N1	-3.08	123.91	128.58
14	8-L	501	ATP	N3-C2-N1	-3.08	123.91	128.58
14	9-L	501	ATP	N3-C2-N1	-3.08	123.91	128.58
14	10-L	501	ATP	N3-C2-N1	-3.08	123.91	128.58
12	6-K	1502	ADP	N3-C2-N1	-3.08	123.92	128.58
12	2-K	1502	ADP	C2'-C1'-N9	-3.00	105.86	113.30
12	6-K	1502	ADP	C4-N9-C8	2.94	108.82	105.74
12	1-K	1502	ADP	C4-N9-C8	2.90	108.78	105.74
12	5-K	1502	ADP	C5-N7-C8	2.76	107.79	103.45
12	7-K	1502	ADP	C5-N7-C8	2.75	107.78	103.45
12	10-K	1502	ADP	C5-N7-C8	2.72	107.72	103.45
12	3-K	1502	ADP	C5-N7-C8	2.69	107.68	103.45
12	1-K	1502	ADP	C5-N7-C8	2.68	107.66	103.45
12	6-K	1502	ADP	C5-N7-C8	2.67	107.64	103.45
12	9-K	1502	ADP	C5-N7-C8	2.63	107.58	103.45
12	8-K	1502	ADP	C5-N7-C8	2.62	107.57	103.45
14	1-L	501	ATP	O3G-PG-O2G	2.62	117.61	107.80
14	2-L	501	ATP	O3G-PG-O2G	2.62	117.61	107.80
14	3-L	501	ATP	O3G-PG-O2G	2.62	117.61	107.80
14	4-L	501	ATP	O3G-PG-O2G	2.62	117.61	107.80
14	5-L	501	ATP	O3G-PG-O2G	2.62	117.61	107.80
14	6-L	501	ATP	O3G-PG-O2G	2.62	117.61	107.80
14	7-L	501	ATP	O3G-PG-O2G	2.62	117.61	107.80
14	8-L	501	ATP	O3G-PG-O2G	2.62	117.61	107.80
14	9-L	501	ATP	O3G-PG-O2G	2.62	117.61	107.80
14	10-L	501	ATP	O3G-PG-O2G	2.62	117.61	107.80
12	2-K	1502	ADP	C5-N7-C8	2.51	107.40	103.45
14	1-L	501	ATP	C3'-C2'-C1'	2.48	106.15	101.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	2-L	501	ATP	C3'-C2'-C1'	2.48	106.15	101.46
14	3-L	501	ATP	C3'-C2'-C1'	2.48	106.15	101.46
14	4-L	501	ATP	C3'-C2'-C1'	2.48	106.15	101.46
14	5-L	501	ATP	C3'-C2'-C1'	2.48	106.15	101.46
14	6-L	501	ATP	C3'-C2'-C1'	2.48	106.15	101.46
14	7-L	501	ATP	C3'-C2'-C1'	2.48	106.15	101.46
14	8-L	501	ATP	C3'-C2'-C1'	2.48	106.15	101.46
14	9-L	501	ATP	C3'-C2'-C1'	2.48	106.15	101.46
14	10-L	501	ATP	C3'-C2'-C1'	2.48	106.15	101.46
14	1-L	501	ATP	C4-N9-C8	2.46	108.32	105.74
14	2-L	501	ATP	C4-N9-C8	2.46	108.32	105.74
14	3-L	501	ATP	C4-N9-C8	2.46	108.32	105.74
14	4-L	501	ATP	C4-N9-C8	2.46	108.32	105.74
14	5-L	501	ATP	C4-N9-C8	2.46	108.32	105.74
14	6-L	501	ATP	C4-N9-C8	2.46	108.32	105.74
14	7-L	501	ATP	C4-N9-C8	2.46	108.32	105.74
14	8-L	501	ATP	C4-N9-C8	2.46	108.32	105.74
14	9-L	501	ATP	C4-N9-C8	2.46	108.32	105.74
14	10-L	501	ATP	C4-N9-C8	2.46	108.32	105.74
12	1-K	1502	ADP	C3'-C2'-C1'	2.46	106.12	101.46
12	8-K	1502	ADP	N9-C8-N7	-2.41	110.52	113.94
12	4-K	1502	ADP	C5-N7-C8	2.37	107.17	103.45
12	2-K	1502	ADP	N9-C8-N7	-2.36	110.58	113.94
12	7-K	1502	ADP	N9-C8-N7	-2.36	110.59	113.94
12	5-K	1502	ADP	N9-C8-N7	-2.31	110.66	113.94
12	5-K	1502	ADP	C6-C5-N7	2.30	136.53	132.09
12	2-K	1502	ADP	C6-C5-N7	2.29	136.50	132.09
14	1-L	501	ATP	C5-N7-C8	2.27	107.01	103.45
14	2-L	501	ATP	C5-N7-C8	2.27	107.01	103.45
14	3-L	501	ATP	C5-N7-C8	2.27	107.01	103.45
14	4-L	501	ATP	C5-N7-C8	2.27	107.01	103.45
14	5-L	501	ATP	C5-N7-C8	2.27	107.01	103.45
14	6-L	501	ATP	C5-N7-C8	2.27	107.01	103.45
14	7-L	501	ATP	C5-N7-C8	2.27	107.01	103.45
14	8-L	501	ATP	C5-N7-C8	2.27	107.01	103.45
14	9-L	501	ATP	C5-N7-C8	2.27	107.01	103.45
14	10-L	501	ATP	C5-N7-C8	2.27	107.01	103.45
12	3-K	1502	ADP	C2'-C1'-N9	-2.26	107.69	113.30
12	3-K	1502	ADP	N9-C8-N7	-2.26	110.73	113.94
12	6-K	1502	ADP	C2'-C1'-N9	-2.24	107.73	113.30
12	9-K	1502	ADP	C2'-C1'-N9	-2.23	107.76	113.30
12	9-K	1502	ADP	N9-C8-N7	-2.21	110.79	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	4-K	1502	ADP	N9-C8-N7	-2.21	110.81	113.94
12	10-K	1502	ADP	N9-C8-N7	-2.20	110.81	113.94
12	10-K	1502	ADP	C6-C5-N7	2.14	136.22	132.09
12	1-K	1502	ADP	N9-C8-N7	-2.14	110.90	113.94
12	8-K	1502	ADP	C6-C5-N7	2.13	136.20	132.09
12	2-K	1502	ADP	O2A-PA-O1A	2.13	122.37	112.44
12	7-K	1502	ADP	C2'-C1'-N9	-2.13	108.01	113.30
12	4-K	1502	ADP	C6-C5-N7	2.10	136.13	132.09
12	6-K	1502	ADP	C3'-C2'-C1'	2.08	105.41	101.46
12	10-K	1502	ADP	C2-N1-C6	2.07	122.14	118.73
12	6-K	1502	ADP	N9-C8-N7	-2.05	111.02	113.94
14	1-L	501	ATP	O2B-PB-O1B	2.05	121.97	112.44
14	2-L	501	ATP	O2B-PB-O1B	2.05	121.97	112.44
14	3-L	501	ATP	O2B-PB-O1B	2.05	121.97	112.44
14	4-L	501	ATP	O2B-PB-O1B	2.05	121.97	112.44
14	5-L	501	ATP	O2B-PB-O1B	2.05	121.97	112.44
14	6-L	501	ATP	O2B-PB-O1B	2.05	121.97	112.44
14	7-L	501	ATP	O2B-PB-O1B	2.05	121.97	112.44
14	8-L	501	ATP	O2B-PB-O1B	2.05	121.97	112.44
14	9-L	501	ATP	O2B-PB-O1B	2.05	121.97	112.44
14	10-L	501	ATP	O2B-PB-O1B	2.05	121.97	112.44
12	5-K	1502	ADP	C2-N1-C6	2.03	122.07	118.73
12	10-K	1502	ADP	O2A-PA-O1A	2.02	121.83	112.44
12	4-K	1502	ADP	O3B-PB-O2B	2.02	115.36	107.80
12	10-K	1502	ADP	C2'-C1'-N9	-2.01	108.30	113.30

There are no chirality outliers.

