



Full wwPDB EM Validation Report ⓘ

Nov 7, 2022 – 02:11 PM JST

PDB ID : 5X0Y
EMDB ID : EMD-6700
Title : Complex of Snf2-Nucleosome complex with Snf2 bound to SHL2 of the nucleosome
Authors : Li, M.; Liu, X.; Xia, X.; Chen, Z.; Li, X.
Deposited on : 2017-01-23
Resolution : 4.69 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

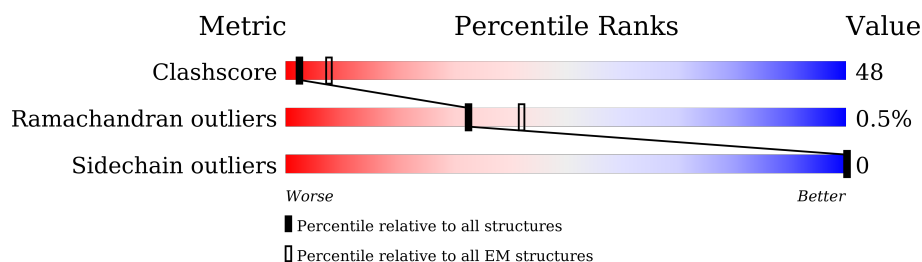
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.69 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	135	<div> <div>22%</div> <div>30%</div> <div>42%</div> <div>27%</div> </div>
1	E	135	<div> <div>19%</div> <div>33%</div> <div>36%</div> <div>30%</div> </div>
2	B	102	<div> <div>25%</div> <div>33%</div> <div>51%</div> <div>15%</div> </div>
2	F	102	<div> <div>23%</div> <div>46%</div> <div>38%</div> <div>16%</div> </div>
3	C	129	<div> <div>35%</div> <div>40%</div> <div>42%</div> <div>17%</div> </div>
3	G	129	<div> <div>23%</div> <div>43%</div> <div>40%</div> <div>17%</div> </div>
4	D	122	<div> <div>17%</div> <div>46%</div> <div>30%</div> <div>24%</div> </div>
4	H	122	<div> <div>7%</div> <div>41%</div> <div>35%</div> <div>24%</div> </div>

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Mol	Chain	Length	Quality of chain
5	I	167	<div><div><div></div><div></div><div></div></div><div><div>10%</div><div>9%</div><div>75%</div><div>13%</div></div></div>
6	J	167	<div><div><div></div><div></div><div></div></div><div><div>11%</div><div>5%</div><div>79%</div><div>13%</div></div></div>
7	O	735	<div><div><div></div><div></div><div></div></div><div><div>41%</div><div>18%</div><div>61%</div><div>21%</div></div></div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 16798 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 H3.2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	98	Total	C	N	O	S	0	0
			800	505	153	139	3		
1	E	95	Total	C	N	O	S	0	0
			778	491	148	136	3		

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	87	Total	C	N	O	S	0	0
			703	443	142	117	1		
2	F	86	Total	C	N	O	S	0	0
			672	424	130	117	1		

- Molecule 3 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	107	Total	C	N	O	0	0
			811	510	158	143		
3	G	107	Total	C	N	O	0	0
			815	513	159	143		

- Molecule 4 is a protein called Histone H2B 1.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	93	Total	C	N	O	S	0	0
			718	451	128	137	2		
4	H	93	Total	C	N	O	S	0	0
			726	457	130	137	2		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	29	THR	SER	see sequence details	UNP P02281

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Chain	Residue	Modelled	Actual	Comment	Reference
H	29	THR	SER	see sequence details	UNP P02281

- Molecule 5 is a DNA chain called DNA (167-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	146	Total	C	N	O	P	0	0
			2975	1413	540	876	146		

- Molecule 6 is a DNA chain called DNA (167-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	146	Total	C	N	O	P	0	0
			3011	1425	564	876	146		

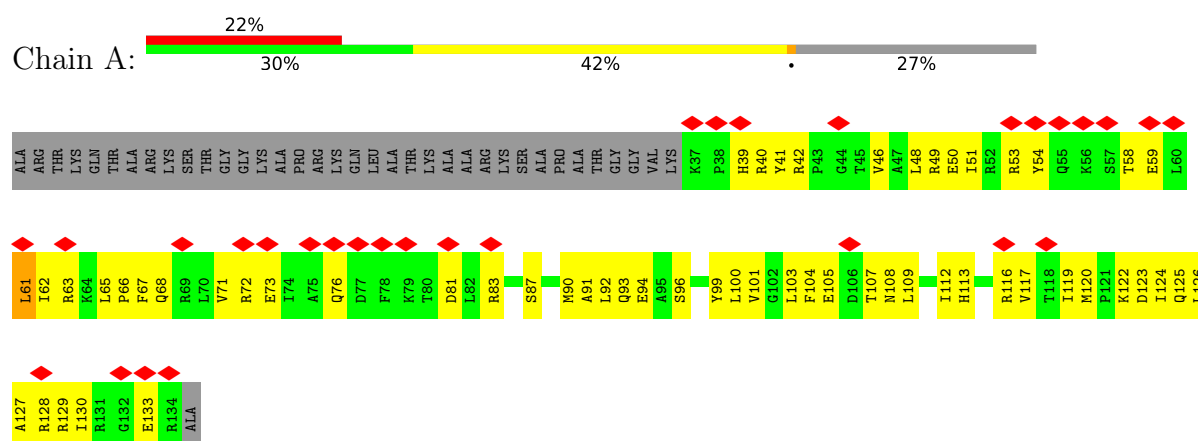
- Molecule 7 is a protein called Transcription regulatory protein SNF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	O	583	Total	C	N	O	S	0	0
			4789	3045	846	881	17		

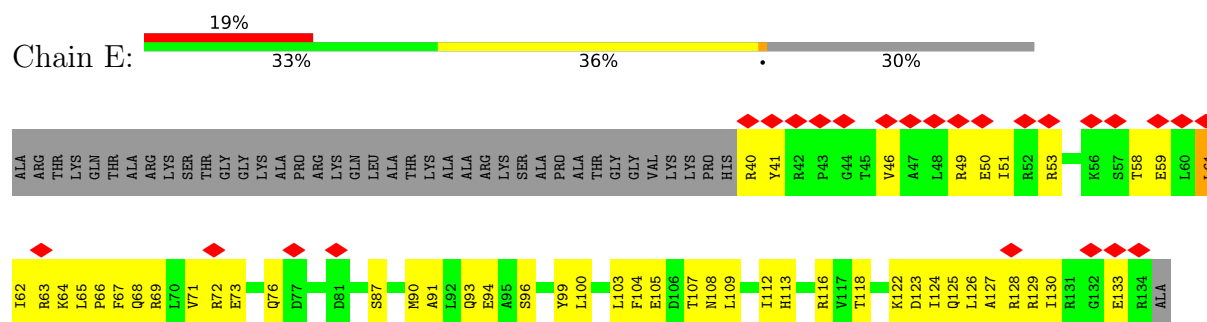
3 Residue-property plots [i](#)

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.

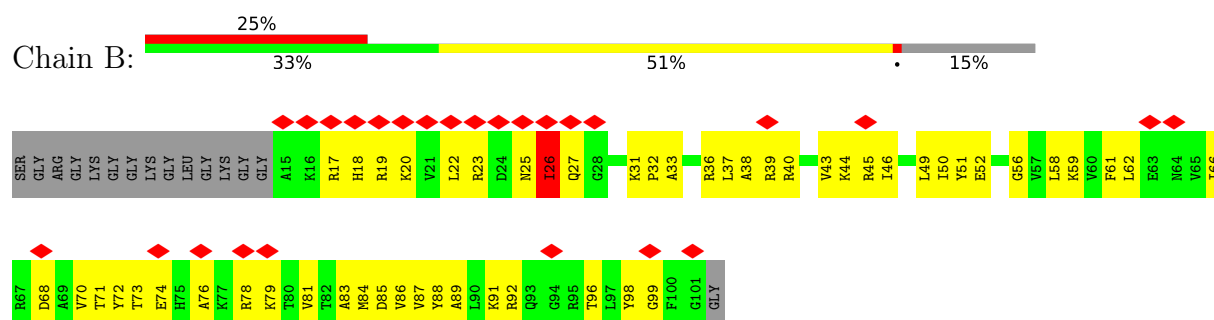
• Molecule 1: Histone H3.2



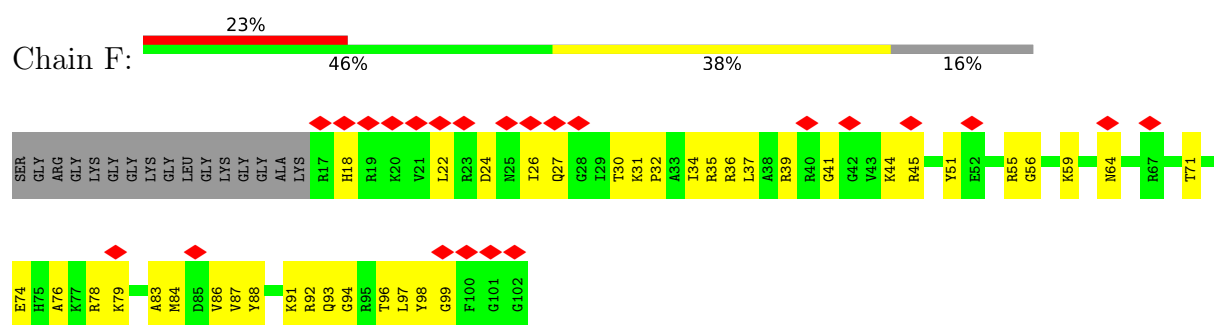
• Molecule 1: Histone H3.2



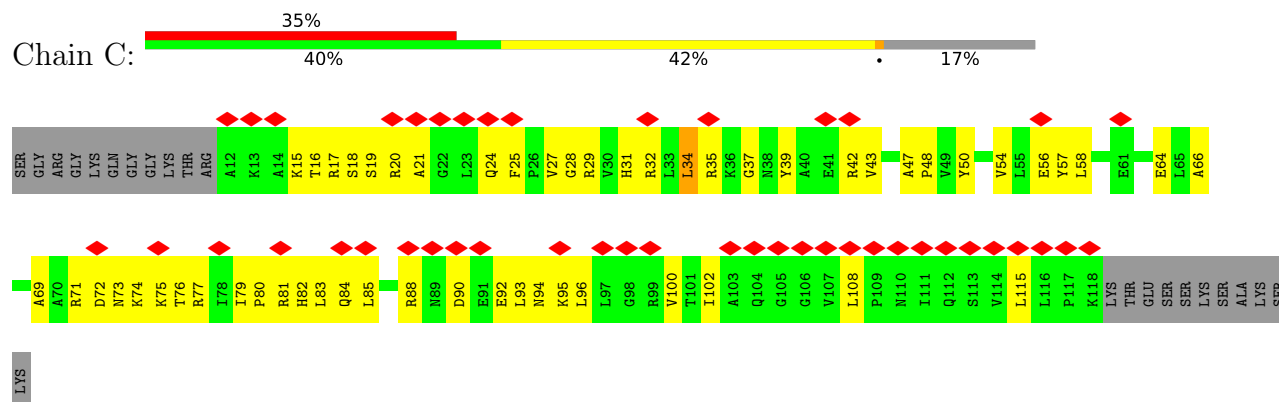
• Molecule 2: Histone H4



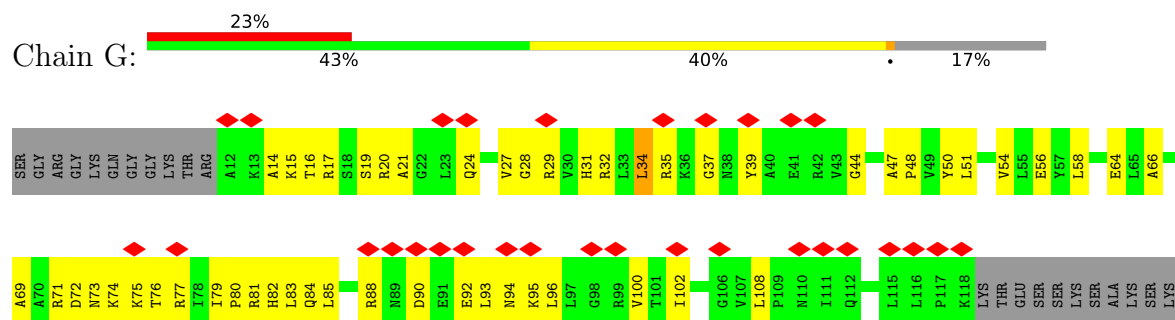
• Molecule 2: Histone H4



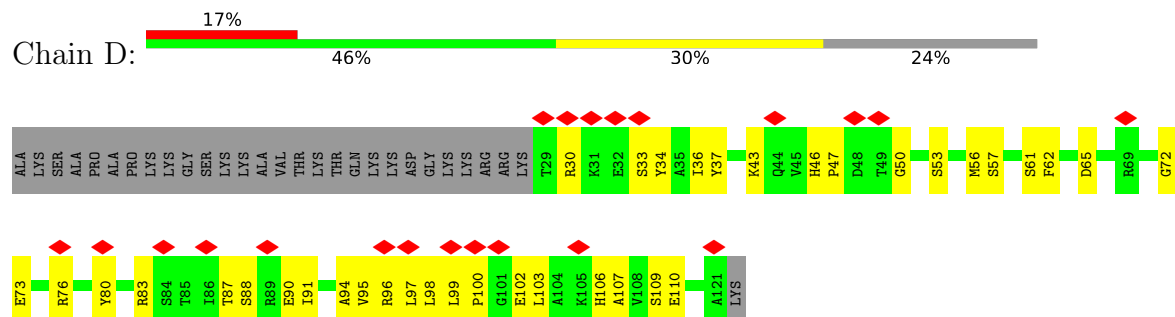
- Molecule 3: Histone H2A



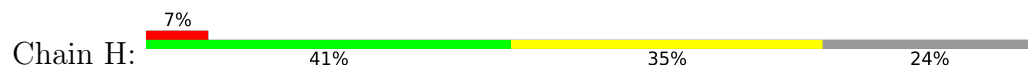
- Molecule 3: Histone H2A

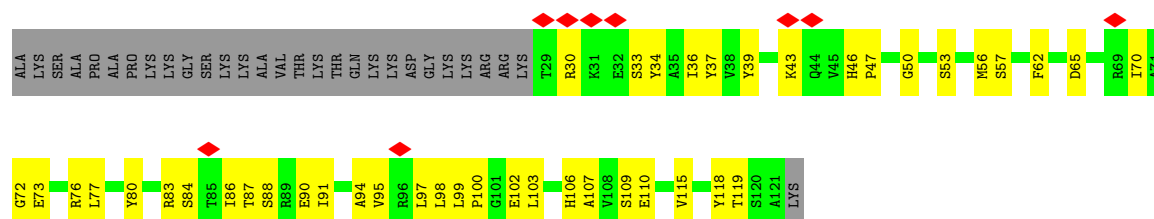


- Molecule 4: Histone H2B 1.1

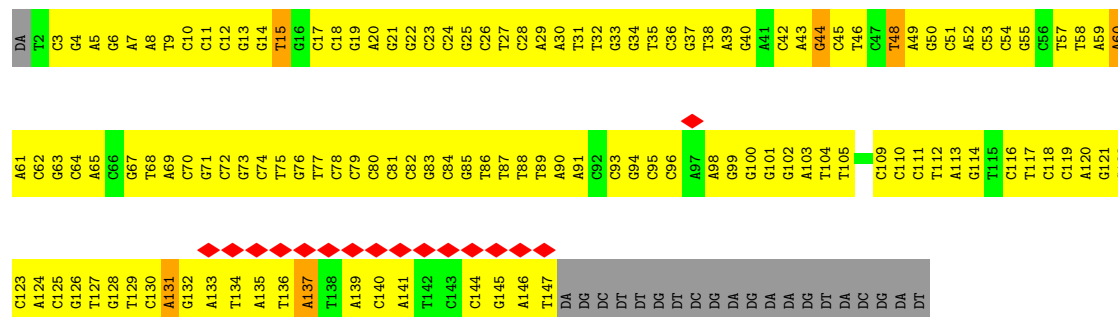
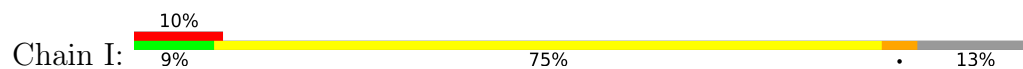


- Molecule 4: Histone H2B 1.1

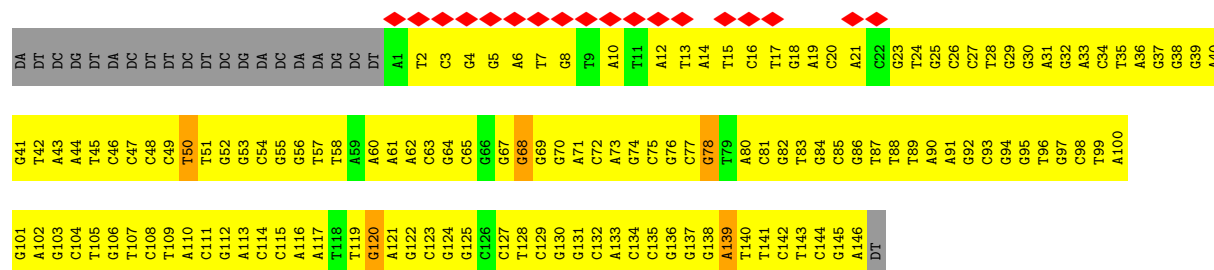
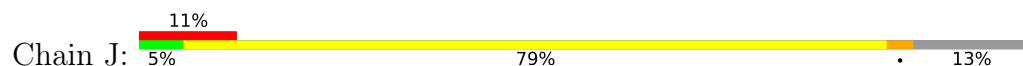




• Molecule 5: DNA (167-MER)



• Molecule 6: DNA (167-MER)



• Molecule 7: Transcription regulatory protein SNF2





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	90725	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	22500	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.093	Depositor
Minimum map value	-0.039	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0341	Depositor
Map size (Å)	337.92, 337.92, 337.92	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.32, 1.32, 1.32	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.57	0/812	0.67	1/1091 (0.1%)
1	E	0.57	0/788	0.67	1/1057 (0.1%)
2	B	0.62	0/711	0.68	0/950
2	F	0.62	0/680	0.66	0/912
3	C	0.49	0/821	0.63	1/1112 (0.1%)
3	G	0.48	0/825	0.64	1/1116 (0.1%)
4	D	0.59	0/729	0.61	0/985
4	H	0.59	0/737	0.62	0/993
5	I	1.34	0/3333	1.11	6/5137 (0.1%)
6	J	1.36	1/3381 (0.0%)	1.04	4/5221 (0.1%)
7	O	0.45	0/4864	0.65	2/6536 (0.0%)
All	All	0.93	1/17681 (0.0%)	0.85	16/25110 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	E	0	1
2	B	0	1
7	O	0	5
All	All	0	8

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	J	68	DG	C3'-O3'	-5.87	1.36	1.44

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	J	120	DG	O4'-C4'-C3'	-7.85	101.29	106.00
5	I	15	DT	O4'-C4'-C3'	-7.37	101.55	104.50
5	I	48	DT	O4'-C4'-C3'	-7.21	101.61	104.50
5	I	60	DA	O4'-C1'-N9	6.42	112.50	108.00
5	I	44	DG	O4'-C4'-C3'	-6.09	102.06	104.50
7	O	959	PRO	N-CA-CB	5.90	110.38	103.30
1	A	61	LEU	CA-CB-CG	-5.76	102.05	115.30
1	E	61	LEU	CA-CB-CG	-5.75	102.07	115.30
6	J	50	DT	O4'-C4'-C3'	-5.62	102.25	104.50
5	I	137	DA	O4'-C4'-C3'	-5.57	102.27	104.50
6	J	139	DA	O4'-C4'-C3'	-5.24	102.41	104.50
3	G	34	LEU	CA-CB-CG	-5.23	103.28	115.30
3	C	34	LEU	CA-CB-CG	-5.21	103.32	115.30
6	J	78	DG	O4'-C4'-C3'	-5.20	102.42	104.50
5	I	131	DA	O4'-C1'-N9	-5.09	104.43	108.00
7	O	1185	TRP	C-N-CA	5.07	134.37	121.70

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	58	THR	Peptide
2	B	26	ILE	Peptide
1	E	58	THR	Peptide
7	O	1046	ARG	Peptide
7	O	768	LYS	Peptide
7	O	839	ALA	Peptide
7	O	931	LEU	Peptide
7	O	976	THR	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	A	800	0	829	60	0
1	E	778	0	813	45	0
2	B	703	0	757	74	0
2	F	672	0	698	44	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	811	0	849	62	0
3	G	815	0	860	51	0
4	D	718	0	725	53	0
4	H	726	0	747	45	0
5	I	2975	0	1639	262	0
6	J	3011	0	1639	309	0
7	O	4789	0	4882	638	0
All	All	16798	0	14438	1477	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 48.

