



Full wwPDB EM Validation Report ⓘ

Sep 28, 2024 – 01:51 PM EDT

PDB ID : 8TB9
EMDB ID : EMD-41146
Title : PRC2-J119-450 monomer bound to H1-nucleosome
Authors : Sauer, P.V.; Cookis, T.; Pavlenko, E.; Nogales, E.; Poepsel, S.
Deposited on : 2023-06-28
Resolution : 4.00 Å (reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

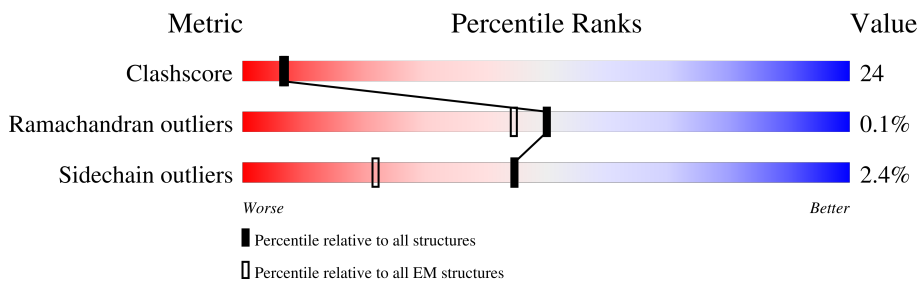
EMDB validation analysis : 0.0.1.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

1 Overall quality at a glance

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

The reported resolution of this entry is 4.00 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	197	
2	B	334	
3	D	619	
4	E	753	
5	G	441	
6	H	215	
7	I	136	
7	W	136	

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Mol	Chain	Length	Quality of chain
8	J	106	<p>6% 52% 25% 17%</p>
8	X	106	<p>8% 56% 26% 10%</p>
9	O	425	<p>12% 50% 41% 7%</p>
10	R	133	<p>1% 50% 31% 18%</p>
10	U	133	<p>1% 50% 31% 18%</p>
11	S	123	<p>1% 45% 33% 21%</p>
11	V	123	<p>1% 38% 39% 22%</p>
12	T	215	<p>7% 40% 46% 10%</p>
13	Y	303	<p>28% 24% 16% 32%</p>

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 30224 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Histone H1.0.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	74	568	354	107	106	1	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP P07305
A	-2	SER	-	expression tag	UNP P07305
A	-1	HIS	-	expression tag	UNP P07305

- Molecule 2 is a protein called Protein Jumonji.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	29	196	121	36	38	1	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	117	MET	-	initiating methionine	UNP Q92833
B	118	VAL	-	expression tag	UNP Q92833

- Molecule 3 is a protein called Polycomb protein SUZ12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	443	3653	2321	656	649	27	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	67	MET	-	initiating methionine	UNP Q15022

- Molecule 4 is a protein called Histone-lysine N-methyltransferase EZH2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	570	4580	2871	821	846	42	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	SER	-	expression tag	UNP Q15910
E	0	ASN	-	expression tag	UNP Q15910
E	1	ALA	-	expression tag	UNP Q15910
E	14	ALA	CYS	conflict	UNP Q15910
E	15	CYS	TRP	conflict	UNP Q15910

- Molecule 5 is a protein called Polycomb protein EED.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	G	362	2930	1855	513	541	21	0	0

- Molecule 6 is a DNA chain called DNA (226-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
6	H	193	3972	1873	761	1145	193	0	0

- Molecule 7 is a protein called Histone H3.2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	I	114	917	576	179	159	3	0	0
7	W	99	817	515	158	141	3	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	102	ALA	GLY	conflict	UNP P84233
W	102	ALA	GLY	conflict	UNP P84233

- Molecule 8 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	83	Total	C	N	O	S	0	0
			661	418	129	113	1		
8	X	87	Total	C	N	O	S	0	0
			666	419	129	117	1		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	103	SER	-	expression tag	UNP P62799
J	104	SER	-	expression tag	UNP P62799
J	105	GLY	-	expression tag	UNP P62799
X	103	SER	-	expression tag	UNP P62799
X	104	SER	-	expression tag	UNP P62799
X	105	GLY	-	expression tag	UNP P62799

- Molecule 9 is a protein called Histone-binding protein RBBP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	O	395	Total	C	N	O	S	0	0
			3139	1981	535	613	10		

- Molecule 10 is a protein called Histone H2A type 1.

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

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	-3	SER	-	expression tag	UNP P06897
R	-2	ASN	-	expression tag	UNP P06897
R	-1	ALA	-	expression tag	UNP P06897
R	99	ARG	GLY	conflict	UNP P06897
R	119	CYS	LYS	conflict	UNP P06897
R	123	SER	ALA	conflict	UNP P06897
U	-3	SER	-	expression tag	UNP P06897
U	-2	ASN	-	expression tag	UNP P06897
U	-1	ALA	-	expression tag	UNP P06897
U	99	ARG	GLY	conflict	UNP P06897
U	119	CYS	LYS	conflict	UNP P06897

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Chain	Residue	Modelled	Actual	Comment	Reference
U	123	SER	ALA	conflict	UNP P06897

- Molecule 11 is a protein called Histone H2B 1.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	S	96	742	466	133	141	2	0	0
11	V	95	737	463	132	140	2	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	0	MET	-	initiating methionine	UNP P02281
S	29	THR	SER	conflict	UNP P02281
V	0	MET	-	initiating methionine	UNP P02281
V	29	THR	SER	conflict	UNP P02281

- Molecule 12 is a DNA chain called DNA (226-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
12	T	193	3919	1853	724	1149	193	0	0

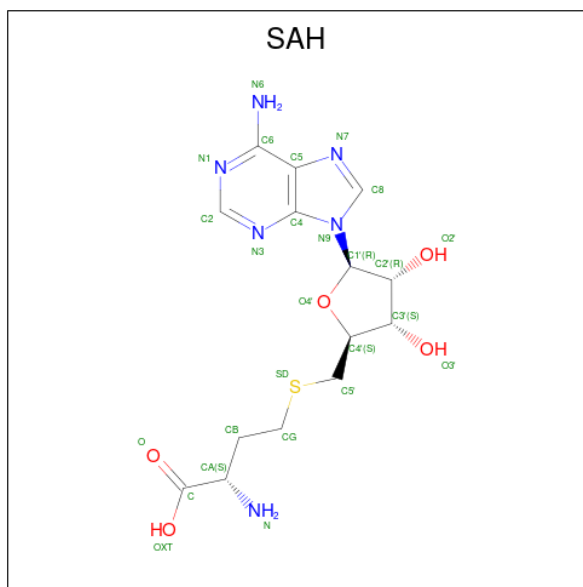
- Molecule 13 is a protein called Zinc finger protein AEBP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	Y	126	1047	664	206	174	3	0	0

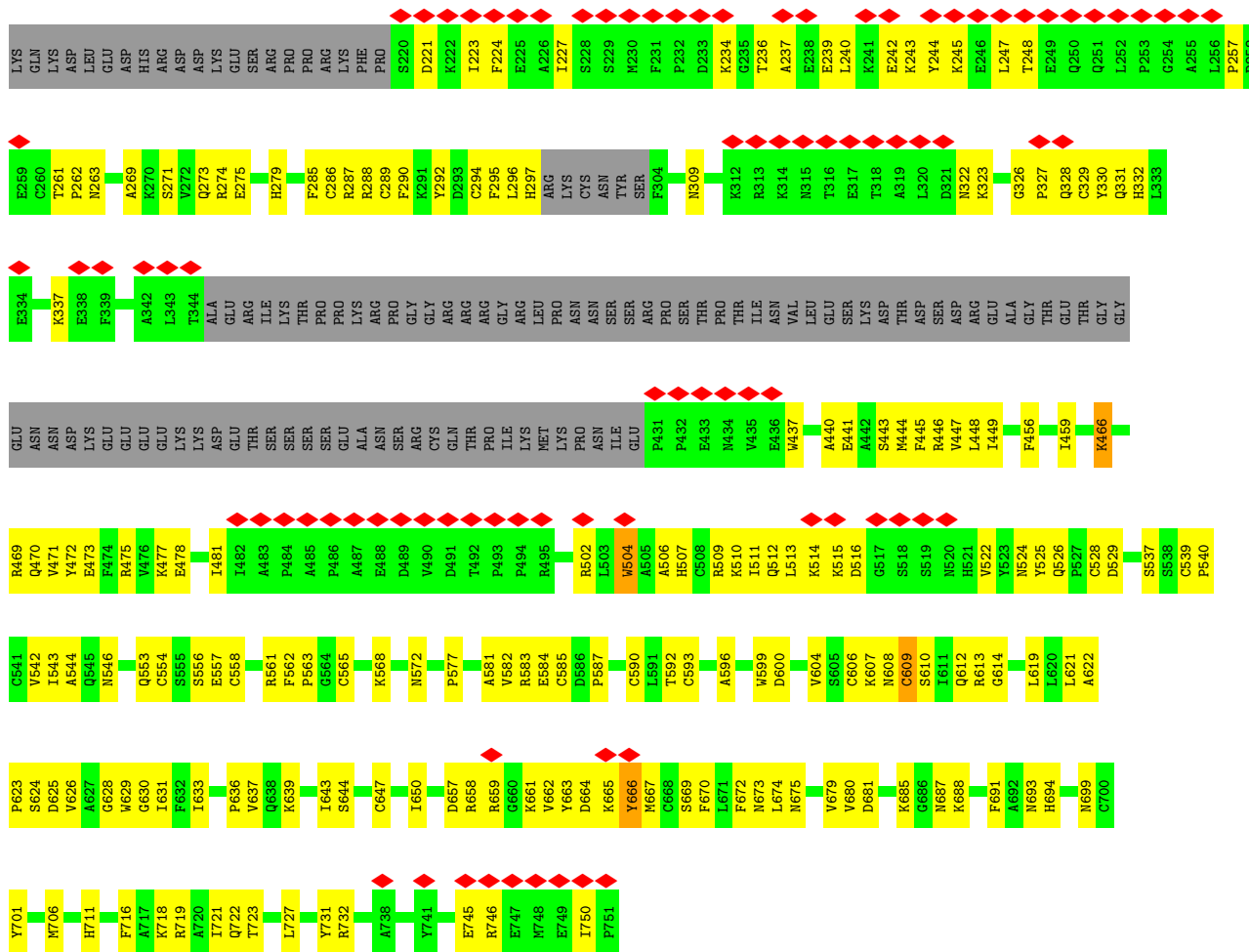
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	7	SER	-	expression tag	UNP Q6ZN18
Y	8	ASN	-	expression tag	UNP Q6ZN18
Y	9	ALA	-	expression tag	UNP Q6ZN18

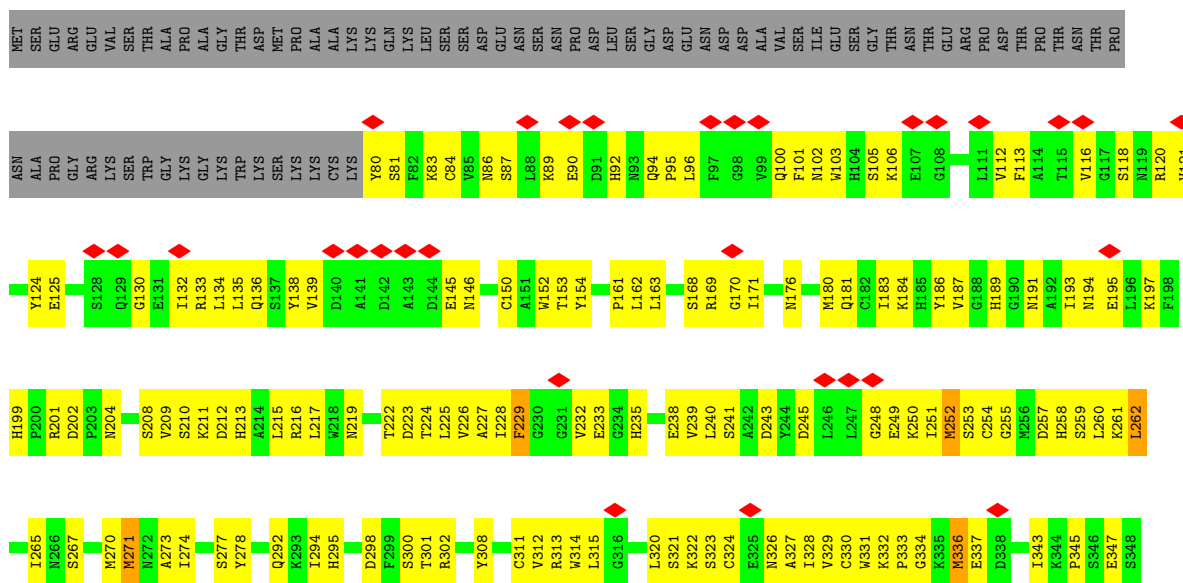
- Molecule 14 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: C₁₄H₂₀N₆O₅S) (labeled as "Ligand of Interest" by depositor).

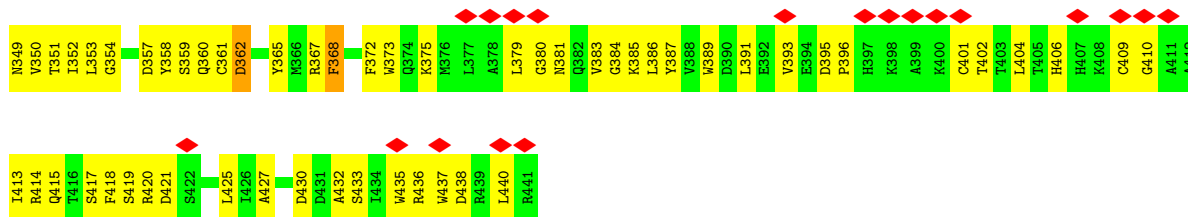


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
14	E	1	26	14	6	5	1	0

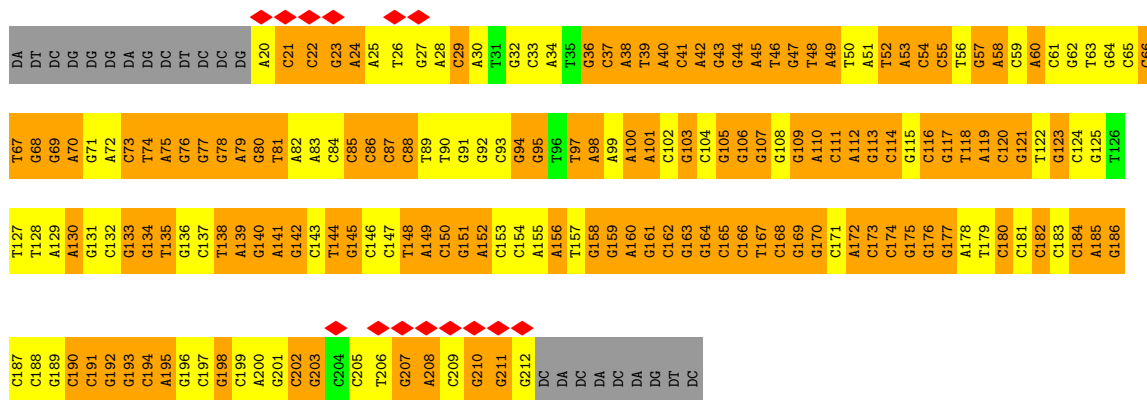


• Molecule 5: Polycomb protein EED

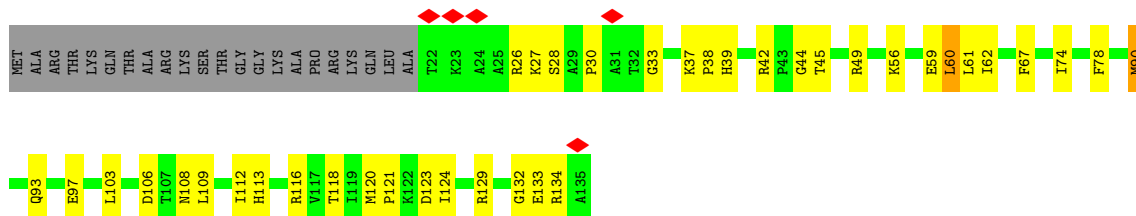




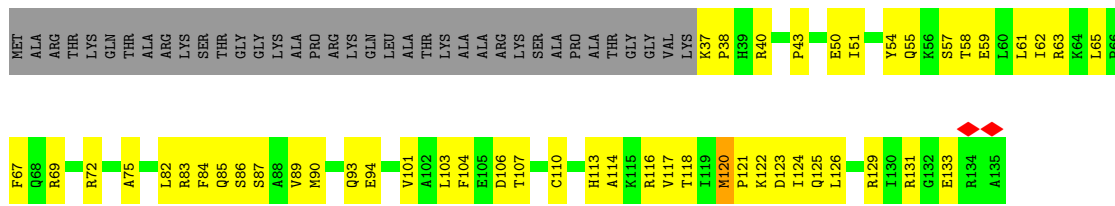
• Molecule 6: DNA (226-MER)



• Molecule 7: Histone H3.2

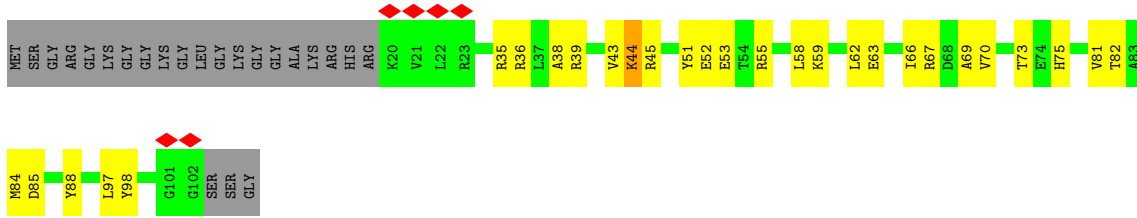


• Molecule 7: Histone H3.2

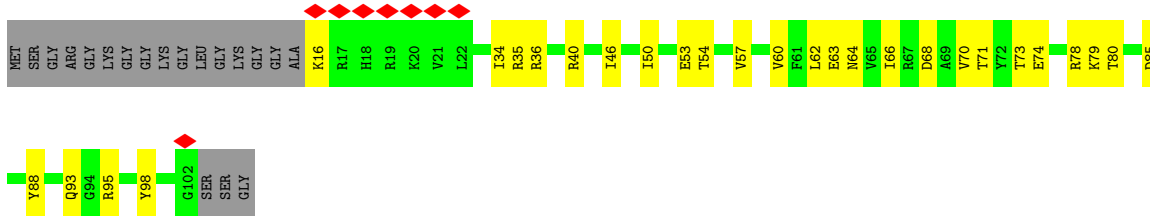


• Molecule 8: Histone H4

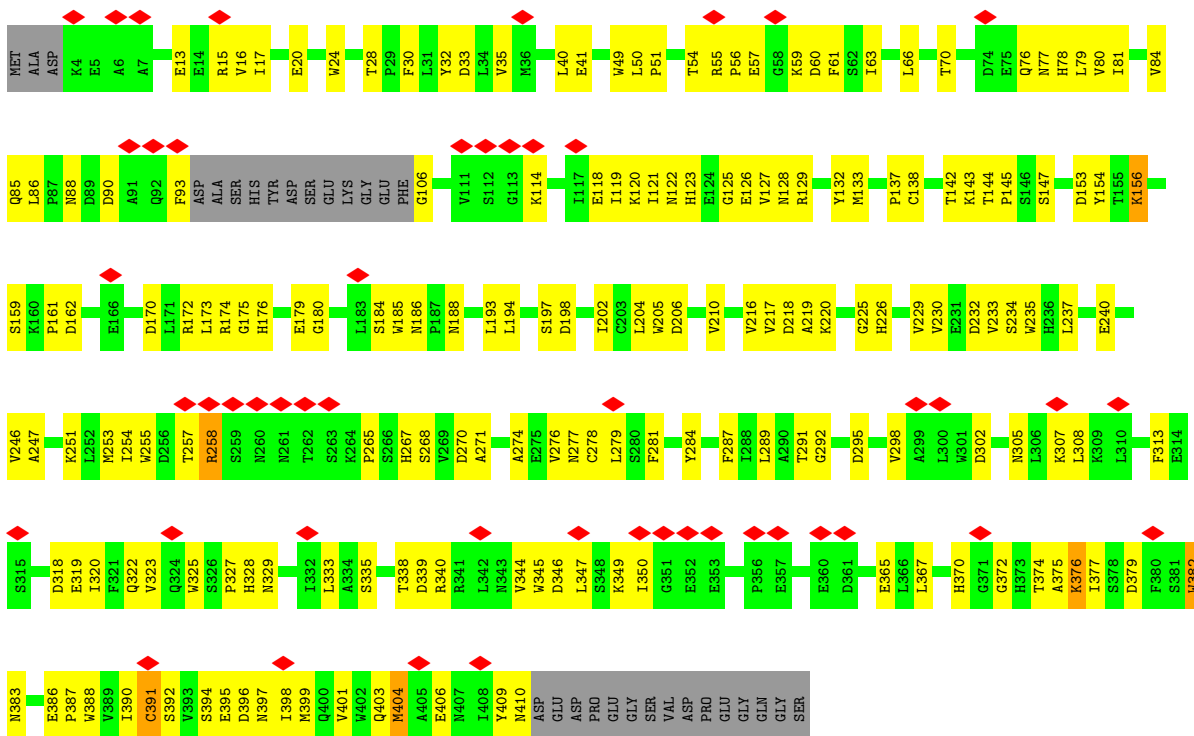




• Molecule 8: Histone H4



• Molecule 9: Histone-binding protein RBBP4

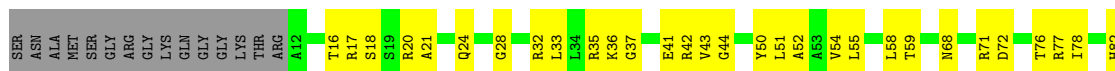


• Molecule 10: Histone H2A type 1

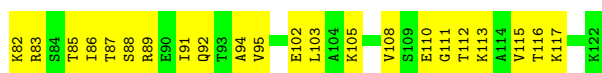
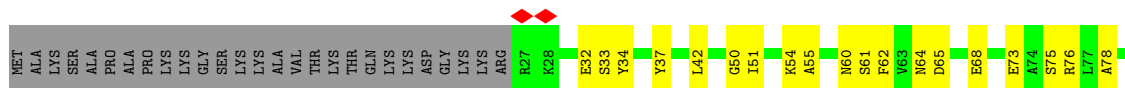




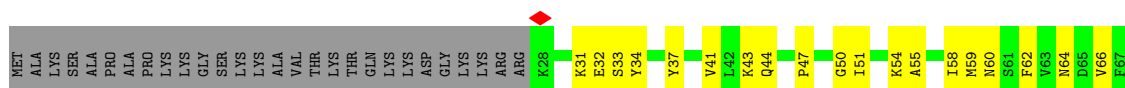
• Molecule 10: Histone H2A type 1



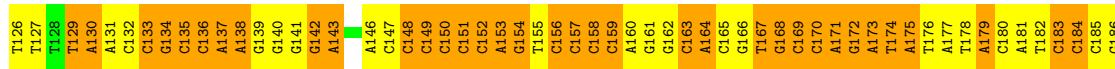
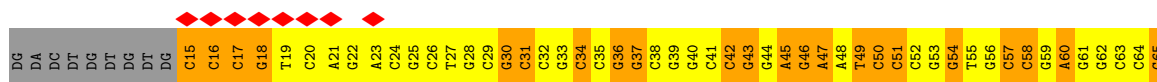
• Molecule 11: Histone H2B 1.1



• Molecule 11: Histone H2B 1.1

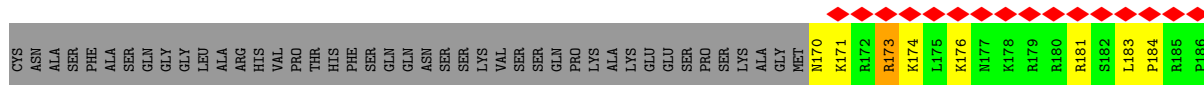
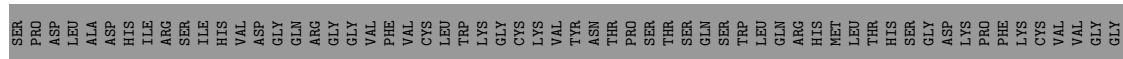
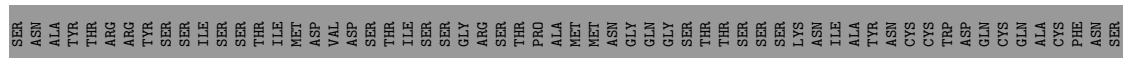


• Molecule 12: DNA (226-MER)





• Molecule 13: Zinc finger protein AEBP2



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	55918	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.735	Depositor
Minimum map value	-0.244	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.030	Depositor
Recommended contour level	0.18	Depositor
Map size (Å)	360.96, 360.96, 360.96	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.94, 0.94, 0.94	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	A	0.25	0/574	0.52	0/765
2	B	0.24	0/199	0.57	0/270
3	D	0.26	0/3733	0.50	0/5020
4	E	0.29	0/4682	0.52	0/6308
5	G	0.27	0/3005	0.51	0/4070
6	H	0.59	0/4463	1.57	283/6888 (4.1%)
7	I	0.30	0/930	0.60	1/1246 (0.1%)
7	W	0.30	0/829	0.57	0/1111
8	J	0.33	0/668	0.58	0/894
8	X	0.31	0/673	0.57	0/904
9	O	0.25	0/3225	0.48	0/4394
10	R	0.29	0/839	0.55	0/1132
10	U	0.28	0/835	0.55	0/1128
11	S	0.31	0/753	0.53	0/1014
11	V	0.32	0/748	0.52	0/1007
12	T	0.60	0/4391	1.58	268/6763 (4.0%)
13	Y	0.24	0/1070	0.58	0/1437
All	All	0.39	0/31617	0.98	552/44351 (1.2%)

There are no bond length outliers.