All (60) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	1-K	1502	ADP	C5'-O5'-PA-O1A
12	1-K	1502	ADP	C4'-C5'-O5'-PA
12	2-K	1502	ADP	C5'-O5'-PA-O1A
12	3-K	1502	ADP	PA-O3A-PB-O2B
12	3-K	1502	ADP	PA-O3A-PB-O3B
12	3-K	1502	ADP	C5'-O5'-PA-O3A
12	4-K	1502	ADP	C5'-O5'-PA-O3A
12	4-K	1502	ADP	C4'-C5'-O5'-PA
12	5-K	1502	ADP	C5'-O5'-PA-O1A
12	6-K	1502	ADP	PA-O3A-PB-O3B
12	6-K	1502	ADP	C5'-O5'-PA-O1A
12	7-K	1502	ADP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
12	9-K	1502	ADP	PA-O3A-PB-O3B
12	9-K	1502	ADP	C5'-O5'-PA-O1A
12	10-K	1502	ADP	C5'-O5'-PA-O3A
12	10-K	1502	ADP	C4'-C5'-O5'-PA
12	3-K	1502	ADP	C4'-C5'-O5'-PA
12	7-K	1502	ADP	C4'-C5'-O5'-PA
12	5-K	1502	ADP	C4'-C5'-O5'-PA
12	8-K	1502	ADP	C4'-C5'-O5'-PA
12	10-K	1502	ADP	PB-O3A-PA-O5'
14	1-L	501	ATP	C2'-C1'-N9-C8
14	2-L	501	ATP	C2'-C1'-N9-C8
14	3-L	501	ATP	C2'-C1'-N9-C8
14	4-L	501	ATP	C2'-C1'-N9-C8
14	5-L	501	ATP	C2'-C1'-N9-C8
14	6-L	501	ATP	C2'-C1'-N9-C8
14	7-L	501	ATP	C2'-C1'-N9-C8
14	8-L	501	ATP	C2'-C1'-N9-C8
14	9-L	501	ATP	C2'-C1'-N9-C8
14	10-L	501	ATP	C2'-C1'-N9-C8
12	3-K	1502	ADP	PB-O3A-PA-O1A
12	3-K	1502	ADP	C5'-O5'-PA-O1A
12	4-K	1502	ADP	C5'-O5'-PA-O1A
12	8-K	1502	ADP	C5'-O5'-PA-O1A
12	10-K	1502	ADP	C5'-O5'-PA-O1A
12	2-K	1502	ADP	C4'-C5'-O5'-PA
12	5-K	1502	ADP	PB-O3A-PA-O1A
12	7-K	1502	ADP	PB-O3A-PA-O1A
12	6-K	1502	ADP	PA-O3A-PB-O1B
12	9-K	1502	ADP	PA-O3A-PB-O1B
12	6-K	1502	ADP	PA-O3A-PB-O2B
12	9-K	1502	ADP	PA-O3A-PB-O2B
12	10-K	1502	ADP	C3'-C4'-C5'-O5'
12	3-K	1502	ADP	PB-O3A-PA-O2A
12	8-K	1502	ADP	PB-O3A-PA-O1A
14	1-L	501	ATP	PA-O3A-PB-O1B
14	2-L	501	ATP	PA-O3A-PB-O1B
14	3-L	501	ATP	PA-O3A-PB-O1B
14	4-L	501	ATP	PA-O3A-PB-O1B
14	5-L	501	ATP	PA-O3A-PB-O1B
14	6-L	501	ATP	PA-O3A-PB-O1B
14	7-L	501	ATP	PA-O3A-PB-O1B
14	8-L	501	ATP	PA-O3A-PB-O1B

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Mol	Chain	Res	Type	Atoms
14	9-L	501	ATP	PA-O3A-PB-O1B
14	10-L	501	ATP	PA-O3A-PB-O1B
12	1-K	1502	ADP	C2'-C1'-N9-C8
12	5-K	1502	ADP	PB-O3A-PA-O2A
12	7-K	1502	ADP	PB-O3A-PA-O2A
12	8-K	1502	ADP	PB-O3A-PA-O2A

There are no ring outliers.

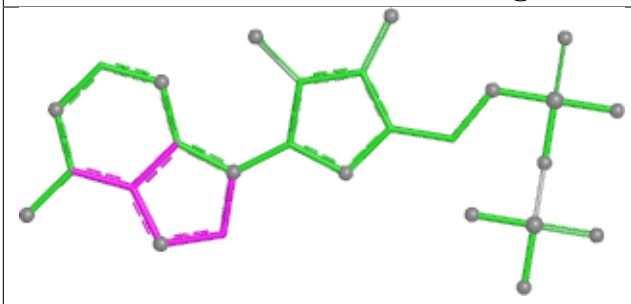
23 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	5-K	1502	ADP	2	0
13	6-K	1503	BEF	1	0
14	3-L	501	ATP	1	0
12	9-K	1502	ADP	3	0
13	9-K	1503	BEF	2	0
14	10-L	501	ATP	1	0
12	1-K	1502	ADP	3	0
12	7-K	1502	ADP	1	0
14	7-L	501	ATP	1	0
12	6-K	1502	ADP	2	0
14	2-L	501	ATP	1	0
14	8-L	501	ATP	1	0
14	5-L	501	ATP	1	0
13	3-K	1503	BEF	3	0
14	9-L	501	ATP	1	0
12	2-K	1502	ADP	1	0
14	1-L	501	ATP	1	0
12	8-K	1502	ADP	2	0
12	10-K	1502	ADP	4	0
14	4-L	501	ATP	1	0
12	4-K	1502	ADP	3	0
14	6-L	501	ATP	1	0
12	3-K	1502	ADP	5	0

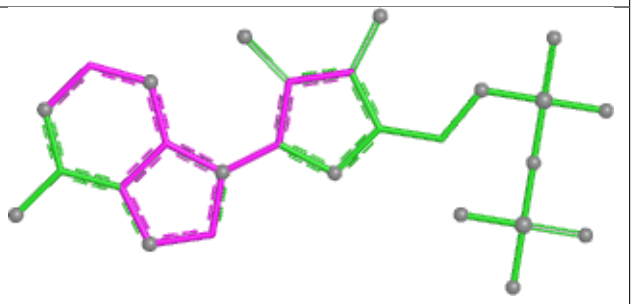
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

