



Full wwPDB EM Validation Report ⓘ

Mar 22, 2025 – 05:46 PM EDT

PDB ID : 6WKR
EMDB ID : EMD-21707
Title : PRC2-AEBP2-JARID2 bound to H2AK119ub1 nucleosome
Authors : Kasinath, V.; Nogales, E.; Beck, C.; Sauer, P.; Poepsel, S.; Kosmatka, J.;
Faini, M.; Toso, D.; Aebersold, R.
Deposited on : 2020-04-16
Resolution : 3.50 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.dev117
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41.4

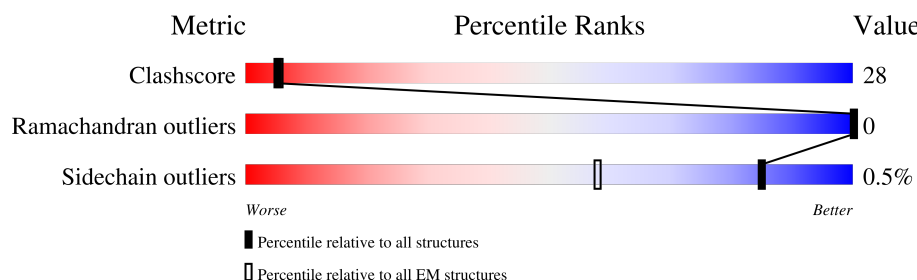
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 Å.

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



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

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	F	76	<div> <div>57%</div> <div>51%</div> <div>49%</div> </div>
1	T	76	<div> <div>84%</div> <div>55%</div> <div>45%</div> </div>
2	A	739	<div> <div>35%</div> <div>25%</div> <div>41%</div> </div>
3	L	441	<div> <div>41%</div> <div>41%</div> <div>18%</div> </div>
4	N	425	<div> <div>42%</div> <div>51%</div> <div>7%</div> </div>
5	C	746	<div> <div>53%</div> <div>28%</div> <div>19%</div> </div>
6	B	450	<div> <div>5%</div> <div>91%</div> </div>
6	E	450	<div> <div>6%</div> <div>7%</div> <div>92%</div> </div>

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Mol	Chain	Length	Quality of chain
7	P	295	
8	H	320	
9	I	136	
9	O	136	
10	J	103	
10	Q	103	
11	K	130	
11	R	130	
12	M	126	
12	S	126	

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 29296 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 Ubiquitin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	T	76	Total	C	N	O	S	0	0
			604	379	105	118	2		
1	F	76	Total	C	N	O	S	0	0
			603	379	105	117	2		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	76	CYS	GLY	engineered mutation	UNP P0CG48
F	76	CYS	GLY	engineered mutation	UNP P0CG48

- Molecule 2 is a protein called Polycomb protein SUZ12.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	439	Total	C	N	O	S	0	0
			3340	2146	603	568	23		

- Molecule 3 is a protein called Polycomb protein EED.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	362	Total	C	N	O	S	0	0
			2874	1822	503	528	21		

- Molecule 4 is a protein called Histone-binding protein RBBP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	N	395	Total	C	N	O	S	0	0
			3080	1950	530	591	9		

- Molecule 5 is a protein called Histone-lysine N-methyltransferase EZH2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	C	606	Total	C	N	O	S	0	0
			4278	2684	779	777	38		

- Molecule 6 is a protein called Protein Jumonji.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	42	Total	C	N	O	S	0	0
			290	181	55	53	1		
6	E	35	Total	C	N	O		0	0
			203	125	39	39			

- Molecule 7 is a protein called Zinc finger protein AEBP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	P	193	Total	C	N	O	S	0	0
			1346	853	260	228	5		

- Molecule 8 is a DNA chain called DNA (314-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	314	Total	C	N	O	P	0	0
			6439	3048	1191	1886	314		

- Molecule 9 is a protein called Histone H3.2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	117	Total	C	N	O	S	0	0
			935	586	183	163	3		
9	O	99	Total	C	N	O	S	0	0
			816	514	158	141	3		

- Molecule 10 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	83	Total	C	N	O	S	0	0
			662	418	129	114	1		
10	Q	87	Total	C	N	O	S	0	0
			667	419	129	118	1		

- Molecule 11 is a protein called Histone H2A type 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	108	Total	C	N	O	S	0	0
			825	519	161	144	1		
11	R	108	Total	C	N	O	S	0	0
			829	522	162	144	1		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	99	ARG	GLY	conflict	UNP P06897
K	119	CYS	LYS	conflict	UNP P06897
R	99	ARG	GLY	conflict	UNP P06897
R	119	CYS	LYS	conflict	UNP P06897

- Molecule 12 is a protein called Histone H2B 1.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	95	Total	C	N	O	S	0	0
			736	463	132	139	2		
12	S	96	Total	C	N	O	S	0	0
			741	466	133	140	2		

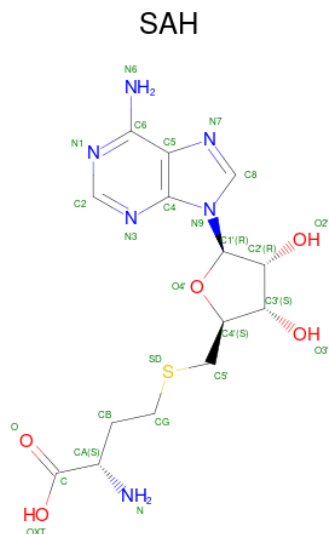
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	29	THR	SER	engineered mutation	UNP P02281
S	29	THR	SER	engineered mutation	UNP P02281

- Molecule 13 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

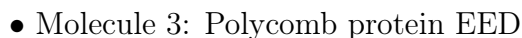
- Molecule 14 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: C₁₄H₂₀N₆O₅S) (labeled as "Ligand of Interest" by depositor).



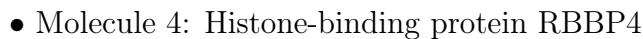
Mol	Chain	Residues	Atoms					AltConf
14	C	1	Total	C	N	O	S	0
			26	14	6	5	1	

- Molecule 15 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
15	P	1	Total Zn 1 1	0

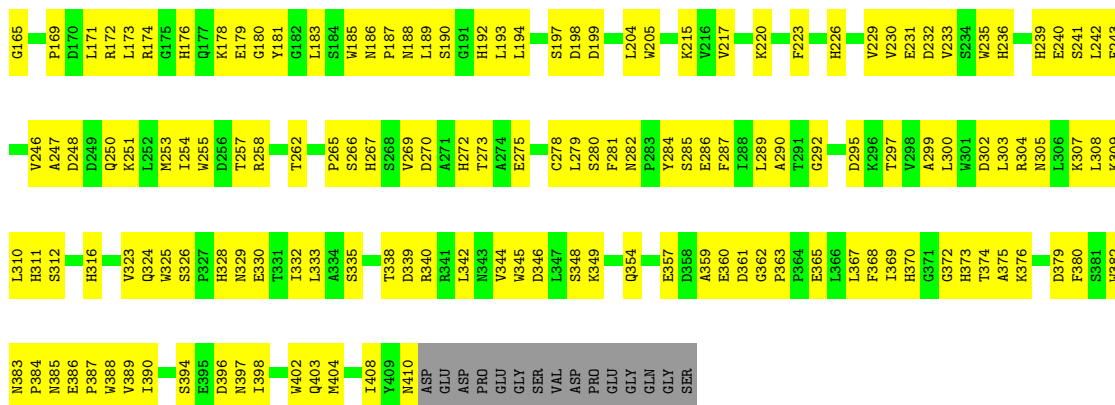


Government	Percentage
Current government	41%
Previous government	41%
Opposition	18%

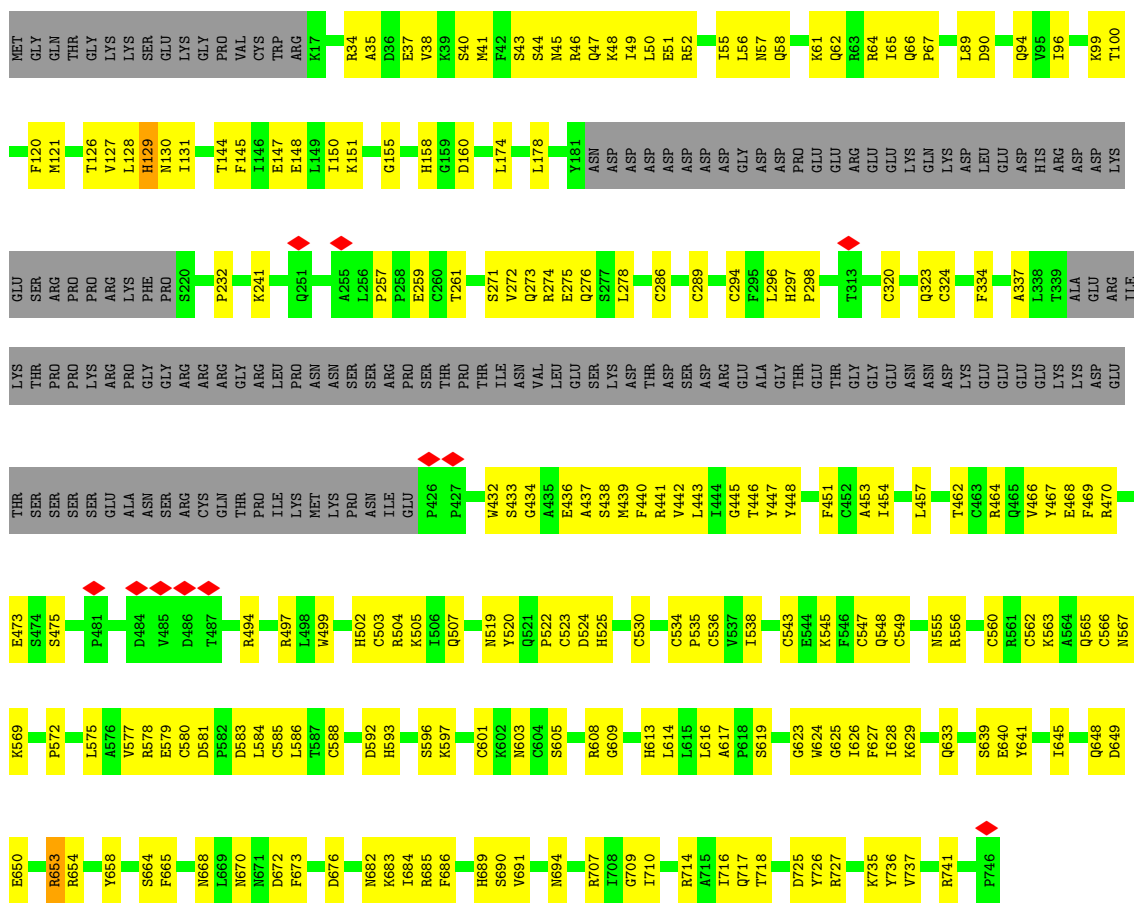


Response	Percentage
Yes, the U.S. should take action to protect the environment	42%
No, the U.S. should not take action to protect the environment	51%
Don't know	7%



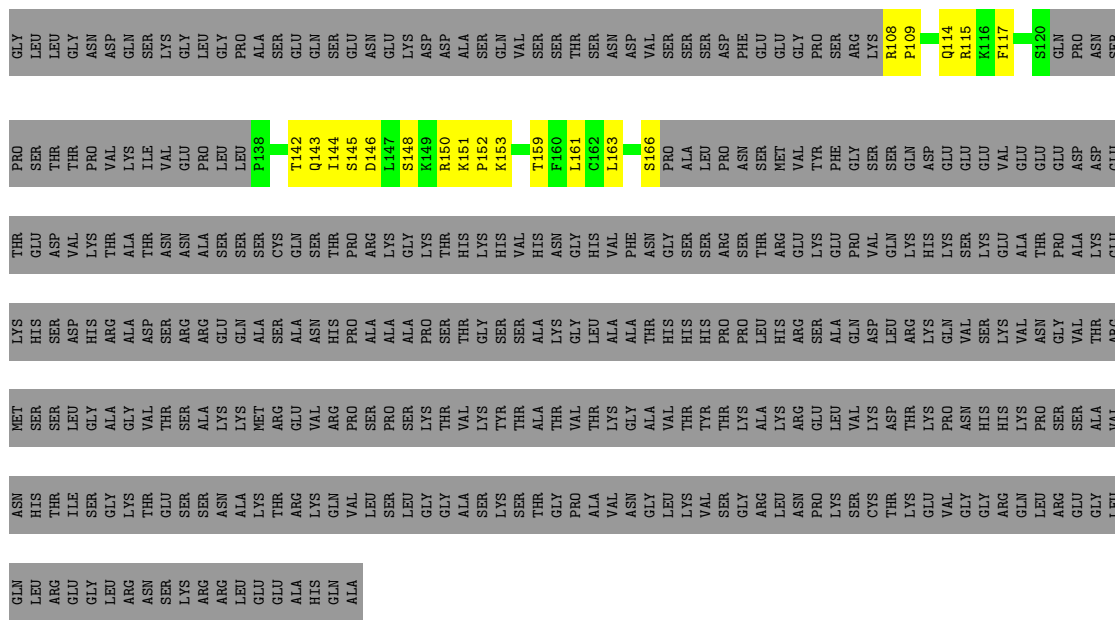


• Molecule 5: Histone-lysine N-methyltransferase EZH2

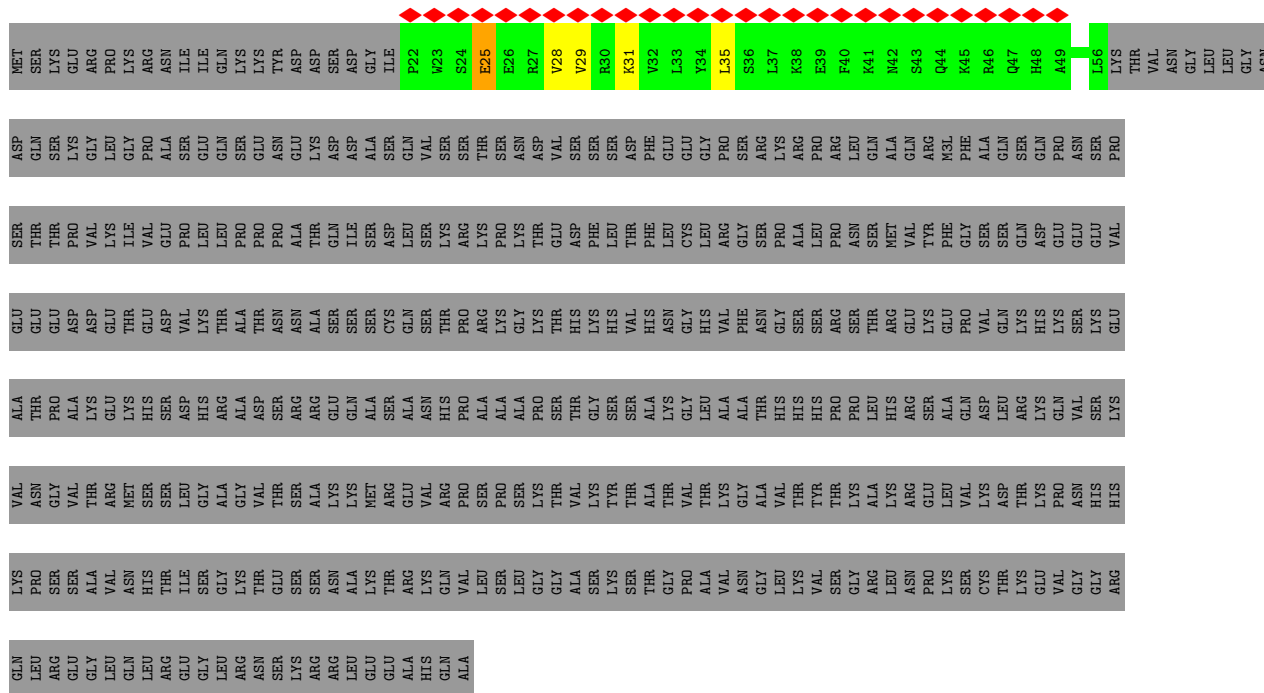


• Molecule 6: Protein Jumonji





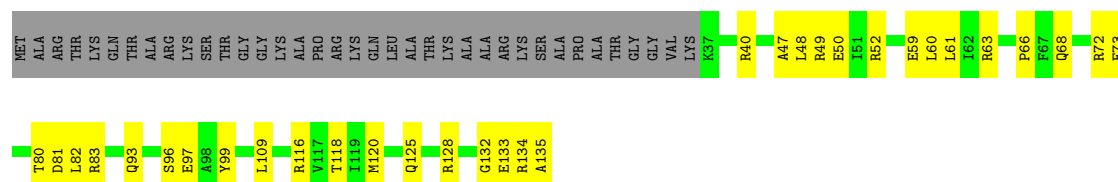
- Molecule 6: Protein Jumonji



- Molecule 7: Zinc finger protein AEBP2



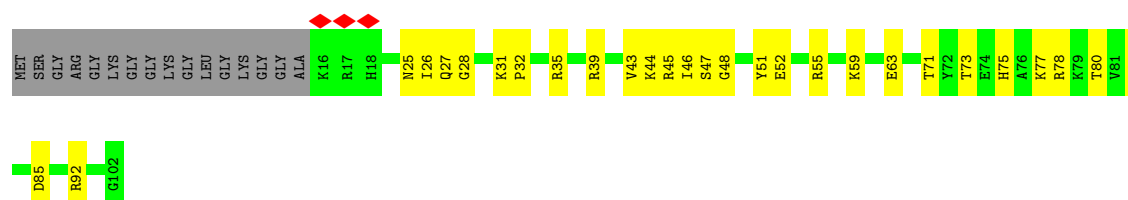




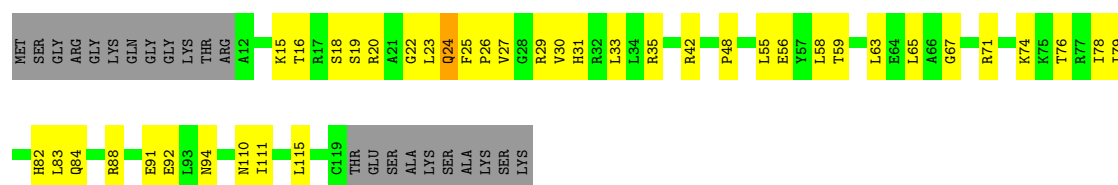
- Molecule 10: Histone H4



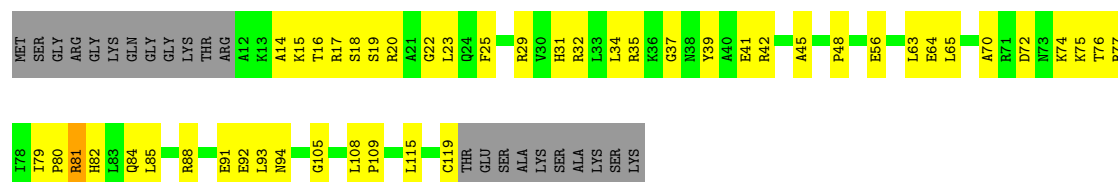
- Molecule 10: Histone H4



- Molecule 11: Histone H2A type 1

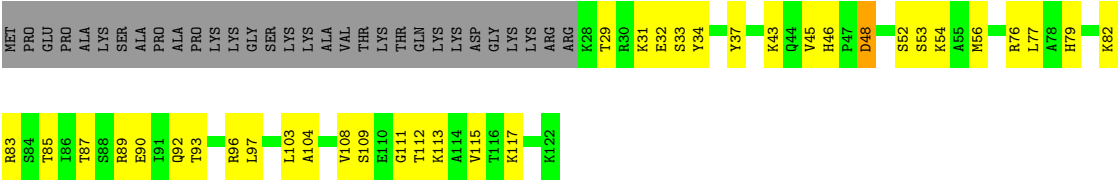


- Molecule 11: Histone H2A type 1



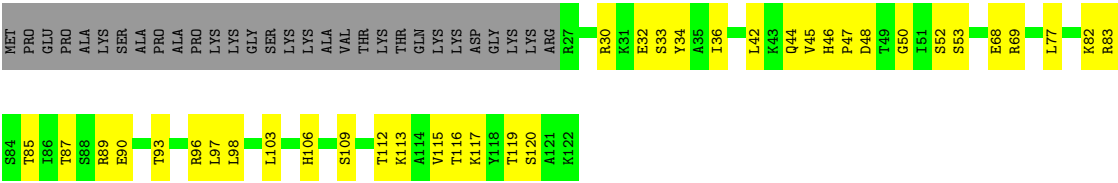
- Molecule 12: Histone H2B 1.1

Chain M: 47% 28% 25%



● Molecule 12: Histone H2B 1.1

Chain S: 47% 29% 24%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	168601	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)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.088	Depositor
Minimum map value	-0.032	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	441.2928, 441.2928, 441.2928	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1492, 1.1492, 1.1492	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: M3L, MG, SAH, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	F	0.25	0/609	0.47	0/819
1	T	0.25	0/610	0.50	0/819
2	A	0.37	0/3419	0.47	0/4636
3	L	0.44	0/2948	0.53	0/4004
4	N	0.37	0/3165	0.50	0/4322
5	C	0.43	0/4375	0.48	0/5964
6	B	0.31	0/282	0.54	0/382
6	E	0.45	0/203	0.57	0/277
7	P	0.32	0/1376	0.49	0/1879
8	H	1.26	0/7222	1.04	6/11143 (0.1%)
9	I	0.62	0/948	0.58	0/1270
9	O	0.61	0/828	0.57	0/1109
10	J	0.75	0/669	0.61	0/894
10	Q	0.73	0/674	0.60	0/904
11	K	0.63	0/835	0.63	1/1128 (0.1%)
11	R	0.67	0/839	0.61	0/1132
12	M	0.68	0/747	0.56	0/1007
12	S	0.71	0/752	0.58	0/1014
All	All	0.74	0/30501	0.69	7/42703 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	296	DC	O4'-C4'-C3'	-7.22	101.61	104.50
8	H	110	DC	O4'-C4'-C3'	-6.96	101.72	104.50
8	H	120	DA	O4'-C4'-C3'	-5.74	102.20	104.50
11	K	24	GLN	C-N-CA	-5.37	108.28	121.70
8	H	111	DG	O4'-C4'-C3'	-5.31	102.37	104.50
8	H	226	DT	C3'-C2'-C1'	-5.11	96.37	102.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	111	DG	C4'-C3'-C2'	-5.02	98.59	103.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	603	0	631	29	0
1	T	604	0	631	29	0
2	A	3340	0	3106	169	0
3	L	2874	0	2735	143	0
4	N	3080	0	2895	226	0
5	C	4278	0	3675	176	0
6	B	290	0	271	19	0
6	E	203	0	154	6	0
7	P	1346	0	1188	77	0
8	H	6439	0	3521	472	0
9	I	935	0	984	43	0
9	O	816	0	856	33	0
10	J	662	0	709	38	0
10	Q	667	0	679	23	0
11	K	825	0	876	45	0
11	R	829	0	887	47	0
12	M	736	0	751	39	0
12	S	741	0	753	36	0
13	A	1	0	0	0	0
14	C	26	0	19	3	0
15	P	1	0	0	0	0
All	All	29296	0	25321	1495	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 28.