All (552) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	T	67	DC	OP1-P-O3'	10.12	127.46	105.20
12	T	109	DA	OP1-P-O3'	9.85	126.87	105.20
6	H	59	DC	OP1-P-O3'	9.58	126.28	105.20
12	T	104	DC	OP1-P-O3'	9.56	126.23	105.20
12	T	82	DC	OP1-P-O3'	9.52	126.15	105.20
12	T	150	DC	OP1-P-O3'	9.44	125.96	105.20
6	H	92	DG	OP1-P-O3'	9.10	125.22	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	T	93	DC	OP1-P-O3'	9.09	125.19	105.20
12	T	68	DC	OP1-P-OP2	-9.08	105.98	119.60
12	T	117	DT	OP1-P-O3'	9.08	125.17	105.20
12	T	110	DC	OP1-P-OP2	-9.01	106.08	119.60
12	T	58	DC	OP1-P-O3'	8.98	124.95	105.20
6	H	174	DC	OP1-P-O3'	8.97	124.92	105.20
12	T	151	DC	OP1-P-OP2	-8.89	106.26	119.60
12	T	46	DG	OP1-P-O3'	8.85	124.68	105.20
12	T	98	DT	OP1-P-O3'	8.71	124.37	105.20
12	T	83	DA	OP1-P-OP2	-8.70	106.55	119.60
12	T	61	DG	OP1-P-O3'	8.70	124.34	105.20
12	T	47	DA	OP1-P-OP2	-8.66	106.60	119.60
6	H	60	DA	OP1-P-OP2	-8.55	106.77	119.60
12	T	59	DG	OP1-P-OP2	-8.54	106.78	119.60
12	T	105	DA	OP1-P-OP2	-8.54	106.80	119.60
12	T	94	DC	OP1-P-OP2	-8.41	106.98	119.60
12	T	99	DA	OP1-P-OP2	-8.34	107.09	119.60
6	H	93	DC	OP1-P-OP2	-8.26	107.21	119.60
12	T	62	DG	OP1-P-OP2	-8.25	107.23	119.60
6	H	175	DG	OP1-P-OP2	-8.13	107.40	119.60
6	H	104	DC	OP1-P-O3'	8.12	123.07	105.20
6	H	87	DC	OP1-P-O3'	8.12	123.05	105.20
6	H	50	DT	OP1-P-O3'	8.06	122.93	105.20
12	T	80	DG	OP1-P-OP2	-8.01	107.59	119.60
12	T	81	DA	OP1-P-OP2	-8.00	107.59	119.60
6	H	51	DA	OP1-P-OP2	-7.93	107.71	119.60
12	T	80	DG	OP1-P-O3'	7.92	122.63	105.20
12	T	118	DC	OP1-P-OP2	-7.89	107.76	119.60
6	H	76	DG	OP1-P-O3'	7.82	122.41	105.20
6	H	88	DC	OP1-P-OP2	-7.79	107.91	119.60
12	T	79	DA	OP1-P-O3'	7.74	122.24	105.20
6	H	118	DT	OP1-P-O3'	7.70	122.13	105.20
6	H	77	DG	OP1-P-OP2	-7.68	108.07	119.60
12	T	111	DG	OP1-P-OP2	-7.57	108.25	119.60
6	H	119	DA	OP1-P-OP2	-7.54	108.29	119.60
6	H	105	DG	OP1-P-OP2	-7.51	108.34	119.60
6	H	58	DA	OP1-P-O3'	7.40	121.47	105.20
12	T	170	DC	OP1-P-OP2	-7.37	108.54	119.60
12	T	77	DG	OP1-P-OP2	-7.32	108.62	119.60
6	H	48	DT	OP1-P-OP2	-7.30	108.66	119.60
6	H	61	DC	OP1-P-OP2	-7.27	108.69	119.60
12	T	134	DG	OP1-P-OP2	-7.26	108.72	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	T	123	DG	OP1-P-OP2	-7.24	108.74	119.60
12	T	45	DA	OP1-P-OP2	-7.22	108.77	119.60
12	T	141	DG	OP1-P-O3'	7.22	121.08	105.20
12	T	60	DA	OP1-P-OP2	-7.20	108.80	119.60
6	H	68	DG	OP1-P-OP2	-7.19	108.82	119.60
12	T	133	DC	OP1-P-O3'	7.19	121.01	105.20
6	H	59	DC	OP1-P-OP2	-7.18	108.83	119.60
12	T	196	DA	OP1-P-OP2	-7.17	108.85	119.60
6	H	110	DA	OP1-P-OP2	-7.16	108.87	119.60
12	T	119	DC	OP1-P-OP2	-7.16	108.87	119.60
12	T	43	DG	OP1-P-OP2	-7.15	108.88	119.60
6	H	150	DC	OP1-P-OP2	-7.14	108.88	119.60
6	H	87	DC	OP1-P-OP2	-7.14	108.90	119.60
12	T	163	DC	OP1-P-OP2	-7.13	108.91	119.60
6	H	139	DA	OP1-P-OP2	-7.12	108.91	119.60
6	H	171	DC	OP1-P-OP2	-7.12	108.93	119.60
6	H	91	DG	OP1-P-OP2	-7.10	108.95	119.60
12	T	150	DC	OP1-P-OP2	-7.09	108.96	119.60
12	T	38	DC	OP1-P-OP2	-7.09	108.97	119.60
12	T	40	DG	OP1-P-OP2	-7.08	108.97	119.60
12	T	110	DC	OP1-P-O3'	7.08	120.78	105.20
12	T	76	DC	OP1-P-OP2	-7.08	108.98	119.60
6	H	67	DT	OP1-P-O3'	7.05	120.72	105.20
12	T	162	DG	OP1-P-OP2	-7.05	109.03	119.60
6	H	80	DG	OP1-P-OP2	-7.05	109.03	119.60
12	T	116	DG	OP1-P-OP2	-7.04	109.03	119.60
12	T	137	DA	OP1-P-OP2	-7.04	109.04	119.60
6	H	198	DG	OP1-P-OP2	-7.04	109.05	119.60
6	H	132	DC	OP1-P-OP2	-7.03	109.05	119.60
12	T	172	DG	OP1-P-OP2	-7.02	109.08	119.60
6	H	190	DC	OP1-P-OP2	-7.01	109.08	119.60
6	H	108	DG	OP1-P-OP2	-7.01	109.09	119.60
6	H	22	DC	OP1-P-OP2	-7.00	109.10	119.60
6	H	172	DA	OP1-P-OP2	-6.98	109.12	119.60
12	T	191	DC	OP1-P-OP2	-6.98	109.13	119.60
6	H	37	DC	OP1-P-OP2	-6.97	109.14	119.60
6	H	50	DT	OP1-P-OP2	-6.97	109.14	119.60
12	T	29	DC	OP1-P-OP2	-6.97	109.14	119.60
12	T	161	DG	OP1-P-OP2	-6.97	109.15	119.60
12	T	205	DG	OP1-P-OP2	-6.97	109.15	119.60
12	T	138	DA	OP1-P-OP2	-6.96	109.16	119.60
12	T	173	DA	OP1-P-OP2	-6.96	109.17	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	53	DA	OP1-P-OP2	-6.95	109.17	119.60
6	H	42	DA	OP1-P-OP2	-6.95	109.18	119.60
12	T	149	DC	OP1-P-O3'	6.95	120.48	105.20
12	T	95	DG	OP1-P-OP2	-6.94	109.19	119.60
12	T	41	DC	OP1-P-OP2	-6.94	109.19	119.60
6	H	162	DC	OP1-P-OP2	-6.94	109.19	119.60
12	T	136	DC	OP1-P-OP2	-6.94	109.19	119.60
12	T	33	DG	OP1-P-OP2	-6.93	109.20	119.60
12	T	30	DG	OP1-P-OP2	-6.93	109.21	119.60
6	H	73	DC	OP1-P-OP2	-6.92	109.22	119.60
12	T	63	DC	OP1-P-OP2	-6.90	109.24	119.60
6	H	130	DA	OP1-P-OP2	-6.90	109.25	119.60
6	H	207	DG	OP1-P-OP2	-6.90	109.25	119.60
6	H	145	DG	OP1-P-OP2	-6.90	109.25	119.60
12	T	42	DC	OP1-P-OP2	-6.90	109.25	119.60
12	T	142	DG	OP1-P-OP2	-6.90	109.26	119.60
6	H	86	DC	OP1-P-OP2	-6.89	109.26	119.60
12	T	164	DA	OP1-P-OP2	-6.89	109.26	119.60
6	H	33	DC	OP1-P-OP2	-6.89	109.26	119.60
6	H	44	DG	OP1-P-OP2	-6.89	109.27	119.60
6	H	28	DA	OP1-P-OP2	-6.89	109.27	119.60
6	H	143	DC	OP1-P-OP2	-6.88	109.27	119.60
6	H	153	DC	OP1-P-OP2	-6.88	109.28	119.60
6	H	199	DC	OP1-P-OP2	-6.88	109.28	119.60
12	T	190	DG	OP1-P-OP2	-6.88	109.28	119.60
6	H	196	DG	OP1-P-OP2	-6.88	109.28	119.60
12	T	104	DC	OP1-P-OP2	-6.88	109.28	119.60
6	H	161	DG	OP1-P-OP2	-6.88	109.28	119.60
6	H	211	DG	OP1-P-OP2	-6.88	109.28	119.60
12	T	34	DC	OP1-P-OP2	-6.88	109.28	119.60
12	T	160	DA	OP1-P-O3'	6.88	120.32	105.20
12	T	17	DC	OP1-P-OP2	-6.87	109.30	119.60
6	H	41	DC	OP1-P-OP2	-6.87	109.30	119.60
12	T	75	DT	OP1-P-O3'	6.87	120.31	105.20
12	T	121	DC	OP1-P-OP2	-6.87	109.30	119.60
6	H	170	DG	OP1-P-OP2	-6.86	109.31	119.60
6	H	23	DG	OP1-P-OP2	-6.86	109.31	119.60
12	T	44	DG	OP1-P-O3'	6.86	120.29	105.20
6	H	49	DA	OP1-P-OP2	-6.86	109.31	119.60
6	H	92	DG	OP1-P-OP2	-6.86	109.32	119.60
12	T	19	DT	OP1-P-OP2	-6.86	109.32	119.60
12	T	22	DG	OP1-P-OP2	-6.84	109.34	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	34	DA	OP1-P-OP2	-6.83	109.35	119.60
12	T	31	DC	OP1-P-OP2	-6.83	109.35	119.60
6	H	173	DC	OP1-P-OP2	-6.83	109.35	119.60
6	H	178	DA	OP1-P-OP2	-6.83	109.36	119.60
6	H	131	DG	OP1-P-OP2	-6.83	109.36	119.60
12	T	39	DG	OP1-P-OP2	-6.82	109.37	119.60
12	T	25	DG	OP1-P-OP2	-6.82	109.37	119.60
12	T	26	DC	OP1-P-OP2	-6.82	109.37	119.60
12	T	125	DG	OP1-P-OP2	-6.81	109.39	119.60
6	H	29	DC	OP1-P-OP2	-6.81	109.39	119.60
6	H	155	DA	OP1-P-OP2	-6.81	109.39	119.60
6	H	159	DG	OP1-P-OP2	-6.81	109.39	119.60
6	H	197	DC	OP1-P-OP2	-6.81	109.39	119.60
6	H	202	DC	OP1-P-OP2	-6.81	109.39	119.60
12	T	201	DA	OP1-P-OP2	-6.81	109.39	119.60
12	T	171	DA	OP1-P-OP2	-6.80	109.40	119.60
6	H	154	DC	OP1-P-OP2	-6.80	109.40	119.60
12	T	64	DC	OP1-P-OP2	-6.80	109.40	119.60
12	T	93	DC	OP1-P-OP2	-6.80	109.40	119.60
6	H	83	DA	OP1-P-OP2	-6.80	109.40	119.60
6	H	151	DG	OP1-P-OP2	-6.80	109.40	119.60
12	T	21	DA	OP1-P-OP2	-6.79	109.42	119.60
6	H	187	DC	OP1-P-OP2	-6.79	109.42	119.60
12	T	32	DC	OP1-P-OP2	-6.79	109.42	119.60
12	T	101	DA	OP1-P-OP2	-6.78	109.43	119.60
12	T	109	DA	OP1-P-OP2	-6.78	109.43	119.60
6	H	181	DC	OP1-P-OP2	-6.78	109.43	119.60
12	T	24	DC	OP1-P-OP2	-6.78	109.43	119.60
12	T	91	DC	OP1-P-OP2	-6.78	109.43	119.60
12	T	54	DG	OP1-P-OP2	-6.78	109.43	119.60
6	H	101	DA	OP1-P-OP2	-6.78	109.44	119.60
12	T	37	DG	OP1-P-OP2	-6.78	109.44	119.60
12	T	179	DA	OP1-P-OP2	-6.78	109.44	119.60
6	H	24	DA	OP1-P-OP2	-6.77	109.44	119.60
12	T	36	DG	OP1-P-OP2	-6.77	109.44	119.60
12	T	168	DG	OP1-P-OP2	-6.77	109.44	119.60
6	H	212	DG	OP1-P-OP2	-6.77	109.45	119.60
12	T	23	DA	OP1-P-OP2	-6.77	109.45	119.60
6	H	20	DA	OP1-P-OP2	-6.76	109.45	119.60
6	H	120	DC	OP1-P-OP2	-6.76	109.46	119.60
6	H	191	DC	OP1-P-OP2	-6.76	109.46	119.60
6	H	194	DC	OP1-P-OP2	-6.76	109.46	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	T	165	DC	OP1-P-OP2	-6.76	109.46	119.60
6	H	210	DG	OP1-P-OP2	-6.76	109.47	119.60
12	T	122	DC	OP1-P-OP2	-6.76	109.47	119.60
12	T	166	DG	OP1-P-OP2	-6.75	109.47	119.60
6	H	109	DG	OP1-P-OP2	-6.75	109.47	119.60
6	H	174	DC	OP1-P-OP2	-6.75	109.47	119.60
12	T	149	DC	OP1-P-OP2	-6.75	109.47	119.60
12	T	184	DC	OP1-P-OP2	-6.75	109.48	119.60
12	T	194	DG	OP1-P-OP2	-6.75	109.47	119.60
12	T	65	DG	OP1-P-OP2	-6.74	109.49	119.60
6	H	125	DG	OP1-P-OP2	-6.74	109.49	119.60
12	T	158	DC	OP1-P-OP2	-6.74	109.49	119.60
6	H	134	DG	OP1-P-OP2	-6.74	109.49	119.60
12	T	195	DC	OP1-P-OP2	-6.74	109.50	119.60
12	T	35	DC	OP1-P-OP2	-6.73	109.50	119.60
6	H	27	DG	OP1-P-OP2	-6.73	109.50	119.60
12	T	57	DC	OP1-P-OP2	-6.73	109.50	119.60
6	H	138	DT	OP1-P-O3'	6.72	119.99	105.20
6	H	208	DA	OP1-P-OP2	-6.72	109.52	119.60
12	T	154	DG	OP1-P-OP2	-6.72	109.52	119.60
12	T	118	DC	OP1-P-O3'	6.72	119.97	105.20
12	T	180	DC	OP1-P-OP2	-6.71	109.53	119.60
12	T	53	DG	OP1-P-OP2	-6.71	109.53	119.60
12	T	59	DG	OP1-P-O3'	6.71	119.96	105.20
12	T	156	DC	OP1-P-OP2	-6.71	109.54	119.60
6	H	209	DC	OP1-P-OP2	-6.71	109.54	119.60
12	T	198	DA	OP1-P-OP2	-6.71	109.54	119.60
6	H	46	DT	OP1-P-OP2	-6.70	109.55	119.60
6	H	69	DG	OP1-P-OP2	-6.70	109.55	119.60
6	H	107	DG	OP1-P-O3'	6.70	119.94	105.20
6	H	21	DC	OP1-P-OP2	-6.70	109.55	119.60
6	H	200	DA	OP1-P-OP2	-6.70	109.55	119.60
6	H	201	DG	OP1-P-OP2	-6.70	109.55	119.60
12	T	15	DC	OP1-P-OP2	-6.70	109.56	119.60
6	H	26	DT	OP1-P-OP2	-6.69	109.56	119.60
6	H	165	DC	OP1-P-OP2	-6.69	109.56	119.60
12	T	74	DG	OP1-P-OP2	-6.69	109.56	119.60
12	T	132	DC	OP1-P-OP2	-6.69	109.56	119.60
6	H	38	DA	OP1-P-OP2	-6.69	109.57	119.60
12	T	20	DC	OP1-P-OP2	-6.69	109.57	119.60
6	H	25	DA	OP1-P-OP2	-6.68	109.57	119.60
6	H	205	DC	OP1-P-OP2	-6.68	109.57	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	T	16	DC	OP1-P-OP2	-6.68	109.58	119.60
12	T	27	DT	OP1-P-OP2	-6.68	109.57	119.60
12	T	61	DG	OP1-P-OP2	-6.68	109.57	119.60
12	T	188	DA	OP1-P-OP2	-6.68	109.57	119.60
6	H	183	DC	OP1-P-OP2	-6.68	109.58	119.60
12	T	135	DC	OP1-P-OP2	-6.68	109.58	119.60
6	H	32	DG	OP1-P-OP2	-6.67	109.59	119.60
6	H	36	DG	OP1-P-OP2	-6.67	109.59	119.60
6	H	75	DA	OP1-P-OP2	-6.67	109.59	119.60
6	H	115	DG	OP1-P-OP2	-6.67	109.59	119.60
6	H	40	DA	OP1-P-OP2	-6.66	109.60	119.60
6	H	99	DA	OP1-P-OP2	-6.66	109.61	119.60
12	T	92	DA	OP1-P-OP2	-6.66	109.61	119.60
6	H	30	DA	OP1-P-OP2	-6.66	109.61	119.60
12	T	40	DG	OP1-P-O3'	6.66	119.86	105.20
12	T	52	DC	OP1-P-OP2	-6.66	109.61	119.60
6	H	62	DG	OP1-P-OP2	-6.66	109.61	119.60
6	H	160	DA	OP1-P-OP2	-6.66	109.61	119.60
12	T	120	DC	OP1-P-OP2	-6.66	109.61	119.60
6	H	47	DG	OP1-P-OP2	-6.66	109.62	119.60
6	H	156	DA	OP1-P-OP2	-6.66	109.62	119.60
12	T	50	DC	OP1-P-OP2	-6.66	109.62	119.60
12	T	206	DA	OP1-P-OP2	-6.65	109.62	119.60
12	T	159	DC	OP1-P-OP2	-6.65	109.62	119.60
6	H	86	DC	OP1-P-O3'	6.65	119.83	105.20
12	T	58	DC	OP1-P-OP2	-6.65	109.62	119.60
6	H	79	DA	OP1-P-OP2	-6.65	109.63	119.60
6	H	195	DA	OP1-P-OP2	-6.65	109.63	119.60
6	H	70	DA	OP1-P-OP2	-6.64	109.63	119.60
6	H	193	DG	OP1-P-OP2	-6.64	109.64	119.60
12	T	96	DC	OP1-P-OP2	-6.64	109.64	119.60
12	T	84	DG	OP1-P-OP2	-6.64	109.64	119.60
6	H	43	DG	OP1-P-OP2	-6.64	109.65	119.60
6	H	111	DC	OP1-P-OP2	-6.64	109.64	119.60
12	T	186	DG	OP1-P-OP2	-6.64	109.64	119.60
6	H	133	DG	OP1-P-OP2	-6.63	109.65	119.60
6	H	124	DC	OP1-P-OP2	-6.63	109.65	119.60
6	H	166	DC	OP1-P-OP2	-6.63	109.65	119.60
12	T	51	DC	OP1-P-OP2	-6.63	109.66	119.60
6	H	137	DC	OP1-P-OP2	-6.62	109.66	119.60
12	T	200	DC	OP1-P-OP2	-6.61	109.68	119.60
6	H	176	DG	OP1-P-OP2	-6.61	109.68	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	102	DC	OP1-P-OP2	-6.61	109.69	119.60
12	T	103	DG	OP1-P-OP2	-6.61	109.69	119.60
6	H	55	DC	OP1-P-OP2	-6.60	109.69	119.60
12	T	46	DG	OP1-P-OP2	-6.60	109.70	119.60
12	T	130	DA	OP1-P-OP2	-6.60	109.70	119.60
12	T	113	DG	OP1-P-OP2	-6.60	109.70	119.60
12	T	82	DC	OP1-P-OP2	-6.60	109.70	119.60
6	H	147	DC	OP1-P-OP2	-6.60	109.71	119.60
6	H	188	DC	OP1-P-OP2	-6.59	109.71	119.60
12	T	106	DC	OP1-P-OP2	-6.59	109.72	119.60
6	H	65	DC	OP1-P-OP2	-6.59	109.72	119.60
6	H	94	DG	OP1-P-OP2	-6.59	109.72	119.60
6	H	104	DC	OP1-P-OP2	-6.59	109.72	119.60
6	H	163	DG	OP1-P-OP2	-6.58	109.72	119.60