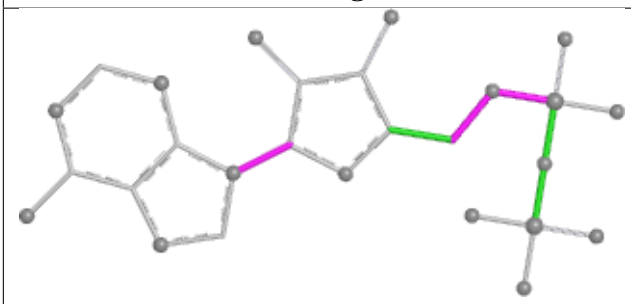
Ligand ADP K 1502



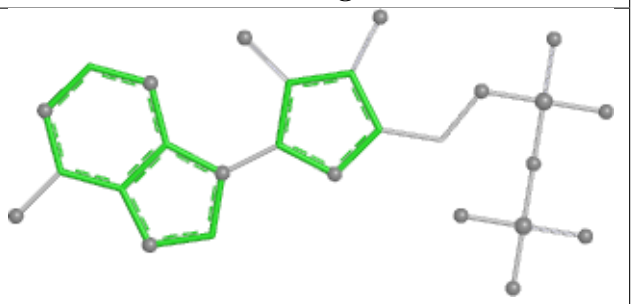
Bond lengths



Bond angles

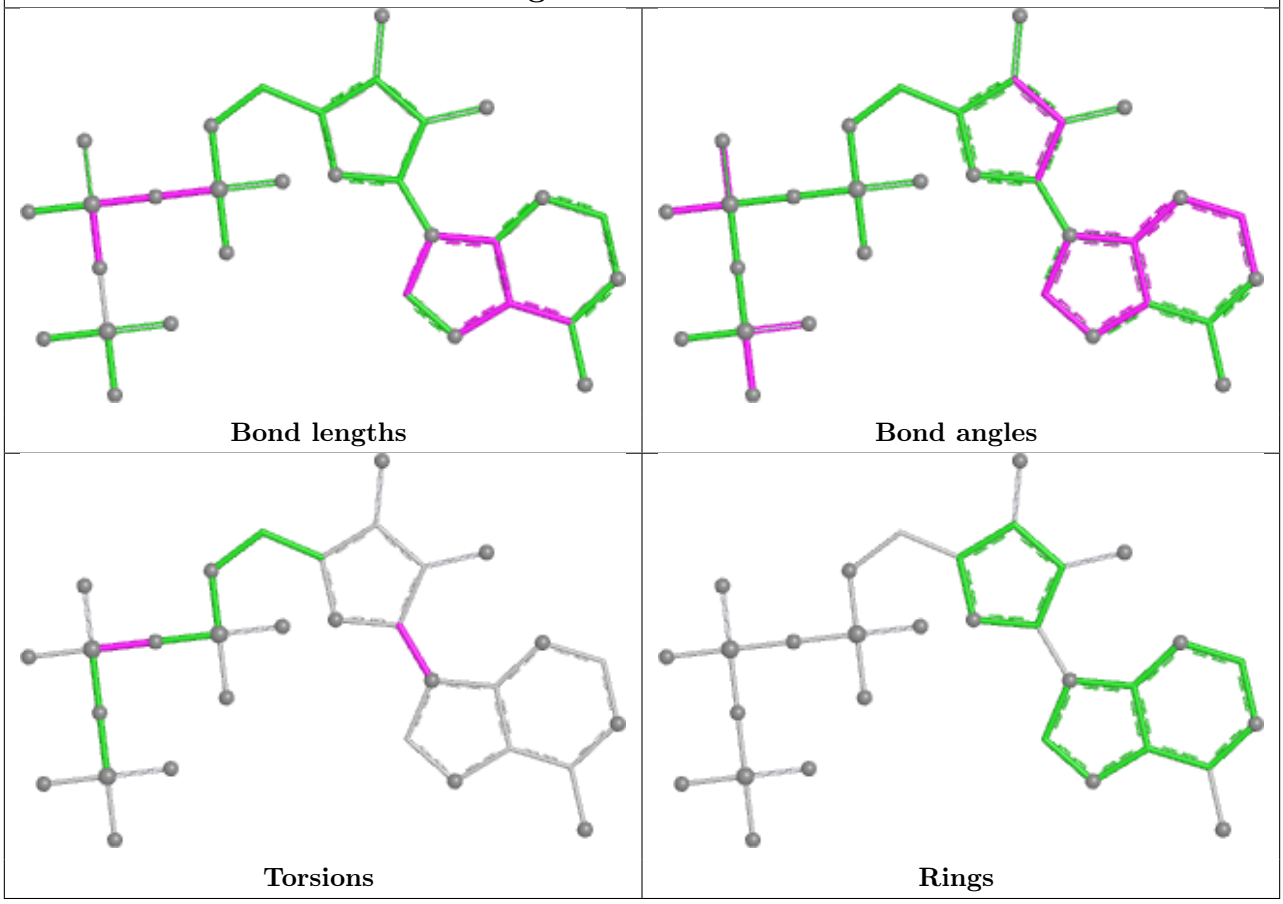


Torsions



Rings

Ligand ATP L 501



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

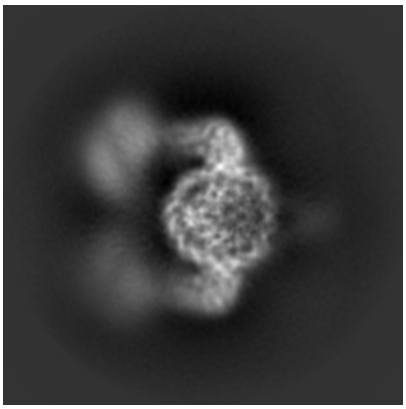
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-21484. These allow visual inspection of the internal detail of the map and identification of artifacts.

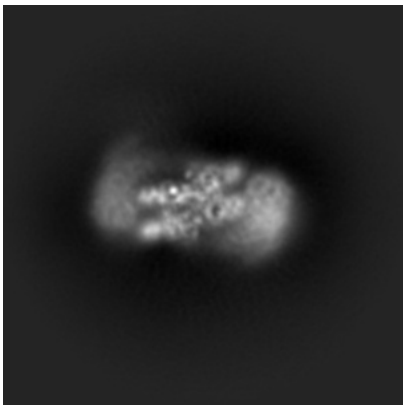
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