All (1495) 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)
8:H:103:DC:O2	8:H:212:DG:N2	1.92	1.02
8:H:110:DC:O2	8:H:205:DG:N2	1.94	1.01
8:H:154:DC:O2	8:H:161:DG:N2	1.96	0.98
8:H:53:DC:O2	8:H:262:DG:N2	1.98	0.97
8:H:110:DC:N3	8:H:205:DG:N1	2.13	0.96
1:T:47:GLY:HA2	6:E:25:GLU:HG2	1.50	0.94
8:H:137:DG:N2	8:H:178:DC:O2	2.00	0.93
8:H:134:DC:O2	8:H:181:DG:N2	2.01	0.93
8:H:124:DG:N2	8:H:191:DC:O2	2.02	0.91
8:H:53:DC:N3	8:H:262:DG:N1	2.19	0.91
8:H:124:DG:N1	8:H:191:DC:N3	2.21	0.88
8:H:238:DC:H2'	8:H:239:DG:H8	1.39	0.87
8:H:238:DC:H2'	8:H:239:DG:C8	2.09	0.87
5:C:294:CYS:SG	5:C:297:HIS:ND1	2.48	0.86
8:H:93:DG:N1	8:H:222:DC:N3	2.23	0.86
10:J:31:LYS:HE2	10:J:35:ARG:HH22	1.37	0.86
8:H:94:DG:N1	8:H:221:DC:N3	2.22	0.86
8:H:114:DC:O2	8:H:201:DG:N2	2.07	0.86
8:H:298:DC:H2''	8:H:299:DA:H5''	1.54	0.86
8:H:103:DC:N3	8:H:212:DG:N1	2.22	0.85
8:H:114:DC:N3	8:H:201:DG:N1	2.22	0.85
8:H:136:DG:N2	8:H:180:DC:O2	2.08	0.85
9:I:68:GLN:HE21	9:I:72:ARG:HE	1.24	0.84
2:A:130:LYS:HD3	4:N:348:SER:HA	1.59	0.84
8:H:16:DT:O4	8:H:298:DC:N4	2.10	0.84
4:N:61:PHE:HA	4:N:88:ASN:H	1.44	0.83
8:H:137:DG:N1	8:H:178:DC:N3	2.27	0.82
8:H:199:DT:OP1	11:R:20:ARG:NH2	2.13	0.82
11:R:42:ARG:HB2	12:S:85:THR:HG22	1.61	0.81
8:H:135:DG:N1	8:H:180:DC:N3	2.27	0.81
9:I:116:ARG:NH1	9:I:120:MET:SD	2.53	0.81
2:A:98:ARG:HD2	2:A:101:ARG:HH12	1.46	0.80
8:H:126:DC:H2''	8:H:127:DT:H5'	1.61	0.80
8:H:135:DG:N2	8:H:180:DC:O2	2.14	0.80
8:H:280:DT:H2''	8:H:281:DA:H8	1.46	0.80
9:O:116:ARG:NH1	9:O:120:MET:SD	2.55	0.80
5:C:504:ARG:NH1	9:I:36:LYS:O	2.14	0.80
12:M:90:GLU:OE1	12:M:90:GLU:N	2.13	0.80
4:N:223:PHE:HA	4:N:262:THR:HB	1.62	0.79
11:R:41:GLU:HG2	11:R:42:ARG:HG3	1.63	0.79
8:H:299:DA:H2'	8:H:300:DG:O4'	1.82	0.79
8:H:50:DT:O3'	9:I:83:ARG:NH2	2.16	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:82:PHE:HB3	3:L:437:TRP:HB3	1.63	0.79
8:H:134:DC:N3	8:H:181:DG:N1	2.31	0.79
12:M:87:THR:N	12:M:90:GLU:OE2	2.12	0.79
6:B:151:LYS:HG3	6:B:152:PRO:HD3	1.65	0.78
8:H:94:DG:N2	8:H:221:DC:O2	2.16	0.78
8:H:93:DG:N2	8:H:222:DC:O2	2.17	0.78
10:J:77:LYS:HE2	12:M:89:ARG:HH12	1.47	0.78
11:K:42:ARG:HG3	12:M:85:THR:HG22	1.65	0.78
8:H:259:DA:OP1	9:I:63:ARG:NH2	2.16	0.77
8:H:15:DC:H2'	8:H:16:DT:H71	1.66	0.77
8:H:94:DG:O6	8:H:221:DC:N4	2.18	0.77
8:H:154:DC:N3	8:H:161:DG:N1	2.32	0.77
3:L:133:ARG:HA	5:C:94:GLN:HE22	1.51	0.76
3:L:381:ASN:HD22	3:L:385:LYS:HB2	1.50	0.76
8:H:297:DT:H2''	8:H:298:DC:C2	2.20	0.76
10:Q:75:HIS:O	12:S:89:ARG:NH2	2.17	0.76
8:H:19:DG:H1'	8:H:20:DA:N7	1.99	0.76
5:C:58:GLN:O	5:C:62:GLN:NE2	2.14	0.76
8:H:18:DA:N6	8:H:297:DT:O4	2.18	0.76
8:H:120:DA:H1'	8:H:121:DG:C5	2.20	0.76
2:A:456:ASN:ND2	4:N:357:GLU:OE2	2.17	0.76
8:H:256:DT:OP1	10:J:20:LYS:NZ	2.19	0.76
12:M:29:THR:O	12:M:31:LYS:NZ	2.18	0.76
3:L:190:GLY:N	3:L:212:ASP:OD2	2.16	0.75
5:C:320:CYS:N	5:C:324:CYS:SG	2.59	0.75
2:A:103:ARG:NH1	7:P:283:ASN:O	2.19	0.75
5:C:524:ASP:HA	5:C:548:GLN:HB2	1.67	0.75
9:O:59:GLU:OE1	9:O:59:GLU:N	2.19	0.75
2:A:588:ASP:OD2	2:A:593:ARG:NH1	2.18	0.75
3:L:312:VAL:O	3:L:313:ARG:NH1	2.20	0.75
4:N:323:VAL:O	4:N:324:GLN:NE2	2.19	0.74
8:H:124:DG:H2'	8:H:125:DC:C6	2.22	0.74
5:C:624:TRP:N	14:C:801:SAH:O	2.20	0.74
5:C:613:HIS:HD2	5:C:629:LYS:HD2	1.52	0.74
1:T:41:GLN:HB3	1:T:69:LEU:HD11	1.69	0.74
10:J:51:TYR:O	10:J:55:ARG:NH1	2.20	0.74
1:T:39:ASP:HA	1:T:74:ARG:HH21	1.52	0.73
8:H:53:DC:H2'	8:H:54:DG:C8	2.23	0.73
4:N:342:LEU:HB3	4:N:370:HIS:HB3	1.70	0.73
9:I:59:GLU:N	9:I:59:GLU:OE1	2.21	0.73
11:K:115:LEU:HD13	10:Q:44:LYS:HB2	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:291:SER:OG	3:L:292:GLN:N	2.21	0.73
7:P:281:ASP:HB3	7:P:284:ILE:HG13	1.70	0.73
5:C:462:THR:O	5:C:466:VAL:N	2.22	0.72
9:O:68:GLN:HE21	9:O:72:ARG:HE	1.35	0.72
5:C:286:CYS:SG	5:C:297:HIS:ND1	2.61	0.72
3:L:149:THR:HG21	3:L:195:GLU:HA	1.72	0.72
4:N:47:ALA:O	4:N:131:ARG:NH1	2.22	0.72
4:N:178:LYS:HB2	4:N:198:ASP:HB2	1.71	0.72
4:N:76:GLN:NE2	4:N:77:ASN:O	2.23	0.72
8:H:17:DG:H1'	8:H:18:DA:C5	2.25	0.72
7:P:239:LEU:N	7:P:254:VAL:O	2.22	0.72
8:H:250:DC:OP1	9:I:44:GLY:N	2.21	0.72
7:P:259:ARG:NE	7:P:260:HIS:H	1.88	0.71
1:F:43:LEU:HD23	1:F:67:LEU:HD22	1.72	0.71
8:H:208:DG:H2''	8:H:209:DA:H8	1.53	0.71
2:A:103:ARG:O	2:A:107:ALA:N	2.21	0.71
11:K:31:HIS:HD1	11:K:48:PRO:HG3	1.54	0.71
10:Q:39:ARG:NH1	10:Q:43:VAL:O	2.22	0.71
4:N:287:PHE:HA	4:N:303:LEU:HG	1.73	0.71
3:L:339:ASP:H	3:L:342:LYS:HE3	1.56	0.71
3:L:184:LYS:NZ	3:L:220:ILE:O	2.21	0.70
11:R:91:GLU:OE1	11:R:91:GLU:N	2.24	0.70
8:H:180:DC:H2''	8:H:181:DG:C8	2.25	0.70
3:L:219:ASN:ND2	3:L:222:THR:OG1	2.24	0.70
5:C:52:ARG:HA	5:C:55:ILE:HD12	1.74	0.70
5:C:545:LYS:NZ	5:C:583:ASP:OD2	2.23	0.70
8:H:93:DG:O6	8:H:222:DC:N4	2.23	0.70
8:H:135:DG:N2	8:H:180:DC:C2	2.58	0.70
4:N:204:LEU:O	4:N:220:LYS:N	2.24	0.70
5:C:650:GLU:HA	5:C:653:ARG:HH21	1.57	0.70
8:H:257:DA:OP1	10:J:23:ARG:NH2	2.17	0.69
3:L:116:VAL:HG12	3:L:121:VAL:HG12	1.74	0.69
2:A:431:GLN:HE21	2:A:439:ARG:HD2	1.57	0.69
1:T:15:LEU:HD11	1:T:30:ILE:HD11	1.74	0.69
2:A:473:ARG:NH2	4:N:19:GLU:OE2	2.25	0.69
12:S:33:SER:OG	12:S:34:TYR:N	2.25	0.69
4:N:10:ASP:OD1	7:P:286:ARG:NH2	2.26	0.69
5:C:129:HIS:HA	5:C:158:HIS:HB3	1.73	0.69
5:C:443:LEU:O	5:C:446:THR:OG1	2.11	0.69
2:A:249:SER:HA	2:A:300:THR:HA	1.74	0.68
11:K:18:SER:O	11:K:22:GLY:N	2.24	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:S:87:THR:HG22	12:S:90:GLU:HG2	1.75	0.68
1:T:44:ILE:CG2	6:E:25:GLU:OE2	2.42	0.68
2:A:429:PHE:HA	2:A:443:GLU:HA	1.75	0.68
9:I:128:ARG:HH11	9:I:134:ARG:HH21	1.42	0.68
2:A:607:ASN:ND2	5:C:261:THR:O	2.22	0.68
3:L:245:ASP:OD2	3:L:250:LYS:N	2.25	0.68
5:C:502:HIS:HA	5:C:505:LYS:HD2	1.74	0.68
5:C:543:CYS:HB2	5:C:556:ARG:HA	1.75	0.68
5:C:593:HIS:CG	5:C:596:SER:HB2	2.29	0.68
8:H:94:DG:H2'	8:H:95:DT:H71	1.74	0.68
10:Q:51:TYR:O	10:Q:55:ARG:NH1	2.27	0.67
9:I:48:LEU:O	9:I:52:ARG:HD3	1.95	0.67
11:K:20:ARG:O	12:M:117:LYS:NZ	2.28	0.67
12:M:48:ASP:N	12:M:48:ASP:OD1	2.22	0.67
8:H:197:DA:H2''	8:H:198:DA:C8	2.30	0.67
8:H:32:DA:OP1	11:K:20:ARG:NH2	2.26	0.67
9:O:73:GLU:OE1	10:Q:25:ASN:ND2	2.28	0.67
2:A:191:VAL:O	2:A:246:LYS:N	2.27	0.67
8:H:111:DG:H1'	8:H:112:DA:C8	2.30	0.67
4:N:287:PHE:HD2	4:N:303:LEU:HB2	1.60	0.67
5:C:147:GLU:HA	5:C:150:ILE:HD12	1.75	0.67
3:L:364:TRP:CD1	6:B:114:GLN:HG3	2.30	0.67
11:R:72:ASP:O	11:R:74:LYS:NZ	2.26	0.66
1:T:26:VAL:HA	1:T:29:LYS:HE2	1.76	0.66
2:A:252:PHE:HB2	2:A:297:ALA:HB3	1.77	0.66
7:P:227:ILE:N	7:P:240:LEU:O	2.27	0.66
5:C:605:SER:O	5:C:609:GLY:N	2.25	0.66
4:N:15:ARG:HB3	7:P:190:PHE:CE1	2.31	0.66
6:B:146:ASP:OD1	6:B:150:ARG:NH2	2.28	0.66
2:A:183:THR:OG1	2:A:211:LYS:O	2.11	0.66
2:A:530:VAL:H	4:N:35:VAL:HB	1.61	0.66
8:H:14:DT:H2'	8:H:15:DC:C6	2.30	0.66
10:Q:26:ILE:HG13	10:Q:55:ARG:HD3	1.76	0.66
2:A:103:ARG:NH2	4:N:13:GLU:OE2	2.28	0.66
2:A:429:PHE:HB2	2:A:486:ARG:HG3	1.78	0.66
3:L:123:LEU:HD22	3:L:136:GLN:HB2	1.78	0.66
11:K:79:ILE:HG12	11:K:82:HIS:CE1	2.30	0.66
4:N:253:MET:HB2	4:N:255:TRP:HE1	1.61	0.66
5:C:148:GLU:HA	5:C:151:LYS:HD2	1.76	0.65
8:H:123:DG:H4'	12:S:30:ARG:HD2	1.77	0.65
2:A:440:GLN:NE2	2:A:441:GLN:O	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:344:VAL:HG12	4:N:367:LEU:HB3	1.77	0.65
12:S:106:HIS:O	12:S:109:SER:OG	2.10	0.65
7:P:94:CYS:SG	7:P:110:HIS:NE2	2.69	0.65
8:H:93:DG:O6	8:H:221:DC:N4	2.29	0.65
11:K:16:THR:O	11:K:19:SER:OG	2.14	0.65
5:C:273:GLN:NE2	5:C:275:GLU:OE2	2.30	0.65
4:N:141:ALA:HB3	4:N:183:LEU:HD21	1.77	0.65
3:L:204:ASN:ND2	3:L:278:TYR:OH	2.28	0.65
4:N:33:ASP:N	4:N:403:GLN:O	2.29	0.65
8:H:27:DT:H2''	8:H:28:DG:N7	2.11	0.65
2:A:97:TYR:CE1	2:A:471:HIS:HA	2.32	0.65
4:N:226:HIS:NE2	4:N:251:LYS:O	2.19	0.65
5:C:100:THR:O	7:P:193:GLN:NE2	2.30	0.65
8:H:19:DG:H1'	8:H:20:DA:C5	2.32	0.65
1:T:23:ILE:HB	1:T:52:ASP:HA	1.78	0.65
3:L:81:SER:O	3:L:440:LEU:N	2.24	0.65
3:L:245:ASP:OD2	3:L:249:GLU:N	2.27	0.65
4:N:92:GLN:HA	7:P:171:LYS:HE2	1.79	0.65
10:Q:92:ARG:NH2	12:S:97:LEU:O	2.30	0.65
4:N:33:ASP:HB2	4:N:403:GLN:HG2	1.79	0.64
4:N:171:LEU:HA	4:N:215:LYS:HA	1.79	0.64
3:L:391:LEU:O	5:C:46:ARG:NH1	2.30	0.64
4:N:171:LEU:H	4:N:215:LYS:HE3	1.63	0.64
5:C:433:SER:O	5:C:437:ALA:N	2.29	0.64
8:H:130:DG:H1'	8:H:131:DC:C4	2.32	0.64
2:A:458:ARG:NH2	4:N:357:GLU:OE1	2.30	0.64
3:L:199:HIS:NE2	3:L:248:GLY:O	2.31	0.64
3:L:333:PRO:HA	3:L:350:VAL:HG13	1.80	0.64
3:L:339:ASP:HB3	3:L:342:LYS:HG2	1.79	0.64
2:A:508:ARG:NH1	2:A:512:PHE:O	2.31	0.64
10:J:77:LYS:HE2	12:M:89:ARG:NH1	2.12	0.64
5:C:619:SER:N	5:C:623:GLY:O	2.28	0.64
8:H:102:DG:H2''	8:H:103:DC:H5'	1.80	0.64
3:L:339:ASP:OD1	3:L:340:ILE:N	2.30	0.64
7:P:239:LEU:O	7:P:254:VAL:N	2.28	0.64
7:P:259:ARG:HE	7:P:260:HIS:H	1.44	0.64
8:H:208:DG:H2''	8:H:209:DA:C8	2.32	0.64
8:H:224:DC:H2'	8:H:225:DT:C6	2.33	0.64
8:H:13:DA:H2'	8:H:14:DT:C6	2.33	0.64
8:H:71:DC:H2''	8:H:72:DA:C8	2.33	0.64
8:H:187:DG:H5''	8:H:187:DG:H8	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:197:DA:H2''	8:H:198:DA:H8	1.62	0.64
5:C:274:ARG:HD2	5:C:442:VAL:HA	1.79	0.64
3:L:408:LYS:HB2	3:L:435:TRP:HH2	1.62	0.63
4:N:382:TRP:HA	4:N:390:ILE:HG12	1.79	0.63
8:H:198:DA:C2'	8:H:199:DT:H71	2.28	0.63
2:A:314:GLU:HA	2:A:358:THR:HA	1.80	0.63
8:H:13:DA:H2'	8:H:14:DT:H6	1.62	0.63
8:H:41:DT:H2''	8:H:42:DA:C8	2.34	0.63
8:H:111:DG:H1'	8:H:112:DA:N7	2.13	0.63
3:L:364:TRP:HD1	6:B:114:GLN:HG3	1.62	0.63
5:C:535:PRO:HA	5:C:538:ILE:HG12	1.80	0.63
8:H:49:DT:H2''	8:H:50:DT:H71	1.79	0.63
2:A:191:VAL:HG22	2:A:203:ILE:HG12	1.81	0.63
2:A:192:CYS:HB2	2:A:202:PRO:HG2	1.80	0.63
8:H:116:DA:H1'	8:H:117:DT:H5''	1.81	0.63
4:N:335:SER:HB3	4:N:345:TRP:HE1	1.63	0.63
8:H:90:DA:H2''	8:H:91:DG:C8	2.34	0.63
2:A:112:HIS:HA	2:A:115:LEU:HD13	1.80	0.62
8:H:101:DA:H2''	8:H:102:DG:H8	1.64	0.62
8:H:209:DA:H2'	8:H:210:DC:C6	2.34	0.62
7:P:102:THR:OG1	12:S:44:GLN:O	2.15	0.62
5:C:289:CYS:HB2	5:C:294:CYS:SG	2.40	0.62
2:A:428:ILE:HB	2:A:444:ALA:HB3	1.81	0.62
2:A:646:LYS:O	2:A:650:LYS:N	2.31	0.62
5:C:670:ASN:OD1	5:C:673:PHE:N	2.31	0.62
4:N:48:GLN:HB3	4:N:67:VAL:HB	1.82	0.62
8:H:22:DG:H2'	8:H:23:DT:H71	1.81	0.62
4:N:205:TRP:HD1	4:N:217:VAL:HG12	1.64	0.62
5:C:694:ASN:HB3	5:C:714:ARG:NH2	2.15	0.62
11:K:115:LEU:O	10:Q:44:LYS:NZ	2.31	0.62
11:R:16:THR:O	11:R:19:SER:OG	2.15	0.62
5:C:40:SER:O	5:C:43:SER:OG	2.18	0.62
5:C:129:HIS:HA	5:C:158:HIS:H	1.65	0.62
12:S:52:SER:OG	12:S:53:SER:N	2.33	0.62
5:C:579:GLU:HA	5:C:603:ASN:ND2	2.15	0.62
5:C:593:HIS:O	5:C:608:ARG:NH1	2.32	0.62
3:L:150:CYS:HB2	3:L:163:LEU:HD11	1.81	0.62
4:N:370:HIS:CD2	4:N:372:GLY:H	2.17	0.62
9:I:61:LEU:HD21	10:J:40:ARG:HH21	1.65	0.62
1:F:22:THR:HA	1:F:55:THR:HA	1.82	0.62
3:L:118:SER:OG	3:L:119:ASN:OD1	2.18	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:P:268:HIS:HB3	7:P:271:LYS:HZ3	1.65	0.61
2:A:116:THR:O	2:A:119:SER:OG	2.10	0.61
2:A:681:LEU:HG	2:A:682:ARG:HG3	1.82	0.61
4:N:138:CYS:HA	4:N:154:TYR:CE2	2.35	0.61
5:C:66:GLN:OE1	5:C:67:PRO:HD2	2.00	0.61
2:A:105:LEU:HD13	7:P:269:LEU:HD12	1.81	0.61
3:L:332:LYS:HD3	3:L:336:MET:HA	1.82	0.61
4:N:186:ASN:HD22	4:N:189:LEU:HB2	1.63	0.61
8:H:139:DT:H2''	8:H:140:DT:H5''	1.82	0.61
8:H:157:DC:N3	8:H:158:DG:N1	2.49	0.61
8:H:173:DA:OP1	9:I:36:LYS:NZ	2.33	0.61
8:H:298:DC:H2''	8:H:299:DA:C5'	2.29	0.61
5:C:46:ARG:HA	5:C:49:ILE:HD12	1.80	0.61
7:P:188:ASP:OD1	7:P:189:PHE:N	2.33	0.61
3:L:323:SER:HB3	3:L:325:GLU:HG2	1.81	0.61
8:H:32:DA:H5'	8:H:32:DA:C8	2.35	0.61
8:H:281:DA:H2''	8:H:282:DG:H8	1.64	0.61
11:K:78:ILE:O	12:M:52:SER:OG	2.17	0.61
11:K:92:GLU:HG2	12:M:103:LEU:HG	1.83	0.61
1:T:51:GLU:O	1:T:59:TYR:OH	2.19	0.61
2:A:162:THR:H	2:A:357:PHE:HA	1.65	0.61
8:H:196:DC:OP1	12:S:30:ARG:NH2	2.34	0.61
2:A:318:ALA:HA	2:A:354:THR:HA	1.82	0.61
5:C:499:TRP:HA	5:C:502:HIS:CD2	2.36	0.61
5:C:534:CYS:SG	5:C:536:CYS:HB2	2.41	0.61
2:A:450:CYS:HB3	2:A:455:LEU:H	1.65	0.61
10:J:44:LYS:NZ	11:R:115:LEU:O	2.33	0.61
4:N:67:VAL:HA	4:N:81:ILE:HG12	1.83	0.60
4:N:198:ASP:HA	4:N:229:VAL:HG13	1.83	0.60
8:H:17:DG:H1'	8:H:18:DA:N7	2.15	0.60
11:R:20:ARG:O	12:S:117:LYS:NZ	2.34	0.60
6:B:163:LEU:O	6:B:166:SER:OG	2.16	0.60
3:L:408:LYS:HB2	3:L:435:TRP:CH2	2.36	0.60
7:P:228:ALA:H	7:P:240:LEU:HB3	1.66	0.60
2:A:647:ILE:O	2:A:651:ASN:N	2.34	0.60
3:L:125:GLU:HB2	3:L:135:LEU:HD11	1.83	0.60
5:C:443:LEU:HB3	5:C:454:ILE:HG12	1.84	0.60
8:H:236:DT:H2''	8:H:237:DA:C8	2.36	0.60
7:P:294:LYS:HG3	7:P:295:ARG:H	1.66	0.60
2:A:458:ARG:HB2	2:A:459:LYS:HZ3	1.66	0.60
5:C:46:ARG:O	5:C:50:LEU:HG	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:523:CYS:HB2	5:C:525:HIS:CE1	2.36	0.60
11:K:91:GLU:OE1	11:K:91:GLU:N	2.24	0.60
4:N:253:MET:HB2	4:N:255:TRP:NE1	2.17	0.60
8:H:124:DG:H2'	8:H:125:DC:H6	1.64	0.60
2:A:589:PRO:HG2	2:A:592:LEU:HB2	1.84	0.60
7:P:215:GLY:HA3	7:P:219:SER:O	2.02	0.60
8:H:152:DG:H2''	8:H:153:DG:C8	2.37	0.60
2:A:428:ILE:O	2:A:444:ALA:N	2.30	0.59
2:A:526:THR:OG1	4:N:38:HIS:ND1	2.34	0.59
5:C:126:THR:HG23	5:C:127:VAL:HG23	1.84	0.59
7:P:224:SER:HB2	7:P:241:LEU:HD22	1.83	0.59
3:L:188:GLY:O	3:L:216:ARG:NH1	2.35	0.59
3:L:388:VAL:HB	3:L:402:THR:HB	1.84	0.59
4:N:188:ASN:HB2	4:N:240:GLU:HB3	1.84	0.59
12:M:33:SER:OG	12:M:34:TYR:N	2.34	0.59
3:L:431:ASP:OD1	3:L:433:SER:OG	2.18	0.59
8:H:72:DA:H1'	8:H:73:DG:H5'	1.85	0.59
8:H:135:DG:O6	8:H:180:DC:N4	2.36	0.59
8:H:283:DT:H1'	8:H:284:DC:H5'	1.84	0.59
8:H:294:DG:H2''	8:H:295:DT:H5''	1.83	0.59
8:H:305:DA:H3'	8:H:306:DT:H71	1.85	0.59
9:I:128:ARG:HD3	9:I:134:ARG:HH21	1.67	0.59
3:L:302:ARG:NH2	5:C:129:HIS:O	2.35	0.59
8:H:196:DC:H2''	8:H:197:DA:C8	2.36	0.59
3:L:335:LYS:N	3:L:338:ASP:OD2	2.32	0.59
4:N:50:LEU:HD12	4:N:65:ARG:HB2	1.83	0.59
1:F:27:LYS:O	1:F:41:GLN:NE2	2.35	0.59
3:L:118:SER:OG	3:L:119:ASN:N	2.34	0.59
7:P:206:ASN:O	7:P:210:HIS:N	2.30	0.59
3:L:134:LEU:HG	5:C:96:ILE:HD12	1.83	0.59
8:H:280:DT:H2''	8:H:281:DA:C8	2.34	0.59
11:R:119:CYS:HA	1:F:76:CYS:HB3	1.84	0.59
3:L:404:LEU:HB3	3:L:437:TRP:CZ3	2.38	0.59
7:P:109:ARG:O	7:P:113:THR:HG23	2.02	0.59
8:H:259:DA:P	9:I:63:ARG:HH21	2.25	0.59
2:A:136:ASP:O	2:A:140:LYS:N	2.34	0.58
2:A:657:MET:O	2:A:661:VAL:HG23	2.03	0.58
3:L:376:MET:HE3	3:L:388:VAL:HG13	1.84	0.58
5:C:128:LEU:O	5:C:129:HIS:ND1	2.32	0.58
1:T:27:LYS:NZ	1:T:38:PRO:O	2.35	0.58
4:N:126:GLU:HG2	4:N:145:PRO:HG3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:169:PRO:HG2	4:N:172:ARG:HH21	1.68	0.58
4:N:329:ASN:HD21	4:N:388:TRP:HE1	1.51	0.58
5:C:737:VAL:HG13	14:C:801:SAH:C6	2.32	0.58
8:H:9:DA:H3'	8:H:10:DT:H71	1.83	0.58
4:N:284:TYR:HB2	4:N:330:GLU:HG3	1.83	0.58
3:L:100:GLN:O	3:L:152:TRP:NE1	2.33	0.58
3:L:113:PHE:CE1	3:L:124:TYR:HB2	2.37	0.58
3:L:123:LEU:HB2	3:L:136:GLN:H	1.67	0.58
4:N:61:PHE:HA	4:N:88:ASN:N	2.14	0.58
4:N:231:GLU:HB2	4:N:246:VAL:HG12	1.85	0.58
8:H:67:DG:H2''	8:H:68:DG:N7	2.19	0.58
8:H:101:DA:H2''	8:H:102:DG:C8	2.38	0.58
2:A:102:THR:HA	2:A:105:LEU:HD12	1.84	0.58
7:P:106:TRP:CH2	12:S:47:PRO:HD2	2.39	0.58
11:R:29:ARG:NH2	12:S:32:GLU:HB3	2.19	0.58
2:A:192:CYS:HA	2:A:245:VAL:HA	1.85	0.58
2:A:250:LEU:N	2:A:299:MET:O	2.20	0.58
6:E:31:LYS:O	6:E:35:LEU:HG	2.03	0.58
5:C:271:SER:HB2	5:C:434:GLY:HA2	1.85	0.58
7:P:281:ASP:OD1	7:P:283:ASN:N	2.34	0.58
8:H:155:DA:H61	8:H:159:DC:H42	1.52	0.58
8:H:268:DG:H1'	8:H:269:DG:C8	2.38	0.58
4:N:186:ASN:HD21	4:N:240:GLU:HB2	1.69	0.58
5:C:614:LEU:O	5:C:683:LYS:NZ	2.35	0.58
8:H:8:DT:H2'	8:H:9:DA:C8	2.39	0.58
1:T:42:ARG:HD2	1:T:72:ARG:HH21	1.69	0.58
2:A:249:SER:OG	2:A:299:MET:O	2.17	0.58
3:L:269:ARG:NE	3:L:292:GLN:OE1	2.32	0.58
5:C:649:ASP:N	5:C:649:ASP:OD1	2.36	0.58
4:N:89:ASP:OD1	4:N:90:ASP:N	2.37	0.57
5:C:275:GLU:HG3	5:C:276:GLN:H	1.69	0.57
8:H:46:DC:N4	8:H:268:DG:O6	2.36	0.57
8:H:53:DC:N4	8:H:262:DG:O6	2.36	0.57
8:H:296:DC:H2''	8:H:297:DT:H5''	1.86	0.57
2:A:164:PHE:HD1	2:A:355:LEU:HB2	1.69	0.57
6:B:115:ARG:HH21	6:B:117:PHE:HB2	1.68	0.57
8:H:21:DC:H2''	8:H:22:DG:H8	1.69	0.57
8:H:220:DA:H2''	8:H:221:DC:O5'	2.04	0.57
10:J:70:VAL:O	10:J:73:THR:OG1	2.20	0.57
11:R:77:ARG:HG2	12:S:50:GLY:HA3	1.87	0.57
3:L:82:PHE:CZ	3:L:439:ARG:HB2	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:336:MET:SD	3:L:336:MET:N	2.77	0.57
5:C:130:ASN:OD1	5:C:131:ILE:N	2.37	0.57
1:F:15:LEU:HD22	1:F:26:VAL:HG13	1.86	0.57
8:H:20:DA:H2''	8:H:21:DC:H5''	1.86	0.57
3:L:381:ASN:OD1	3:L:382:GLN:N	2.37	0.57
8:H:10:DT:H2'	8:H:11:DA:C8	2.39	0.57
4:N:269:VAL:HG12	4:N:270:ASP:H	1.70	0.57
4:N:326:SER:HB2	4:N:382:TRP:CH2	2.40	0.57
3:L:274:ILE:O	3:L:277:SER:OG	2.12	0.56
8:H:154:DC:C2	8:H:161:DG:N2	2.73	0.56
8:H:234:DC:H1'	8:H:235:DG:C5	2.39	0.56
11:K:29:ARG:NE	12:M:32:GLU:OE2	2.38	0.56
3:L:136:GLN:NE2	3:L:180:MET:SD	2.78	0.56
9:I:61:LEU:HD12	10:J:37:LEU:HD23	1.87	0.56
10:J:44:LYS:HB2	11:R:115:LEU:HD13	1.87	0.56
4:N:300:LEU:HG	4:N:310:LEU:HD12	1.86	0.56
5:C:560:CYS:HB2	5:C:585:CYS:HB2	1.88	0.56
8:H:103:DC:C2	8:H:212:DG:N2	2.57	0.56
8:H:144:DC:H4'	8:H:145:DA:OP1	2.05	0.56
2:A:492:ASN:OD1	2:A:493:GLU:N	2.38	0.56
4:N:76:GLN:NE2	4:N:123:HIS:H	2.04	0.56
5:C:323:GLN:O	5:C:464:ARG:N	2.35	0.56
11:R:29:ARG:NH2	12:S:32:GLU:OE1	2.38	0.56
3:L:245:ASP:HA	3:L:314:TRP:CG	2.40	0.56
5:C:566:CYS:HB2	5:C:601:CYS:SG	2.45	0.56
6:B:142:THR:OG1	6:B:143:GLN:N	2.39	0.56
3:L:225:LEU:HD12	3:L:226:VAL:H	1.69	0.56
8:H:109:DA:H2''	8:H:110:DC:C5	2.41	0.56
5:C:694:ASN:HB2	5:C:716:ILE:HD11	1.87	0.56
8:H:71:DC:H2''	8:H:72:DA:N7	2.21	0.56
12:S:109:SER:O	12:S:112:THR:OG1	2.22	0.56
2:A:583:SER:HA	5:C:613:HIS:HE1	1.71	0.56
7:P:211:ILE:HG23	7:P:219:SER:O	2.05	0.56
11:R:64:GLU:HB3	12:S:45:VAL:HG11	1.88	0.56
3:L:90:GLU:HB2	3:L:432:ALA:HB1	1.88	0.56
4:N:46:THR:OG1	4:N:69:GLY:N	2.38	0.56
8:H:137:DG:H2''	8:H:138:DA:C8	2.41	0.56
8:H:251:DG:O4'	9:I:40:ARG:NH2	2.39	0.56
10:J:47:SER:OG	10:J:48:GLY:N	2.35	0.56
12:M:53:SER:OG	12:M:54:LYS:N	2.37	0.55
10:Q:31:LYS:HE2	10:Q:35:ARG:HD2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:115:THR:O	3:L:122:THR:OG1	2.21	0.55
5:C:432:TRP:HH2	5:C:466:VAL:HA	1.71	0.55
5:C:682:ASN:O	5:C:685:ARG:HG2	2.07	0.55
2:A:302:PHE:O	2:A:309:GLN:NE2	2.39	0.55
4:N:28:THR:HA	4:N:31:LEU:HD12	1.89	0.55
4:N:235:TRP:HA	4:N:243:PHE:HB3	1.87	0.55
5:C:57:ASN:O	5:C:61:LYS:HG3	2.07	0.55
8:H:173:DA:H4'	8:H:174:DG:OP1	2.07	0.55
8:H:288:DA:H2''	8:H:289:DG:C8	2.41	0.55
5:C:523:CYS:HB3	5:C:536:CYS:H	1.70	0.55
8:H:152:DG:H2''	8:H:153:DG:H8	1.70	0.55
8:H:178:DC:H5'	8:H:178:DC:C6	2.40	0.55
12:M:76:ARG:O	12:M:79:HIS:N	2.39	0.55
8:H:269:DG:H2''	8:H:270:DG:H8	1.71	0.55
8:H:301:DA:H5''	8:H:302:DT:H71	1.89	0.55
2:A:133:LYS:HD2	4:N:304:ARG:HH22	1.71	0.55
7:P:108:GLN:O	7:P:112:LEU:HG	2.05	0.55
8:H:120:DA:H1'	8:H:121:DG:C6	2.41	0.55
11:K:84:GLN:NE2	11:K:88:ARG:HE	2.04	0.55
8:H:14:DT:H2'	8:H:15:DC:H6	1.72	0.55
8:H:287:DC:H2''	8:H:288:DA:N7	2.20	0.55
9:I:91:ALA:HB2	10:J:100:PHE:CD2	2.41	0.55
10:J:39:ARG:O	10:J:42:GLY:N	2.40	0.55
3:L:311:CYS:SG	3:L:313:ARG:NH1	2.80	0.55
5:C:274:ARG:HG3	5:C:442:VAL:HG13	1.89	0.55
8:H:23:DT:H2''	8:H:24:DG:H5''	1.88	0.55
8:H:62:DC:H2''	8:H:63:DG:C8	2.41	0.55
9:O:60:LEU:HD13	9:O:93:GLN:NE2	2.22	0.55
2:A:113:ARG:NH1	4:N:361:ASP:OD1	2.40	0.55
8:H:93:DG:H2''	8:H:94:DG:H8	1.73	0.55
8:H:218:DG:H2''	8:H:219:DC:H5'	1.89	0.55
1:T:44:ILE:HG21	6:E:25:GLU:OE2	2.07	0.54
2:A:432:PHE:N	2:A:440:GLN:O	2.35	0.54
2:A:468:LYS:HG2	2:A:476:PHE:HD1	1.71	0.54
4:N:287:PHE:CD2	4:N:303:LEU:HB2	2.39	0.54
8:H:128:DG:C6	8:H:186:DC:N4	2.75	0.54
11:R:79:ILE:HB	11:R:82:HIS:CE1	2.42	0.54
3:L:186:TYR:OH	3:L:223:ASP:OD1	2.18	0.54
8:H:155:DA:H61	8:H:159:DC:N4	2.04	0.54
9:O:96:SER:OG	9:O:97:GLU:OE1	2.24	0.54
2:A:133:LYS:HE3	4:N:287:PHE:CD1	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:P:218:HIS:HB2	7:P:268:HIS:CE1	2.42	0.54
5:C:503:CYS:HB3	9:I:35:VAL:HG21	1.89	0.54
8:H:94:DG:C2	8:H:95:DT:C2	2.96	0.54
8:H:140:DT:H2''	8:H:141:DC:C6	2.43	0.54
2:A:647:ILE:HA	2:A:650:LYS:HB2	1.89	0.54
3:L:261:LYS:HB2	3:L:263:TRP:CZ3	2.43	0.54
8:H:11:DA:H2'	8:H:12:DT:H71	1.89	0.54
1:T:26:VAL:O	1:T:30:ILE:HG12	2.08	0.54
4:N:188:ASN:HD22	4:N:240:GLU:HB3	1.72	0.54
8:H:224:DC:C6	8:H:225:DT:H72	2.43	0.54
8:H:3:DG:H2''	8:H:4:DG:C8	2.43	0.54
8:H:79:DA:H1'	8:H:80:DC:C5	2.43	0.54
8:H:100:DG:H2''	8:H:101:DA:C8	2.42	0.54
8:H:109:DA:OP2	8:H:109:DA:H2'	2.07	0.54
8:H:118:DT:O4	8:H:196:DC:N4	2.40	0.54
11:K:19:SER:O	11:K:22:GLY:N	2.40	0.54
2:A:126:ASN:HD22	4:N:410:ASN:H	1.56	0.54
2:A:521:LYS:HB2	4:N:42:TRP:CZ2	2.43	0.54
4:N:357:GLU:HA	4:N:360:GLU:HG2	1.89	0.54
8:H:89:DT:H3	8:H:226:DT:H3	1.54	0.54
8:H:155:DA:N6	8:H:159:DC:H42	2.05	0.54
8:H:207:DA:H2''	8:H:208:DG:H8	1.73	0.54
3:L:96:LEU:HB2	3:L:428:VAL:HG11	1.90	0.54
4:N:189:LEU:HB3	4:N:192:HIS:CE1	2.43	0.54
5:C:174:LEU:O	5:C:178:LEU:N	2.33	0.54
8:H:5:DA:H1'	8:H:6:DT:O4'	2.08	0.54
5:C:52:ARG:O	5:C:56:LEU:HG	2.08	0.54
7:P:275:ASP:OD1	7:P:275:ASP:N	2.40	0.54
8:H:2:DA:H2''	8:H:3:DG:C8	2.44	0.54
8:H:300:DG:H2'	8:H:301:DA:O4'	2.08	0.54
10:J:62:LEU:O	10:J:66:ILE:HG13	2.07	0.54
11:R:70:ALA:HA	11:R:82:HIS:CD2	2.42	0.54
4:N:15:ARG:HD3	7:P:194:THR:HG21	1.90	0.53
8:H:187:DG:C2	8:H:188:DA:C4	2.96	0.53
8:H:199:DT:C2'	8:H:200:DT:H71	2.38	0.53
2:A:497:GLY:HA2	4:N:22:LYS:HE2	1.91	0.53
3:L:339:ASP:N	3:L:342:LYS:HE3	2.23	0.53
4:N:133:MET:HA	4:N:185:TRP:CD1	2.44	0.53
2:A:428:ILE:HG12	2:A:485:ALA:HB3	1.90	0.53
4:N:236:HIS:HB3	4:N:239:HIS:O	2.09	0.53
5:C:464:ARG:O	5:C:468:GLU:N	2.36	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:P:211:ILE:O	7:P:216:LYS:N	2.42	0.53
8:H:32:DA:H5'	8:H:32:DA:H8	1.74	0.53
8:H:132:DA:H1'	8:H:133:DC:H5'	1.90	0.53
2:A:133:LYS:HE3	4:N:287:PHE:HD1	1.73	0.53
4:N:302:ASP:OD1	4:N:303:LEU:N	2.41	0.53
5:C:581:ASP:OD1	5:C:583:ASP:N	2.34	0.53
8:H:218:DG:H4'	9:O:83:ARG:HH22	1.73	0.53
8:H:297:DT:H4'	8:H:297:DT:OP1	2.09	0.53
2:A:502:ASN:HA	2:A:522:ARG:HH11	1.72	0.53
2:A:589:PRO:HB2	2:A:591:TRP:CD1	2.44	0.53
4:N:232:ASP:OD1	4:N:233:VAL:N	2.40	0.53
5:C:90:ASP:N	5:C:90:ASP:OD1	2.37	0.53