12	T	177	DA	OP1-P-OP2	-6.58	109.73	119.60
6	H	142	DG	OP1-P-O3'	6.58	119.67	105.20
12	T	146	DA	OP1-P-OP2	-6.58	109.73	119.60
12	T	141	DG	OP1-P-OP2	-6.58	109.74	119.60
6	H	106	DG	OP1-P-OP2	-6.57	109.74	119.60
6	H	141	DA	OP1-P-OP2	-6.57	109.74	119.60
12	T	112	DC	OP1-P-OP2	-6.57	109.74	119.60
12	T	147	DC	OP1-P-OP2	-6.57	109.74	119.60
6	H	158	DG	OP1-P-O3'	6.57	119.65	105.20
12	T	204	DC	OP1-P-OP2	-6.57	109.75	119.60
6	H	168	DC	OP1-P-OP2	-6.57	109.75	119.60
6	H	117	DG	OP1-P-OP2	-6.56	109.76	119.60
12	T	160	DA	OP1-P-OP2	-6.56	109.75	119.60
12	T	100	DA	OP1-P-OP2	-6.56	109.76	119.60
6	H	203	DG	OP1-P-OP2	-6.56	109.77	119.60
6	H	136	DG	OP1-P-OP2	-6.55	109.77	119.60
12	T	39	DG	OP1-P-O3'	6.55	119.62	105.20
6	H	152	DA	OP1-P-OP2	-6.55	109.77	119.60
12	T	28	DG	OP1-P-OP2	-6.55	109.77	119.60
12	T	48	DA	OP1-P-OP2	-6.55	109.77	119.60
6	H	114	DC	OP1-P-OP2	-6.54	109.79	119.60
12	T	18	DG	OP1-P-OP2	-6.54	109.78	119.60
6	H	82	DA	OP1-P-OP2	-6.54	109.79	119.60
12	T	114	DC	OP1-P-OP2	-6.54	109.80	119.60
6	H	186	DG	OP1-P-OP2	-6.53	109.80	119.60
6	H	72	DA	OP1-P-OP2	-6.53	109.81	119.60
6	H	113	DG	OP1-P-OP2	-6.53	109.80	119.60
12	T	133	DC	OP1-P-OP2	-6.53	109.80	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	64	DG	OP1-P-OP2	-6.53	109.81	119.60
6	H	153	DC	OP1-P-O3'	6.53	119.56	105.20
6	H	184	DC	OP1-P-OP2	-6.53	109.81	119.60
12	T	87	DC	OP1-P-OP2	-6.53	109.81	119.60
12	T	66	DC	OP1-P-OP2	-6.53	109.81	119.60
12	T	107	DG	OP1-P-OP2	-6.53	109.81	119.60
6	H	189	DG	OP1-P-OP2	-6.52	109.83	119.60
12	T	85	DC	OP1-P-OP2	-6.50	109.85	119.60
6	H	140	DG	OP1-P-O3'	6.50	119.50	105.20
6	H	76	DG	OP1-P-OP2	-6.50	109.86	119.60
12	T	140	DG	OP1-P-OP2	-6.49	109.86	119.60
12	T	124	DC	OP1-P-OP2	-6.49	109.86	119.60
12	T	190	DG	OP1-P-O3'	6.49	119.48	105.20
6	H	60	DA	OP1-P-O3'	6.49	119.47	105.20
12	T	73	DG	OP1-P-OP2	-6.49	109.87	119.60
6	H	177	DG	OP1-P-OP2	-6.47	109.89	119.60
12	T	181	DA	OP1-P-OP2	-6.47	109.89	119.60
6	H	66	DC	OP1-P-OP2	-6.47	109.89	119.60
6	H	100	DA	OP1-P-OP2	-6.47	109.89	119.60
6	H	103	DG	OP1-P-OP2	-6.47	109.89	119.60
6	H	149	DA	OP1-P-O3'	6.47	119.44	105.20
12	T	175	DA	OP1-P-OP2	-6.47	109.89	119.60
6	H	192	DG	OP1-P-OP2	-6.46	109.90	119.60
12	T	44	DG	OP1-P-OP2	-6.46	109.91	119.60
6	H	43	DG	OP1-P-O3'	6.46	119.40	105.20
6	H	85	DC	OP1-P-OP2	-6.45	109.93	119.60
12	T	131	DA	OP1-P-OP2	-6.45	109.93	119.60
12	T	56	DG	OP1-P-OP2	-6.44	109.93	119.60
6	H	71	DG	OP1-P-OP2	-6.44	109.94	119.60
12	T	37	DG	OP1-P-O3'	6.44	119.37	105.20
12	T	79	DA	OP1-P-OP2	-6.43	109.95	119.60
12	T	70	DA	OP1-P-OP2	-6.42	109.97	119.60
12	T	103	DG	OP1-P-O3'	6.41	119.30	105.20
6	H	152	DA	OP1-P-O3'	6.41	119.29	105.20
12	T	139	DG	OP1-P-OP2	-6.40	110.00	119.60
6	H	149	DA	OP1-P-OP2	-6.40	110.00	119.60
12	T	38	DC	OP1-P-O3'	6.40	119.28	105.20
6	H	169	DG	OP1-P-OP2	-6.39	110.01	119.60
6	H	116	DC	OP1-P-OP2	-6.39	110.02	119.60
6	H	100	DA	OP1-P-O3'	6.38	119.23	105.20
12	T	90	DG	OP1-P-OP2	-6.37	110.04	119.60
12	T	31	DC	OP1-P-O3'	6.37	119.21	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	T	153	DA	OP1-P-OP2	-6.37	110.05	119.60
6	H	190	DC	OP1-P-O3'	6.37	119.21	105.20
12	T	192	DA	OP1-P-OP2	-6.37	110.05	119.60
12	T	92	DA	OP1-P-O3'	6.36	119.19	105.20
6	H	45	DA	OP1-P-OP2	-6.35	110.07	119.60
6	H	185	DA	OP1-P-OP2	-6.35	110.07	119.60
6	H	98	DA	OP1-P-OP2	-6.35	110.08	119.60
12	T	102	DC	OP1-P-OP2	-6.34	110.09	119.60
12	T	89	DA	OP1-P-OP2	-6.34	110.09	119.60
6	H	90	DT	OP1-P-O3'	6.34	119.14	105.20
6	H	167	DT	OP1-P-O3'	6.32	119.10	105.20
6	H	142	DG	OP1-P-OP2	-6.32	110.12	119.60
12	T	49	DT	OP1-P-O3'	6.32	119.09	105.20
6	H	107	DG	OP1-P-OP2	-6.31	110.13	119.60
6	H	78	DG	OP1-P-OP2	-6.29	110.16	119.60
6	H	121	DG	OP1-P-OP2	-6.28	110.18	119.60
6	H	169	DG	OP1-P-O3'	6.28	119.02	105.20
12	T	36	DG	OP1-P-O3'	6.27	119.00	105.20
6	H	123	DG	OP1-P-OP2	-6.27	110.20	119.60
12	T	42	DC	OP1-P-O3'	6.27	118.99	105.20
6	H	32	DG	OP1-P-O3'	6.26	118.97	105.20
6	H	95	DG	OP1-P-OP2	-6.26	110.22	119.60
12	T	135	DC	OP1-P-O3'	6.26	118.96	105.20
12	T	187	DT	OP1-P-O3'	6.25	118.96	105.20
6	H	129	DA	OP1-P-OP2	-6.25	110.22	119.60
6	H	91	DG	OP1-P-O3'	6.24	118.92	105.20
6	H	47	DG	OP1-P-O3'	6.22	118.89	105.20
6	H	58	DA	OP1-P-OP2	-6.21	110.28	119.60
6	H	119	DA	OP1-P-O3'	6.18	118.79	105.20
12	T	169	DC	OP1-P-O3'	6.17	118.78	105.20
6	H	36	DG	OP1-P-O3'	6.17	118.77	105.20
6	H	109	DG	OP1-P-O3'	6.16	118.76	105.20
6	H	164	DG	OP1-P-OP2	-6.16	110.36	119.60
12	T	183	DC	OP1-P-OP2	-6.16	110.36	119.60
12	T	56	DG	OP1-P-O3'	6.13	118.69	105.20
12	T	120	DC	OP1-P-O3'	6.13	118.68	105.20
6	H	182	DC	OP1-P-O3'	6.11	118.65	105.20
12	T	152	DC	OP1-P-O3'	6.11	118.65	105.20
12	T	32	DC	OP1-P-O3'	6.09	118.61	105.20
6	H	57	DG	OP1-P-OP2	-6.08	110.48	119.60
12	T	129	DT	OP1-P-O3'	6.07	118.55	105.20
6	H	79	DA	OP1-P-O3'	6.06	118.54	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	82	DA	OP1-P-O3'	6.06	118.52	105.20
6	H	140	DG	OP1-P-OP2	-6.05	110.52	119.60
6	H	186	DG	OP1-P-O3'	6.05	118.52	105.20
6	H	189	DG	OP1-P-O3'	6.04	118.48	105.20
12	T	157	DC	OP1-P-O3'	6.04	118.48	105.20
12	T	195	DC	OP1-P-O3'	6.03	118.47	105.20
6	H	78	DG	OP1-P-O3'	6.03	118.47	105.20
12	T	153	DA	OP1-P-O3'	6.03	118.46	105.20
6	H	193	DG	OP1-P-O3'	6.02	118.45	105.20
6	H	173	DC	OP1-P-O3'	6.01	118.43	105.20
6	H	129	DA	OP1-P-O3'	6.01	118.42	105.20
6	H	197	DC	OP1-P-O3'	6.01	118.42	105.20
12	T	172	DG	OP1-P-O3'	6.01	118.42	105.20
12	T	176	DT	OP1-P-O3'	6.01	118.42	105.20
6	H	112	DA	OP1-P-OP2	-6.01	110.59	119.60
6	H	180	DC	OP1-P-O3'	6.00	118.41	105.20
6	H	61	DC	OP1-P-O3'	5.99	118.39	105.20
6	H	108	DG	OP1-P-O3'	5.98	118.35	105.20
6	H	103	DG	OP1-P-O3'	5.97	118.33	105.20
6	H	130	DA	OP1-P-O3'	5.96	118.31	105.20
6	H	154	DC	OP1-P-O3'	5.96	118.31	105.20
6	H	132	DC	OP1-P-O3'	5.95	118.29	105.20
12	T	158	DC	OP1-P-O3'	5.95	118.28	105.20
6	H	112	DA	OP1-P-O3'	5.95	118.28	105.20
12	T	143	DA	OP1-P-OP2	-5.94	110.69	119.60
6	H	23	DG	OP1-P-O3'	5.93	118.25	105.20
12	T	197	DC	OP1-P-O3'	5.92	118.23	105.20
6	H	183	DC	OP1-P-O3'	5.92	118.23	105.20
6	H	33	DC	OP1-P-O3'	5.91	118.21	105.20
6	H	52	DT	OP1-P-O3'	5.89	118.17	105.20
12	T	121	DC	OP1-P-O3'	5.88	118.14	105.20
6	H	194	DC	OP1-P-O3'	5.88	118.13	105.20
6	H	71	DG	OP1-P-O3'	5.87	118.10	105.20
12	T	174	DT	OP1-P-O3'	5.86	118.10	105.20
6	H	101	DA	OP1-P-O3'	5.85	118.07	105.20
12	T	34	DC	OP1-P-O3'	5.85	118.07	105.20
6	H	199	DC	OP1-P-O3'	5.85	118.07	105.20
6	H	45	DA	OP1-P-O3'	5.84	118.05	105.20
12	T	162	DG	OP1-P-O3'	5.83	118.03	105.20
12	T	170	DC	OP1-P-O3'	5.83	118.03	105.20
12	T	148	DC	OP1-P-O3'	5.83	118.02	105.20
6	H	75	DA	OP1-P-O3'	5.82	118.00	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	T	163	DC	OP1-P-O3'	5.82	118.01	105.20
6	H	22	DC	OP1-P-O3'	5.82	118.00	105.20
6	H	46	DT	OP1-P-O3'	5.82	117.99	105.20
6	H	187	DC	OP1-P-O3'	5.81	117.98	105.20
12	T	140	DG	OP1-P-O3'	5.81	117.98	105.20
12	T	21	DA	OP1-P-O3'	5.81	117.98	105.20
6	H	135	DT	OP1-P-O3'	5.79	117.94	105.20
12	T	47	DA	OP1-P-O3'	5.79	117.95	105.20
12	T	139	DG	OP1-P-O3'	5.77	117.89	105.20
12	T	101	DA	OP1-P-O3'	5.77	117.89	105.20
12	T	108	DT	OP1-P-O3'	5.76	117.88	105.20
6	H	41	DC	OP1-P-O3'	5.76	117.88	105.20
6	H	201	DG	OP1-P-O3'	5.75	117.85	105.20
6	H	172	DA	OP1-P-O3'	5.74	117.83	105.20
12	T	167	DT	OP1-P-O3'	5.74	117.83	105.20
6	H	124	DC	OP1-P-O3'	5.74	117.82	105.20
6	H	74	DT	OP1-P-O3'	5.73	117.81	105.20
6	H	161	DG	OP1-P-O3'	5.73	117.80	105.20
12	T	86	DC	OP1-P-O3'	5.72	117.78	105.20
12	T	179	DA	OP1-P-O3'	5.72	117.78	105.20
6	H	26	DT	OP1-P-O3'	5.70	117.74	105.20
12	T	130	DA	OP1-P-O3'	5.70	117.74	105.20
6	H	141	DA	OP1-P-O3'	5.68	117.71	105.20
7	I	60	LEU	CA-CB-CG	5.68	128.35	115.30
12	T	119	DC	OP1-P-O3'	5.67	117.67	105.20
12	T	95	DG	OP1-P-O3'	5.66	117.66	105.20
6	H	207	DG	OP1-P-O3'	5.66	117.65	105.20
6	H	151	DG	OP1-P-O3'	5.66	117.64	105.20
12	T	84	DG	OP1-P-O3'	5.65	117.63	105.20
12	T	193	DC	OP1-P-O3'	5.65	117.63	105.20
6	H	64	DG	OP1-P-O3'	5.64	117.61	105.20
12	T	24	DC	OP1-P-O3'	5.63	117.58	105.20
12	T	29	DC	OP1-P-O3'	5.63	117.58	105.20
12	T	102	DC	OP1-P-O3'	5.63	117.58	105.20
12	T	51	DC	OP1-P-O3'	5.62	117.57	105.20
6	H	133	DG	OP1-P-O3'	5.62	117.56	105.20
12	T	99	DA	OP1-P-O3'	5.60	117.52	105.20
12	T	136	DC	OP1-P-O3'	5.60	117.52	105.20
6	H	146	DC	OP1-P-O3'	5.60	117.51	105.20
12	T	106	DC	OP1-P-O3'	5.59	117.51	105.20
6	H	69	DG	OP1-P-O3'	5.58	117.47	105.20
6	H	29	DC	OP1-P-O3'	5.57	117.44	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	131	DG	OP1-P-O3'	5.57	117.44	105.20
6	H	211	DG	OP1-P-O3'	5.57	117.44	105.20
6	H	159	DG	OP1-P-O3'	5.56	117.44	105.20
12	T	57	DC	OP1-P-O3'	5.56	117.43	105.20
12	T	50	DC	OP1-P-O3'	5.54	117.39	105.20
6	H	198	DG	OP1-P-O3'	5.51	117.33	105.20
6	H	65	DC	OP1-P-O3'	5.50	117.29	105.20
12	T	60	DA	OP1-P-O3'	5.49	117.28	105.20
6	H	144	DT	OP1-P-O3'	5.47	117.24	105.20
6	H	202	DC	OP1-P-O3'	5.47	117.24	105.20
12	T	191	DC	OP1-P-O3'	5.47	117.24	105.20
6	H	70	DA	OP1-P-O3'	5.47	117.23	105.20
6	H	102	DC	OP1-P-O3'	5.47	117.22	105.20
12	T	81	DA	OP1-P-O3'	5.45	117.19	105.20
12	T	23	DA	OP1-P-O3'	5.45	117.18	105.20
12	T	41	DC	OP1-P-O3'	5.44	117.18	105.20
6	H	93	DC	OP1-P-O3'	5.43	117.16	105.20
6	H	110	DA	OP1-P-O3'	5.43	117.16	105.20
6	H	123	DG	OP1-P-O3'	5.43	117.15	105.20
6	H	206	DT	OP1-P-O3'	5.42	117.13	105.20
12	T	134	DG	OP1-P-O3'	5.42	117.12	105.20
6	H	81	DT	OP1-P-O3'	5.42	117.12	105.20
12	T	27	DT	OP1-P-O3'	5.41	117.11	105.20
6	H	84	DC	OP1-P-O3'	5.41	117.10	105.20
12	T	64	DC	OP1-P-O3'	5.41	117.10	105.20
12	T	63	DC	OP1-P-O3'	5.38	117.03	105.20
12	T	17	DC	OP1-P-O3'	5.37	117.02	105.20
12	T	19	DT	OP1-P-O3'	5.37	117.01	105.20
6	H	165	DC	OP1-P-O3'	5.36	116.99	105.20
6	H	200	DA	OP1-P-O3'	5.36	116.98	105.20
12	T	159	DC	OP1-P-O3'	5.35	116.98	105.20
12	T	204	DC	OP1-P-O3'	5.35	116.96	105.20
12	T	131	DA	OP1-P-O3'	5.34	116.95	105.20
6	H	57	DG	OP1-P-O3'	5.33	116.94	105.20
12	T	113	DG	OP1-P-O3'	5.33	116.94	105.20
12	T	146	DA	OP1-P-O3'	5.33	116.94	105.20
6	H	44	DG	OP1-P-O3'	5.33	116.92	105.20
12	T	94	DC	OP1-P-O3'	5.33	116.92	105.20
12	T	105	DA	OP1-P-O3'	5.33	116.92	105.20
12	T	203	DT	OP1-P-O3'	5.32	116.91	105.20
6	H	196	DG	OP1-P-O3'	5.31	116.89	105.20
6	H	54	DC	OP1-P-O3'	5.31	116.89	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	63	DT	OP1-P-O3'	5.30	116.87	105.20
6	H	176	DG	OP1-P-O3'	5.28	116.82	105.20
6	H	39	DT	OP1-P-O3'	5.28	116.82	105.20
6	H	49	DA	OP1-P-O3'	5.28	116.81	105.20
12	T	132	DC	OP1-P-O3'	5.28	116.81	105.20
6	H	208	DA	OP1-P-O3'	5.26	116.78	105.20
12	T	18	DG	OP1-P-O3'	5.25	116.75	105.20
12	T	26	DC	OP1-P-O3'	5.25	116.75	105.20
6	H	24	DA	OP1-P-O3'	5.24	116.72	105.20
6	H	20	DA	OP1-P-O3'	5.23	116.71	105.20
12	T	52	DC	OP1-P-O3'	5.23	116.70	105.20
6	H	164	DG	OP1-P-O3'	5.22	116.69	105.20
6	H	209	DC	OP1-P-O3'	5.22	116.69	105.20
12	T	123	DG	OP1-P-O3'	5.22	116.68	105.20
12	T	43	DG	OP1-P-O3'	5.21	116.66	105.20
12	T	90	DG	OP1-P-O3'	5.20	116.64	105.20
6	H	148	DT	OP1-P-O3'	5.19	116.61	105.20
12	T	33	DG	OP1-P-O3'	5.18	116.60	105.20
6	H	25	DA	OP1-P-O3'	5.18	116.59	105.20
6	H	97	DT	OP1-P-O3'	5.18	116.59	105.20
6	H	99	DA	OP1-P-O3'	5.17	116.58	105.20
6	H	150	DC	OP1-P-O3'	5.16	116.56	105.20
12	T	200	DC	OP1-P-O3'	5.15	116.53	105.20
6	H	48	DT	OP1-P-O3'	5.14	116.50	105.20
6	H	155	DA	OP1-P-O3'	5.13	116.50	105.20
12	T	89	DA	OP1-P-O3'	5.13	116.49	105.20
12	T	35	DC	OP1-P-O3'	5.12	116.47	105.20
12	T	55	DT	OP1-P-O3'	5.12	116.46	105.20
6	H	21	DC	OP1-P-O3'	5.09	116.40	105.20
6	H	68	DG	OP1-P-O3'	5.08	116.38	105.20
12	T	164	DA	OP1-P-O3'	5.08	116.37	105.20
6	H	184	DC	OP1-P-O3'	5.07	116.35	105.20
12	T	182	DT	OP1-P-O3'	5.06	116.32	105.20
6	H	37	DC	OP1-P-O3'	5.05	116.30	105.20
6	H	191	DC	OP1-P-O3'	5.05	116.30	105.20
12	T	15	DC	OP1-P-O3'	5.05	116.30	105.20
12	T	194	DG	OP1-P-O3'	5.03	116.26	105.20
6	H	115	DG	OP1-P-O3'	5.03	116.26	105.20
12	T	65	DG	OP1-P-O3'	5.02	116.25	105.20
6	H	188	DC	OP1-P-O3'	5.01	116.22	105.20
12	T	180	DC	OP1-P-O3'	5.01	116.22	105.20