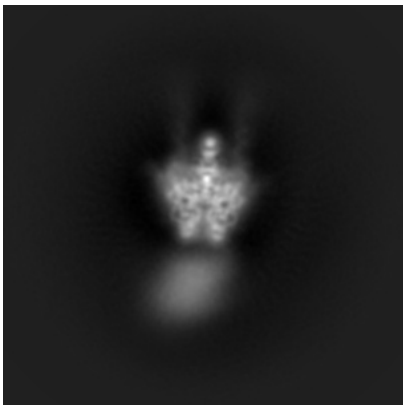
6.1.1 Primary map



X

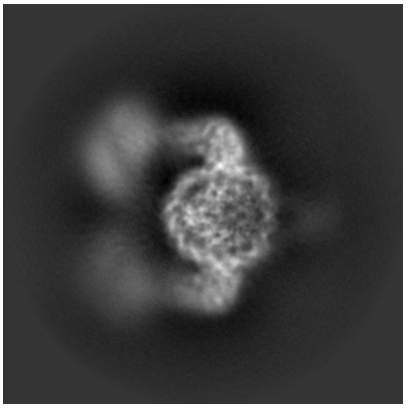


Y

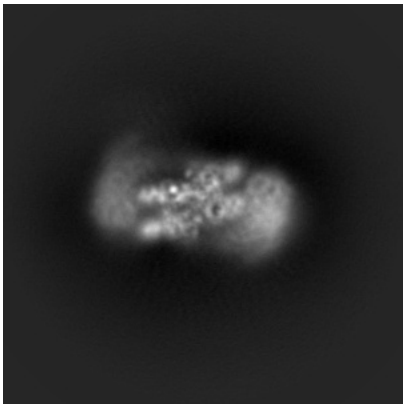


Z

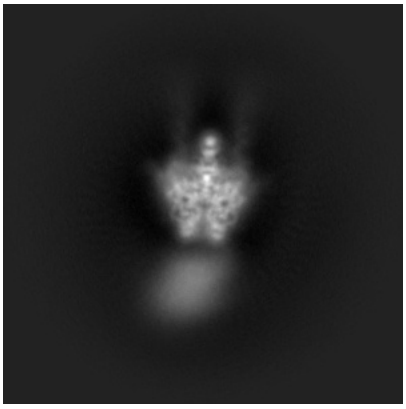
6.1.2 Raw map



X



Y

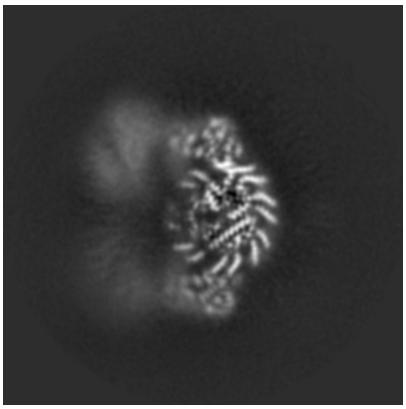


Z

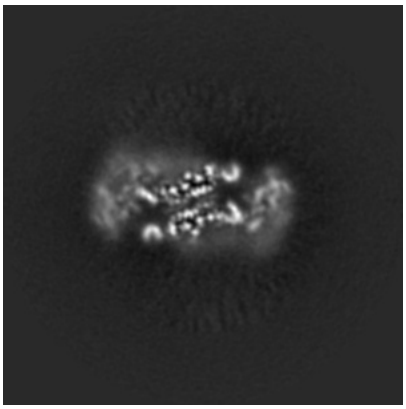
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

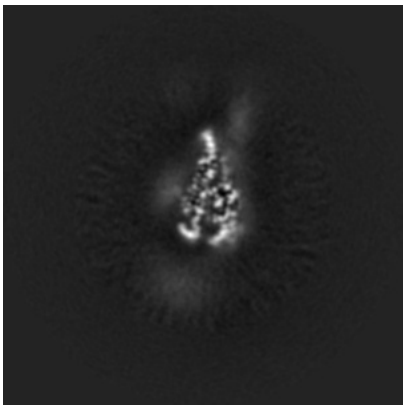
6.2.1 Primary map



X Index: 150

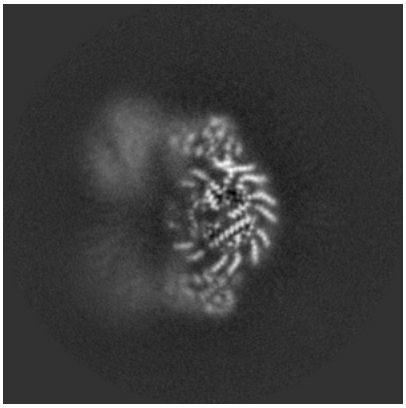


Y Index: 150

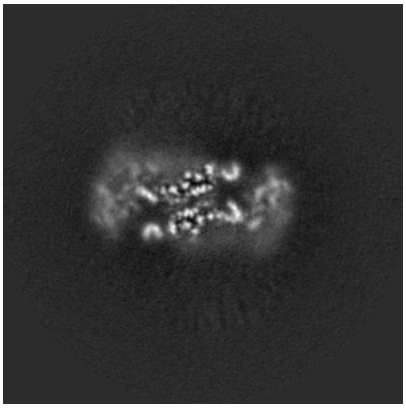


Z Index: 150

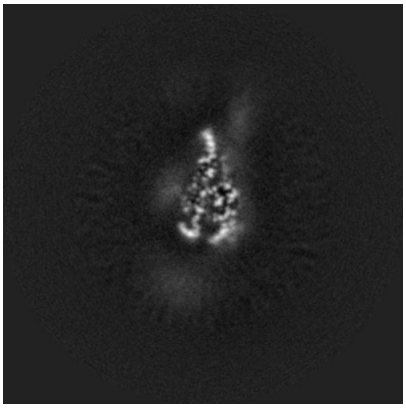
6.2.2 Raw map



X Index: 150



Y Index: 150

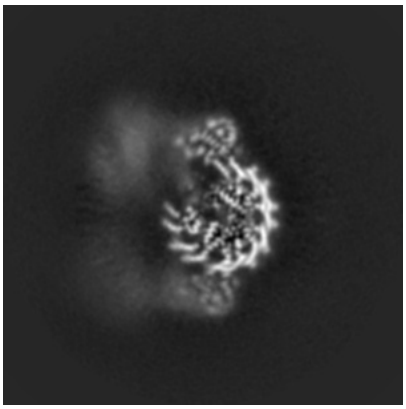


Z Index: 150

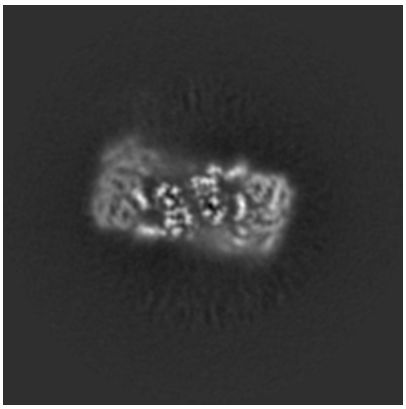
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

