Full wwPDB EM Validation Report

May 26, 2025 – 04:51 PM EDT

PDB ID	:	6WKR / pdb_00006wkr
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:

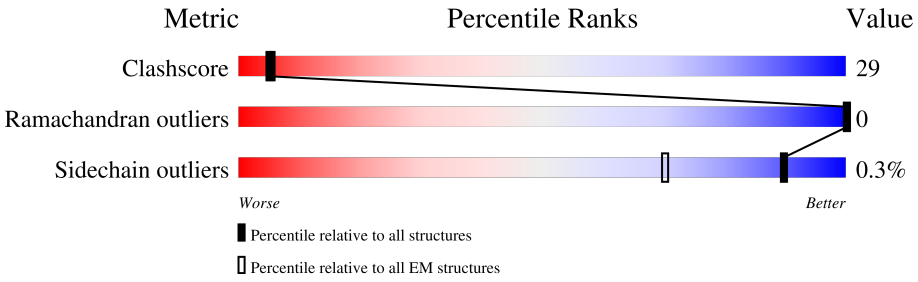
EMDB validation analysis	:	0.0.1.dev118
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0rc1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

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 <=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	57% 47% 53%
1	T	76	84% 55% 45%
2	A	739	34% 25% 41%
3	L	441	41% 41% 18%
4	N	425	41% 52% 7%
5	C	746	53% 28% 19%
6	B	450	5% 91%
6	E	450	6% 7% 92%

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Mol	Chain	Length	Quality of chain
7	P	295	17% 39% 27% 35%
8	H	320	11% 87%
9	I	136	55% 31% 14%
9	O	136	46% 27% 27%
10	J	103	45% 36% 19%
10	Q	103	57% 27% 16%
11	K	130	49% 34% 17%
11	R	130	45% 38% 17%
12	M	126	44% 31% 25%
12	S	126	44% 32% 24%

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		

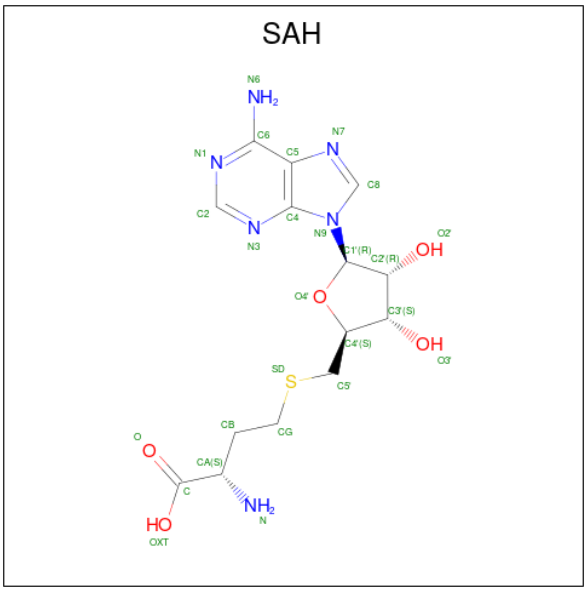
There are 2 discrepancies between the modelled and reference sequences:

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 (CCD ID: 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 (CCD ID: SAH) (formula: $C_{14}H_{20}N_6O_5S$) (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 (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

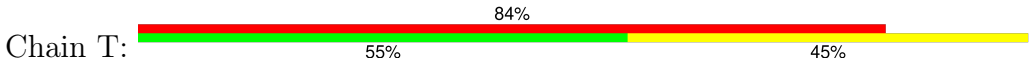
Mol	Chain	Residues	Atoms		AltConf
15	P	1	Total	Zn	0
			1	1	

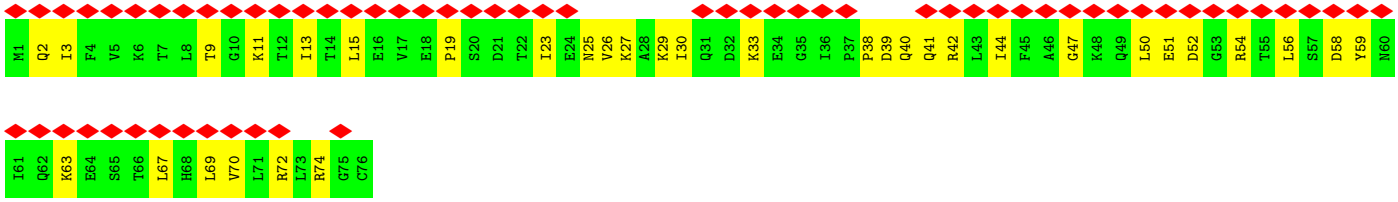
3 Residue-property plots (i)

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

• Molecule 1: Ubiquitin

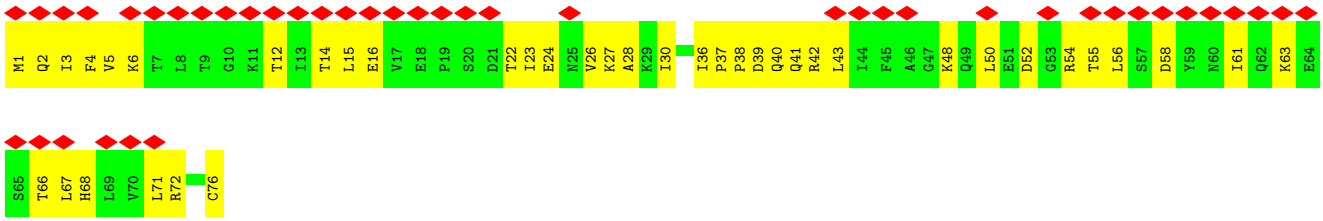
Chain T:





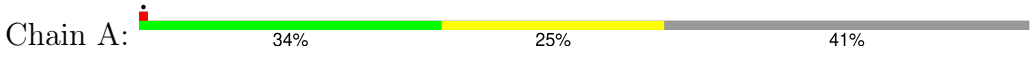
• Molecule 1: Ubiquitin

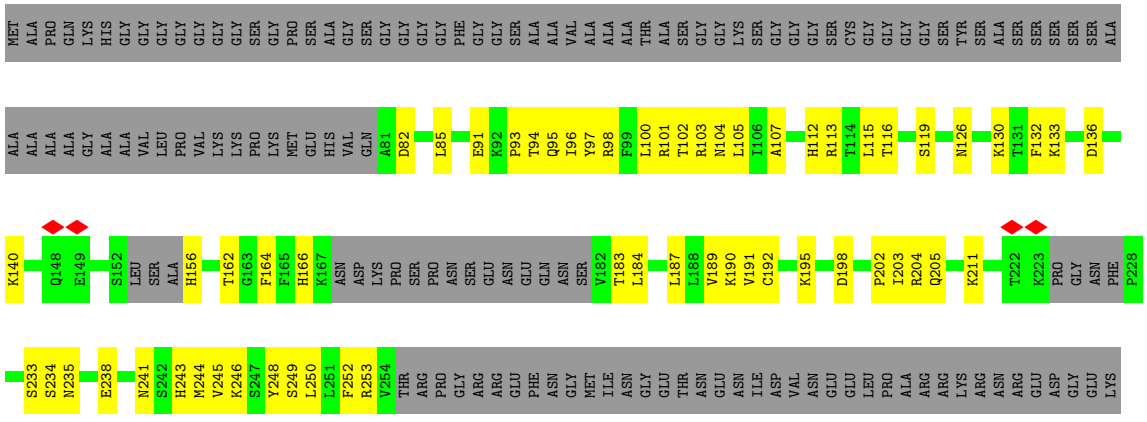
Chain F:

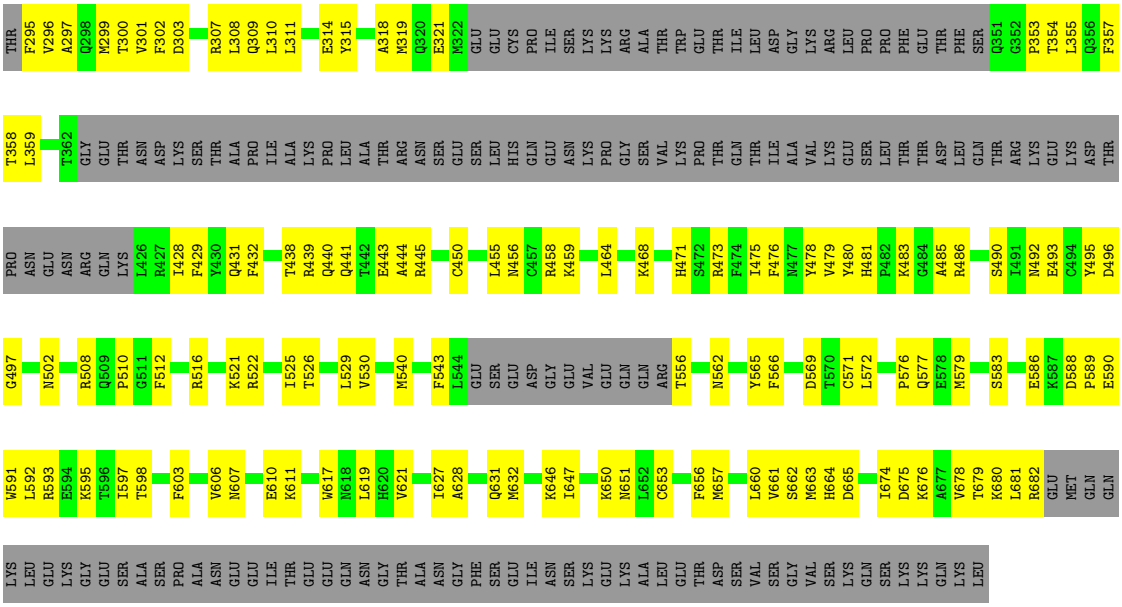


• Molecule 2: Polycomb protein SUZ12

Chain A:

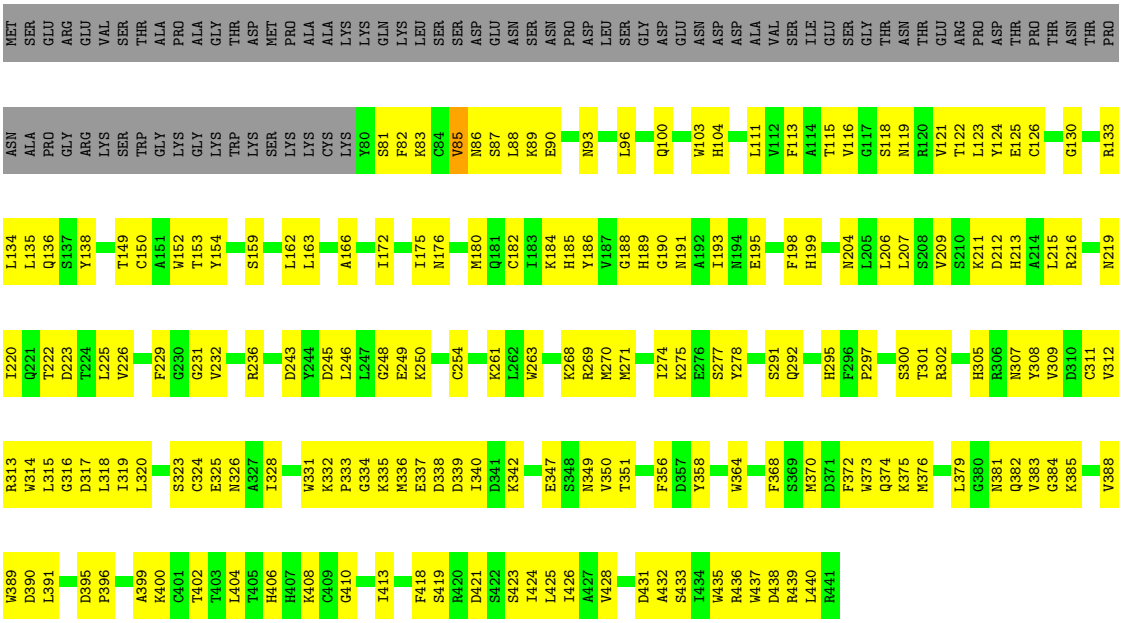






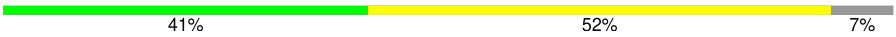
• Molecule 3: Polycomb protein EED

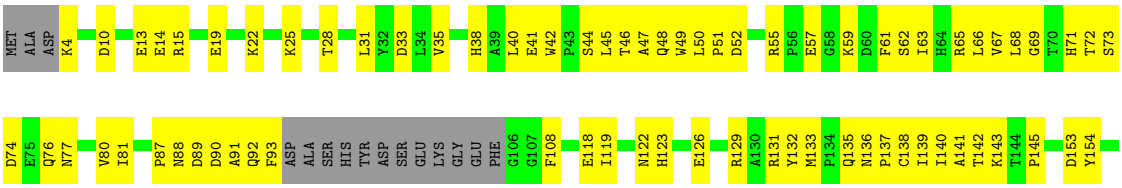
Chain L:

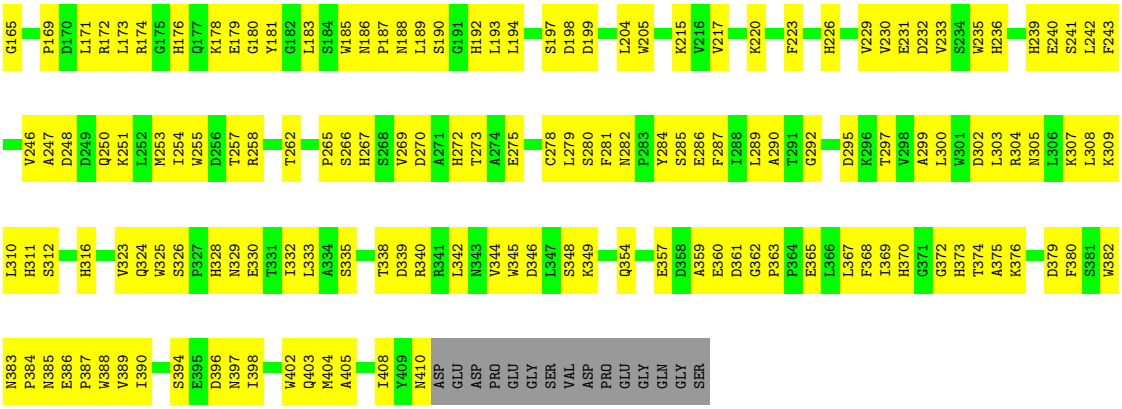


• Molecule 4: Histone-binding protein RBBP4

Chain N:

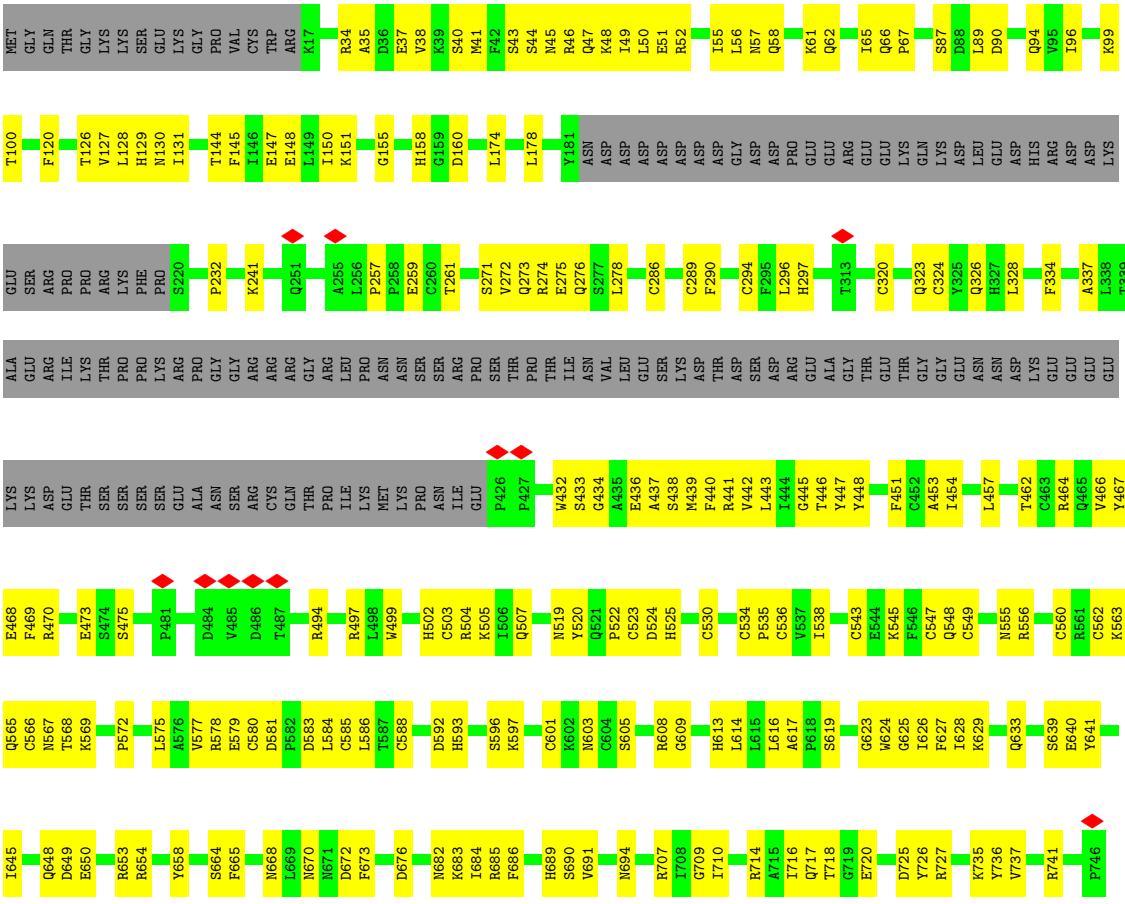






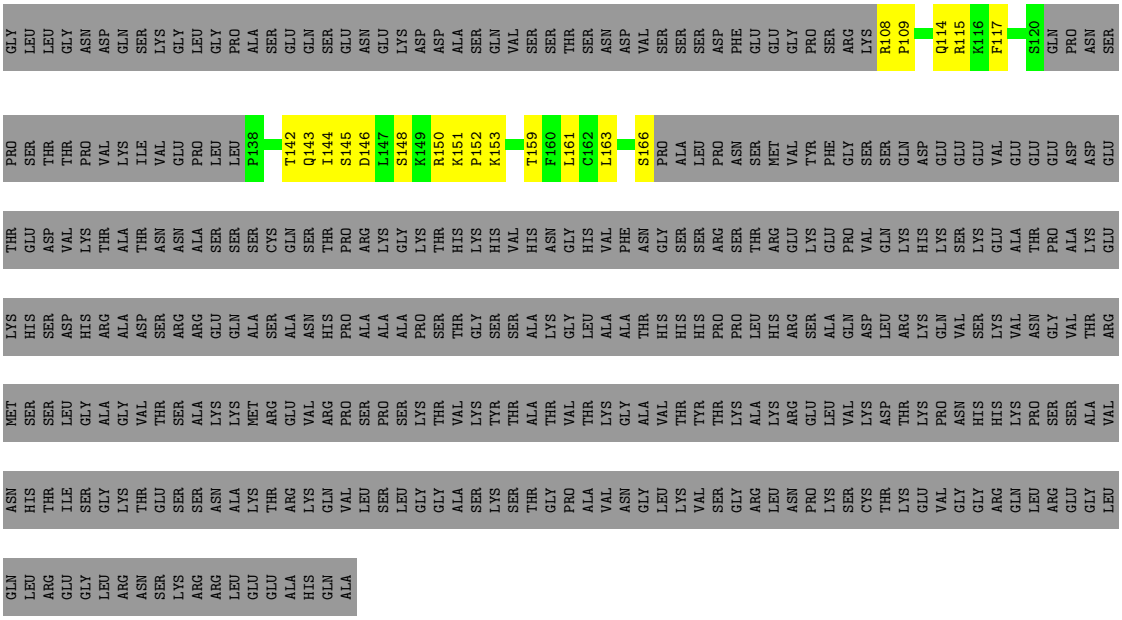
• Molecule 5: Histone-lysine N-methyltransferase EZH2

Chain C:



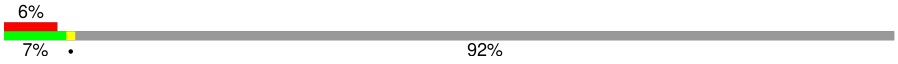
• Molecule 6: Protein Jumonji

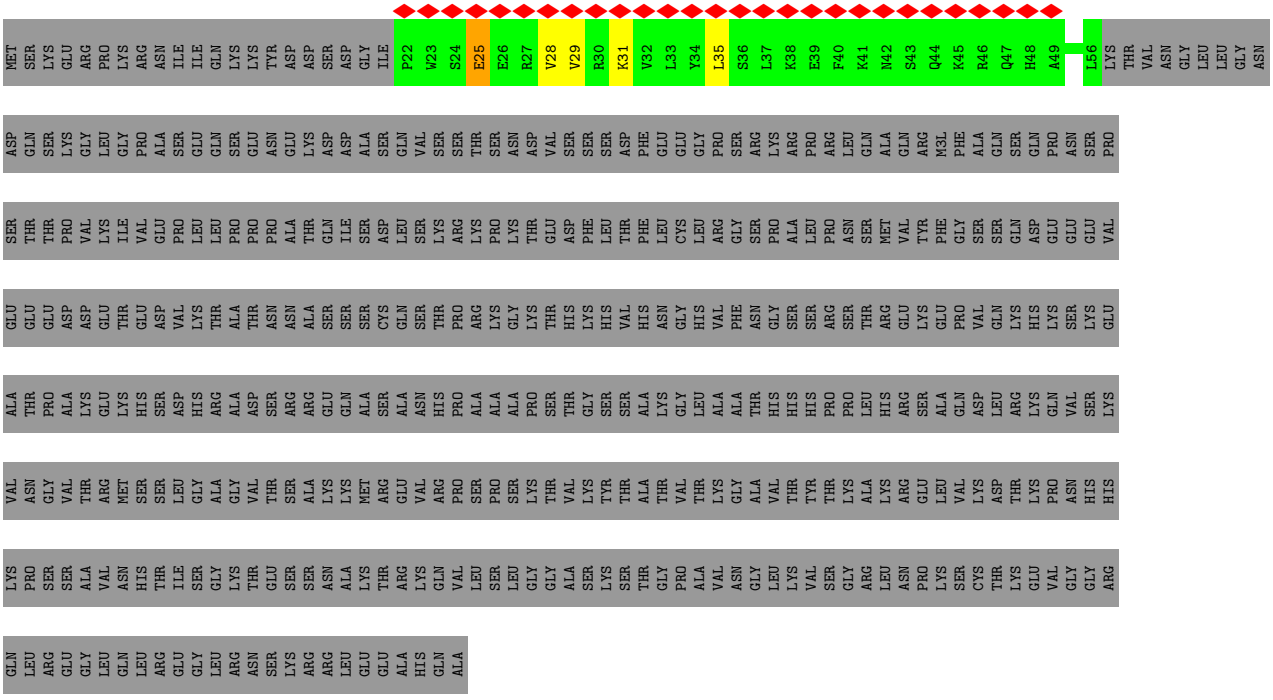
Chain B:



• Molecule 6: Protein Jumonji

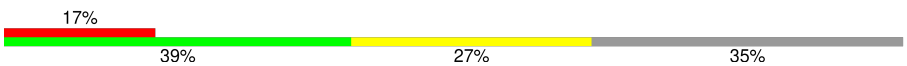
Chain E:

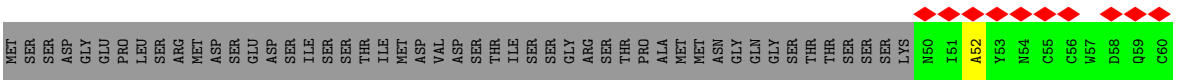


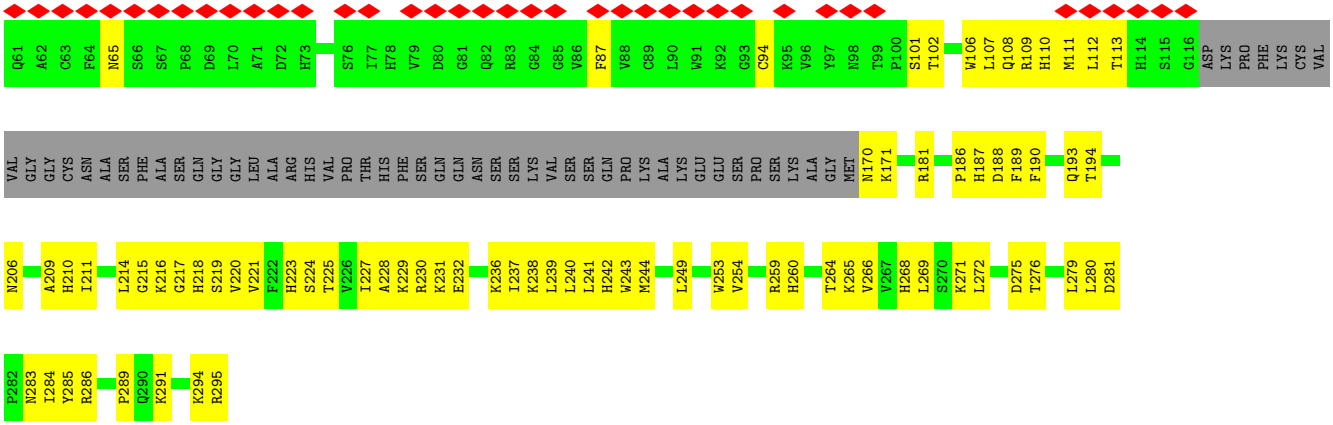


• Molecule 7: Zinc finger protein AEBP2

Chain P:

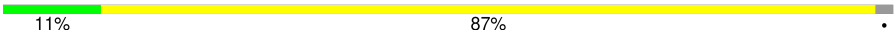


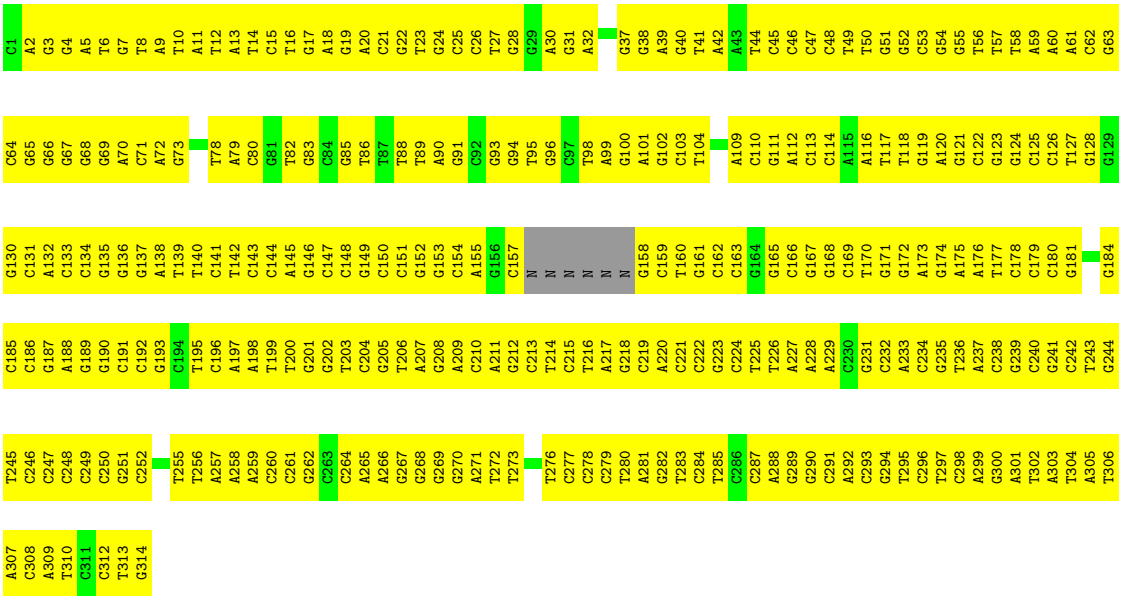




• Molecule 8: DNA (314-MER)

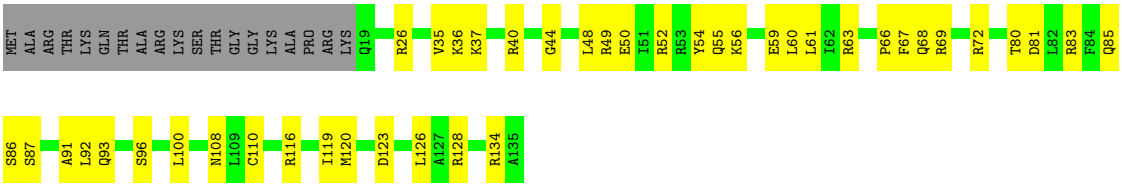
Chain H:





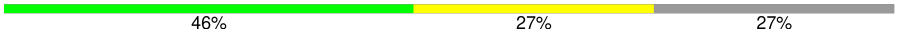
• Molecule 9: Histone H3.2

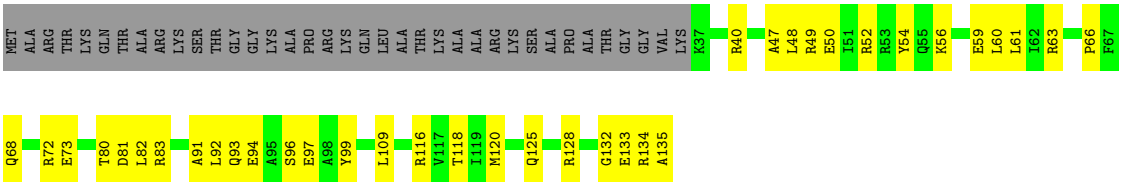
Chain I:



• Molecule 9: Histone H3.2

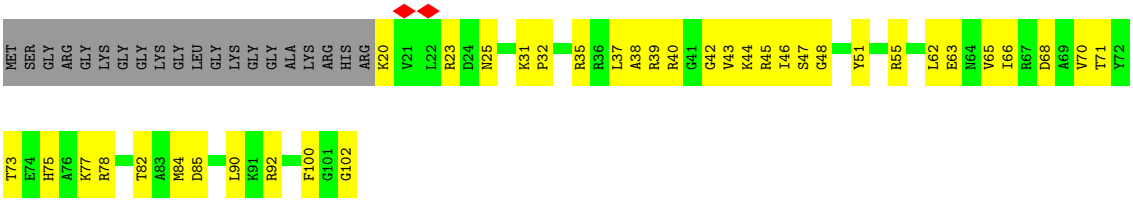
Chain O:





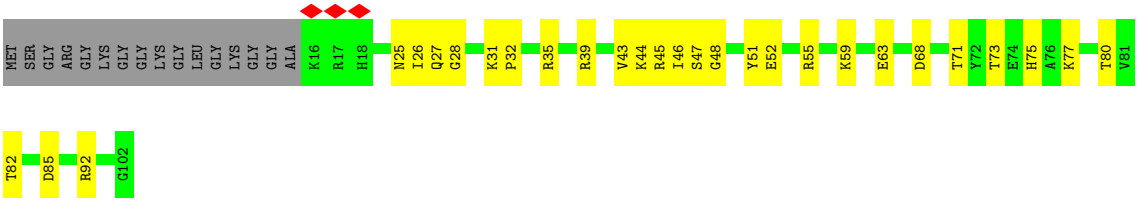
• Molecule 10: Histone H4

Chain J:



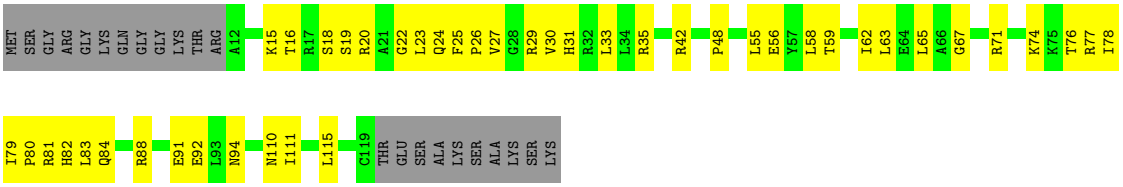
• Molecule 10: Histone H4

Chain Q:



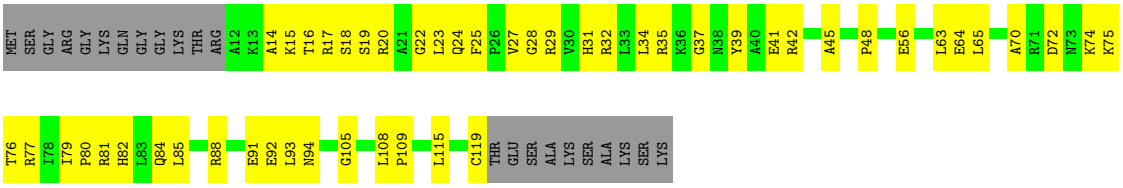
• Molecule 11: Histone H2A type 1

Chain K:



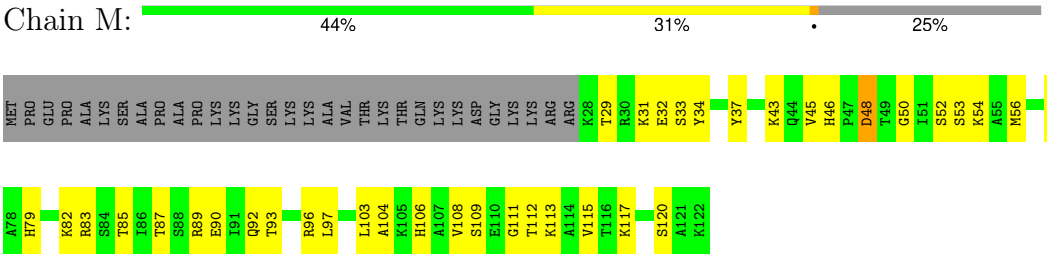
• Molecule 11: Histone H2A type 1

Chain R:



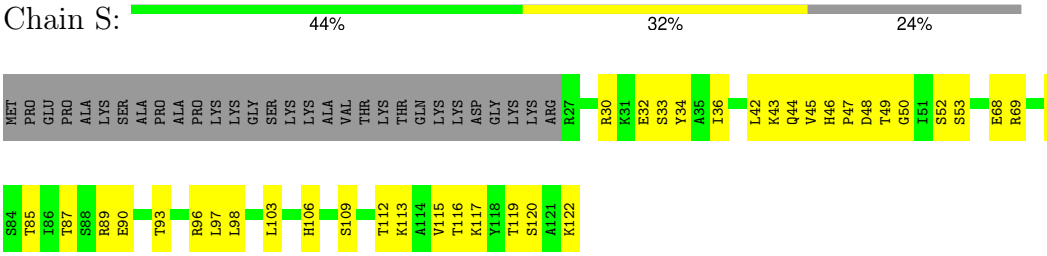
• Molecule 12: Histone H2B 1.1

Chain M:



• Molecule 12: Histone H2B 1.1

Chain S:



4 Experimental information (i)

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 ($e^-/Å^2$)	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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: M3L, ZN, MG, SAH

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	0.15	0/609	0.36	0/819
1	T	0.15	0/610	0.39	0/819
2	A	0.32	0/3419	0.50	0/4636
3	L	0.40	0/2948	0.56	1/4004 (0.0%)
4	N	0.32	0/3165	0.49	0/4322
5	C	0.38	0/4375	0.52	0/5964
6	B	0.27	0/282	0.63	0/382
6	E	0.64	0/203	1.01	0/277
7	P	0.28	0/1376	0.52	0/1879
8	H	0.57	0/7222	0.53	0/11143
9	I	0.65	0/948	0.66	0/1270
9	O	0.63	0/828	0.65	0/1109
10	J	0.72	0/669	0.67	0/894
10	Q	0.70	0/674	0.64	0/904
11	K	0.66	0/835	0.69	0/1128
11	R	0.71	1/839 (0.1%)	0.67	0/1132
12	M	0.69	0/747	0.66	0/1007
12	S	0.73	0/752	0.70	0/1014
All	All	0.49	1/30501 (0.0%)	0.56	1/42703 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	R	24	GLN	C-N	-6.35	1.23	1.33

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	L	85	VAL	N-CA-C	-5.06	108.04	112.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	603	0	631	31	0
1	T	604	0	631	29	0
2	A	3340	0	3106	173	0
3	L	2874	0	2735	143	0
4	N	3080	0	2895	229	0
5	C	4278	0	3675	182	0
6	B	290	0	271	20	0
6	E	203	0	154	6	0
7	P	1346	0	1188	76	0
8	H	6439	0	3521	473	0
9	I	935	0	984	44	0
9	O	816	0	856	36	0
10	J	662	0	709	38	0
10	Q	667	0	679	23	0
11	K	825	0	876	48	0
11	R	829	0	887	50	0
12	M	736	0	751	46	0
12	S	741	0	753	38	0
13	A	1	0	0	0	0
14	C	26	0	19	4	0
15	P	1	0	0	0	0
All	All	29296	0	25321	1527	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 29.

All (1527) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:L:82:PHE:HB3	3:L:437:TRP:HB3	1.63	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:L:291:SER:OG	3:L:292:GLN:N	2.21	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
8:H:213:DC:H2'	8:H:214:DT:H71	1.73	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
4:N:253:MET:HE2	4:N:265:PRO:HG3	1.75	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: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
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
4:N:280:SER:HG	4:N:325:TRP:CD1	2.15	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
2:A:183:THR:OG1	2:A:211:LYS:O	2.11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:187:DG:H5”	8:H:187:DG:H8	1.62	0.64
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
3:L:376:MET:HE3	3:L:388:VAL:HG13	1.80	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:657:MET:HE3	2:A:678:VAL:HG21	1.80	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
7:P:268:HIS:HB3	7:P:271:LYS:HZ3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
10:J:44:LYS:NZ	11:R:115:LEU:O	2.33	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
5:C:37:GLU:O	5:C:40:SER:OG	2.16	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:C:46:ARG:O	5:C:50:LEU:HG	2.01	0.60
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
5:C:128:LEU:O	5:C:129:HIS:ND1	2.32	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
12:S:113:LYS:O	12:S:116:THR:OG1	2.20	0.58
4:N:284:TYR:HB2	4:N:330:GLU:HG3	1.83	0.58
12:M:117:LYS:O	12:M:120:SER:OG	2.21	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
11:K:16:THR:O	11:K:19:SER:OG	2.14	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
3:L:82:PHE:C	3:L:83:LYS:HZ2	2.12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
7:P:289:PRO:C	7:P:291:LYS:H	2.13	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
2:A:133:LYS:HD2	4:N:304:ARG:HH22	1.71	0.55
5:C:48:LYS:HA	5:C:51:GLU:CD	2.32	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
2:A:603:PHE:O	2:A:611:LYS:NZ	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
3:L:115:THR:O	3:L:122:THR:OG1	2.21	0.53
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:565:GLN:HB2	5:C:567:ASN:CG	2.33	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
9:I:80:THR:OG1	9:I:81:ASP:OD1	2.20	0.53
10:J:84:MET:HE1	10:J:102:GLY:HA2	1.90	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
12:M:87:THR:H	12:M:90:GLU:CD	2.13	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
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
6:B:142:THR:OG1	6:B:143:GLN:N	2.39	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
2:A:565:TYR:C	2:A:566:PHE:HD1	2.18	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:95:GLN:H	2:A:95:GLN:CD	2.17	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:54:ARG:HE	1:F:58:ASP:CG	2.18	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
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
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
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
3:L:374:GLN:C	3:L:391:LEU:HD12	2.36	0.51
4:N:236:HIS:CE1	4:N:239:HIS:HD2	2.29	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
12:M:106:HIS:O	12:M:109:SER:OG	2.29	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
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
5:C:682:ASN:OD1	5:C:682:ASN:N	2.41	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:250:DC:H2”	8:H:251:DG:C8	2.47	0.50
9:I:54:TYR:C	9:I:56:LYS:H	2.19	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
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
3:L:419:SER:OG	3:L:421:ASP:OD1	2.29	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
5:C:717:GLN:H	5:C:717:GLN:CD	2.20	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
8:H:301:DA:C8	8:H:302:DT:H72	2.46	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:346:ASP:OD1	4:N:348:SER:OG	2.22	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
12:S:43:LYS:NZ	12:S:49:THR:O	2.35	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:85:VAL:HG21	3:L:438:ASP:CG	2.37	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
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: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
4:N:346:ASP:CG	4:N:349:LYS:HG3	2.38	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:268:LYS:HA	3:L:271:MET:HE2	1.95	0.48
4:N:71:HIS:ND1	4:N:126:GLU:OE1	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:309:GLN:C	2:A:310:LEU:HD12	2.39	0.47
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
3:L:261:LYS:HB3	3:L:297:PRO:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
4:N:340:ARG:HG2	4:N:375:ALA:C	2.39	0.47
8:H:51:DG:P	9:I:72:ARG:HH22	2.38	0.47
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
5:C:664:SER:H	14:C:801:SAH:HO3'	1.61	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
4:N:176:HIS:CG	4:N:197:SER:HG	2.31	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
2:A:100:LEU:O	2:A:104:ASN:ND2	2.49	0.46
2:A:458:ARG:C	2:A:459:LYS:HD3	2.41	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
3:L:245:ASP:CG	3:L:248:GLY:H	2.23	0.46
5:C:145:PHE:HA	5:C:148:GLU:CD	2.40	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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
4:N:387:PRO:C	4:N:388:TRP:HD1	2.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:213:HIS:HD2	3:L:236:ARG:C	2.25	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:K:77:ARG:HG3	12:M:50:GLY:C	2.42	0.45
11:R:20:ARG:HD3	12:S:122:LYS:C	2.42	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
2:A:445:ARG:HD3	6:B:143:GLN:CD	2.42	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
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:583:ASP:C	5:C:584:LEU:HD23	2.43	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:C:326:GLN:C	5:C:328:LEU:H	2.25	0.44
8:H:15:DC:H2"	8:H:16:DT:H6	1.82	0.44
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:33:ASP:CG	4:N:405:ALA:HA	2.43	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
12:M:59:MET:HB3	12:M:59:MET:HE3	1.64	0.44
11:R:23:LEU:HD23	11:R:23:LEU:HA	1.77	0.44
11:R:79:ILE:O	11:R:80:PRO:C	2.60	0.44
2:A:126:ASN:HB3	4:N:410:ASN:H	1.82	0.44
3:L:113:PHE:CZ	3:L:124:TYR:HD2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:C:672:ASP:C	5:C:673:PHE:HD1	2.26	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:A:679:THR:OG1	2:A:680:LYS:N	2.51	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
5:C:87:SER:OG	5:C:89:LEU:O	2.28	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
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
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
5:C:716:ILE:HG23	5:C:720:GLU:CD	2.44	0.42
8:H:37:DG:O3'	8:H:38:DG:C8	2.71	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:213:HIS:CD2	3:L:236:ARG:C	2.97	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
9:O:93:GLN:O	9:O:94:GLU:C	2.62	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:93:PHE:C	4:N:108:PHE:HA	2.43	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
11:R:27:VAL:O	11:R:28:GLY:C	2.62	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
12:M:46:HIS:C	12:M:48:ASP:H	2.27	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:F:1:MET:HE1	1:F:3:ILE:HG23	2.02	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:J:68:ASP:OD1	10:J:68:ASP:N	2.49	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:132:DA:H3'	11:R:75:LYS:HZ2	1.84	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
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
9:O:54:TYR:C	9:O:56:LYS:H	2.28	0.41
12:S:48:ASP:OD1	12:S:48:ASP:N	2.51	0.41
2:A:521:LYS:HZ2	2:A:577:GLN:HG3	1.84	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
4:N:302:ASP:OD1	4:N:302:ASP:C	2.63	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
12:S:115:VAL:O	12:S:116:THR:C	2.63	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: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
12:M:76:ARG:O	12:M:77:LEU:C	2.63	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
4:N:338:THR:HA	4:N:376:LYS:HG3	2.02	0.41
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
2:A:663:MET:HE3	2:A:663:MET:HB3	1.89	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
9:I:60:LEU:HD13	9:I:93:GLN:CD	2.46	0.41
9:O:91:ALA:O	9:O:92:LEU:C	2.62	0.41
2:A:632:MET:HE3	5:C:290:PHE:CG	2.56	0.41
4:N:241:SER:OG	4:N:258:ARG:NH1	2.53	0.41
5:C:259:GLU:O	5:C:261:THR:HG23	2.21	0.41
5:C:684:ILE:C	5:C:686:PHE:N	2.78	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
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
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
11:K:80:PRO:O	11:K:81:ARG:C	2.64	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
11:K:79:ILE:O	11:K:80:PRO:C	2.64	0.40
1:F:1:MET:HE2	1:F:63:LYS:HA	2.03	0.40
3:L:82:PHE:HA	3:L:438:ASP:O	2.22	0.40
3:L:320:LEU:HD23	3:L:320:LEU:HA	1.92	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	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%)	372 (100%)	1 (0%)	91	96
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%)	96 (100%)	0	100	100
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%)	83 (99%)	1 (1%)	67	82
11	R	85/101 (84%)	85 (100%)	0	100	100
12	M	79/106 (74%)	78 (99%)	1 (1%)	65	81
12	S	79/106 (74%)	79 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2266/4049 (56%)	2259 (100%)	7 (0%)	90 96

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	C	563	LYS
10	J	85	ASP
11	K	62	ILE
12	M	48	ASP
10	Q	68	ASP
6	E	25	GLU
6	E	29	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	T	25	ASN
1	T	41	GLN
1	T	62	GLN
2	A	104	ASN
2	A	126	ASN
2	A	241	ASN
2	A	243	HIS
2	A	431	GLN
2	A	481	HIS
2	A	507	HIS
3	L	136	GLN
3	L	189	HIS
3	L	204	ASN
3	L	221	GLN
3	L	235	HIS
3	L	407	HIS
4	N	76	GLN
4	N	88	ASN
4	N	123	HIS
4	N	128	ASN
4	N	135	GLN
4	N	188	ASN
4	N	239	HIS
4	N	329	ASN
4	N	370	HIS

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Mol	Chain	Res	Type
4	N	397	ASN
5	C	94	GLN
5	C	117	GLN
5	C	273	GLN
5	C	507	GLN
5	C	593	HIS
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	81	ASN
12	M	92	GLN
9	O	39	HIS
9	O	68	GLN
9	O	113	HIS
10	Q	75	HIS
11	R	24	GLN
11	R	31	HIS
11	R	84	GLN
12	S	46	HIS
12	S	60	ASN
12	S	79	HIS
1	F	25	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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 (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

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(^{o})	Ideal(^{o})
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
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.