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	A	568	0	597	27	0
2	B	196	0	188	9	0
3	D	3653	0	3636	134	0
4	E	4580	0	4483	200	0
5	G	2930	0	2839	155	0
6	H	3972	0	2154	138	0
7	I	917	0	971	43	0
7	W	817	0	858	45	0
8	J	661	0	709	31	0
8	X	666	0	679	26	0
9	O	3139	0	2986	131	0
10	R	829	0	887	41	0
10	U	825	0	876	40	0
11	S	742	0	753	36	0
11	V	737	0	751	50	0
12	T	3919	0	2153	126	0
13	Y	1047	0	1102	51	0
14	E	26	0	19	2	0
All	All	30224	0	26641	1092	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 24.

All (1092) 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)
10:R:112:GLN:HE21	10:R:114:VAL:H	1.16	0.90
10:R:78:ILE:HG22	11:S:51:ILE:HA	1.55	0.86
6:H:75:DA:H61	12:T:152:DC:H42	1.27	0.81
4:E:674:LEU:HD11	4:E:711:HIS:HB3	1.63	0.81
5:G:222:THR:HG21	5:G:278:TYR:HA	1.63	0.80
10:R:80:PRO:HD3	11:S:55:ALA:HB2	1.64	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:673:ASN:HA	4:E:679:VAL:HG22	1.66	0.78
6:H:158:DG:H1	12:T:69:DT:H3	1.31	0.78
5:G:132:ILE:HD11	5:G:436:ARG:HD3	1.66	0.77
4:E:286:CYS:SG	4:E:297:HIS:ND1	2.57	0.77
8:J:52:GLU:OE2	8:J:52:GLU:N	2.18	0.77
7:W:82:LEU:HA	8:X:79:LYS:HD2	1.67	0.76
4:E:326:GLY:O	4:E:328:GLN:N	2.19	0.76
3:D:311:LEU:HD11	13:Y:232:GLU:HG3	1.66	0.76
5:G:330:CYS:H	5:G:354:GLY:HA3	1.49	0.76
6:H:85:DC:O2	12:T:142:DG:N2	2.19	0.76
5:G:215:LEU:HB3	5:G:229:PHE:HD2	1.52	0.75
7:I:129:ARG:O	7:I:129:ARG:NH1	2.19	0.75
8:J:84:MET:SD	8:J:84:MET:N	2.60	0.74
3:D:612:GLU:HA	3:D:615:LYS:HD2	1.67	0.74
5:G:153:THR:HB	5:G:162:LEU:HB2	1.69	0.74
6:H:21:DC:H42	12:T:206:DA:H61	1.36	0.74
6:H:184:DC:O2	12:T:43:DG:N2	2.17	0.74
6:H:173:DC:O2	12:T:54:DG:N2	2.18	0.73
4:E:448:LEU:HB3	4:E:459:ILE:HG12	1.69	0.73
11:V:68:GLU:OE1	11:V:68:GLU:N	2.18	0.73
12:T:167:DT:H2''	12:T:168:DG:C8	2.22	0.73
5:G:217:LEU:HB3	5:G:226:VAL:HB	1.70	0.73
6:H:179:DT:H2''	6:H:180:DC:H5'	1.71	0.72
5:G:332:LYS:HD3	5:G:336:MET:HA	1.71	0.72
7:I:61:LEU:O	8:J:36:ARG:NH2	2.23	0.71
10:U:17:ARG:HH21	10:U:28:GLY:HA2	1.56	0.71
5:G:271:MET:SD	5:G:271:MET:N	2.63	0.71
13:Y:224:SER:OG	13:Y:259:ARG:NH1	2.23	0.71
6:H:211:DG:O6	12:T:15:DC:N4	2.24	0.71
1:A:72:LYS:HD3	1:A:88:ALA:HB2	1.71	0.71
3:D:137:MET:HA	3:D:140:LYS:HG3	1.71	0.70
5:G:233:GLU:O	5:G:261:LYS:NZ	2.24	0.70
1:A:74:LEU:HD11	1:A:80:LEU:HD13	1.74	0.70
11:V:60:ASN:O	11:V:64:ASN:ND2	2.24	0.70
1:A:74:LEU:HD21	1:A:80:LEU:HD22	1.74	0.70
4:E:475:ARG:NH2	4:E:478:GLU:OE1	2.25	0.70
3:D:307:ARG:HH12	3:D:309:GLN:HA	1.56	0.70
4:E:647:CYS:SG	4:E:687:ASN:ND2	2.65	0.69
7:W:59:GLU:N	7:W:59:GLU:OE2	2.22	0.69
5:G:270:MET:SD	5:G:270:MET:N	2.64	0.69
10:U:32:ARG:NH2	11:V:32:GLU:OE1	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:305:ASN:HD21	3:D:307:ARG:HE	1.39	0.69
7:W:129:ARG:O	7:W:129:ARG:NH1	2.25	0.69
4:E:544:ALA:O	4:E:546:ASN:ND2	2.25	0.69
8:X:60:VAL:O	8:X:64:ASN:ND2	2.24	0.69
5:G:86:ASN:ND2	5:G:130:GLY:O	2.25	0.69
5:G:125:GLU:OE1	5:G:133:ARG:NH2	2.24	0.69
11:S:60:ASN:O	11:S:64:ASN:ND2	2.26	0.69
11:S:73:GLU:HA	11:S:76:ARG:HE	1.56	0.69
7:W:57:SER:OG	8:X:40:ARG:NH2	2.26	0.69
3:D:81:ALA:N	3:D:437:ASN:OD1	2.26	0.68
8:X:53:GLU:OE2	8:X:53:GLU:N	2.26	0.68
4:E:624:SER:HB3	4:E:630:GLY:HA3	1.76	0.68
6:H:42:DA:H61	12:T:185:DC:H42	1.40	0.68
13:Y:239:LEU:N	13:Y:254:VAL:O	2.20	0.68
4:E:631:ILE:HD11	4:E:691:PHE:HB2	1.76	0.68
9:O:76:GLN:NE2	9:O:77:ASN:O	2.26	0.67
9:O:80:VAL:HG12	9:O:120:LYS:HG2	1.77	0.67
10:R:39:TYR:O	11:S:75:SER:OG	2.10	0.67
6:H:184:DC:N3	12:T:43:DG:N1	2.34	0.67
10:R:42:ARG:HB2	11:S:85:THR:HG22	1.76	0.67
4:E:82:GLU:HA	4:E:97:PRO:HA	1.76	0.67
4:E:554:CYS:HB3	4:E:558:CYS:HB2	1.77	0.67
7:I:44:GLY:N	12:T:123:DG:OP1	2.28	0.67
3:D:100:LEU:HA	3:D:103:ARG:HH12	1.60	0.67
12:T:133:DC:H2'	12:T:134:DG:C8	2.29	0.67
5:G:273:ALA:O	5:G:277:SER:N	2.26	0.67
7:I:116:ARG:NH2	7:I:123:ASP:OD2	2.27	0.67
8:X:34:ILE:HD12	8:X:34:ILE:H	1.60	0.67
5:G:191:ASN:HB2	5:G:211:LYS:HB3	1.77	0.66
11:V:80:TYR:O	11:V:82:LYS:NZ	2.25	0.66
5:G:436:ARG:NH2	5:G:438:ASP:OD2	2.29	0.66
3:D:607:ASN:ND2	4:E:261:THR:O	2.28	0.66
8:J:75:HIS:O	11:V:89:ARG:NH2	2.28	0.66
9:O:338:THR:HA	9:O:376:LYS:HG3	1.76	0.66
9:O:32:TYR:OH	9:O:370:HIS:ND1	2.25	0.66
10:R:85:LEU:O	10:R:89:ASN:ND2	2.29	0.66
4:E:639:LYS:HE2	4:E:719:ARG:HA	1.78	0.66
4:E:624:SER:N	4:E:628:GLY:O	2.29	0.66
5:G:92:HIS:O	5:G:94:GLN:NE2	2.29	0.66
3:D:358:THR:OG1	3:D:360:ARG:NH2	2.30	0.66
4:E:96:ILE:HD12	5:G:134:LEU:HG	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:90:MET:SD	7:I:90:MET:N	2.68	0.66
11:S:87:THR:HG23	11:S:89:ARG:H	1.60	0.66
3:D:597:ILE:HD11	3:D:619:LEU:HD11	1.78	0.65
6:H:85:DC:N3	12:T:142:DG:N1	2.43	0.65
11:V:55:ALA:HA	11:V:58:ILE:HD12	1.77	0.65
7:I:37:LYS:HD2	7:I:38:PRO:HD2	1.78	0.65
9:O:133:MET:HB2	9:O:185:TRP:CD2	2.32	0.65
4:E:288:ARG:HB3	4:E:297:HIS:CE1	2.32	0.65
6:H:208:DA:N6	12:T:18:DG:O6	2.29	0.65
9:O:377:ILE:HA	9:O:394:SER:HA	1.79	0.65
12:T:172:DG:H2'	12:T:173:DA:O4'	1.97	0.65
1:A:91:SER:OG	12:T:116:DG:OP1	2.12	0.65
3:D:192:CYS:SG	3:D:195:LYS:NZ	2.70	0.65
4:E:525:TYR:O	4:E:526:GLN:NE2	2.30	0.65
9:O:305:ASN:HD21	9:O:308:LEU:HD12	1.61	0.65
3:D:610:GLU:OE2	3:D:610:GLU:N	2.24	0.65
4:E:289:CYS:HB2	4:E:297:HIS:HE1	1.62	0.65
4:E:568:LYS:HA	4:E:592:THR:HB	1.78	0.65
9:O:232:ASP:HB3	9:O:246:VAL:HB	1.78	0.65
5:G:252:MET:SD	5:G:253:SER:N	2.70	0.64
11:V:68:GLU:O	11:V:72:GLY:N	2.28	0.64
6:H:182:DC:H42	12:T:45:DA:H61	1.45	0.64
4:E:558:CYS:HB3	4:E:561:ARG:HE	1.61	0.64
10:U:71:ARG:NH1	10:U:72:ASP:OD1	2.31	0.64
5:G:183:ILE:HG13	5:G:184:LYS:HD3	1.80	0.64
5:G:312:VAL:O	5:G:313:ARG:NE	2.27	0.64
4:E:46:ARG:HH22	5:G:375:LYS:HG2	1.63	0.64
11:V:33:SER:OG	11:V:34:TYR:N	2.29	0.64
11:V:43:LYS:HE3	11:V:47:PRO:HA	1.78	0.64
8:J:39:ARG:NH1	8:J:44:LYS:O	2.31	0.63
9:O:198:ASP:HA	9:O:229:VAL:HG13	1.79	0.63
9:O:292:GLY:HA2	9:O:298:VAL:HA	1.80	0.63
10:U:85:LEU:O	10:U:89:ASN:ND2	2.27	0.63
3:D:567:HIS:N	3:D:572:LEU:O	2.25	0.63
9:O:79:LEU:HG	9:O:123:HIS:HB2	1.80	0.63
3:D:312:ASP:O	3:D:360:ARG:NH2	2.31	0.63
9:O:237:LEU:HG	9:O:281:PHE:HB2	1.80	0.63
5:G:145:GLU:OE1	5:G:168:SER:N	2.31	0.63
5:G:226:VAL:HG12	5:G:227:ALA:H	1.62	0.63
9:O:271:ALA:HB3	9:O:276:VAL:HG21	1.80	0.63
5:G:202:ASP:OD1	5:G:204:ASN:ND2	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:O:106:GLY:O	13:Y:170:ASN:N	2.32	0.63
3:D:659:HIS:HD1	4:E:292:TYR:HH	1.47	0.63
4:E:529:ASP:HA	4:E:553:GLN:HB2	1.80	0.63
6:H:148:DT:H2''	6:H:149:DA:C8	2.34	0.63
13:Y:261:GLN:OE1	13:Y:261:GLN:N	2.31	0.63
7:W:85:GLN:NE2	7:W:87:SER:H	1.97	0.62
4:E:672:PHE:HB3	4:E:680:VAL:HG12	1.80	0.62
6:H:66:DC:H2''	6:H:67:DT:C5	2.35	0.62
9:O:40:LEU:HD12	9:O:41:GLU:H	1.64	0.62
9:O:204:LEU:O	9:O:220:LYS:N	2.33	0.62
8:X:63:GLU:HA	8:X:66:ILE:HD12	1.80	0.62
9:O:404:MET:SD	9:O:404:MET:N	2.64	0.62
4:E:528:CYS:HB2	4:E:540:PRO:HD2	1.80	0.62
9:O:32:TYR:HH	9:O:370:HIS:HD1	1.36	0.62
6:H:110:DA:C8	6:H:110:DA:H5'	2.35	0.62
6:H:60:DA:OP1	10:U:77:ARG:NH2	2.27	0.62
6:H:192:DG:O6	12:T:34:DC:N4	2.33	0.62
4:E:24:MET:SD	4:E:31:ARG:NH2	2.72	0.62
4:E:329:CYS:SG	4:E:330:TYR:N	2.73	0.62
9:O:49:TRP:CD2	9:O:383:ASN:HB3	2.35	0.62
3:D:568:SER:OG	3:D:584:GLU:OE1	2.16	0.61
9:O:93:PHE:HB2	13:Y:171:LYS:HD3	1.80	0.61
5:G:116:VAL:HG12	5:G:121:VAL:HG12	1.81	0.61
6:H:56:DT:O2	12:T:172:DG:N2	2.33	0.61
9:O:77:ASN:ND2	9:O:125:GLY:O	2.33	0.61
10:U:104:GLN:N	7:W:94:GLU:OE2	2.32	0.61
12:T:153:DA:OP1	10:U:43:VAL:N	2.27	0.61
5:G:80:TYR:HA	5:G:402:THR:HG21	1.81	0.61
12:T:158:DC:H2''	12:T:159:DC:C5	2.35	0.61
8:X:93:GLN:HE22	8:X:95:ARG:HG3	1.66	0.61
5:G:232:VAL:HG13	5:G:233:GLU:HG2	1.82	0.61
12:T:193:DC:H2'	12:T:194:DG:C8	2.35	0.61
3:D:158:GLN:HB3	3:D:230:LEU:HD11	1.83	0.61
4:E:273:GLN:HA	4:E:446:ARG:HD2	1.82	0.60
6:H:172:DA:OP2	10:R:75:LYS:NZ	2.27	0.60
9:O:76:GLN:NE2	9:O:123:HIS:O	2.34	0.60
13:Y:244:MET:SD	13:Y:245:PRO:HD3	2.40	0.60
7:W:83:ARG:HB2	8:X:80:THR:HG22	1.83	0.60
1:A:27:TYR:OH	12:T:194:DG:OP1	2.20	0.60
4:E:60:TRP:NE1	5:G:105:SER:O	2.35	0.60
4:E:329:CYS:HB3	4:E:332:HIS:HD2	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:60:LEU:HD23	7:I:62:ILE:H	1.66	0.60
12:T:50:DC:H2''	12:T:51:DC:H5''	1.83	0.60
1:A:81:LYS:O	1:A:93:ARG:N	2.33	0.60
4:E:289:CYS:HB2	4:E:297:HIS:CE1	2.36	0.60
4:E:449:ILE:HB	4:E:475:ARG:CZ	2.32	0.60
3:D:89:ALA:O	3:D:92:LYS:NZ	2.32	0.59
6:H:163:DG:H2'	6:H:164:DG:C8	2.37	0.59
6:H:173:DC:N3	12:T:54:DG:N1	2.40	0.59
7:I:59:GLU:OE2	7:I:59:GLU:N	2.28	0.59
4:E:39:LYS:NZ	5:G:393:VAL:O	2.35	0.59
9:O:174:ARG:NH1	9:O:218:ASP:OD1	2.30	0.59
12:T:153:DA:OP2	10:U:35:ARG:NH2	2.35	0.59
6:H:57:DG:O6	12:T:169:DC:N4	2.35	0.59
8:J:75:HIS:HD2	11:V:93:THR:HG21	1.67	0.59
9:O:253:MET:HG3	9:O:255:TRP:HE1	1.68	0.59
9:O:127:VAL:HG13	9:O:142:THR:HG23	1.85	0.59
9:O:251:LYS:HA	9:O:270:ASP:HA	1.83	0.59
12:T:100:DA:H5''	7:W:63:ARG:HH12	1.68	0.59
3:D:502:ASN:HD21	3:D:504:GLN:HB3	1.66	0.58
4:E:636:PRO:HB3	4:E:722:GLN:HA	1.85	0.58
9:O:174:ARG:N	9:O:217:VAL:O	2.28	0.58
11:S:68:GLU:N	11:S:68:GLU:OE2	2.36	0.58
13:Y:255:ASN:N	13:Y:258:GLU:OE1	2.32	0.58
9:O:81:ILE:HB	9:O:119:ILE:HB	1.85	0.58
10:R:29:ARG:NH1	11:S:33:SER:O	2.22	0.58
5:G:92:HIS:HD2	5:G:120:ARG:HD2	1.68	0.58
6:H:158:DG:H22	12:T:69:DT:H3	1.50	0.58
9:O:327:PRO:HD3	9:O:382:TRP:CD1	2.39	0.58
10:U:33:LEU:O	10:U:37:GLY:N	2.36	0.58
3:D:666:PHE:HB3	4:E:287:ARG:HE	1.67	0.58
6:H:169:DG:H1'	6:H:170:DG:C5	2.38	0.58
4:E:40:SER:OG	4:E:41:MET:SD	2.62	0.58
5:G:334:GLY:O	5:G:351:THR:OG1	2.20	0.58
5:G:89:LYS:HA	5:G:433:SER:HA	1.84	0.58
10:R:72:ASP:O	10:R:74:LYS:NZ	2.33	0.58
3:D:586:GLU:HG2	3:D:588:ASP:H	1.69	0.58
9:O:49:TRP:CG	9:O:383:ASN:HB3	2.39	0.58
3:D:303:ASP:OD2	3:D:307:ARG:NH2	2.37	0.57
4:E:271:SER:HA	4:E:443:SER:HB2	1.86	0.57
5:G:233:GLU:HB2	5:G:295:HIS:O	2.03	0.57
7:W:61:LEU:O	8:X:36:ARG:NH2	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:O:382:TRP:HE3	9:O:390:ILE:HG12	1.70	0.57
5:G:332:LYS:NZ	5:G:333:PRO:O	2.38	0.57
1:A:49:ILE:HG22	1:A:53:ILE:HD13	1.86	0.57
4:E:470:GLN:HA	4:E:473:GLU:HB2	1.85	0.57
4:E:610:SER:O	4:E:614:GLY:N	2.38	0.57
6:H:43:DG:O6	12:T:183:DC:N4	2.37	0.57
10:U:84:GLN:HE21	10:U:88:ARG:HE	1.53	0.57
11:V:99:LEU:HD12	11:V:99:LEU:H	1.70	0.57
9:O:251:LYS:HE2	9:O:268:SER:HB3	1.85	0.57
10:R:78:ILE:N	11:S:50:GLY:O	2.32	0.57
10:U:41:GLU:OE2	10:U:42:ARG:HG3	2.04	0.57
3:D:319:MET:HG3	3:D:353:PRO:HB2	1.85	0.57
3:D:582:ASP:OD1	3:D:582:ASP:N	2.28	0.57
4:E:585:CYS:HB2	4:E:590:CYS:HB2	1.87	0.57
12:T:126:DT:H2''	12:T:127:DT:H5'	1.85	0.57
3:D:157:LEU:HB3	3:D:233:SER:HB3	1.87	0.57
4:E:58:GLN:O	4:E:62:GLN:NE2	2.31	0.57
5:G:249:GLU:O	5:G:265:ILE:N	2.34	0.57
13:Y:223:HIS:ND1	13:Y:263:LYS:O	2.34	0.56
3:D:464:LEU:HD23	3:D:467:LEU:HD12	1.86	0.56
4:E:175:VAL:HA	4:E:178:LEU:HG	1.87	0.56
9:O:188:ASN:HB2	9:O:240:GLU:HB3	1.86	0.56
4:E:262:PRO:HD2	4:E:269:ALA:HA	1.88	0.56
4:E:663:TYR:HA	4:E:666:TYR:CE1	2.40	0.56
6:H:163:DG:H2'	6:H:164:DG:H8	1.68	0.56
6:H:174:DC:H2'	6:H:175:DG:C8	2.40	0.56
8:J:88:TYR:CG	11:V:80:TYR:HE1	2.24	0.56
10:R:92:GLU:OE1	11:S:102:GLU:HB3	2.05	0.56
2:B:150:ARG:NH2	3:D:87:LEU:O	2.38	0.56
6:H:117:DG:H1	12:T:110:DC:H42	1.53	0.56
8:J:98:TYR:OH	11:S:65:ASP:OD2	2.22	0.56
13:Y:240:LEU:HG	13:Y:251:ASP:OD1	2.05	0.56
3:D:214:PRO:HD2	3:D:217:PRO:HG3	1.88	0.56
10:U:36:LYS:HE3	10:U:36:LYS:HA	1.87	0.56
6:H:52:DT:H2'	6:H:53:DA:H8	1.71	0.56
9:O:350:ILE:HA	9:O:365:GLU:HB3	1.88	0.56
11:V:78:ALA:O	11:V:83:ARG:N	2.37	0.56
3:D:143:LYS:HG3	9:O:308:LEU:HD22	1.87	0.56
4:E:584:GLU:HA	4:E:608:ASN:HD21	1.71	0.56
9:O:226:HIS:NE2	9:O:251:LYS:O	2.36	0.56
12:T:89:DA:H1'	12:T:90:DG:C8	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:V:95:VAL:HG13	11:V:99:LEU:HD13	1.88	0.56
6:H:29:DC:H42	12:T:197:DC:H42	1.54	0.56
6:H:202:DC:H2''	6:H:203:DG:C8	2.41	0.56
12:T:104:DC:H2''	12:T:105:DA:H8	1.71	0.56
12:T:129:DT:H2''	12:T:130:DA:C8	2.41	0.56
7:W:133:GLU:N	7:W:133:GLU:OE2	2.38	0.56
5:G:315:LEU:HD22	5:G:320:LEU:HD21	1.87	0.55
8:J:38:ALA:HB1	8:J:43:VAL:HB	1.88	0.55
10:R:92:GLU:OE1	11:S:103:LEU:HD22	2.06	0.55
3:D:471:HIS:HB2	3:D:476:PHE:CZ	2.41	0.55
5:G:257:ASP:O	5:G:302:ARG:NE	2.30	0.55
3:D:182:VAL:HG23	3:D:215:LEU:HD13	1.89	0.55
4:E:289:CYS:HB3	4:E:294:CYS:SG	2.46	0.55
5:G:90:GLU:N	5:G:432:ALA:O	2.36	0.55
5:G:245:ASP:OD1	5:G:248:GLY:N	2.39	0.55
7:I:106:ASP:OD2	7:I:106:ASP:N	2.39	0.55
12:T:163:DC:H2''	12:T:164:DA:C8	2.40	0.55
10:U:110:ASN:H	7:W:55:GLN:NE2	2.04	0.55
3:D:465:LYS:HD3	3:D:468:LYS:HZ2	1.71	0.55
4:E:99:LYS:HZ1	5:G:181:GLN:HG2	1.71	0.55
5:G:100:GLN:HB3	5:G:152:TRP:CD1	2.40	0.55
8:X:68:ASP:N	8:X:68:ASP:OD1	2.38	0.55
4:E:600:ASP:OD1	4:E:600:ASP:N	2.38	0.55
6:H:210:DG:O6	12:T:16:DC:N4	2.39	0.55
4:E:105:ALA:HA	13:Y:187:HIS:HE1	1.71	0.55
7:W:85:GLN:HE22	7:W:87:SER:H	1.55	0.55
13:Y:243:TRP:HB2	13:Y:248:ILE:HG12	1.89	0.55
3:D:502:ASN:ND2	3:D:505:ASP:OD1	2.33	0.55
9:O:55:ARG:NH2	9:O:386:GLU:OE2	2.40	0.55
12:T:191:DC:H2''	12:T:192:DA:C8	2.42	0.55
6:H:165:DC:H2''	6:H:166:DC:H5'	1.89	0.55
8:J:75:HIS:CD2	11:V:93:THR:HG21	2.42	0.55
9:O:40:LEU:HD12	9:O:41:GLU:N	2.22	0.55
8:X:46:ILE:HB	8:X:50:ILE:HD11	1.88	0.55
3:D:94:THR:HG23	3:D:452:TRP:HE1	1.72	0.55
6:H:161:DG:N2	12:T:67:DC:O2	2.40	0.55
12:T:97:DC:H2'	12:T:98:DT:C6	2.42	0.55
3:D:359:LEU:O	3:D:360:ARG:NE	2.40	0.55
5:G:229:PHE:HD1	5:G:294:ILE:HD12	1.72	0.55
6:H:111:DC:H2''	6:H:112:DA:H8	1.72	0.55
6:H:141:DA:H2''	6:H:142:DG:H8	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:97:DT:H4'	6:H:98:DA:H5'	1.88	0.54
7:I:116:ARG:NH1	7:I:120:MET:SD	2.80	0.54
9:O:56:PRO:HG2	9:O:59:LYS:HB2	1.89	0.54
11:S:33:SER:OG	11:S:34:TYR:N	2.39	0.54
9:O:118:GLU:O	9:O:159:SER:OG	2.24	0.54
4:E:285:PHE:HA	4:E:292:TYR:HA	1.88	0.54
5:G:373:TRP:HB3	5:G:375:LYS:HE3	1.88	0.54
9:O:51:PRO:HD3	9:O:132:TYR:CZ	2.42	0.54
12:T:152:DC:H5''	10:U:44:GLY:HA2	1.89	0.54
3:D:191:VAL:HG13	3:D:203:ILE:HG12	1.88	0.54
9:O:377:ILE:HD13	9:O:392:SER:HB2	1.88	0.54
1:A:30:MET:H	1:A:30:MET:HE2	1.73	0.54
6:H:57:DG:H1'	6:H:58:DA:H5'	1.89	0.54
13:Y:244:MET:SD	13:Y:244:MET:N	2.81	0.54
3:D:305:ASN:ND2	3:D:307:ARG:HE	2.06	0.54
3:D:605:ASP:HA	4:E:257:PRO:HD3	1.90	0.54
5:G:375:LYS:HA	5:G:391:LEU:HB2	1.90	0.54
6:H:159:DG:H1'	6:H:160:DA:C5	2.42	0.54
9:O:173:LEU:HB3	9:O:205:TRP:CE2	2.43	0.54
13:Y:238:LYS:HA	13:Y:255:ASN:HA	1.89	0.54
13:Y:240:LEU:HD13	13:Y:253:TRP:CE2	2.42	0.54
3:D:532:ARG:HB2	9:O:90:ASP:HB3	1.90	0.54
4:E:477:LYS:HE3	4:E:481:ILE:HD11	1.90	0.54
9:O:254:ILE:HB	9:O:267:HIS:HB2	1.90	0.54
12:T:77:DG:H2''	12:T:78:DT:H72	1.90	0.54
5:G:113:PHE:CZ	5:G:124:TYR:HB2	2.43	0.54
9:O:40:LEU:O	9:O:397:ASN:ND2	2.28	0.54
9:O:49:TRP:CZ2	9:O:391:CYS:HB3	2.43	0.54
9:O:123:HIS:HE1	9:O:144:THR:HG22	1.73	0.54
12:T:93:DC:OP1	8:X:16:LYS:N	2.40	0.53
11:V:68:GLU:HA	11:V:71:ALA:HB3	1.90	0.53
5:G:334:GLY:HA2	5:G:349:ASN:HB2	1.90	0.53
12:T:122:DC:H2'	12:T:123:DG:C8	2.43	0.53
9:O:257:THR:O	9:O:258:ARG:NH1	2.41	0.53
5:G:194:ASN:ND2	5:G:239:VAL:O	2.41	0.53
5:G:215:LEU:HB3	5:G:229:PHE:CD2	2.40	0.53
6:H:106:DG:H2''	6:H:107:DG:N7	2.23	0.53
6:H:138:DT:H4'	6:H:139:DA:H5'	1.91	0.53
3:D:577:GLN:OE1	3:D:577:GLN:N	2.38	0.53
4:E:289:CYS:HB2	4:E:296:LEU:HD21	1.90	0.53
5:G:414:ARG:HB3	5:G:415:GLN:OE1	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:127:DT:H2''	6:H:128:DT:H72	1.90	0.53
7:I:106:ASP:HA	7:I:109:LEU:HD13	1.90	0.53
10:U:17:ARG:HA	10:U:20:ARG:HD2	1.90	0.53
1:A:44:SER:N	1:A:92:PHE:O	2.42	0.53
5:G:189:HIS:NE2	5:G:208:SER:OG	2.39	0.53
3:D:565:TYR:HB2	3:D:574:LEU:HD12	1.89	0.53
3:D:607:ASN:HB2	3:D:610:GLU:OE2	2.08	0.53
4:E:236:THR:O	4:E:240:LEU:N	2.41	0.53
4:E:329:CYS:HB3	4:E:332:HIS:CD2	2.43	0.53
5:G:212:ASP:N	5:G:212:ASP:OD1	2.35	0.53
6:H:190:DC:N4	12:T:36:DG:O6	2.41	0.53
9:O:24:TRP:O	9:O:28:THR:OG1	2.15	0.53
9:O:132:TYR:HB2	9:O:137:PRO:HA	1.91	0.53
12:T:122:DC:H4'	12:T:123:DG:OP1	2.09	0.53
11:V:58:ILE:O	11:V:62:PHE:N	2.34	0.53
3:D:126:ASN:HB3	3:D:128:LYS:HE3	1.90	0.53
3:D:512:PHE:O	3:D:515:SER:OG	2.26	0.53
6:H:52:DT:H2'	6:H:53:DA:C8	2.43	0.53
6:H:191:DC:H2''	6:H:192:DG:C8	2.43	0.53
13:Y:222:PHE:N	13:Y:265:LYS:O	2.35	0.53
1:A:49:ILE:HD12	1:A:49:ILE:H	1.72	0.53
4:E:120:PHE:CE1	4:E:295:PHE:HB3	2.44	0.53
8:X:62:LEU:HG	8:X:66:ILE:HD11	1.90	0.53