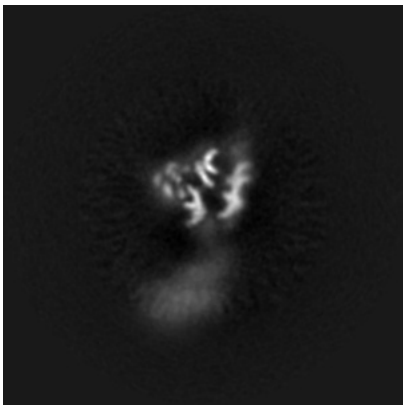
6.3.1 Primary map



X Index: 154

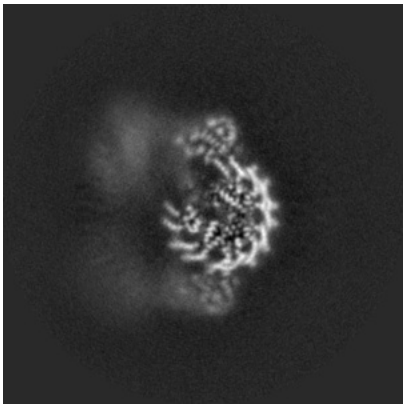


Y Index: 163

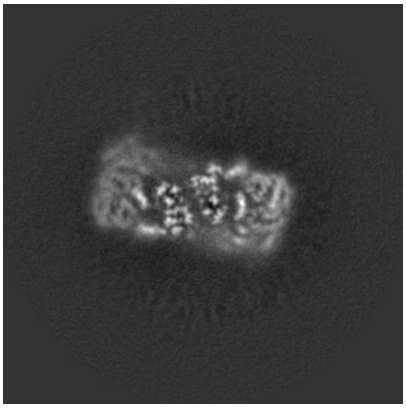


Z Index: 174

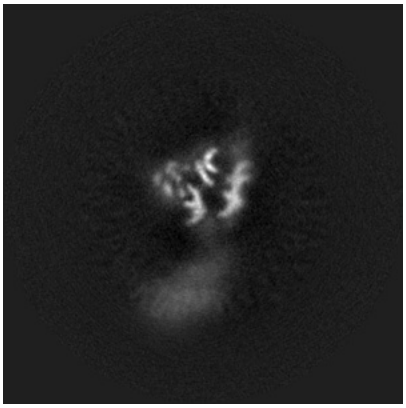
6.3.2 Raw map



X Index: 154



Y Index: 163

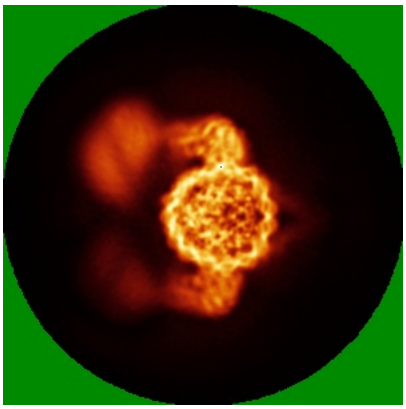


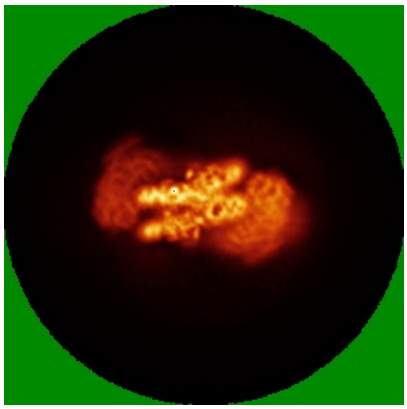
Z Index: 174

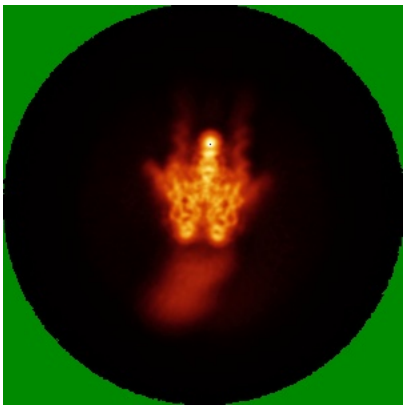
The images above show the largest variance slices of the map in three orthogonal directions.

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

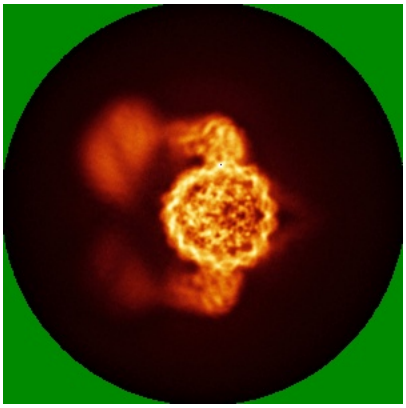
6.4.1 Primary map

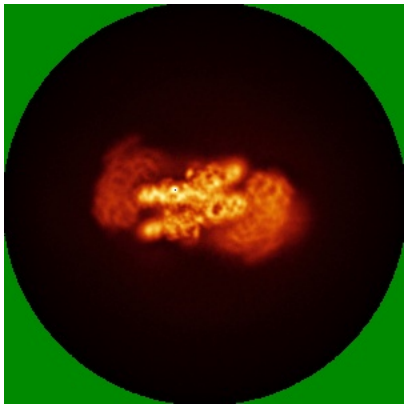

X

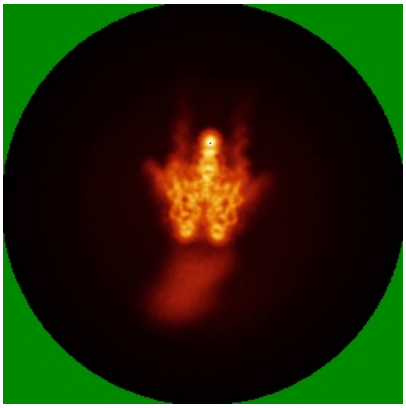

Y


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

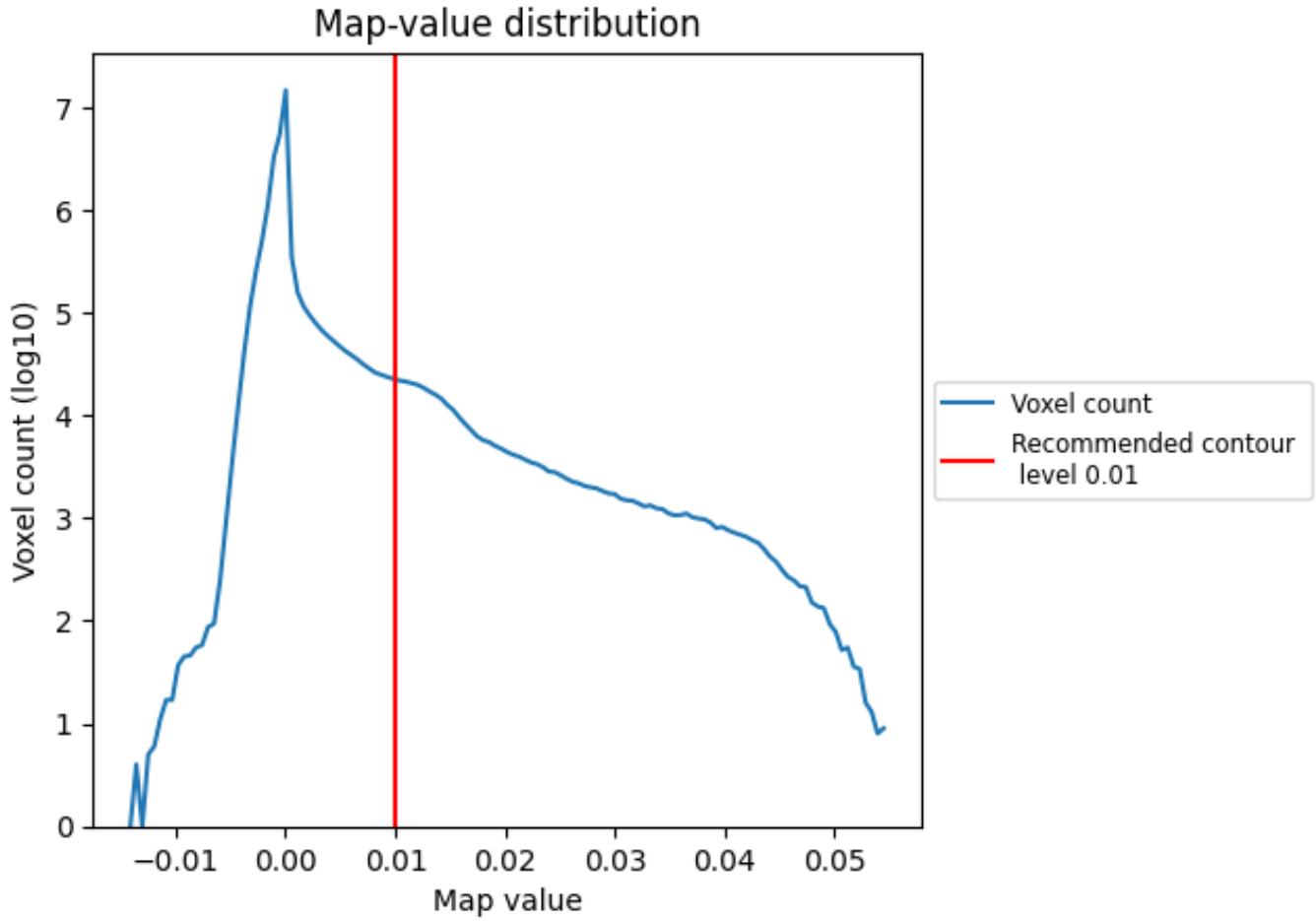
6.6 Mask visualisation (i)