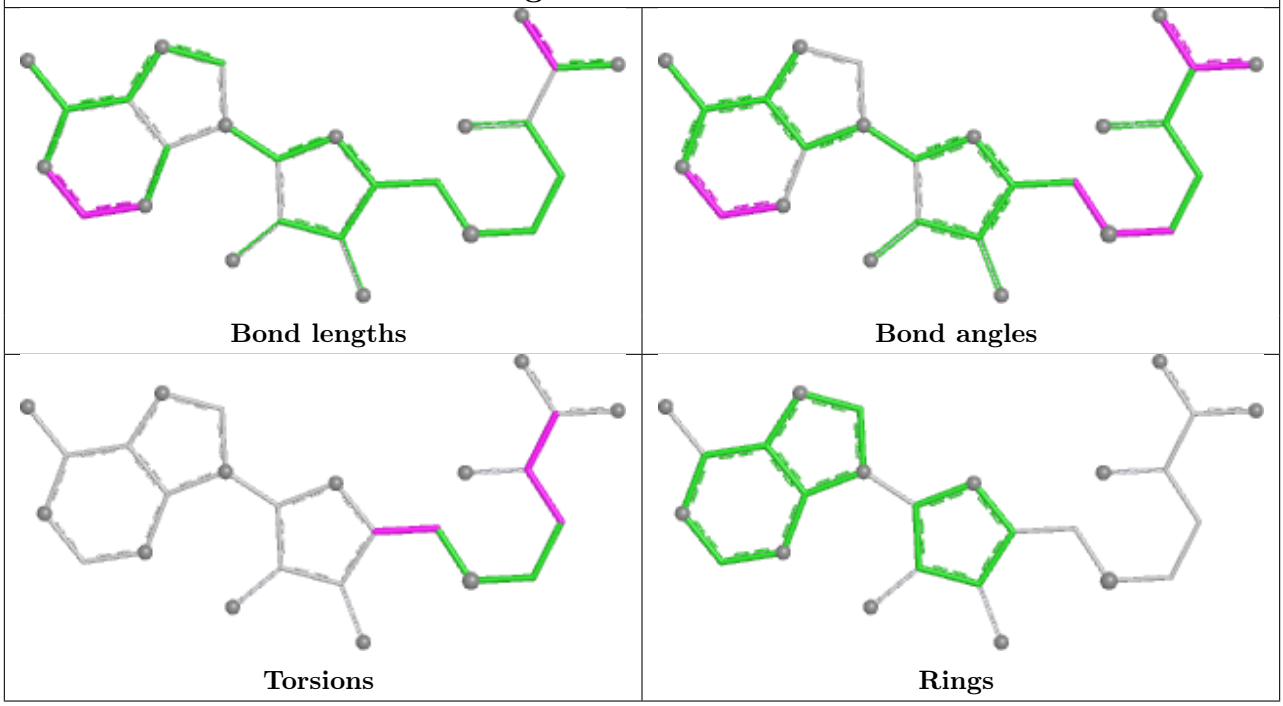
1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	C	801	SAH	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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

Ligand SAH C 801



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

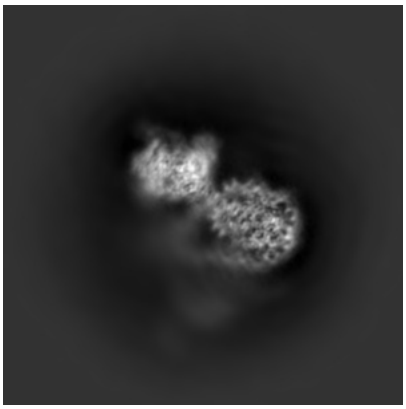
6 Map visualisation

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

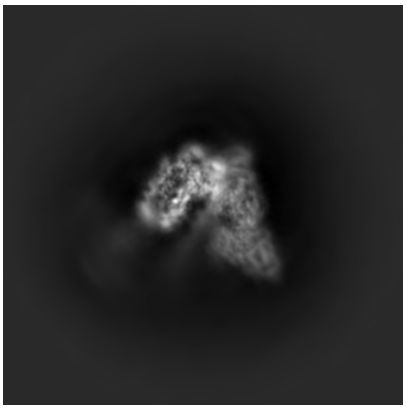
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

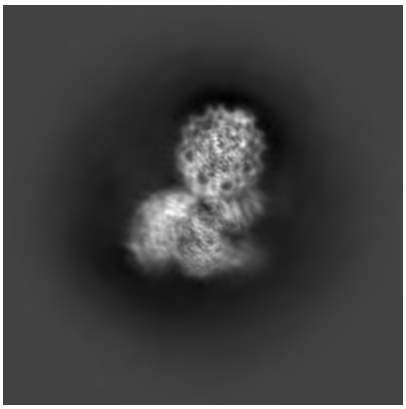
6.1.1 Primary map



X

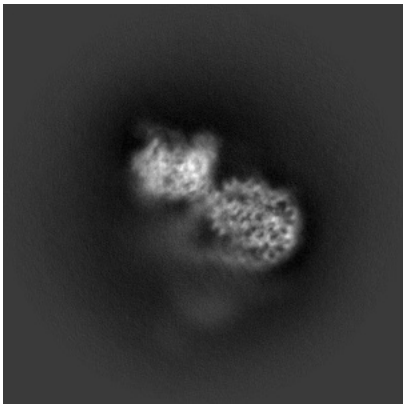


Y

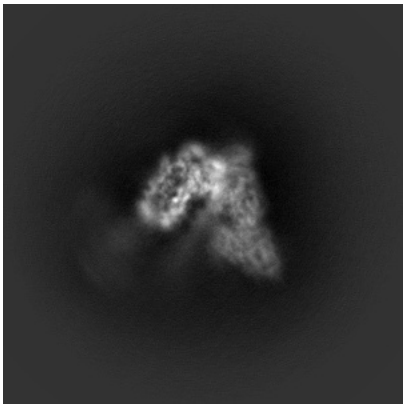


Z

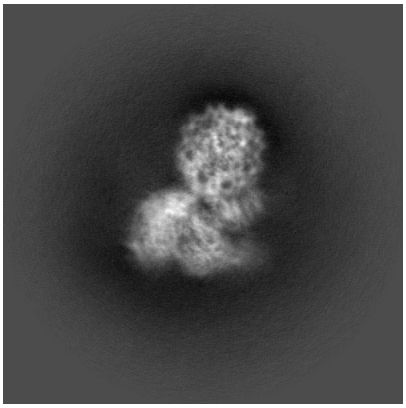
6.1.2 Raw map



X



Y

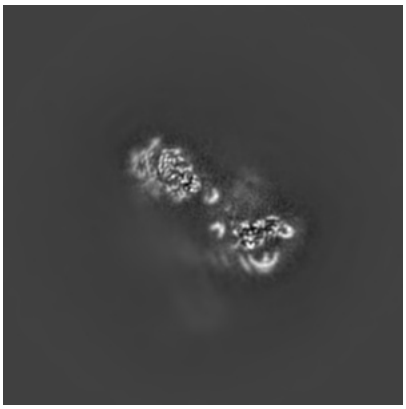


Z

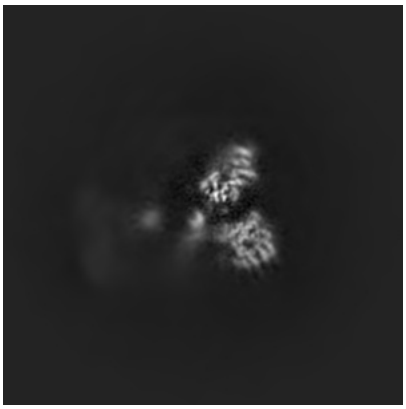
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map



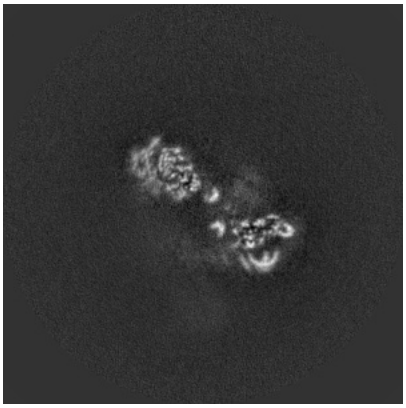
X Index: 192



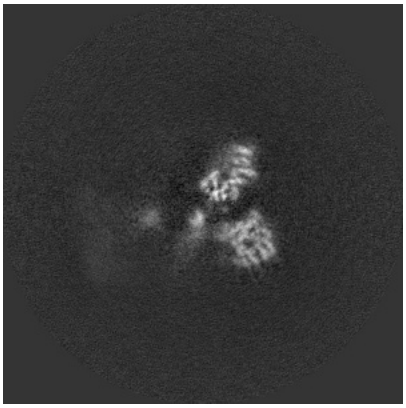
Y Index: 192

Z Index: 192

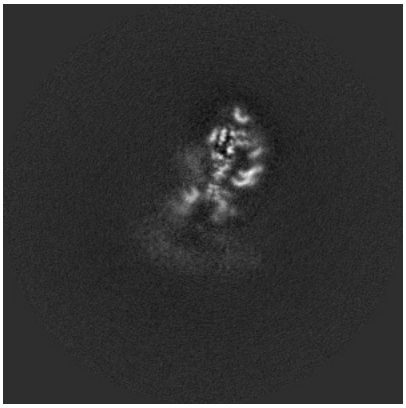
6.2.2 Raw map



X Index: 192



Y Index: 192

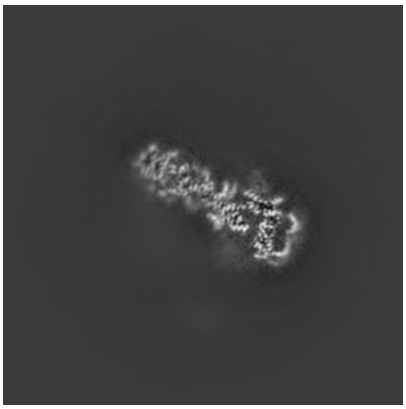


Z Index: 192

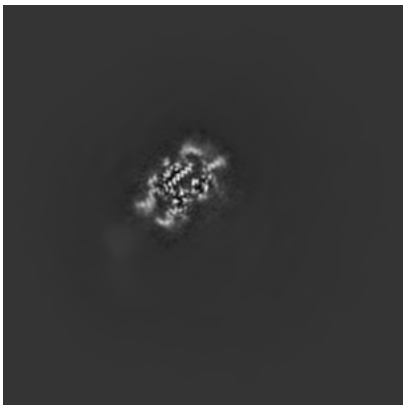
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