4:E:699:ASN:O	4:E:718:LYS:N	2.41	0.53
6:H:56:DT:H1'	6:H:57:DG:C5	2.44	0.53
3:D:637:MET:HA	3:D:640:VAL:HG22	1.91	0.52
4:E:116:LEU:HD22	4:E:685:LYS:HB3	1.91	0.52
6:H:106:DG:N2	12:T:122:DC:O2	2.42	0.52
12:T:184:DC:H1'	12:T:185:DC:H5'	1.90	0.52
3:D:318:ALA:HB3	13:Y:227:ILE:HD12	1.90	0.52
6:H:56:DT:H1'	6:H:57:DG:C4	2.45	0.52
11:S:75:SER:HA	11:S:86:ILE:HD11	1.91	0.52
11:S:102:GLU:HA	11:S:105:LYS:NZ	2.24	0.52
6:H:77:DG:H2''	6:H:78:DG:N7	2.24	0.52
6:H:121:DG:P	8:X:35:ARG:HH22	2.32	0.52
11:V:102:GLU:HA	11:V:105:LYS:NZ	2.24	0.52
4:E:121:MET:HA	4:E:650:ILE:HB	1.90	0.52
4:E:577:PRO:O	4:E:581:ALA:N	2.32	0.52
4:E:629:TRP:N	14:E:801:SAH:OXT	2.43	0.52
5:G:384:GLY:HA3	5:G:410:GLY:HA2	1.92	0.52
8:J:51:TYR:HB3	8:J:55:ARG:HH12	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:X:73:THR:HG23	8:X:78:ARG:HB2	1.91	0.52
1:A:74:LEU:O	1:A:77:THR:OG1	2.24	0.52
3:D:193:HIS:HA	3:D:246:LYS:NZ	2.24	0.52
4:E:699:ASN:HB2	4:E:721:ILE:HD11	1.92	0.52
5:G:260:LEU:HD23	5:G:301:THR:HG23	1.92	0.52
9:O:122:ASN:ND2	9:O:162:ASP:O	2.37	0.52
5:G:189:HIS:HA	5:G:216:ARG:NH2	2.25	0.52
5:G:232:VAL:HG12	5:G:295:HIS:CG	2.43	0.52
6:H:75:DA:H2''	6:H:76:DG:C8	2.45	0.52
10:U:43:VAL:HA	11:V:86:ILE:HG22	1.92	0.52
10:U:78:ILE:H	11:V:51:ILE:HA	1.75	0.52
3:D:124:ARG:HG3	9:O:349:LYS:HE2	1.91	0.52
5:G:260:LEU:O	5:G:300:SER:HA	2.09	0.52
9:O:128:ASN:ND2	9:O:179:GLU:OE1	2.40	0.52
9:O:406:GLU:HA	9:O:409:TYR:CZ	2.45	0.52
10:R:79:ILE:HG22	10:R:82:HIS:CE1	2.44	0.52
12:T:68:DC:H4'	12:T:69:DT:OP1	2.08	0.52
7:I:129:ARG:HA	7:I:134:ARG:HB3	1.92	0.52
9:O:162:ASP:OD1	9:O:162:ASP:N	2.38	0.52
9:O:375:ALA:HB1	9:O:395:GLU:HB2	1.92	0.52
13:Y:258:GLU:HB2	13:Y:261:GLN:HE22	1.75	0.52
3:D:481:HIS:HB3	3:D:484:GLY:H	1.75	0.52
4:E:672:PHE:CD2	7:I:27:LYS:HB2	2.45	0.52
6:H:168:DC:H2''	6:H:169:DG:C8	2.45	0.52
4:E:504:TRP:HA	4:E:507:HIS:CD2	2.45	0.51
4:E:511:ILE:HG23	4:E:515:LYS:HE2	1.92	0.51
4:E:732:ARG:NH2	7:I:28:SER:OG	2.42	0.51
5:G:387:TYR:HB3	5:G:389:TRP:CH2	2.45	0.51
3:D:116:THR:O	3:D:119:SER:OG	2.20	0.51
5:G:120:ARG:HA	5:G:139:VAL:HA	1.93	0.51
5:G:154:TYR:HA	5:G:161:PRO:HA	1.92	0.51
12:T:170:DC:H2''	12:T:171:DA:N9	2.25	0.51
5:G:241:SER:HB3	5:G:254:CYS:SG	2.50	0.51
9:O:70:THR:OG1	9:O:78:HIS:O	2.19	0.51
9:O:253:MET:HG3	9:O:255:TRP:NE1	2.25	0.51
6:H:80:DG:N2	12:T:148:DC:O2	2.43	0.51
8:J:58:LEU:O	8:J:62:LEU:HD22	2.11	0.51
7:W:75:ALA:HB1	7:W:82:LEU:HD21	1.91	0.51
4:E:626:VAL:HA	13:Y:183:LEU:HD22	1.91	0.51
6:H:122:DT:O2	7:W:40:ARG:NH2	2.26	0.51
6:H:140:DG:O6	12:T:86:DC:N4	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:T:46:DG:H1'	12:T:47:DA:C8	2.45	0.51
12:T:111:DG:P	7:W:117:VAL:H	2.34	0.51
1:A:90:GLY:HA2	12:T:115:DC:H4'	1.93	0.51
5:G:358:TYR:HE2	5:G:361:CYS:HB3	1.74	0.51
9:O:61:PHE:HB2	9:O:85:GLN:HB3	1.93	0.51
9:O:156:LYS:NZ	9:O:170:ASP:HB2	2.26	0.51
12:T:57:DC:H2''	12:T:58:DC:C2	2.46	0.51
1:A:47:GLN:O	1:A:51:LYS:HG3	2.10	0.51
3:D:568:SER:HA	4:E:621:LEU:HD23	1.93	0.51
4:E:178:LEU:HB3	4:E:240:LEU:HG	1.92	0.51
6:H:110:DA:OP1	7:I:118:THR:N	2.33	0.51
9:O:284:TYR:OH	9:O:328:HIS:N	2.44	0.51
10:R:57:TYR:HB2	11:S:110:GLU:HG3	1.93	0.51
11:V:102:GLU:OE2	11:V:102:GLU:N	2.42	0.51
7:W:50:GLU:HB3	7:W:54:TYR:CE2	2.45	0.51
13:Y:240:LEU:HD13	13:Y:253:TRP:CD2	2.46	0.51
7:W:51:ILE:O	7:W:55:GLN:HG3	2.11	0.51
10:R:41:GLU:N	10:R:41:GLU:OE2	2.43	0.51
13:Y:223:HIS:HB2	13:Y:244:MET:CE	2.40	0.51
4:E:661:LYS:HG2	4:E:665:LYS:HZ1	1.76	0.51
5:G:336:MET:SD	5:G:337:GLU:N	2.84	0.51
6:H:159:DG:H4'	6:H:160:DA:H5'	1.93	0.51
3:D:672:MET:SD	3:D:672:MET:N	2.72	0.50
10:R:16:THR:HA	12:T:71:DT:H5''	1.92	0.50
3:D:666:PHE:O	4:E:287:ARG:NH2	2.39	0.50
7:I:67:PHE:CD2	7:I:93:GLN:HG3	2.46	0.50
12:T:118:DC:H2''	12:T:119:DC:C4	2.46	0.50
3:D:427:ARG:HG2	3:D:483:LYS:HG3	1.93	0.50
4:E:65:ILE:HG12	5:G:106:LYS:HG2	1.93	0.50
3:D:321:GLU:O	3:D:322:MET:HG3	2.11	0.50
4:E:29:LEU:HA	4:E:32:PHE:CZ	2.47	0.50
4:E:60:TRP:HE1	5:G:105:SER:H	1.60	0.50
4:E:245:LYS:O	4:E:248:THR:OG1	2.29	0.50
4:E:633:ILE:HB	4:E:727:LEU:HD21	1.93	0.50
5:G:222:THR:HG1	5:G:224:THR:HG1	1.57	0.50
10:R:63:LEU:HA	10:R:66:ALA:HB3	1.93	0.50
3:D:632:MET:HG2	3:D:668:LEU:HB3	1.93	0.50
4:E:83:CYS:HB3	4:E:98:LEU:HD21	1.93	0.50
4:E:558:CYS:HB3	4:E:561:ARG:NE	2.26	0.50
9:O:175:GLY:HA3	9:O:219:ALA:HB2	1.93	0.50
9:O:320:ILE:HG21	9:O:335:SER:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:79:DA:OP1	11:V:84:SER:N	2.30	0.50
6:H:109:DG:N2	12:T:119:DC:O2	2.44	0.50
8:J:70:VAL:O	8:J:73:THR:OG1	2.25	0.50
9:O:325:TRP:CE2	9:O:333:LEU:HD13	2.47	0.50
10:U:54:VAL:O	10:U:58:LEU:HG	2.11	0.50
7:W:54:TYR:O	8:X:40:ARG:NH2	2.43	0.50
3:D:157:LEU:HD11	3:D:359:LEU:HD11	1.92	0.50
3:D:190:LYS:N	3:D:204:ARG:O	2.33	0.50
4:E:30:LYS:HA	4:E:33:ARG:HG2	1.94	0.50
4:E:437:TRP:CE2	4:E:466:LYS:HE3	2.46	0.50
4:E:510:LYS:O	4:E:513:LEU:HG	2.12	0.50
6:H:130:DA:OP1	7:W:69:ARG:NH1	2.44	0.50
8:J:35:ARG:O	8:J:39:ARG:HG2	2.12	0.50
10:R:88:ARG:HB3	10:R:108:LEU:HD11	1.93	0.50
12:T:171:DA:H2''	12:T:172:DG:O4'	2.11	0.50
13:Y:288:MET:O	13:Y:290:GLN:HG2	2.12	0.50
3:D:161:PHE:CD2	3:D:229:SER:HB2	2.47	0.50
4:E:237:ALA:HA	4:E:240:LEU:HD22	1.94	0.50
5:G:211:LYS:HA	5:G:238:GLU:HG3	1.93	0.50
6:H:117:DG:H1	12:T:110:DC:N4	2.10	0.50
10:R:79:ILE:HG22	10:R:82:HIS:ND1	2.27	0.50
12:T:168:DG:H2''	12:T:169:DC:C4	2.47	0.50
13:Y:275:ASP:OD2	13:Y:276:THR:N	2.45	0.50
4:E:661:LYS:O	4:E:665:LYS:NZ	2.42	0.50
8:J:62:LEU:HB3	8:J:66:ILE:HD11	1.93	0.50
10:U:55:LEU:HA	10:U:58:LEU:HD12	1.93	0.50
3:D:112:HIS:HA	3:D:115:LEU:HD13	1.93	0.49
5:G:358:TYR:CE2	5:G:361:CYS:HB3	2.47	0.49
4:E:88:ASP:OD2	5:G:87:SER:OG	2.30	0.49
4:E:732:ARG:CZ	7:I:30:PRO:HD3	2.43	0.49
10:R:18:SER:OG	10:R:23:LEU:O	2.27	0.49
12:T:111:DG:H2''	12:T:112:DC:O5'	2.12	0.49
3:D:497:GLY:O	13:Y:188:ASP:HA	2.13	0.49
5:G:171:ILE:HG23	5:G:187:VAL:HG22	1.94	0.49
5:G:386:LEU:HD12	5:G:404:LEU:HB2	1.94	0.49
6:H:166:DC:N3	12:T:60:DA:N6	2.61	0.49
9:O:279:LEU:HD12	9:O:291:THR:HG22	1.95	0.49
12:T:112:DC:H2''	12:T:113:DG:H8	1.77	0.49
13:Y:259:ARG:O	13:Y:260:HIS:HB3	2.12	0.49
1:A:85:GLY:HA3	1:A:90:GLY:HA3	1.93	0.49
3:D:100:LEU:HA	3:D:103:ARG:NH1	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:45:DA:C8	6:H:46:DT:H72	2.47	0.49
6:H:77:DG:H2''	6:H:78:DG:C8	2.47	0.49
6:H:85:DC:H4'	6:H:86:DC:OP1	2.12	0.49
6:H:112:DA:H61	12:T:115:DC:H42	1.59	0.49
12:T:152:DC:H2''	12:T:153:DA:C8	2.48	0.49
4:E:171:PHE:O	4:E:175:VAL:HG23	2.12	0.49
9:O:307:LYS:HG3	9:O:308:LEU:HG	1.94	0.49
12:T:105:DA:H2''	12:T:106:DC:H5''	1.94	0.49
3:D:478:TYR:OH	3:D:484:GLY:O	2.20	0.49
3:D:565:TYR:HD1	4:E:622:ALA:HB2	1.77	0.49
4:E:31:ARG:HG3	4:E:34:ARG:HH21	1.78	0.49
5:G:229:PHE:CD1	5:G:294:ILE:HD12	2.47	0.49
9:O:49:TRP:HA	9:O:66:LEU:HD13	1.94	0.49
9:O:172:ARG:HG3	9:O:216:VAL:HG13	1.94	0.49
1:A:88:ALA:HA	1:A:92:PHE:HZ	1.78	0.49
4:E:643:ILE:HG22	4:E:644:SER:H	1.76	0.49
6:H:113:DG:H1'	6:H:114:DC:H5'	1.95	0.49
7:W:72:ARG:HA	7:W:84:PHE:HE2	1.78	0.49
3:D:158:GLN:HB2	3:D:360:ARG:HB2	1.94	0.49
4:E:502:ARG:NH1	7:I:39:HIS:HB3	2.28	0.49
4:E:673:ASN:HB2	7:I:26:ARG:HB3	1.95	0.49
4:E:44:SER:O	4:E:47:GLN:HG2	2.13	0.49
12:T:178:DT:H2''	12:T:179:DA:H8	1.78	0.49
7:W:116:ARG:NH2	7:W:120:MET:SD	2.86	0.49
13:Y:225:THR:O	13:Y:242:HIS:N	2.40	0.49
3:D:187:LEU:HB2	3:D:251:LEU:HB2	1.95	0.48
4:E:65:ILE:HG21	5:G:105:SER:HA	1.95	0.48
5:G:323:SER:O	5:G:358:TYR:OH	2.30	0.48
5:G:360:GLN:OE1	5:G:381:ASN:ND2	2.46	0.48
11:V:102:GLU:HA	11:V:105:LYS:HZ3	1.78	0.48
4:E:28:GLN:HG3	4:E:32:PHE:CD1	2.48	0.48
4:E:621:LEU:HD12	4:E:622:ALA:N	2.28	0.48
5:G:406:HIS:HB2	5:G:437:TRP:HZ2	1.77	0.48
9:O:85:GLN:HB2	9:O:114:LYS:HB3	1.94	0.48
9:O:345:TRP:HA	9:O:367:LEU:H	1.77	0.48
11:V:54:LYS:HA	11:V:54:LYS:HE2	1.95	0.48
5:G:170:GLY:HA2	5:G:193:ILE:HG12	1.95	0.48
7:I:56:LYS:NZ	10:R:81:ARG:HH21	2.10	0.48
11:S:83:ARG:NH2	12:T:80:DG:H3'	2.28	0.48
1:A:46:ARG:HD2	1:A:89:SER:HA	1.95	0.48
7:I:113:HIS:CD2	7:W:126:LEU:HD22	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:T:168:DG:H2''	12:T:169:DC:C2	2.49	0.48
7:W:103:LEU:O	7:W:107:THR:HG23	2.13	0.48
5:G:150:CYS:HB2	5:G:163:LEU:HD21	1.96	0.48
6:H:111:DC:H2''	6:H:112:DA:C8	2.48	0.48
12:T:111:DG:H2'	12:T:112:DC:C6	2.48	0.48
11:V:87:THR:OG1	11:V:90:GLU:OE1	2.22	0.48
3:D:528:ILE:HB	3:D:557:TYR:HB3	1.95	0.48
3:D:606:VAL:HB	3:D:611:LYS:HE3	1.95	0.48
4:E:445:PHE:CZ	4:E:475:ARG:HG2	2.49	0.48
5:G:86:ASN:HB3	5:G:436:ARG:HB3	1.96	0.48
9:O:346:ASP:N	9:O:365:GLU:O	2.32	0.48
8:X:78:ARG:HH22	8:X:85:ASP:CG	2.17	0.48
3:D:471:HIS:HB2	3:D:476:PHE:HZ	1.78	0.48
4:E:565:CYS:O	4:E:590:CYS:HA	2.13	0.48
9:O:298:VAL:O	9:O:313:PHE:N	2.37	0.48
1:A:25:PRO:HG2	1:A:30:MET:SD	2.54	0.48
5:G:311:CYS:SG	5:G:367:ARG:HA	2.54	0.48
8:J:98:TYR:CE2	10:R:100:VAL:HG11	2.49	0.48
3:D:189:VAL:HA	3:D:205:GLN:HA	1.96	0.47
4:E:584:GLU:HG3	4:E:608:ASN:O	2.13	0.47
6:H:116:DC:H2''	6:H:117:DG:C8	2.49	0.47
10:U:92:GLU:HG2	11:V:103:LEU:HD21	1.96	0.47
13:Y:215:GLY:HA3	13:Y:219:SER:O	2.14	0.47
1:A:45:SER:HA	1:A:91:SER:HA	1.96	0.47
4:E:99:LYS:HD2	5:G:138:TYR:HD2	1.79	0.47
5:G:240:LEU:HD23	5:G:255:GLY:HA2	1.96	0.47
5:G:243:ASP:OD2	5:G:314:TRP:N	2.38	0.47
6:H:70:DA:H61	12:T:157:DC:H42	1.62	0.47
9:O:340:ARG:HH21	9:O:374:THR:HA	1.78	0.47
11:S:91:ILE:HA	11:S:94:ALA:HB3	1.97	0.47
10:U:52:ALA:HA	10:U:55:LEU:HD12	1.97	0.47
3:D:101:ARG:HD3	3:D:452:TRP:O	2.14	0.47
3:D:164:PHE:HB2	3:D:213:VAL:HG11	1.96	0.47
3:D:192:CYS:HA	3:D:245:VAL:HB	1.96	0.47
5:G:360:GLN:OE1	5:G:385:LYS:NZ	2.25	0.47
10:U:78:ILE:HB	11:V:51:ILE:HG22	1.95	0.47
11:V:37:TYR:O	11:V:41:VAL:HG22	2.13	0.47
3:D:307:ARG:HH22	3:D:309:GLN:HG2	1.78	0.47
4:E:171:PHE:O	4:E:175:VAL:N	2.46	0.47
4:E:604:VAL:HG21	4:E:609:CYS:SG	2.54	0.47
6:H:73:DC:H2'	6:H:74:DT:C6	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:O:186:ASN:HD21	9:O:240:GLU:HB2	1.80	0.47
12:T:88:DC:H2''	12:T:89:DA:C8	2.49	0.47
3:D:657:MET:SD	3:D:657:MET:N	2.88	0.47
4:E:170:ILE:O	4:E:174:LEU:N	2.43	0.47
5:G:96:LEU:HG	5:G:432:ALA:HA	1.97	0.47
5:G:219:ASN:O	5:G:223:ASP:N	2.47	0.47
5:G:352:ILE:O	5:G:353:LEU:HD23	2.14	0.47
9:O:129:ARG:N	9:O:143:LYS:HB2	2.29	0.47
11:V:77:LEU:HA	11:V:80:TYR:HB2	1.95	0.47
8:X:93:GLN:NE2	8:X:95:ARG:HG3	2.30	0.47
3:D:183:THR:OG1	3:D:211:LYS:O	2.32	0.47
4:E:673:ASN:N	7:I:27:LYS:O	2.42	0.47
11:V:91:ILE:O	11:V:95:VAL:HG23	2.15	0.47
7:W:121:PRO:HB3	8:X:53:GLU:HG2	1.96	0.47
5:G:383:VAL:HG23	5:G:385:LYS:HG3	1.95	0.47
6:H:80:DG:OP2	11:V:83:ARG:NH1	2.48	0.47
6:H:94:DG:H2''	6:H:95:DG:C8	2.49	0.47
6:H:158:DG:N2	12:T:69:DT:H3	2.13	0.47
7:I:121:PRO:O	7:I:124:ILE:HG22	2.15	0.47
9:O:185:TRP:CE3	9:O:193:LEU:HB3	2.50	0.47
3:D:591:TRP:CE3	5:G:232:VAL:HG11	2.49	0.47
5:G:329:VAL:HG23	5:G:354:GLY:O	2.15	0.47
11:S:108:VAL:O	11:S:112:THR:HG23	2.15	0.47
3:D:460:LEU:HD12	3:D:463:LEU:HD22	1.97	0.47
4:E:174:LEU:HD21	4:E:227:ILE:HG23	1.97	0.47
4:E:466:LYS:HB3	4:E:471:VAL:HG23	1.96	0.47
4:E:637:VAL:O	4:E:721:ILE:N	2.26	0.47
4:E:694:HIS:HB2	4:E:731:TYR:CZ	2.50	0.47
4:E:24:MET:O	4:E:28:GLN:N	2.45	0.47
4:E:44:SER:HA	4:E:47:GLN:OE1	2.15	0.47
8:J:66:ILE:HA	8:J:69:ALA:HB3	1.97	0.47
9:O:344:VAL:O	9:O:367:LEU:N	2.48	0.47
13:Y:258:GLU:CA	13:Y:261:GLN:HE22	2.28	0.47
4:E:657:ASP:O	4:E:661:LYS:N	2.36	0.46
6:H:56:DT:H6	6:H:56:DT:H2''	1.60	0.46
7:W:65:LEU:HG	7:W:69:ARG:HH11	1.81	0.46
6:H:46:DT:H2''	6:H:47:DG:C8	2.51	0.46
7:I:133:GLU:N	7:I:133:GLU:OE1	2.48	0.46
9:O:318:ASP:HB2	9:O:339:ASP:HB3	1.97	0.46
3:D:184:LEU:HD12	3:D:254:VAL:HG22	1.96	0.46
3:D:590:GLU:OE1	3:D:593:ARG:NH2	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:609:CYS:SG	4:E:613:ARG:NH1	2.88	0.46
4:E:745:GLU:O	4:E:746:ARG:HG3	2.16	0.46
6:H:169:DG:H1'	6:H:170:DG:N7	2.30	0.46
8:J:53:GLU:CD	8:J:53:GLU:H	2.17	0.46
10:R:25:PHE:CZ	10:R:59:THR:HG21	2.51	0.46
13:Y:258:GLU:HA	13:Y:261:GLN:HE22	1.80	0.46
13:Y:258:GLU:OE2	13:Y:258:GLU:N	2.35	0.46
3:D:564:LEU:HD12	3:D:565:TYR:H	1.79	0.46
4:E:273:GLN:HE21	4:E:275:GLU:HB3	1.80	0.46
4:E:274:ARG:HA	4:E:447:VAL:HG22	1.97	0.46
4:E:584:GLU:HA	4:E:608:ASN:ND2	2.31	0.46
5:G:267:SER:O	5:G:270:MET:HG2	2.16	0.46
10:R:26:PRO:HB2	10:R:29:ARG:HB3	1.97	0.46
12:T:119:DC:H2''	12:T:120:DC:C5	2.50	0.46
10:U:92:GLU:OE2	11:V:102:GLU:N	2.49	0.46
3:D:617:TRP:O	3:D:621:VAL:HG23	2.15	0.46
6:H:211:DG:N2	12:T:17:DC:O2	2.49	0.46
10:R:91:GLU:CD	10:R:91:GLU:H	2.19	0.46
11:V:31:LYS:NZ	11:V:32:GLU:O	2.48	0.46
2:B:150:ARG:HH22	3:D:90:PHE:C	2.19	0.46
4:E:669:SER:HB3	14:E:801:SAH:H3'	1.97	0.46
7:I:49:ARG:NH1	12:T:49:DT:OP1	2.47	0.46
9:O:202:ILE:HG21	9:O:233:VAL:HG21	1.97	0.46
12:T:65:DG:C8	12:T:65:DG:H5'	2.51	0.46
10:U:55:LEU:O	10:U:59:THR:HG22	2.15	0.46
5:G:311:CYS:HB3	5:G:368:PHE:CE2	2.51	0.46
6:H:78:DG:H2''	6:H:79:DA:C8	2.51	0.46
9:O:328:HIS:O	9:O:329:ASN:ND2	2.48	0.46
1:A:63:ALA:O	1:A:67:ILE:HG12	2.16	0.46
2:B:150:ARG:HB3	3:D:87:LEU:HD22	1.98	0.46
5:G:312:VAL:HG12	5:G:321:SER:HA	1.97	0.46
5:G:359:SER:HB3	5:G:360:GLN:NE2	2.30	0.46
4:E:71:LEU:HB2	5:G:136:GLN:HB3	1.97	0.46
4:E:512:GLN:HA	4:E:516:ASP:HB2	1.98	0.46
6:H:54:DC:H42	12:T:173:DA:N6	2.14	0.46
9:O:84:VAL:HG13	9:O:86:LEU:HD11	1.98	0.46
10:R:50:TYR:O	10:R:54:VAL:HG23	2.16	0.46
12:T:133:DC:N4	12:T:134:DG:O6	2.48	0.46
12:T:137:DA:H1'	12:T:138:DA:H5'	1.97	0.46
10:U:78:ILE:HB	11:V:51:ILE:HA	1.98	0.46
3:D:163:GLY:CA	3:D:221:GLN:HE22	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:195:LYS:N	3:D:198:ASP:OD2	2.45	0.46
4:E:554:CYS:HB3	4:E:558:CYS:CB	2.45	0.46
5:G:176:ASN:O	5:G:180:MET:N	2.47	0.46
6:H:151:DG:H2''	6:H:152:DA:C8	2.50	0.46
6:H:160:DA:H61	12:T:67:DC:H42	1.63	0.46
7:I:103:LEU:HG	7:I:124:ILE:HD11	1.98	0.46
9:O:49:TRP:HZ2	9:O:391:CYS:HB3	1.81	0.46
10:U:112:GLN:HB2	10:U:115:LEU:HG	1.98	0.46
11:V:73:GLU:OE2	11:V:73:GLU:N	2.48	0.46
4:E:562:PHE:CG	4:E:563:PRO:HD2	2.51	0.45
4:E:636:PRO:HD3	4:E:723:THR:OG1	2.15	0.45
9:O:56:PRO:HB2	9:O:59:LYS:HD2	1.98	0.45
10:U:76:THR:O	11:V:50:GLY:N	2.40	0.45
11:V:66:VAL:O	11:V:70:ILE:HG22	2.15	0.45
3:D:86:PHE:CD1	3:D:434:TYR:HB2	2.52	0.45
4:E:106:SER:HB2	5:G:169:ARG:HH21	1.81	0.45
4:E:110:MET:HB3	4:E:629:TRP:NE1	2.32	0.45
5:G:213:HIS:N	5:G:213:HIS:CD2	2.84	0.45
6:H:47:DG:C8	6:H:48:DT:H72	2.51	0.45
6:H:140:DG:P	7:W:83:ARG:HH21	2.40	0.45
9:O:120:LYS:HB3	9:O:161:PRO:HB3	1.98	0.45
9:O:184:SER:O	9:O:235:TRP:NE1	2.47	0.45
10:R:29:ARG:NE	11:S:32:GLU:OE2	2.49	0.45
12:T:97:DC:H2'	12:T:98:DT:C5	2.51	0.45
7:W:107:THR:HG21	7:W:124:ILE:HG13	1.98	0.45
13:Y:222:PHE:HB2	13:Y:265:LYS:HB3	1.96	0.45
1:A:27:TYR:OH	1:A:66:GLN:OE1	2.22	0.45
6:H:156:DA:H2'	6:H:157:DT:H71	1.98	0.45
10:R:56:GLU:HA	10:R:59:THR:HG22	1.98	0.45
8:J:88:TYR:CD1	11:V:80:TYR:HE1	2.34	0.45
9:O:57:GLU:O	9:O:59:LYS:HG3	2.16	0.45
13:Y:223:HIS:HB2	13:Y:244:MET:HE1	1.97	0.45
3:D:540:MET:HG3	3:D:544:LEU:HG	1.97	0.45
5:G:331:TRP:CE3	5:G:350:VAL:HG13	2.52	0.45
6:H:43:DG:C6	6:H:44:DG:C6	3.04	0.45
7:I:42:ARG:O	7:I:45:THR:HG22	2.16	0.45
7:I:60:LEU:HD23	7:I:62:ILE:N	2.30	0.45
12:T:153:DA:H2''	12:T:154:DG:H8	1.81	0.45
12:T:155:DT:H1'	12:T:156:DC:H5'	1.99	0.45
13:Y:226:VAL:HG21	13:Y:239:LEU:HD13	1.99	0.45
3:D:86:PHE:CE1	3:D:434:TYR:HB2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:468:LYS:HA	3:D:476:PHE:CE2	2.51	0.45
3:D:499:TYR:HB2	13:Y:189:PHE:CD1	2.52	0.45
11:S:113:LYS:O	11:S:116:THR:OG1	2.28	0.45
7:W:124:ILE:HD12	7:W:124:ILE:H	1.81	0.45
13:Y:278:LEU:HD21	13:Y:285:TYR:HB3	1.99	0.45
4:E:537:SER:HA	4:E:542:VAL:HG11	1.98	0.45
4:E:637:VAL:HG22	4:E:721:ILE:HB	1.99	0.45
5:G:226:VAL:HG12	5:G:227:ALA:N	2.30	0.45
6:H:117:DG:N2	12:T:110:DC:N3	2.60	0.45
9:O:230:VAL:HA	9:O:247:ALA:HB2	1.98	0.45
9:O:396:ASP:HB3	9:O:398:ILE:HG12	1.98	0.45
12:T:80:DG:H2''	12:T:81:DA:H8	1.80	0.45
7:W:86:SER:O	7:W:89:VAL:HG12	2.17	0.45
4:E:46:ARG:NH2	5:G:375:LYS:HG2	2.29	0.45
4:E:239:GLU:OE1	4:E:242:GLU:HB2	2.15	0.45
12:T:122:DC:H2''	12:T:123:DG:O5'	2.17	0.45
4:E:35:ALA:HA	4:E:38:VAL:HG22	1.99	0.45
4:E:99:LYS:HB3	5:G:138:TYR:CD2	2.51	0.45
4:E:667:MET:SD	4:E:667:MET:N	2.89	0.45
6:H:87:DC:H2''	6:H:88:DC:C5	2.51	0.45
8:J:66:ILE:HG22	8:J:70:VAL:HG23	1.99	0.45
9:O:281:PHE:CD2	9:O:289:LEU:HD13	2.51	0.45
11:S:88:SER:HA	11:S:91:ILE:HD11	1.99	0.45
