Full wwPDB EM Validation Report ⓘ

Sep 19, 2024 – 04:15 PM EDT

PDB ID	:	8TAS
EMDB ID	:	EMD-41141
Title	:	PRC2 monomer bound to nucleosome
Authors	:	Sauer, P.V.; Pavlenko, E.; Nogales, E.; Poepsel, S.
Deposited on	:	2023-06-27
Resolution	:	4.10 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:

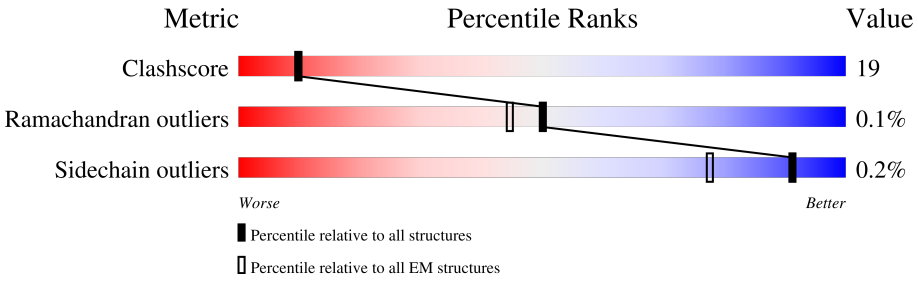
EMDB validation analysis	:	0.0.1.dev112
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.38.3

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.10 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	D	619	35% 51% 20% 29%
2	E	753	48% 28% 24%
3	G	441	39% 44% 18%
4	I	136	52% 32% 16%
4	W	136	43% 29% 27%
5	H	215	37% 51% 10%
6	J	106	54% 25% 22%
6	X	106	58% 24% 18%

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Mol	Chain	Length	Quality of chain
7	R	133	54% 27% 19%
7	U	133	53% 28% 19%
8	S	123	58% 20% 22%
8	V	123	51% 26% 23%
9	T	215	38% 50% 10%
10	O	425	43% 60% 32% 7%
11	Y	303	35% 31% 11% 58%

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 29440 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 Polycomb protein SUZ12.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D	439	Total	C	N	O	S	0	0
			3633	2309	652	645	27		

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 2 is a protein called Histone-lysine N-methyltransferase EZH2.

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

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 3 is a protein called Polycomb protein EED.

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

- Molecule 4 is a protein called Histone H3.2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	I	114	Total 917	C 576	N 179	O 159	S 3	0	0
4	W	99	Total 817	C 515	N 158	O 141	S 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 5 is a DNA chain called DNA (226-MER).

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

- Molecule 6 is a protein called Histone H4.

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

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 7 is a protein called Histone H2A.

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

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	-3	SER	-	expression tag	UNP Q6AZJ8
R	-2	ASN	-	expression tag	UNP Q6AZJ8
R	-1	ALA	-	expression tag	UNP Q6AZJ8
R	119	CYS	LYS	conflict	UNP Q6AZJ8
U	-3	SER	-	expression tag	UNP Q6AZJ8
U	-2	ASN	-	expression tag	UNP Q6AZJ8
U	-1	ALA	-	expression tag	UNP Q6AZJ8
U	119	CYS	LYS	conflict	UNP Q6AZJ8

- Molecule 8 is a protein called Histone H2B 1.1.

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

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 9 is a DNA chain called DNA (226-MER).

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

- Molecule 10 is a protein called Histone-binding protein RBBP4.

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

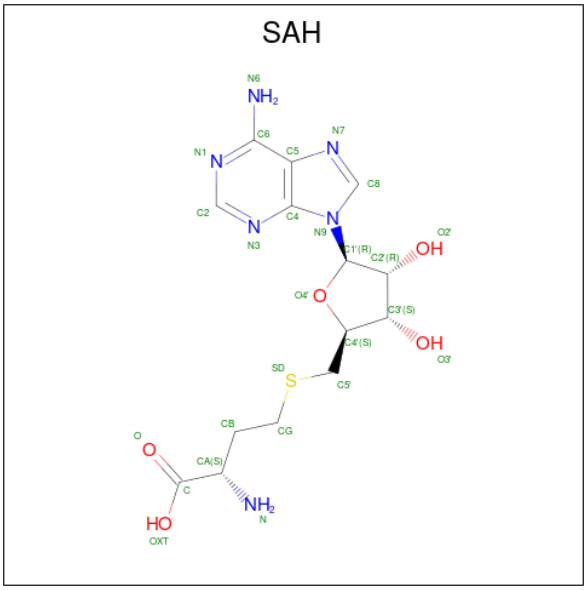
- Molecule 11 is a protein called Zinc finger protein AEBP2.

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

There are 9 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
Y	10	TYR	-	expression tag	UNP Q6ZN18
Y	11	THR	-	expression tag	UNP Q6ZN18
Y	12	ARG	-	expression tag	UNP Q6ZN18
Y	13	ARG	-	expression tag	UNP Q6ZN18
Y	14	TYR	-	expression tag	UNP Q6ZN18
Y	15	SER	-	expression tag	UNP Q6ZN18

- Molecule 12 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: $C_{14}H_{20}N_6O_5S$) (labeled as "Ligand of Interest" by depositor).