8:H:288:DA:H2''	8:H:289:DG:H8	1.73	0.53
9:O:128:ARG:HH21	9:O:134:ARG:HB2	1.73	0.53
10:Q:52:GLU:OE2	10:Q:55:ARG:NH1	2.42	0.53
2:A:243:HIS:HE1	4:N:272:HIS:O	1.92	0.53
8:H:24:DG:H2''	8:H:25:DC:H5''	1.90	0.53
8:H:114:DC:N4	8:H:201:DG:O6	2.42	0.53
8:H:172:DG:H2''	8:H:173:DA:C8	2.44	0.53
8:H:250:DC:P	9:I:44:GLY:H	2.32	0.53
11:K:110:ASN:OD1	11:K:111:ILE:N	2.42	0.53
9:O:125:GLN:HG2	9:O:134:ARG:HH12	1.74	0.53
2:A:238:GLU:H	2:A:241:ASN:ND2	2.06	0.53
4:N:239:HIS:CG	4:N:242:LEU:HD12	2.44	0.53
7:P:221:VAL:HG12	7:P:266:VAL:HG22	1.91	0.53
9:O:93:GLN:O	9:O:96:SER:OG	2.27	0.53
12:S:45:VAL:HG12	12:S:46:HIS:CD2	2.44	0.53
1:T:44:ILE:HD11	1:T:70:VAL:HG12	1.91	0.53
4:N:305:ASN:OD1	4:N:307:LYS:NZ	2.40	0.53
5:C:47:GLN:O	5:C:51:GLU:HG3	2.09	0.53
5:C:438:SER:O	5:C:442:VAL:HG23	2.09	0.53
5:C:658:TYR:HB3	5:C:664:SER:HB2	1.91	0.53
5:C:668:ASN:HB2	9:I:26:ARG:HD3	1.91	0.53
8:H:49:DT:H1'	8:H:50:DT:C6	2.44	0.53
8:H:85:DG:H2''	8:H:86:DT:H71	1.89	0.53
8:H:99:DA:H2''	8:H:100:DG:C8	2.44	0.53
8:H:110:DC:H1'	8:H:111:DG:C5	2.44	0.53
8:H:256:DT:H2''	8:H:257:DA:C8	2.42	0.53
8:H:295:DT:H2''	8:H:296:DC:H5''	1.90	0.53
1:T:47:GLY:CA	6:E:25:GLU:HG2	2.32	0.52
2:A:104:ASN:HA	2:A:107:ALA:O	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:379:ASP:OD1	4:N:380:PHE:N	2.42	0.52
3:L:319:ILE:HG21	3:L:331:TRP:CZ2	2.45	0.52
4:N:257:THR:O	4:N:258:ARG:HG2	2.09	0.52
6:B:151:LYS:CG	6:B:152:PRO:HD3	2.39	0.52
8:H:135:DG:N1	8:H:181:DG:C6	2.78	0.52
8:H:203:DT:H1'	8:H:204:DC:C2	2.44	0.52
2:A:607:ASN:N	2:A:610:GLU:OE1	2.23	0.52
3:L:347:GLU:OE2	3:L:349:ASN:N	2.42	0.52
5:C:275:GLU:HG3	5:C:276:GLN:N	2.23	0.52
8:H:271:DA:H2'	8:H:272:DT:H71	1.92	0.52
2:A:308:LEU:HG	2:A:310:LEU:H	1.75	0.52
4:N:282:ASN:OD1	4:N:285:SER:N	2.31	0.52
4:N:382:TRP:CD2	4:N:390:ILE:HD11	2.45	0.52
2:A:443:GLU:O	6:B:143:GLN:HA	2.10	0.52
5:C:51:GLU:O	5:C:55:ILE:HG13	2.09	0.52
8:H:269:DG:H2''	8:H:270:DG:C8	2.45	0.52
8:H:295:DT:H2''	8:H:296:DC:C2	2.45	0.52
11:K:74:LYS:HD2	11:K:74:LYS:O	2.09	0.52
2:A:308:LEU:HD11	2:A:310:LEU:HB2	1.92	0.52
4:N:280:SER:O	4:N:290:ALA:N	2.36	0.52
4:N:390:ILE:HB	4:N:402:TRP:CH2	2.45	0.52
8:H:18:DA:H2''	8:H:19:DG:C8	2.44	0.52
8:H:247:DC:H1'	8:H:248:DC:C5	2.45	0.52
9:I:69:ARG:HB3	10:J:25:ASN:ND2	2.24	0.52
4:N:311:HIS:CG	4:N:312:SER:N	2.77	0.52
5:C:470:ARG:O	5:C:475:SER:N	2.42	0.52
5:C:580:CYS:HB3	5:C:585:CYS:HB2	1.90	0.52
8:H:98:DT:H2''	8:H:99:DA:C8	2.45	0.52
8:H:175:DA:O3'	9:I:49:ARG:NH2	2.41	0.52
1:F:56:LEU:HD22	1:F:61:ILE:HD12	1.92	0.52
3:L:82:PHE:CE2	3:L:439:ARG:HB2	2.45	0.52
3:L:86:ASN:ND2	3:L:130:GLY:O	2.31	0.52
3:L:231:GLY:HA3	3:L:295:HIS:ND1	2.25	0.52
3:L:315:LEU:O	3:L:318:LEU:N	2.28	0.52
5:C:640:GLU:HG2	5:C:641:TYR:N	2.25	0.52
5:C:682:ASN:OD1	5:C:682:ASN:N	2.41	0.52
8:H:79:DA:C6	8:H:235:DG:C6	2.98	0.52
8:H:191:DC:H1'	8:H:192:DC:H5'	1.92	0.52
8:H:232:DC:H1'	8:H:233:DA:C8	2.45	0.52
8:H:234:DC:O2	8:H:235:DG:C2	2.63	0.52
11:K:26:PRO:HD3	12:M:37:TYR:CE1	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:15:LEU:HD21	1:T:30:ILE:HD13	1.92	0.52
1:T:39:ASP:O	1:T:74:ARG:NE	2.43	0.52
2:A:234:SER:OG	2:A:235:ASN:N	2.42	0.52
4:N:136:ASN:ND2	4:N:139:ILE:HG13	2.25	0.52
8:H:271:DA:C2'	8:H:272:DT:H71	2.39	0.52
8:H:280:DT:OP2	11:K:35:ARG:NH2	2.34	0.52
11:R:25:PHE:HE2	11:R:56:GLU:HA	1.74	0.52
8:H:175:DA:H2''	8:H:176:DA:C8	2.45	0.52
5:C:543:CYS:SG	5:C:555:ASN:HB3	2.50	0.51
7:P:170:ASN:OD1	7:P:171:LYS:N	2.43	0.51
8:H:30:DA:H2''	8:H:31:DG:H8	1.74	0.51
9:I:63:ARG:O	9:I:66:PRO:HD2	2.09	0.51
12:S:93:THR:O	12:S:96:ARG:N	2.43	0.51
4:N:349:LYS:HB2	4:N:365:GLU:HA	1.90	0.51
5:C:640:GLU:OE1	5:C:707:ARG:NH1	2.43	0.51
8:H:25:DC:H2''	8:H:26:DC:C6	2.45	0.51
8:H:93:DG:N2	8:H:222:DC:C2	2.78	0.51
8:H:228:DA:P	9:O:63:ARG:HH22	2.33	0.51
2:A:113:ARG:HH11	4:N:361:ASP:HB3	1.75	0.51
2:A:597:ILE:HD11	2:A:619:LEU:HD11	1.92	0.51
4:N:145:PRO:HA	4:N:179:GLU:OE1	2.09	0.51
1:F:5:VAL:HG22	1:F:67:LEU:HB2	1.90	0.51
4:N:129:ARG:HB3	4:N:143:LYS:HB2	1.92	0.51
5:C:37:GLU:O	5:C:40:SER:OG	2.16	0.51
12:M:89:ARG:O	12:M:92:GLN:HB3	2.10	0.51
2:A:529:LEU:HB2	4:N:35:VAL:HG11	1.91	0.51
4:N:236:HIS:CE1	4:N:239:HIS:HD2	2.29	0.51
5:C:639:SER:OG	5:C:684:ILE:HG13	2.11	0.51
8:H:16:DT:C2	8:H:17:DG:C5	2.98	0.51
8:H:146:DG:OP1	9:I:37:LYS:NZ	2.36	0.51
9:I:48:LEU:HD11	10:J:44:LYS:HZ2	1.76	0.51
4:N:176:HIS:CG	4:N:197:SER:HG	2.28	0.51
7:P:211:ILE:HD12	7:P:219:SER:O	2.11	0.51
7:P:241:LEU:HD11	7:P:259:ARG:HH22	1.76	0.51
8:H:15:DC:H6	8:H:15:DC:H5''	1.75	0.51
8:H:250:DC:H2''	8:H:251:DG:H8	1.75	0.51
8:H:258:DA:H2''	8:H:259:DA:H8	1.75	0.51
9:O:128:ARG:NH2	9:O:134:ARG:HB2	2.26	0.51
11:R:81:ARG:NH1	11:R:85:LEU:HD21	2.26	0.51
2:A:445:ARG:HE	6:B:144:ILE:HG12	1.76	0.51
7:P:223:HIS:ND1	7:P:264:THR:OG1	2.34	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:P:289:PRO:C	7:P:291:LYS:H	2.13	0.51
8:H:178:DC:H1'	8:H:179:DC:H5'	1.92	0.51
8:H:207:DA:H4'	8:H:208:DG:OP1	2.11	0.51
2:A:603:PHE:O	2:A:611:LYS:NZ	2.28	0.51
8:H:112:DA:H1'	8:H:113:DC:H5'	1.92	0.51
8:H:189:DG:H2''	8:H:190:DG:C8	2.45	0.51
8:H:299:DA:N6	8:H:300:DG:C6	2.79	0.51
1:F:42:ARG:NE	1:F:72:ARG:HD3	2.26	0.51
3:L:384:GLY:HA3	3:L:410:GLY:HA2	1.93	0.51
4:N:41:GLU:HG3	4:N:42:TRP:CD1	2.46	0.51
7:P:280:LEU:HB2	7:P:284:ILE:HD11	1.94	0.51
8:H:148:DC:H2''	8:H:149:DG:C8	2.46	0.51
8:H:215:DC:C6	8:H:216:DT:H72	2.46	0.51
12:S:113:LYS:O	12:S:116:THR:OG1	2.20	0.51
3:L:396:PRO:HA	3:L:399:ALA:HB2	1.93	0.50
5:C:257:PRO:HG2	5:C:259:GLU:O	2.11	0.50
8:H:169:DC:H1'	8:H:170:DT:H5'	1.92	0.50
8:H:184:DG:H4'	8:H:185:DC:OP1	2.11	0.50
10:J:31:LYS:HG3	10:J:51:TYR:CE1	2.46	0.50
11:K:29:ARG:NH1	12:M:33:SER:O	2.44	0.50
12:M:87:THR:OG1	12:M:90:GLU:OE1	2.26	0.50
10:Q:25:ASN:O	10:Q:28:GLY:N	2.35	0.50
2:A:675:ASP:OD1	2:A:676:LYS:N	2.43	0.50
4:N:49:TRP:CD2	4:N:383:ASN:HB3	2.46	0.50
4:N:390:ILE:HB	4:N:402:TRP:CZ2	2.46	0.50
8:H:173:DA:H2''	8:H:174:DG:O5'	2.11	0.50
10:Q:82:THR:N	10:Q:85:ASP:OD2	2.44	0.50
2:A:675:ASP:O	2:A:679:THR:HG23	2.11	0.50
5:C:48:LYS:HA	5:C:51:GLU:CD	2.32	0.50
7:P:107:LEU:O	7:P:111:MET:HG2	2.11	0.50
8:H:15:DC:H2''	8:H:16:DT:H5'	1.92	0.50
8:H:213:DC:C6	8:H:214:DT:H72	2.46	0.50
8:H:250:DC:H2''	8:H:251:DG:C8	2.47	0.50
9:O:97:GLU:OE1	9:O:97:GLU:N	2.43	0.50
11:R:15:LYS:HG3	11:R:20:ARG:HE	1.76	0.50
2:A:510:PRO:HD3	3:L:185:HIS:NE2	2.26	0.50
4:N:72:THR:HG22	4:N:77:ASN:OD1	2.12	0.50
5:C:562:CYS:SG	5:C:572:PRO:HD2	2.52	0.50
8:H:54:DG:H1'	8:H:55:DG:OP2	2.12	0.50
10:J:38:ALA:HB1	10:J:43:VAL:HG11	1.93	0.50
12:S:115:VAL:O	12:S:119:THR:HG23	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:173:LEU:HD13	4:N:205:TRP:CD2	2.47	0.50
8:H:117:DT:H2'	8:H:118:DT:H71	1.94	0.50
8:H:187:DG:H5''	8:H:187:DG:C8	2.44	0.50
8:H:292:DA:H1'	8:H:293:DC:H5''	1.93	0.50
11:K:42:ARG:O	12:M:85:THR:HA	2.12	0.50
2:A:136:ASP:N	2:A:136:ASP:OD1	2.41	0.50
3:L:166:ALA:HB1	3:L:193:ILE:HD12	1.93	0.50
8:H:13:DA:C2	8:H:303:DA:C2	3.00	0.50
8:H:231:DG:H4'	8:H:232:DC:OP1	2.11	0.50
9:O:80:THR:HG22	9:O:81:ASP:H	1.77	0.50
2:A:91:GLU:O	2:A:95:GLN:NE2	2.45	0.50
3:L:389:TRP:NE1	3:L:400:LYS:O	2.44	0.50
4:N:269:VAL:HG12	4:N:270:ASP:N	2.26	0.50
5:C:525:HIS:HE1	5:C:535:PRO:HD2	1.77	0.50
8:H:197:DA:OP1	11:R:32:ARG:NH1	2.44	0.50
11:K:115:LEU:HB3	10:Q:44:LYS:HD2	1.93	0.50
9:O:48:LEU:HG	9:O:52:ARG:HH21	1.77	0.50
8:H:8:DT:O3'	9:O:49:ARG:NH1	2.44	0.50
8:H:153:DG:H2''	8:H:154:DC:H5'	1.92	0.50
8:H:161:DG:H1'	8:H:162:DC:O5'	2.11	0.50
10:J:78:ARG:NH1	10:J:82:THR:OG1	2.45	0.50
9:O:99:TYR:OH	9:O:133:GLU:OE1	2.29	0.50
5:C:150:ILE:HG23	5:C:155:GLY:HA2	1.94	0.50
5:C:567:ASN:OD1	5:C:568:THR:N	2.45	0.50
6:B:150:ARG:O	6:B:153:LYS:HG3	2.12	0.50
8:H:306:DT:H2''	8:H:307:DA:C8	2.47	0.50
2:A:93:PRO:HA	2:A:96:ILE:HD12	1.93	0.49
4:N:138:CYS:HA	4:N:154:TYR:CZ	2.47	0.49
8:H:16:DT:H1'	8:H:17:DG:O5'	2.12	0.49
8:H:103:DC:H2'	8:H:104:DT:H71	1.94	0.49
12:S:119:THR:OG1	12:S:120:SER:N	2.45	0.49
1:F:37:PRO:O	1:F:41:GLN:HG3	2.13	0.49
4:N:389:VAL:HG12	4:N:403:GLN:HB2	1.92	0.49
10:J:46:ILE:HG22	10:J:47:SER:O	2.13	0.49
11:K:92:GLU:OE2	12:M:103:LEU:N	2.43	0.49
4:N:176:HIS:ND1	4:N:197:SER:OG	2.41	0.49
8:H:199:DT:H2''	8:H:200:DT:H71	1.94	0.49
9:O:118:THR:HG22	10:Q:45:ARG:HB3	1.95	0.49
2:A:166:HIS:HD2	2:A:353:PRO:HG3	1.77	0.49
2:A:195:LYS:H	2:A:198:ASP:HB2	1.77	0.49
2:A:521:LYS:HD3	2:A:577:GLN:HE21	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:P:211:ILE:HA	7:P:215:GLY:H	1.77	0.49
7:P:269:LEU:O	7:P:272:LEU:HG	2.12	0.49
8:H:240:DC:C2	8:H:241:DG:N7	2.80	0.49
3:L:368:PHE:HB3	3:L:379:LEU:HD13	1.94	0.49
3:L:419:SER:OG	3:L:421:ASP:OD1	2.29	0.49
4:N:73:SER:OG	4:N:74:ASP:N	2.46	0.49
4:N:344:VAL:N	4:N:368:PHE:O	2.46	0.49
5:C:38:VAL:HA	5:C:41:MET:HG2	1.94	0.49
5:C:507:GLN:HE22	9:I:35:VAL:H	1.59	0.49
8:H:10:DT:H2'	8:H:11:DA:H8	1.76	0.49
8:H:103:DC:C2'	8:H:104:DT:H71	2.42	0.49
2:A:132:PHE:HE2	4:N:330:GLU:HG2	1.78	0.49
2:A:525:ILE:HG21	2:A:562:ASN:OD1	2.13	0.49
3:L:189:HIS:CE1	3:L:216:ARG:HG3	2.48	0.49
5:C:690:SER:OG	5:C:691:VAL:N	2.45	0.49
8:H:180:DC:H2'	8:H:180:DC:OP2	2.12	0.49
8:H:200:DT:C2	8:H:201:DG:N7	2.80	0.49
8:H:279:DC:H2''	8:H:280:DT:H71	1.94	0.49
10:J:38:ALA:O	10:J:43:VAL:HG12	2.13	0.49
2:A:82:ASP:O	2:A:85:LEU:HG	2.13	0.49
5:C:46:ARG:HD2	5:C:49:ILE:HD12	1.95	0.49
7:P:101:SER:OG	12:S:45:VAL:O	2.30	0.49
8:H:200:DT:C2	8:H:201:DG:C8	3.01	0.49
2:A:525:ILE:HD13	2:A:562:ASN:OD1	2.12	0.49
3:L:89:LYS:HA	3:L:433:SER:HA	1.94	0.49
3:L:383:VAL:HG23	3:L:385:LYS:HG3	1.94	0.49
4:N:329:ASN:HB3	4:N:332:ILE:HD12	1.94	0.49
4:N:338:THR:HG22	4:N:376:LYS:HG3	1.95	0.49
8:H:159:DC:H2''	8:H:160:DT:H72	1.95	0.49
2:A:516:ARG:NH1	4:N:374:THR:O	2.45	0.49
4:N:132:TYR:HA	4:N:140:ILE:HG22	1.94	0.49
4:N:181:TYR:CE2	7:P:295:ARG:HD3	2.48	0.49
4:N:287:PHE:HB3	4:N:303:LEU:H	1.77	0.49
5:C:569:LYS:O	5:C:575:LEU:HD11	2.12	0.49
8:H:119:DG:H2''	8:H:120:DA:N7	2.28	0.49
8:H:248:DC:H2''	8:H:249:DC:C5	2.48	0.49
10:Q:47:SER:OG	10:Q:48:GLY:N	2.45	0.48
2:A:468:LYS:HG2	2:A:476:PHE:CD1	2.48	0.48
2:A:664:HIS:CD2	2:A:674:ILE:HD11	2.48	0.48
3:L:153:THR:HG21	3:L:198:PHE:CE2	2.47	0.48
5:C:35:ALA:HA	5:C:38:VAL:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:P:214:LEU:HD12	7:P:221:VAL:HG11	1.94	0.48
2:A:184:LEU:HD23	2:A:184:LEU:H	1.78	0.48
2:A:525:ILE:O	4:N:38:HIS:ND1	2.38	0.48
2:A:676:LYS:O	2:A:679:THR:OG1	2.18	0.48
3:L:232:VAL:HG12	3:L:295:HIS:HB3	1.94	0.48
3:L:373:TRP:HB3	3:L:375:LYS:HD2	1.96	0.48
4:N:172:ARG:HG2	4:N:215:LYS:O	2.12	0.48
4:N:273:THR:OG1	4:N:295:ASP:OD2	2.31	0.48
5:C:565:GLN:HB2	5:C:567:ASN:CG	2.33	0.48
5:C:579:GLU:HG2	5:C:603:ASN:OD1	2.13	0.48
8:H:100:DG:H2'	8:H:100:DG:OP2	2.14	0.48
8:H:267:DG:H1'	8:H:268:DG:C8	2.48	0.48
11:R:18:SER:O	11:R:22:GLY:N	2.46	0.48
3:L:103:TRP:CZ3	3:L:372:PHE:HB2	2.48	0.48
5:C:453:ALA:O	5:C:457:LEU:HG	2.13	0.48
5:C:629:LYS:O	5:C:718:THR:HG23	2.13	0.48
7:P:225:THR:HG23	7:P:227:ILE:HD11	1.95	0.48
9:I:61:LEU:HD21	10:J:40:ARG:NH2	2.28	0.48
3:L:191:ASN:HB3	3:L:211:LYS:HD3	1.94	0.48
4:N:255:TRP:CD2	4:N:265:PRO:HB3	2.48	0.48
4:N:404:MET:HG2	4:N:408:ILE:HD13	1.96	0.48
5:C:525:HIS:NE2	5:C:549:CYS:SG	2.86	0.48
5:C:596:SER:O	5:C:597:LYS:HE2	2.13	0.48
2:A:303:ASP:N	2:A:307:ARG:O	2.47	0.48
3:L:82:PHE:C	3:L:83:LYS:HZ2	2.15	0.48
4:N:71:HIS:ND1	4:N:126:GLU:OE1	2.46	0.48
5:C:296:LEU:HD12	5:C:297:HIS:CD2	2.49	0.48
6:B:142:THR:O	6:B:143:GLN:HG3	2.13	0.48
8:H:246:DC:H2''	8:H:247:DC:C5	2.48	0.48
8:H:300:DG:C6	8:H:301:DA:C5	3.01	0.48
2:A:458:ARG:HB2	2:A:459:LYS:NZ	2.29	0.48
2:A:595:LYS:O	2:A:598:THR:OG1	2.32	0.48
4:N:316:HIS:ND1	4:N:339:ASP:OD2	2.37	0.48
8:H:47:DC:H2''	8:H:48:DC:C6	2.47	0.48
8:H:165:DG:N3	8:H:166:DC:H5'	2.29	0.48
8:H:313:DT:H2'	8:H:314:DG:C8	2.49	0.48
3:L:104:HIS:CD2	3:L:154:TYR:HD1	2.32	0.48
3:L:153:THR:HG21	3:L:198:PHE:CD2	2.49	0.48
4:N:284:TYR:OH	4:N:329:ASN:N	2.47	0.48
4:N:325:TRP:HA	4:N:333:LEU:HD12	1.96	0.48
4:N:396:ASP:O	4:N:398:ILE:HG12	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:689:HIS:HB3	5:C:737:VAL:HG11	1.95	0.48
7:P:241:LEU:HD11	7:P:259:ARG:NH2	2.29	0.48
8:H:12:DT:H2''	8:H:13:DA:H8	1.77	0.48
8:H:21:DC:H2''	8:H:22:DG:C8	2.48	0.48
8:H:120:DA:H1'	8:H:121:DG:N7	2.29	0.48
8:H:189:DG:H2''	8:H:190:DG:H8	1.79	0.48
4:N:122:ASN:ND2	4:N:165:GLY:O	2.47	0.48
4:N:382:TRP:CE3	4:N:390:ILE:HD11	2.49	0.48
5:C:45:ASN:HA	5:C:48:LYS:HD2	1.96	0.48
5:C:568:THR:OG1	5:C:569:LYS:N	2.44	0.48
8:H:90:DA:H2''	8:H:91:DG:H8	1.76	0.48
11:R:79:ILE:HG23	11:R:80:PRO:HD2	1.95	0.48
2:A:521:LYS:HG3	4:N:41:GLU:HB2	1.96	0.48
4:N:324:GLN:HB3	4:N:382:TRP:HE1	1.78	0.48
8:H:22:DG:C2	8:H:294:DG:C2	3.01	0.48
8:H:55:DG:H2''	8:H:56:DT:H5''	1.95	0.48
8:H:103:DC:H5'	8:H:103:DC:H6	1.79	0.48
8:H:242:DC:H2''	8:H:243:DT:OP2	2.14	0.48
2:A:315:TYR:HB2	2:A:357:PHE:CZ	2.49	0.47
3:L:406:HIS:CE1	3:L:408:LYS:HG2	2.48	0.47
4:N:325:TRP:O	4:N:382:TRP:NE1	2.46	0.47
5:C:717:GLN:N	5:C:717:GLN:OE1	2.44	0.47
8:H:218:DG:P	9:O:72:ARG:HH22	2.37	0.47
11:R:92:GLU:OE1	12:S:103:LEU:HG	2.14	0.47
2:A:565:TYR:C	2:A:566:PHE:HD1	2.18	0.47
3:L:261:LYS:HB3	3:L:297:PRO:HB3	1.96	0.47
4:N:281:PHE:CE2	4:N:289:LEU:HD13	2.49	0.47
5:C:334:PHE:HA	5:C:337:ALA:HB3	1.96	0.47
7:P:224:SER:HB3	7:P:243:TRP:CE2	2.49	0.47
8:H:62:DC:H2''	8:H:63:DG:H8	1.79	0.47
8:H:220:DA:H4'	8:H:221:DC:OP1	2.14	0.47
8:H:282:DG:H2''	8:H:283:DT:H71	1.96	0.47
10:Q:46:ILE:HG22	10:Q:47:SER:O	2.14	0.47
11:R:31:HIS:HE1	11:R:35:ARG:CZ	2.27	0.47
2:A:95:GLN:H	2:A:95:GLN:CD	2.17	0.47
8:H:210:DC:H2''	8:H:211:DA:H8	1.78	0.47
8:H:281:DA:H2''	8:H:282:DG:C8	2.48	0.47
9:I:120:MET:N	9:I:123:ASP:OD2	2.27	0.47
3:L:326:ASN:HA	3:L:358:TYR:CE2	2.49	0.47
3:L:370:MET:HG2	3:L:391:LEU:HD11	1.96	0.47
8:H:51:DG:P	9:I:72:ARG:HH22	2.38	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:65:DG:H2''	8:H:66:DG:C8	2.48	0.47
8:H:85:DG:C2'	8:H:86:DT:H71	2.44	0.47
8:H:277:DC:H1'	8:H:278:DC:C5	2.49	0.47
1:F:2:GLN:NE2	1:F:16:GLU:OE2	2.36	0.47
3:L:175:ILE:HA	3:L:182:CYS:HA	1.95	0.47
4:N:50:LEU:HA	4:N:50:LEU:HD23	1.70	0.47
8:H:59:DA:H2''	8:H:60:DA:C8	2.50	0.47
8:H:131:DC:H2''	8:H:132:DA:C8	2.50	0.47
8:H:132:DA:H3'	11:R:75:LYS:NZ	2.29	0.47
8:H:217:DA:H2''	8:H:218:DG:H8	1.80	0.47
8:H:272:DT:H2''	8:H:273:DT:H71	1.95	0.47
10:J:71:THR:HG21	12:M:97:LEU:HD21	1.96	0.47
4:N:255:TRP:CE2	4:N:265:PRO:HB3	2.50	0.47
4:N:295:ASP:HB3	4:N:297:THR:OG1	2.15	0.47
5:C:436:GLU:O	5:C:439:MET:HB3	2.14	0.47
8:H:13:DA:C2	8:H:14:DT:C2	3.03	0.47
8:H:44:DT:H2'	8:H:45:DC:C6	2.49	0.47
8:H:298:DC:C2'	8:H:299:DA:C8	2.97	0.47
11:R:15:LYS:HG2	11:R:20:ARG:HH21	1.80	0.47
3:L:176:ASN:O	3:L:180:MET:N	2.47	0.47
4:N:40:LEU:O	4:N:397:ASN:HB3	2.15	0.47
5:C:443:LEU:HD13	5:C:454:ILE:HA	1.96	0.47
5:C:689:HIS:HB2	5:C:726:TYR:CZ	2.50	0.47
8:H:83:DG:N3	9:O:40:ARG:NH2	2.43	0.47
8:H:109:DA:C6	8:H:205:DG:C5	3.03	0.47
8:H:248:DC:O4'	10:J:45:ARG:NH2	2.48	0.47
8:H:291:DC:C2	8:H:292:DA:C5	3.02	0.47
12:M:43:LYS:HA	12:M:43:LYS:HD3	1.59	0.47
2:A:94:THR:O	2:A:98:ARG:HG2	2.14	0.47
8:H:219:DC:C2	8:H:220:DA:C8	3.03	0.47
11:K:25:PHE:O	11:K:27:VAL:N	2.47	0.47
1:F:6:LYS:HG2	1:F:66:THR:HG23	1.97	0.47
2:A:164:PHE:CD1	2:A:355:LEU:HB2	2.48	0.47
2:A:479:VAL:HG21	2:A:486:ARG:HH21	1.80	0.47
3:L:119:ASN:OD1	3:L:119:ASN:N	2.48	0.47
4:N:295:ASP:O	4:N:297:THR:HG23	2.14	0.47
8:H:103:DC:N3	8:H:212:DG:C2	2.83	0.47
8:H:298:DC:H4'	8:H:299:DA:OP1	2.15	0.47
11:K:84:GLN:HE22	11:K:88:ARG:HE	1.62	0.47
12:M:111:GLY:O	12:M:115:VAL:HG12	2.14	0.47
12:S:77:LEU:HD23	12:S:77:LEU:HA	1.67	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:311:LEU:O	2:A:315:TYR:OH	2.24	0.47
2:A:516:ARG:NH2	4:N:14:GLU:OE1	2.48	0.47
3:L:153:THR:O	3:L:162:LEU:N	2.43	0.47
5:C:121:MET:HE1	5:C:298:PRO:HD3	1.96	0.47
5:C:577:VAL:O	5:C:578:ARG:HG3	2.15	0.47
8:H:57:DT:H4'	8:H:58:DT:OP1	2.15	0.47
8:H:251:DG:H2''	8:H:252:DC:C6	2.50	0.47
9:I:100:LEU:HA	9:I:100:LEU:HD23	1.62	0.47
11:K:67:GLY:HA3	12:M:46:HIS:CE1	2.49	0.47
1:T:54:ARG:HE	1:T:58:ASP:HB3	1.81	0.46
2:A:126:ASN:HD22	4:N:410:ASN:N	2.13	0.46
2:A:445:ARG:NH1	6:B:145:SER:OG	2.48	0.46
3:L:390:ASP:OD1	3:L:390:ASP:N	2.48	0.46
4:N:173:LEU:HB3	4:N:205:TRP:NE1	2.30	0.46
4:N:178:LYS:N	4:N:199:ASP:OD1	2.48	0.46
4:N:250:GLN:HG2	4:N:275:GLU:HA	1.97	0.46
4:N:280:SER:O	4:N:289:LEU:HD12	2.15	0.46
4:N:386:GLU:OE1	4:N:387:PRO:HD2	2.16	0.46
7:P:227:ILE:HD11	7:P:242:HIS:HB3	1.97	0.46
8:H:52:DG:N1	8:H:264:DC:N3	2.62	0.46
8:H:238:DC:H2''	8:H:239:DG:O5'	2.14	0.46
10:J:77:LYS:HG2	12:M:89:ARG:HH22	1.79	0.46
2:A:187:LEU:HD11	2:A:253:ARG:NH2	2.30	0.46
2:A:244:MET:SD	2:A:244:MET:N	2.88	0.46
2:A:315:TYR:CD1	7:P:230:ARG:HB2	2.50	0.46
3:L:87:SER:O	3:L:88:LEU:HD23	2.16	0.46
3:L:261:LYS:HG2	3:L:300:SER:OG	2.14	0.46
3:L:374:GLN:C	3:L:391:LEU:HD12	2.36	0.46
4:N:176:HIS:CE1	4:N:197:SER:HG	2.30	0.46
7:P:294:LYS:HG3	7:P:295:ARG:N	2.30	0.46
8:H:155:DA:H2	8:H:160:DT:O2	1.98	0.46
8:H:195:DT:H6	8:H:195:DT:H2'	1.60	0.46
2:A:133:LYS:HD2	4:N:304:ARG:NH2	2.29	0.46
4:N:49:TRP:HA	4:N:66:LEU:HD13	1.96	0.46
4:N:185:TRP:CD2	4:N:193:LEU:HD12	2.51	0.46
5:C:613:HIS:CD2	5:C:629:LYS:HD2	2.41	0.46
6:B:144:ILE:HG13	6:B:145:SER:N	2.31	0.46
8:H:189:DG:C2	8:H:190:DG:C5	3.03	0.46
11:R:17:ARG:O	11:R:20:ARG:N	2.48	0.46
8:H:217:DA:O3'	9:O:83:ARG:NH1	2.48	0.46
8:H:240:DC:H2''	8:H:241:DG:H8	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:15:LYS:HB2	11:K:20:ARG:HE	1.79	0.46
2:A:190:LYS:O	2:A:204:ARG:N	2.35	0.46
3:L:246:LEU:HD12	3:L:316:GLY:HA2	1.98	0.46
4:N:49:TRP:CE2	4:N:66:LEU:HD11	2.50	0.46
7:P:231:LYS:HA	7:P:237:ILE:HA	1.97	0.46
8:H:142:DT:H2''	8:H:143:DC:C5	2.50	0.46
8:H:270:DG:H2''	8:H:271:DA:C8	2.50	0.46
2:A:252:PHE:O	2:A:297:ALA:N	2.48	0.46
8:H:121:DG:H1'	8:H:122:DC:C6	2.50	0.46
8:H:298:DC:C4	8:H:299:DA:C6	3.03	0.46
9:I:85:GLN:HE22	10:J:82:THR:HG23	1.81	0.46
12:M:45:VAL:HG12	12:M:46:HIS:CD2	2.51	0.46
1:T:2:GLN:HE22	1:T:63:LYS:HB3	1.80	0.46
5:C:741:ARG:O	5:C:741:ARG:HG2	2.16	0.46
7:P:231:LYS:HG2	7:P:232:GLU:O	2.16	0.46
8:H:191:DC:C2	8:H:192:DC:C4	3.04	0.46
1:F:54:ARG:HE	1:F:58:ASP:CG	2.18	0.46
2:A:100:LEU:O	2:A:104:ASN:ND2	2.49	0.46
5:C:507:GLN:NE2	9:I:35:VAL:HG23	2.31	0.46
7:P:276:THR:O	7:P:279:LEU:HG	2.16	0.46
8:H:270:DG:C2	8:H:271:DA:C5	3.04	0.46
2:A:295:PHE:N	2:A:321:GLU:HA	2.31	0.46
5:C:497:ARG:NE	8:H:252:DC:OP1	2.44	0.46
8:H:12:DT:H2''	8:H:13:DA:C8	2.51	0.46
8:H:93:DG:H2''	8:H:94:DG:C8	2.50	0.46
8:H:170:DT:H1'	8:H:171:DG:O4'	2.16	0.46
8:H:176:DA:H1'	8:H:177:DT:H5'	1.98	0.46
8:H:243:DT:H2''	8:H:244:DG:N7	2.30	0.46
8:H:276:DT:H2''	8:H:277:DC:C5	2.51	0.46
1:F:4:PHE:CD1	1:F:14:THR:HG22	2.51	0.46
2:A:653:CYS:O	2:A:656:PHE:HB3	2.16	0.46
4:N:344:VAL:HB	4:N:368:PHE:HB3	1.97	0.46
5:C:494:ARG:O	5:C:497:ARG:HG3	2.17	0.46
8:H:102:DG:H2''	8:H:103:DC:C6	2.51	0.46
8:H:207:DA:H2''	8:H:208:DG:C8	2.51	0.46
8:H:238:DC:H2''	8:H:239:DG:C5'	2.46	0.46
9:I:54:TYR:C	9:I:56:LYS:H	2.19	0.46
3:L:245:ASP:OD1	3:L:248:GLY:N	2.44	0.45
4:N:135:GLN:HE21	4:N:190:SER:HA	1.81	0.45
5:C:469:PHE:O	5:C:473:GLU:N	2.28	0.45
7:P:211:ILE:HD12	7:P:220:VAL:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:198:DA:H2''	8:H:199:DT:H71	1.99	0.45
11:R:25:PHE:CE2	11:R:56:GLU:HA	2.51	0.45
2:A:627:ILE:HG13	2:A:628:ALA:N	2.31	0.45
5:C:48:LYS:O	5:C:52:ARG:HG3	2.15	0.45
8:H:135:DG:N1	8:H:180:DC:C2	2.83	0.45
8:H:154:DC:H2''	8:H:155:DA:N7	2.31	0.45
8:H:175:DA:H2''	8:H:176:DA:H8	1.81	0.45
11:K:91:GLU:HG2	11:K:92:GLU:N	2.31	0.45
4:N:126:GLU:OE2	7:P:294:LYS:NZ	2.39	0.45
5:C:648:GLN:HG2	5:C:672:ASP:O	2.16	0.45
12:S:82:LYS:HE3	12:S:82:LYS:HB2	1.83	0.45
4:N:173:LEU:HD13	4:N:205:TRP:CG	2.52	0.45
5:C:717:GLN:H	5:C:717:GLN:CD	2.20	0.45
8:H:20:DA:C4	8:H:21:DC:C5	3.04	0.45
8:H:48:DC:H2''	8:H:49:DT:C5	2.51	0.45
8:H:68:DG:H2''	8:H:69:DG:N7	2.31	0.45
9:I:93:GLN:O	9:I:96:SER:OG	2.28	0.45
11:R:65:LEU:HD23	11:R:65:LEU:HA	1.78	0.45
1:T:3:ILE:HD12	1:T:67:LEU:HD13	1.99	0.45
1:T:38:PRO:HA	1:T:41:GLN:OE1	2.16	0.45
3:L:313:ARG:HD3	3:L:313:ARG:HA	1.62	0.45
6:B:148:SER:HA	6:B:151:LYS:NZ	2.31	0.45
7:P:52:ALA:HA	7:P:65:ASN:HA	1.99	0.45
8:H:8:DT:H2'	8:H:9:DA:O4'	2.15	0.45
8:H:181:DG:OP2	8:H:181:DG:H2'	2.17	0.45
8:H:185:DC:H4'	8:H:186:DC:OP1	2.14	0.45
8:H:197:DA:C4	8:H:198:DA:N7	2.85	0.45
8:H:259:DA:H2''	8:H:260:DC:C6	2.51	0.45
12:M:113:LYS:HE2	12:M:113:LYS:HB3	1.74	0.45
1:F:15:LEU:HD21	1:F:30:ILE:HG12	1.98	0.45
1:F:24:GLU:HB2	1:F:52:ASP:HB3	1.99	0.45
1:T:3:ILE:HD11	1:T:15:LEU:HD12	1.99	0.45
2:A:656:PHE:CE2	2:A:660:LEU:HD11	2.52	0.45
4:N:143:LYS:HE2	4:N:180:GLY:O	2.16	0.45
5:C:654:ARG:NH1	5:C:676:ASP:OD2	2.49	0.45
6:B:148:SER:HA	6:B:151:LYS:HZ3	1.81	0.45
8:H:135:DG:P	8:H:135:DG:H3'	2.57	0.45
9:I:86:SER:OG	9:I:87:SER:N	2.49	0.45
11:K:24:GLN:N	11:K:24:GLN:OE1	2.50	0.45
1:F:6:LYS:HD2	1:F:12:THR:HG22	1.98	0.45
1:F:36:ILE:O	1:F:41:GLN:NE2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:268:LYS:HA	3:L:271:MET:HE2	1.98	0.45
5:C:625:GLY:HA2	5:C:686:PHE:O	2.17	0.45
6:B:163:LEU:HD12	6:B:163:LEU:H	1.82	0.45
8:H:302:DT:H2'	8:H:303:DA:C8	2.52	0.45
2:A:653:CYS:O	2:A:657:MET:HG3	2.17	0.45
4:N:123:HIS:CE1	4:N:142:THR:HG21	2.52	0.45
7:P:106:TRP:CZ2	12:S:47:PRO:HD2	2.52	0.45
8:H:172:DG:H2''	8:H:173:DA:H8	1.81	0.45
8:H:192:DC:H6	8:H:192:DC:H2'	1.68	0.45
11:K:23:LEU:HD23	11:K:23:LEU:HA	1.82	0.45
11:K:55:LEU:O	11:K:59:THR:HG22	2.17	0.45
1:F:48:LYS:HE3	1:F:54:ARG:HH22	1.82	0.45
3:L:85:VAL:HG21	3:L:438:ASP:CG	2.37	0.45
3:L:123:LEU:HB2	3:L:136:GLN:N	2.32	0.45
3:L:229:PHE:HB3	3:L:263:TRP:NE1	2.31	0.45
4:N:81:ILE:O	4:N:118:GLU:HG2	2.17	0.45
4:N:284:TYR:OH	4:N:328:HIS:N	2.49	0.45
4:N:340:ARG:HH12	7:P:285:TYR:HE1	1.63	0.45
7:P:211:ILE:HG22	7:P:217:GLY:H	1.82	0.45
8:H:135:DG:C2	8:H:180:DC:C2	3.05	0.45
8:H:167:DG:H4'	8:H:168:DG:OP1	2.16	0.45
11:K:25:PHE:CD2	11:K:56:GLU:HB2	2.52	0.45
11:R:45:ALA:O	11:R:48:PRO:HD2	2.17	0.45
3:L:381:ASN:H	3:L:413:ILE:HB	1.81	0.45