All (1477) 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:O:1233:GLY:O	7:O:1237:GLN:HB2	1.22	1.32
7:O:876:ILE:O	7:O:880:ARG:HB2	1.41	1.17
7:O:1232:ASP:O	7:O:1236:ILE:HB	1.42	1.16
7:O:1301:ASP:O	7:O:1305:SER:HB2	1.60	1.02
5:I:111:DC:O2	6:J:37:DG:N2	1.93	1.01
7:O:807:THR:O	7:O:811:GLU:HB2	1.62	0.99
2:B:71:THR:O	2:B:74:GLU:HB2	1.61	0.98
7:O:1340:SER:O	7:O:1344:ALA:HB2	1.62	0.98
5:I:111:DC:N3	6:J:37:DG:N1	2.14	0.96
5:I:60:DA:N6	6:J:87:DT:O4	1.99	0.95
5:I:28:DC:N4	6:J:119:DT:C4	2.36	0.94
7:O:1129:LYS:HD3	7:O:1155:GLU:HB3	1.51	0.93
7:O:1222:LEU:O	7:O:1226:TYR:HB3	1.68	0.93
5:I:10:DC:N3	6:J:138:DG:N1	2.16	0.93
7:O:977:LEU:O	7:O:981:ARG:HB2	1.68	0.92
7:O:1339:GLU:O	7:O:1343:ALA:HB3	1.69	0.91
7:O:1055:LEU:HB3	7:O:1217:VAL:HG11	1.52	0.91
7:O:1222:LEU:O	7:O:1226:TYR:CB	2.19	0.91
7:O:1233:GLY:O	7:O:1237:GLN:CB	2.17	0.89
7:O:945:ILE:O	7:O:949:VAL:HB	1.69	0.89
7:O:978:LEU:O	7:O:982:ARG:HB2	1.70	0.89
7:O:1018:LEU:HA	7:O:1022:MET:HB2	1.53	0.89
2:F:51:TYR:HB3	2:F:55:ARG:HH12	1.34	0.88
7:O:1055:LEU:O	7:O:1059:CYS:HB2	1.72	0.88
7:O:1173:GLN:NE2	7:O:1199:ARG:O	2.06	0.88
7:O:744:TYR:HE1	7:O:944:LYS:HZ1	1.18	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:1255:ARG:O	7:O:1259:ASP:HB2	1.75	0.87
7:O:1004:PRO:HG3	7:O:1203:LYS:HA	1.58	0.86
7:O:1207:ARG:HH12	7:O:1287:LEU:HA	1.39	0.86
7:O:897:HIS:O	7:O:900:LYS:HB3	1.74	0.86
7:O:1228:LYS:HA	7:O:1231:ILE:HB	1.57	0.86
1:E:68:GLN:HE21	1:E:72:ARG:HE	1.24	0.86
7:O:1013:CYS:HB2	7:O:1213:THR:HG22	1.59	0.85
7:O:1105:ARG:NH2	7:O:1149:PHE:O	2.09	0.85
7:O:858:GLN:NE2	7:O:879:GLU:OE2	2.10	0.85
7:O:771:GLN:HA	7:O:994:ARG:HH12	1.40	0.85
7:O:1051:GLN:HA	7:O:1055:LEU:HD12	1.60	0.84
7:O:791:ALA:O	7:O:993:ARG:NH1	2.11	0.84
5:I:10:DC:O2	6:J:138:DG:N2	2.10	0.84
7:O:895:GLU:OE2	7:O:897:HIS:NE2	2.11	0.83
4:D:65:ASP:OD2	2:F:98:TYR:OH	1.96	0.83
1:A:68:GLN:HE21	1:A:72:ARG:HE	1.23	0.83
7:O:1299:ARG:HA	7:O:1302:GLU:HG2	1.60	0.82
7:O:832:SER:HA	7:O:835:PHE:HD2	1.44	0.82
6:J:90:DA:H1'	6:J:91:DA:C8	2.16	0.81
7:O:949:VAL:HA	7:O:952:PHE:HB2	1.61	0.81
7:O:1026:MET:HG2	7:O:1029:TYR:HD2	1.45	0.81
5:I:28:DC:N4	6:J:119:DT:N3	2.29	0.80
7:O:1223:GLU:HA	7:O:1226:TYR:HB3	1.62	0.80
7:O:1020:GLN:O	7:O:1024:GLN:N	2.14	0.80
7:O:1109:PHE:HB3	7:O:1163:THR:HG22	1.64	0.80
5:I:111:DC:C2	6:J:37:DG:N2	2.50	0.79
7:O:931:LEU:HD22	7:O:934:LEU:HG	1.64	0.79
7:O:1301:ASP:O	7:O:1305:SER:CB	2.30	0.79
7:O:1084:ARG:HH21	7:O:1315:SER:HB2	1.46	0.79
7:O:810:TYR:CD1	7:O:816:ARG:HA	2.19	0.78
7:O:1022:MET:O	7:O:1026:MET:N	2.15	0.78
7:O:1116:MET:O	7:O:1119:MET:HB3	1.84	0.78
7:O:1081:ASP:HA	7:O:1084:ARG:HB2	1.66	0.78
7:O:1113:THR:HG22	7:O:1132:ARG:HH21	1.49	0.77
7:O:1063:PHE:HB2	7:O:1066:GLU:HA	1.67	0.77
7:O:1340:SER:O	7:O:1344:ALA:CB	2.32	0.77
7:O:1028:LYS:O	7:O:1032:LEU:N	2.17	0.77
7:O:1055:LEU:HD13	7:O:1217:VAL:HG21	1.65	0.77
7:O:929:ASN:HD21	7:O:1232:ASP:HA	1.49	0.77
7:O:744:TYR:O	7:O:748:ALA:N	2.12	0.77
7:O:1069:GLU:O	7:O:1073:ASN:N	2.18	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:1135:GLY:O	7:O:1142:ARG:NH2	2.18	0.76
5:I:85:DG:H2'	5:I:86:DT:H71	1.67	0.76
1:A:63:ARG:NH2	6:J:61:DA:OP1	2.19	0.76
2:F:51:TYR:HB3	2:F:55:ARG:NH1	2.01	0.76
7:O:939:ASN:HB3	7:O:946:PHE:HB3	1.65	0.76
7:O:1168:LEU:O	7:O:1196:ARG:NH2	2.19	0.76
3:G:77:ARG:HH21	5:I:20:DA:H4'	1.50	0.75
7:O:843:ARG:HH12	7:O:865:GLU:HB3	1.51	0.75
7:O:671:LEU:HB3	7:O:955:TRP:CH2	2.22	0.75
4:D:53:SER:N	6:J:20:DC:OP1	2.19	0.74
7:O:1212:ILE:HG13	7:O:1222:LEU:HD22	1.68	0.74
7:O:1226:TYR:O	7:O:1264:ARG:NH1	2.20	0.74
7:O:807:THR:O	7:O:811:GLU:CB	2.35	0.74
7:O:952:PHE:HA	7:O:955:TRP:HB2	1.68	0.74
7:O:1212:ILE:HG23	7:O:1218:GLU:HG3	1.69	0.74
5:I:7:DA:H1'	5:I:8:DA:H5'	1.68	0.74
7:O:1023:TYR:HA	7:O:1026:MET:HB2	1.69	0.74
7:O:1255:ARG:HA	7:O:1258:LEU:HG	1.69	0.74
7:O:845:ILE:O	7:O:870:LEU:N	2.20	0.73
7:O:1173:GLN:HE22	7:O:1200:ILE:C	1.91	0.73
1:E:64:LYS:N	6:J:92:DG:OP1	2.19	0.73
5:I:118:DC:H2''	5:I:119:DC:C5	2.24	0.73
7:O:771:GLN:NE2	7:O:796:LEU:O	2.21	0.73
7:O:882:LEU:HD12	7:O:885:LYS:HD2	1.68	0.73
7:O:997:LYS:HA	7:O:1001:LYS:HA	1.70	0.73
7:O:1015:MET:HB2	7:O:1020:GLN:HG3	1.69	0.73
7:O:1099:LEU:O	7:O:1103:GLY:N	2.21	0.73
2:B:45:ARG:HE	5:I:81:DC:H4'	1.54	0.72
7:O:1105:ARG:N	7:O:1176:ASP:OD1	2.21	0.72
7:O:672:ASP:OD2	7:O:982:ARG:NH2	2.22	0.72
7:O:1062:PRO:HG3	7:O:1085:VAL:HG11	1.71	0.72
6:J:58:DT:OP1	7:O:878:LYS:NZ	2.23	0.72
7:O:1026:MET:O	7:O:1030:ARG:HG3	1.89	0.72
2:F:45:ARG:HG3	6:J:82:DG:H5''	1.72	0.72
7:O:891:MET:O	7:O:919:ARG:HA	1.89	0.72
7:O:1230:ASP:OD2	7:O:1264:ARG:NE	2.19	0.72
5:I:28:DC:H4'	5:I:29:DA:H5'	1.70	0.72
7:O:672:ASP:HA	7:O:675:LYS:HD2	1.70	0.71
7:O:1218:GLU:O	7:O:1222:LEU:CB	2.37	0.71
3:C:16:THR:HA	6:J:31:DA:H5''	1.71	0.71
7:O:938:LEU:HG	7:O:945:ILE:HG21	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:1309:GLU:OE2	7:O:1314:LYS:N	2.22	0.71
7:O:686:THR:HA	7:O:689:PHE:HD2	1.53	0.71
7:O:1113:THR:HG21	7:O:1134:ASP:HB3	1.73	0.71
5:I:10:DC:N4	6:J:138:DG:O6	2.17	0.71
7:O:891:MET:HB3	7:O:919:ARG:HG2	1.71	0.71
4:H:102:GLU:OE1	4:H:106:HIS:NE2	2.24	0.71
7:O:1017:ALA:O	7:O:1022:MET:N	2.24	0.71
7:O:1151:ALA:HB3	7:O:1154:SER:HB2	1.72	0.71
7:O:1207:ARG:HB3	7:O:1209:LEU:HD21	1.72	0.71
7:O:754:ASP:HB3	7:O:776:GLN:HE21	1.55	0.71
7:O:1218:GLU:O	7:O:1222:LEU:HB2	1.91	0.71
4:D:102:GLU:OE1	4:D:106:HIS:NE2	2.24	0.70
5:I:44:DG:H2'	5:I:45:DC:C6	2.25	0.70
7:O:953:ASP:O	7:O:957:ASN:CB	2.39	0.70
7:O:761:ILE:HD11	7:O:807:THR:HB	1.73	0.70
7:O:1083:TRP:HA	7:O:1089:PHE:HB3	1.73	0.70
7:O:1003:LEU:HD12	7:O:1004:PRO:HD2	1.73	0.70
7:O:1232:ASP:O	7:O:1236:ILE:CB	2.33	0.70
3:G:16:THR:HA	5:I:31:DT:H5''	1.73	0.70
5:I:121:DG:H1'	5:I:122:DG:C8	2.26	0.70
7:O:1226:TYR:HD1	7:O:1229:LEU:HD12	1.57	0.70
7:O:1081:ASP:HB3	7:O:1318:LEU:HD21	1.74	0.69
4:D:103:LEU:O	4:D:107:ALA:HB3	1.92	0.69
7:O:919:ARG:HH12	7:O:941:VAL:HA	1.57	0.69
7:O:931:LEU:N	7:O:933:GLU:OE1	2.26	0.69
7:O:1026:MET:HA	7:O:1029:TYR:HB2	1.73	0.69
7:O:1092:LEU:HD23	7:O:1095:ILE:HD11	1.74	0.69
5:I:96:DC:OP2	7:O:901:ASN:ND2	2.23	0.69
2:B:18:HIS:HB3	7:O:1076:ARG:HH21	1.56	0.69
4:D:90:GLU:OE1	4:D:90:GLU:N	2.24	0.69
4:D:103:LEU:O	4:D:107:ALA:CB	2.41	0.69
4:H:103:LEU:O	4:H:107:ALA:HB3	1.92	0.69
7:O:1019:GLN:HE22	7:O:1086:ALA:HB2	1.58	0.69
4:H:103:LEU:O	4:H:107:ALA:CB	2.41	0.69
7:O:1016:SER:O	7:O:1020:GLN:N	2.25	0.69
3:C:90:ASP:OD2	3:C:93:LEU:N	2.20	0.69
2:B:68:ASP:O	2:B:71:THR:HB	1.93	0.68
5:I:99:DG:OP1	7:O:1051:GLN:NE2	2.26	0.68
7:O:1222:LEU:O	7:O:1226:TYR:HB2	1.92	0.68
5:I:87:DT:H2''	5:I:88:DT:H73	1.76	0.68
7:O:982:ARG:HA	7:O:985:LYS:HB3	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:32:ARG:NE	6:J:30:DG:OP1	2.25	0.68
6:J:120:DG:H1'	6:J:121:DA:N7	2.09	0.68
7:O:967:ASP:O	7:O:971:LEU:N	2.27	0.68
2:B:88:TYR:O	2:B:91:LYS:N	2.27	0.67
6:J:44:DA:H2'	6:J:45:DT:C6	2.29	0.67
3:G:92:GLU:HB3	4:H:103:LEU:HD11	1.75	0.67
7:O:1232:ASP:OD1	7:O:1233:GLY:N	2.26	0.67
7:O:952:PHE:HB3	7:O:956:PHE:CD2	2.29	0.67
3:G:32:ARG:HA	3:G:35:ARG:HH21	1.59	0.67
7:O:832:SER:HA	7:O:835:PHE:CD2	2.28	0.67
3:C:92:GLU:HB3	4:D:103:LEU:HD11	1.74	0.67
6:J:27:DC:H1'	6:J:28:DT:C2	2.29	0.67
7:O:969:ILE:HA	7:O:973:GLU:HB3	1.77	0.67
2:B:17:ARG:NH1	7:O:1121:ASP:OD2	2.20	0.67
2:B:70:VAL:O	2:B:74:GLU:N	2.24	0.67
5:I:102:DG:H2''	5:I:103:DA:H8	1.60	0.67
7:O:1063:PHE:HB3	7:O:1068:VAL:HB	1.77	0.67
7:O:1095:ILE:HG13	7:O:1096:LEU:H	1.59	0.67
3:C:16:THR:O	3:C:19:SER:OG	2.10	0.67
7:O:771:GLN:HG2	7:O:801:GLN:HE21	1.60	0.67
5:I:59:DA:H61	6:J:88:DT:H3	1.40	0.67
3:G:90:ASP:OD2	3:G:93:LEU:N	2.20	0.66
5:I:111:DC:H2'	5:I:112:DT:H6	1.60	0.66
7:O:671:LEU:O	7:O:674:THR:OG1	2.14	0.66
7:O:780:SER:OG	7:O:784:ASN:ND2	2.27	0.66
3:G:17:ARG:HH21	3:G:28:GLY:HA2	1.61	0.66
6:J:104:DC:H2'	6:J:105:DT:H71	1.77	0.66
3:C:32:ARG:HA	3:C:35:ARG:HH21	1.59	0.66
7:O:1007:VAL:HG13	7:O:1207:ARG:HD3	1.77	0.66
7:O:1057:LYS:HB3	7:O:1064:VAL:HG11	1.77	0.66
7:O:1081:ASP:OD1	7:O:1084:ARG:HD3	1.93	0.66
1:A:42:ARG:NH2	6:J:69:DG:OP1	2.28	0.66
7:O:910:LEU:HA	7:O:913:HIS:HB3	1.77	0.66
1:A:39:HIS:HE1	1:A:41:TYR:CZ	2.13	0.66
2:F:26:ILE:HD11	2:F:55:ARG:HB3	1.78	0.66
6:J:99:DT:H4'	6:J:100:DA:H5'	1.77	0.66
7:O:676:ASP:HA	7:O:679:ILE:HD12	1.77	0.66
5:I:71:DG:H5'	5:I:71:DG:C8	2.32	0.65
6:J:49:DC:H2''	6:J:50:DT:H73	1.78	0.65
6:J:113:DA:H5'	6:J:113:DA:H8	1.61	0.65
7:O:1046:ARG:HB3	7:O:1048:PHE:HB2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:17:ARG:HH21	3:C:28:GLY:HA2	1.61	0.65
2:F:79:LYS:HG3	6:J:101:DG:H3'	1.79	0.65
6:J:18:DG:H1'	6:J:19:DA:C8	2.32	0.65
5:I:82:DC:H1'	5:I:83:DG:H5'	1.79	0.65
7:O:1265:ARG:O	7:O:1268:ARG:HG2	1.96	0.65
3:C:100:VAL:HG11	2:F:98:TYR:CE2	2.30	0.65
6:J:71:DA:H2''	6:J:72:DC:H2'	1.79	0.65
7:O:1215:ASN:N	7:O:1219:GLU:OE2	2.29	0.65
7:O:1289:ARG:N	7:O:1293:GLU:OE1	2.23	0.65
7:O:785:HIS:ND1	7:O:918:TYR:OH	2.30	0.65
7:O:1014:LYS:HB3	7:O:1317:LEU:HD11	1.78	0.65
7:O:1253:LEU:HA	7:O:1256:SER:HB2	1.79	0.65
7:O:1345:VAL:HG12	7:O:1349:ARG:HH22	1.61	0.65
1:A:124:ILE:HD11	2:B:50:ILE:HG23	1.78	0.65
3:C:15:LYS:N	6:J:32:DG:OP1	2.30	0.65
3:C:100:VAL:HG22	2:F:96:THR:HB	1.78	0.65
4:H:90:GLU:OE1	4:H:90:GLU:N	2.24	0.65
5:I:44:DG:H2'	5:I:45:DC:H6	1.60	0.65
5:I:68:DT:H4'	5:I:69:DA:H5'	1.79	0.64
7:O:968:LYS:O	7:O:973:GLU:N	2.27	0.64
7:O:1171:ASN:HD21	7:O:1173:GLN:NE2	1.96	0.64
7:O:1223:GLU:O	7:O:1227:LYS:HG3	1.97	0.64
1:E:40:ARG:HG2	6:J:84:DG:H5'	1.78	0.64
2:F:36:ARG:NH1	5:I:61:DA:OP1	2.30	0.64
6:J:53:DG:H5'	7:O:1112:MET:HA	1.79	0.64
7:O:1105:ARG:HB2	7:O:1175:ALA:HA	1.77	0.64
7:O:1247:SER:O	7:O:1250:GLN:HG2	1.97	0.64
7:O:679:ILE:HG12	7:O:744:TYR:CE2	2.31	0.64
7:O:844:THR:HA	7:O:868:VAL:HB	1.78	0.64
7:O:1207:ARG:HG2	7:O:1289:ARG:HH21	1.62	0.64
3:G:16:THR:O	3:G:19:SER:OG	2.10	0.64
5:I:146:DA:H2'	5:I:147:DT:H71	1.79	0.64
7:O:747:VAL:HA	7:O:750:ARG:HG3	1.80	0.64
7:O:880:ARG:HH22	7:O:912:THR:HG21	1.62	0.64
7:O:935:TRP:HH2	7:O:953:ASP:HA	1.62	0.64
7:O:1255:ARG:HG2	7:O:1258:LEU:HD11	1.79	0.64
7:O:988:ARG:HE	7:O:1241:PHE:HE1	1.46	0.64
7:O:975:GLU:N	7:O:975:GLU:OE1	2.29	0.64
7:O:1251:GLU:HA	7:O:1254:LEU:HG	1.79	0.64
7:O:1175:ALA:O	7:O:1202:GLN:NE2	2.31	0.64
2:B:18:HIS:NE2	7:O:1076:ARG:O	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:38:DT:H2''	5:I:39:DA:N7	2.13	0.64
7:O:985:LYS:HA	7:O:988:ARG:HG3	1.80	0.64
5:I:125:DC:H2''	5:I:126:DG:H8	1.62	0.63
7:O:1090:GLU:OE2	7:O:1094:ARG:NE	2.18	0.63
7:O:1168:LEU:HG	7:O:1169:GLY:H	1.63	0.63
7:O:1012:LYS:HA	7:O:1212:ILE:O	1.97	0.63
4:D:30:ARG:HB3	5:I:124:DA:H5''	1.80	0.63
5:I:37:DG:H2'	5:I:38:DT:H71	1.79	0.63
7:O:1301:ASP:OD1	7:O:1304:ARG:NH2	2.31	0.63
2:B:18:HIS:CG	7:O:1076:ARG:HD3	2.33	0.63
5:I:59:DA:H8	5:I:59:DA:OP2	1.81	0.63
1:A:50:GLU:O	1:A:53:ARG:N	2.32	0.63
1:E:50:GLU:O	1:E:53:ARG:N	2.32	0.63
6:J:113:DA:H5'	6:J:113:DA:C8	2.33	0.63
2:F:79:LYS:N	6:J:102:DA:OP1	2.29	0.63
7:O:1237:GLN:HE22	7:O:1257:LEU:N	1.96	0.63
7:O:686:THR:HA	7:O:689:PHE:CD2	2.34	0.63
7:O:1023:TYR:O	7:O:1027:LEU:N	2.32	0.63
6:J:34:DC:H2'	6:J:35:DT:H71	1.80	0.62
7:O:1062:PRO:HG2	7:O:1063:PHE:CE2	2.34	0.62
7:O:1198:HIS:HA	7:O:1202:GLN:HB3	1.80	0.62
7:O:1263:GLU:HA	7:O:1266:LYS:HD2	1.80	0.62
7:O:845:ILE:HG21	7:O:861:ILE:HD11	1.79	0.62
7:O:1025:GLN:NE2	7:O:1029:TYR:OH	2.32	0.62
7:O:1188:HIS:HA	7:O:1191:LEU:HD12	1.80	0.62
7:O:1337:ARG:O	7:O:1340:SER:OG	2.13	0.62
7:O:1237:GLN:HG3	7:O:1253:LEU:HD22	1.82	0.62
7:O:755:ILE:H	7:O:776:GLN:HG3	1.64	0.62
7:O:753:GLU:OE1	7:O:783:ASN:ND2	2.33	0.62
1:A:59:GLU:OE1	1:A:59:GLU:N	2.28	0.62
2:B:18:HIS:CE1	7:O:1076:ARG:HB2	2.35	0.62
5:I:34:DG:H3'	5:I:35:DT:H71	1.80	0.62
5:I:11:DC:N4	6:J:136:DG:O6	2.33	0.61
7:O:810:TYR:HD1	7:O:816:ARG:HA	1.64	0.61
7:O:1018:LEU:O	7:O:1023:TYR:N	2.33	0.61
7:O:768:LYS:N	7:O:771:GLN:OE1	2.29	0.61
7:O:928:GLN:HB2	7:O:933:GLU:OE2	2.00	0.61
7:O:743:ASP:OD1	7:O:744:TYR:N	2.33	0.61
7:O:794:MET:HA	7:O:798:LYS:NZ	2.15	0.61
5:I:42:DC:H2''	5:I:43:DA:C8	2.35	0.61
5:I:132:DG:N2	6:J:17:DT:O2	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:5:DG:H2''	6:J:6:DA:C8	2.36	0.61
6:J:69:DG:H2''	6:J:70:DG:C8	2.36	0.61
7:O:1112:MET:O	7:O:1114:GLN:N	2.33	0.61
7:O:1113:THR:HG23	7:O:1116:MET:SD	2.41	0.61
5:I:67:DG:H2'	5:I:68:DT:H71	1.83	0.61
6:J:141:DT:H2''	6:J:142:DC:C5	2.36	0.61
7:O:1080:ASP:OD2	7:O:1314:LYS:NZ	2.24	0.61
7:O:1164:ARG:HB2	7:O:1189:GLN:OE1	2.01	0.61
7:O:976:THR:HB	7:O:980:ILE:HB	1.82	0.61
6:J:135:DC:H2''	6:J:136:DG:C8	2.36	0.60
3:C:66:ALA:O	3:C:69:ALA:N	2.35	0.60
7:O:999:VAL:HG23	7:O:1000:GLU:H	1.65	0.60
5:I:18:DC:H2''	5:I:19:DG:N7	2.16	0.60
5:I:84:DC:H2''	5:I:85:DG:H8	1.67	0.60
7:O:1088:LYS:O	7:O:1092:LEU:HG	2.01	0.60
7:O:1117:ASP:OD1	7:O:1132:ARG:NH2	2.30	0.60
3:G:88:ARG:NH1	3:G:94:ASN:OD1	2.34	0.60
7:O:808:TYR:HA	7:O:811:GLU:HB3	1.83	0.60
3:G:66:ALA:O	3:G:69:ALA:N	2.35	0.60
7:O:1137:THR:O	7:O:1142:ARG:NE	2.34	0.60
3:C:93:LEU:O	3:C:96:LEU:N	2.35	0.60
5:I:84:DC:H2''	5:I:85:DG:C8	2.37	0.60
7:O:1088:LYS:HD3	7:O:1181:PHE:HD1	1.65	0.60
7:O:1105:ARG:HG2	7:O:1157:LEU:HA	1.83	0.60
1:A:113:HIS:NE2	1:E:123:ASP:OD1	2.35	0.60
2:F:30:THR:HB	2:F:32:PRO:HD2	1.84	0.60
6:J:27:DC:H2''	6:J:28:DT:C5	2.37	0.60
3:C:42:ARG:NH1	6:J:39:DG:H4'	2.17	0.60
4:D:57:SER:OG	2:F:99:GLY:O	2.18	0.60
3:G:88:ARG:HB3	3:G:108:LEU:HD11	1.84	0.60
2:B:25:ASN:C	2:B:27:GLN:H	2.05	0.60
4:H:115:VAL:O	4:H:119:THR:OG1	2.12	0.60
7:O:943:PRO:HA	7:O:946:PHE:CE2	2.36	0.60
7:O:1091:LEU:O	7:O:1094:ARG:N	2.32	0.60
3:C:42:ARG:HH21	5:I:112:DT:H4'	1.67	0.60
1:E:59:GLU:OE1	1:E:59:GLU:N	2.28	0.60
7:O:973:GLU:OE1	7:O:974:GLU:HG3	2.01	0.60
5:I:24:DC:H2''	5:I:25:DG:C8	2.37	0.59
7:O:1017:ALA:O	7:O:1021:ILE:N	2.35	0.59
7:O:1029:TYR:HD1	7:O:1032:LEU:HB2	1.67	0.59
3:G:93:LEU:O	3:G:96:LEU:N	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:1084:ARG:NH2	7:O:1317:LEU:O	2.35	0.59
7:O:1234:LYS:O	7:O:1237:GLN:HB3	2.01	0.59
2:B:62:LEU:HD22	2:B:66:ILE:HD11	1.85	0.59
3:C:88:ARG:NH1	3:C:94:ASN:OD1	2.34	0.59
7:O:931:LEU:HD23	7:O:933:GLU:HB2	1.84	0.59
7:O:983:LEU:O	7:O:986:VAL:HB	2.02	0.59
5:I:144:DC:H2''	5:I:145:DG:C8	2.37	0.59
6:J:139:DA:H2'	6:J:140:DT:C6	2.37	0.59
7:O:934:LEU:O	7:O:938:LEU:HB2	2.03	0.59
7:O:1283:ILE:HA	7:O:1286:ILE:HG12	1.85	0.59
7:O:771:GLN:HG2	7:O:801:GLN:NE2	2.18	0.59
7:O:888:TRP:HB3	7:O:916:ALA:HB2	1.85	0.59
7:O:935:TRP:CH2	7:O:953:ASP:HA	2.37	0.59
7:O:1098:LYS:NZ	7:O:1284:ASN:OD1	2.33	0.59
7:O:1278:LEU:HD11	7:O:1283:ILE:HG13	1.85	0.59
5:I:8:DA:H2'	5:I:9:DT:H71	1.85	0.59
5:I:36:DC:H2''	5:I:37:DG:C8	2.37	0.59
7:O:1173:GLN:O	7:O:1202:GLN:NE2	2.36	0.58
3:C:88:ARG:HB3	3:C:108:LEU:HD11	1.84	0.58
7:O:987:LEU:HA	7:O:990:PHE:HD2	1.69	0.58
5:I:99:DG:H2''	5:I:100:DG:OP2	2.03	0.58
7:O:1124:ARG:C	7:O:1127:ASN:H	2.06	0.58
7:O:1237:GLN:NE2	7:O:1253:LEU:O	2.35	0.58
2:B:73:THR:N	2:B:85:ASP:OD2	2.36	0.58
3:C:20:ARG:NH2	6:J:32:DG:OP1	2.29	0.58
5:I:88:DT:H2'	5:I:89:DT:H72	1.84	0.58
7:O:686:THR:HG21	7:O:942:LEU:HD13	1.85	0.58
7:O:1019:GLN:NE2	7:O:1085:VAL:HG22	2.18	0.58
7:O:1095:ILE:HG13	7:O:1096:LEU:N	2.18	0.58
1:A:124:ILE:O	1:A:127:ALA:N	2.37	0.58
6:J:47:DC:H1'	6:J:48:DC:C5	2.38	0.58
7:O:690:LEU:HD21	7:O:785:HIS:HB3	1.84	0.58
1:A:46:VAL:HG21	5:I:83:DG:H3'	1.85	0.58
4:D:62:PHE:HA	2:F:98:TYR:CE1	2.39	0.58
5:I:94:DG:H2'	5:I:95:DC:O4'	2.02	0.58
7:O:859:ALA:O	7:O:863:ALA:N	2.36	0.58
7:O:971:LEU:O	7:O:975:GLU:HB2	2.03	0.58
7:O:1010:VAL:HG12	7:O:1210:ARG:HB3	1.85	0.58
3:G:84:GLN:HA	3:G:102:ILE:HD12	1.86	0.58
7:O:682:LEU:O	7:O:686:THR:HG23	2.04	0.58
7:O:1144:GLU:OE2	7:O:1147:ARG:NH2	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:84:MET:O	2:B:87:VAL:N	2.36	0.58
3:C:29:ARG:NH2	5:I:123:DC:OP1	2.33	0.58
5:I:100:DG:H2''	5:I:101:DG:C8	2.39	0.58
7:O:951:SER:O	7:O:955:TRP:HD1	1.86	0.58
7:O:1009:LYS:HE2	7:O:1286:ILE:HD12	1.86	0.58
7:O:1028:LYS:HB3	7:O:1032:LEU:HD12	1.85	0.58
7:O:1108:ILE:HG12	7:O:1179:ILE:HB	1.85	0.58
7:O:1179:ILE:HG12	7:O:1209:LEU:HD12	1.86	0.58
7:O:1295:ALA:O	7:O:1298:THR:OG1	2.20	0.58
7:O:785:HIS:HA	7:O:918:TYR:HE1	1.69	0.58