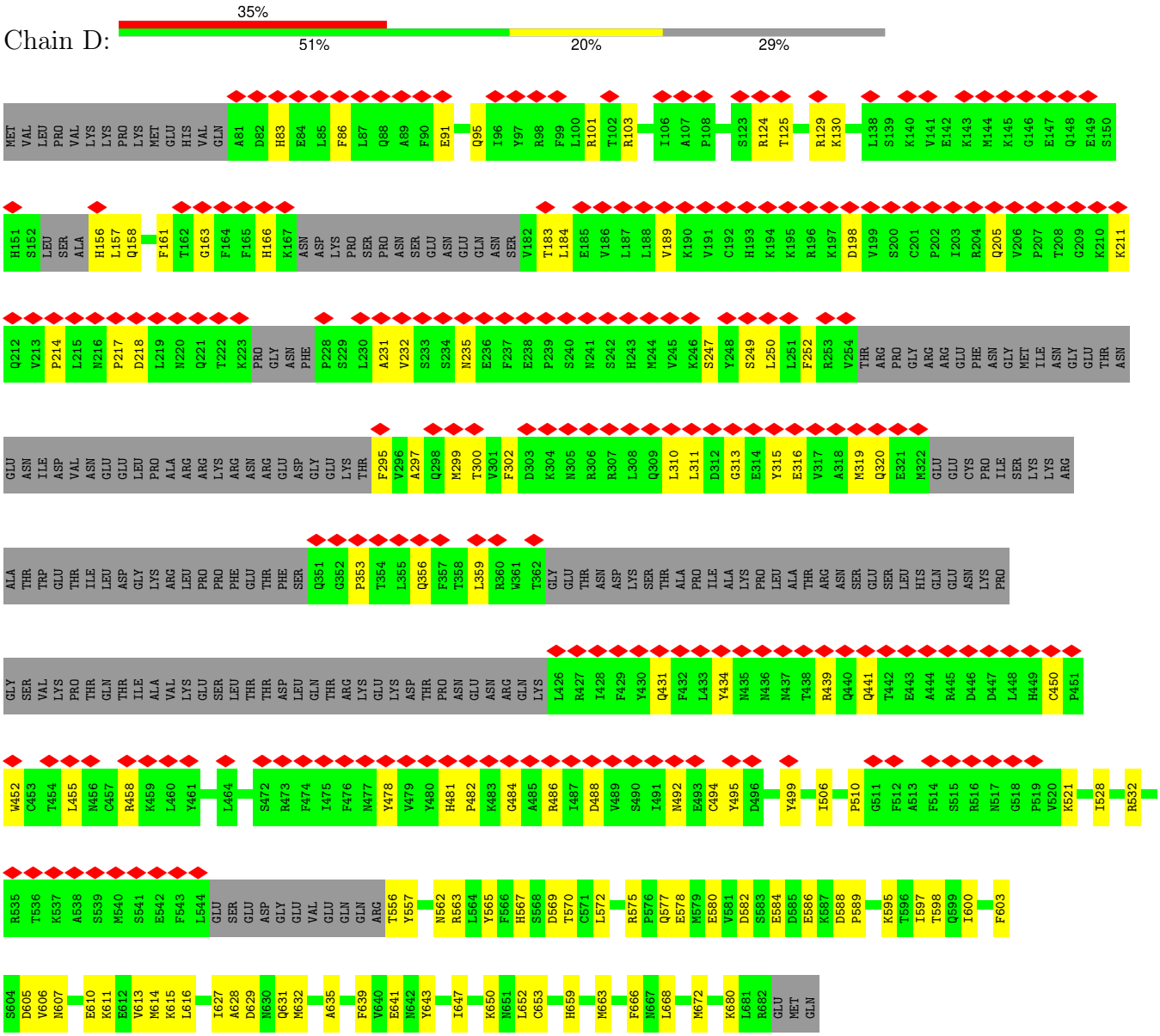
Mol	Chain	Residues	Atoms					AltConf
12	E	1	Total	C	N	O	S	0
			26	14	6	5	1	

3 Residue-property plots (i)

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

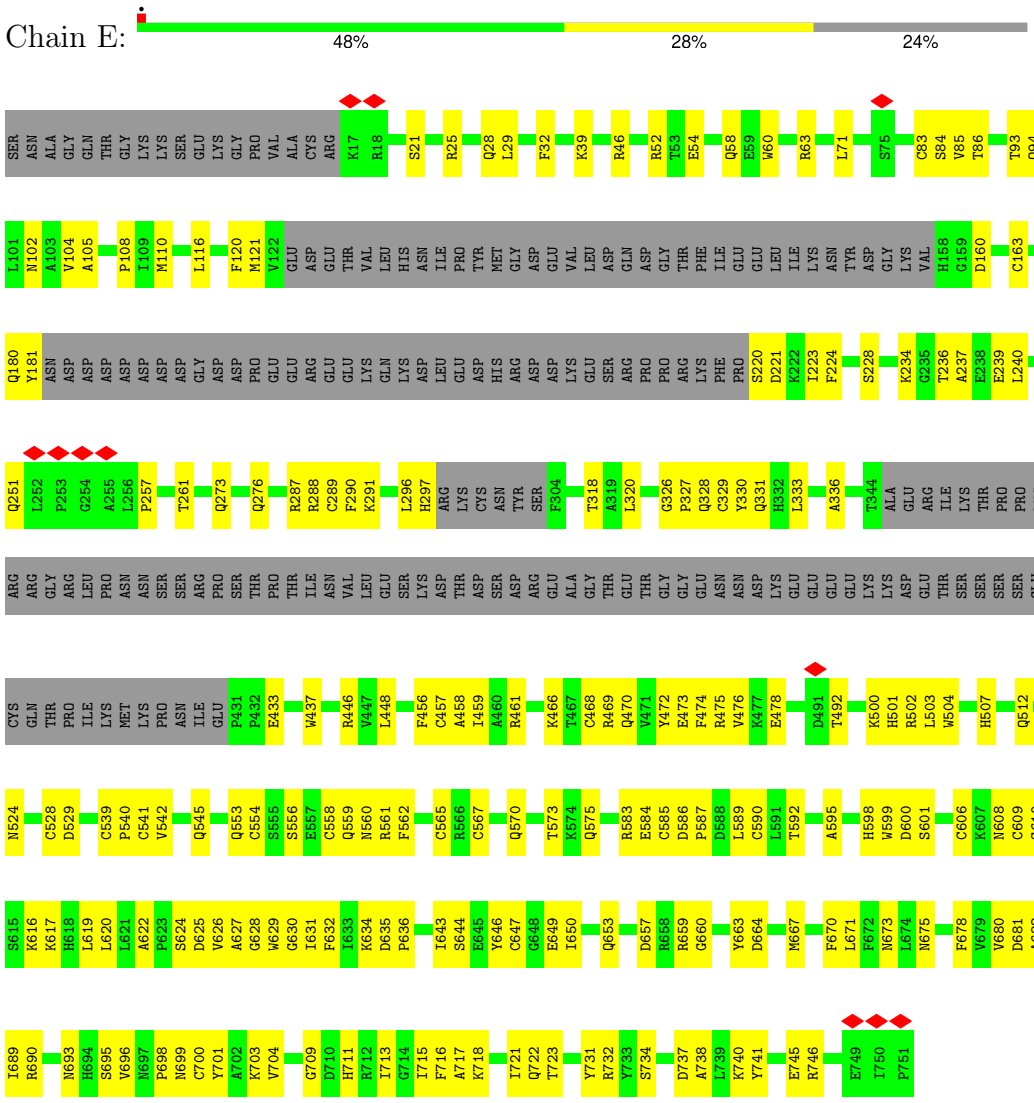
• Molecule 1: Polycomb protein SUZ12

Chain D:



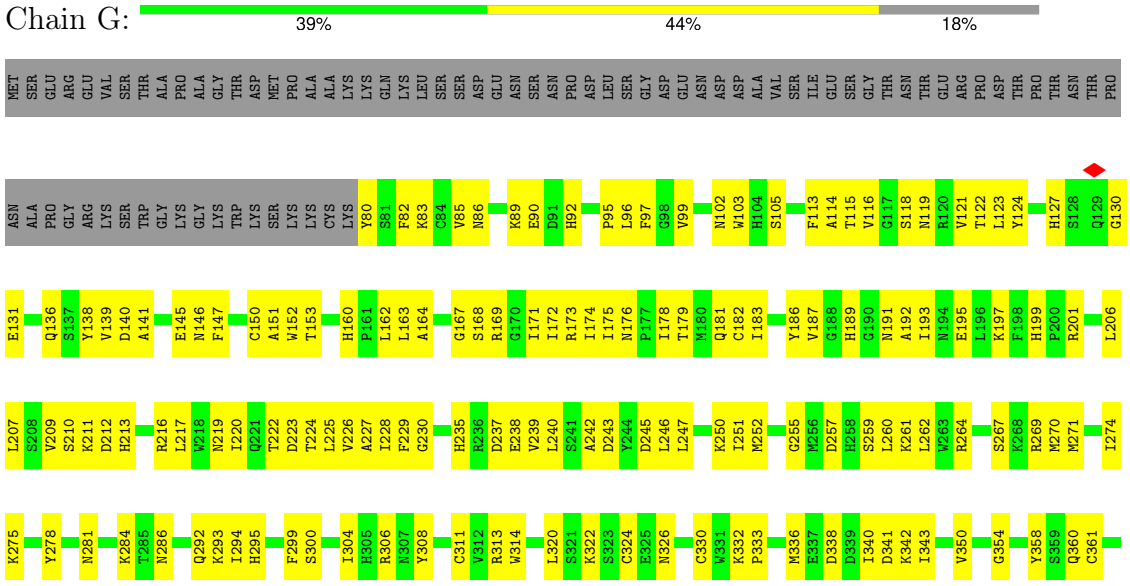
• Molecule 2: Histone-lysine N-methyltransferase EZH2