3:D:351:GLN:N	3:D:351:GLN:OE1	2.50	0.45
6:H:207:DG:H2''	6:H:208:DA:C8	2.52	0.45
9:O:180:GLY:HA3	9:O:197:SER:HA	1.98	0.45
1:A:27:TYR:HE1	12:T:194:DG:H5''	1.81	0.44
3:D:218:ASP:N	3:D:218:ASP:OD1	2.49	0.44
4:E:289:CYS:N	4:E:297:HIS:HE1	2.15	0.44
5:G:409:CYS:HB2	5:G:435:TRP:CE2	2.52	0.44
6:H:36:DG:C2	6:H:37:DC:C2	3.05	0.44
4:E:178:LEU:HD22	4:E:240:LEU:HD12	1.99	0.44
4:E:296:LEU:HD23	4:E:296:LEU:H	1.83	0.44
6:H:130:DA:H61	12:T:97:DC:H42	1.63	0.44
9:O:153:ASP:O	9:O:156:LYS:HG2	2.18	0.44
12:T:107:DG:H1'	12:T:108:DT:C2	2.51	0.44
7:W:51:ILE:HG22	7:W:55:GLN:OE1	2.17	0.44
13:Y:244:MET:O	13:Y:246:GLU:HG3	2.17	0.44
3:D:307:ARG:NH1	3:D:309:GLN:HA	2.30	0.44
4:E:328:GLN:O	4:E:469:ARG:N	2.45	0.44
5:G:145:GLU:HB2	5:G:168:SER:OG	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:O:59:LYS:HB3	9:O:61:PHE:CE2	2.52	0.44
9:O:287:PHE:HB3	9:O:302:ASP:OD1	2.17	0.44
10:U:110:ASN:H	7:W:55:GLN:HE22	1.65	0.44
13:Y:222:PHE:HB3	13:Y:243:TRP:CE3	2.51	0.44
2:B:147:LEU:O	2:B:150:ARG:HG2	2.17	0.44
4:E:41:MET:HA	4:E:44:SER:OG	2.18	0.44
4:E:587:PRO:O	4:E:596:ALA:HB2	2.17	0.44
5:G:103:TRP:CZ3	5:G:372:PHE:HA	2.53	0.44
5:G:227:ALA:HA	5:G:292:GLN:H	1.82	0.44
6:H:39:DT:H2''	6:H:40:DA:H8	1.83	0.44
6:H:139:DA:H2''	6:H:140:DG:C8	2.53	0.44
6:H:192:DG:N2	12:T:36:DG:N3	2.65	0.44
9:O:225:GLY:HA3	9:O:255:TRP:CZ2	2.52	0.44
10:R:26:PRO:HD3	11:S:37:TYR:CG	2.53	0.44
11:S:113:LYS:O	11:S:117:LYS:HG3	2.17	0.44
12:T:104:DC:H4'	12:T:105:DA:OP1	2.16	0.44
11:V:108:VAL:O	11:V:112:THR:HG23	2.17	0.44
3:D:159:LEU:HG	3:D:231:ALA:HB3	1.99	0.44
4:E:625:ASP:O	13:Y:184:PRO:HD2	2.17	0.44
6:H:119:DA:H1'	6:H:120:DC:C2	2.53	0.44
6:H:210:DG:H2''	6:H:211:DG:H8	1.83	0.44
7:I:108:ASN:HD21	8:J:43:VAL:HA	1.82	0.44
9:O:129:ARG:H	9:O:143:LYS:HB2	1.82	0.44
9:O:387:PRO:HG2	9:O:388:TRP:CD1	2.53	0.44
12:T:173:DA:H3'	12:T:174:DT:H71	1.99	0.44
11:V:58:ILE:HG23	8:X:98:TYR:HB3	1.99	0.44
4:E:224:PHE:HB3	4:E:236:THR:HA	1.99	0.44
5:G:112:VAL:HG13	5:G:135:LEU:HD12	1.99	0.44
5:G:225:LEU:HD21	5:G:228:ILE:HD11	2.00	0.44
9:O:325:TRP:CZ3	9:O:347:LEU:HD11	2.52	0.44
10:R:26:PRO:HB3	11:S:37:TYR:CZ	2.53	0.44
12:T:142:DG:C6	12:T:143:DA:C6	3.05	0.44
10:U:68:ASN:OD1	10:U:71:ARG:NH1	2.47	0.44
13:Y:286:ARG:HG3	13:Y:286:ARG:HH11	1.82	0.44
3:D:535:ARG:NH1	9:O:30:PHE:O	2.44	0.44
3:D:556:THR:HG1	13:Y:173:ARG:HH21	1.61	0.44
4:E:121:MET:HE1	4:E:297:HIS:N	2.33	0.44
4:E:662:VAL:HA	4:E:665:LYS:HE2	1.99	0.44
6:H:48:DT:H2''	6:H:49:DA:H8	1.83	0.44
9:O:126:GLU:O	9:O:145:PRO:HD3	2.17	0.44
8:X:54:THR:HA	8:X:57:VAL:HB	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Y:275:ASP:O	13:Y:279:LEU:HG	2.17	0.44
4:E:512:GLN:NE2	7:I:33:GLY:O	2.51	0.44
7:I:109:LEU:HA	7:I:112:ILE:HG12	1.99	0.44
9:O:33:ASP:HB2	9:O:403:GLN:HG2	2.00	0.44
3:D:103:ARG:O	3:D:107:ALA:N	2.24	0.44
3:D:529:LEU:HD12	9:O:35:VAL:HG11	2.00	0.44
3:D:659:HIS:CE1	4:E:292:TYR:HH	2.36	0.44
4:E:46:ARG:HD2	4:E:49:ILE:HD12	2.00	0.44
4:E:322:ASN:O	4:E:331:GLN:NE2	2.47	0.44
4:E:469:ARG:NH1	4:E:473:GLU:OE2	2.51	0.44
9:O:138:CYS:HA	9:O:154:TYR:CE2	2.53	0.44
10:R:97:LEU:HD11	11:S:62:PHE:CE2	2.53	0.44
13:Y:214:LEU:HD12	13:Y:221:VAL:HG21	1.99	0.44
2:B:147:LEU:O	2:B:151:LYS:HE2	2.18	0.43
3:D:448:LEU:O	3:D:457:CYS:N	2.51	0.43
3:D:481:HIS:ND1	3:D:486:ARG:HD3	2.33	0.43
4:E:111:TYR:CE1	5:G:212:ASP:HA	2.53	0.43
4:E:510:LYS:HB3	4:E:514:LYS:HE2	2.00	0.43
6:H:162:DC:H2''	6:H:163:DG:C8	2.53	0.43
9:O:147:SER:HB3	9:O:176:HIS:O	2.18	0.43
9:O:194:LEU:HG	9:O:235:TRP:CZ2	2.52	0.43
11:S:102:GLU:HA	11:S:105:LYS:HZ1	1.81	0.43
1:A:62:ASN:O	1:A:66:GLN:HG3	2.17	0.43
3:D:161:PHE:CG	3:D:211:LYS:HD3	2.53	0.43
4:E:59:GLU:HA	4:E:62:GLN:HG2	2.00	0.43
4:E:110:MET:HB3	4:E:629:TRP:HE1	1.83	0.43
4:E:522:VAL:O	4:E:675:ASN:ND2	2.47	0.43
5:G:210:SER:OG	5:G:212:ASP:OD1	2.22	0.43
6:H:198:DG:C2	12:T:30:DG:C2	3.06	0.43
8:J:98:TYR:CE2	11:S:62:PHE:HD2	2.36	0.43
9:O:81:ILE:HD12	9:O:119:ILE:HD13	2.00	0.43
10:U:21:ALA:HB2	11:V:118:TYR:HB2	2.00	0.43
4:E:74:VAL:O	4:E:78:ARG:HD2	2.18	0.43
4:E:540:PRO:HA	4:E:543:ILE:HG12	2.00	0.43
5:G:83:LYS:NZ	5:G:84:CYS:O	2.47	0.43
5:G:326:ASN:HA	5:G:358:TYR:CE2	2.52	0.43
6:H:144:DT:H2''	6:H:145:DG:H8	1.83	0.43
6:H:194:DC:H2''	6:H:195:DA:C8	2.53	0.43
9:O:79:LEU:HD12	9:O:121:ILE:O	2.18	0.43
10:R:97:LEU:HD11	11:S:62:PHE:HE2	1.83	0.43
13:Y:173:ARG:HD3	13:Y:174:LYS:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:655:ASN:OD1	4:E:263:ASN:HB2	2.18	0.43
4:E:623:PRO:HA	4:E:629:TRP:HA	2.00	0.43
7:I:62:ILE:HG21	7:I:67:PHE:CE1	2.53	0.43
3:D:618:ASN:O	3:D:621:VAL:N	2.39	0.43
5:G:323:SER:OG	5:G:324:CYS:N	2.52	0.43
5:G:384:GLY:HA2	5:G:413:ILE:HG13	2.00	0.43
6:H:192:DG:H2''	6:H:193:DG:H8	1.83	0.43
9:O:277:ASN:N	9:O:277:ASN:OD1	2.50	0.43
12:T:36:DG:C6	12:T:37:DG:C6	3.07	0.43
12:T:82:DC:H4'	12:T:83:DA:OP1	2.17	0.43
11:V:86:ILE:HD12	11:V:86:ILE:HA	1.83	0.43
2:B:150:ARG:NH1	3:D:91:GLU:HA	2.33	0.43
5:G:235:HIS:CE1	5:G:259:SER:HB2	2.54	0.43
10:R:79:ILE:HG22	10:R:82:HIS:CG	2.53	0.43
4:E:30:LYS:H	4:E:30:LYS:HD3	1.83	0.43
4:E:244:TYR:HA	4:E:247:LEU:HD12	2.00	0.43
4:E:701:TYR:CZ	4:E:716:PHE:HB2	2.53	0.43
6:H:133:DG:C4	6:H:134:DG:C8	3.06	0.43
10:R:80:PRO:HA	10:R:83:LEU:HB2	2.00	0.43
10:U:95:LYS:HD3	10:U:95:LYS:HA	1.62	0.43
7:W:83:ARG:O	8:X:80:THR:HA	2.18	0.43
8:X:70:VAL:HG12	8:X:74:GLU:OE1	2.18	0.43
1:A:27:TYR:CE1	12:T:194:DG:H5''	2.54	0.43
3:D:193:HIS:ND1	3:D:246:LYS:HG2	2.33	0.43
6:H:41:DC:H2''	6:H:42:DA:C8	2.54	0.43
6:H:121:DG:OP1	8:X:46:ILE:HG13	2.19	0.43
6:H:141:DA:H2''	6:H:142:DG:C8	2.51	0.43
12:T:45:DA:C6	12:T:46:DG:C6	3.07	0.43
12:T:69:DT:H2''	12:T:70:DA:C8	2.54	0.43
12:T:118:DC:H2''	12:T:119:DC:C5	2.54	0.43
10:U:82:HIS:HA	10:U:85:LEU:HD12	2.01	0.43
10:U:104:GLN:O	7:W:58:THR:OG1	2.34	0.43
11:V:115:VAL:O	11:V:119:THR:HG23	2.19	0.43
7:W:106:ASP:OD2	7:W:131:ARG:NH2	2.51	0.43
8:X:63:GLU:CD	8:X:63:GLU:H	2.22	0.43
3:D:100:LEU:HD23	3:D:103:ARG:HH12	1.84	0.43
3:D:122:ASN:HA	3:D:124:ARG:NH1	2.34	0.43
3:D:127:ILE:HD12	3:D:127:ILE:H	1.82	0.43
4:E:54:GLU:OE2	4:E:58:GLN:NE2	2.36	0.43
4:E:57:ASN:OD1	5:G:420:ARG:NH2	2.42	0.43
5:G:184:LYS:HB3	5:G:186:TYR:CE2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:259:SER:HA	5:G:302:ARG:HG2	2.00	0.43
5:G:271:MET:HA	5:G:274:ILE:HB	2.01	0.43
5:G:389:TRP:CD1	5:G:401:CYS:HA	2.54	0.43
9:O:322:GLN:NE2	9:O:379:ASP:OD1	2.51	0.43
10:R:17:ARG:HG2	10:R:20:ARG:HH21	1.84	0.43
12:T:134:DG:C5	12:T:135:DC:C4	3.07	0.43
4:E:221:ASP:HA	4:E:224:PHE:CD2	2.54	0.43
4:E:584:GLU:HG2	4:E:612:GLN:NE2	2.34	0.43
5:G:418:PHE:CD1	5:G:425:LEU:HD13	2.54	0.43
5:G:427:ALA:O	5:G:435:TRP:N	2.49	0.43
10:R:13:LYS:O	10:R:15:LYS:NZ	2.52	0.43
10:R:79:ILE:HG13	10:R:80:PRO:HD2	1.99	0.43
12:T:129:DT:H2''	12:T:130:DA:N7	2.34	0.43
11:V:82:LYS:HD3	11:V:82:LYS:N	2.34	0.43
7:W:62:ILE:HB	7:W:93:GLN:HE21	1.84	0.43
7:W:110:CYS:O	7:W:114:ALA:N	2.52	0.43
8:X:71:THR:HA	8:X:74:GLU:OE1	2.19	0.43
3:D:254:VAL:HB	3:D:295:PHE:CG	2.54	0.42
3:D:295:PHE:N	3:D:322:MET:H	2.17	0.42
5:G:404:LEU:HB3	5:G:437:TRP:CZ3	2.54	0.42
6:H:174:DC:H2''	6:H:175:DG:O5'	2.19	0.42
7:I:37:LYS:HD2	7:I:37:LYS:HA	1.90	0.42
7:I:124:ILE:HD12	7:I:124:ILE:HA	1.86	0.42
9:O:60:ASP:O	9:O:88:ASN:N	2.28	0.42
1:A:30:MET:H	1:A:30:MET:CE	2.32	0.42
3:D:92:LYS:H	3:D:92:LYS:HG3	1.57	0.42
3:D:585:ASP:OD2	4:E:688:LYS:HE3	2.19	0.42
5:G:343:ILE:HD13	5:G:343:ILE:HA	1.87	0.42
6:H:89:DT:H6	6:H:89:DT:H2'	1.69	0.42
9:O:253:MET:HB2	9:O:265:PRO:CB	2.49	0.42
12:T:75:DT:H2''	12:T:76:DC:C6	2.55	0.42
7:W:122:LYS:HA	7:W:125:GLN:OE1	2.18	0.42
3:D:161:PHE:CE1	3:D:231:ALA:HB2	2.55	0.42
3:D:664:HIS:CD2	3:D:669:ILE:HG22	2.54	0.42
5:G:199:HIS:HB3	5:G:202:ASP:O	2.20	0.42
6:H:158:DG:H2''	6:H:159:DG:N7	2.34	0.42
9:O:226:HIS:CD2	9:O:247:ALA:HB3	2.54	0.42
11:S:111:GLY:O	11:S:115:VAL:HG23	2.19	0.42
12:T:93:DC:H4'	12:T:94:DC:OP1	2.17	0.42
10:U:50:TYR:OH	11:V:108:VAL:HA	2.19	0.42
7:W:110:CYS:HA	7:W:113:HIS:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:122:ASN:OD1	3:D:124:ARG:NH1	2.44	0.42
3:D:563:ARG:NH1	4:E:625:ASP:OD1	2.37	0.42
3:D:664:HIS:HD2	3:D:674:ILE:HD11	1.84	0.42
5:G:298:ASP:O	5:G:345:PRO:HA	2.19	0.42
7:I:60:LEU:HD23	7:I:61:LEU:N	2.34	0.42
9:O:184:SER:CB	9:O:234:SER:HA	2.50	0.42
9:O:323:VAL:HG12	9:O:335:SER:HB3	2.02	0.42
12:T:42:DC:H2''	12:T:43:DG:C8	2.55	0.42
12:T:111:DG:OP1	7:W:118:THR:N	2.27	0.42
13:Y:191:ASP:HB3	13:Y:194:THR:HG22	2.00	0.42
3:D:525:ILE:HA	3:D:525:ILE:HD12	1.77	0.42
3:D:617:TRP:O	3:D:620:HIS:HB3	2.19	0.42
4:E:239:GLU:OE1	4:E:243:LYS:HE3	2.18	0.42
5:G:186:TYR:OH	5:G:223:ASP:OD1	2.36	0.42
5:G:253:SER:OG	5:G:261:LYS:O	2.19	0.42
12:T:30:DG:C2	12:T:31:DC:C2	3.08	0.42
3:D:193:HIS:CE1	3:D:246:LYS:HG2	2.54	0.42
4:E:506:ALA:O	4:E:510:LYS:HG3	2.19	0.42
4:E:572:ASN:HB2	4:E:607:LYS:HB2	2.02	0.42
9:O:370:HIS:CE1	9:O:372:GLY:H	2.37	0.42
10:U:51:LEU:O	10:U:55:LEU:HG	2.19	0.42
7:W:116:ARG:HH22	7:W:123:ASP:CG	2.23	0.42
4:E:539:CYS:HB3	4:E:542:VAL:HB	2.01	0.42
4:E:619:LEU:HD12	4:E:631:ILE:HG22	2.00	0.42
4:E:637:VAL:N	4:E:721:ILE:O	2.47	0.42
4:E:670:PHE:O	4:E:681:ASP:HA	2.20	0.42
5:G:419:SER:C	5:G:421:ASP:H	2.23	0.42
8:J:82:THR:OG1	8:J:85:ASP:OD2	2.27	0.42
9:O:40:LEU:H	9:O:397:ASN:HB3	1.84	0.42
10:U:78:ILE:N	11:V:50:GLY:O	2.48	0.42
4:E:181:TYR:HD1	4:E:223:ILE:HD12	1.84	0.42
4:E:441:GLU:O	4:E:445:PHE:HB2	2.19	0.42
6:H:54:DC:H2''	6:H:55:DC:H5'	2.02	0.42
6:H:185:DA:H1'	6:H:186:DG:H5'	2.02	0.42
8:J:51:TYR:O	8:J:55:ARG:NH1	2.52	0.42
9:O:234:SER:HB3	9:O:281:PHE:HE1	1.85	0.42
1:A:69:LEU:HA	1:A:72:LYS:HB2	2.01	0.42
3:D:103:ARG:NH1	3:D:103:ARG:HB3	2.34	0.42
3:D:629:ASP:N	3:D:629:ASP:OD2	2.53	0.42
5:G:251:ILE:O	5:G:262:LEU:HA	2.20	0.42
5:G:308:TYR:HB2	5:G:324:CYS:SG	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:80:DG:C2	6:H:81:DT:C2	3.07	0.42
6:H:179:DT:C2'	6:H:180:DC:H5'	2.47	0.42
6:H:185:DA:C6	6:H:186:DG:C6	3.07	0.42
7:I:62:ILE:HD12	7:I:97:GLU:OE2	2.20	0.42
8:J:73:THR:HG21	8:J:81:VAL:HA	2.01	0.42
12:T:109:DA:H5'	7:W:43:PRO:HG2	2.02	0.42
2:B:151:LYS:HG2	2:B:152:PRO:HD3	2.02	0.42
3:D:165:PHE:HB2	3:D:354:THR:HG23	2.01	0.42
4:E:583:ARG:HA	4:E:706:MET:HB3	2.01	0.42
5:G:95:PRO:HA	5:G:430:ASP:O	2.20	0.42
5:G:100:GLN:C	5:G:152:TRP:HE1	2.24	0.42
6:H:100:DA:H2''	6:H:101:DA:H8	1.85	0.42
8:J:88:TYR:CD2	11:V:80:TYR:HE1	2.38	0.42
9:O:24:TRP:CZ2	9:O:370:HIS:HE1	2.38	0.42
9:O:226:HIS:CE1	9:O:253:MET:HG2	2.55	0.42
10:R:63:LEU:O	10:R:67:GLY:N	2.38	0.42
13:Y:237:ILE:HD12	13:Y:237:ILE:H	1.85	0.42
4:E:105:ALA:HA	13:Y:187:HIS:CE1	2.52	0.41
4:E:322:ASN:H	4:E:322:ASN:ND2	2.18	0.41
4:E:473:GLU:OE1	4:E:473:GLU:N	2.52	0.41
4:E:515:LYS:HE3	4:E:542:VAL:O	2.20	0.41
4:E:556:SER:OG	4:E:557:GLU:OE2	2.33	0.41
4:E:582:VAL:O	4:E:706:MET:N	2.42	0.41
5:G:102:ASN:HB2	5:G:152:TRP:CZ2	2.55	0.41
5:G:257:ASP:OD1	5:G:257:ASP:N	2.53	0.41
6:H:157:DT:H2''	6:H:158:DG:C8	2.55	0.41
11:S:78:ALA:O	11:S:82:LYS:N	2.53	0.41
3:D:126:ASN:H	9:O:410:ASN:HD21	1.67	0.41
3:D:457:CYS:C	3:D:459:LYS:H	2.23	0.41
6:H:23:DG:H2''	6:H:24:DA:C8	2.55	0.41
9:O:185:TRP:CH2	9:O:193:LEU:HD13	2.55	0.41
4:E:502:ARG:HH11	7:I:39:HIS:HB3	1.84	0.41
5:G:195:GLU:HB3	5:G:209:VAL:HB	2.02	0.41
6:H:38:DA:H2'	6:H:39:DT:H71	2.03	0.41
6:H:151:DG:H2''	6:H:152:DA:H8	1.85	0.41
6:H:162:DC:H2''	6:H:163:DG:H8	1.85	0.41
7:I:61:LEU:HD13	8:J:36:ARG:HB3	2.02	0.41
11:S:91:ILE:O	11:S:95:VAL:HG13	2.20	0.41
10:U:24:GLN:HE21	11:V:44:GLN:NE2	2.18	0.41
11:V:112:THR:O	11:V:116:THR:HG22	2.21	0.41
1:A:67:ILE:O	1:A:71:ILE:HG13	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:163:GLY:HA3	3:D:221:GLN:HE22	1.85	0.41
5:G:86:ASN:O	5:G:436:ARG:N	2.51	0.41
6:H:68:DG:H1'	6:H:69:DG:C8	2.55	0.41
6:H:118:DT:H2''	6:H:119:DA:C8	2.54	0.41
12:T:67:DC:H4'	12:T:68:DC:OP1	2.19	0.41
12:T:174:DT:H2'	12:T:175:DA:O4'	2.19	0.41
10:U:16:THR:HG22	10:U:18:SER:H	1.86	0.41
4:E:30:LYS:HD3	4:E:30:LYS:N	2.36	0.41
6:H:109:DG:H4'	8:J:45:ARG:NH1	2.36	0.41
6:H:123:DG:O4'	7:W:40:ARG:NH2	2.54	0.41
9:O:15:ARG:HH22	13:Y:191:ASP:HB2	1.85	0.41
4:E:45:ASN:ND2	5:G:315:LEU:O	2.53	0.41
4:E:177:ALA:HB1	4:E:227:ILE:HG12	2.03	0.41
4:E:177:ALA:O	4:E:180:GLN:HG2	2.21	0.41
4:E:323:LYS:HE2	4:E:323:LYS:HB2	1.95	0.41
4:E:456:PHE:CD2	4:E:472:TYR:HB2	2.55	0.41
5:G:417:SER:O	5:G:425:LEU:HD12	2.20	0.41
6:H:22:DC:N4	6:H:23:DG:O6	2.54	0.41
7:I:78:PHE:CE2	8:J:67:ARG:HB2	2.56	0.41
10:R:26:PRO:HD3	11:S:37:TYR:CD1	2.55	0.41
5:G:92:HIS:HB2	5:G:94:GLN:HG2	2.02	0.41
5:G:395:ASP:HB3	5:G:396:PRO:HD2	2.02	0.41
6:H:105:DG:C6	6:H:106:DG:C6	3.08	0.41
9:O:206:ASP:O	9:O:210:VAL:HG23	2.21	0.41
9:O:376:LYS:O	9:O:395:GLU:HG3	2.20	0.41
12:T:98:DT:H2''	12:T:99:DA:C8	2.55	0.41
12:T:142:DG:H2''	12:T:143:DA:H8	1.85	0.41
12:T:150:DC:H4'	12:T:151:DC:OP1	2.17	0.41
4:E:750:ILE:HG23	13:Y:174:LYS:HE2	2.03	0.41
10:R:63:LEU:HD12	11:S:42:LEU:HD13	2.03	0.41
12:T:196:DA:H2''	12:T:197:DC:H6	1.85	0.41
2:B:151:LYS:CG	2:B:152:PRO:HD3	2.51	0.41
4:E:28:GLN:OE1	4:E:31:ARG:NE	2.41	0.41
4:E:309:ASN:O	4:E:309:ASN:ND2	2.54	0.41
4:E:440:ALA:O	4:E:444:MET:HG3	2.20	0.41
4:E:524:ASN:HA	4:E:711:HIS:CD2	2.56	0.41
4:E:699:ASN:OD1	4:E:699:ASN:N	2.50	0.41
5:G:189:HIS:ND1	5:G:210:SER:HB3	2.36	0.41
5:G:379:LEU:HD12	5:G:380:GLY:N	2.36	0.41
6:H:47:DG:C2	6:H:48:DT:C2	3.09	0.41
6:H:67:DT:H2''	6:H:68:DG:C8	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:134:DG:C6	6:H:135:DT:C4	3.09	0.41
7:I:74:ILE:HD13	7:I:74:ILE:HA	1.89	0.41
8:J:97:LEU:HD12	8:J:97:LEU:HA	1.76	0.41
9:O:50:LEU:HD23	9:O:50:LEU:HA	1.94	0.41
9:O:54:THR:HG23	9:O:63:ILE:HB	2.03	0.41
12:T:163:DC:H2''	12:T:164:DA:H8	1.83	0.41
10:U:83:LEU:HD21	11:V:59:MET:CE	2.51	0.41
7:W:37:LYS:HB3	7:W:38:PRO:HD3	2.02	0.41
4:E:37:GLU:O	4:E:40:SER:OG	2.28	0.41
4:E:234:LYS:O	4:E:236:THR:N	2.45	0.41
4:E:693:ASN:ND2	4:E:694:HIS:H	2.19	0.41
12:T:173:DA:H2'	12:T:174:DT:O4'	2.21	0.41
7:W:67:PHE:CE2	7:W:93:GLN:HB2	2.56	0.41
7:W:101:VAL:HA	7:W:104:PHE:CD2	2.56	0.41
5:G:81:SER:O	5:G:440:LEU:N	2.39	0.40
5:G:233:GLU:H	5:G:295:HIS:HB3	1.86	0.40
5:G:274:ILE:O	5:G:277:SER:OG	2.27	0.40
5:G:425:LEU:HD12	5:G:425:LEU:HA	1.92	0.40
6:H:192:DG:C2	12:T:36:DG:C2	3.09	0.40
7:I:37:LYS:NZ	7:I:38:PRO:HG2	2.36	0.40
9:O:13:GLU:O	9:O:17:ILE:HG12	2.21	0.40
12:T:135:DC:H2''	12:T:136:DC:H6	1.86	0.40
3:D:158:GLN:HE22	3:D:232:VAL:HG13	1.87	0.40
3:D:473:ARG:HA	3:D:495:TYR:CD1	2.57	0.40
3:D:481:HIS:CG	3:D:482:PRO:HD2	2.56	0.40
3:D:496:ASP:OD1	3:D:496:ASP:N	2.32	0.40
3:D:556:THR:HG23	13:Y:176:LYS:HB3	2.02	0.40
4:E:511:ILE:HA	4:E:514:LYS:HE3	2.02	0.40
4:E:593:CYS:HB2	4:E:606:CYS:HB2	2.03	0.40
4:E:593:CYS:SG	4:E:606:CYS:HB2	2.61	0.40
4:E:745:GLU:HB3	13:Y:181:ARG:HH12	1.86	0.40
5:G:118:SER:O	5:G:146:ASN:HA	2.21	0.40
5:G:322:LYS:HB2	5:G:328:ILE:HG12	2.01	0.40
6:H:176:DG:H2''	6:H:177:DG:C8	2.57	0.40
7:I:129:ARG:O	7:I:132:GLY:N	2.51	0.40
11:S:83:ARG:HH21	12:T:80:DG:P	2.44	0.40
12:T:111:DG:H4'	12:T:112:DC:OP1	2.21	0.40
12:T:149:DC:H2''	12:T:150:DC:C6	2.56	0.40
2:B:149:LYS:HG2	2:B:162:CYS:HB2	2.03	0.40
5:G:249:GLU:HB3	5:G:250:LYS:NZ	2.37	0.40
5:G:326:ASN:HA	5:G:358:TYR:CZ	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:327:ALA:HA	5:G:357:ASP:HA	2.03	0.40
6:H:103:DG:C8	6:H:103:DG:H5'	2.55	0.40
6:H:149:DA:H2''	6:H:150:DC:C5	2.56	0.40
6:H:167:DT:H2''	6:H:168:DC:C5	2.56	0.40
7:I:93:GLN:O	7:I:97:GLU:N	2.42	0.40
9:O:15:ARG:NH2	13:Y:191:ASP:HB2	2.37	0.40
9:O:399:MET:SD	9:O:401:VAL:HG23	2.62	0.40
10:R:16:THR:HG23	10:R:19:SER:H	1.86	0.40
3:D:464:LEU:O	3:D:468:LYS:HG2	2.20	0.40
5:G:197:LYS:NZ	5:G:243:ASP:OD1	2.32	0.40
5:G:324:CYS:O	5:G:362:ASP:HA	2.21	0.40
5:G:343:ILE:HD12	5:G:347:GLU:HG2	2.02	0.40
6:H:57:DG:O6	12:T:169:DC:C4	2.75	0.40
6:H:69:DG:OP2	10:U:32:ARG:HD3	2.22	0.40
6:H:175:DG:C6	6:H:176:DG:C6	3.09	0.40
1:A:71:ILE:HG13	1:A:71:ILE:H	1.75	0.40
5:G:406:HIS:HB2	5:G:437:TRP:CZ2	2.56	0.40
8:J:59:LYS:O	8:J:63:GLU:HG2	2.22	0.40
9:O:16:VAL:O	9:O:20:GLU:HG2	2.21	0.40
9:O:274:ALA:HB3	9:O:295:ASP:HB2	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	A	72/197 (36%)	70 (97%)	2 (3%)	0	100	100
2	B	27/334 (8%)	18 (67%)	9 (33%)	0	100	100
3	D	427/619 (69%)	406 (95%)	21 (5%)	0	100	100
4	E	560/753 (74%)	519 (93%)	40 (7%)	1 (0%)	44	76