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

7 Map analysis

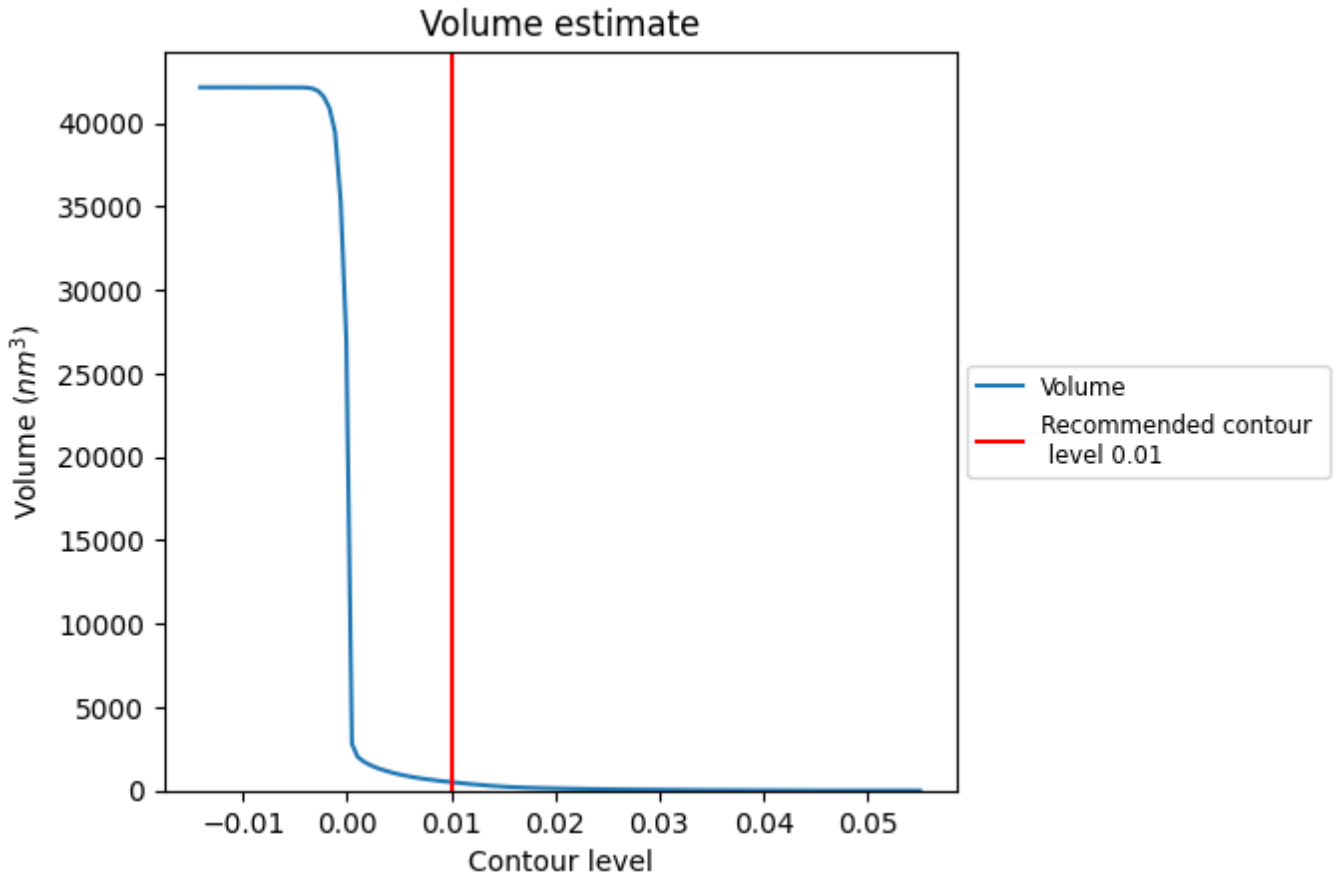
This section contains the results of statistical analysis of the map.

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.