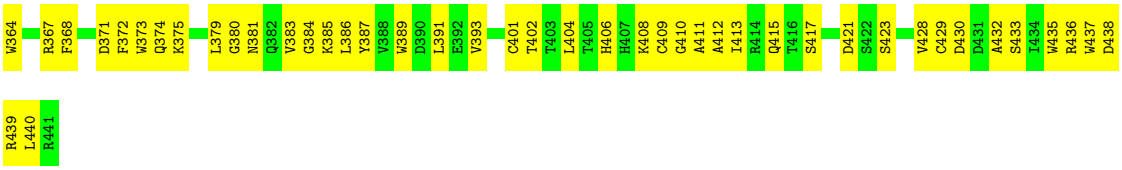
Chain E:



• Molecule 3: Polycomb protein EED

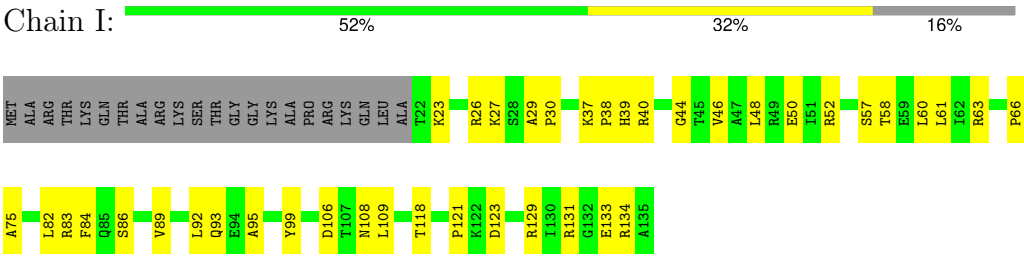
Chain G:





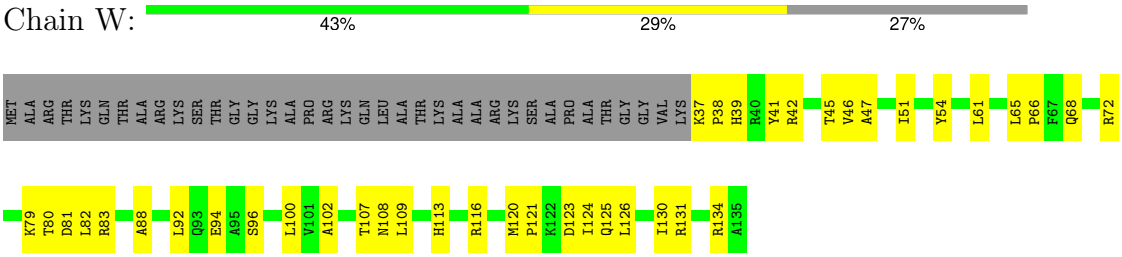
• Molecule 4: Histone H3.2

Chain I:



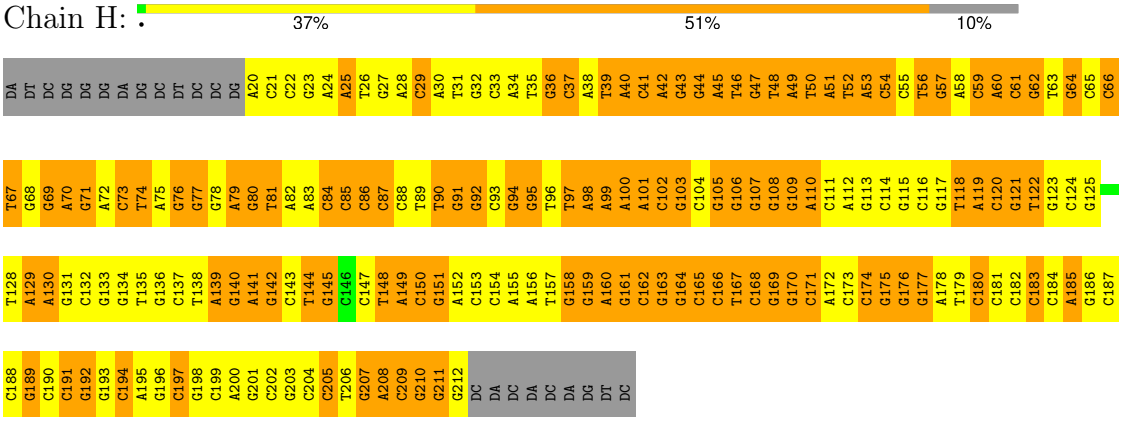
• Molecule 4: Histone H3.2

Chain W:



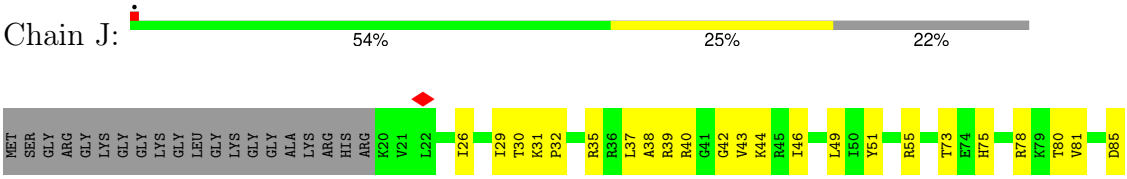
• Molecule 5: DNA (226-MER)

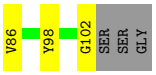
Chain H:



• Molecule 6: Histone H4

Chain J:



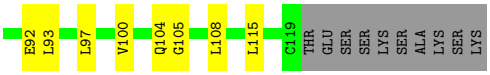


• Molecule 6: Histone H4

Chain X:

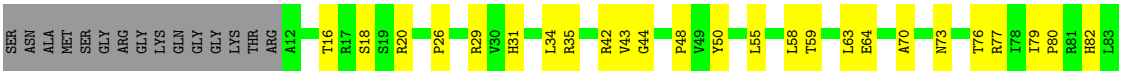
• Molecule 7: Histone H2A

Chain R:



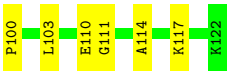
• Molecule 7: Histone H2A

Chain U:



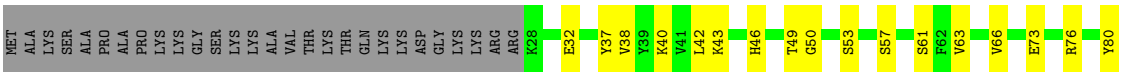
• Molecule 8: Histone H2B 1.1

Chain S:



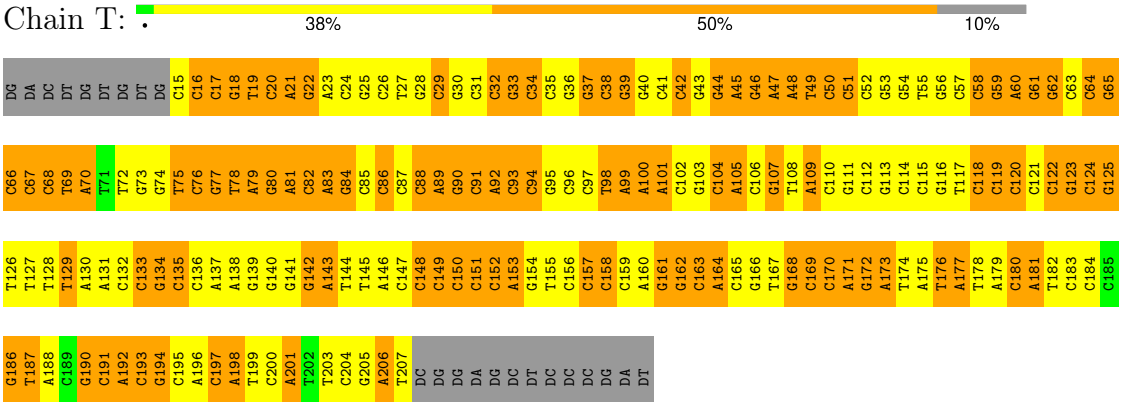
• Molecule 8: Histone H2B 1.1

Chain V:



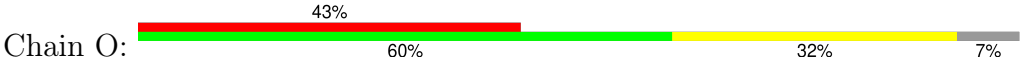
• Molecule 9: DNA (226-MER)

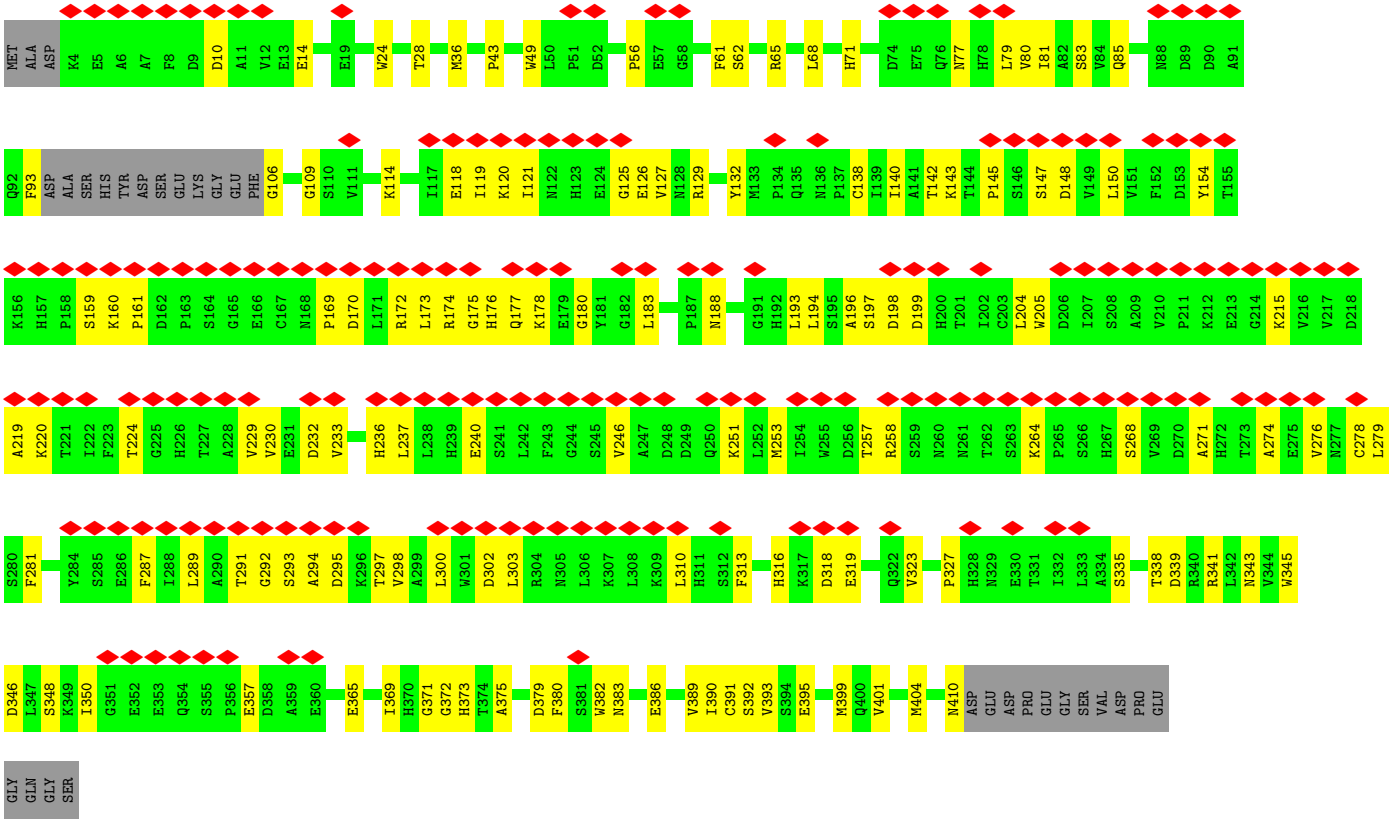
Chain T:



• Molecule 10: Histone-binding protein RBBP4

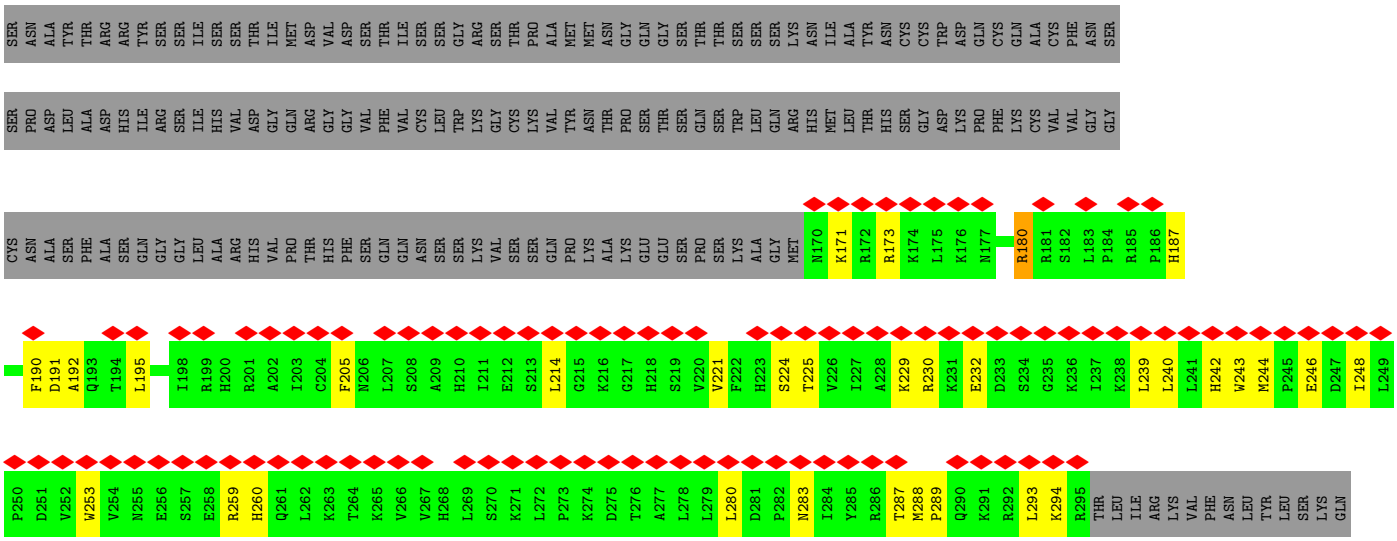
Chain O:





• Molecule 11: Zinc finger protein AEBP2

Chain Y:


SER ASN ALA TYR THR ARG ARG TYR SER SER ILE SER SER THR ILE MET ASP VAL ASP SER THR ILE SER SER GLY ARG SER THR PRO ALA MET MET ASN GLY GLN GLY SER THR THR SER SER SER LYS ASN ILE ALA TYR ASN CYS CYS TRP ASP GLN CYS GLN ALA CYS PHE ASN SER
SER PRO ASP LEU ALA ASP HIS ILE ARG SER ILE HIS VAL ASP GLY GLN ARG GLY GLY VAL PHE VAL CYS LEU TRP LYS GLY CYS LYS VAL TYR ASN THR PRO SER THR SER GLN SER TRP LEU GLN ARG HIS MET LEU THR HIS SER GLY ASP LYS PRO PHE LYS CYS VAL VAL GLY GLY
CYS ASN ALA SER PHE ALA SER GLN GLY GLY LEU ALA ARG HIS VAL PRO THR HIS PHE SER GLN GLN ASN SER SER LYS VAL SER SER GLN PRO LYS ALA LYS GLU GLU SER PRO SER LYS ALA GLY MET N170 K171 R172 R173 K174 L175 K176 N177 R180 R181 S182 L183 P184 R185 P186 H187
F190 D191 A192 Q193 T194 L195 I198 R199 H200 R201 A202 I203 C204 F205 N206 L207 S208 A209 H210 I211 E212 S213 L214 G215 K216 G217 H218 S219 V220 V221 F222 H223 S224 T225 V226 I227 A228 K229 R230 K231 E232 D233 S234 G235 K236 I237 K238 L239 L240 L241 H242 W243 M244 P245 E246 D247 I248 L249
P250 D251 V252 W253 V254 N255 E256 S257 E258 R259 H260 Q261 L262 K263 T264 K265 V266 V267 H268 L269 S270 K271 L272 P273 K274 D275 T276 A277 L278 L279 L280 D281 P282 N283 I284 Y285 R286 T287 M288 P289 Q290 K291 R292 L293 K294 R295 THR LEU ILE ARG LYS VAL PHE ASN LEU TYR LEU SER LYS GLN

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	69000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.135	Depositor
Minimum map value	-0.069	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	505.88998, 505.88998, 505.88998	wwPDB
Map dimensions	330, 330, 330	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.533, 1.533, 1.533	Depositor

5 Model quality

5.1 Standard geometry

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	D	0.25	0/3713	0.49	0/4992
2	E	0.30	0/4682	0.50	0/6308
3	G	0.26	0/3005	0.52	0/4070
4	I	0.38	0/930	0.60	0/1246
4	W	0.44	0/829	0.62	0/1111
5	H	0.65	0/4463	1.55	276/6888 (4.0%)
6	J	0.50	0/668	0.64	0/894
6	X	0.51	0/673	0.60	0/904
7	R	0.47	0/839	0.61	0/1132
7	U	0.44	0/835	0.62	0/1128
8	S	0.47	0/753	0.55	0/1014
8	V	0.49	0/748	0.57	0/1007
9	T	0.66	0/4391	1.59	276/6763 (4.1%)
10	O	0.24	0/3225	0.47	0/4394
11	Y	0.23	0/1070	0.52	0/1437
All	All	0.45	0/30824	0.98	552/43288 (1.3%)

There are no bond length outliers.