1:A:40:ARG:HG2	5:I:84:DC:H5'	1.86	0.57
3:C:84:GLN:HA	3:C:102:ILE:HD12	1.86	0.57
6:J:61:DA:H1'	6:J:62:DA:H5'	1.86	0.57
6:J:87:DT:H3'	6:J:88:DT:H71	1.85	0.57
6:J:89:DT:H2''	6:J:90:DA:C8	2.39	0.57
7:O:771:GLN:O	7:O:775:LEU:HB2	2.04	0.57
7:O:802:THR:O	7:O:805:LEU:HB3	2.04	0.57
3:C:92:GLU:OE2	4:D:102:GLU:N	2.37	0.57
3:G:77:ARG:NH2	5:I:20:DA:H4'	2.18	0.57
5:I:132:DG:H1'	5:I:133:DA:N7	2.19	0.57
7:O:843:ARG:N	7:O:867:ASP:OD2	2.29	0.57
5:I:109:DC:H2''	5:I:110:DC:C5	2.39	0.57
5:I:134:DT:H2''	5:I:135:DA:H8	1.69	0.57
6:J:83:DT:H2''	6:J:84:DG:C8	2.38	0.57
7:O:858:GLN:HB3	7:O:862:ARG:NH1	2.19	0.57
7:O:1061:HIS:HE1	7:O:1088:LYS:HB2	1.69	0.57
1:E:124:ILE:O	1:E:127:ALA:N	2.37	0.57
3:G:76:THR:O	4:H:50:GLY:N	2.26	0.57
5:I:72:DC:H2''	5:I:73:DG:C8	2.40	0.57
7:O:1182:ASP:O	7:O:1210:ARG:NH1	2.36	0.57
1:A:65:LEU:O	1:A:68:GLN:N	2.38	0.57
1:E:65:LEU:O	1:E:68:GLN:N	2.37	0.57
7:O:944:LYS:O	7:O:948:SER:OG	2.11	0.57
7:O:1050:ASN:O	7:O:1054:GLN:N	2.37	0.57
1:A:63:ARG:HH21	6:J:61:DA:P	2.27	0.57
5:I:120:DA:H2''	5:I:121:DG:N7	2.20	0.57
7:O:792:ASP:HB2	7:O:798:LYS:HD3	1.86	0.57
5:I:144:DC:H2''	5:I:145:DG:H8	1.70	0.57
7:O:1124:ARG:O	7:O:1127:ASN:N	2.37	0.57
2:F:84:MET:HB3	2:F:88:TYR:HE2	1.69	0.57
5:I:111:DC:H2'	5:I:112:DT:C6	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:130:DG:H2''	6:J:131:DG:N7	2.19	0.57
7:O:913:HIS:O	7:O:913:HIS:ND1	2.38	0.57
6:J:120:DG:OP2	6:J:120:DG:H2'	2.05	0.56
7:O:1084:ARG:NH2	7:O:1315:SER:HB2	2.19	0.56
7:O:1120:GLU:OE2	7:O:1132:ARG:NH1	2.33	0.56
5:I:9:DT:H1'	5:I:10:DC:H5'	1.87	0.56
5:I:17:DC:H2''	5:I:18:DC:C5	2.39	0.56
6:J:145:DG:H2''	6:J:146:DA:C8	2.41	0.56
7:O:1131:LEU:HB2	7:O:1159:PHE:HD1	1.70	0.56
2:B:39:ARG:NH1	2:B:43:VAL:O	2.38	0.56
2:B:71:THR:HA	2:B:74:GLU:CD	2.25	0.56
3:C:17:ARG:NH2	3:C:28:GLY:HA2	2.20	0.56
3:G:15:LYS:HB3	3:G:20:ARG:NH2	2.20	0.56
6:J:35:DT:H2''	6:J:36:DA:C8	2.40	0.56
6:J:41:DG:H2'	6:J:42:DT:H71	1.87	0.56
6:J:105:DT:H2''	6:J:106:DG:N7	2.21	0.56
7:O:976:THR:HA	7:O:979:VAL:HB	1.87	0.56
7:O:983:LEU:O	7:O:987:LEU:HG	2.06	0.56
7:O:1255:ARG:O	7:O:1259:ASP:CB	2.51	0.56
3:C:77:ARG:HH21	6:J:20:DC:H4'	1.70	0.56
5:I:73:DG:H8	5:I:73:DG:OP2	1.89	0.56
6:J:121:DA:H2''	6:J:122:DG:OP2	2.06	0.56
4:H:43:LYS:HA	4:H:47:PRO:HA	1.88	0.56
7:O:751:ILE:HD12	7:O:784:ASN:HA	1.87	0.56
3:C:15:LYS:HB3	3:C:20:ARG:NH2	2.20	0.56
3:G:84:GLN:HE21	3:G:88:ARG:HG3	1.71	0.56
5:I:112:DT:H2'	5:I:113:DA:C8	2.41	0.56
7:O:1090:GLU:O	7:O:1093:ASP:HB3	2.05	0.56
2:F:64:ASN:HB3	2:F:93:GLN:HE22	1.70	0.56
5:I:4:DG:H2''	5:I:5:DA:C8	2.40	0.56
6:J:75:DC:OP2	6:J:75:DC:H2'	2.05	0.56
6:J:139:DA:H2'	6:J:140:DT:H6	1.70	0.56
7:O:679:ILE:HA	7:O:744:TYR:CE1	2.40	0.56
1:A:73:GLU:OE1	2:B:25:ASN:ND2	2.32	0.56
4:H:90:GLU:H	4:H:90:GLU:CD	2.08	0.56
5:I:89:DT:H1'	5:I:90:DA:C8	2.41	0.56
7:O:1029:TYR:CD1	7:O:1348:GLY:HA2	2.41	0.56
4:H:106:HIS:O	4:H:110:GLU:HG2	2.06	0.56
7:O:821:VAL:HG23	7:O:870:LEU:HA	1.88	0.56
6:J:116:DA:H2''	6:J:117:DA:H8	1.71	0.56
7:O:794:MET:SD	7:O:798:LYS:NZ	2.66	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:25:ASN:O	2:B:26:ILE:HG12	2.07	0.55
7:O:1029:TYR:HA	7:O:1032:LEU:HB2	1.87	0.55
2:B:56:GLY:O	2:B:59:LYS:HB3	2.05	0.55
2:B:96:THR:O	3:G:100:VAL:HG13	2.07	0.55
1:E:128:ARG:NE	1:E:133:GLU:OE1	2.39	0.55
2:F:71:THR:O	2:F:74:GLU:HB2	2.06	0.55
7:O:843:ARG:HH11	7:O:866:PHE:HA	1.71	0.55
6:J:20:DC:H2''	6:J:21:DA:C8	2.42	0.55
6:J:129:DC:H1'	6:J:130:DG:C5	2.41	0.55
7:O:880:ARG:HH11	7:O:913:HIS:HB2	1.72	0.55
7:O:1013:CYS:H	7:O:1213:THR:HA	1.70	0.55
7:O:1121:ASP:O	7:O:1125:TYR:N	2.38	0.55
1:A:128:ARG:NE	1:A:133:GLU:OE1	2.39	0.55
4:D:43:LYS:HA	4:D:47:PRO:HA	1.88	0.55
4:D:99:LEU:HB3	4:D:103:LEU:HB3	1.89	0.55
3:G:17:ARG:NH2	3:G:28:GLY:HA2	2.20	0.55
7:O:979:VAL:O	7:O:983:LEU:HG	2.06	0.55
7:O:1224:ARG:O	7:O:1227:LYS:HB2	2.06	0.55
6:J:145:DG:H2''	6:J:146:DA:H8	1.72	0.55
7:O:785:HIS:HA	7:O:918:TYR:CE1	2.42	0.55
7:O:1217:VAL:O	7:O:1220:VAL:N	2.39	0.55
3:C:84:GLN:OE1	3:C:102:ILE:HB	2.07	0.55
7:O:675:LYS:O	7:O:679:ILE:HG13	2.07	0.55
7:O:1258:LEU:O	7:O:1262:GLU:HG3	2.07	0.55
2:B:31:LYS:HE2	2:B:51:TYR:CE2	2.42	0.55
4:D:90:GLU:H	4:D:90:GLU:CD	2.08	0.55
5:I:28:DC:C4	6:J:119:DT:N3	2.75	0.55
3:C:76:THR:O	4:D:50:GLY:N	2.33	0.55
2:B:33:ALA:HA	2:B:36:ARG:CZ	2.37	0.55
2:B:83:ALA:O	2:B:87:VAL:HG23	2.07	0.55
2:B:92:ARG:NH2	4:D:98:LEU:HD23	2.22	0.55
4:D:106:HIS:O	4:D:110:GLU:HG2	2.06	0.55
4:H:99:LEU:HB3	4:H:103:LEU:HB3	1.88	0.55
7:O:680:THR:O	7:O:684:ARG:HG2	2.07	0.55
7:O:950:LYS:C	7:O:953:ASP:H	2.09	0.55
2:B:92:ARG:HH21	4:D:98:LEU:HD23	1.72	0.55
2:F:71:THR:HA	2:F:74:GLU:CD	2.27	0.55
7:O:1084:ARG:NE	7:O:1315:SER:O	2.26	0.55
7:O:1173:GLN:HG2	7:O:1202:GLN:HB2	1.88	0.55
3:G:84:GLN:OE1	3:G:102:ILE:HB	2.07	0.54
6:J:12:DA:H2'	6:J:13:DT:H71	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:929:ASN:HD21	7:O:1232:ASP:CA	2.20	0.54
1:A:105:GLU:O	1:A:108:ASN:HB3	2.07	0.54
4:D:61:SER:HB3	2:F:98:TYR:HD1	1.73	0.54
1:E:46:VAL:HG22	1:E:49:ARG:HH22	1.72	0.54
5:I:130:DC:H2''	5:I:131:DA:N7	2.23	0.54
6:J:131:DG:H8	6:J:131:DG:P	2.31	0.54
7:O:787:ASN:OD1	7:O:919:ARG:N	2.34	0.54
7:O:1090:GLU:O	7:O:1094:ARG:HG2	2.08	0.54
1:E:105:GLU:O	1:E:108:ASN:HB3	2.07	0.54
6:J:73:DA:H2''	6:J:74:DG:OP2	2.07	0.54
1:A:40:ARG:HG2	5:I:84:DC:C5'	2.38	0.54
5:I:125:DC:H2''	5:I:126:DG:C8	2.42	0.54
7:O:939:ASN:ND2	7:O:946:PHE:HA	2.23	0.54
7:O:1000:GLU:O	7:O:1002:GLU:HG3	2.08	0.54
3:C:84:GLN:HE21	3:C:88:ARG:HG3	1.71	0.54
3:G:31:HIS:HA	3:G:34:LEU:HD12	1.90	0.54
7:O:683:LEU:HG	7:O:944:LYS:NZ	2.22	0.54
7:O:1094:ARG:NH2	7:O:1304:ARG:HD2	2.23	0.54
3:C:27:VAL:HG13	3:C:48:PRO:HB2	1.90	0.54
2:F:79:LYS:NZ	6:J:101:DG:OP1	2.41	0.54
5:I:3:DC:H1'	5:I:4:DG:O5'	2.08	0.54
5:I:60:DA:C4	5:I:61:DA:N7	2.76	0.54
6:J:70:DG:H2''	6:J:71:DA:C8	2.43	0.54
6:J:89:DT:H2''	6:J:90:DA:H8	1.73	0.54
7:O:1121:ASP:HA	7:O:1124:ARG:HB2	1.90	0.54
7:O:1250:GLN:HA	7:O:1253:LEU:HB2	1.89	0.54
2:F:76:ALA:HB1	2:F:78:ARG:HE	1.71	0.53
7:O:914:TYR:CG	7:O:915:HIS:N	2.76	0.53
1:A:46:VAL:HG22	1:A:49:ARG:HH22	1.72	0.53
5:I:129:DT:H2''	5:I:130:DC:C5	2.43	0.53
7:O:769:ASP:HB3	7:O:772:ILE:HD12	1.91	0.53
7:O:891:MET:HB2	7:O:916:ALA:HB3	1.90	0.53
2:B:45:ARG:HE	5:I:81:DC:C4'	2.21	0.53
5:I:90:DA:H1'	5:I:91:DA:C8	2.43	0.53
6:J:138:DG:C2	6:J:139:DA:C4	2.97	0.53
4:H:84:SER:N	5:I:40:DG:OP1	2.32	0.53
6:J:44:DA:H3'	6:J:45:DT:H71	1.89	0.53
7:O:782:PHE:HD1	7:O:918:TYR:CD1	2.26	0.53
7:O:1067:GLU:O	7:O:1071:GLN:HB2	2.08	0.53
7:O:1114:GLN:O	7:O:1117:ASP:HB2	2.08	0.53
7:O:1126:ILE:HD12	7:O:1128:ILE:HD11	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:18:HIS:HB3	7:O:1076:ARG:NH2	2.24	0.53
3:C:69:ALA:HA	3:C:72:ASP:OD2	2.08	0.53
4:D:62:PHE:O	4:D:65:ASP:HB3	2.08	0.53
5:I:63:DG:H1'	5:I:64:DC:O4'	2.08	0.53
6:J:54:DC:H2''	6:J:55:DG:C8	2.44	0.53
2:F:91:LYS:O	2:F:94:GLY:N	2.37	0.53
3:G:69:ALA:HA	3:G:72:ASP:OD2	2.08	0.53
4:H:62:PHE:O	4:H:65:ASP:HB3	2.08	0.53
5:I:58:DT:H2''	5:I:59:DA:C8	2.43	0.53
5:I:111:DC:C2	6:J:37:DG:N1	2.76	0.53
7:O:825:LEU:HA	7:O:872:THR:HG21	1.89	0.53
7:O:1164:ARG:HH11	7:O:1189:GLN:HA	1.74	0.53
7:O:1247:SER:O	7:O:1251:GLU:HG3	2.09	0.53
2:B:20:LYS:HD3	7:O:1076:ARG:HH12	1.73	0.53
1:E:63:ARG:NH2	5:I:61:DA:OP1	2.42	0.53
3:G:88:ARG:HD3	3:G:94:ASN:OD1	2.08	0.53
5:I:93:DC:H2''	5:I:94:DG:C8	2.43	0.53
6:J:81:DC:OP2	6:J:81:DC:H2'	2.07	0.53
6:J:122:DG:C4	6:J:123:DC:C5	2.96	0.53
7:O:1102:THR:HB	7:O:1104:HIS:CD2	2.44	0.53
7:O:1258:LEU:HA	7:O:1261:GLU:OE1	2.09	0.53
3:G:27:VAL:HG13	3:G:48:PRO:HB2	1.90	0.53
6:J:18:DG:H1'	6:J:19:DA:N9	2.23	0.53
7:O:769:ASP:O	7:O:772:ILE:HB	2.09	0.53
7:O:809:LEU:HA	7:O:813:LYS:HB2	1.90	0.53
1:A:117:VAL:N	6:J:71:DA:OP1	2.41	0.53
3:C:31:HIS:HA	3:C:34:LEU:HD12	1.90	0.53
4:D:102:GLU:HB3	4:D:106:HIS:CD2	2.44	0.53
6:J:98:DC:H2'	6:J:99:DT:C5	2.44	0.53
6:J:107:DT:H2''	6:J:108:DC:C5	2.43	0.53
7:O:771:GLN:O	7:O:775:LEU:CB	2.57	0.53
7:O:778:MET:HG2	7:O:781:LEU:HD12	1.90	0.53
7:O:1198:HIS:HB3	7:O:1206:VAL:HG21	1.90	0.53
7:O:1344:ALA:O	7:O:1348:GLY:N	2.42	0.53
5:I:111:DC:N4	6:J:36:DA:N1	2.56	0.53
7:O:1138:LYS:O	7:O:1142:ARG:HG3	2.09	0.53
7:O:1250:GLN:HA	7:O:1253:LEU:HD12	1.90	0.53
6:J:86:DG:H1'	6:J:87:DT:O4'	2.08	0.52
6:J:100:DA:C5	6:J:101:DG:C5	2.98	0.52
6:J:124:DG:H8	6:J:124:DG:OP2	1.93	0.52
7:O:1083:TRP:CE2	7:O:1084:ARG:HG3	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:1238:ALA:HA	7:O:1241:PHE:CE2	2.45	0.52
2:B:25:ASN:O	2:B:27:GLN:N	2.39	0.52
3:C:73:ASN:HB3	3:C:75:LYS:HE2	1.91	0.52
5:I:28:DC:H1'	5:I:29:DA:C8	2.44	0.52
7:O:1015:MET:HE3	7:O:1019:GLN:HB3	1.90	0.52
7:O:782:PHE:CE1	7:O:787:ASN:HA	2.44	0.52
7:O:822:ILE:HA	7:O:871:THR:O	2.09	0.52
5:I:89:DT:C2	5:I:90:DA:C5	2.98	0.52
6:J:43:DA:H2''	6:J:44:DA:C8	2.44	0.52
7:O:1227:LYS:O	7:O:1231:ILE:N	2.42	0.52
2:B:17:ARG:HA	7:O:1117:ASP:HB3	1.92	0.52
2:B:49:LEU:O	2:B:52:GLU:HB3	2.10	0.52
3:C:88:ARG:HD3	3:C:94:ASN:OD1	2.08	0.52
3:C:92:GLU:O	3:C:95:LYS:HB3	2.10	0.52
4:H:106:HIS:O	4:H:109:SER:HB2	2.10	0.52
7:O:777:TRP:CE3	7:O:778:MET:HG3	2.44	0.52
7:O:835:PHE:HE2	7:O:870:LEU:HD22	1.75	0.52
7:O:880:ARG:HA	7:O:883:LEU:HD12	1.92	0.52
7:O:939:ASN:HD22	7:O:945:ILE:HG22	1.74	0.52
4:D:76:ARG:HB3	4:D:80:TYR:CZ	2.45	0.52
4:H:76:ARG:HB3	4:H:80:TYR:CZ	2.45	0.52
4:H:102:GLU:HB3	4:H:106:HIS:CD2	2.44	0.52
7:O:804:SER:O	7:O:807:THR:OG1	2.23	0.52
7:O:1085:VAL:HG13	7:O:1086:ALA:H	1.74	0.52
7:O:1106:VAL:N	7:O:1157:LEU:O	2.29	0.52
7:O:1218:GLU:O	7:O:1222:LEU:HB3	2.10	0.52
1:A:48:LEU:HD21	2:B:44:LYS:HD2	1.90	0.52
3:C:18:SER:OG	3:C:25:PHE:O	2.22	0.52
7:O:896:GLY:O	7:O:899:MET:HB2	2.09	0.52
7:O:942:LEU:HB2	7:O:945:ILE:HG13	1.92	0.52
7:O:982:ARG:O	7:O:986:VAL:HG23	2.10	0.52
7:O:1060:ASN:HB3	7:O:1061:HIS:CD2	2.45	0.52
7:O:1225:ALA:O	7:O:1228:LYS:HB2	2.09	0.52
2:F:31:LYS:HB3	2:F:32:PRO:HD3	1.91	0.51
5:I:10:DC:H2''	5:I:11:DC:OP2	2.08	0.51
5:I:13:DG:OP2	5:I:13:DG:H2'	2.10	0.51
6:J:56:DG:H1'	6:J:57:DT:H5'	1.91	0.51
6:J:124:DG:C6	6:J:125:DG:C6	2.98	0.51
7:O:858:GLN:HB3	7:O:862:ARG:HH12	1.74	0.51
7:O:908:LEU:HA	7:O:911:ASN:OD1	2.10	0.51
7:O:939:ASN:ND2	7:O:945:ILE:HG22	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:1030:ARG:HG2	7:O:1054:GLN:HG3	1.91	0.51
7:O:1131:LEU:HD12	7:O:1149:PHE:HB2	1.92	0.51
6:J:103:DG:C4	6:J:104:DC:C5	2.98	0.51
7:O:827:THR:O	7:O:831:TRP:HD1	1.93	0.51
7:O:1062:PRO:HG3	7:O:1085:VAL:CG1	2.40	0.51
4:D:33:SER:OG	4:D:34:TYR:N	2.43	0.51
5:I:33:DG:H2''	5:I:34:DG:H5''	1.92	0.51
7:O:854:ARG:NH1	7:O:875:TYR:OH	2.43	0.51
7:O:939:ASN:HD22	7:O:945:ILE:C	2.13	0.51
7:O:1027:LEU:O	7:O:1030:ARG:HB2	2.10	0.51
7:O:1173:GLN:NE2	7:O:1200:ILE:O	2.31	0.51
1:A:123:ASP:OD1	1:E:113:HIS:NE2	2.43	0.51
6:J:119:DT:H2''	6:J:120:DG:N7	2.25	0.51
5:I:34:DG:C6	5:I:35:DT:C4	2.98	0.51
5:I:132:DG:H1'	5:I:133:DA:C8	2.45	0.51
6:J:53:DG:H8	6:J:53:DG:OP2	1.92	0.51
7:O:855:LYS:HA	7:O:858:GLN:OE1	2.10	0.51
7:O:939:ASN:ND2	7:O:945:ILE:O	2.43	0.51
7:O:1116:MET:HB2	7:O:1132:ARG:NH2	2.25	0.51
7:O:1190:ASP:O	7:O:1194:GLN:HG3	2.10	0.51
5:I:104:DT:H2'	5:I:105:DT:H71	1.93	0.51
7:O:797:GLY:O	7:O:801:GLN:HG3	2.11	0.51
1:E:51:ILE:HG12	2:F:39:ARG:O	2.11	0.51
4:H:76:ARG:HB3	4:H:80:TYR:CE2	2.45	0.51
5:I:77:DT:H2''	5:I:78:DC:C6	2.46	0.51
5:I:101:DG:H2'	5:I:101:DG:OP2	2.10	0.51
6:J:61:DA:C2	6:J:62:DA:C5	2.99	0.51
6:J:97:DG:C4	6:J:98:DC:C5	2.99	0.51
7:O:848:LYS:HA	7:O:875:TYR:HE2	1.74	0.51
7:O:1006:LYS:HA	7:O:1206:VAL:HB	1.93	0.51
7:O:1007:VAL:N	7:O:1206:VAL:O	2.42	0.51
7:O:1083:TRP:HA	7:O:1089:PHE:CB	2.41	0.51
3:G:73:ASN:HB3	3:G:75:LYS:HE2	1.92	0.51
6:J:46:DC:H2''	6:J:47:DC:OP2	2.10	0.51
1:A:40:ARG:NH1	5:I:84:DC:O4'	2.44	0.51
4:D:76:ARG:HB3	4:D:80:TYR:CE2	2.45	0.51
3:G:14:ALA:HA	5:I:32:DT:OP1	2.11	0.51
3:G:17:ARG:HH21	3:G:28:GLY:CA	2.24	0.51
5:I:102:DG:C2'	5:I:103:DA:H8	2.24	0.51
6:J:109:DT:H1'	6:J:110:DA:C8	2.46	0.51
6:J:123:DC:H2''	6:J:124:DG:C8	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:142:DC:C2	6:J:143:DT:C4	2.99	0.51
7:O:837:LYS:HB2	7:O:838:TRP:CD1	2.46	0.51
7:O:843:ARG:HD2	7:O:866:PHE:HA	1.92	0.51
7:O:854:ARG:O	7:O:858:GLN:HG3	2.10	0.51
7:O:945:ILE:O	7:O:949:VAL:CB	2.52	0.51
7:O:978:LEU:HD22	7:O:982:ARG:HH12	1.75	0.51
7:O:980:ILE:HG12	7:O:983:LEU:HD12	1.92	0.51
7:O:1106:VAL:HG11	7:O:1179:ILE:HD12	1.92	0.51
7:O:1159:PHE:CE2	7:O:1161:LEU:HD21	2.46	0.51
3:G:37:GLY:HA3	3:G:39:TYR:CE2	2.46	0.50
3:G:92:GLU:O	3:G:95:LYS:HB3	2.10	0.50
6:J:17:DT:H2''	6:J:18:DG:OP2	2.09	0.50
6:J:63:DC:H2''	6:J:64:DG:H8	1.76	0.50
7:O:928:GLN:HE22	7:O:1228:LYS:HD3	1.76	0.50
7:O:1133:LEU:HD11	7:O:1142:ARG:HG2	1.92	0.50
3:C:17:ARG:HH21	3:C:28:GLY:CA	2.24	0.50
3:C:77:ARG:NE	6:J:20:DC:H5''	2.26	0.50
1:E:72:ARG:O	1:E:76:GLN:HG3	2.11	0.50
4:H:107:ALA:O	4:H:110:GLU:N	2.44	0.50
5:I:111:DC:C2	6:J:37:DG:C2	3.00	0.50
6:J:128:DT:H1'	6:J:129:DC:C2	2.46	0.50
7:O:683:LEU:HD11	7:O:744:TYR:HD1	1.76	0.50
7:O:684:ARG:HH12	7:O:747:VAL:HG21	1.76	0.50
7:O:835:PHE:CG	7:O:844:THR:HG21	2.46	0.50
7:O:1262:GLU:O	7:O:1266:LYS:HG3	2.11	0.50
1:A:72:ARG:O	1:A:76:GLN:HG3	2.11	0.50
4:D:106:HIS:O	4:D:109:SER:HB2	2.10	0.50
5:I:103:DA:H2'	5:I:104:DT:H6	1.76	0.50
6:J:41:DG:C5	6:J:42:DT:C4	2.99	0.50
6:J:71:DA:H1'	6:J:72:DC:H5'	1.93	0.50
6:J:101:DG:H2''	6:J:102:DA:C8	2.46	0.50
6:J:123:DC:C2	6:J:124:DG:C5	2.99	0.50
4:D:107:ALA:O	4:D:110:GLU:N	2.44	0.50
1:E:68:GLN:NE2	1:E:72:ARG:HE	2.03	0.50
4:H:33:SER:OG	4:H:34:TYR:N	2.43	0.50
5:I:90:DA:H1'	5:I:91:DA:N7	2.27	0.50
6:J:42:DT:C2	6:J:43:DA:C8	2.99	0.50
7:O:781:LEU:O	7:O:786:LEU:N	2.45	0.50
7:O:1085:VAL:HA	7:O:1318:LEU:HG	1.94	0.50
7:O:1254:LEU:O	7:O:1257:LEU:HB3	2.10	0.50
3:C:37:GLY:HA3	3:C:39:TYR:CE2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:111:DC:O2	6:J:37:DG:C2	2.64	0.50
7:O:1108:ILE:HG23	7:O:1179:ILE:O	2.10	0.50
7:O:1113:THR:HG21	7:O:1134:ASP:CB	2.41	0.50
7:O:1236:ILE:O	7:O:1240:LYS:HG3	2.10	0.50
5:I:64:DC:H2''	5:I:65:DA:N7	2.27	0.50
6:J:37:DG:H1'	6:J:38:DG:C5	2.47	0.50
6:J:73:DA:H2''	6:J:74:DG:H8	1.75	0.50
6:J:76:DG:C4	6:J:77:DC:C4	2.99	0.50
6:J:120:DG:H1'	6:J:121:DA:C5	2.47	0.50
7:O:744:TYR:CE2	7:O:986:VAL:HG13	2.47	0.50
7:O:753:GLU:OE1	7:O:813:LYS:NZ	2.30	0.50
7:O:908:LEU:HD12	7:O:909:THR:HG23	1.94	0.50
5:I:60:DA:OP2	5:I:60:DA:H2'	2.12	0.50
5:I:110:DC:N3	6:J:37:DG:C2	2.80	0.50
5:I:136:DT:H2''	5:I:137:DA:H5'	1.93	0.50
6:J:111:DC:H2''	6:J:112:DG:C8	2.46	0.50
2:B:20:LYS:CD	7:O:1076:ARG:HH12	2.24	0.50
2:B:25:ASN:C	2:B:27:GLN:N	2.65	0.50
3:C:50:TYR:O	3:C:54:VAL:HG23	2.12	0.50
5:I:122:DG:H2'	5:I:122:DG:OP2	2.12	0.50
7:O:1064:VAL:HG23	7:O:1065:PHE:CD2	2.47	0.50
3:C:42:ARG:HH21	5:I:112:DT:C4'	2.25	0.50
3:G:50:TYR:O	3:G:54:VAL:HG23	2.12	0.50
6:J:81:DC:H2''	6:J:82:DG:N7	2.27	0.50
7:O:1237:GLN:NE2	7:O:1256:SER:HB2	2.27	0.50
6:J:142:DC:H1'	6:J:143:DT:H5'	1.93	0.49
7:O:767:LEU:HB3	7:O:771:GLN:HB2	1.94	0.49
7:O:1091:LEU:O	7:O:1095:ILE:HG12	2.11	0.49
2:B:84:MET:HB3	2:B:88:TYR:HE2	1.76	0.49
5:I:20:DA:H1'	5:I:21:DG:O4'	2.12	0.49
6:J:7:DT:H2''	6:J:8:DG:N7	2.27	0.49
6:J:15:DT:H4'	6:J:16:DC:OP1	2.12	0.49
2:B:71:THR:HA	2:B:74:GLU:OE1	2.13	0.49
2:F:88:TYR:O	2:F:92:ARG:CB	2.60	0.49
5:I:59:DA:H2''	5:I:60:DA:O4'	2.13	0.49
5:I:74:DC:C6	5:I:75:DT:H72	2.47	0.49
5:I:145:DG:C6	5:I:146:DA:C6	2.99	0.49
6:J:32:DG:H2''	6:J:33:DA:H8	1.77	0.49
6:J:98:DC:H2'	6:J:99:DT:H72	1.93	0.49
6:J:133:DA:H1'	6:J:134:DC:H5'	1.94	0.49
7:O:1015:MET:SD	7:O:1213:THR:HG21	2.52	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:16:THR:O	3:C:20:ARG:HG3	2.12	0.49
5:I:126:DG:H2'	5:I:127:DT:C6	2.47	0.49
6:J:116:DA:H2''	6:J:117:DA:C8	2.47	0.49
7:O:987:LEU:HA	7:O:990:PHE:CD2	2.47	0.49
7:O:989:PRO:HG2	7:O:990:PHE:CD2	2.48	0.49
3:G:16:THR:O	3:G:20:ARG:HG3	2.12	0.49
5:I:44:DG:OP2	5:I:44:DG:H8	1.95	0.49
5:I:111:DC:N4	6:J:37:DG:O6	2.46	0.49
5:I:121:DG:H2''	5:I:122:DG:OP2	2.12	0.49
7:O:1015:MET:HB2	7:O:1020:GLN:CG	2.39	0.49
7:O:1023:TYR:OH	7:O:1055:LEU:HD23	2.12	0.49
7:O:1340:SER:OG	7:O:1341:GLU:OE1	2.30	0.49
1:A:91:ALA:HB1	2:B:86:VAL:HG11	1.94	0.49
5:I:33:DG:H2''	5:I:34:DG:H8	1.77	0.49