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	G	360/441 (82%)	335 (93%)	25 (7%)	0	100	100
7	I	112/136 (82%)	108 (96%)	4 (4%)	0	100	100
7	W	97/136 (71%)	93 (96%)	4 (4%)	0	100	100
8	J	81/106 (76%)	77 (95%)	4 (5%)	0	100	100
8	X	85/106 (80%)	82 (96%)	3 (4%)	0	100	100
9	O	391/425 (92%)	375 (96%)	16 (4%)	0	100	100
10	R	106/133 (80%)	105 (99%)	1 (1%)	0	100	100
10	U	106/133 (80%)	106 (100%)	0	0	100	100
11	S	94/123 (76%)	91 (97%)	3 (3%)	0	100	100
11	V	93/123 (76%)	89 (96%)	4 (4%)	0	100	100
13	Y	124/303 (41%)	113 (91%)	10 (8%)	1 (1%)	16	53
All	All	2735/4068 (67%)	2587 (95%)	146 (5%)	2 (0%)	50	81

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	E	327	PRO
13	Y	187	HIS

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	A	61/160 (38%)	60 (98%)	1 (2%)	58	74
2	B	20/286 (7%)	20 (100%)	0	100	100
3	D	411/575 (72%)	400 (97%)	11 (3%)	40	60
4	E	507/672 (75%)	491 (97%)	16 (3%)	34	55
5	G	324/392 (83%)	313 (97%)	11 (3%)	32	54
7	I	95/111 (86%)	94 (99%)	1 (1%)	70	80
7	W	86/111 (78%)	84 (98%)	2 (2%)	45	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	J	68/81 (84%)	67 (98%)	1 (2%)	60	75
8	X	64/81 (79%)	63 (98%)	1 (2%)	58	74
9	O	351/375 (94%)	343 (98%)	8 (2%)	45	64
10	R	85/104 (82%)	85 (100%)	0	100	100
10	U	84/104 (81%)	84 (100%)	0	100	100
11	S	79/103 (77%)	76 (96%)	3 (4%)	28	51
11	V	79/103 (77%)	78 (99%)	1 (1%)	65	77
13	Y	117/271 (43%)	114 (97%)	3 (3%)	41	61
All	All	2431/3529 (69%)	2372 (98%)	59 (2%)	45	63

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	MET
3	D	129	ARG
3	D	149	GLU
3	D	198	ASP
3	D	322	MET
3	D	468	LYS
3	D	496	ASP
3	D	522	ARG
3	D	540	MET
3	D	569	ASP
3	D	637	MET
3	D	672	MET
4	E	32	PHE
4	E	41	MET
4	E	111	TYR
4	E	163	CYS
4	E	279	HIS
4	E	290	PHE
4	E	337	LYS
4	E	466	LYS
4	E	504	TRP
4	E	509	ARG
4	E	599	TRP
4	E	609	CYS
4	E	658	ARG
4	E	659	ARG

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Mol	Chain	Res	Type
4	E	664	ASP
4	E	666	TYR
5	G	101	PHE
5	G	201	ARG
5	G	229	PHE
5	G	252	MET
5	G	258	HIS
5	G	262	LEU
5	G	271	MET
5	G	336	MET
5	G	362	ASP
5	G	365	TYR
5	G	368	PHE
7	I	90	MET
8	J	44	LYS
9	O	156	LYS
9	O	258	ARG
9	O	278	CYS
9	O	319	GLU
9	O	376	LYS
9	O	382	TRP
9	O	391	CYS
9	O	404	MET
11	S	54	LYS
11	S	61	SER
11	S	92	GLN
11	V	79	HIS
7	W	90	MET
7	W	120	MET
8	X	88	TYR
13	Y	173	ARG
13	Y	232	GLU
13	Y	242	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	GLN
1	A	50	GLN
1	A	82	GLN
3	D	221	GLN
3	D	351	GLN

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Mol	Chain	Res	Type
3	D	517	ASN
4	E	273	GLN
4	E	512	GLN
4	E	520	ASN
4	E	526	GLN
4	E	608	ASN
4	E	618	HIS
4	E	687	ASN
4	E	693	ASN
5	G	94	GLN
5	G	157	ASN
5	G	181	GLN
5	G	213	HIS
5	G	382	GLN
5	G	415	GLN
7	I	113	HIS
9	O	329	ASN
9	O	343	ASN
9	O	385	ASN
10	R	89	ASN
10	R	94	ASN
10	R	112	GLN
10	U	110	ASN
10	U	112	GLN
11	V	44	GLN
8	X	27	GLN
8	X	75	HIS
13	Y	187	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

1 ligand 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
14	SAH	E	801	-	23,28,28	1.27	3 (13%)	22,40,40	1.83	4 (18%)

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	E	801	-	-	6/11/31/31	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	E	801	SAH	C2-N3	4.21	1.38	1.32
14	E	801	SAH	C2-N1	2.44	1.38	1.33
14	E	801	SAH	OXT-C	-2.28	1.23	1.30

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	E	801	SAH	N3-C2-N1	-6.07	120.43	128.67
14	E	801	SAH	C5'-SD-CG	-3.71	91.24	102.26
14	E	801	SAH	OXT-C-O	-2.61	118.15	124.08
14	E	801	SAH	C4'-O4'-C1'	2.10	111.85	109.92

There are no chirality outliers.

All (6) torsion outliers are listed below:

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

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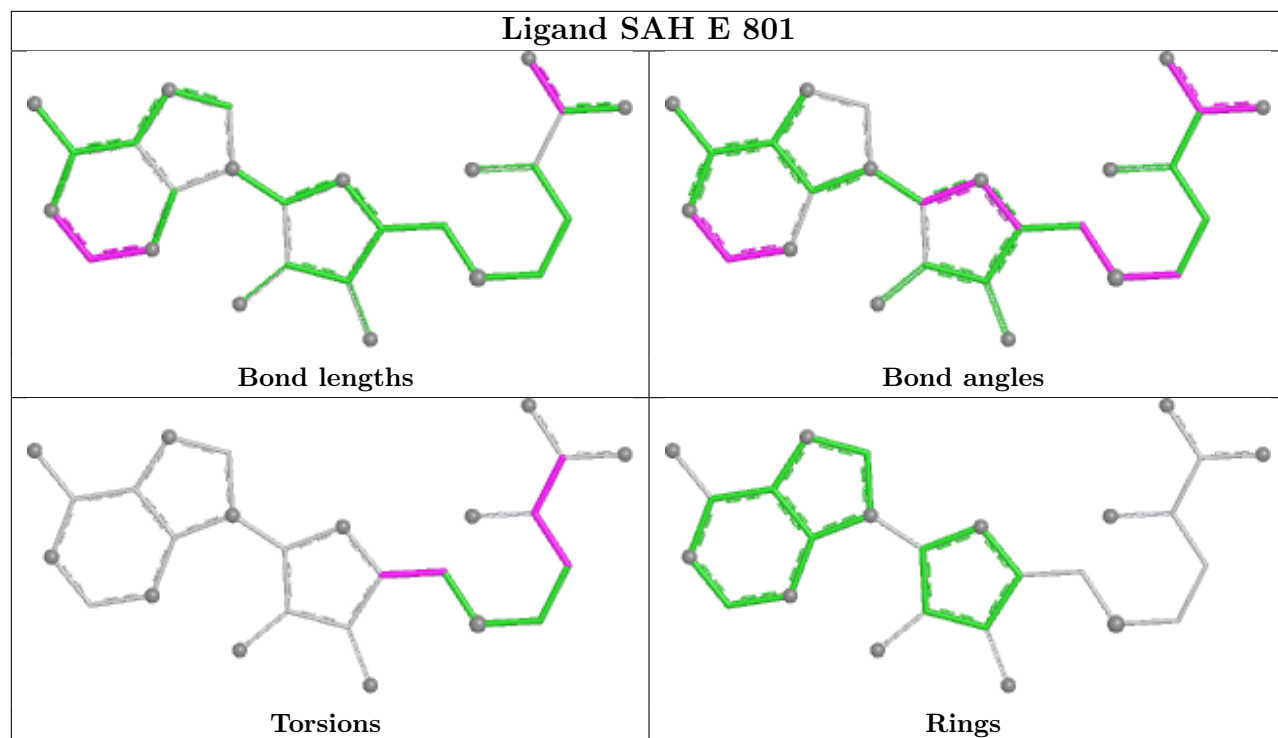
Mol	Chain	Res	Type	Atoms
14	E	801	SAH	O4'-C4'-C5'-SD
14	E	801	SAH	C3'-C4'-C5'-SD
14	E	801	SAH	C-CA-CB-CG
14	E	801	SAH	OXT-C-CA-N
14	E	801	SAH	O-C-CA-N

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	E	801	SAH	2	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

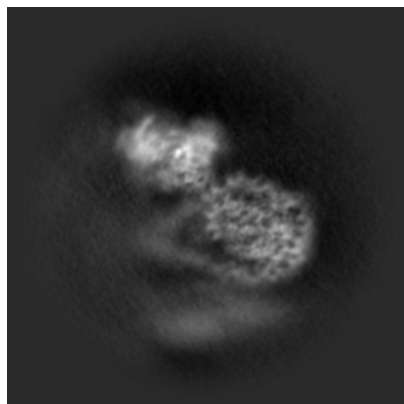
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-41146. These allow visual inspection of the internal detail of the map and identification of artifacts.

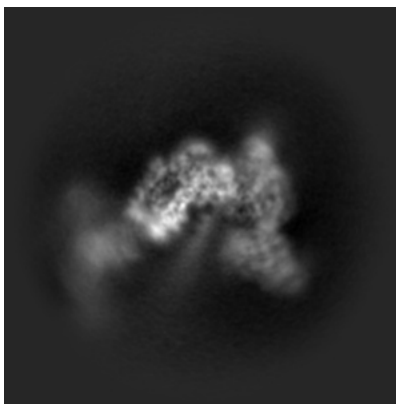
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

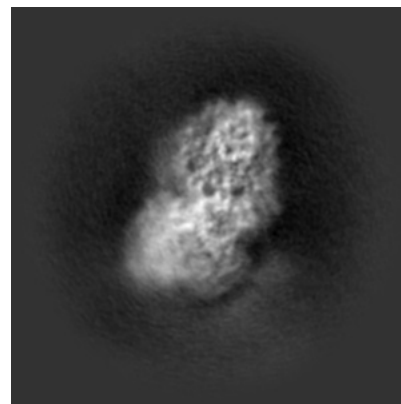
6.1.1 Primary map



X

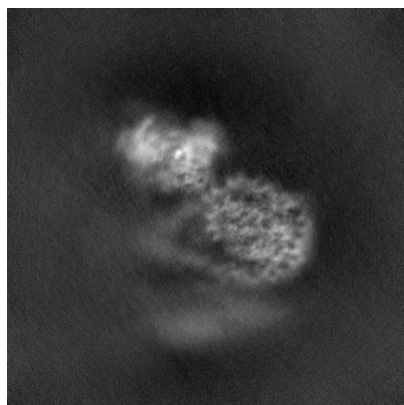


Y

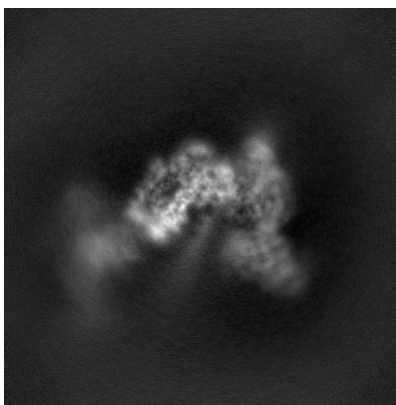


Z

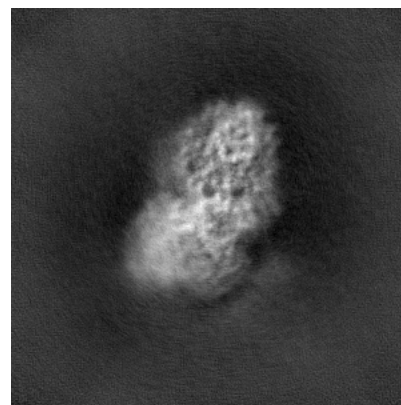
6.1.2 Raw map



X



Y

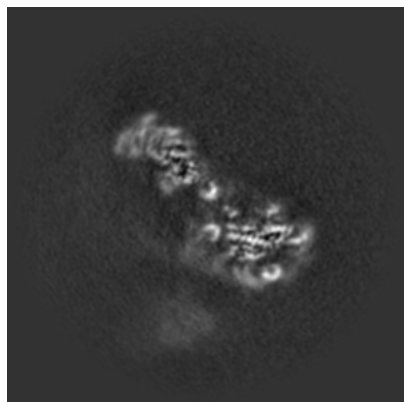


Z

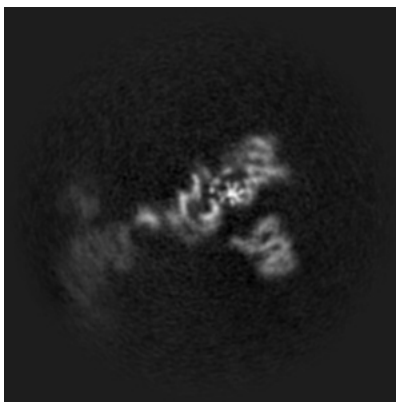
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

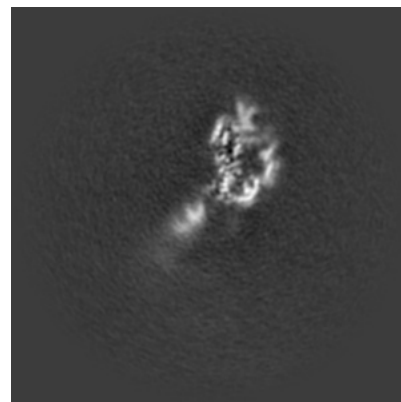
6.2.1 Primary map



X Index: 192

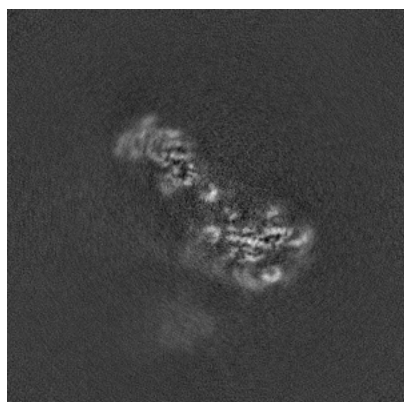


Y Index: 192

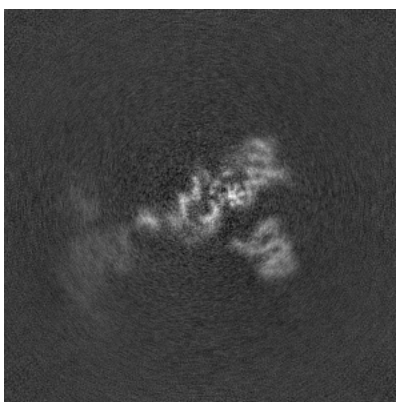


Z Index: 192

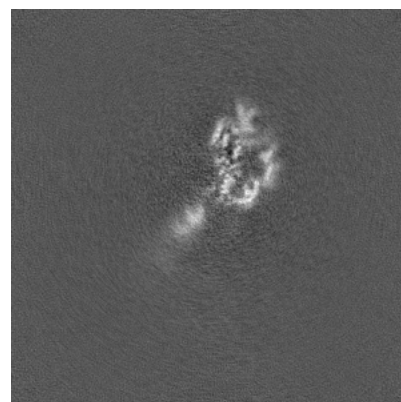
6.2.2 Raw map



X Index: 192



Y Index: 192

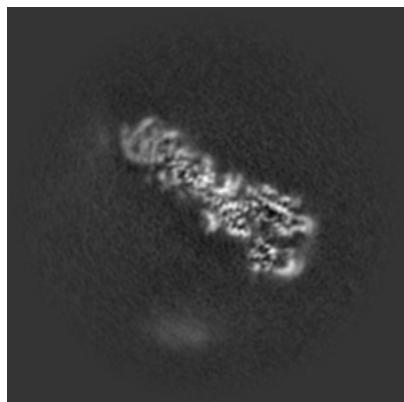


Z Index: 192

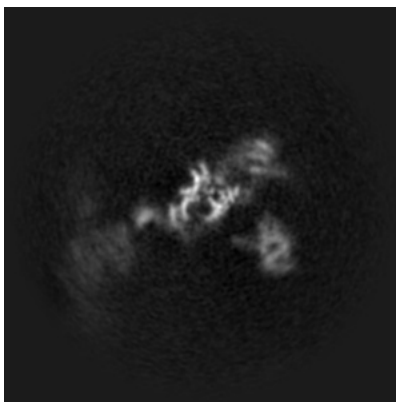
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

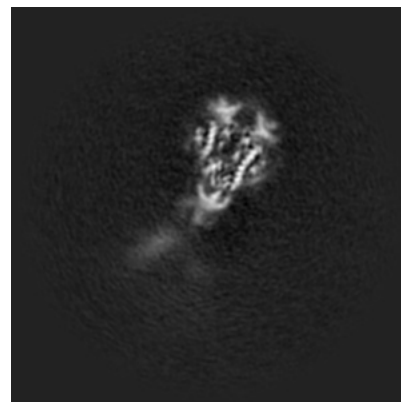
6.3.1 Primary map



X Index: 206

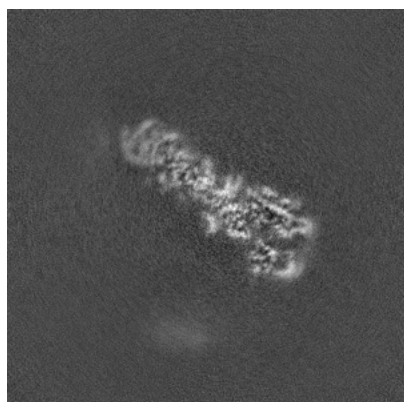


Y Index: 197

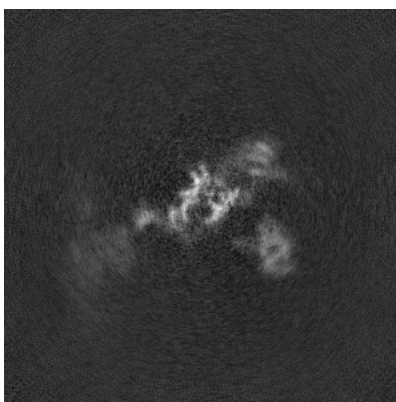


Z Index: 171

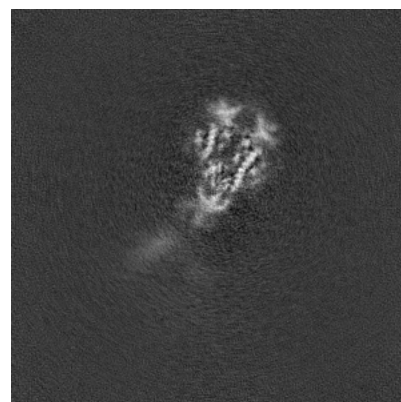
6.3.2 Raw map



X Index: 206



Y Index: 197

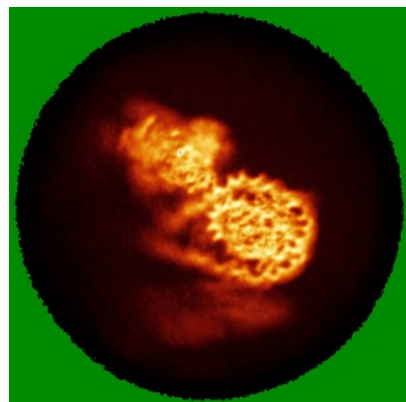


Z Index: 171

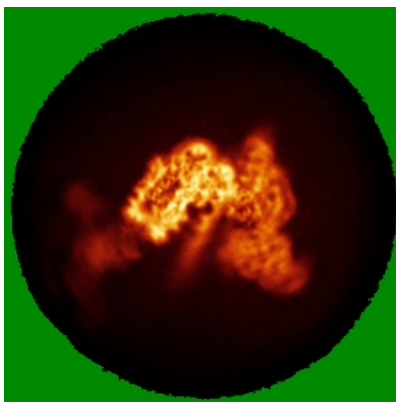
The images above show the largest variance slices of the map in three orthogonal directions.

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

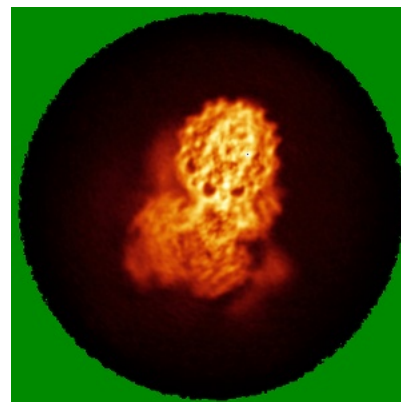
6.4.1 Primary map



X

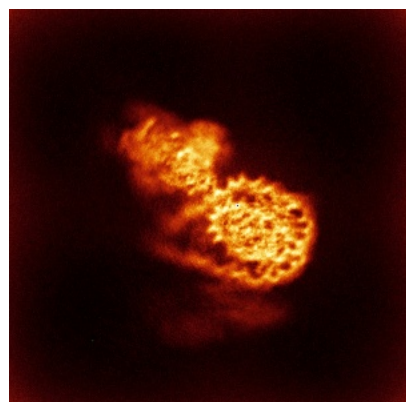


Y

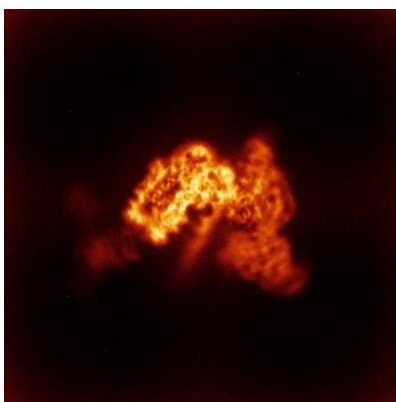


Z

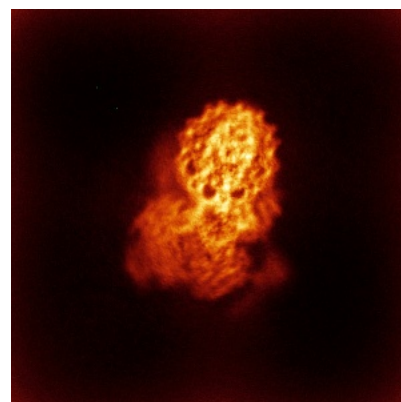
6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

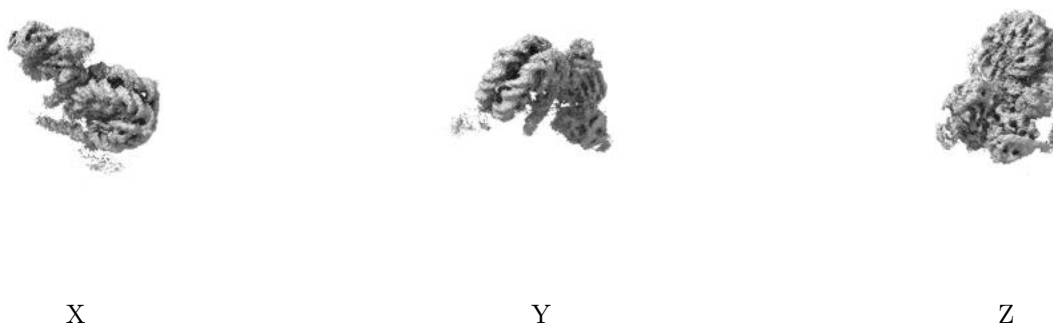
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.18. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

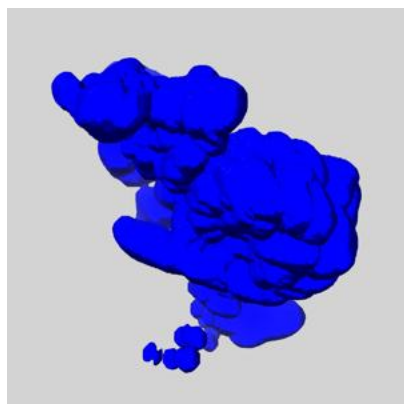
6.6 Mask visualisation [i](#)