All (552) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	T	67	DC	OP1-P-O3'	10.30	127.86	105.20
9	T	46	DG	OP1-P-O3'	9.92	127.03	105.20
9	T	150	DC	OP1-P-O3'	9.89	126.96	105.20
5	H	104	DC	OP1-P-O3'	9.77	126.69	105.20
9	T	120	DC	OP1-P-O3'	9.68	126.50	105.20
9	T	109	DA	OP1-P-O3'	9.65	126.43	105.20
5	H	174	DC	OP1-P-O3'	9.39	125.86	105.20
9	T	80	DG	OP1-P-O3'	9.23	125.51	105.20
9	T	61	DG	OP1-P-O3'	9.22	125.49	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	T	58	DC	OP1-P-O3'	9.21	125.47	105.20
9	T	104	DC	OP1-P-O3'	9.20	125.44	105.20
9	T	68	DC	OP1-P-OP2	-9.17	105.85	119.60
9	T	47	DA	OP1-P-OP2	-9.13	105.91	119.60
9	T	151	DC	OP1-P-OP2	-9.03	106.06	119.60
9	T	110	DC	OP1-P-OP2	-8.98	106.14	119.60
9	T	57	DC	OP1-P-O3'	8.67	124.28	105.20
9	T	93	DC	OP1-P-O3'	8.64	124.20	105.20
9	T	105	DA	OP1-P-OP2	-8.62	106.67	119.60
9	T	62	DG	OP1-P-OP2	-8.55	106.78	119.60
9	T	82	DC	OP1-P-O3'	8.50	123.91	105.20
5	H	175	DG	OP1-P-OP2	-8.41	106.98	119.60
9	T	117	DT	OP1-P-O3'	8.40	123.69	105.20
9	T	83	DA	OP1-P-OP2	-8.37	107.05	119.60
9	T	59	DG	OP1-P-OP2	-8.31	107.14	119.60
5	H	105	DG	OP1-P-OP2	-8.30	107.15	119.60
9	T	133	DC	OP1-P-O3'	8.29	123.43	105.20
9	T	98	DT	OP1-P-O3'	8.28	123.41	105.20
9	T	94	DC	OP1-P-OP2	-8.25	107.23	119.60
9	T	171	DA	OP1-P-OP2	-8.20	107.30	119.60
9	T	58	DC	OP1-P-OP2	-8.18	107.33	119.60
9	T	99	DA	OP1-P-OP2	-8.15	107.37	119.60
9	T	81	DA	OP1-P-OP2	-8.07	107.49	119.60
9	T	170	DC	OP1-P-O3'	8.07	122.96	105.20
9	T	118	DC	OP1-P-OP2	-8.02	107.57	119.60
9	T	59	DG	OP1-P-O3'	8.01	122.83	105.20
9	T	134	DG	OP1-P-OP2	-7.95	107.68	119.60
5	H	93	DC	OP1-P-OP2	-7.79	107.92	119.60
5	H	87	DC	OP1-P-O3'	7.78	122.31	105.20
5	H	107	DG	OP1-P-O3'	7.72	122.18	105.20
5	H	92	DG	OP1-P-O3'	7.71	122.15	105.20
9	T	121	DC	OP1-P-OP2	-7.69	108.07	119.60
9	T	60	DA	OP1-P-OP2	-7.63	108.15	119.60
5	H	109	DG	OP1-P-O3'	7.60	121.92	105.20
5	H	131	DG	OP1-P-OP2	-7.59	108.21	119.60
5	H	110	DA	OP1-P-OP2	-7.59	108.22	119.60
9	T	170	DC	OP1-P-OP2	-7.59	108.22	119.60
9	T	168	DG	OP1-P-OP2	-7.58	108.22	119.60
5	H	88	DC	OP1-P-OP2	-7.53	108.30	119.60
5	H	51	DA	OP1-P-OP2	-7.50	108.35	119.60
5	H	50	DT	OP1-P-O3'	7.46	121.60	105.20
5	H	108	DG	OP1-P-OP2	-7.44	108.43	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	H	98	DA	OP1-P-OP2	-7.41	108.49	119.60
9	T	129	DT	OP1-P-O3'	7.39	121.46	105.20
5	H	151	DG	OP1-P-OP2	-7.38	108.53	119.60
9	T	80	DG	OP1-P-OP2	-7.36	108.56	119.60
5	H	100	DA	OP1-P-OP2	-7.35	108.58	119.60
9	T	160	DA	OP1-P-O3'	7.30	121.25	105.20
5	H	108	DG	OP1-P-O3'	7.29	121.24	105.20
5	H	109	DG	OP1-P-OP2	-7.29	108.67	119.60
5	H	87	DC	OP1-P-OP2	-7.27	108.69	119.60
5	H	97	DT	OP1-P-O3'	7.27	121.20	105.20
5	H	80	DG	OP1-P-OP2	-7.25	108.72	119.60
9	T	112	DC	OP1-P-OP2	-7.24	108.73	119.60
9	T	57	DC	OP1-P-OP2	-7.23	108.75	119.60
5	H	101	DA	OP1-P-OP2	-7.22	108.76	119.60
9	T	130	DA	OP1-P-OP2	-7.16	108.86	119.60
9	T	56	DG	OP1-P-O3'	7.15	120.94	105.20
9	T	125	DG	OP1-P-OP2	-7.15	108.87	119.60
5	H	28	DA	OP1-P-OP2	-7.12	108.93	119.60
9	T	172	DG	OP1-P-OP2	-7.12	108.93	119.60
5	H	59	DC	OP1-P-O3'	7.10	120.82	105.20
9	T	70	DA	OP1-P-OP2	-7.10	108.96	119.60
9	T	154	DG	OP1-P-OP2	-7.08	108.98	119.60
9	T	161	DG	OP1-P-OP2	-7.04	109.03	119.60
5	H	86	DC	OP1-P-OP2	-7.03	109.05	119.60
5	H	171	DC	OP1-P-OP2	-7.02	109.06	119.60
9	T	195	DC	OP1-P-OP2	-7.02	109.06	119.60
5	H	26	DT	OP1-P-OP2	-7.01	109.08	119.60
5	H	163	DG	OP1-P-OP2	-7.00	109.09	119.60
9	T	77	DG	OP1-P-OP2	-7.00	109.09	119.60
9	T	111	DG	OP1-P-OP2	-7.00	109.09	119.60
9	T	124	DC	OP1-P-OP2	-7.00	109.10	119.60
5	H	22	DC	OP1-P-OP2	-6.99	109.12	119.60
5	H	164	DG	OP1-P-OP2	-6.99	109.12	119.60
5	H	150	DC	OP1-P-OP2	-6.98	109.13	119.60
9	T	84	DG	OP1-P-OP2	-6.97	109.14	119.60
5	H	203	DG	OP1-P-OP2	-6.95	109.17	119.60
5	H	33	DC	OP1-P-OP2	-6.94	109.19	119.60
5	H	94	DG	OP1-P-OP2	-6.93	109.20	119.60
9	T	52	DC	OP1-P-OP2	-6.93	109.21	119.60
5	H	130	DA	OP1-P-O3'	6.93	120.44	105.20
5	H	119	DA	OP1-P-OP2	-6.91	109.24	119.60
5	H	76	DG	OP1-P-OP2	-6.90	109.25	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	T	21	DA	OP1-P-OP2	-6.90	109.25	119.60
9	T	38	DC	OP1-P-OP2	-6.89	109.26	119.60
9	T	66	DC	OP1-P-OP2	-6.89	109.27	119.60
9	T	30	DG	OP1-P-OP2	-6.89	109.27	119.60
5	H	86	DC	OP1-P-O3'	6.88	120.35	105.20
9	T	201	DA	OP1-P-OP2	-6.88	109.28	119.60
9	T	85	DC	OP1-P-OP2	-6.88	109.29	119.60
5	H	92	DG	OP1-P-OP2	-6.87	109.29	119.60