6:J:131:DG:H8	6:J:131:DG:O5'	1.95	0.49
6:J:134:DC:H2''	6:J:135:DC:C6	2.48	0.49
7:O:1084:ARG:NH1	7:O:1318:LEU:HD23	2.27	0.49
1:A:67:PHE:O	1:A:71:VAL:HG23	2.12	0.49
2:B:58:LEU:O	2:B:61:PHE:HB3	2.12	0.49
6:J:98:DC:H2'	6:J:99:DT:C6	2.48	0.49
6:J:142:DC:H1'	6:J:143:DT:C5'	2.42	0.49
7:O:828:LEU:HD11	7:O:870:LEU:HG	1.95	0.49
7:O:909:THR:O	7:O:913:HIS:HB2	2.12	0.49
7:O:921:ILE:HG21	7:O:937:LEU:HD22	1.94	0.49
7:O:939:ASN:HA	7:O:945:ILE:HB	1.95	0.49
6:J:43:DA:C4	6:J:44:DA:N7	2.81	0.49
6:J:72:DC:H1'	6:J:73:DA:C8	2.48	0.49
2:B:91:LYS:HD3	4:D:76:ARG:HH22	1.78	0.49
4:H:72:GLY:O	4:H:76:ARG:HG3	2.13	0.49
5:I:33:DG:C6	5:I:34:DG:C6	3.01	0.49
5:I:50:DG:H2''	5:I:51:DC:H5'	1.95	0.49
6:J:32:DG:H2''	6:J:33:DA:OP2	2.11	0.49
7:O:981:ARG:HD2	7:O:1238:ALA:HB2	1.94	0.49
7:O:1116:MET:HB2	7:O:1132:ARG:HH21	1.78	0.49
7:O:1235:VAL:O	7:O:1238:ALA:HB3	2.12	0.49
2:B:22:LEU:HD12	2:B:23:ARG:H	1.77	0.48
2:B:39:ARG:HH12	2:B:46:ILE:HG13	1.78	0.48
2:B:79:LYS:NZ	5:I:101:DG:OP1	2.45	0.48
5:I:30:DA:H2'	5:I:31:DT:H71	1.94	0.48
7:O:744:TYR:HB2	7:O:989:PRO:HG3	1.94	0.48
7:O:774:GLY:HA3	7:O:992:LEU:HD22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:820:LEU:HD12	7:O:821:VAL:N	2.28	0.48
7:O:1016:SER:HB2	7:O:1318:LEU:HB2	1.95	0.48
3:C:64:GLU:HA	4:D:46:HIS:NE2	2.28	0.48
4:H:30:ARG:HE	6:J:123:DC:H4'	1.78	0.48
5:I:54:DC:H2''	5:I:55:DG:C8	2.48	0.48
5:I:95:DC:OP1	7:O:904:SER:HA	2.13	0.48
6:J:30:DG:H2''	6:J:31:DA:H8	1.78	0.48
7:O:889:VAL:C	7:O:916:ALA:HB1	2.32	0.48
7:O:1104:HIS:C	7:O:1157:LEU:HD22	2.34	0.48
7:O:1163:THR:OG1	7:O:1164:ARG:N	2.45	0.48
5:I:103:DA:H2'	5:I:104:DT:C6	2.48	0.48
5:I:122:DG:N2	6:J:27:DC:O2	2.46	0.48
7:O:882:LEU:HA	7:O:885:LYS:HE3	1.95	0.48
7:O:989:PRO:HG2	7:O:990:PHE:CE2	2.48	0.48
7:O:1105:ARG:HD3	7:O:1174:THR:O	2.12	0.48
7:O:1108:ILE:HG22	7:O:1109:PHE:H	1.78	0.48
3:G:21:ALA:HA	4:H:118:TYR:HB2	1.95	0.48
6:J:3:DC:H1'	6:J:4:DG:O4'	2.13	0.48
7:O:1019:GLN:NE2	7:O:1086:ALA:HB2	2.27	0.48
7:O:1055:LEU:O	7:O:1059:CYS:CB	2.54	0.48
4:D:72:GLY:O	4:D:76:ARG:HG3	2.13	0.48
5:I:69:DA:H2''	5:I:70:DC:C5	2.49	0.48
6:J:108:DC:H2'	6:J:108:DC:OP2	2.13	0.48
6:J:136:DG:H2''	6:J:137:DG:OP2	2.13	0.48
7:O:768:LYS:HB3	7:O:770:TYR:CE2	2.49	0.48
7:O:782:PHE:HA	7:O:786:LEU:H	1.79	0.48
7:O:789:ILE:HG12	7:O:921:ILE:HB	1.95	0.48
7:O:860:LYS:O	7:O:863:ALA:HB3	2.13	0.48
5:I:32:DT:C4	5:I:33:DG:C6	3.02	0.48
7:O:794:MET:HA	7:O:798:LYS:HZ1	1.79	0.48
7:O:809:LEU:O	7:O:813:LYS:HB2	2.13	0.48
7:O:845:ILE:N	7:O:868:VAL:O	2.47	0.48
7:O:980:ILE:HA	7:O:983:LEU:HD12	1.95	0.48
7:O:1021:ILE:HA	7:O:1024:GLN:OE1	2.13	0.48
1:E:67:PHE:O	1:E:71:VAL:HG23	2.12	0.48
2:F:18:HIS:NE2	5:I:52:DA:O3'	2.46	0.48
5:I:12:DC:H2''	5:I:13:DG:N7	2.28	0.48
6:J:75:DC:H2''	6:J:76:DG:C8	2.48	0.48
6:J:115:DC:H2''	6:J:116:DA:H8	1.78	0.48
6:J:131:DG:C4	6:J:132:DC:C5	3.02	0.48
7:O:754:ASP:CB	7:O:776:GLN:HE21	2.25	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:834:GLU:O	7:O:838:TRP:HD1	1.97	0.48
7:O:984:HIS:O	7:O:988:ARG:N	2.47	0.48
7:O:1051:GLN:O	7:O:1055:LEU:HB2	2.13	0.48
6:J:37:DG:OP2	6:J:37:DG:H8	1.96	0.48
2:B:71:THR:HG21	4:D:97:LEU:HD21	1.95	0.48
6:J:41:DG:C2	6:J:42:DT:C2	3.02	0.48
7:O:671:LEU:HB3	7:O:955:TRP:HH2	1.77	0.48
7:O:672:ASP:O	7:O:675:LYS:HB2	2.14	0.48
7:O:778:MET:HA	7:O:781:LEU:HD12	1.95	0.48
7:O:950:LYS:O	7:O:953:ASP:N	2.46	0.48
5:I:96:DC:N4	6:J:53:DG:O6	2.46	0.48
7:O:778:MET:O	7:O:781:LEU:HB2	2.14	0.48
7:O:1136:HIS:O	7:O:1136:HIS:ND1	2.45	0.48
6:J:64:DG:C5	6:J:65:DC:C4	3.01	0.47
6:J:67:DG:C2	6:J:68:DG:C2	3.02	0.47
6:J:111:DC:OP2	6:J:111:DC:H2'	2.14	0.47
7:O:903:GLN:OE1	7:O:903:GLN:N	2.42	0.47
7:O:951:SER:O	7:O:954:GLU:HB2	2.14	0.47
7:O:1003:LEU:HD13	7:O:1198:HIS:HD2	1.79	0.47
1:E:72:ARG:NH2	5:I:51:DC:OP2	2.48	0.47
6:J:72:DC:C2	6:J:73:DA:C5	3.02	0.47
7:O:675:LYS:HE2	7:O:983:LEU:HD21	1.96	0.47
7:O:823:VAL:HG22	7:O:828:LEU:HD12	1.97	0.47
7:O:929:ASN:ND2	7:O:1231:ILE:HG22	2.29	0.47
7:O:1014:LYS:HE3	7:O:1317:LEU:CD1	2.44	0.47
7:O:1238:ALA:HA	7:O:1241:PHE:CD2	2.49	0.47
7:O:1244:LYS:O	7:O:1245:SER:OG	2.25	0.47
2:F:56:GLY:O	2:F:59:LYS:HB3	2.13	0.47
3:G:14:ALA:HB2	5:I:32:DT:H5''	1.96	0.47
5:I:120:DA:OP2	5:I:120:DA:H8	1.97	0.47
6:J:137:DG:OP2	6:J:137:DG:H8	1.97	0.47
7:O:1096:LEU:HA	7:O:1099:LEU:HD12	1.96	0.47
7:O:1297:LEU:O	7:O:1300:MET:HB2	2.13	0.47
2:B:32:PRO:O	2:B:36:ARG:HG3	2.14	0.47
1:E:69:ARG:HB3	2:F:22:LEU:HD13	1.96	0.47
6:J:82:DG:C4	6:J:83:DT:C5	3.01	0.47
7:O:908:LEU:HD12	7:O:909:THR:N	2.28	0.47
7:O:914:TYR:C	7:O:915:HIS:CG	2.87	0.47
7:O:947:ASN:HA	7:O:950:LYS:NZ	2.30	0.47
7:O:1088:LYS:HD3	7:O:1181:PHE:CD1	2.48	0.47
1:A:109:LEU:HA	1:A:112:ILE:HD12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:73:GLU:O	4:D:76:ARG:HB2	2.15	0.47
2:F:31:LYS:O	2:F:35:ARG:HG3	2.15	0.47
6:J:116:DA:OP2	6:J:116:DA:H2'	2.15	0.47
7:O:1120:GLU:O	7:O:1123:LEU:HB2	2.14	0.47
7:O:1216:SER:O	7:O:1219:GLU:HB2	2.14	0.47
7:O:1226:TYR:CD1	7:O:1229:LEU:HD12	2.46	0.47
1:E:87:SER:O	1:E:90:MET:HB2	2.15	0.47
4:H:87:THR:O	4:H:91:ILE:HG12	2.15	0.47
6:J:52:DG:C2	6:J:53:DG:C5	3.02	0.47
4:D:73:GLU:HA	4:D:76:ARG:HD3	1.97	0.47
1:E:104:PHE:CE2	2:F:37:LEU:HB3	2.50	0.47
6:J:53:DG:H5'	7:O:1112:MET:HG2	1.96	0.47
6:J:63:DC:H2''	6:J:64:DG:C8	2.50	0.47
6:J:68:DG:H2''	6:J:69:DG:C8	2.50	0.47
6:J:98:DC:H2'	6:J:99:DT:C7	2.44	0.47
7:O:759:PRO:HB2	7:O:811:GLU:OE2	2.15	0.47
7:O:771:GLN:HA	7:O:994:ARG:NH1	2.20	0.47
7:O:1025:GLN:HG2	7:O:1029:TYR:CE2	2.49	0.47
4:D:87:THR:O	4:D:91:ILE:HG12	2.15	0.47
4:D:91:ILE:O	4:D:95:VAL:HG23	2.15	0.47
1:E:104:PHE:O	1:E:107:THR:N	2.48	0.47
3:G:17:ARG:O	3:G:21:ALA:N	2.46	0.47
4:H:98:LEU:HA	4:H:98:LEU:HD23	1.74	0.47
5:I:33:DG:O6	6:J:114:DC:N4	2.47	0.47
6:J:73:DA:H2''	6:J:74:DG:C8	2.50	0.47
7:O:780:SER:O	7:O:784:ASN:ND2	2.45	0.47
7:O:872:THR:O	7:O:876:ILE:HG12	2.15	0.47
7:O:1053:MET:HG3	7:O:1054:GLN:NE2	2.30	0.47
7:O:1080:ASP:HA	7:O:1083:TRP:HE1	1.80	0.47
1:A:68:GLN:O	1:A:71:VAL:N	2.48	0.47
2:B:98:TYR:CE2	3:G:100:VAL:HG11	2.49	0.47
5:I:95:DC:H2'	5:I:96:DC:C6	2.49	0.47
6:J:37:DG:H2''	6:J:38:DG:N7	2.30	0.47
7:O:968:LYS:HA	7:O:972:SER:H	1.80	0.47
7:O:999:VAL:HG23	7:O:1000:GLU:N	2.28	0.47
7:O:1225:ALA:HA	7:O:1228:LYS:HD2	1.96	0.47
7:O:1226:TYR:O	7:O:1229:LEU:HB2	2.14	0.47
2:B:74:GLU:OE2	4:D:96:ARG:NH2	2.48	0.47
2:B:92:ARG:NH2	4:D:98:LEU:HA	2.30	0.47
6:J:67:DG:H1'	6:J:68:DG:C8	2.50	0.47
1:A:113:HIS:HE1	1:E:122:LYS:HG3	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:17:ARG:O	3:C:21:ALA:N	2.46	0.46
2:F:31:LYS:HG3	2:F:51:TYR:CZ	2.50	0.46
3:G:80:PRO:HA	3:G:83:LEU:HD12	1.98	0.46
4:H:91:ILE:O	4:H:95:VAL:HG23	2.15	0.46
5:I:132:DG:H4'	5:I:133:DA:OP1	2.14	0.46
6:J:37:DG:H21	6:J:38:DG:N2	2.13	0.46
7:O:1227:LYS:O	7:O:1231:ILE:HG13	2.15	0.46
1:A:46:VAL:HB	5:I:83:DG:P	2.54	0.46
1:E:68:GLN:O	1:E:71:VAL:N	2.48	0.46
1:E:109:LEU:HA	1:E:112:ILE:HD12	1.97	0.46
5:I:39:DA:H2''	5:I:40:DG:C8	2.50	0.46
5:I:44:DG:C2	5:I:45:DC:C2	3.03	0.46
5:I:127:DT:H2''	5:I:128:DG:N7	2.30	0.46
7:O:897:HIS:O	7:O:900:LYS:CB	2.57	0.46
1:A:87:SER:O	1:A:90:MET:HB2	2.15	0.46
2:F:34:ILE:HA	2:F:37:LEU:HD12	1.96	0.46
4:H:73:GLU:O	4:H:76:ARG:HB2	2.15	0.46
5:I:124:DA:H1'	5:I:125:DC:H5'	1.98	0.46
6:J:53:DG:H2''	6:J:54:DC:H5'	1.96	0.46
7:O:744:TYR:HB3	7:O:748:ALA:HB2	1.97	0.46
7:O:890:HIS:CE1	7:O:892:ILE:HG13	2.50	0.46
7:O:978:LEU:O	7:O:982:ARG:CB	2.54	0.46
7:O:995:LEU:O	7:O:999:VAL:HG22	2.14	0.46
4:H:39:TYR:HE1	5:I:21:DG:OP2	1.97	0.46
5:I:12:DC:C2	5:I:13:DG:C6	3.03	0.46
5:I:119:DC:C2	5:I:120:DA:C5	3.04	0.46
6:J:122:DG:C4	6:J:123:DC:C4	3.03	0.46
6:J:128:DT:H2''	6:J:129:DC:C5	2.51	0.46
7:O:679:ILE:O	7:O:683:LEU:HB2	2.15	0.46
7:O:1288:ALA:HB2	7:O:1294:MET:HG2	1.98	0.46
1:A:91:ALA:CB	2:B:86:VAL:HG11	2.46	0.46
3:C:80:PRO:HA	3:C:83:LEU:HD12	1.98	0.46
1:E:109:LEU:HA	1:E:109:LEU:HD23	1.66	0.46
2:F:24:ASP:HB3	2:F:27:GLN:HG2	1.96	0.46
5:I:13:DG:C4	5:I:14:DG:C5	3.03	0.46
6:J:139:DA:C6	6:J:140:DT:C4	3.03	0.46
7:O:671:LEU:O	7:O:675:LYS:HG3	2.15	0.46
7:O:754:ASP:HB3	7:O:776:GLN:NE2	2.28	0.46
7:O:880:ARG:HH22	7:O:912:THR:CG2	2.26	0.46
7:O:1094:ARG:HH21	7:O:1304:ARG:HD2	1.80	0.46
5:I:20:DA:H5'	5:I:20:DA:C8	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:47:DC:OP2	6:J:47:DC:H2'	2.15	0.46
6:J:121:DA:C4	6:J:122:DG:C5	3.03	0.46
7:O:1067:GLU:OE1	7:O:1067:GLU:N	2.40	0.46
7:O:1223:GLU:HG2	7:O:1226:TYR:HD2	1.80	0.46
1:A:104:PHE:O	1:A:107:THR:N	2.48	0.46
2:B:33:ALA:O	2:B:36:ARG:N	2.48	0.46
5:I:99:DG:C6	5:I:100:DG:C6	3.03	0.46
7:O:931:LEU:HA	7:O:933:GLU:HB2	1.98	0.46
2:F:84:MET:O	2:F:87:VAL:N	2.49	0.46
5:I:46:DT:H6	5:I:46:DT:O5'	1.98	0.46
5:I:57:DT:OP1	5:I:57:DT:H3'	2.15	0.46
5:I:141:DA:C2	6:J:8:DG:C2	3.04	0.46
6:J:83:DT:H2''	6:J:84:DG:N7	2.30	0.46
6:J:136:DG:H1'	6:J:137:DG:O5'	2.16	0.46
7:O:996:LYS:O	7:O:1000:GLU:N	2.49	0.46
7:O:1004:PRO:HG3	7:O:1203:LYS:CA	2.39	0.46
7:O:1020:GLN:O	7:O:1024:GLN:HG3	2.16	0.46
3:C:71:ARG:C	3:C:74:LYS:H	2.19	0.46
3:C:84:GLN:HE21	3:C:88:ARG:CG	2.29	0.46
4:D:83:ARG:HD2	6:J:40:DA:H5''	1.97	0.46
5:I:100:DG:H2''	5:I:101:DG:N7	2.31	0.46
6:J:90:DA:OP2	6:J:90:DA:H2'	2.16	0.46
7:O:920:LEU:HD21	7:O:922:LEU:HD21	1.96	0.46
7:O:943:PRO:HA	7:O:946:PHE:CD2	2.49	0.46
2:B:31:LYS:HG3	2:B:51:TYR:CZ	2.51	0.46
4:H:73:GLU:HA	4:H:76:ARG:HD3	1.97	0.46
5:I:27:DT:H4'	5:I:28:DC:OP1	2.15	0.46
5:I:94:DG:H5''	7:O:905:LYS:CE	2.46	0.46
6:J:39:DG:H1'	6:J:40:DA:O4'	2.16	0.46
7:O:950:LYS:O	7:O:953:ASP:HB3	2.15	0.46
7:O:1026:MET:HG2	7:O:1029:TYR:CD2	2.37	0.46
7:O:1026:MET:HA	7:O:1029:TYR:CB	2.44	0.46
6:J:73:DA:H8	6:J:73:DA:OP2	1.98	0.45
6:J:82:DG:C2	6:J:83:DT:C2	3.04	0.45
6:J:105:DT:H2''	6:J:106:DG:C8	2.51	0.45
7:O:676:ASP:O	7:O:679:ILE:HB	2.16	0.45
7:O:685:GLN:O	7:O:688:ALA:HB3	2.17	0.45
7:O:778:MET:O	7:O:782:PHE:HD2	1.99	0.45
7:O:780:SER:C	7:O:784:ASN:HD22	2.20	0.45
7:O:1053:MET:HG3	7:O:1054:GLN:HE21	1.81	0.45
7:O:1207:ARG:NH2	7:O:1288:ALA:O	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:ARG:HD2	6:J:50:DT:H4'	1.98	0.45
3:C:28:GLY:HA3	6:J:30:DG:H3'	1.98	0.45
1:E:73:GLU:HB2	2:F:22:LEU:HB2	1.98	0.45
5:I:22:DG:C6	5:I:23:DC:N4	2.84	0.45
6:J:78:DG:H2'	6:J:78:DG:OP2	2.15	0.45
7:O:1092:LEU:HB3	7:O:1096:LEU:CD1	2.46	0.45
3:G:81:ARG:CZ	3:G:85:LEU:HD21	2.46	0.45
6:J:32:DG:H5'	6:J:32:DG:H8	1.82	0.45
7:O:1080:ASP:OD1	7:O:1125:TYR:OH	2.32	0.45
7:O:1086:ALA:HB3	7:O:1089:PHE:CE2	2.51	0.45
4:D:98:LEU:HD23	4:D:98:LEU:HA	1.74	0.45
3:G:47:ALA:HA	4:H:88:SER:HA	1.98	0.45
5:I:22:DG:C4	5:I:23:DC:C5	3.05	0.45
6:J:62:DA:C4	6:J:63:DC:C5	3.04	0.45
6:J:74:DG:C5	6:J:75:DC:C4	3.04	0.45
2:B:72:TYR:HB2	2:B:85:ASP:CG	2.36	0.45
5:I:61:DA:C4	5:I:62:DC:C5	3.04	0.45
6:J:16:DC:H1'	6:J:17:DT:C2	2.52	0.45
6:J:52:DG:N1	6:J:53:DG:C6	2.85	0.45
6:J:117:DA:H8	6:J:117:DA:OP2	1.99	0.45
6:J:121:DA:C5	6:J:122:DG:C6	3.04	0.45
6:J:133:DA:C4	6:J:134:DC:C5	3.05	0.45
6:J:137:DG:C6	6:J:138:DG:C6	3.04	0.45
6:J:139:DA:OP2	6:J:139:DA:H8	1.99	0.45
7:O:834:GLU:OE1	7:O:838:TRP:NE1	2.50	0.45
7:O:1062:PRO:HG2	7:O:1063:PHE:CD2	2.51	0.45
3:C:81:ARG:CZ	3:C:85:LEU:HD21	2.46	0.45
3:G:71:ARG:C	3:G:74:LYS:H	2.19	0.45
3:G:84:GLN:HE21	3:G:88:ARG:CG	2.29	0.45
5:I:24:DC:H2''	5:I:25:DG:N7	2.31	0.45
6:J:102:DA:H2''	6:J:103:DG:H8	1.82	0.45
7:O:768:LYS:HB2	7:O:770:TYR:CZ	2.52	0.45
7:O:874:GLU:O	7:O:877:ILE:HB	2.16	0.45
7:O:952:PHE:HB3	7:O:956:PHE:CE2	2.52	0.45
7:O:1133:LEU:HB3	7:O:1161:LEU:CD2	2.47	0.45
7:O:1179:ILE:HA	7:O:1209:LEU:HB2	1.99	0.45
1:A:61:LEU:HD23	1:A:61:LEU:HA	1.73	0.45
2:B:99:GLY:O	4:H:57:SER:OG	2.22	0.45
5:I:135:DA:C8	5:I:136:DT:H72	2.52	0.45
6:J:80:DA:OP2	6:J:80:DA:H8	1.99	0.45
7:O:674:THR:O	7:O:677:THR:OG1	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:884:SER:HB3	7:O:913:HIS:HA	1.99	0.45
7:O:1237:GLN:HE21	7:O:1253:LEU:HB3	1.82	0.45
4:D:36:ILE:HG13	4:D:37:TYR:N	2.32	0.45
4:D:97:LEU:HD23	4:D:97:LEU:HA	1.74	0.45
5:I:34:DG:H2'	5:I:35:DT:C6	2.52	0.45
6:J:143:DT:C6	6:J:144:DC:C4	3.05	0.45
7:O:907:SER:OG	7:O:908:LEU:N	2.50	0.45
7:O:938:LEU:CG	7:O:945:ILE:HG21	2.45	0.45
7:O:971:LEU:O	7:O:976:THR:HG23	2.17	0.45
7:O:1063:PHE:HB3	7:O:1069:GLU:H	1.82	0.45
2:B:62:LEU:HB3	2:B:66:ILE:HD12	1.98	0.45
1:E:116:ARG:NH2	1:E:122:LYS:HE3	2.32	0.45
5:I:52:DA:H1'	5:I:53:DC:H5'	1.99	0.45
5:I:85:DG:H2''	5:I:86:DT:O5'	2.17	0.45
6:J:74:DG:C4	6:J:75:DC:C4	3.05	0.45
6:J:92:DG:H1'	6:J:93:DC:H5'	1.99	0.45
6:J:138:DG:C4	6:J:139:DA:C5	3.05	0.45
7:O:1025:GLN:HG2	7:O:1029:TYR:CZ	2.51	0.45
4:H:36:ILE:HG13	4:H:37:TYR:N	2.32	0.45
5:I:68:DT:H2''	5:I:69:DA:C8	2.51	0.45
6:J:16:DC:H1'	6:J:17:DT:O4'	2.17	0.45
6:J:44:DA:H2'	6:J:45:DT:H6	1.78	0.45
7:O:682:LEU:C	7:O:944:LYS:HD2	2.37	0.45
7:O:935:TRP:HZ2	7:O:956:PHE:HB2	1.82	0.45
7:O:1016:SER:N	7:O:1019:GLN:HB2	2.32	0.45
7:O:1029:TYR:OH	7:O:1344:ALA:HB1	2.16	0.45
7:O:1093:ASP:OD2	7:O:1094:ARG:CZ	2.65	0.45
7:O:1164:ARG:HH11	7:O:1189:GLN:CA	2.30	0.45
3:C:88:ARG:HB2	3:C:108:LEU:HD21	1.99	0.44
5:I:67:DG:C2'	5:I:68:DT:H71	2.46	0.44
6:J:91:DA:C4	6:J:92:DG:C8	3.05	0.44
7:O:751:ILE:HB	7:O:784:ASN:HA	1.98	0.44
7:O:798:LYS:HA	7:O:801:GLN:OE1	2.17	0.44
7:O:1139:SER:O	7:O:1142:ARG:HB2	2.17	0.44
7:O:1230:ASP:CG	7:O:1264:ARG:HH11	2.19	0.44
7:O:1281:SER:O	7:O:1284:ASN:HB2	2.16	0.44
1:A:48:LEU:HG	2:B:44:LYS:HE3	2.00	0.44
1:A:116:ARG:NH2	1:A:122:LYS:HE3	2.32	0.44
2:B:45:ARG:HH21	5:I:81:DC:C4'	2.30	0.44
1:E:62:ILE:HB	1:E:93:GLN:HE21	1.83	0.44
6:J:74:DG:C2	6:J:75:DC:C2	3.05	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:82:DG:C5	6:J:83:DT:C4	3.05	0.44
7:O:876:ILE:O	7:O:880:ARG:CB	2.35	0.44
7:O:883:LEU:O	7:O:886:VAL:HG22	2.16	0.44
7:O:1207:ARG:NH1	7:O:1287:LEU:HA	2.20	0.44
1:A:54:TYR:HB3	2:B:40:ARG:HB2	1.99	0.44
2:F:32:PRO:HA	2:F:35:ARG:HD3	1.98	0.44
3:G:88:ARG:HB2	3:G:108:LEU:HD21	1.99	0.44
5:I:5:DA:H2''	5:I:6:DG:OP2	2.17	0.44
5:I:60:DA:H2''	5:I:61:DA:C8	2.52	0.44
5:I:88:DT:H2''	5:I:89:DT:O5'	2.17	0.44
5:I:96:DC:N3	6:J:53:DG:N1	2.65	0.44
5:I:127:DT:OP2	5:I:127:DT:H2'	2.17	0.44
7:O:1007:VAL:O	7:O:1207:ARG:HA	2.17	0.44
7:O:1063:PHE:CB	7:O:1068:VAL:HB	2.46	0.44
7:O:1096:LEU:HD23	7:O:1099:LEU:HD12	1.98	0.44
7:O:1299:ARG:HG2	7:O:1302:GLU:HG2	1.99	0.44
1:E:50:GLU:O	1:E:53:ARG:HB3	2.18	0.44
1:E:118:THR:HG23	2:F:45:ARG:O	2.17	0.44
5:I:33:DG:C2	5:I:34:DG:C4	3.06	0.44
5:I:79:DC:H2''	5:I:80:DC:C5	2.52	0.44
7:O:976:THR:HG22	7:O:979:VAL:HB	1.99	0.44
7:O:1047:GLY:HA2	7:O:1054:GLN:NE2	2.33	0.44
7:O:1149:PHE:CD1	7:O:1159:PHE:HB2	2.53	0.44
1:A:68:GLN:HE21	1:A:72:ARG:NE	2.04	0.44
1:A:130:ILE:HD13	1:A:130:ILE:HA	1.73	0.44
5:I:8:DA:C4	5:I:9:DT:C5	3.06	0.44
5:I:13:DG:H2''	5:I:14:DG:OP2	2.18	0.44
6:J:8:DG:O5'	6:J:8:DG:H8	2.01	0.44
6:J:139:DA:H2'	6:J:140:DT:O4'	2.18	0.44
7:O:830:ASN:O	7:O:833:SER:HB3	2.17	0.44
7:O:845:ILE:HB	7:O:869:VAL:HA	2.00	0.44
7:O:1086:ALA:HB3	7:O:1089:PHE:CD2	2.53	0.44
7:O:1226:TYR:CD2	7:O:1264:ARG:NH2	2.84	0.44
1:A:62:ILE:HB	1:A:93:GLN:HE21	1.83	0.44
1:A:68:GLN:NE2	1:A:72:ARG:HE	2.03	0.44
5:I:28:DC:H1'	5:I:29:DA:N9	2.32	0.44
5:I:76:DG:H2''	5:I:77:DT:OP2	2.17	0.44
5:I:78:DC:OP2	5:I:78:DC:H2'	2.18	0.44
6:J:38:DG:H1'	6:J:39:DG:H5'	2.00	0.44
6:J:100:DA:H2''	6:J:101:DG:OP2	2.17	0.44
6:J:140:DT:H2'	6:J:141:DT:C6	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:753:GLU:HB3	7:O:783:ASN:HD22	1.81	0.44
7:O:1283:ILE:O	7:O:1286:ILE:HG12	2.17	0.44
1:A:51:ILE:HG12	2:B:39:ARG:O	2.18	0.44
4:D:98:LEU:O	4:D:100:PRO:HD3	2.18	0.44
5:I:14:DG:C4	5:I:15:DT:C6	3.05	0.44
5:I:57:DT:H6	5:I:57:DT:H2'	1.60	0.44
6:J:107:DT:H2''	6:J:108:DC:C6	2.53	0.44
7:O:1062:PRO:HD3	7:O:1089:PHE:HE2	1.83	0.44
7:O:1170:LEU:HB2	7:O:1196:ARG:HD2	2.00	0.44
2:B:83:ALA:O	2:B:86:VAL:HB	2.18	0.44
3:C:100:VAL:HG13	2:F:96:THR:O	2.18	0.44
4:H:94:ALA:O	4:H:97:LEU:HB2	2.18	0.44
4:H:103:LEU:O	4:H:107:ALA:HB2	2.18	0.44
5:I:18:DC:OP2	5:I:18:DC:H2'	2.18	0.44
5:I:49:DA:OP2	5:I:49:DA:H2'	2.18	0.44
6:J:36:DA:C2	6:J:37:DG:C6	3.06	0.44
7:O:799:THR:HG21	7:O:834:GLU:HG3	2.00	0.44
7:O:805:LEU:O	7:O:808:TYR:HB3	2.18	0.44
7:O:935:TRP:HB3	7:O:939:ASN:OD1	2.18	0.44
7:O:1171:ASN:HB2	7:O:1199:ARG:HD2	1.98	0.44