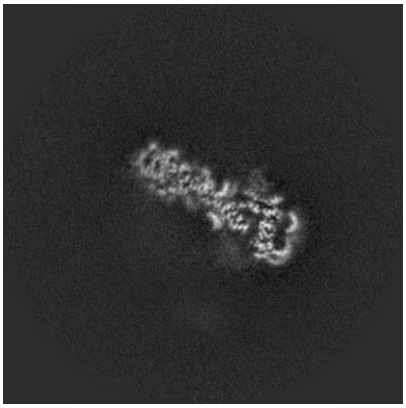
X Index: 205



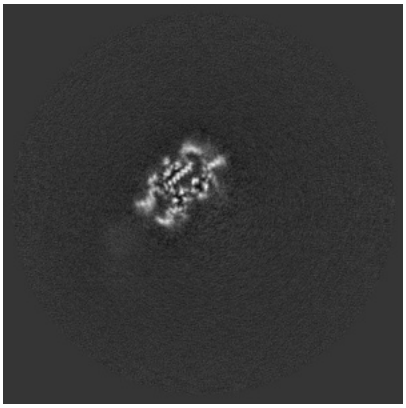
Y Index: 252

Z Index: 206

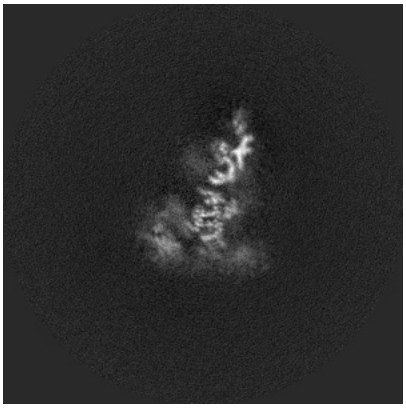
6.3.2 Raw map



X Index: 204



Y Index: 252

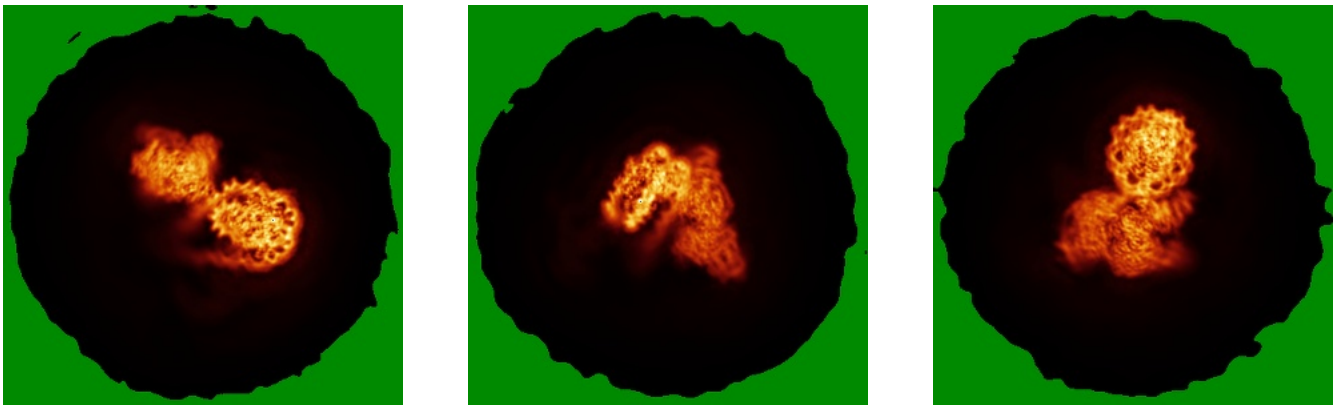


Z Index: 206

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

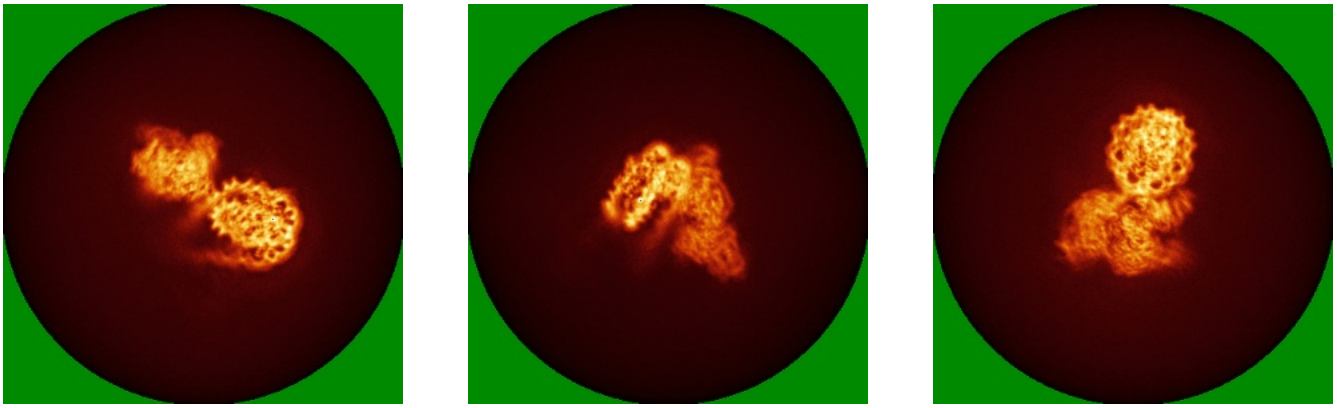
6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map



X Y Z

6.4.2 Raw map

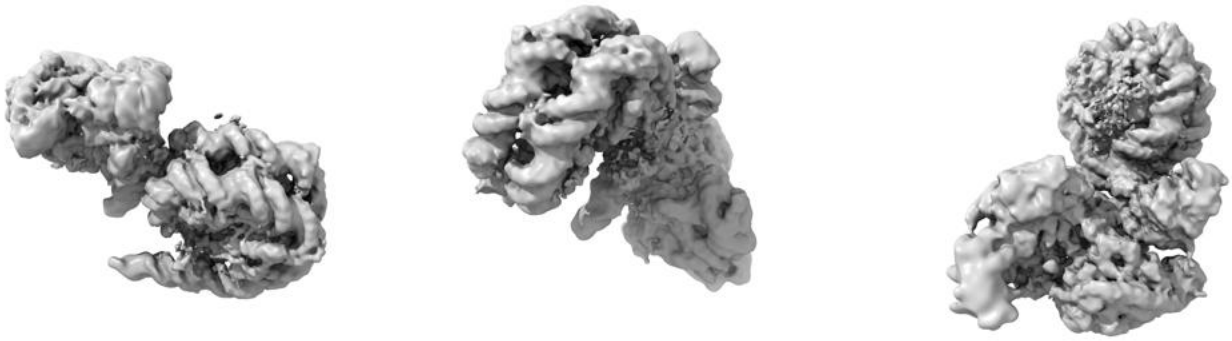


X Y Z

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



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

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

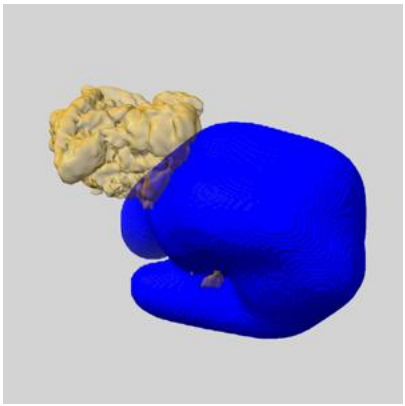
6.6 Mask visualisation (i)

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

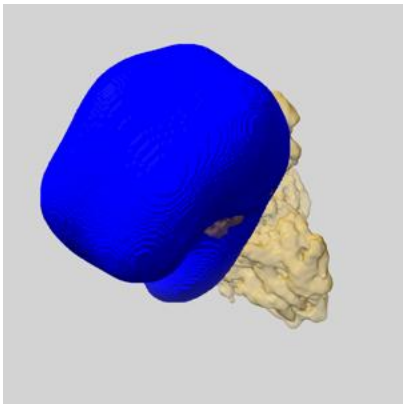
A mask typically either:

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

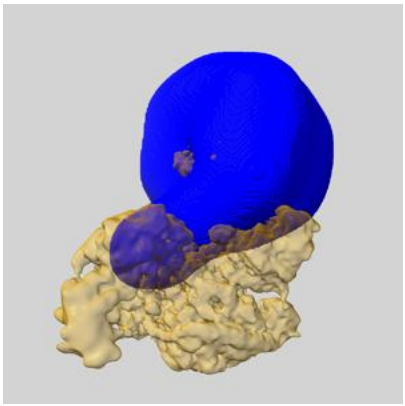
6.6.1 emd_21707_msk_2.map (i)



X

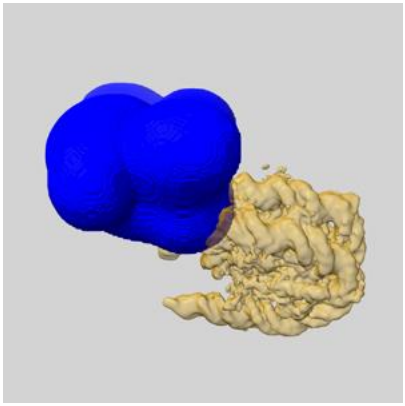


Y

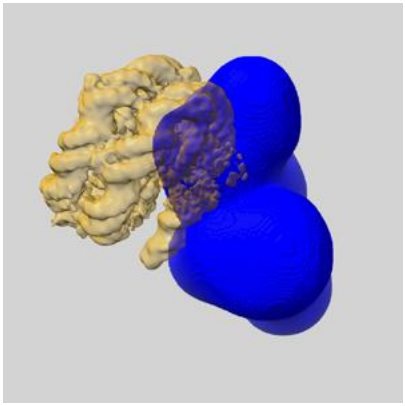


Z

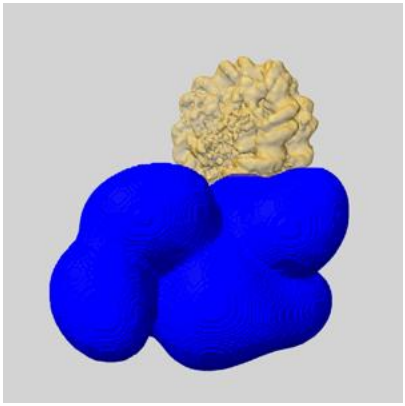
6.6.2 emd_21707_msk_1.map (i)