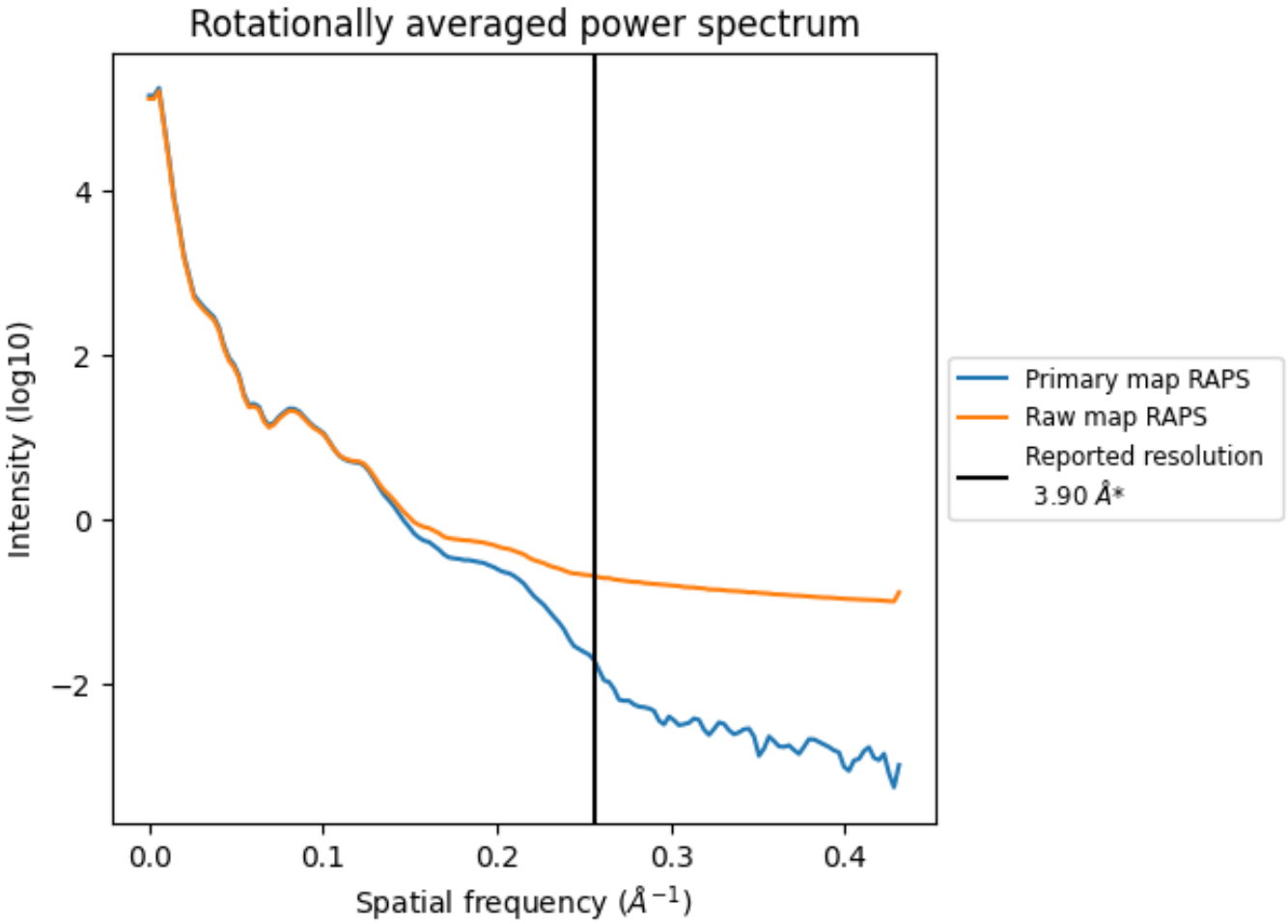
7.2 Volume estimate



The volume at the recommended contour level is 505 nm^3; this corresponds to an approximate mass of 456 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)

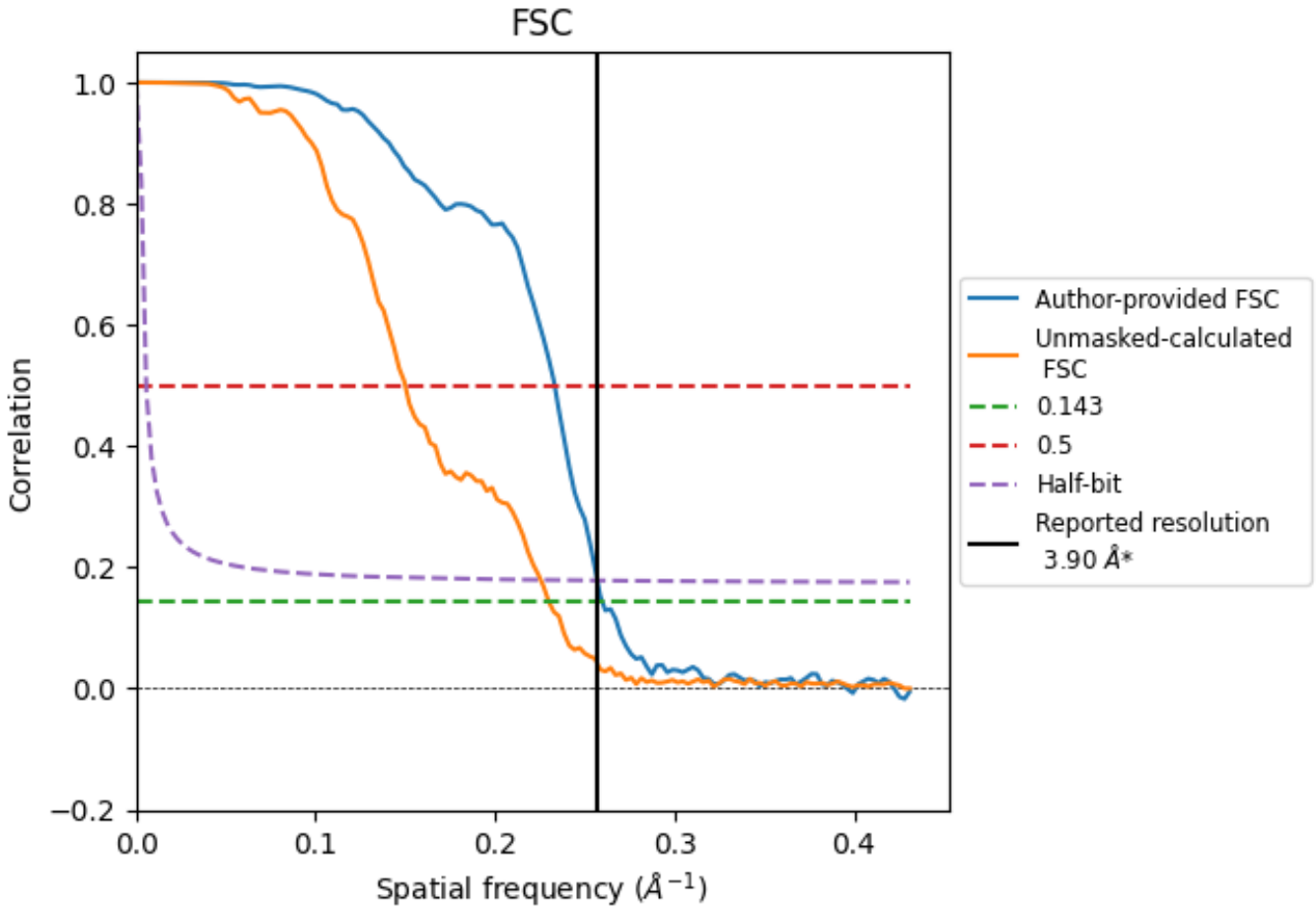


*Reported resolution corresponds to spatial frequency of 0.256 $Å^{-1}$

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 0.256 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.85	4.29	3.89
Unmasked-calculated*	4.35	6.67	4.43

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.35 differs from the reported value 3.9 by more than 10 %

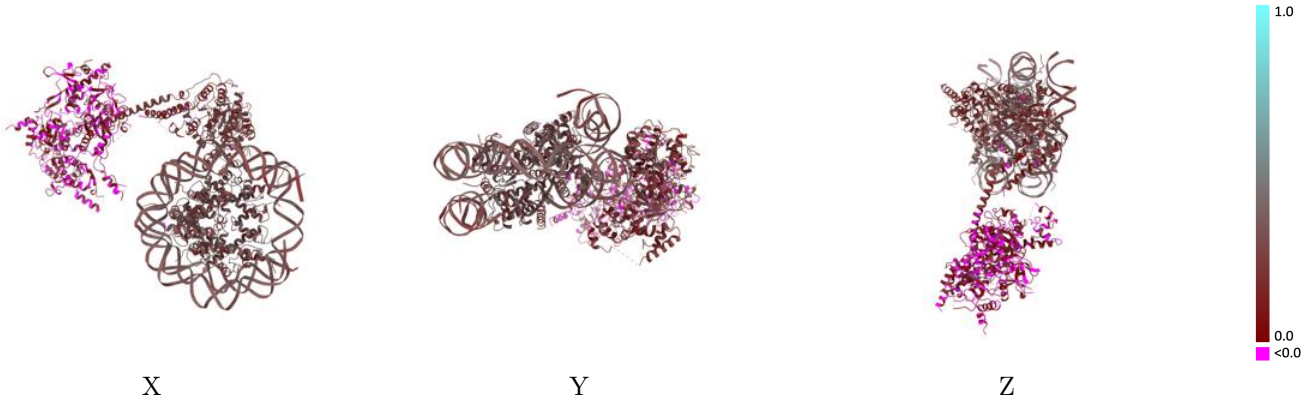
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-21484 and PDB model 6VZ4. Per-residue inclusion information can be found in section 3 on page 21.