4:N:62:SER:OG	4:N:63:ILE:N	2.50	0.45
4:N:189:LEU:HG	4:N:240:GLU:HB2	1.98	0.45
4:N:278:CYS:SG	4:N:292:GLY:HA3	2.57	0.45
4:N:284:TYR:CD1	4:N:330:GLU:HA	2.52	0.45
7:P:218:HIS:O	7:P:268:HIS:ND1	2.50	0.45
7:P:220:VAL:O	7:P:266:VAL:HA	2.16	0.45
8:H:15:DC:C2'	8:H:16:DT:H6	2.30	0.45
8:H:224:DC:H2'	8:H:225:DT:H6	1.81	0.45
9:I:50:GLU:OE1	10:J:39:ARG:NE	2.46	0.45
11:R:15:LYS:HZ3	11:R:20:ARG:NH2	2.15	0.45
1:F:27:LYS:HA	1:F:41:GLN:OE1	2.17	0.45
2:A:431:GLN:HG3	2:A:441:GLN:HG2	1.99	0.44
3:L:373:TRP:HB3	3:L:375:LYS:NZ	2.32	0.44
4:N:282:ASN:HB2	4:N:325:TRP:CH2	2.52	0.44
5:C:519:ASN:OD1	5:C:520:TYR:N	2.50	0.44
5:C:633:GLN:N	5:C:633:GLN:OE1	2.50	0.44
8:H:20:DA:H8	8:H:20:DA:H5''	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:88:DT:H1'	8:H:89:DT:H5'	1.98	0.44
8:H:248:DC:H5''	8:H:248:DC:H6	1.83	0.44
3:L:83:LYS:O	3:L:85:VAL:HG13	2.17	0.44
5:C:241:LYS:HA	5:C:241:LYS:HD3	1.68	0.44
5:C:437:ALA:O	5:C:441:ARG:HG3	2.17	0.44
5:C:725:ASP:OD1	5:C:727:ARG:N	2.28	0.44
8:H:309:DA:H4'	8:H:310:DT:OP1	2.17	0.44
11:K:83:LEU:HD23	11:K:83:LEU:HA	1.72	0.44
6:E:28:VAL:HA	6:E:31:LYS:HD2	1.99	0.44
2:A:521:LYS:NZ	2:A:577:GLN:HG3	2.33	0.44
2:A:590:GLU:HA	2:A:593:ARG:HE	1.82	0.44
4:N:169:PRO:CG	4:N:172:ARG:HH21	2.30	0.44
4:N:324:GLN:HB3	4:N:382:TRP:NE1	2.33	0.44
5:C:650:GLU:HA	5:C:653:ARG:NH2	2.30	0.44
8:H:130:DG:H1'	8:H:131:DC:C5	2.52	0.44
8:H:144:DC:H2''	8:H:145:DA:O5'	2.16	0.44
8:H:175:DA:H5'	8:H:175:DA:H8	1.83	0.44
8:H:195:DT:H4'	8:H:196:DC:OP1	2.18	0.44
8:H:294:DG:C2'	8:H:295:DT:H5''	2.47	0.44
11:K:58:LEU:HD23	11:K:58:LEU:HA	1.76	0.44
12:M:82:LYS:HB2	12:M:82:LYS:HE2	1.78	0.44
4:N:55:ARG:NH2	4:N:385:ASN:O	2.50	0.44
5:C:44:SER:O	5:C:47:GLN:HB3	2.18	0.44
8:H:147:DC:H2''	8:H:148:DC:O5'	2.17	0.44
8:H:178:DC:H5'	8:H:178:DC:H6	1.82	0.44
8:H:198:DA:O3'	11:R:14:ALA:HB1	2.16	0.44
8:H:223:DG:H2''	8:H:224:DC:H6	1.83	0.44
8:H:301:DA:C6	8:H:302:DT:C4	3.06	0.44
10:J:31:LYS:N	10:J:32:PRO:HD2	2.33	0.44
1:T:23:ILE:HG13	1:T:50:LEU:HB3	1.98	0.44
2:A:650:LYS:HA	2:A:650:LYS:HD3	1.69	0.44
8:H:66:DG:H2''	8:H:67:DG:C8	2.53	0.44
8:H:308:DC:H2''	8:H:309:DA:N7	2.32	0.44
11:K:26:PRO:O	11:K:29:ARG:N	2.51	0.44
1:F:43:LEU:O	1:F:50:LEU:HB2	2.18	0.44
1:T:27:LYS:HB3	1:T:38:PRO:HB3	1.99	0.44
2:A:495:TYR:O	2:A:497:GLY:N	2.50	0.44
3:L:138:TYR:CD2	5:C:99:LYS:HB3	2.52	0.44
3:L:302:ARG:HH12	5:C:129:HIS:HB2	1.83	0.44
4:N:324:GLN:HB2	4:N:380:PHE:CZ	2.52	0.44
8:H:15:DC:H2''	8:H:16:DT:H6	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:16:DT:H2''	8:H:17:DG:C8	2.52	0.44
8:H:50:DT:C2	8:H:51:DG:C5	3.05	0.44
10:Q:71:THR:HG21	12:S:97:LEU:HD21	2.00	0.44
2:A:496:ASP:HA	7:P:186:PRO:HG3	1.99	0.44
4:N:230:VAL:HA	4:N:247:ALA:HA	2.00	0.44
8:H:258:DA:OP1	9:I:69:ARG:NH2	2.51	0.44
8:H:266:DA:H2''	8:H:267:DG:C8	2.53	0.44
8:H:270:DG:C4	8:H:271:DA:N7	2.86	0.44
11:R:84:GLN:HG2	11:R:105:GLY:O	2.18	0.44
4:N:76:GLN:HE22	4:N:123:HIS:H	1.64	0.44
4:N:186:ASN:OD1	4:N:187:PRO:HD2	2.17	0.44
5:C:144:THR:O	5:C:148:GLU:HG3	2.17	0.44
8:H:48:DC:C4	8:H:266:DA:C6	3.06	0.44
8:H:160:DT:H1'	8:H:161:DG:O4'	2.18	0.44
11:R:23:LEU:HD23	11:R:23:LEU:HA	1.77	0.44
2:A:126:ASN:HB3	4:N:410:ASN:H	1.82	0.44
2:A:679:THR:OG1	2:A:680:LYS:N	2.51	0.44
3:L:113:PHE:CZ	3:L:124:TYR:HD2	2.36	0.44
3:L:189:HIS:CE1	3:L:210:SER:HG	2.36	0.44
4:N:185:TRP:CE2	4:N:193:LEU:HD12	2.52	0.44
4:N:190:SER:O	4:N:192:HIS:ND1	2.44	0.44
7:P:181:ARG:HA	7:P:181:ARG:HD3	1.86	0.44
8:H:11:DA:H2'	8:H:12:DT:C6	2.52	0.44
8:H:176:DA:C2'	8:H:177:DT:H71	2.48	0.44
8:H:201:DG:H2''	8:H:202:DG:C8	2.53	0.44
8:H:303:DA:H3'	8:H:304:DT:H73	2.00	0.44
2:A:101:ARG:HG2	2:A:105:LEU:HD11	1.99	0.43
3:L:81:SER:OG	3:L:440:LEU:HB2	2.18	0.43
3:L:335:LYS:HA	3:L:351:THR:OG1	2.17	0.43
4:N:346:ASP:CG	4:N:349:LYS:HG3	2.38	0.43
8:H:41:DT:H2''	8:H:42:DA:N7	2.32	0.43
8:H:161:DG:H2''	8:H:162:DC:H2'	2.00	0.43
8:H:180:DC:H2''	8:H:181:DG:H8	1.82	0.43
8:H:187:DG:H4'	11:R:77:ARG:NH1	2.33	0.43
11:R:31:HIS:HE1	11:R:35:ARG:NE	2.16	0.43
12:S:98:LEU:HD23	12:S:98:LEU:HA	1.76	0.43
1:T:9:THR:OG1	1:T:11:LYS:HG2	2.18	0.43
4:N:89:ASP:OD1	4:N:91:ALA:N	2.46	0.43
4:N:328:HIS:ND1	4:N:387:PRO:HA	2.32	0.43
5:C:34:ARG:O	5:C:38:VAL:HG13	2.18	0.43
8:H:82:DT:H2''	8:H:83:DG:C8	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:15:LYS:HB2	11:K:20:ARG:NE	2.33	0.43
11:K:91:GLU:O	11:K:94:ASN:N	2.51	0.43
12:M:77:LEU:HA	12:M:77:LEU:HD12	1.70	0.43
4:N:77:ASN:HB2	4:N:123:HIS:O	2.19	0.43
4:N:132:TYR:HD2	4:N:137:PRO:HA	1.81	0.43
4:N:311:HIS:CG	4:N:312:SER:H	2.37	0.43
5:C:584:LEU:O	5:C:586:LEU:N	2.49	0.43
7:P:240:LEU:HD13	7:P:253:TRP:CE2	2.54	0.43
8:H:10:DT:C2	8:H:11:DA:C8	3.06	0.43
8:H:137:DG:O6	8:H:178:DC:N4	2.50	0.43
8:H:137:DG:OP2	8:H:137:DG:H2'	2.19	0.43
8:H:142:DT:O2	8:H:174:DG:N2	2.51	0.43
8:H:162:DC:H4'	8:H:163:DC:OP1	2.16	0.43
8:H:276:DT:H1'	8:H:277:DC:C2	2.53	0.43
8:H:299:DA:O5'	11:K:76:THR:HG21	2.18	0.43
9:I:67:PHE:CZ	9:I:93:GLN:HA	2.54	0.43
1:T:25:ASN:O	1:T:29:LYS:HG3	2.18	0.43
2:A:481:HIS:CD2	2:A:483:LYS:H	2.37	0.43
3:L:375:LYS:HA	3:L:391:LEU:HB2	1.99	0.43
3:L:395:ASP:O	3:L:399:ALA:N	2.51	0.43
4:N:300:LEU:HD21	4:N:311:HIS:HB3	2.01	0.43
4:N:373:HIS:ND1	4:N:394:SER:HB3	2.34	0.43
5:C:565:GLN:O	5:C:567:ASN:N	2.48	0.43
8:H:39:DA:C4	8:H:40:DG:C5	3.06	0.43
8:H:123:DG:C2	8:H:193:DG:N2	2.86	0.43
8:H:157:DC:N3	8:H:158:DG:C6	2.87	0.43
8:H:228:DA:C8	8:H:228:DA:H5'	2.54	0.43
8:H:291:DC:C2	8:H:292:DA:N7	2.85	0.43
9:O:48:LEU:O	9:O:52:ARG:NE	2.48	0.43
10:Q:31:LYS:N	10:Q:32:PRO:HD2	2.33	0.43
2:A:241:ASN:HB3	2:A:245:VAL:HG22	1.99	0.43
3:L:172:ILE:O	3:L:185:HIS:HA	2.17	0.43
4:N:49:TRP:CD2	4:N:66:LEU:HD11	2.53	0.43
4:N:52:ASP:OD2	4:N:65:ARG:NH1	2.48	0.43
4:N:174:ARG:H	4:N:205:TRP:HE1	1.66	0.43
4:N:408:ILE:HD12	4:N:408:ILE:H	1.83	0.43
7:P:211:ILE:HG22	7:P:217:GLY:N	2.33	0.43
9:I:110:CYS:SG	9:I:126:LEU:HD23	2.59	0.43
12:M:104:ALA:O	12:M:108:VAL:HG12	2.19	0.43
2:A:438:THR:OG1	2:A:439:ARG:N	2.50	0.43
2:A:576:PRO:O	2:A:579:MET:HG2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:418:PHE:CE2	3:L:425:LEU:HD13	2.53	0.43
4:N:133:MET:HG2	4:N:136:ASN:H	1.84	0.43
4:N:285:SER:OG	4:N:286:GLU:N	2.51	0.43
6:B:159:THR:O	6:B:161:LEU:N	2.52	0.43
8:H:195:DT:OP2	8:H:195:DT:H3'	2.19	0.43
8:H:264:DC:H2''	8:H:265:DA:OP2	2.18	0.43
10:J:68:ASP:OD1	10:J:68:ASP:N	2.49	0.43
3:L:261:LYS:HG2	3:L:300:SER:CB	2.49	0.43
4:N:248:ASP:HA	4:N:275:GLU:HB3	2.01	0.43
4:N:340:ARG:HG2	4:N:375:ALA:C	2.39	0.43
4:N:346:ASP:OD1	4:N:348:SER:N	2.50	0.43
7:P:223:HIS:O	7:P:244:MET:N	2.48	0.43
12:M:93:THR:O	12:M:96:ARG:N	2.52	0.43
9:O:80:THR:HG22	9:O:81:ASP:N	2.33	0.43
2:A:309:GLN:C	2:A:310:LEU:HD12	2.39	0.43
3:L:206:LEU:HD12	3:L:207:LEU:N	2.33	0.43
5:C:443:LEU:HD23	5:C:443:LEU:HA	1.79	0.43
5:C:628:ILE:HG12	5:C:629:LYS:N	2.34	0.43
8:H:22:DG:C2	8:H:294:DG:N2	2.87	0.43
8:H:103:DC:H5'	8:H:103:DC:C6	2.54	0.43
8:H:240:DC:C2	8:H:241:DG:C8	3.06	0.43
10:J:75:HIS:HB2	12:M:93:THR:HG21	2.01	0.43
11:R:63:LEU:HD13	12:S:42:LEU:HD13	2.01	0.43
2:A:189:VAL:HA	2:A:205:GLN:HA	2.01	0.43
3:L:126:CYS:HB3	3:L:436:ARG:HH12	1.84	0.43
3:L:243:ASP:OD2	3:L:314:TRP:N	2.30	0.43
4:N:68:LEU:HD23	4:N:68:LEU:HA	1.77	0.43
5:C:451:PHE:CZ	5:C:467:TYR:HA	2.54	0.43
5:C:685:ARG:HG3	5:C:686:PHE:CD1	2.54	0.43
7:P:242:HIS:CG	7:P:243:TRP:N	2.86	0.43
8:H:15:DC:C2	8:H:16:DT:C5	3.07	0.43
8:H:55:DG:H2''	8:H:56:DT:H6	1.84	0.43
8:H:138:DA:OP2	8:H:138:DA:H8	2.01	0.43
11:R:29:ARG:HH21	12:S:32:GLU:HB3	1.84	0.43
2:A:98:ARG:O	2:A:101:ARG:HB3	2.19	0.43
2:A:156:HIS:HB3	2:A:233:SER:O	2.19	0.43
2:A:296:VAL:O	2:A:319:MET:HB2	2.19	0.43
5:C:51:GLU:HG3	5:C:51:GLU:H	1.61	0.43
8:H:242:DC:H1'	8:H:243:DT:O5'	2.18	0.43
9:I:108:ASN:ND2	10:J:42:GLY:O	2.52	0.43
10:J:90:LEU:HD23	10:J:90:LEU:HA	1.69	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:O:82:LEU:HD23	9:O:82:LEU:HA	1.67	0.43
9:O:109:LEU:HD23	9:O:109:LEU:HA	1.74	0.43
3:L:93:ASN:HA	3:L:432:ALA:HB3	2.01	0.42
5:C:735:LYS:HG2	5:C:736:TYR:CD1	2.54	0.42
8:H:125:DC:H2''	8:H:126:DC:C6	2.54	0.42
8:H:198:DA:H2'	8:H:199:DT:H71	2.01	0.42
8:H:203:DT:H4'	8:H:204:DC:OP1	2.18	0.42
3:L:315:LEU:N	3:L:318:LEU:O	2.48	0.42
3:L:337:GLU:H	3:L:337:GLU:HG2	1.70	0.42
5:C:120:PHE:O	5:C:645:ILE:HG12	2.18	0.42
5:C:530:CYS:HA	5:C:534:CYS:HB2	2.00	0.42
8:H:48:DC:H2''	8:H:49:DT:C7	2.49	0.42
8:H:104:DT:OP1	12:M:29:THR:HG21	2.19	0.42
8:H:216:DT:H2''	8:H:217:DA:C8	2.55	0.42
8:H:223:DG:C4	8:H:224:DC:C5	3.07	0.42
9:I:55:GLN:OE1	11:R:109:PRO:HA	2.19	0.42
11:R:84:GLN:NE2	11:R:88:ARG:HE	2.16	0.42
4:N:123:HIS:HE1	4:N:142:THR:HG21	1.84	0.42
4:N:180:GLY:HA3	4:N:197:SER:HA	1.99	0.42
5:C:579:GLU:HA	5:C:603:ASN:HD21	1.84	0.42
5:C:592:ASP:O	5:C:608:ARG:NH2	2.52	0.42
5:C:665:PHE:CE1	5:C:685:ARG:HB2	2.54	0.42
8:H:37:DG:O3'	8:H:38:DG:C8	2.71	0.42
8:H:47:DC:H2''	8:H:48:DC:H5'	2.01	0.42
8:H:64:DC:H2''	8:H:65:DG:C8	2.55	0.42
8:H:117:DT:H1'	8:H:118:DT:H5'	2.00	0.42
8:H:185:DC:H6	8:H:185:DC:H2'	1.60	0.42
8:H:197:DA:C2	8:H:198:DA:C5	3.08	0.42
12:M:53:SER:O	12:M:56:MET:HB3	2.19	0.42
1:F:39:ASP:OD1	1:F:39:ASP:N	2.52	0.42
2:A:101:ARG:O	2:A:105:LEU:HG	2.19	0.42
2:A:311:LEU:O	2:A:359:LEU:HD22	2.20	0.42
2:A:627:ILE:HG13	2:A:628:ALA:H	1.83	0.42
7:P:230:ARG:HD3	7:P:253:TRP:CZ2	2.54	0.42
7:P:230:ARG:HE	7:P:238:LYS:CB	2.32	0.42
8:H:4:DG:N2	8:H:312:DC:O2	2.52	0.42
8:H:188:DA:C2	8:H:189:DG:C4	3.08	0.42
8:H:267:DG:C2	8:H:268:DG:C2	3.07	0.42
9:I:92:LEU:HD23	9:I:92:LEU:HA	1.65	0.42
11:K:67:GLY:HA3	12:M:46:HIS:ND1	2.33	0.42
9:O:132:GLY:HA2	9:O:135:ALA:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:13:ILE:HD11	1:T:30:ILE:HD12	2.02	0.42
3:L:166:ALA:HB2	3:L:172:ILE:HG12	2.02	0.42
3:L:301:THR:HG21	3:L:350:VAL:HG21	2.01	0.42
4:N:254:ILE:O	4:N:265:PRO:HB2	2.18	0.42
4:N:278:CYS:O	4:N:292:GLY:N	2.52	0.42
4:N:289:LEU:HD12	4:N:290:ALA:H	1.84	0.42
5:C:525:HIS:CE1	5:C:535:PRO:HD2	2.53	0.42
7:P:187:HIS:O	7:P:187:HIS:ND1	2.52	0.42
8:H:135:DG:H2''	8:H:136:DG:C8	2.54	0.42
8:H:140:DT:H2''	8:H:141:DC:H5'	2.02	0.42
8:H:168:DG:H2''	8:H:169:DC:OP2	2.17	0.42
8:H:186:DC:H1'	8:H:187:DG:C8	2.55	0.42
8:H:188:DA:C6	8:H:189:DG:C6	3.07	0.42
9:I:119:ILE:HD13	10:J:43:VAL:HG21	2.00	0.42
2:A:248:TYR:O	2:A:301:VAL:HG12	2.19	0.42
3:L:111:LEU:HB2	3:L:126:CYS:HB2	2.02	0.42
3:L:426:ILE:HG23	3:L:435:TRP:O	2.20	0.42
4:N:4:LYS:HE3	4:N:4:LYS:HB3	1.87	0.42
4:N:308:LEU:HD23	4:N:308:LEU:HA	1.92	0.42
5:C:34:ARG:HA	5:C:37:GLU:OE1	2.19	0.42
8:H:47:DC:N4	8:H:267:DG:O6	2.51	0.42
8:H:110:DC:H1'	8:H:111:DG:N7	2.35	0.42
8:H:278:DC:H2''	8:H:279:DC:C5	2.55	0.42
11:K:71:ARG:O	11:K:74:LYS:N	2.36	0.42
10:Q:26:ILE:HG23	10:Q:27:GLN:HE21	1.84	0.42
11:R:34:LEU:HD23	11:R:34:LEU:HA	1.80	0.42
2:A:478:TYR:CZ	2:A:480:TYR:HB2	2.54	0.42
2:A:656:PHE:O	2:A:660:LEU:HG	2.20	0.42
3:L:209:VAL:HG22	3:L:215:LEU:HG	2.02	0.42
4:N:80:VAL:HA	4:N:119:ILE:O	2.19	0.42
6:B:108:ARG:N	6:B:109:PRO:HD2	2.35	0.42
8:H:14:DT:C2	8:H:15:DC:C5	3.08	0.42
8:H:58:DT:C2	8:H:59:DA:C6	3.08	0.42
8:H:95:DT:C2	8:H:96:DG:C8	3.07	0.42
8:H:99:DA:N6	8:H:215:DC:N4	2.68	0.42
8:H:123:DG:OP2	12:S:36:ILE:HD11	2.19	0.42
8:H:132:DA:OP1	11:R:76:THR:N	2.47	0.42
8:H:228:DA:C4	8:H:229:DA:N7	2.87	0.42
8:H:260:DC:H4'	8:H:261:DC:OP1	2.19	0.42
10:J:92:ARG:NH1	10:J:92:ARG:HG2	2.35	0.42
11:K:79:ILE:HG12	11:K:82:HIS:ND1	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:46:HIS:O	12:M:48:ASP:N	2.53	0.42
9:O:68:GLN:HE21	9:O:72:ARG:NE	2.11	0.42
12:S:68:GLU:OE1	12:S:69:ARG:N	2.53	0.42
2:A:569:ASP:OD1	2:A:569:ASP:N	2.50	0.42
4:N:72:THR:OG1	4:N:73:SER:N	2.53	0.42
5:C:628:ILE:HG12	5:C:629:LYS:H	1.84	0.42
5:C:694:ASN:HB3	5:C:714:ARG:CZ	2.49	0.42
7:P:227:ILE:O	7:P:229:LYS:NZ	2.50	0.42
8:H:8:DT:H2'	8:H:9:DA:H8	1.82	0.42
8:H:132:DA:C4	8:H:133:DC:C5	3.07	0.42
8:H:206:DT:H2''	8:H:207:DA:O4'	2.20	0.42
8:H:269:DG:C4	8:H:270:DG:N7	2.88	0.42
1:F:28:ALA:HA	1:F:38:PRO:HG3	2.02	0.42
1:T:13:ILE:HD12	1:T:33:LYS:HD3	2.02	0.42
2:A:428:ILE:HA	2:A:485:ALA:O	2.19	0.42
2:A:662:SER:OG	5:C:278:LEU:HD22	2.20	0.42
3:L:328:ILE:O	3:L:356:PHE:N	2.42	0.42
4:N:132:TYR:HA	4:N:140:ILE:HA	2.02	0.42
4:N:278:CYS:SG	4:N:323:VAL:HG22	2.60	0.42
4:N:299:ALA:HB2	4:N:309:LYS:HE2	2.00	0.42
5:C:41:MET:N	5:C:41:MET:SD	2.92	0.42
5:C:443:LEU:HD22	5:C:447:TYR:HE2	1.85	0.42
8:H:196:DC:C4	8:H:197:DA:N6	2.88	0.42
8:H:239:DG:C4	8:H:240:DC:C5	3.08	0.42
8:H:297:DT:H2''	8:H:298:DC:N1	2.35	0.42
8:H:300:DG:H8	8:H:300:DG:H5''	1.85	0.42
12:S:116:THR:O	12:S:119:THR:OG1	2.27	0.42
3:L:162:LEU:HD23	3:L:162:LEU:HA	1.77	0.42
4:N:173:LEU:HB3	4:N:205:TRP:CE2	2.55	0.42
8:H:53:DC:H4'	8:H:54:DG:OP1	2.19	0.42
8:H:214:DT:H1'	8:H:215:DC:C6	2.55	0.42
8:H:269:DG:C4	8:H:270:DG:C5	3.08	0.42
8:H:298:DC:C2'	8:H:299:DA:H5''	2.39	0.42
9:O:83:ARG:O	10:Q:80:THR:HA	2.20	0.42
3:L:270:MET:O	3:L:274:ILE:HG13	2.20	0.41
3:L:334:GLY:N	3:L:350:VAL:HA	2.35	0.41
4:N:25:LYS:O	4:N:28:THR:HG22	2.20	0.41
4:N:49:TRP:CZ3	4:N:66:LEU:HD21	2.55	0.41
4:N:57:GLU:O	4:N:59:LYS:HG3	2.20	0.41
4:N:194:LEU:HG	4:N:235:TRP:NE1	2.34	0.41
4:N:325:TRP:CD2	4:N:333:LEU:HD13	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:46:ARG:O	5:C:49:ILE:HB	2.20	0.41
5:C:585:CYS:SG	5:C:588:CYS:N	2.76	0.41
7:P:209:ALA:HB1	7:P:211:ILE:HD11	2.01	0.41
8:H:269:DG:C6	8:H:270:DG:C6	3.08	0.41
10:J:63:GLU:O	10:J:65:VAL:N	2.52	0.41
9:O:47:ALA:O	9:O:50:GLU:N	2.53	0.41
9:O:61:LEU:HD23	9:O:61:LEU:HA	1.80	0.41
10:Q:31:LYS:O	10:Q:35:ARG:HG3	2.19	0.41
11:R:37:GLY:HA3	11:R:39:TYR:CE1	2.55	0.41
2:A:475:ILE:HG12	2:A:490:SER:O	2.20	0.41
3:L:317:ASP:O	3:L:318:LEU:HD23	2.19	0.41
4:N:253:MET:HB3	4:N:265:PRO:HG3	2.02	0.41
4:N:254:ILE:O	4:N:266:SER:OG	2.37	0.41
5:C:709:GLY:O	5:C:710:ILE:HD13	2.20	0.41
8:H:161:DG:H4'	8:H:162:DC:OP1	2.19	0.41
8:H:222:DC:H2''	8:H:223:DG:H8	1.85	0.41
8:H:227:DA:O3'	9:O:63:ARG:NH1	2.49	0.41
8:H:255:DT:H5'	8:H:255:DT:C6	2.55	0.41
8:H:290:DG:C4	8:H:291:DC:C5	3.08	0.41
8:H:292:DA:C8	8:H:292:DA:H5'	2.55	0.41
10:Q:73:THR:O	10:Q:77:LYS:N	2.53	0.41
11:R:108:LEU:HD23	11:R:108:LEU:HA	1.83	0.41
2:A:97:TYR:O	2:A:101:ARG:N	2.47	0.41
2:A:192:CYS:CB	2:A:202:PRO:HG2	2.50	0.41
2:A:571:CYS:O	2:A:572:LEU:HD23	2.20	0.41
3:L:86:ASN:HA	5:C:89:LEU:HD12	2.02	0.41
3:L:159:SER:OG	5:C:65:ILE:HA	2.19	0.41
4:N:329:ASN:CB	4:N:332:ILE:HD12	2.50	0.41
8:H:154:DC:O2	8:H:161:DG:C2	2.68	0.41
8:H:298:DC:H2''	8:H:299:DA:O4'	2.21	0.41
11:K:30:VAL:O	11:K:33:LEU:N	2.53	0.41
10:Q:59:LYS:O	10:Q:63:GLU:HG3	2.20	0.41
2:A:164:PHE:HE2	2:A:166:HIS:HB2	1.85	0.41
2:A:556:THR:O	2:A:556:THR:OG1	2.26	0.41
2:A:586:GLU:HG2	2:A:588:ASP:H	1.85	0.41
3:L:254:CYS:HB2	3:L:309:VAL:HG13	2.01	0.41
4:N:278:CYS:SG	4:N:323:VAL:HG13	2.61	0.41
5:C:525:HIS:CE1	5:C:534:CYS:SG	3.14	0.41
5:C:626:ILE:HD11	5:C:686:PHE:HB2	2.03	0.41
8:H:7:DG:C2	8:H:8:DT:C2	3.08	0.41
8:H:94:DG:H2''	8:H:95:DT:O5'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:131:DC:C2	8:H:132:DA:C5	3.08	0.41
8:H:211:DA:C4	8:H:212:DG:C8	3.07	0.41
12:S:48:ASP:OD1	12:S:48:ASP:N	2.51	0.41
4:N:311:HIS:NE2	4:N:365:GLU:OE2	2.47	0.41
4:N:354:GLN:NE2	4:N:362:GLY:O	2.52	0.41
5:C:440:PHE:CE1	5:C:454:ILE:HG21	2.56	0.41
8:H:38:DG:C6	8:H:276:DT:C4	3.09	0.41
8:H:64:DC:C2	8:H:65:DG:C5	3.08	0.41
8:H:78:DT:H6	8:H:78:DT:H2'	1.69	0.41
8:H:78:DT:H1'	8:H:79:DA:C5	2.55	0.41
8:H:146:DG:H2''	8:H:147:DC:C6	2.55	0.41
8:H:184:DG:H2''	8:H:185:DC:O5'	2.21	0.41
8:H:226:DT:H2''	8:H:227:DA:N7	2.36	0.41
8:H:296:DC:H6	8:H:296:DC:H2'	1.62	0.41
11:K:65:LEU:HA	11:K:65:LEU:HD23	1.71	0.41
12:M:83:ARG:HA	12:M:83:ARG:HD3	1.89	0.41
1:F:56:LEU:HB3	1:F:61:ILE:HB	2.03	0.41
2:A:458:ARG:C	2:A:459:LYS:HD3	2.41	0.41
2:A:617:TRP:O	2:A:621:VAL:HG23	2.20	0.41
3:L:423:SER:OG	3:L:424:ILE:HG12	2.21	0.41
4:N:138:CYS:O	4:N:153:ASP:HA	2.20	0.41
4:N:223:PHE:HD2	4:N:262:THR:HA	1.84	0.41
5:C:737:VAL:HG13	14:C:801:SAH:N1	2.35	0.41
7:P:243:TRP:CH2	7:P:265:LYS:HB2	2.55	0.41
1:F:27:LYS:HB3	1:F:38:PRO:HA	2.02	0.41
1:F:40:GLN:HB3	1:F:71:LEU:CD1	2.51	0.41
4:N:87:PRO:HB3	4:N:108:PHE:CD2	2.54	0.41
4:N:368:PHE:CG	4:N:369:ILE:N	2.88	0.41
5:C:145:PHE:HA	5:C:148:GLU:CD	2.40	0.41
5:C:272:VAL:H	5:C:438:SER:CB	2.33	0.41
5:C:619:SER:OG	5:C:623:GLY:O	2.36	0.41
8:H:79:DA:H1'	8:H:80:DC:C6	2.55	0.41
8:H:128:DG:N2	8:H:187:DG:C2	2.88	0.41
8:H:175:DA:H5'	8:H:175:DA:C8	2.56	0.41
9:O:49:ARG:O	9:O:52:ARG:HG2	2.21	0.41
1:F:6:LYS:O	1:F:68:HIS:ND1	2.53	0.41
1:F:15:LEU:HD11	1:F:30:ILE:HD11	2.02	0.41
2:A:113:ARG:NH2	4:N:363:PRO:O	2.54	0.41
2:A:678:VAL:O	2:A:681:LEU:HB3	2.21	0.41
3:L:245:ASP:CG	3:L:248:GLY:H	2.23	0.41
4:N:338:THR:HA	4:N:376:LYS:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:95:DT:H2'	8:H:96:DG:O4'	2.21	0.41
8:H:159:DC:H1'	8:H:160:DT:H5'	2.01	0.41
8:H:244:DG:C5	8:H:245:DT:C4	3.09	0.41
8:H:270:DG:H2''	8:H:271:DA:H8	1.86	0.41
11:R:81:ARG:HH12	11:R:85:LEU:HD21	1.83	0.41
2:A:166:HIS:CD2	2:A:353:PRO:HG3	2.55	0.41
2:A:628:ALA:HB3	2:A:631:GLN:HG3	2.02	0.41
3:L:275:LYS:HE2	3:L:275:LYS:HB3	1.93	0.41
3:L:307:ASN:OD1	3:L:308:TYR:N	2.42	0.41
3:L:324:CYS:SG	3:L:364:TRP:HB3	2.61	0.41
4:N:266:SER:HB2	4:N:267:HIS:CE1	2.56	0.41
4:N:279:LEU:HD11	4:N:289:LEU:HD21	2.03	0.41
4:N:287:PHE:O	4:N:302:ASP:HA	2.20	0.41
4:N:354:GLN:NE2	4:N:359:ALA:HA	2.36	0.41
5:C:272:VAL:O	5:C:441:ARG:HD2	2.21	0.41
5:C:626:ILE:HG22	5:C:627:PHE:N	2.36	0.41
5:C:664:SER:OG	5:C:665:PHE:N	2.54	0.41
7:P:232:GLU:N	7:P:236:LYS:O	2.53	0.41
8:H:3:DG:C2	8:H:4:DG:C6	3.09	0.41
8:H:17:DG:O5'	8:H:17:DG:C8	2.74	0.41
8:H:17:DG:H8	8:H:17:DG:OP2	2.04	0.41
8:H:31:DG:N2	8:H:285:DT:O2	2.54	0.41
8:H:86:DT:H6	8:H:86:DT:H2'	1.71	0.41
8:H:189:DG:C4	8:H:190:DG:N7	2.89	0.41
8:H:199:DT:C6	8:H:200:DT:H73	2.56	0.41
8:H:210:DC:H2''	8:H:211:DA:C8	2.55	0.41
8:H:227:DA:C6	8:H:228:DA:C6	3.09	0.41
8:H:238:DC:C2	8:H:239:DG:C8	3.09	0.41
8:H:266:DA:H2''	8:H:267:DG:N7	2.34	0.41
8:H:277:DC:H1'	8:H:278:DC:C4	2.56	0.41
8:H:303:DA:C2	8:H:304:DT:C2	3.08	0.41
4:N:241:SER:OG	4:N:258:ARG:NH1	2.53	0.41
4:N:387:PRO:C	4:N:388:TRP:HD1	2.24	0.41
5:C:259:GLU:O	5:C:261:THR:HG23	2.21	0.41
8:H:82:DT:C4	8:H:83:DG:C6	3.08	0.41
8:H:207:DA:O3'	12:S:83:ARG:NH1	2.52	0.41
8:H:294:DG:OP2	8:H:294:DG:H2'	2.20	0.41
11:K:25:PHE:HD2	11:K:56:GLU:HB2	1.86	0.41
12:M:109:SER:O	12:M:112:THR:OG1	2.36	0.41
11:R:93:LEU:HA	11:R:93:LEU:HD23	1.74	0.41
2:A:521:LYS:HB2	4:N:42:TRP:CE2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:540:MET:HA	2:A:543:PHE:HD1	1.86	0.40
4:N:51:PRO:HA	4:N:384:PRO:HG2	2.03	0.40
4:N:316:HIS:CD2	4:N:335:SER:HG	2.38	0.40
8:H:100:DG:C6	8:H:214:DT:N3	2.88	0.40
8:H:151:DC:C2	8:H:152:DG:C5	3.09	0.40
8:H:289:DG:H2''	8:H:290:DG:C8	2.56	0.40
8:H:300:DG:C6	8:H:301:DA:C6	3.09	0.40
1:T:19:PRO:HA	1:T:56:LEU:HB2	2.03	0.40
2:A:464:LEU:HD23	2:A:464:LEU:HA	1.93	0.40
2:A:586:GLU:OE1	2:A:586:GLU:N	2.54	0.40
2:A:589:PRO:HB2	2:A:591:TRP:NE1	2.35	0.40
2:A:675:ASP:OD1	2:A:675:ASP:N	2.54	0.40
4:N:44:SER:OG	4:N:45:LEU:N	2.53	0.40
4:N:284:TYR:CB	4:N:330:GLU:HG3	2.48	0.40
5:C:522:PRO:HB3	5:C:547:CYS:HA	2.03	0.40
7:P:87:PHE:HA	7:P:107:LEU:HD12	2.02	0.40
7:P:218:HIS:HD1	7:P:219:SER:HG	1.64	0.40
7:P:224:SER:HB3	7:P:243:TRP:CD2	2.55	0.40
8:H:16:DT:H2''	8:H:17:DG:OP2	2.20	0.40
8:H:110:DC:H6	8:H:110:DC:H2'	1.67	0.40
8:H:297:DT:H6	8:H:297:DT:H2'	1.70	0.40
1:F:23:ILE:HG22	1:F:27:LYS:HE3	2.02	0.40
1:F:27:LYS:HD3	1:F:38:PRO:O	2.21	0.40
1:T:39:ASP:OD1	1:T:40:GLN:HG2	2.21	0.40
2:A:450:CYS:SG	2:A:471:HIS:NE2	2.94	0.40
2:A:606:VAL:HB	2:A:611:LYS:HE2	2.04	0.40
3:L:122:THR:HB	3:L:124:TYR:CZ	2.56	0.40
3:L:305:HIS:ND1	3:L:325:GLU:OE2	2.47	0.40
5:C:160:ASP:O	5:C:232:PRO:HG3	2.21	0.40
7:P:243:TRP:HB2	7:P:249:LEU:HD21	2.03	0.40
8:H:135:DG:C2'	8:H:136:DG:C8	3.04	0.40
8:H:150:DC:H1'	8:H:151:DC:H5'	2.03	0.40
9:I:85:GLN:NE2	10:J:82:THR:HA	2.35	0.40
10:J:75:HIS:CD2	12:M:93:THR:HG21	2.57	0.40
2:A:300:THR:O	2:A:310:LEU:HD11	2.22	0.40
2:A:662:SER:O	2:A:665:ASP:HB2	2.22	0.40
4:N:48:GLN:OE1	4:N:131:ARG:NH1	2.48	0.40
4:N:398:ILE:HD13	4:N:398:ILE:HA	1.90	0.40
5:C:445:GLY:HA2	5:C:448:TYR:CE1	2.57	0.40
5:C:614:LEU:HD23	5:C:614:LEU:HA	1.77	0.40
8:H:19:DG:H4'	8:H:20:DA:OP1	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:69:DG:H2''	8:H:70:DA:N7	2.37	0.40
8:H:152:DG:O6	8:H:162:DC:N4	2.54	0.40
8:H:169:DC:H1'	8:H:170:DT:C5'	2.52	0.40
8:H:178:DC:C2	8:H:179:DC:C4	3.09	0.40
8:H:226:DT:H1'	8:H:227:DA:C8	2.57	0.40
8:H:258:DA:C4	8:H:259:DA:N7	2.90	0.40
11:K:63:LEU:HD23	11:K:63:LEU:HA	1.76	0.40
3:L:82:PHE:HA	3:L:438:ASP:O	2.22	0.40
3:L:213:HIS:HD2	3:L:236:ARG:C	2.25	0.40
3:L:320:LEU:HD23	3:L:320:LEU:HA	1.92	0.40
4:N:66:LEU:HD13	4:N:66:LEU:HA	1.91	0.40
5:C:289:CYS:SG	5:C:297:HIS:CE1	3.15	0.40
5:C:616:LEU:HD12	5:C:617:ALA:H	1.85	0.40
8:H:7:DG:N2	8:H:309:DA:C2	2.90	0.40
8:H:60:DA:H2''	8:H:61:DA:C8	2.55	0.40
8:H:186:DC:H6	8:H:186:DC:H2'	1.74	0.40
9:O:63:ARG:O	9:O:66:PRO:HD2	2.21	0.40
11:R:91:GLU:HA	11:R:94:ASN:HB3	2.03	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	F	74/76 (97%)	70 (95%)	4 (5%)	0	100	100
1	T	74/76 (97%)	73 (99%)	1 (1%)	0	100	100
2	A	423/739 (57%)	378 (89%)	45 (11%)	0	100	100
3	L	360/441 (82%)	317 (88%)	43 (12%)	0	100	100
4	N	391/425 (92%)	348 (89%)	43 (11%)	0	100	100
5	C	600/746 (80%)	515 (86%)	85 (14%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	B	37/450 (8%)	27 (73%)	10 (27%)	0	100	100
6	E	33/450 (7%)	30 (91%)	3 (9%)	0	100	100
7	P	189/295 (64%)	163 (86%)	26 (14%)	0	100	100
9	I	115/136 (85%)	107 (93%)	8 (7%)	0	100	100
9	O	97/136 (71%)	85 (88%)	12 (12%)	0	100	100
10	J	81/103 (79%)	66 (82%)	15 (18%)	0	100	100
10	Q	85/103 (82%)	74 (87%)	11 (13%)	0	100	100
11	K	106/130 (82%)	99 (93%)	7 (7%)	0	100	100
11	R	106/130 (82%)	98 (92%)	8 (8%)	0	100	100
12	M	93/126 (74%)	81 (87%)	12 (13%)	0	100	100
12	S	94/126 (75%)	81 (86%)	13 (14%)	0	100	100
All	All	2958/4688 (63%)	2612 (88%)	346 (12%)	0	100	100