X



Y

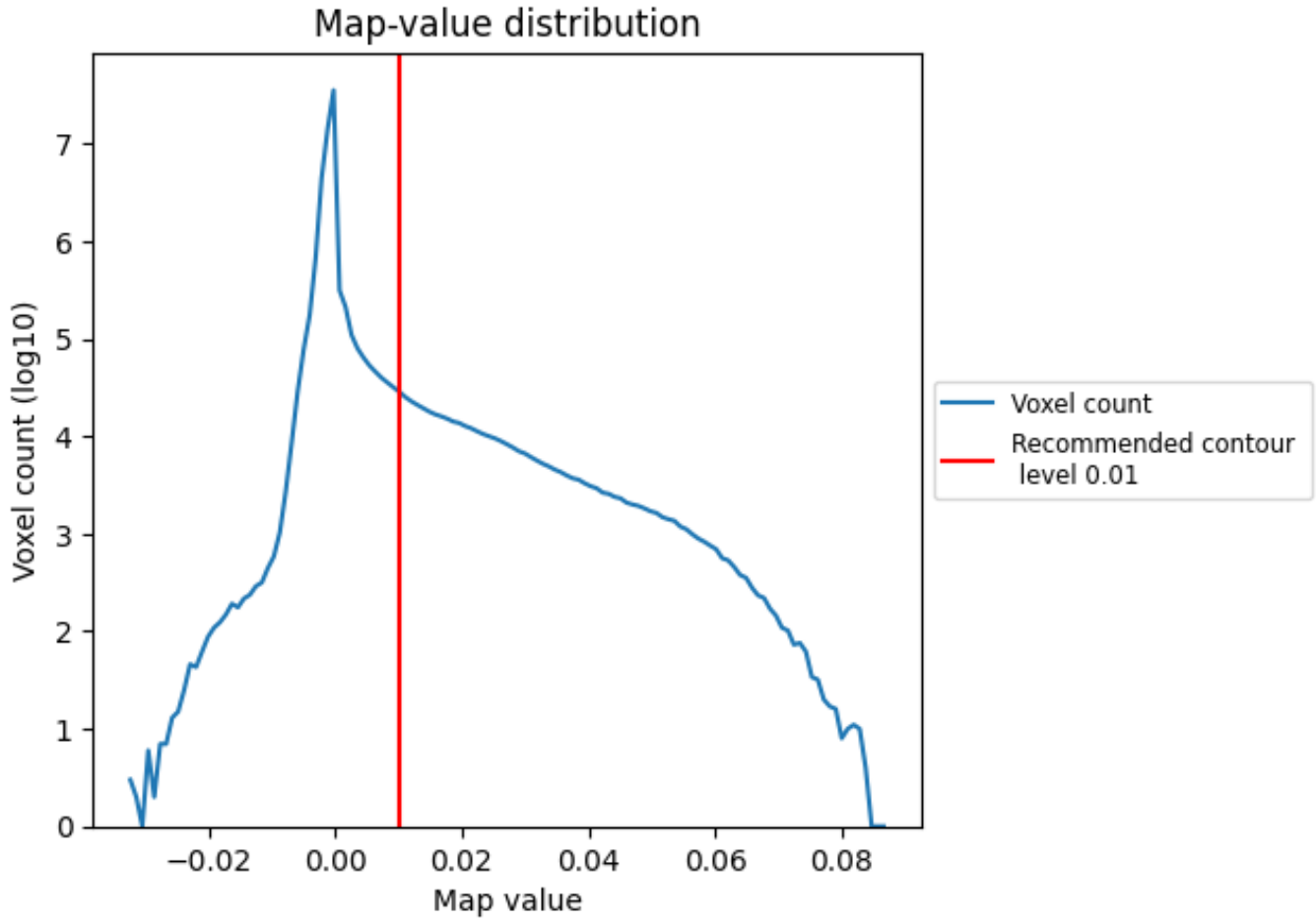


Z

7 Map analysis

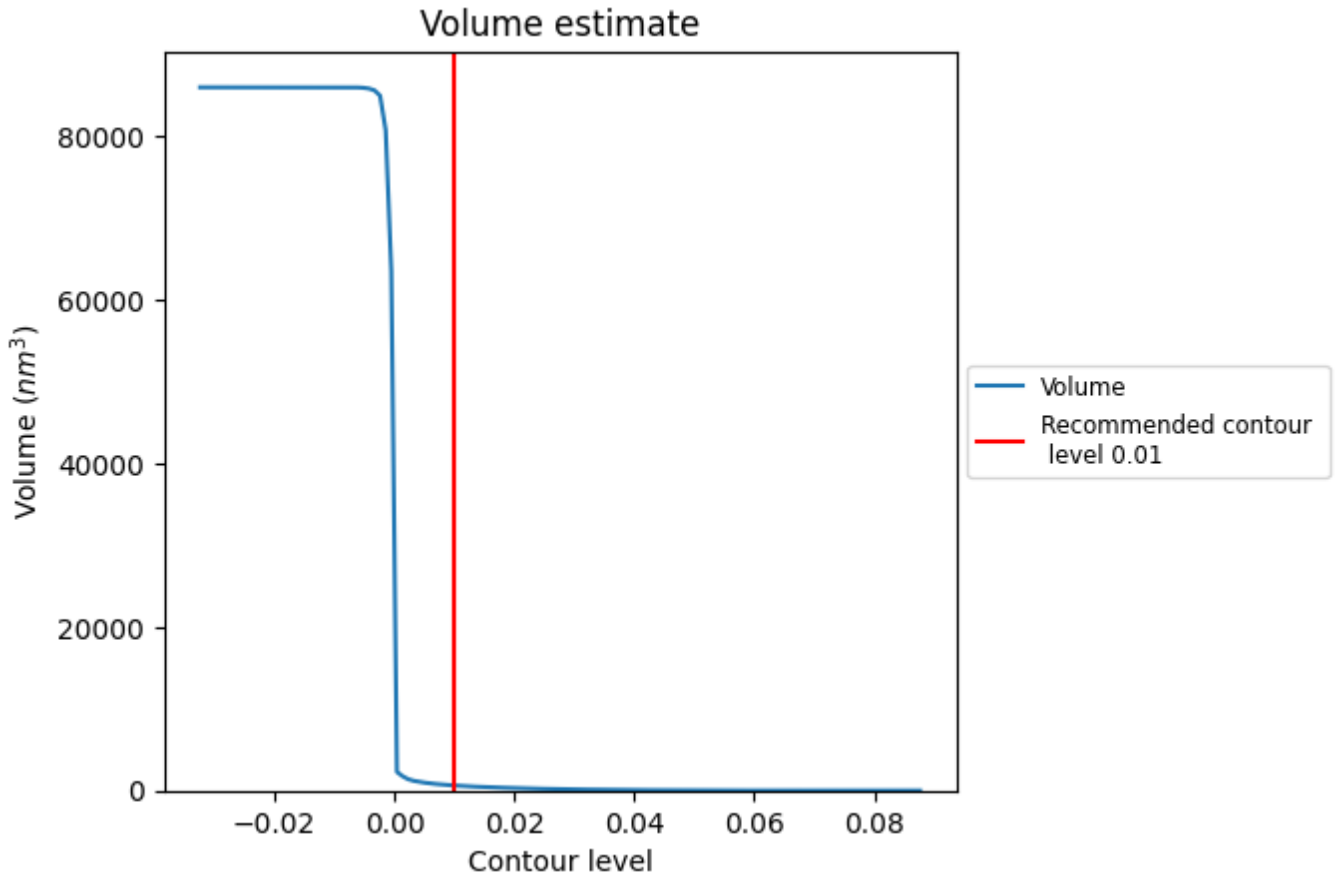
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

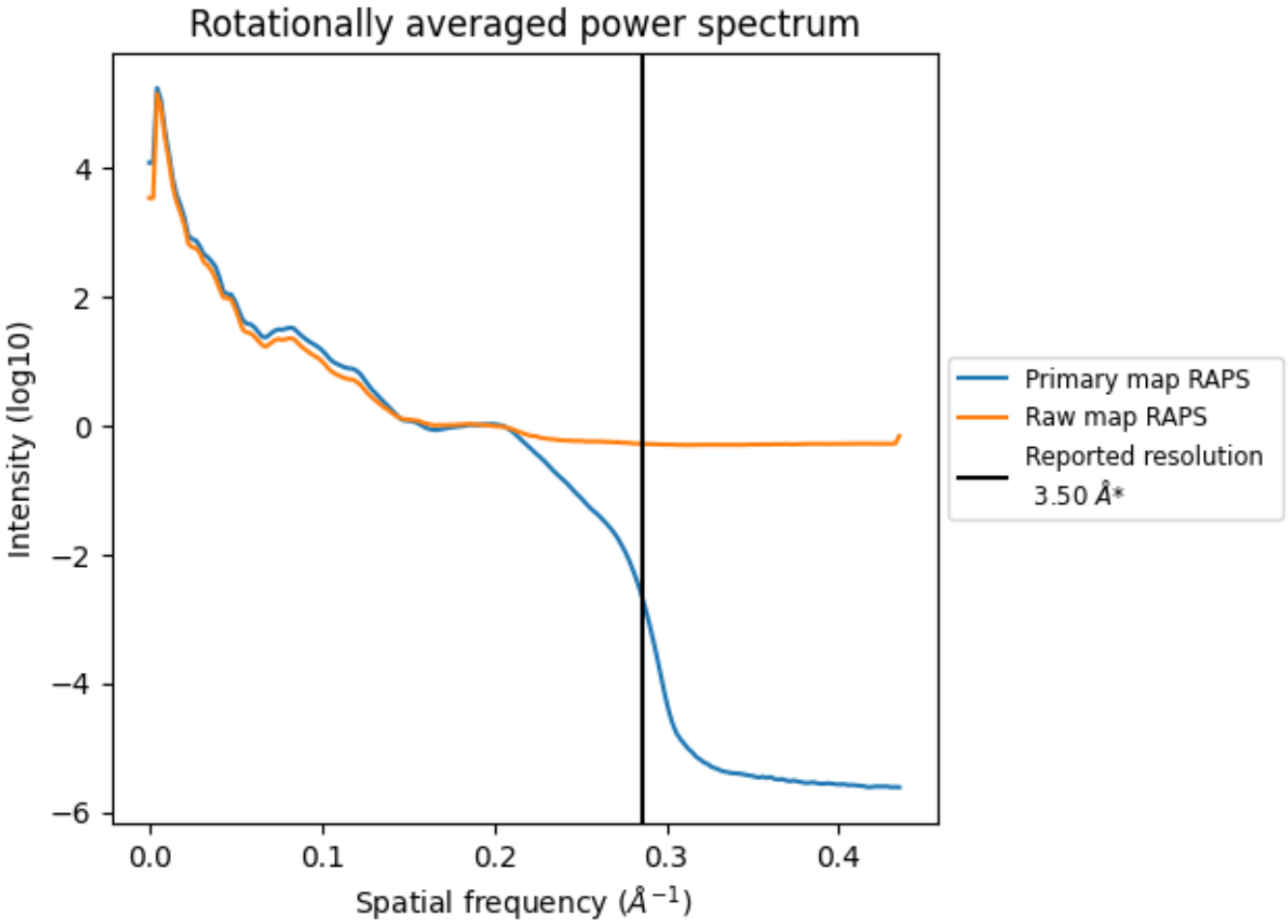
7.2 Volume estimate



The volume at the recommended contour level is 619 nm^3; 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 (i)