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

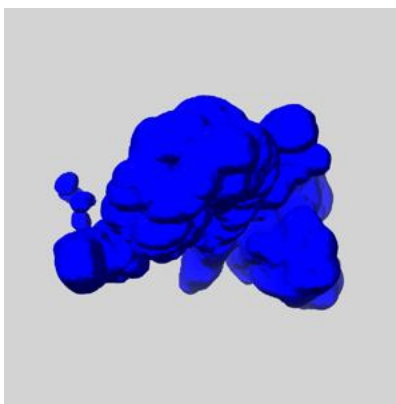
A mask typically either:

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

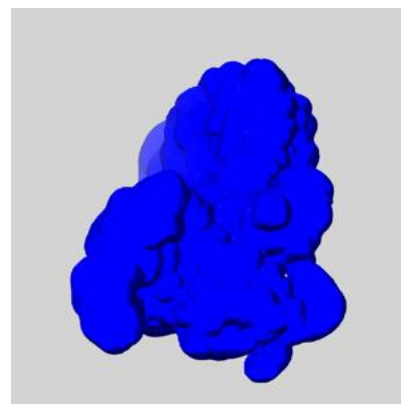
6.6.1 emd_41146_msk_1.map [i](#)



X



Y

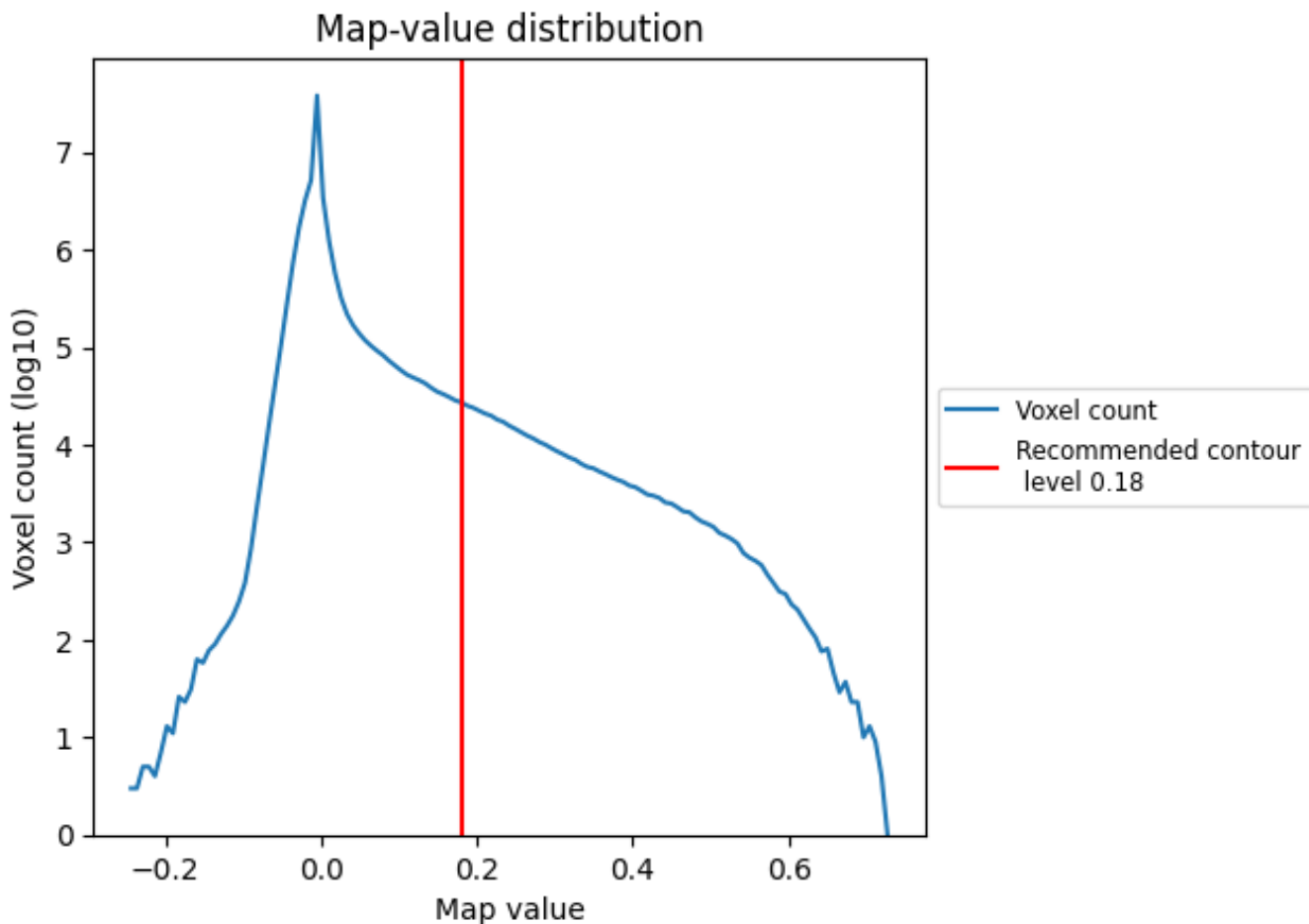


Z

7 Map analysis [i](#)

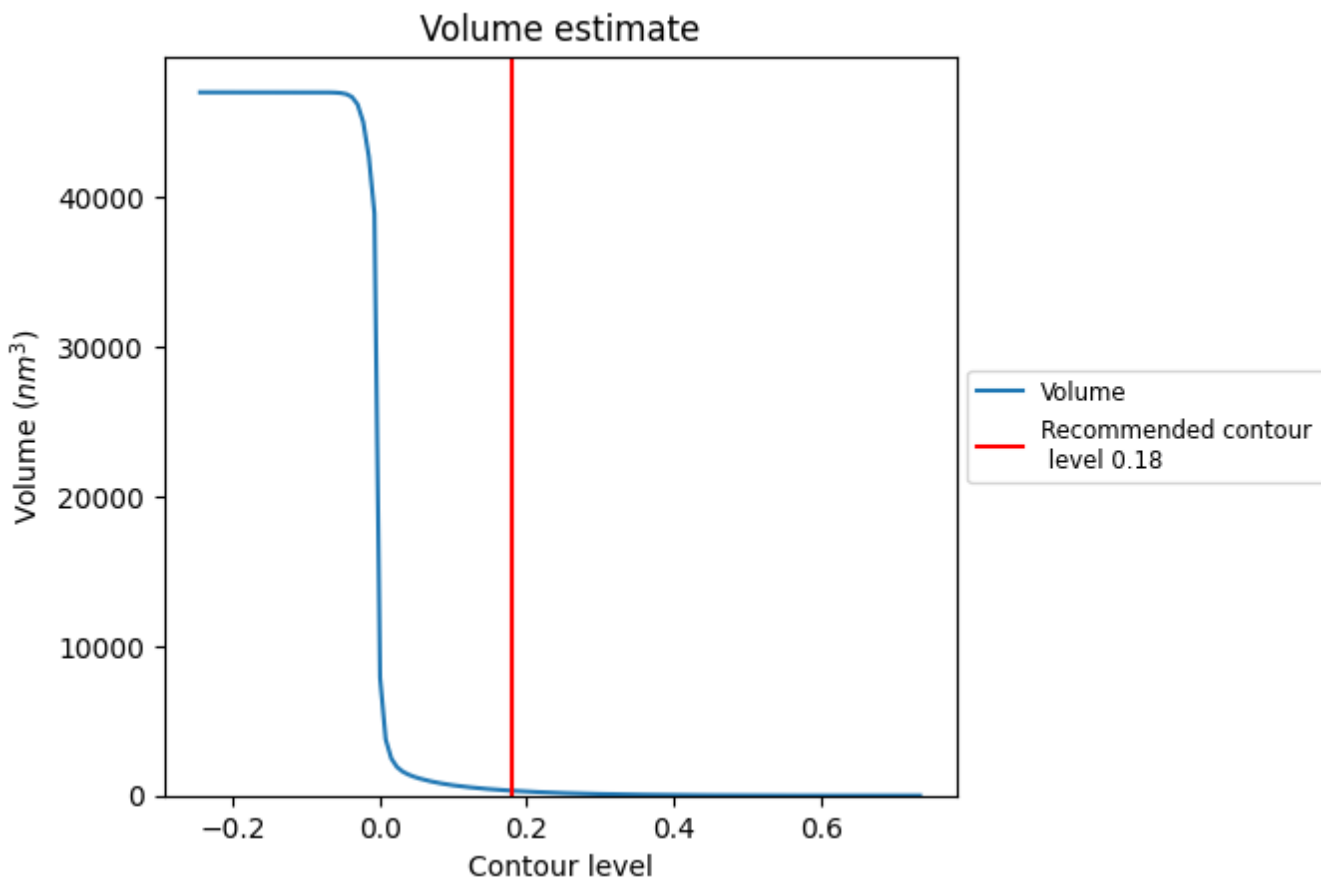
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

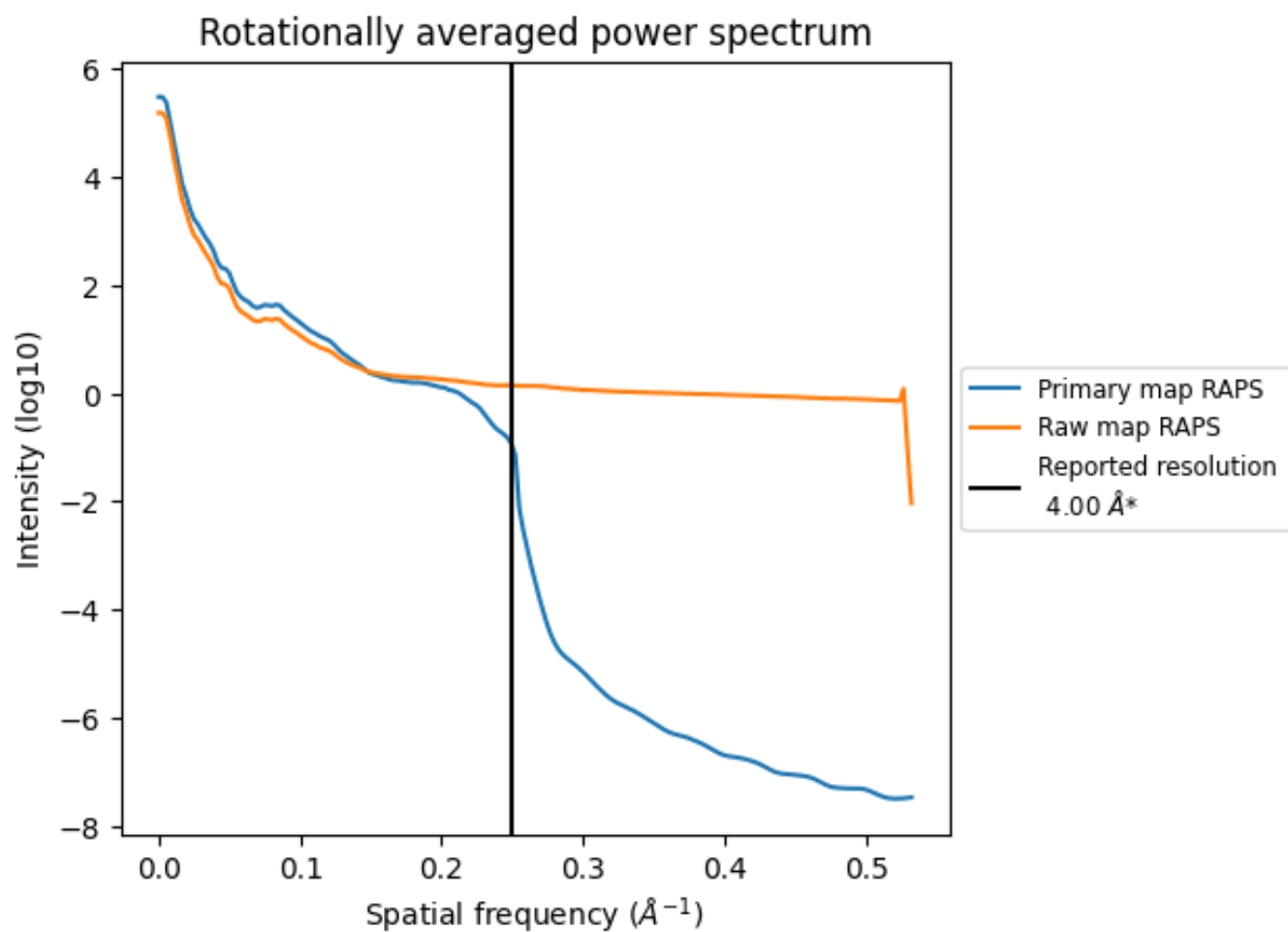
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 325 nm³; this corresponds to an approximate mass of 294 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](#)

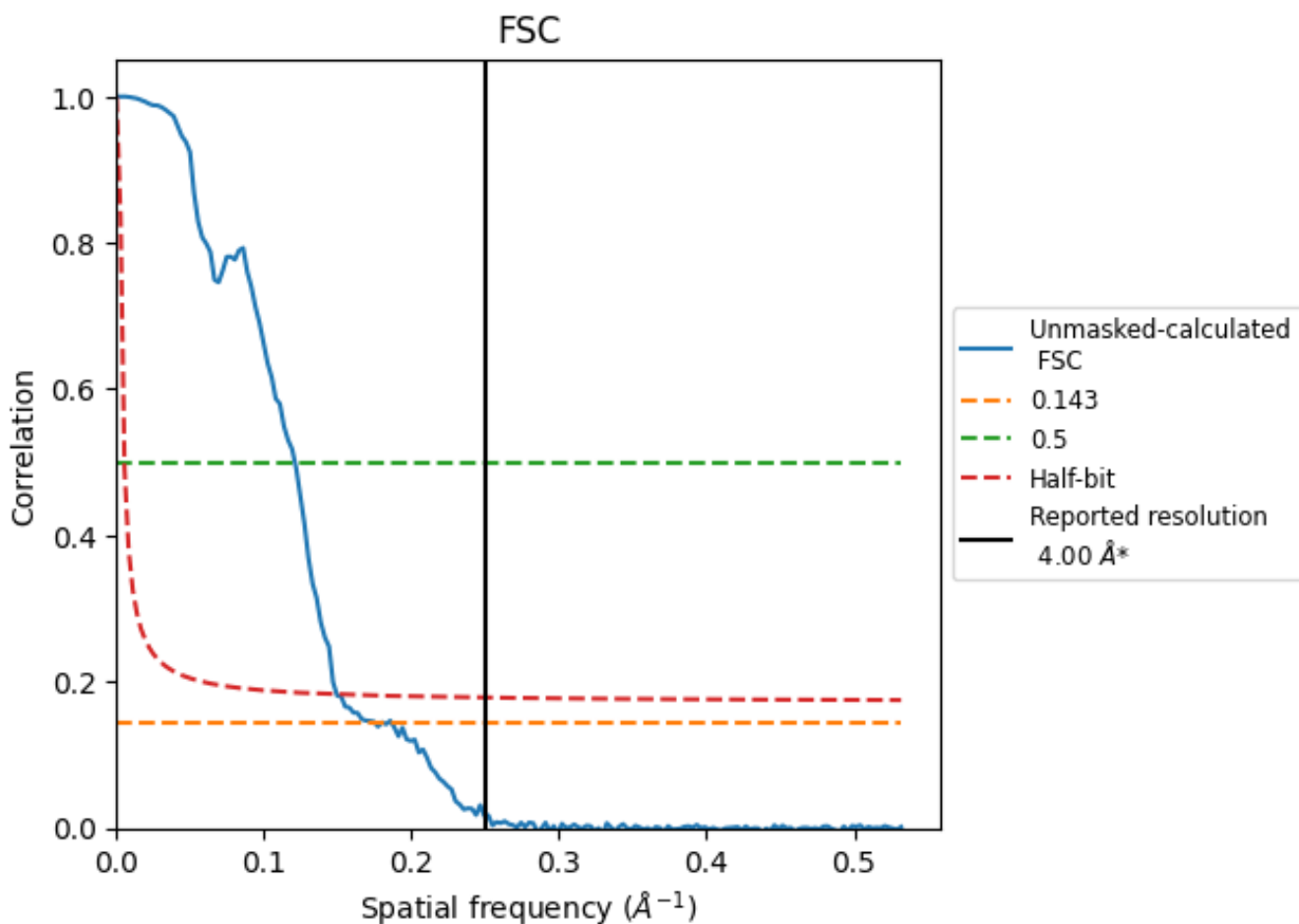


*Reported resolution corresponds to spatial frequency of 0.250 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.250 Å⁻¹

8.2 Resolution estimates [i](#)

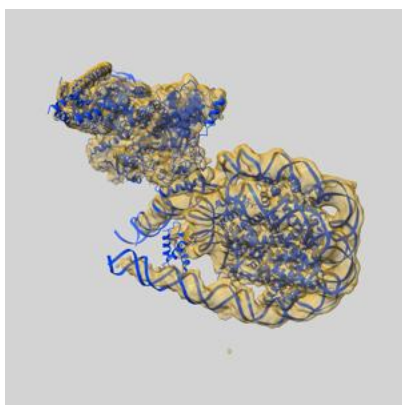
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	5.70	8.26	6.69

*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 5.70 differs from the reported value 4.0 by more than 10 %

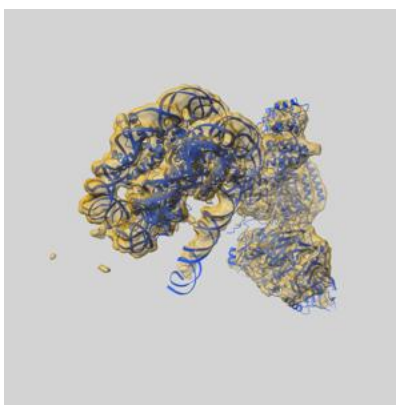
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-41146 and PDB model 8TB9. Per-residue inclusion information can be found in section 3 on page 9.

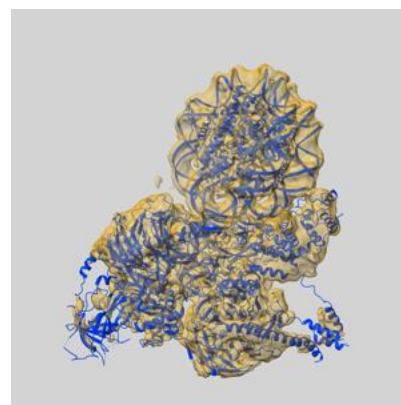
9.1 Map-model overlay [i](#)



X



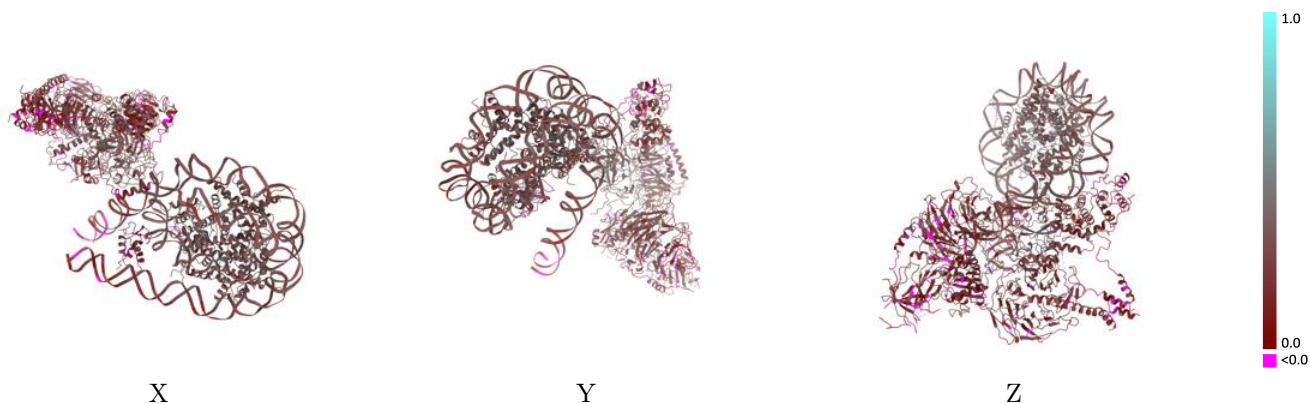
Y



Z

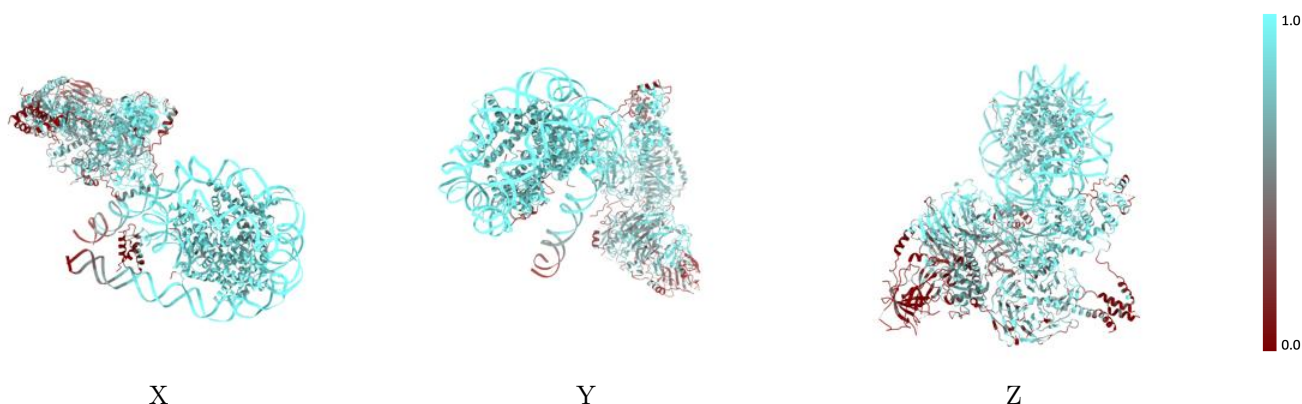
The images above show the 3D surface view of the map at the recommended contour level 0.18 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



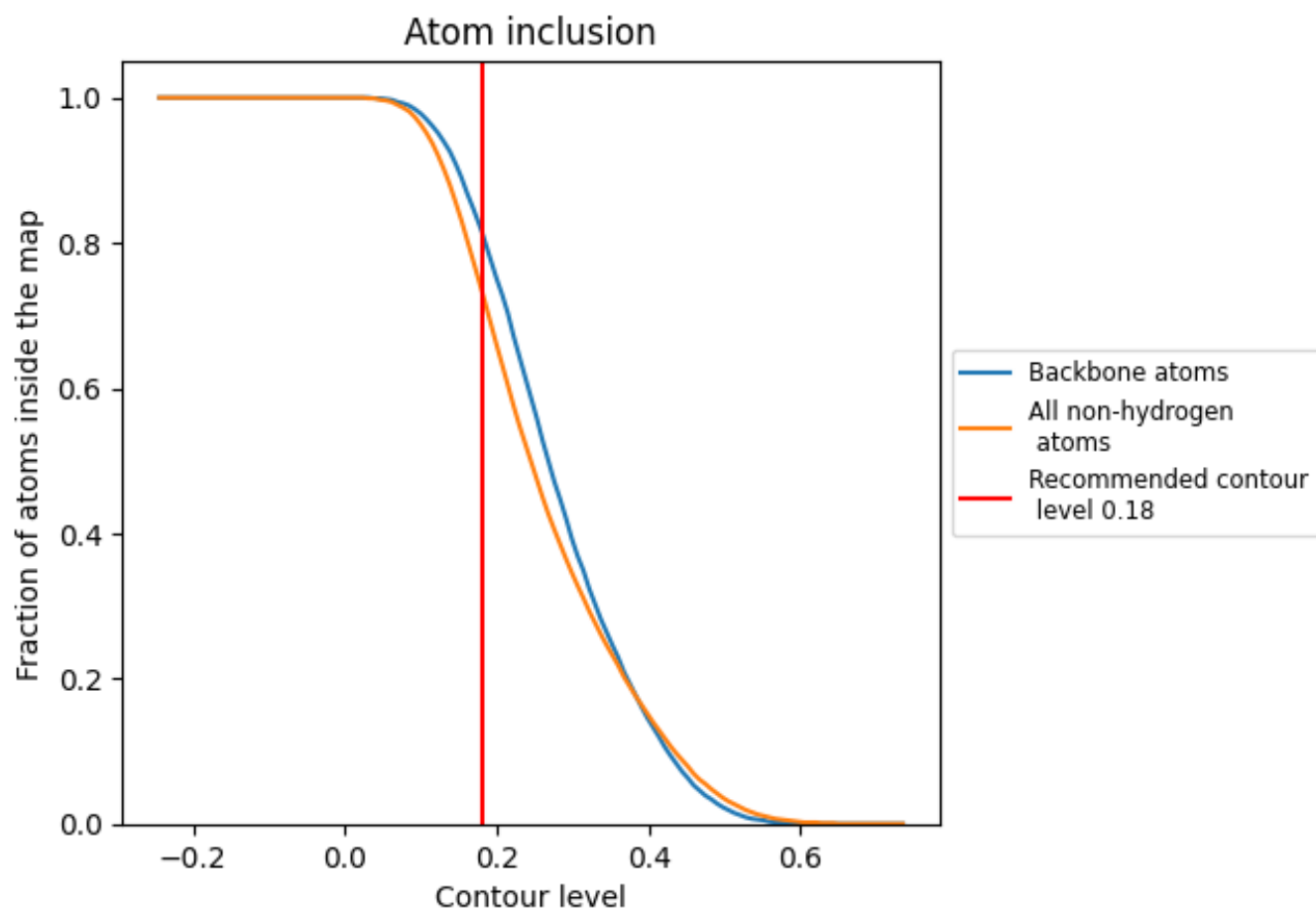
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.18).





































9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 74% 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 (0.18) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7360	 0.2610
A	 0.2850	 0.1670
B	 0.5460	 0.2120
D	 0.5410	 0.2070
E	 0.6380	 0.2340
G	 0.7060	 0.2380
H	 0.8860	 0.2760
I	 0.8630	 0.3610
J	 0.8690	 0.3530
O	 0.7260	 0.2060
R	 0.8920	 0.3720
S	 0.8720	 0.3440
T	 0.8900	 0.2760
U	 0.8700	 0.3580
V	 0.8750	 0.3410
W	 0.8720	 0.3380
X	 0.8550	 0.3620
Y	 0.2690	 0.1930