There are no Ramachandran outliers to report.

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	F	69/69 (100%)	69 (100%)	0	100	100
1	T	69/69 (100%)	69 (100%)	0	100	100
2	A	326/646 (50%)	326 (100%)	0	100	100
3	L	309/392 (79%)	309 (100%)	0	100	100
4	N	332/375 (88%)	332 (100%)	0	100	100
5	C	373/667 (56%)	369 (99%)	4 (1%)	70	83
6	B	25/387 (6%)	25 (100%)	0	100	100
6	E	11/387 (3%)	9 (82%)	2 (18%)	1	7
7	P	111/263 (42%)	111 (100%)	0	100	100
9	I	96/111 (86%)	95 (99%)	1 (1%)	73	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	O	86/111 (78%)	86 (100%)	0	100	100
10	J	68/79 (86%)	67 (98%)	1 (2%)	60	77
10	Q	64/79 (81%)	63 (98%)	1 (2%)	58	76
11	K	84/101 (83%)	84 (100%)	0	100	100
11	R	85/101 (84%)	84 (99%)	1 (1%)	67	82
12	M	79/106 (74%)	78 (99%)	1 (1%)	65	81
12	S	79/106 (74%)	79 (100%)	0	100	100
All	All	2266/4049 (56%)	2255 (100%)	11 (0%)	85	93