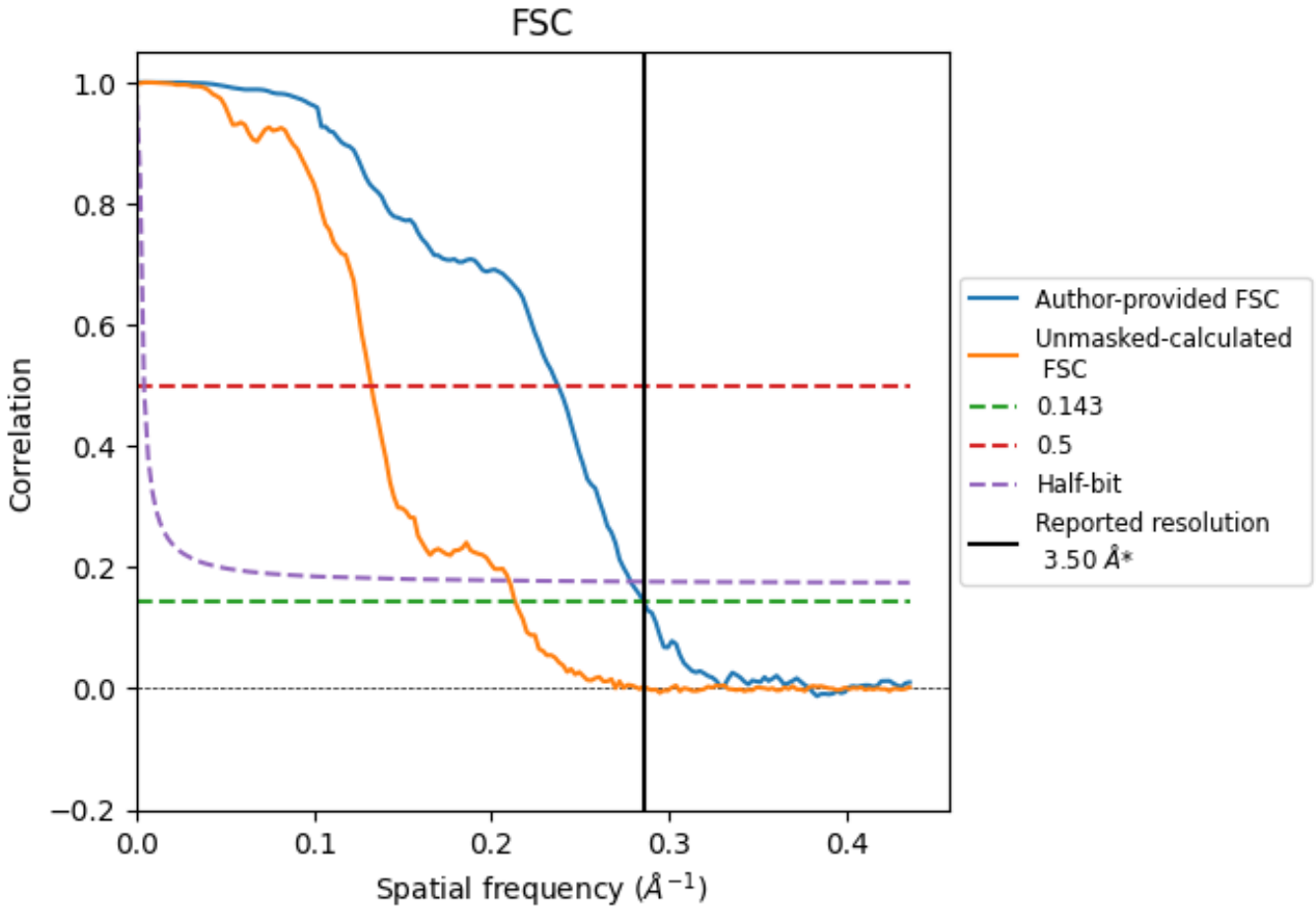


*Reported resolution corresponds to spatial frequency of 0.286 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.286 $Å^{-1}$

8.2 Resolution estimates (i)

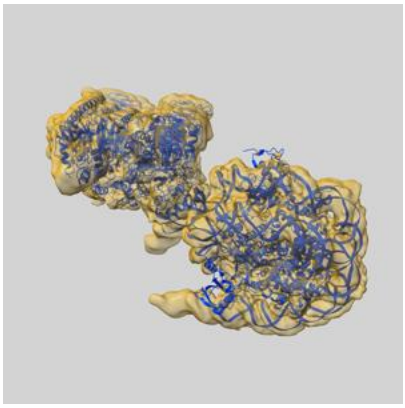
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.50	4.21	3.59
Unmasked-calculated*	4.69	7.56	4.77

*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 %

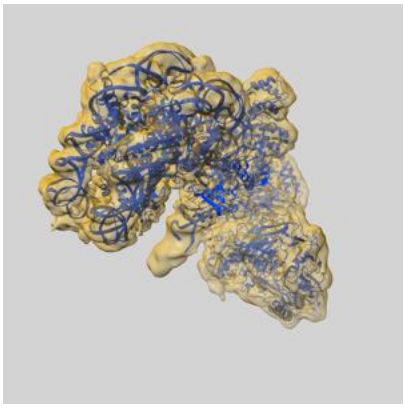
9 Map-model fit

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.

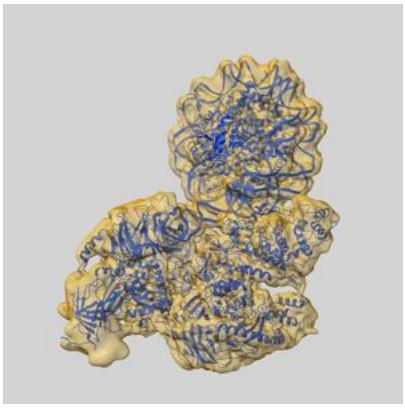
9.1 Map-model overlay



X



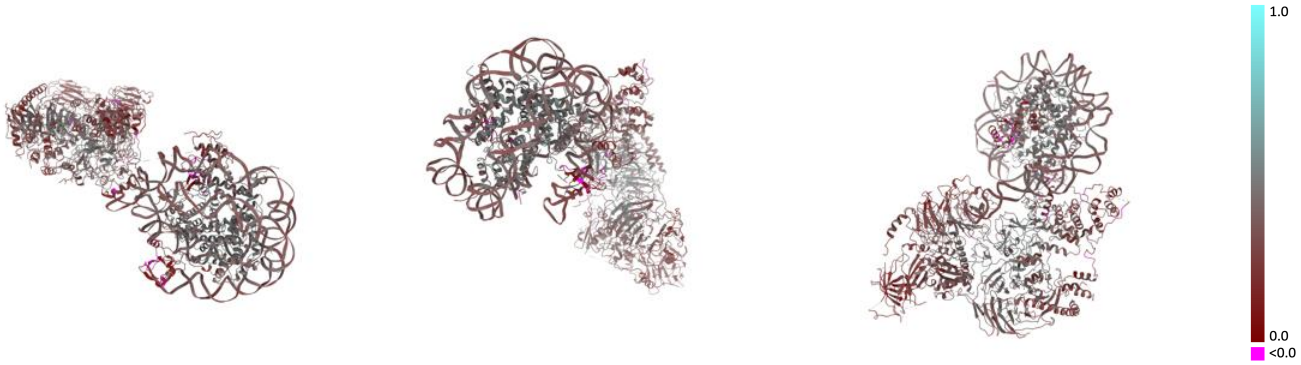
Y



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.

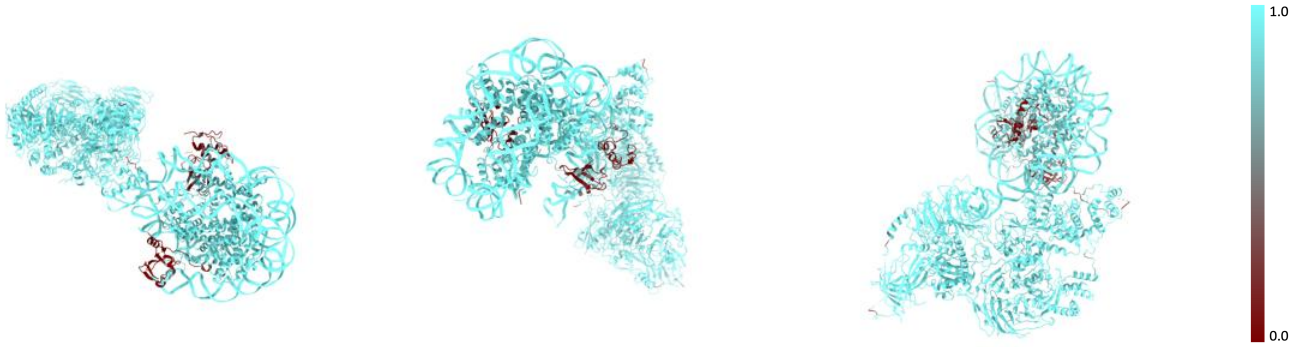
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

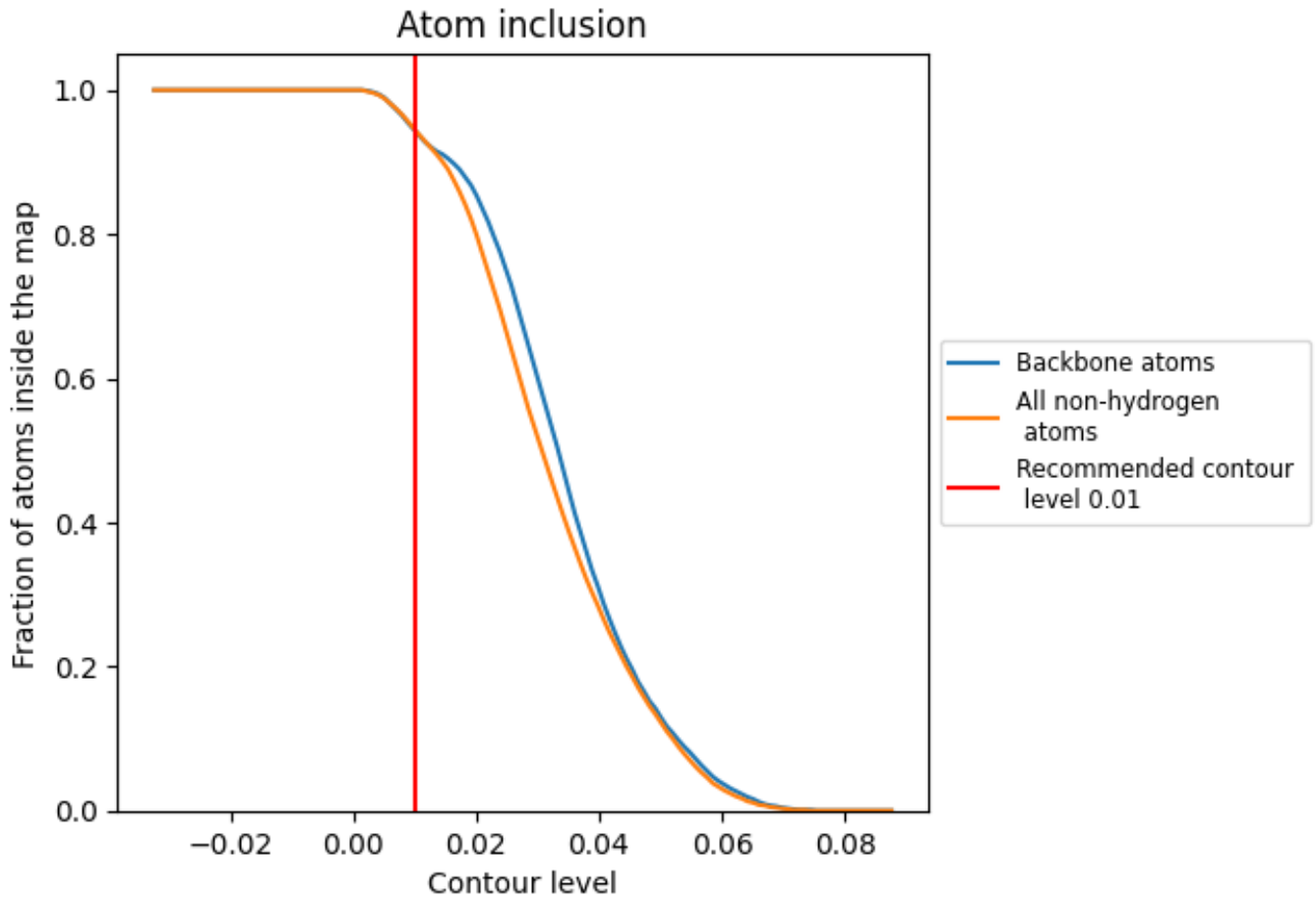
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.01).

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