4:D:103:LEU:O	4:D:107:ALA:HB2	2.18	0.44
4:H:83:ARG:HE	5:I:40:DG:H3'	1.82	0.44
5:I:4:DG:N1	6:J:145:DG:C6	2.86	0.44
5:I:43:DA:C4	5:I:44:DG:C8	3.06	0.44
5:I:59:DA:H2'	5:I:60:DA:H8	1.83	0.44
5:I:78:DC:H2''	5:I:79:DC:C5	2.53	0.44
5:I:88:DT:C2	5:I:89:DT:C4	3.06	0.44
5:I:124:DA:H1'	5:I:125:DC:O4'	2.18	0.44
6:J:50:DT:H2'	6:J:51:DT:C6	2.53	0.44
6:J:82:DG:C2	6:J:83:DT:N3	2.86	0.44
7:O:903:GLN:H	7:O:903:GLN:CD	2.21	0.44
7:O:938:LEU:HG	7:O:945:ILE:HD13	2.00	0.44
7:O:1061:HIS:CE1	7:O:1088:LYS:HD2	2.53	0.44
1:A:104:PHE:CE1	2:B:38:ALA:HB2	2.53	0.43
1:A:122:LYS:HA	1:A:125:GLN:NE2	2.33	0.43
1:E:122:LYS:HA	1:E:125:GLN:NE2	2.33	0.43
5:I:26:DC:C4	6:J:121:DA:N6	2.86	0.43
5:I:38:DT:H2''	5:I:39:DA:C8	2.52	0.43
5:I:139:DA:H1'	5:I:140:DC:C6	2.52	0.43
6:J:42:DT:N3	6:J:43:DA:C5	2.86	0.43
6:J:57:DT:H6	6:J:57:DT:H2'	1.69	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:678:ARG:O	7:O:682:LEU:HB2	2.18	0.43
7:O:910:LEU:O	7:O:914:TYR:N	2.50	0.43
7:O:981:ARG:CD	7:O:1238:ALA:HB2	2.48	0.43
7:O:1109:PHE:CB	7:O:1163:THR:HG22	2.43	0.43
7:O:1237:GLN:HE21	7:O:1253:LEU:CA	2.31	0.43
5:I:75:DT:H2''	5:I:76:DG:C8	2.53	0.43
6:J:69:DG:H2''	6:J:70:DG:N7	2.33	0.43
7:O:679:ILE:HG12	7:O:744:TYR:CZ	2.52	0.43
7:O:745:TYR:O	7:O:749:HIS:HD2	2.01	0.43
7:O:761:ILE:O	7:O:763:VAL:HG23	2.18	0.43
7:O:845:ILE:HB	7:O:869:VAL:HG22	1.99	0.43
7:O:981:ARG:HE	7:O:1241:PHE:HE2	1.66	0.43
7:O:1105:ARG:HG2	7:O:1157:LEU:HD23	2.00	0.43
1:A:40:ARG:NH2	5:I:83:DG:O4'	2.51	0.43
2:B:92:ARG:O	2:B:92:ARG:HG2	2.17	0.43
4:D:76:ARG:HB3	4:D:80:TYR:OH	2.18	0.43
5:I:12:DC:H2'	5:I:12:DC:OP2	2.18	0.43
5:I:80:DC:H1'	5:I:81:DC:C5	2.53	0.43
6:J:53:DG:C5'	7:O:1112:MET:HG2	2.48	0.43
6:J:84:DG:C4	6:J:85:DC:C4	3.07	0.43
6:J:100:DA:C6	6:J:101:DG:C2	3.07	0.43
7:O:843:ARG:HB2	7:O:867:ASP:H	1.83	0.43
7:O:857:LYS:O	7:O:860:LYS:HB3	2.18	0.43
7:O:907:SER:O	7:O:910:LEU:HB2	2.18	0.43
7:O:1021:ILE:O	7:O:1024:GLN:HB2	2.17	0.43
7:O:1113:THR:O	7:O:1132:ARG:NH2	2.51	0.43
7:O:1207:ARG:CG	7:O:1289:ARG:HH21	2.28	0.43
4:H:76:ARG:HB3	4:H:80:TYR:OH	2.18	0.43
5:I:35:DT:OP2	5:I:35:DT:H6	2.01	0.43
6:J:74:DG:OP2	6:J:74:DG:H2'	2.18	0.43
7:O:767:LEU:HD22	7:O:771:GLN:HB3	2.00	0.43
7:O:776:GLN:O	7:O:779:VAL:HB	2.17	0.43
7:O:1216:SER:H	7:O:1219:GLU:CD	2.22	0.43
1:A:50:GLU:O	1:A:53:ARG:HB3	2.18	0.43
1:A:81:ASP:OD1	7:O:1046:ARG:HG2	2.18	0.43
3:C:85:LEU:HD23	3:C:108:LEU:HD23	2.00	0.43
4:D:94:ALA:O	4:D:97:LEU:HB2	2.18	0.43
6:J:32:DG:C2	6:J:33:DA:C5	3.07	0.43
6:J:97:DG:H2''	6:J:98:DC:H6	1.83	0.43
7:O:929:ASN:O	7:O:931:LEU:HG	2.18	0.43
7:O:1056:LYS:O	7:O:1060:ASN:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:1291:ASP:O	7:O:1294:MET:HB2	2.19	0.43
3:G:85:LEU:HD23	3:G:108:LEU:HD23	2.00	0.43
4:H:98:LEU:O	4:H:100:PRO:HD3	2.18	0.43
5:I:18:DC:OP2	5:I:18:DC:H6	2.01	0.43
6:J:25:DG:H1'	6:J:26:DC:C6	2.54	0.43
6:J:91:DA:C6	6:J:92:DG:C6	3.07	0.43
6:J:100:DA:C4	6:J:101:DG:C4	3.06	0.43
7:O:1099:LEU:HD13	7:O:1106:VAL:HG21	1.99	0.43
7:O:1302:GLU:O	7:O:1305:SER:HB3	2.18	0.43
5:I:48:DT:H1'	5:I:49:DA:O4'	2.19	0.43
5:I:68:DT:H2''	5:I:69:DA:N7	2.33	0.43
5:I:87:DT:C6	5:I:88:DT:H72	2.52	0.43
6:J:95:DG:H2''	6:J:96:DT:OP2	2.19	0.43
6:J:113:DA:C4	6:J:114:DC:C5	3.07	0.43
6:J:115:DC:H2''	6:J:116:DA:C8	2.54	0.43
7:O:1184:ASP:HB3	7:O:1186:ASN:O	2.19	0.43
7:O:1187:PRO:O	7:O:1191:LEU:HG	2.18	0.43
2:B:73:THR:HG21	2:B:81:VAL:HG22	2.00	0.43
5:I:52:DA:C4	5:I:53:DC:C5	3.07	0.43
6:J:40:DA:H2''	6:J:41:DG:H8	1.83	0.43
6:J:74:DG:H2'	6:J:74:DG:P	2.57	0.43
6:J:90:DA:H4'	6:J:91:DA:H5'	2.01	0.43
6:J:133:DA:O5'	6:J:133:DA:H8	2.02	0.43
7:O:1192:GLN:HB3	7:O:1196:ARG:NH2	2.33	0.43
1:A:39:HIS:CD2	5:I:7:DA:H5'	2.53	0.43
1:A:104:PHE:O	1:A:105:GLU:C	2.57	0.43
6:J:2:DT:C2	6:J:3:DC:C5	3.07	0.43
6:J:101:DG:H2''	6:J:102:DA:OP2	2.19	0.43
6:J:121:DA:H2''	6:J:122:DG:C8	2.54	0.43
7:O:956:PHE:CZ	7:O:983:LEU:HD13	2.54	0.43
7:O:1227:LYS:O	7:O:1230:ASP:N	2.52	0.43
2:B:76:ALA:O	2:B:78:ARG:HG3	2.18	0.43
2:B:84:MET:HB3	2:B:88:TYR:CE2	2.54	0.43
3:G:32:ARG:CA	3:G:35:ARG:HH21	2.28	0.43
4:H:77:LEU:HD23	4:H:77:LEU:HA	1.79	0.43
5:I:79:DC:N4	6:J:68:DG:O6	2.52	0.43
6:J:32:DG:H2''	6:J:33:DA:C8	2.54	0.43
7:O:744:TYR:O	7:O:747:VAL:N	2.52	0.43
7:O:886:VAL:HG23	7:O:888:TRP:NE1	2.34	0.43
7:O:1025:GLN:NE2	7:O:1344:ALA:HB1	2.33	0.43
5:I:44:DG:N2	6:J:105:DT:C2	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:71:DG:C2	6:J:78:DG:C2	3.07	0.42
5:I:72:DC:H2''	5:I:73:DG:H8	1.83	0.42
5:I:90:DA:H4'	5:I:91:DA:OP1	2.19	0.42
5:I:110:DC:H1'	5:I:111:DC:O4'	2.18	0.42
5:I:128:DG:C8	5:I:129:DT:H72	2.53	0.42
6:J:3:DC:P	6:J:3:DC:H3'	2.58	0.42
6:J:104:DC:C2'	6:J:105:DT:H71	2.48	0.42
7:O:803:ILE:O	7:O:806:LEU:N	2.51	0.42
1:E:65:LEU:HG	6:J:92:DG:OP2	2.19	0.42
2:F:79:LYS:HG3	6:J:101:DG:O5'	2.19	0.42
2:F:97:LEU:HG	2:F:98:TYR:N	2.34	0.42
5:I:8:DA:C2	6:J:141:DT:N3	2.88	0.42
5:I:32:DT:C2	5:I:33:DG:C4	3.07	0.42
5:I:135:DA:H2'	5:I:136:DT:C7	2.49	0.42
6:J:91:DA:C6	6:J:92:DG:C5	3.07	0.42
6:J:124:DG:C4	6:J:125:DG:N7	2.88	0.42
6:J:139:DA:C2	6:J:140:DT:C2	3.07	0.42
7:O:788:GLY:O	7:O:920:LEU:HD12	2.19	0.42
2:B:88:TYR:O	2:B:89:ALA:C	2.58	0.42
3:C:24:GLN:HG2	3:C:56:GLU:OE2	2.19	0.42
4:D:87:THR:H	4:D:90:GLU:CD	2.23	0.42
5:I:98:DA:C6	5:I:99:DG:C6	3.08	0.42
6:J:61:DA:C4	6:J:62:DA:N7	2.88	0.42
6:J:69:DG:OP2	6:J:69:DG:H2'	2.19	0.42
6:J:96:DT:C2	6:J:97:DG:C4	3.07	0.42
6:J:124:DG:C4	6:J:125:DG:C5	3.07	0.42
7:O:1283:ILE:O	7:O:1287:LEU:HG	2.18	0.42
3:C:32:ARG:CA	3:C:35:ARG:HH21	2.28	0.42
1:E:41:TYR:OH	6:J:7:DT:H4'	2.19	0.42
1:E:104:PHE:O	1:E:105:GLU:C	2.57	0.42
5:I:13:DG:C6	5:I:14:DG:C6	3.07	0.42
5:I:111:DC:N4	6:J:36:DA:C6	2.88	0.42
6:J:45:DT:C2	6:J:46:DC:C5	3.07	0.42
6:J:82:DG:H2'	6:J:83:DT:H71	2.01	0.42
7:O:948:SER:O	7:O:952:PHE:HD2	2.02	0.42
7:O:972:SER:HA	7:O:976:THR:CG2	2.49	0.42
7:O:1024:GLN:HA	7:O:1027:LEU:HG	2.01	0.42
7:O:1025:GLN:O	7:O:1028:LYS:HB2	2.19	0.42
1:A:42:ARG:HG2	6:J:144:DC:O5'	2.19	0.42
2:F:88:TYR:O	2:F:92:ARG:HB3	2.19	0.42
3:G:64:GLU:HA	4:H:46:HIS:NE2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:3:DC:H2''	5:I:4:DG:OP2	2.19	0.42
5:I:58:DT:C4	5:I:59:DA:C6	3.07	0.42
6:J:19:DA:H2''	6:J:20:DC:OP2	2.20	0.42
6:J:23:DG:C4	6:J:24:DT:C5	3.08	0.42
6:J:37:DG:OP2	6:J:37:DG:H2'	2.19	0.42
6:J:41:DG:C4	6:J:42:DT:C4	3.07	0.42
6:J:63:DC:C2	6:J:64:DG:N7	2.88	0.42
6:J:91:DA:C5	6:J:92:DG:C5	3.07	0.42
6:J:124:DG:C4	6:J:125:DG:C8	3.07	0.42
7:O:1073:ASN:OD1	7:O:1075:THR:OG1	2.25	0.42
1:A:92:LEU:HA	1:A:92:LEU:HD23	1.70	0.42
1:A:119:ILE:HG13	2:B:50:ILE:HG13	2.00	0.42
5:I:53:DC:C2	5:I:54:DC:C4	3.07	0.42
5:I:59:DA:C6	5:I:60:DA:C6	3.07	0.42
5:I:88:DT:N3	5:I:89:DT:C4	2.88	0.42
5:I:136:DT:C4	5:I:137:DA:N6	2.88	0.42
7:O:929:ASN:C	7:O:931:LEU:HG	2.40	0.42
7:O:1259:ASP:O	7:O:1262:GLU:HB2	2.20	0.42
2:B:37:LEU:HA	2:B:37:LEU:HD23	1.62	0.42
4:D:30:ARG:HD3	5:I:123:DC:H4'	2.02	0.42
3:G:51:LEU:HD13	4:H:70:ILE:HG21	2.02	0.42
6:J:38:DG:H2''	6:J:39:DG:N7	2.35	0.42
6:J:132:DC:H2''	6:J:133:DA:N7	2.34	0.42
6:J:138:DG:C6	6:J:139:DA:C6	3.08	0.42
7:O:973:GLU:O	7:O:977:LEU:HG	2.19	0.42
3:G:79:ILE:HG12	3:G:82:HIS:CE1	2.55	0.42
5:I:101:DG:H2''	5:I:102:DG:C8	2.55	0.42
5:I:123:DC:H2''	5:I:124:DA:C8	2.54	0.42
5:I:139:DA:C4	5:I:140:DC:C4	3.07	0.42
6:J:29:DG:H1'	6:J:30:DG:C8	2.54	0.42
6:J:138:DG:H2''	6:J:139:DA:OP2	2.19	0.42
7:O:745:TYR:O	7:O:749:HIS:CD2	2.72	0.42
3:C:64:GLU:HA	4:D:46:HIS:CD2	2.54	0.42
5:I:34:DG:H5''	5:I:34:DG:H8	1.84	0.42
5:I:126:DG:N1	6:J:23:DG:C6	2.87	0.42
6:J:74:DG:H2''	6:J:75:DC:OP2	2.20	0.42
6:J:112:DG:C4	6:J:113:DA:N7	2.88	0.42
7:O:684:ARG:HH12	7:O:747:VAL:CG2	2.32	0.42
7:O:1098:LYS:HB3	7:O:1297:LEU:HD13	2.02	0.42
7:O:1258:LEU:HD12	7:O:1259:ASP:N	2.35	0.42
1:A:91:ALA:O	1:A:94:GLU:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:19:ARG:O	2:B:19:ARG:HG2	2.20	0.42
2:B:88:TYR:O	2:B:91:LYS:HB3	2.20	0.42
3:C:79:ILE:HG12	3:C:82:HIS:CE1	2.55	0.42
1:E:126:LEU:O	1:E:129:ARG:HB3	2.20	0.42
5:I:9:DT:C2	5:I:10:DC:C5	3.08	0.42
5:I:116:DC:H1'	5:I:117:DT:H5'	2.02	0.42
6:J:39:DG:C6	6:J:40:DA:C6	3.08	0.42
7:O:1230:ASP:O	7:O:1234:LYS:HB2	2.20	0.42
7:O:1293:GLU:O	7:O:1297:LEU:HG	2.20	0.42
3:C:43:VAL:N	5:I:113:DA:OP1	2.39	0.41
5:I:33:DG:H2''	5:I:34:DG:C8	2.55	0.41
5:I:81:DC:H5'	5:I:81:DC:C6	2.55	0.41
6:J:102:DA:C6	6:J:103:DG:C6	3.08	0.41
6:J:127:DC:H2'	6:J:128:DT:H72	2.02	0.41
7:O:1190:ASP:HA	7:O:1193:ALA:HB3	2.02	0.41
7:O:1253:LEU:HA	7:O:1256:SER:CB	2.49	0.41
1:E:103:LEU:HA	1:E:103:LEU:HD12	1.75	0.41
2:F:76:ALA:O	2:F:78:ARG:HG3	2.20	0.41
5:I:102:DG:C4	5:I:103:DA:C8	3.08	0.41
6:J:87:DT:H5''	6:J:88:DT:H71	2.01	0.41
6:J:112:DG:C2	6:J:113:DA:C5	3.08	0.41
7:O:679:ILE:HG23	7:O:744:TYR:CD1	2.56	0.41
7:O:938:LEU:CD1	7:O:945:ILE:HD13	2.50	0.41
7:O:1022:MET:O	7:O:1026:MET:HG3	2.21	0.41
7:O:1244:LYS:HB2	7:O:1249:GLU:HG3	2.02	0.41
2:B:71:THR:HG21	4:D:97:LEU:CD2	2.50	0.41
2:B:73:THR:OG1	2:B:85:ASP:OD2	2.20	0.41
3:G:24:GLN:HG2	3:G:56:GLU:OE2	2.19	0.41
5:I:8:DA:C2'	5:I:9:DT:H71	2.50	0.41
5:I:13:DG:H1'	5:I:14:DG:C8	2.55	0.41
5:I:63:DG:C5	5:I:64:DC:C4	3.08	0.41
6:J:46:DC:C2	6:J:47:DC:C4	3.08	0.41
7:O:890:HIS:HE1	7:O:892:ILE:HG13	1.85	0.41
7:O:901:ASN:HB3	7:O:904:SER:OG	2.19	0.41
7:O:1084:ARG:O	7:O:1317:LEU:HA	2.20	0.41
7:O:1119:MET:O	7:O:1120:GLU:C	2.58	0.41
7:O:1180:ILE:N	7:O:1209:LEU:O	2.52	0.41
7:O:1237:GLN:HA	7:O:1240:LYS:CE	2.50	0.41
1:E:63:ARG:O	1:E:66:PRO:HD2	2.20	0.41
2:F:83:ALA:O	2:F:86:VAL:HB	2.21	0.41
4:H:97:LEU:HD23	4:H:97:LEU:HA	1.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:14:DG:C5	5:I:15:DT:C5	3.09	0.41
6:J:18:DG:C2	6:J:19:DA:C2	3.09	0.41
6:J:49:DC:H2''	6:J:50:DT:OP2	2.21	0.41
6:J:57:DT:H2''	6:J:58:DT:C6	2.55	0.41
6:J:94:DG:C4	6:J:95:DG:C8	3.08	0.41
7:O:851:PRO:O	7:O:854:ARG:HB2	2.20	0.41
7:O:1016:SER:HB3	7:O:1085:VAL:O	2.20	0.41
7:O:1092:LEU:HA	7:O:1095:ILE:CG1	2.51	0.41
7:O:1117:ASP:HA	7:O:1132:ARG:HH12	1.84	0.41
3:C:47:ALA:HA	4:D:88:SER:HA	2.02	0.41
6:J:13:DT:O4	6:J:14:DA:N6	2.53	0.41
6:J:68:DG:C2	6:J:69:DG:C2	3.09	0.41
6:J:124:DG:C2	6:J:125:DG:C4	3.08	0.41
7:O:835:PHE:CD1	7:O:844:THR:HG21	2.55	0.41
7:O:905:LYS:O	7:O:909:THR:OG1	2.39	0.41
7:O:934:LEU:HD23	7:O:934:LEU:HA	1.88	0.41
7:O:935:TRP:O	7:O:936:ALA:C	2.58	0.41
7:O:1018:LEU:CA	7:O:1022:MET:HB2	2.38	0.41
7:O:1121:ASP:HA	7:O:1124:ARG:HD2	2.02	0.41
1:A:63:ARG:O	1:A:66:PRO:HD2	2.20	0.41
2:B:79:LYS:HZ2	5:I:101:DG:P	2.43	0.41
3:C:57:TYR:OH	4:D:106:HIS:HB2	2.19	0.41
3:C:64:GLU:HA	4:D:46:HIS:HE2	1.85	0.41
5:I:10:DC:H1'	5:I:11:DC:O5'	2.21	0.41
5:I:34:DG:C5	5:I:35:DT:C4	3.08	0.41
5:I:46:DT:H73	5:I:46:DT:OP2	2.21	0.41
6:J:13:DT:C4	6:J:14:DA:N6	2.88	0.41
7:O:1093:ASP:O	7:O:1097:PRO:HG2	2.20	0.41
1:E:91:ALA:O	1:E:94:GLU:HB2	2.20	0.41
3:G:44:GLY:N	4:H:86:ILE:O	2.36	0.41
5:I:20:DA:OP2	5:I:20:DA:H2'	2.20	0.41
5:I:49:DA:H2''	5:I:50:DG:OP2	2.20	0.41
5:I:139:DA:C2	6:J:10:DA:C2	3.09	0.41
6:J:42:DT:H2''	6:J:43:DA:O5'	2.19	0.41
6:J:45:DT:H2''	6:J:46:DC:C6	2.56	0.41
6:J:86:DG:H2''	6:J:87:DT:O5'	2.21	0.41
6:J:144:DC:C4	6:J:145:DG:O6	2.74	0.41
7:O:678:ARG:HD3	7:O:948:SER:HB2	2.01	0.41
7:O:791:ALA:HB1	7:O:993:ARG:HH11	1.85	0.41
7:O:1053:MET:O	7:O:1057:LYS:HB2	2.20	0.41
7:O:1080:ASP:HA	7:O:1083:TRP:NE1	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:1099:LEU:HD23	7:O:1099:LEU:HA	1.88	0.41
7:O:1241:PHE:HB3	7:O:1253:LEU:HD12	2.01	0.41
3:C:81:ARG:NE	3:C:85:LEU:HD11	2.36	0.41
3:C:93:LEU:HD23	3:C:93:LEU:HA	1.81	0.41
5:I:6:DG:C6	5:I:7:DA:C6	3.08	0.41
6:J:73:DA:C2	6:J:74:DG:C5	3.09	0.41
7:O:960:PHE:HA	7:O:972:SER:HB3	2.02	0.41
7:O:1027:LEU:HA	7:O:1030:ARG:HD3	2.03	0.41
7:O:1217:VAL:HA	7:O:1220:VAL:HG23	2.03	0.41
1:A:39:HIS:CE1	5:I:7:DA:H4'	2.55	0.41
1:A:120:MET:C	2:B:50:ILE:HD11	2.42	0.41
1:A:126:LEU:O	1:A:129:ARG:HB3	2.20	0.41
4:D:53:SER:O	4:D:56:MET:N	2.54	0.41
1:E:61:LEU:HA	1:E:61:LEU:HD23	1.74	0.41
3:G:93:LEU:HD23	3:G:93:LEU:HA	1.81	0.41
4:H:43:LYS:NZ	4:H:47:PRO:O	2.33	0.41
4:H:87:THR:H	4:H:90:GLU:CD	2.23	0.41
5:I:49:DA:H1'	5:I:50:DG:C8	2.56	0.41
5:I:59:DA:C2'	5:I:60:DA:C8	3.04	0.41
5:I:101:DG:H2''	5:I:102:DG:H8	1.85	0.41
5:I:113:DA:C4	5:I:114:DG:C8	3.08	0.41
6:J:89:DT:H2''	6:J:90:DA:OP2	2.21	0.41
6:J:92:DG:C6	6:J:93:DC:C4	3.09	0.41
6:J:113:DA:H1'	6:J:114:DC:H5'	2.03	0.41
6:J:124:DG:H2''	6:J:125:DG:H8	1.85	0.41
6:J:128:DT:OP2	6:J:128:DT:H2'	2.20	0.41
6:J:137:DG:C2	6:J:138:DG:C4	3.09	0.41
7:O:948:SER:O	7:O:951:SER:OG	2.16	0.41
7:O:1062:PRO:HB3	7:O:1085:VAL:HG21	2.03	0.41
7:O:1110:PHE:O	7:O:1163:THR:HG23	2.20	0.41
7:O:1171:ASN:HD21	7:O:1173:GLN:CD	2.24	0.41
7:O:1229:LEU:HD23	7:O:1229:LEU:HA	1.86	0.41
3:C:115:LEU:HD13	2:F:44:LYS:HB2	2.03	0.41
1:E:96:SER:O	1:E:99:TYR:HB3	2.21	0.41
5:I:25:DG:O5'	5:I:25:DG:H8	2.04	0.41
5:I:100:DG:N2	6:J:49:DC:C2	2.89	0.41
6:J:46:DC:H1'	6:J:47:DC:O5'	2.21	0.41
6:J:110:DA:C4	6:J:111:DC:C5	3.09	0.41
7:O:995:LEU:HD23	7:O:995:LEU:HA	1.84	0.41
7:O:1122:PHE:O	7:O:1125:TYR:HB3	2.21	0.41
7:O:1126:ILE:HB	7:O:1128:ILE:HG13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:1205:GLU:OE1	7:O:1289:ARG:HG2	2.21	0.41
5:I:21:DG:H2''	5:I:22:DG:C8	2.56	0.40
5:I:39:DA:N6	6:J:108:DC:C4	2.89	0.40
5:I:86:DT:H2''	5:I:87:DT:C6	2.55	0.40
6:J:31:DA:C2	6:J:32:DG:C5	3.09	0.40
6:J:134:DC:C2	6:J:135:DC:C4	3.09	0.40
7:O:751:ILE:N	7:O:784:ASN:OD1	2.54	0.40
7:O:835:PHE:CE2	7:O:870:LEU:HD22	2.56	0.40
7:O:1143:SER:HA	7:O:1146:LEU:HD12	2.02	0.40
1:A:96:SER:O	1:A:99:TYR:HB3	2.21	0.40
1:E:65:LEU:HB3	1:E:69:ARG:NH1	2.37	0.40
3:G:54:VAL:O	3:G:58:LEU:HG	2.20	0.40
5:I:37:DG:H8	5:I:37:DG:OP2	2.04	0.40
5:I:60:DA:H2''	5:I:61:DA:H8	1.85	0.40
6:J:56:DG:H1'	6:J:57:DT:C5'	2.51	0.40
7:O:767:LEU:HD12	7:O:772:ILE:HG13	2.03	0.40
7:O:828:LEU:HG	7:O:870:LEU:HD21	2.02	0.40
7:O:1143:SER:O	7:O:1146:LEU:HB2	2.21	0.40
1:A:100:LEU:O	1:A:101:VAL:C	2.60	0.40
3:C:34:LEU:HD23	3:C:34:LEU:HA	1.72	0.40
3:C:54:VAL:O	3:C:58:LEU:HG	2.20	0.40
4:D:43:LYS:O	4:D:47:PRO:HG3	2.22	0.40
1:E:105:GLU:HG2	2:F:41:GLY:O	2.22	0.40
4:H:43:LYS:O	4:H:47:PRO:HG3	2.22	0.40
5:I:110:DC:N3	6:J:37:DG:N2	2.69	0.40
5:I:123:DC:C4	5:I:124:DA:N6	2.89	0.40
6:J:71:DA:C4	6:J:72:DC:C6	3.09	0.40
6:J:142:DC:N3	6:J:143:DT:C4	2.89	0.40
7:O:787:ASN:HB2	7:O:941:VAL:HG13	2.04	0.40
7:O:813:LYS:HB3	7:O:815:ILE:HG13	2.03	0.40
7:O:929:ASN:CG	7:O:1231:ILE:HG22	2.42	0.40
7:O:988:ARG:HA	7:O:1242:ASP:OD1	2.22	0.40
7:O:1184:ASP:OD1	7:O:1190:ASP:HB2	2.21	0.40
7:O:1339:GLU:HA	7:O:1342:SER:OG	2.20	0.40
2:B:50:ILE:O	2:B:51:TYR:C	2.60	0.40
1:E:130:ILE:HD13	1:E:130:ILE:HA	1.73	0.40
4:H:53:SER:O	4:H:56:MET:N	2.54	0.40
5:I:23:DC:H6	5:I:23:DC:O5'	2.03	0.40
5:I:102:DG:C2'	5:I:103:DA:C8	3.04	0.40
5:I:110:DC:C4	6:J:37:DG:N1	2.90	0.40
6:J:60:DA:H2''	6:J:61:DA:C8	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:134:DC:C4	6:J:135:DC:N4	2.89	0.40
7:O:770:TYR:CE1	7:O:771:GLN:HG3	2.56	0.40
7:O:775:LEU:O	7:O:779:VAL:HG23	2.21	0.40
7:O:1148:LEU:HA	7:O:1148:LEU:HD23	1.87	0.40
7:O:1173:GLN:HG2	7:O:1197:ALA:O	2.21	0.40
1:A:103:LEU:HD12	1:A:103:LEU:HA	1.75	0.40
1:E:100:LEU:O	1:E:103:LEU:N	2.55	0.40
3:G:14:ALA:CB	5:I:32:DT:H5''	2.51	0.40
3:G:29:ARG:HG3	3:G:32:ARG:NH2	2.36	0.40
6:J:128:DT:C4'	6:J:129:DC:H5'	2.51	0.40
7:O:678:ARG:CZ	7:O:952:PHE:CE2	3.04	0.40
7:O:758:GLN:HB2	7:O:762:LEU:HD22	2.04	0.40
7:O:884:SER:HB3	7:O:913:HIS:CD2	2.56	0.40
7:O:935:TRP:N	7:O:935:TRP:CD1	2.87	0.40
7:O:981:ARG:NE	7:O:1238:ALA:HB2	2.37	0.40
7:O:1117:ASP:HA	7:O:1132:ARG:NH1	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	96/135 (71%)	88 (92%)	8 (8%)	0	100	100
1	E	93/135 (69%)	85 (91%)	8 (9%)	0	100	100
2	B	85/102 (83%)	69 (81%)	15 (18%)	1 (1%)	13	50
2	F	84/102 (82%)	81 (96%)	3 (4%)	0	100	100
3	C	105/129 (81%)	99 (94%)	6 (6%)	0	100	100
3	G	105/129 (81%)	99 (94%)	6 (6%)	0	100	100
4	D	91/122 (75%)	83 (91%)	8 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	H	91/122 (75%)	83 (91%)	8 (9%)	0	100	100
7	O	569/735 (77%)	483 (85%)	81 (14%)	5 (1%)	17	56
All	All	1319/1711 (77%)	1170 (89%)	143 (11%)	6 (0%)	32	68