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	C	64	ARG
5	C	129	HIS
5	C	563	LYS
5	C	653	ARG
9	I	52	ARG
10	J	85	ASP
12	M	48	ASP
10	Q	78	ARG
11	R	81	ARG
6	E	25	GLU
6	E	29	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	T	41	GLN
1	T	62	GLN
2	A	104	ASN
2	A	126	ASN
2	A	235	ASN
2	A	241	ASN
2	A	243	HIS
2	A	431	GLN
2	A	440	GLN
2	A	481	HIS
2	A	507	HIS

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Mol	Chain	Res	Type
3	L	136	GLN
3	L	189	HIS
3	L	204	ASN
3	L	221	GLN
3	L	382	GLN
4	N	76	GLN
4	N	123	HIS
4	N	128	ASN
4	N	157	HIS
4	N	186	ASN
4	N	188	ASN
4	N	239	HIS
4	N	329	ASN
4	N	370	HIS
4	N	397	ASN
5	C	94	GLN
5	C	117	GLN
5	C	273	GLN
5	C	507	GLN
5	C	688	ASN
7	P	98	ASN
7	P	193	GLN
7	P	210	HIS
7	P	283	ASN
9	I	68	GLN
9	I	85	GLN
10	J	25	ASN
11	K	84	GLN
12	M	46	HIS
12	M	79	HIS
12	M	92	GLN
9	O	39	HIS
9	O	68	GLN
9	O	113	HIS
10	Q	25	ASN
11	R	31	HIS
12	S	46	HIS
12	S	79	HIS
1	F	25	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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	$\# Z > 2$
6	M3L	B	116	6	10,11,12	0.53	0	9,14,16	0.42	0