5	H	197	DC	OP1-P-OP2	-6.87	109.30	119.60
5	H	25	DA	OP1-P-OP2	-6.86	109.31	119.60
5	H	77	DG	OP1-P-OP2	-6.86	109.31	119.60
9	T	39	DG	OP1-P-OP2	-6.86	109.31	119.60
5	H	130	DA	OP1-P-OP2	-6.86	109.31	119.60
9	T	107	DG	OP1-P-OP2	-6.86	109.32	119.60
5	H	68	DG	OP1-P-OP2	-6.85	109.32	119.60
9	T	160	DA	OP1-P-OP2	-6.85	109.33	119.60
9	T	26	DC	OP1-P-OP2	-6.84	109.34	119.60
5	H	117	DG	OP1-P-OP2	-6.84	109.34	119.60
9	T	28	DG	OP1-P-OP2	-6.83	109.35	119.60
9	T	140	DG	OP1-P-OP2	-6.83	109.35	119.60
9	T	206	DA	OP1-P-OP2	-6.83	109.35	119.60
9	T	153	DA	OP1-P-OP2	-6.83	109.36	119.60
5	H	209	DC	OP1-P-OP2	-6.82	109.37	119.60
9	T	180	DC	OP1-P-OP2	-6.82	109.37	119.60
5	H	133	DG	OP1-P-OP2	-6.82	109.37	119.60
5	H	34	DA	OP1-P-OP2	-6.82	109.38	119.60
9	T	165	DC	OP1-P-OP2	-6.81	109.38	119.60
9	T	25	DG	OP1-P-OP2	-6.81	109.38	119.60
9	T	37	DG	OP1-P-OP2	-6.81	109.38	119.60
9	T	27	DT	OP1-P-OP2	-6.81	109.39	119.60
9	T	150	DC	OP1-P-OP2	-6.81	109.39	119.60
5	H	202	DC	OP1-P-OP2	-6.80	109.39	119.60
9	T	96	DC	OP1-P-OP2	-6.80	109.39	119.60
9	T	136	DC	OP1-P-OP2	-6.80	109.40	119.60
5	H	199	DC	OP1-P-OP2	-6.80	109.41	119.60
5	H	193	DG	OP1-P-OP2	-6.79	109.41	119.60
5	H	20	DA	OP1-P-OP2	-6.79	109.41	119.60
9	T	36	DG	OP1-P-OP2	-6.79	109.41	119.60
5	H	36	DG	OP1-P-OP2	-6.79	109.42	119.60
5	H	114	DC	OP1-P-OP2	-6.79	109.42	119.60
9	T	190	DG	OP1-P-OP2	-6.79	109.42	119.60
5	H	46	DT	OP1-P-OP2	-6.79	109.42	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	H	184	DC	OP1-P-OP2	-6.79	109.42	119.60
9	T	142	DG	OP1-P-OP2	-6.79	109.42	119.60
5	H	37	DC	OP1-P-OP2	-6.78	109.43	119.60
5	H	201	DG	OP1-P-OP2	-6.78	109.43	119.60
5	H	32	DG	OP1-P-OP2	-6.78	109.43	119.60
5	H	145	DG	OP1-P-OP2	-6.78	109.43	119.60
9	T	29	DC	OP1-P-OP2	-6.78	109.43	119.60
5	H	198	DG	OP1-P-OP2	-6.78	109.44	119.60
5	H	53	DA	OP1-P-OP2	-6.77	109.44	119.60
5	H	62	DG	OP1-P-OP2	-6.77	109.44	119.60
5	H	212	DG	OP1-P-OP2	-6.77	109.44	119.60
9	T	123	DG	OP1-P-O3'	6.77	120.10	105.20
5	H	172	DA	OP1-P-OP2	-6.77	109.45	119.60
5	H	41	DC	OP1-P-OP2	-6.77	109.45	119.60
5	H	196	DG	OP1-P-OP2	-6.77	109.45	119.60
9	T	22	DG	OP1-P-OP2	-6.76	109.45	119.60
9	T	103	DG	OP1-P-OP2	-6.76	109.46	119.60
9	T	205	DG	OP1-P-OP2	-6.76	109.46	119.60
9	T	179	DA	OP1-P-OP2	-6.75	109.47	119.60
5	H	191	DC	OP1-P-OP2	-6.75	109.47	119.60
9	T	45	DA	OP1-P-OP2	-6.75	109.48	119.60
5	H	48	DT	OP1-P-OP2	-6.75	109.48	119.60
5	H	143	DC	OP1-P-OP2	-6.75	109.48	119.60
9	T	23	DA	OP1-P-OP2	-6.75	109.48	119.60
9	T	87	DC	OP1-P-OP2	-6.75	109.48	119.60
9	T	93	DC	OP1-P-OP2	-6.75	109.48	119.60
5	H	30	DA	OP1-P-OP2	-6.74	109.49	119.60
9	T	24	DC	OP1-P-OP2	-6.74	109.49	119.60
9	T	198	DA	OP1-P-OP2	-6.74	109.49	119.60
9	T	35	DC	OP1-P-OP2	-6.74	109.50	119.60
5	H	61	DC	OP1-P-OP2	-6.73	109.50	119.60
9	T	16	DC	OP1-P-OP2	-6.73	109.50	119.60
9	T	43	DG	OP1-P-OP2	-6.73	109.50	119.60
5	H	189	DG	OP1-P-OP2	-6.73	109.50	119.60
9	T	33	DG	OP1-P-OP2	-6.73	109.50	119.60
9	T	204	DC	OP1-P-OP2	-6.73	109.51	119.60
9	T	166	DG	OP1-P-OP2	-6.72	109.51	119.60
9	T	15	DC	OP1-P-OP2	-6.72	109.52	119.60
5	H	208	DA	OP1-P-OP2	-6.72	109.52	119.60
9	T	102	DC	OP1-P-OP2	-6.72	109.52	119.60
5	H	83	DA	OP1-P-OP2	-6.72	109.53	119.60
5	H	195	DA	OP1-P-OP2	-6.72	109.53	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	H	211	DG	OP1-P-OP2	-6.72	109.52	119.60
5	H	23	DG	OP1-P-OP2	-6.71	109.53	119.60
5	H	116	DC	OP1-P-OP2	-6.71	109.54	119.60
9	T	40	DG	OP1-P-OP2	-6.71	109.54	119.60
5	H	185	DA	OP1-P-OP2	-6.70	109.54	119.60
5	H	194	DC	OP1-P-OP2	-6.70	109.55	119.60
9	T	53	DG	OP1-P-OP2	-6.70	109.54	119.60
5	H	124	DC	OP1-P-OP2	-6.70	109.55	119.60
5	H	192	DG	OP1-P-OP2	-6.70	109.56	119.60
5	H	200	DA	OP1-P-OP2	-6.70	109.56	119.60
9	T	137	DA	OP1-P-OP2	-6.69	109.56	119.60
5	H	64	DG	OP1-P-OP2	-6.69	109.56	119.60
9	T	64	DC	OP1-P-OP2	-6.69	109.56	119.60
5	H	205	DC	OP1-P-OP2	-6.69	109.57	119.60
9	T	138	DA	OP1-P-OP2	-6.69	109.57	119.60
5	H	142	DG	OP1-P-OP2	-6.68	109.57	119.60
5	H	159	DG	OP1-P-OP2	-6.68	109.57	119.60
9	T	95	DG	OP1-P-OP2	-6.68	109.58	119.60
9	T	114	DC	OP1-P-OP2	-6.68	109.58	119.60
9	T	54	DG	OP1-P-OP2	-6.68	109.58	119.60
9	T	191	DC	OP1-P-OP2	-6.68	109.58	119.60
5	H	132	DC	OP1-P-OP2	-6.68	109.58	119.60
9	T	156	DC	OP1-P-OP2	-6.68	109.59	119.60
9	T	34	DC	OP1-P-OP2	-6.67	109.59	119.60
5	H	178	DA	OP1-P-OP2	-6.67	109.59	119.60
5	H	45	DA	OP1-P-OP2	-6.67	109.60	119.60
9	T	42	DC	OP1-P-OP2	-6.67	109.60	119.60