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	26	ILE
7	O	1163	THR
7	O	958	THR
7	O	979	VAL
7	O	679	ILE
7	O	1220	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	84/110 (76%)	84 (100%)	0	100	100
1	E	82/110 (74%)	82 (100%)	0	100	100
2	B	72/78 (92%)	72 (100%)	0	100	100
2	F	67/78 (86%)	67 (100%)	0	100	100
3	C	81/101 (80%)	81 (100%)	0	100	100
3	G	82/101 (81%)	82 (100%)	0	100	100
4	D	77/102 (76%)	77 (100%)	0	100	100
4	H	79/102 (78%)	79 (100%)	0	100	100
7	O	525/667 (79%)	525 (100%)	0	100	100
All	All	1149/1449 (79%)	1149 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	HIS
1	A	68	GLN
3	C	38	ASN
3	C	84	GLN
4	D	79	HIS
1	E	68	GLN
2	F	93	GLN
3	G	38	ASN
3	G	84	GLN
4	H	79	HIS
7	O	749	HIS
7	O	784	ASN
7	O	801	GLN
7	O	928	GLN
7	O	929	ASN
7	O	939	ASN
7	O	1025	GLN
7	O	1051	GLN
7	O	1054	GLN
7	O	1111	GLN
7	O	1171	ASN
7	O	1198	HIS
7	O	1237	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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.