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
6	M3L	B	116	6	-	0/9/10/12	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	SAH	C	801	-	23,28,28	1.28	3 (13%)	22,40,40	1.89	3 (13%)

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
14	SAH	C	801	-	-	8/11/31/31	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	C	801	SAH	C2-N3	3.77	1.37	1.32
14	C	801	SAH	OXT-C	-2.40	1.23	1.30
14	C	801	SAH	C2-N1	2.17	1.37	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	C	801	SAH	N3-C2-N1	-5.83	120.76	128.67
14	C	801	SAH	C5'-SD-CG	-4.13	89.99	102.26
14	C	801	SAH	OXT-C-O	-2.66	118.05	124.08

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	C	801	SAH	N-CA-CB-CG
14	C	801	SAH	O-C-CA-N

Continued on next page...

Continued from previous page...

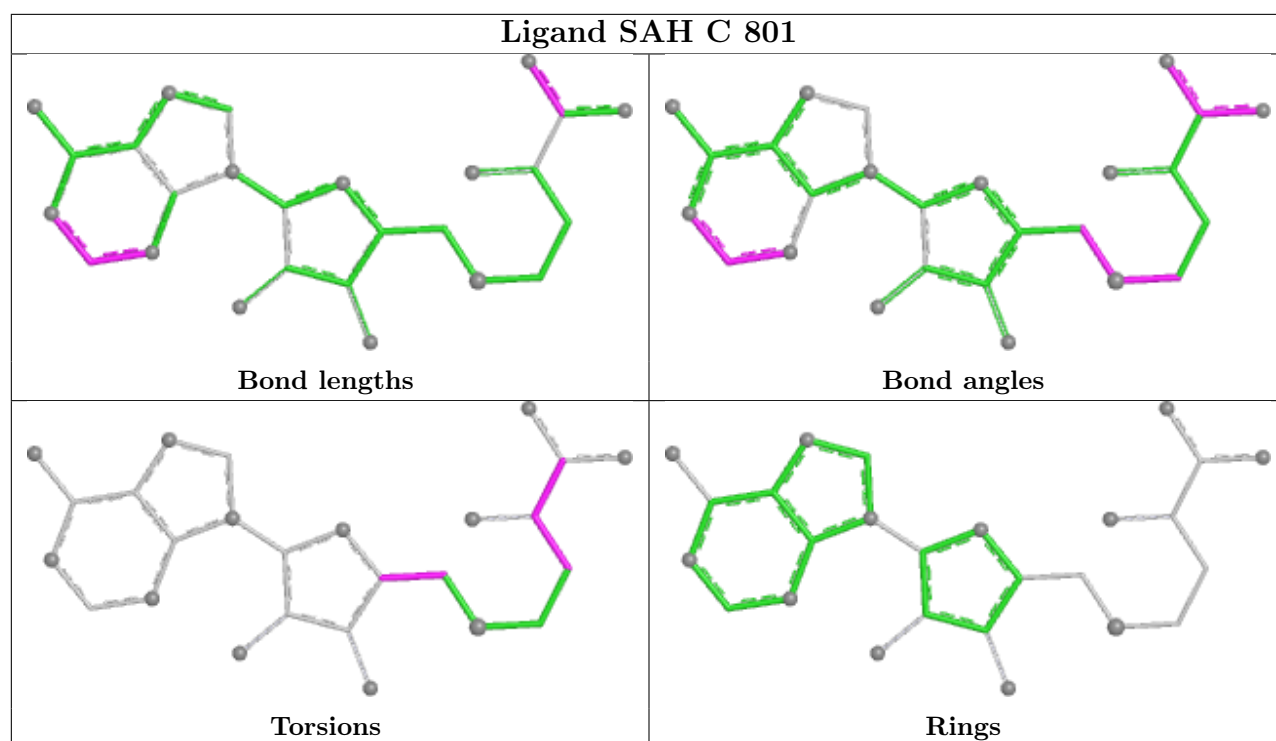
Mol	Chain	Res	Type	Atoms
14	C	801	SAH	OXT-C-CA-N
14	C	801	SAH	C-CA-CB-CG
14	C	801	SAH	O-C-CA-CB
14	C	801	SAH	OXT-C-CA-CB
14	C	801	SAH	C3'-C4'-C5'-SD
14	C	801	SAH	O4'-C4'-C5'-SD

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	C	801	SAH	3	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 than 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.



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.

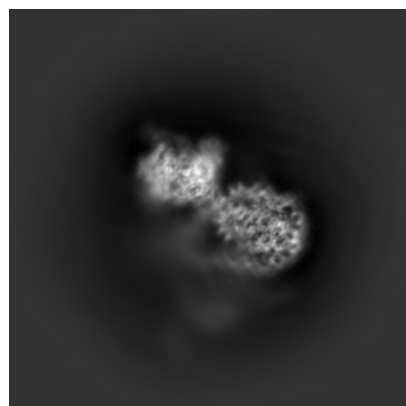
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21707. These allow visual inspection of the internal detail of the map and identification of artifacts.

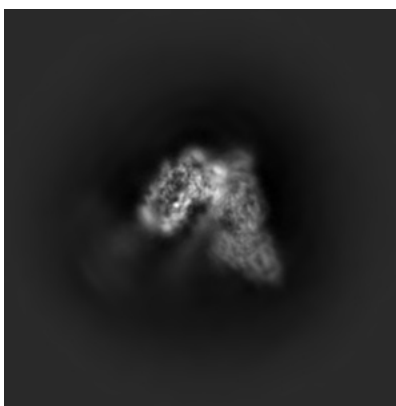
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

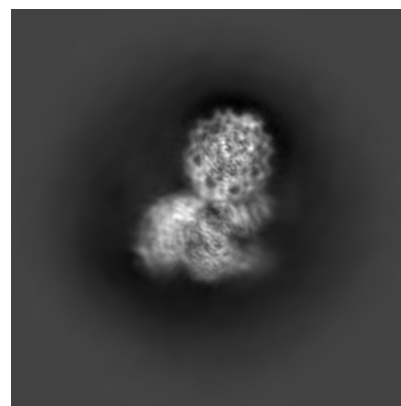
6.1.1 Primary map



X

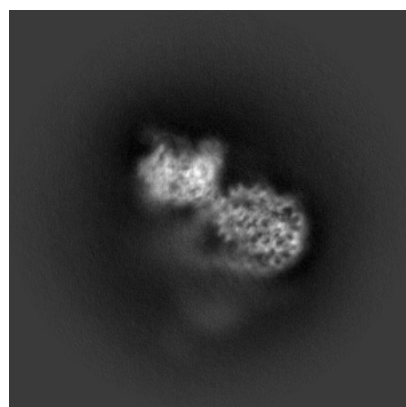


Y

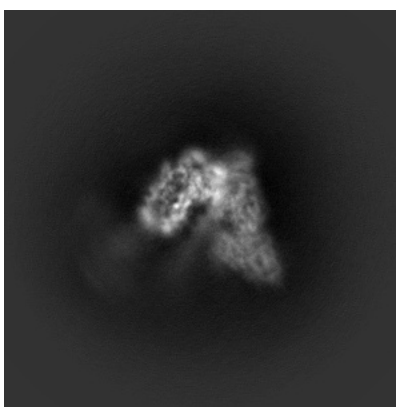


Z

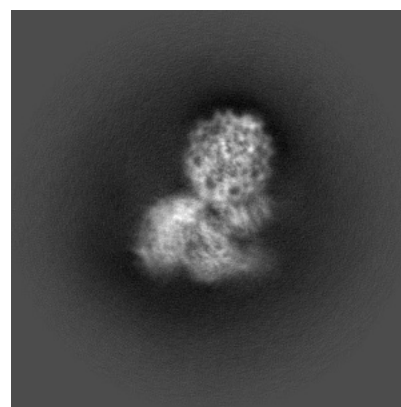
6.1.2 Raw map



X



Y

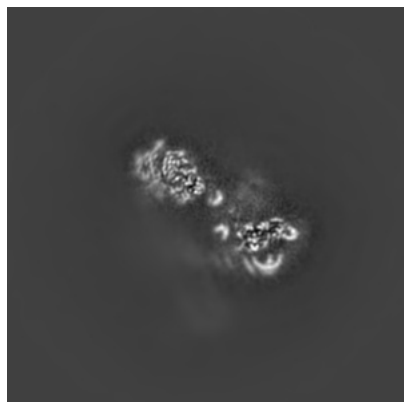


Z

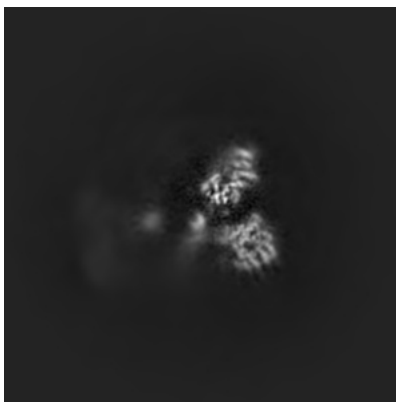
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

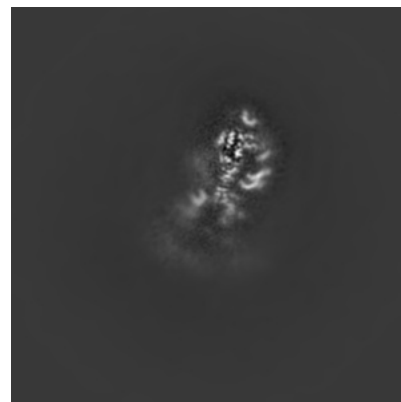
6.2.1 Primary map



X Index: 192

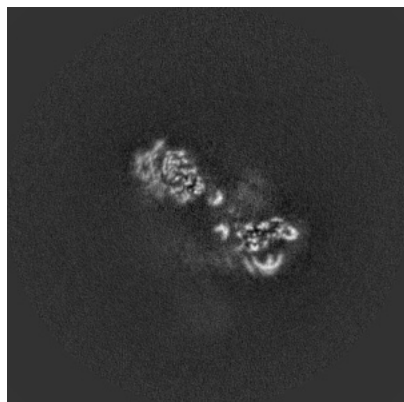


Y Index: 192



Z Index: 192

6.2.2 Raw map



X Index: 192



Y Index: 192

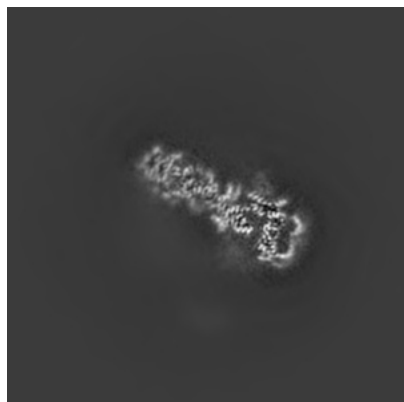


Z Index: 192

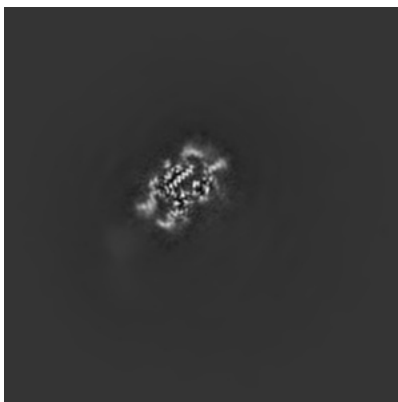
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

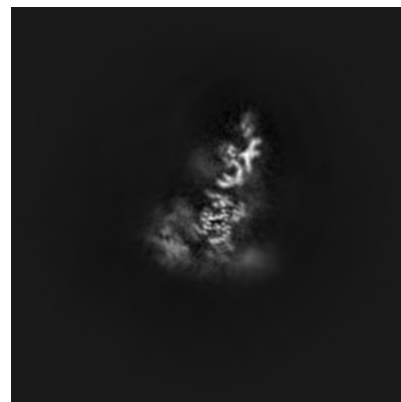
6.3.1 Primary map



X Index: 205

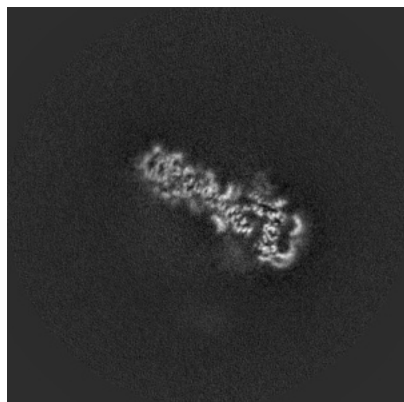


Y Index: 252

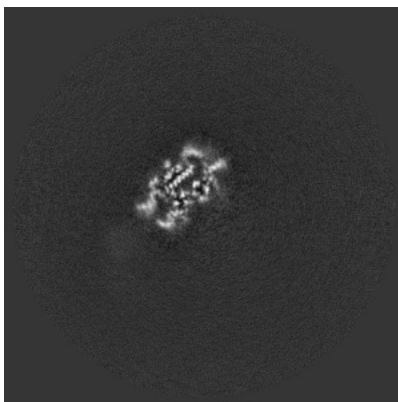


Z Index: 206

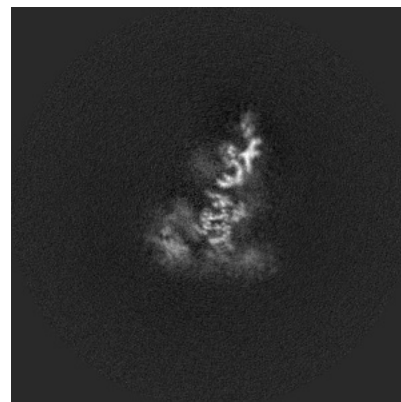
6.3.2 Raw map



X Index: 204



Y Index: 252

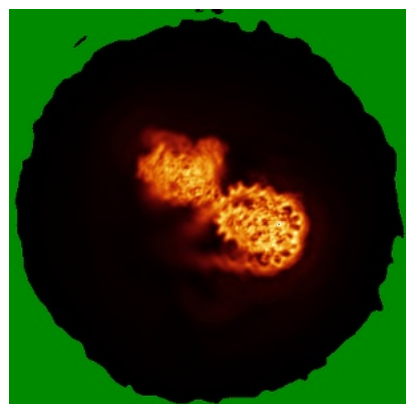


Z Index: 206

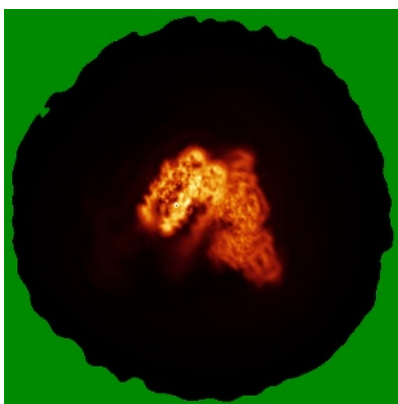
The images above show the largest variance slices of the map in three orthogonal directions.

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

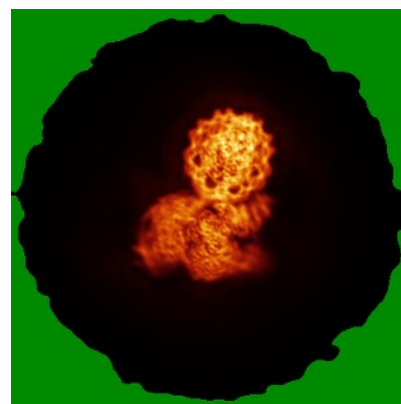
6.4.1 Primary map



X

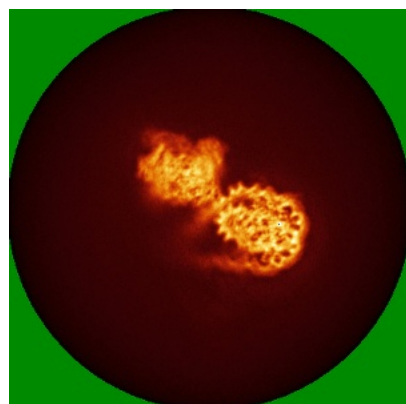


Y



Z

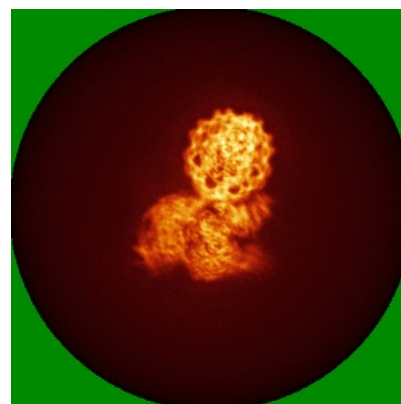
6.4.2 Raw map



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.

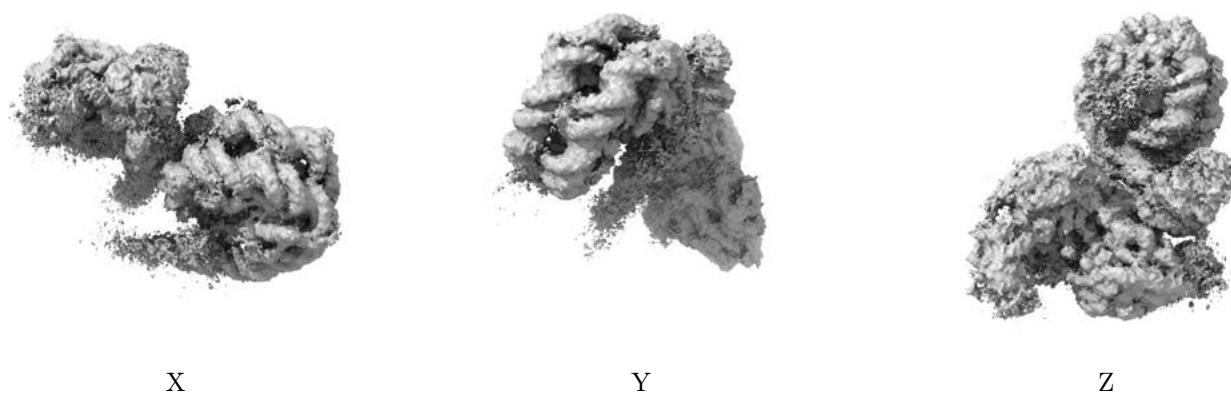
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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.