9.1 Map-model overlay

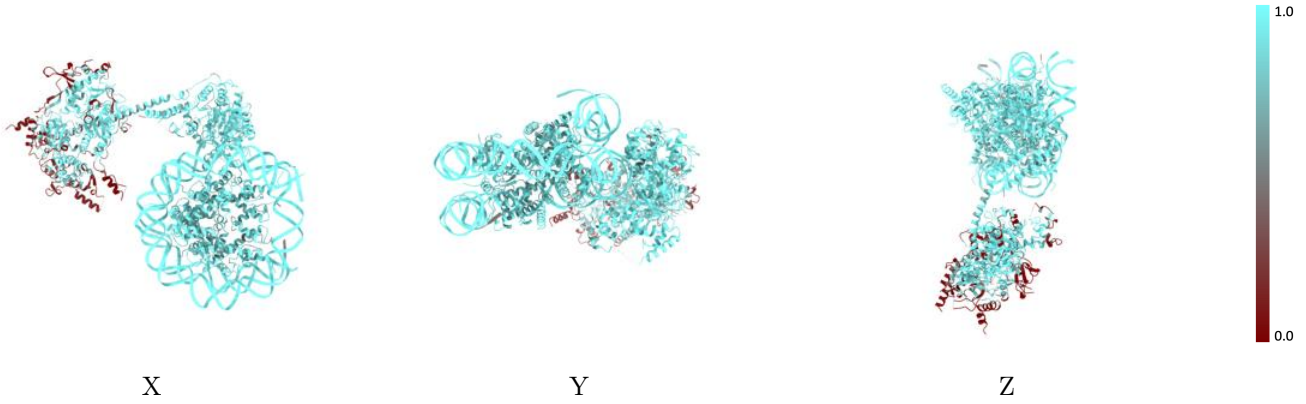
This section was not generated.

9.2 Q-score mapped to coordinate model



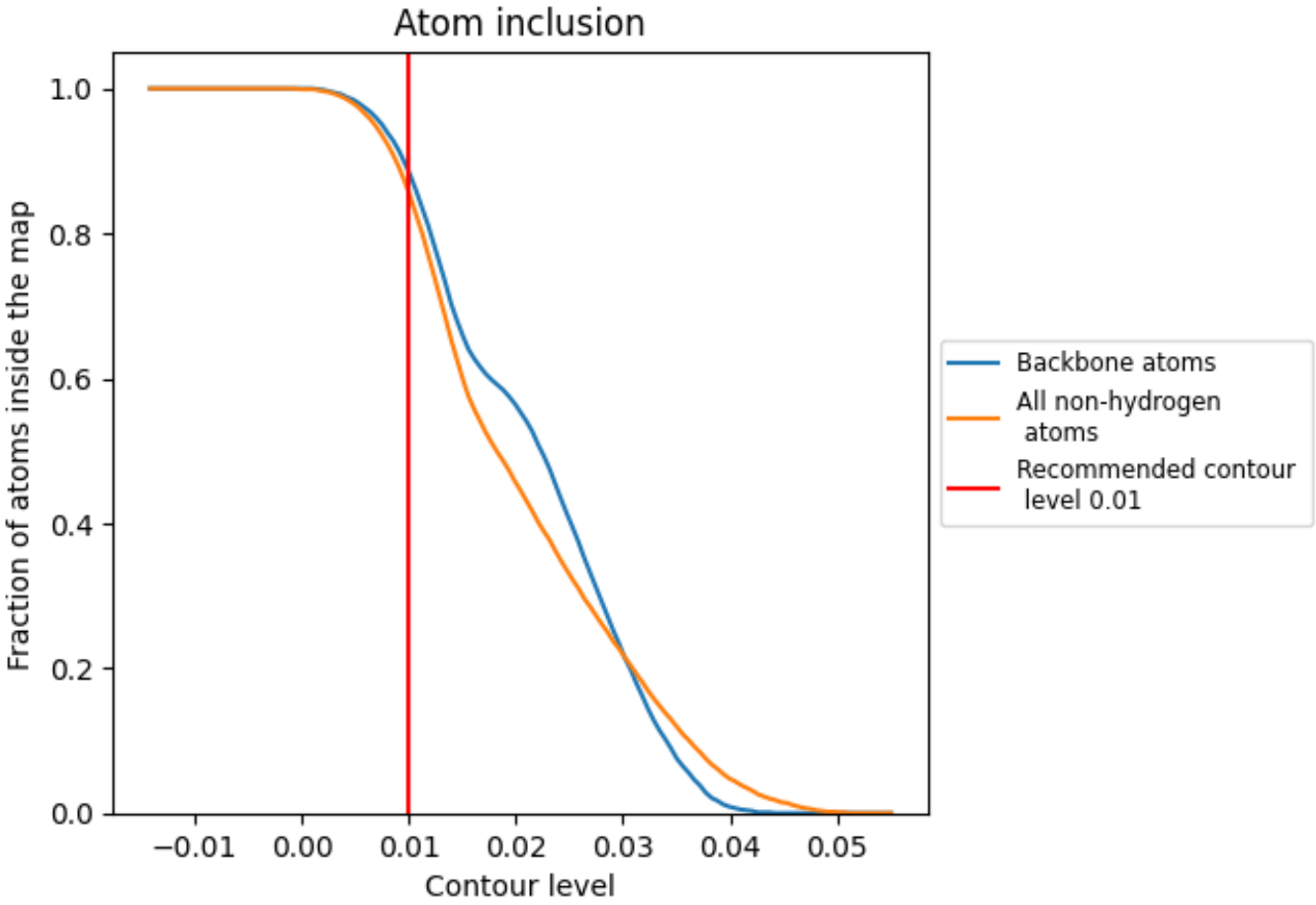
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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 (0.01).

9.4 Atom inclusion (i)



At the recommended contour level, 89% of all backbone atoms, 86% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8580	0.2190
A	0.9150	0.3120
B	0.9170	0.3220
C	0.8930	0.3230
D	0.9330	0.3190
E	0.9120	0.3180
F	0.9140	0.3260
G	0.9100	0.3240
H	0.9300	0.3200
I	0.9930	0.3280
J	0.9910	0.3260
K	0.9210	0.2080
L	0.5700	0.0480
M	0.7540	0.0420
N	0.4050	0.0380