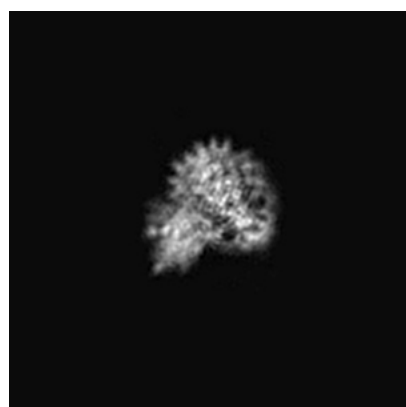
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6700. These allow visual inspection of the internal detail of the map and identification of artifacts.

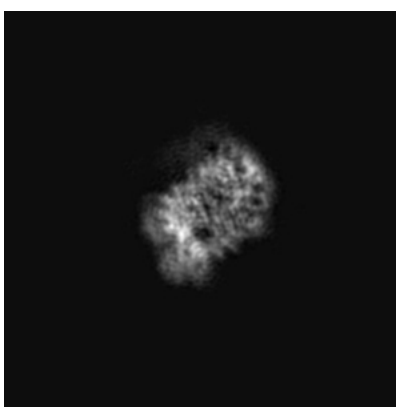
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

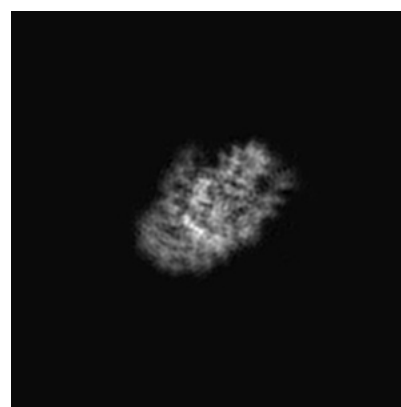
6.1.1 Primary map



X



Y

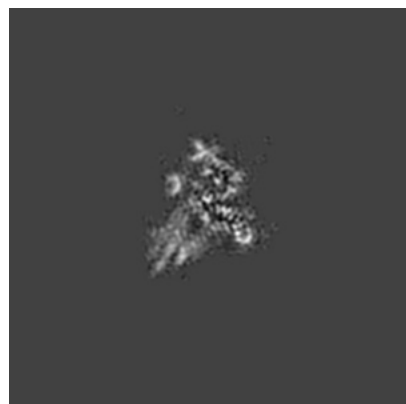


Z

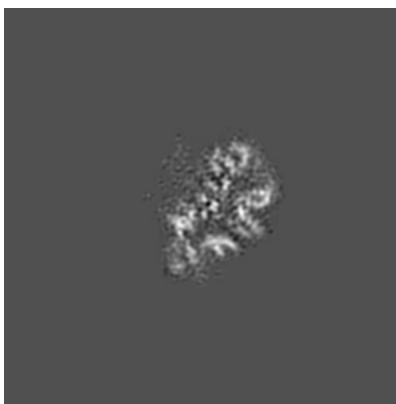
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

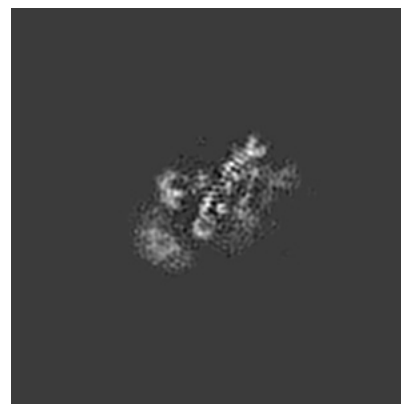
6.2.1 Primary map



X Index: 128



Y Index: 128

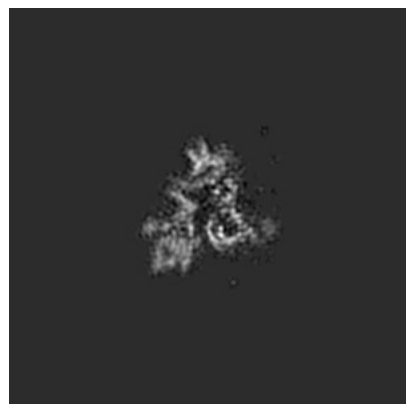


Z Index: 128

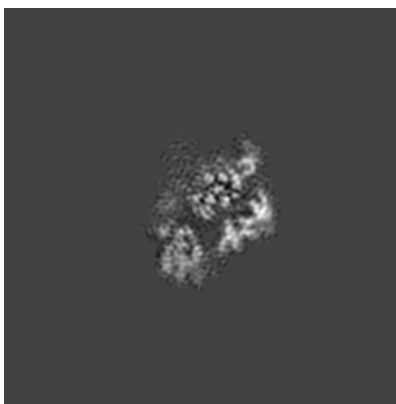
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

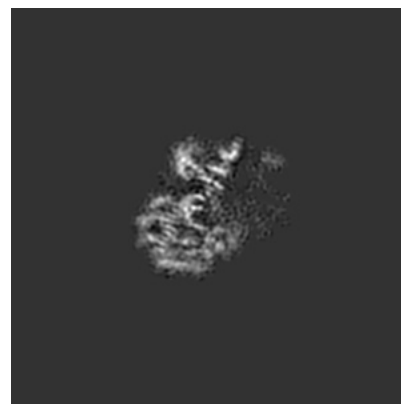
6.3.1 Primary map



X Index: 118



Y Index: 122

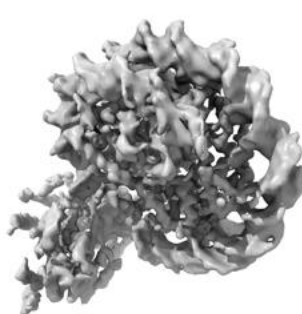


Z Index: 113

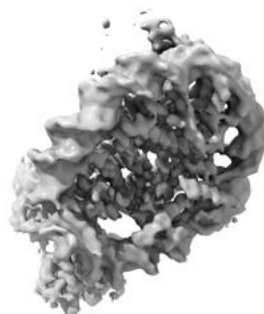
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