6.5.2 Raw map



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

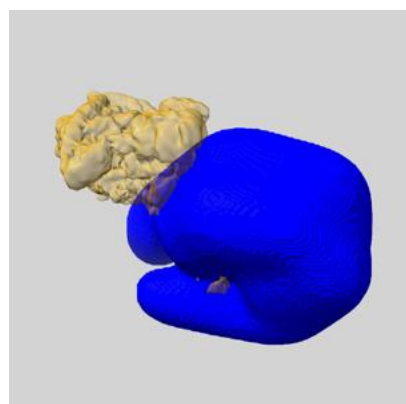
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

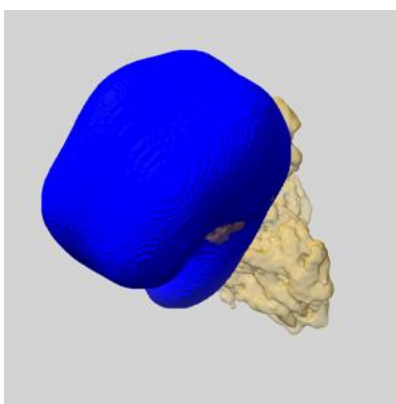
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

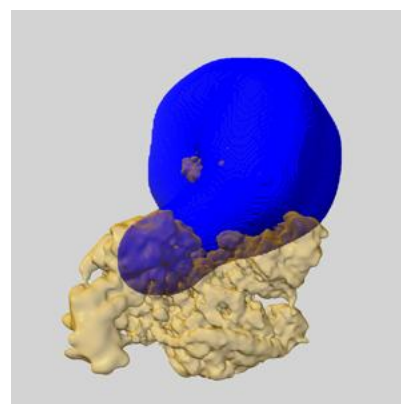
6.6.1 emd_21707_msk_2.map [i](#)



X

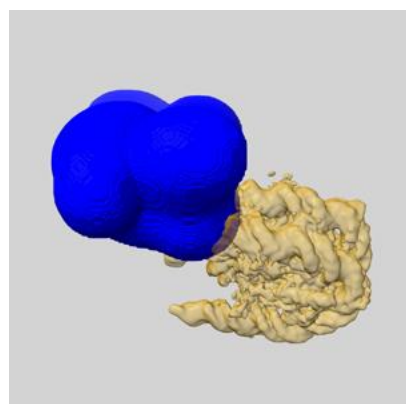


Y

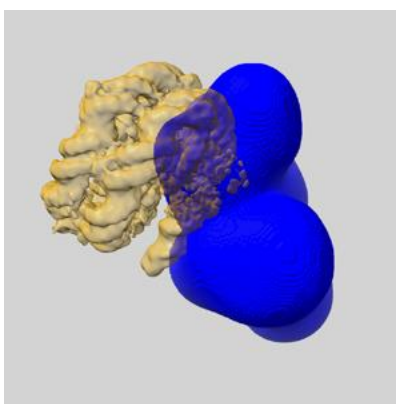


Z

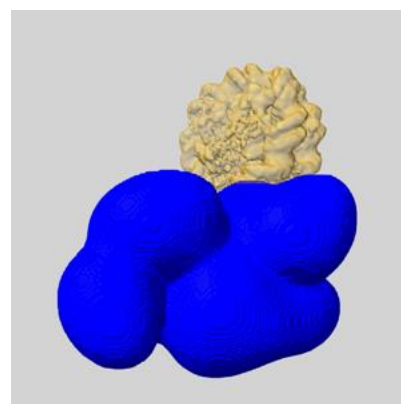
6.6.2 emd_21707_msk_1.map [i](#)



X



Y

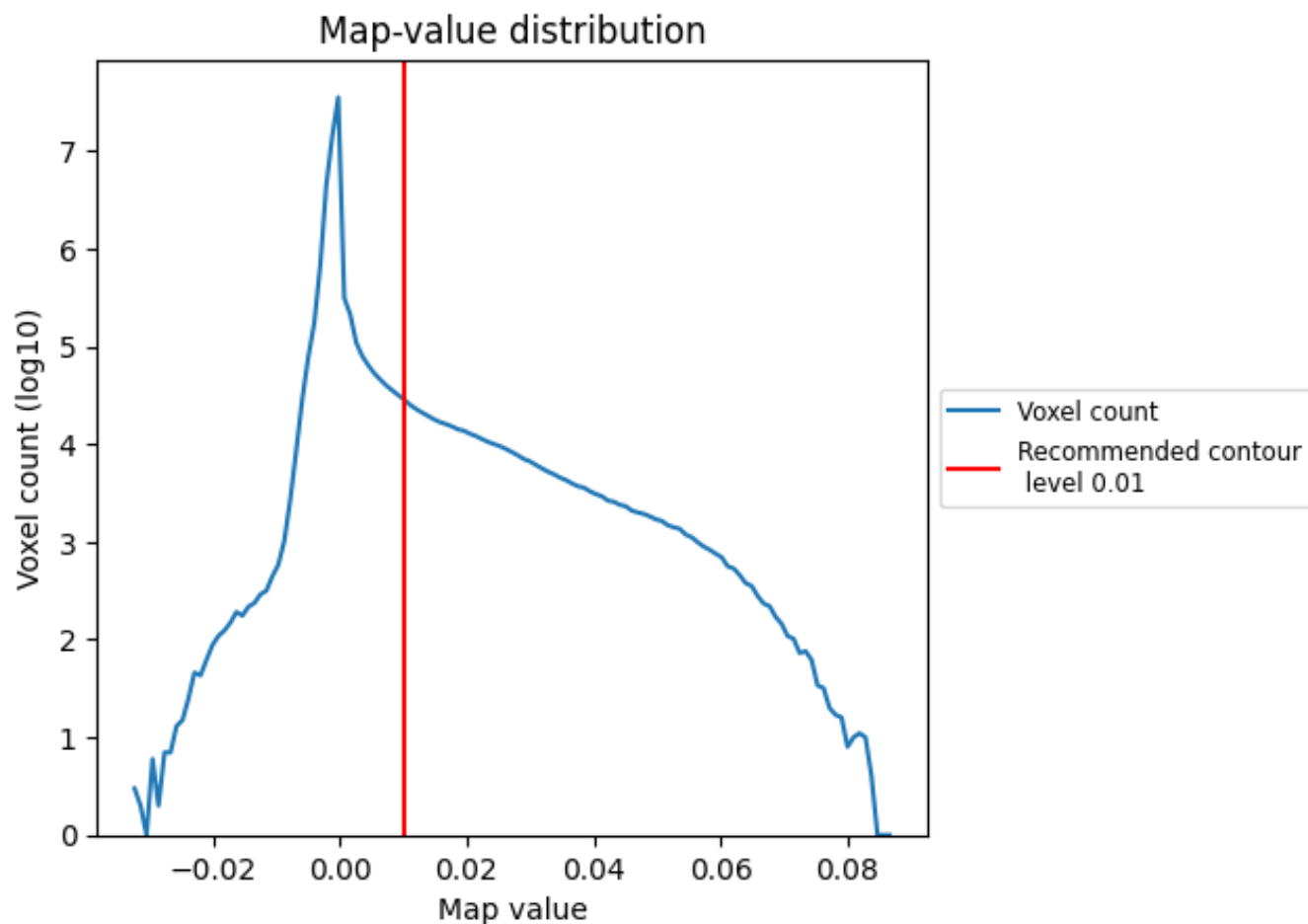


Z

7 Map analysis [i](#)

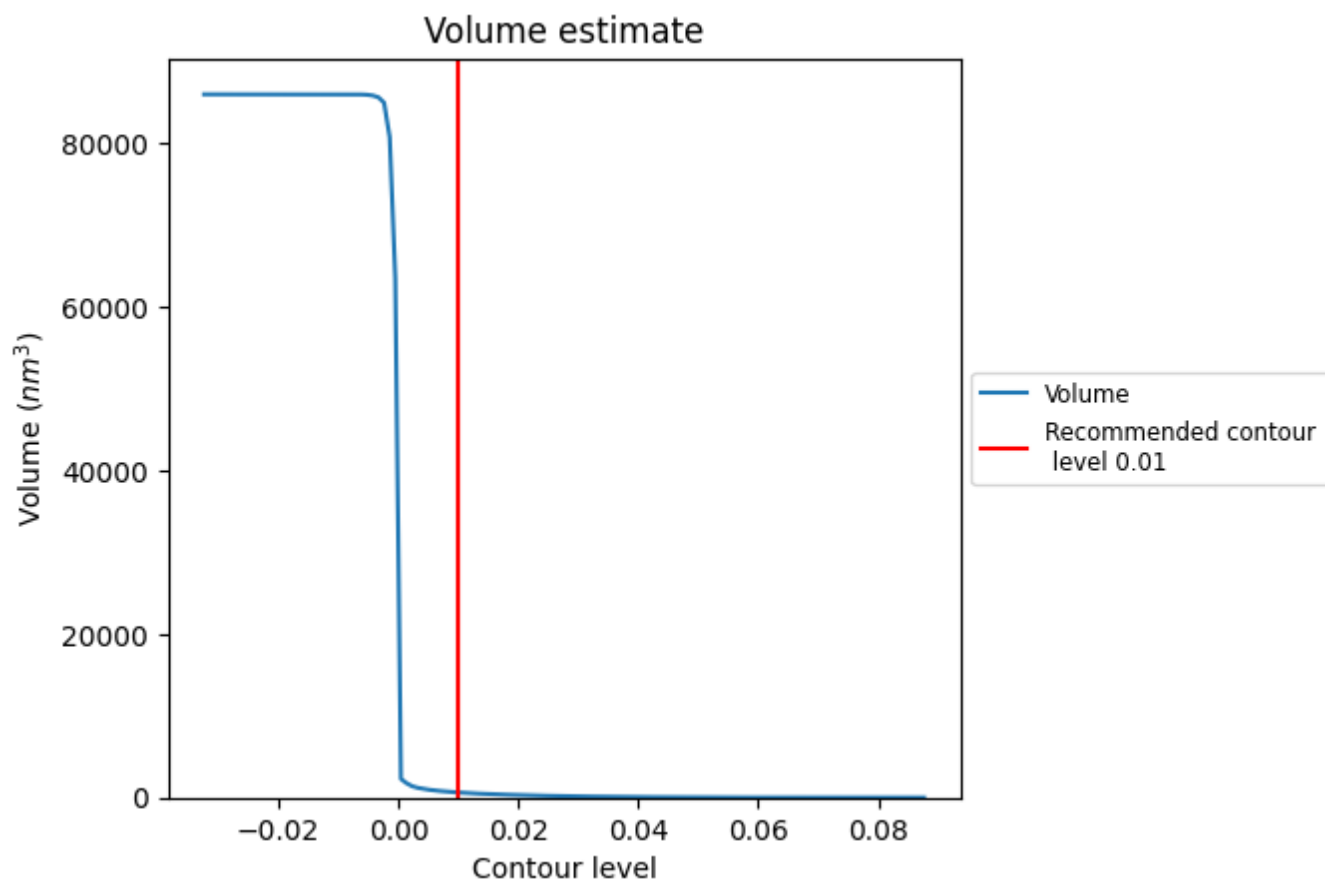
This section contains the results of statistical analysis of the map.

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.

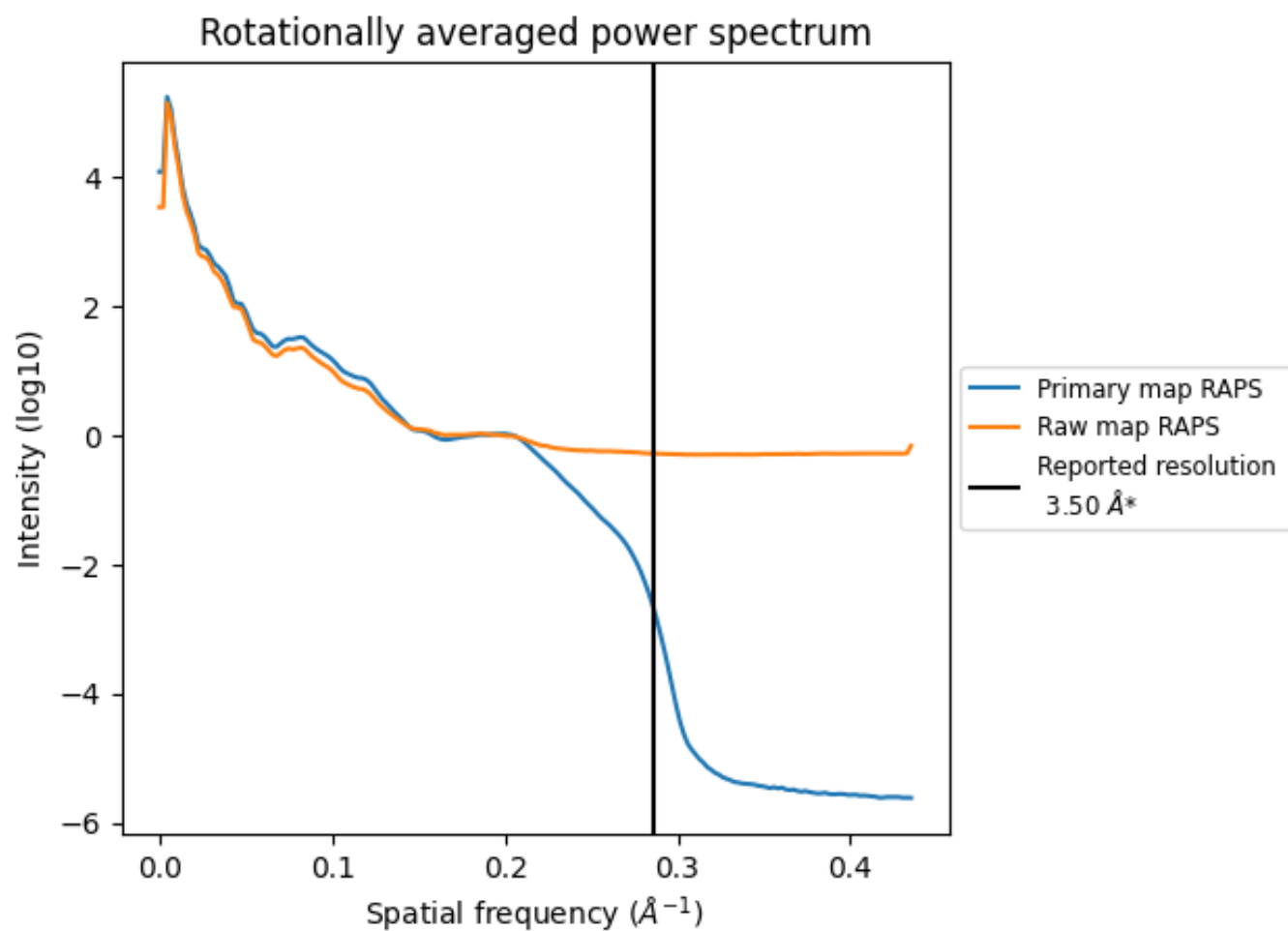
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 619 nm³; this corresponds to an approximate mass of 559 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 ⓘ

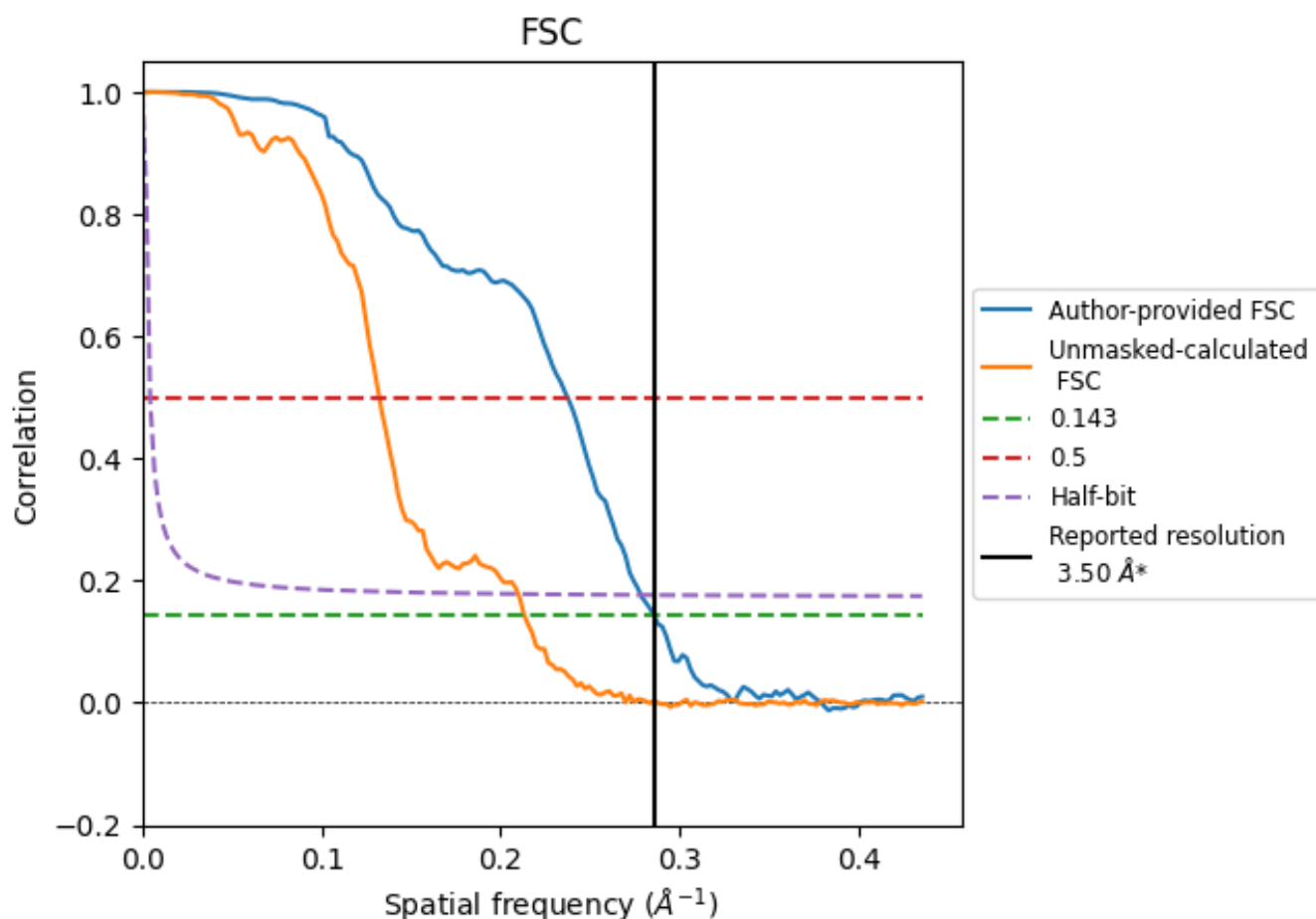


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.286 \AA^{-1}

8.2 Resolution estimates [i](#)

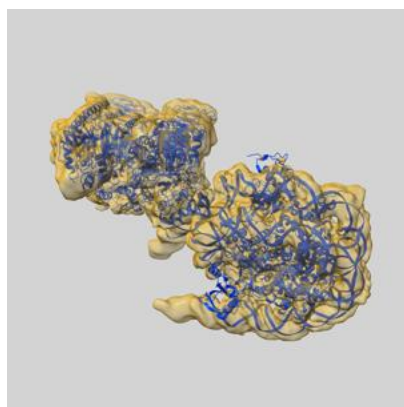
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.50	4.21	3.59
Unmasked-calculated*	4.69	7.56	4.77

*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 4.69 differs from the reported value 3.5 by more than 10 %

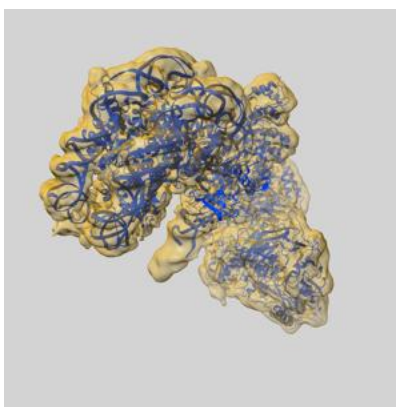
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-21707 and PDB model 6WKR. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

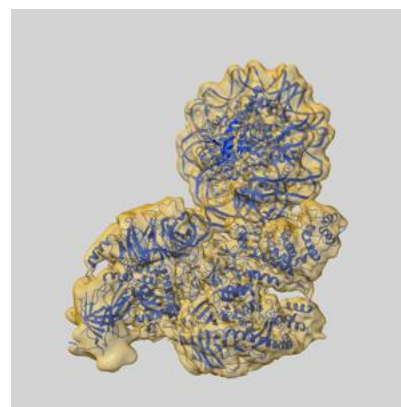
9.1 Map-model overlay [i](#)



X



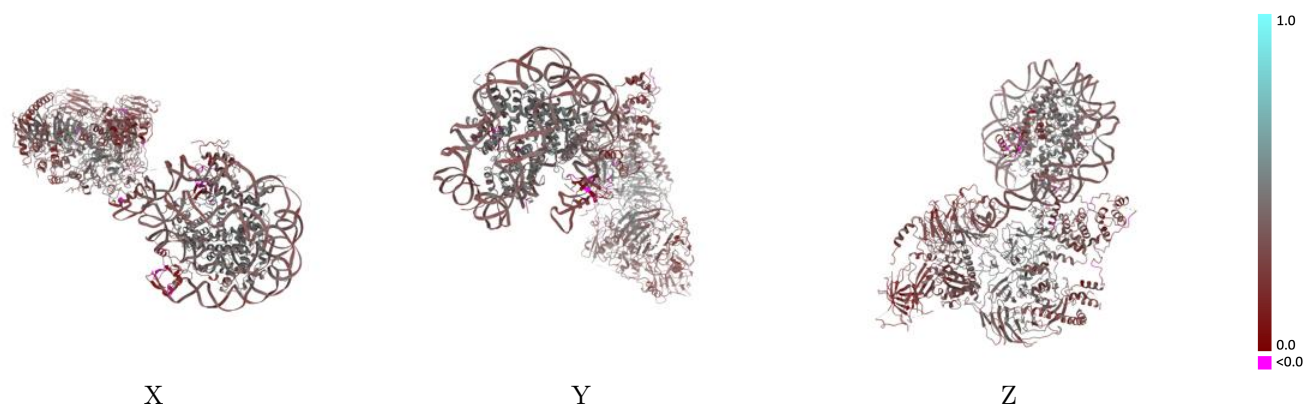
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.01 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](#)



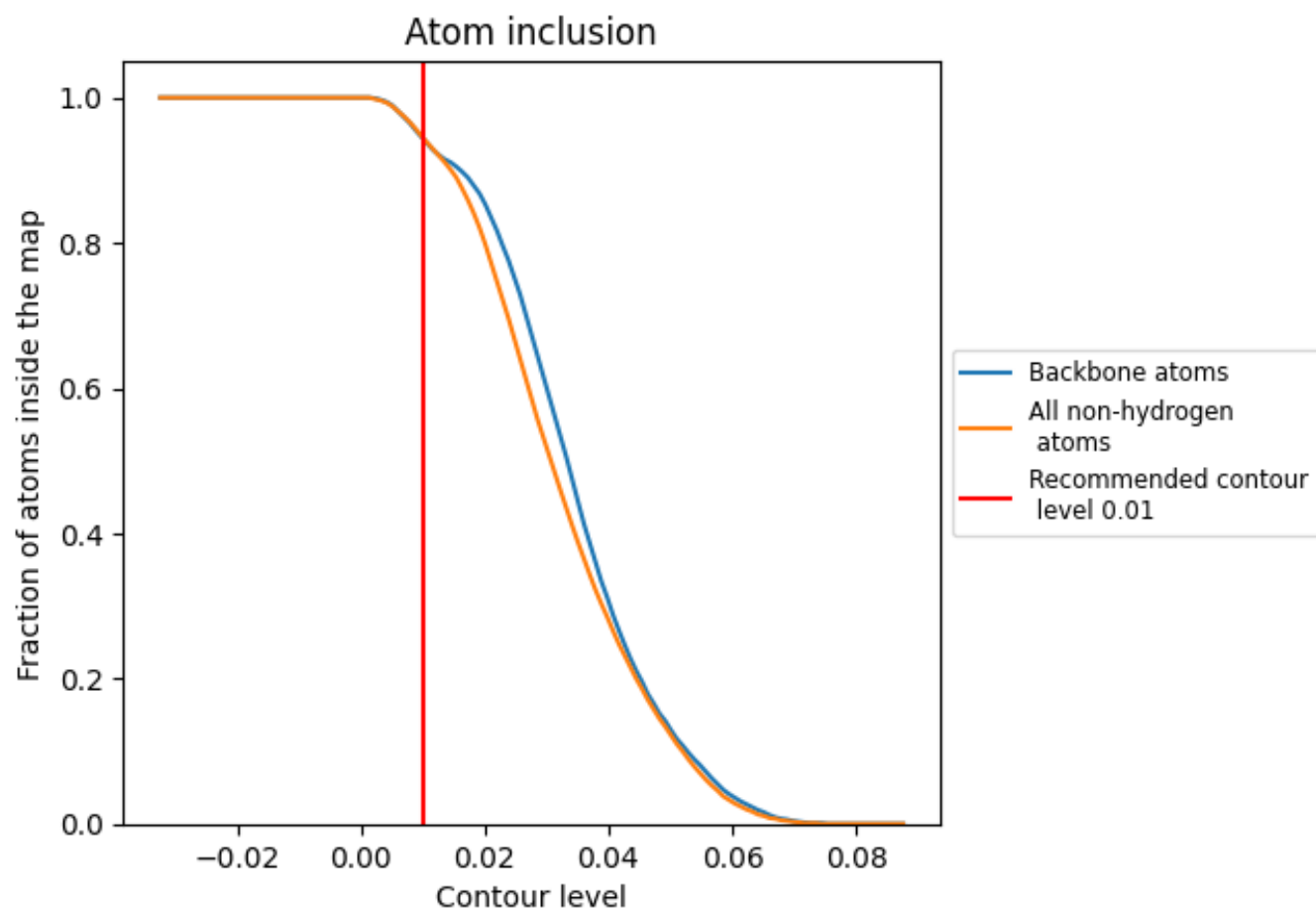
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).







































9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 94% 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	 0.9450	 0.3620
A	 0.9870	 0.3290
B	 1.0000	 0.3330
C	 0.9800	 0.3560
E	 0.1640	 0.2400
F	 0.4090	 0.1670
H	 1.0000	 0.3480
I	 0.9850	 0.4510
J	 0.9610	 0.4460
K	 0.9890	 0.4610
L	 0.9950	 0.4020
M	 0.9930	 0.4610
N	 0.9960	 0.3340
O	 0.9860	 0.4450
P	 0.7700	 0.2980
Q	 0.9720	 0.4610
R	 0.9910	 0.4640
S	 0.9860	 0.4560
T	 0.1430	 0.1450