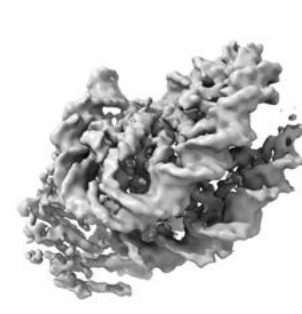
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0341. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

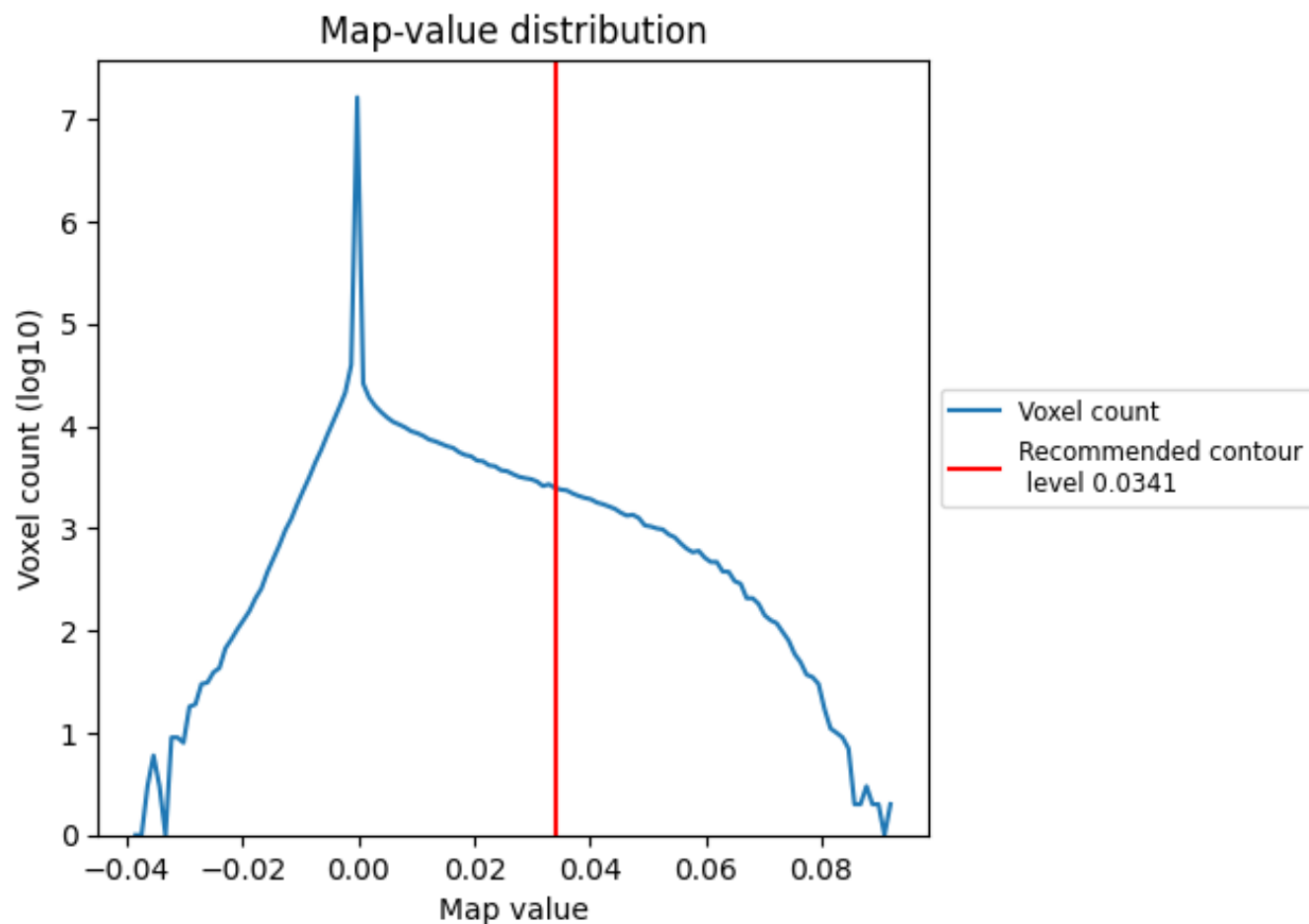
6.5 Mask visualisation

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

7 Map analysis [i](#)

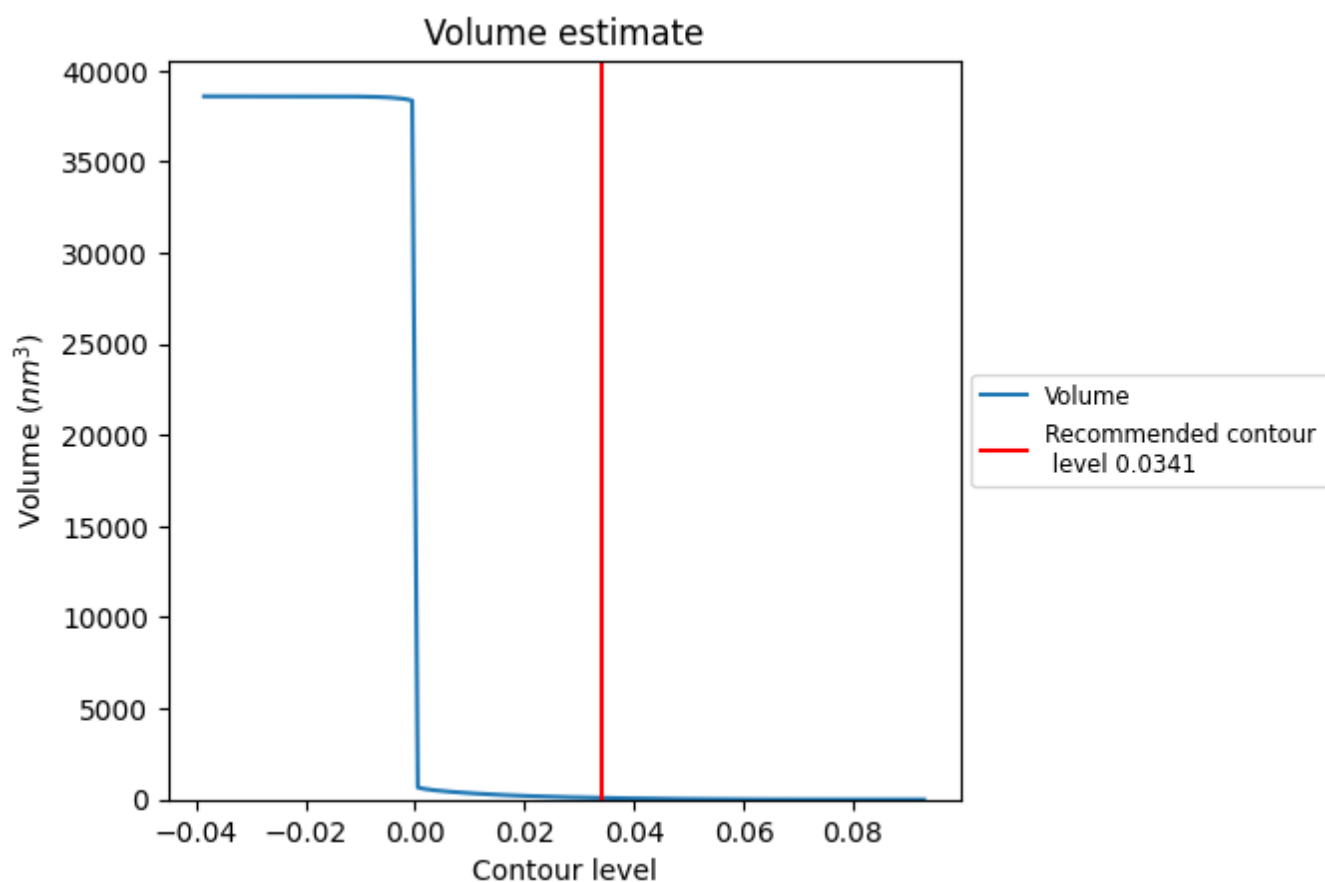
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

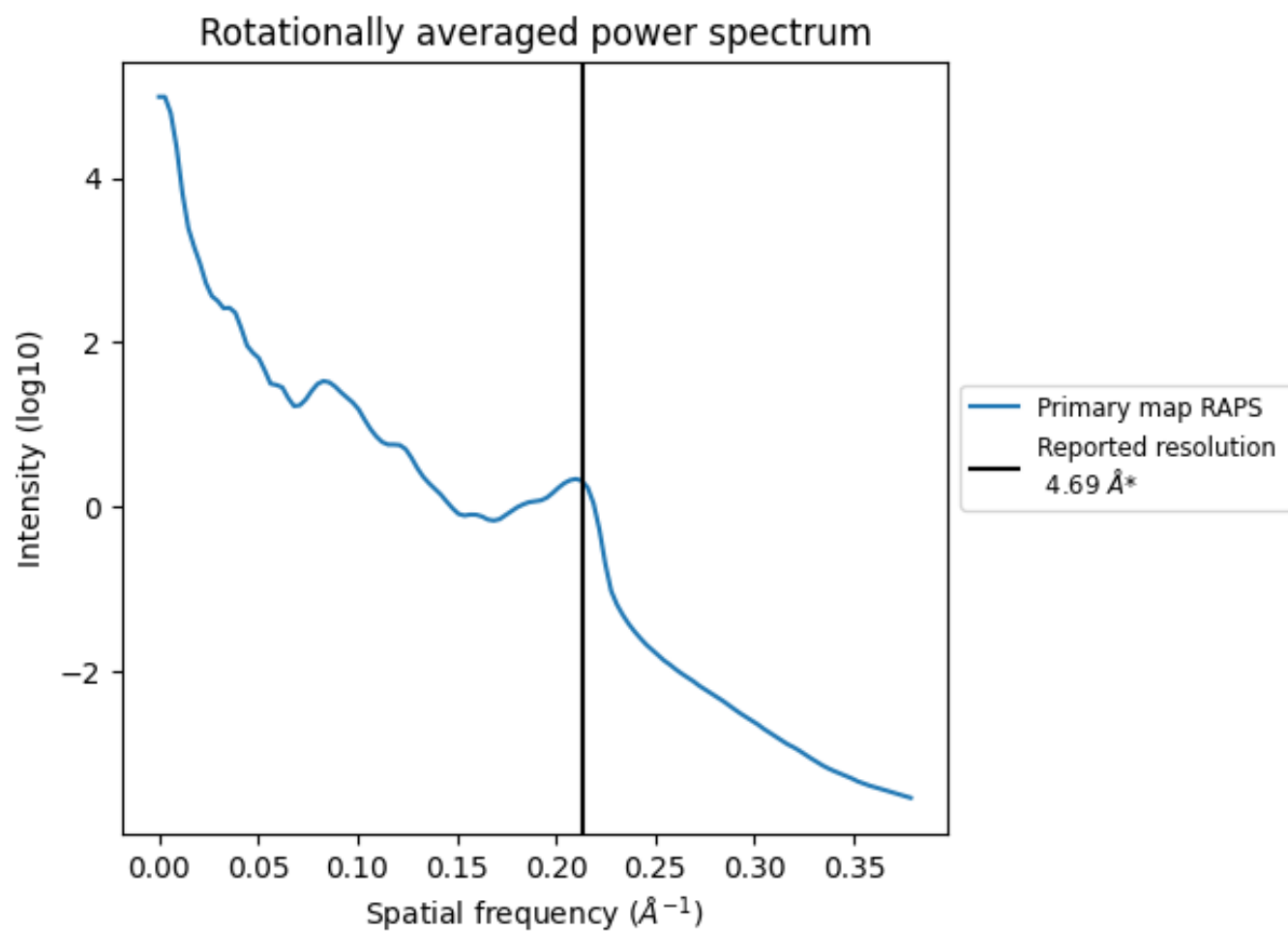
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 91 nm³; this corresponds to an approximate mass of 82 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.213 Å⁻¹

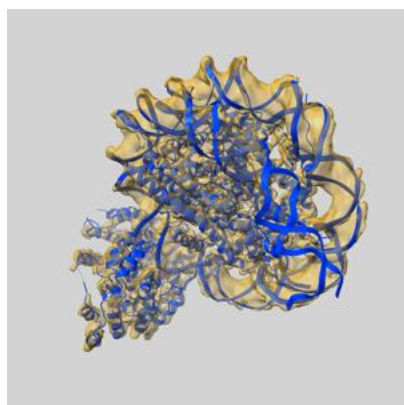
8 Fourier-Shell correlation

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

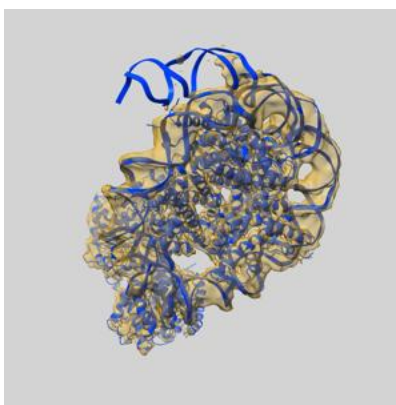
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-6700 and PDB model 5X0Y. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

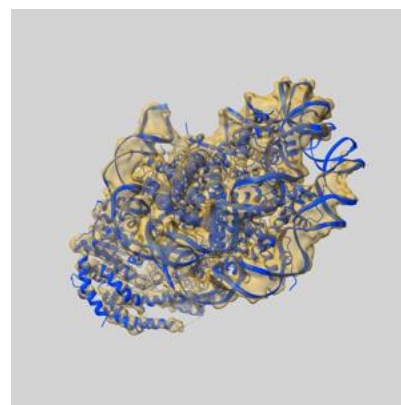
9.1 Map-model overlay [i](#)



X



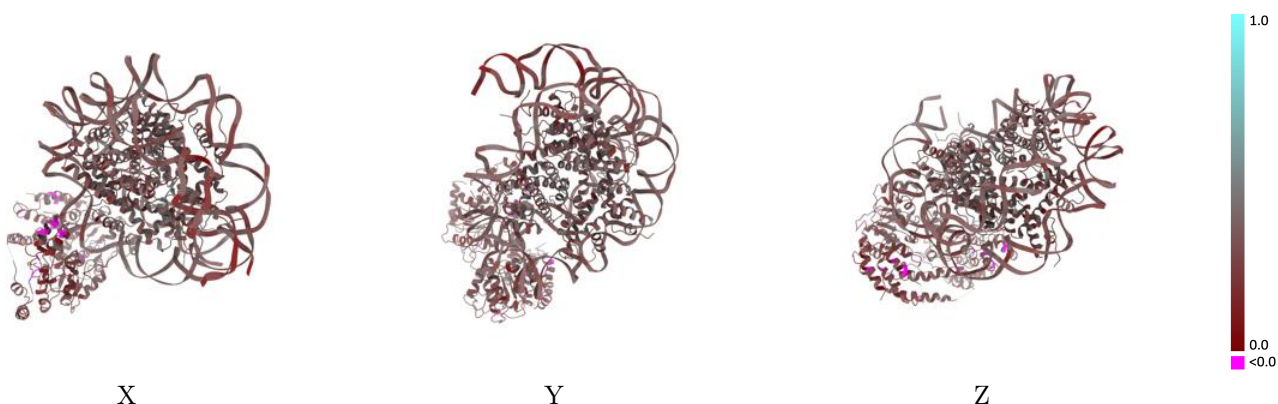
Y



Z

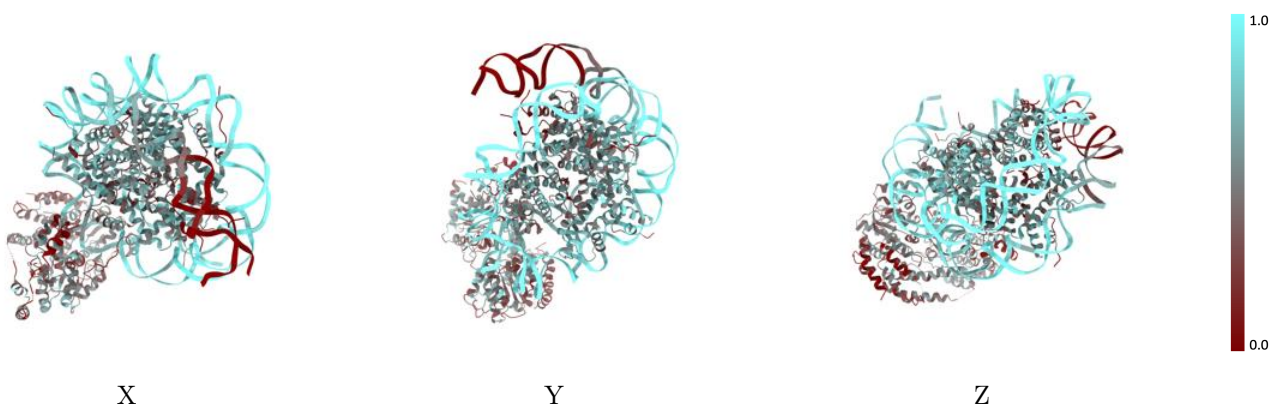
The images above show the 3D surface view of the map at the recommended contour level 0.0341 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



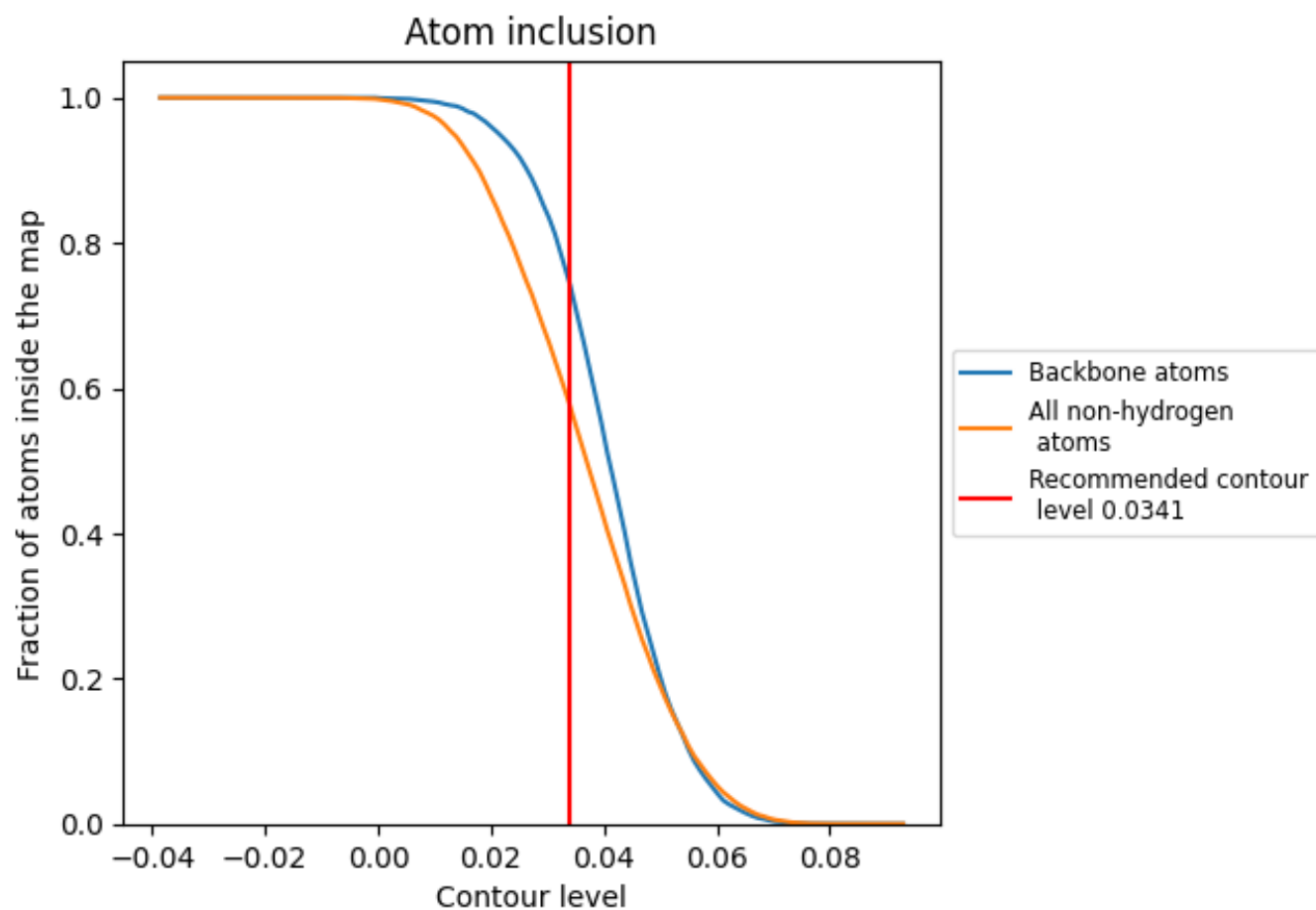
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0341).

9.4 Atom inclusion ⓘ



At the recommended contour level, 74% of all backbone atoms, 57% 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 (0.0341) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.5737	<div></div> 0.3150
A	<div></div> 0.5318	<div></div> 0.3630
B	<div></div> 0.5201	<div></div> 0.3700
C	<div></div> 0.4377	<div></div> 0.3190
D	<div></div> 0.5492	<div></div> 0.3320
E	<div></div> 0.5073	<div></div> 0.3590
F	<div></div> 0.5293	<div></div> 0.3620
G	<div></div> 0.5443	<div></div> 0.3520
H	<div></div> 0.6008	<div></div> 0.3590
I	<div></div> 0.7782	<div></div> 0.3240
J	<div></div> 0.7811	<div></div> 0.3270
O	<div></div> 0.3692	<div></div> 0.2570

1.0

0.0

<0.0