9	T	50	DC	OP1-P-OP2	-6.67	109.60	119.60
5	H	134	DG	OP1-P-OP2	-6.67	109.60	119.60
9	T	139	DG	OP1-P-OP2	-6.67	109.60	119.60
9	T	186	DG	OP1-P-OP2	-6.66	109.61	119.60
9	T	200	DC	OP1-P-OP2	-6.66	109.61	119.60
9	T	163	DC	OP1-P-OP2	-6.66	109.62	119.60
9	T	194	DG	OP1-P-OP2	-6.65	109.62	119.60
5	H	115	DG	OP1-P-OP2	-6.65	109.62	119.60
9	T	32	DC	OP1-P-OP2	-6.65	109.62	119.60
5	H	59	DC	OP1-P-OP2	-6.65	109.63	119.60
5	H	166	DC	OP1-P-OP2	-6.65	109.63	119.60
5	H	38	DA	OP1-P-OP2	-6.65	109.63	119.60
5	H	125	DG	OP1-P-OP2	-6.65	109.63	119.60
9	T	135	DC	OP1-P-OP2	-6.64	109.64	119.60
5	H	49	DA	OP1-P-OP2	-6.64	109.64	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	H	82	DA	OP1-P-OP2	-6.64	109.64	119.60
5	H	57	DG	OP1-P-OP2	-6.64	109.64	119.60
9	T	61	DG	OP1-P-OP2	-6.63	109.65	119.60
9	T	177	DA	OP1-P-OP2	-6.63	109.65	119.60
5	H	40	DA	OP1-P-OP2	-6.63	109.65	119.60
9	T	104	DC	OP1-P-OP2	-6.63	109.66	119.60
5	H	21	DC	OP1-P-OP2	-6.63	109.66	119.60
9	T	17	DC	OP1-P-OP2	-6.62	109.67	119.60
9	T	106	DC	OP1-P-OP2	-6.62	109.67	119.60
5	H	173	DC	OP1-P-OP2	-6.62	109.67	119.60
5	H	50	DT	OP1-P-OP2	-6.61	109.69	119.60
5	H	187	DC	OP1-P-OP2	-6.61	109.69	119.60
5	H	58	DA	OP1-P-OP2	-6.60	109.69	119.60
9	T	158	DC	OP1-P-OP2	-6.60	109.69	119.60
9	T	192	DA	OP1-P-OP2	-6.60	109.69	119.60
5	H	75	DA	OP1-P-OP2	-6.60	109.70	119.60
5	H	95	DG	OP1-P-OP2	-6.60	109.70	119.60
5	H	165	DC	OP1-P-OP2	-6.60	109.70	119.60
5	H	156	DA	OP1-P-OP2	-6.60	109.70	119.60
5	H	102	DC	OP1-P-OP2	-6.59	109.72	119.60
5	H	207	DG	OP1-P-OP2	-6.59	109.72	119.60
9	T	196	DA	OP1-P-OP2	-6.59	109.72	119.60
9	T	31	DC	OP1-P-OP2	-6.58	109.72	119.60
5	H	181	DC	OP1-P-OP2	-6.58	109.72	119.60
5	H	113	DG	OP1-P-OP2	-6.58	109.73	119.60
5	H	43	DG	OP1-P-OP2	-6.58	109.73	119.60
5	H	57	DG	OP1-P-O3'	6.58	119.67	105.20
9	T	143	DA	OP1-P-OP2	-6.58	109.74	119.60
5	H	186	DG	OP1-P-OP2	-6.57	109.75	119.60
5	H	24	DA	OP1-P-OP2	-6.57	109.75	119.60
5	H	149	DA	OP1-P-O3'	6.57	119.65	105.20
9	T	18	DG	OP1-P-OP2	-6.56	109.75	119.60
9	T	48	DA	OP1-P-OP2	-6.56	109.75	119.60
5	H	79	DA	OP1-P-OP2	-6.56	109.76	119.60
9	T	19	DT	OP1-P-OP2	-6.56	109.75	119.60
9	T	147	DC	OP1-P-OP2	-6.56	109.76	119.60
9	T	65	DG	OP1-P-OP2	-6.56	109.76	119.60
5	H	55	DC	OP1-P-OP2	-6.55	109.77	119.60
9	T	51	DC	OP1-P-OP2	-6.55	109.77	119.60
5	H	60	DA	OP1-P-OP2	-6.55	109.78	119.60
9	T	116	DG	OP1-P-OP2	-6.55	109.78	119.60
9	T	141	DG	OP1-P-O3'	6.54	119.60	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	H	121	DG	OP1-P-OP2	-6.54	109.79	119.60
5	H	70	DA	OP1-P-OP2	-6.54	109.79	119.60
5	H	65	DC	OP1-P-OP2	-6.53	109.80	119.60
5	H	169	DG	OP1-P-OP2	-6.53	109.81	119.60
5	H	177	DG	OP1-P-OP2	-6.53	109.81	119.60
9	T	76	DC	OP1-P-OP2	-6.53	109.81	119.60
5	H	139	DA	OP1-P-OP2	-6.52	109.81	119.60
5	H	168	DC	OP1-P-OP2	-6.52	109.81	119.60
9	T	63	DC	OP1-P-OP2	-6.52	109.82	119.60
9	T	44	DG	OP1-P-OP2	-6.52	109.82	119.60
5	H	27	DG	OP1-P-OP2	-6.52	109.83	119.60
9	T	183	DC	OP1-P-OP2	-6.51	109.83	119.60
5	H	155	DA	OP1-P-OP2	-6.51	109.84	119.60
9	T	167	DT	OP1-P-O3'	6.51	119.52	105.20
5	H	73	DC	OP1-P-OP2	-6.51	109.84	119.60
5	H	170	DG	OP1-P-OP2	-6.50	109.84	119.60
5	H	152	DA	OP1-P-OP2	-6.50	109.85	119.60
5	H	190	DC	OP1-P-OP2	-6.50	109.85	119.60
9	T	188	DA	OP1-P-OP2	-6.50	109.85	119.60
9	T	173	DA	OP1-P-OP2	-6.50	109.86	119.60
5	H	91	DG	OP1-P-OP2	-6.49	109.86	119.60
9	T	149	DC	OP1-P-OP2	-6.49	109.86	119.60
5	H	136	DG	OP1-P-OP2	-6.49	109.86	119.60
9	T	82	DC	OP1-P-OP2	-6.49	109.86	119.60
9	T	175	DA	OP1-P-OP2	-6.49	109.87	119.60
5	H	176	DG	OP1-P-OP2	-6.49	109.87	119.60
9	T	56	DG	OP1-P-OP2	-6.48	109.88	119.60
9	T	89	DA	OP1-P-O3'	6.48	119.45	105.20
5	H	42	DA	OP1-P-OP2	-6.47	109.89	119.60
9	T	120	DC	OP1-P-OP2	-6.47	109.90	119.60
5	H	129	DA	OP1-P-OP2	-6.46	109.90	119.60
5	H	103	DG	OP1-P-OP2	-6.46	109.91	119.60
5	H	112	DA	OP1-P-OP2	-6.46	109.91	119.60
5	H	107	DG	OP1-P-OP2	-6.46	109.91	119.60
9	T	79	DA	OP1-P-OP2	-6.46	109.91	119.60
9	T	69	DT	OP1-P-O3'	6.45	119.40	105.20
9	T	73	DG	OP1-P-OP2	-6.45	109.92	119.60
9	T	181	DA	OP1-P-OP2	-6.45	109.93	119.60
9	T	92	DA	OP1-P-OP2	-6.44	109.94	119.60
9	T	113	DG	OP1-P-OP2	-6.44	109.95	119.60
9	T	141	DG	OP1-P-OP2	-6.43	109.95	119.60
5	H	106	DG	OP1-P-OP2	-6.43	109.95	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	H	44	DG	OP1-P-OP2	-6.42	109.96	119.60
5	H	137	DC	OP1-P-OP2	-6.42	109.96	119.60
5	H	188	DC	OP1-P-OP2	-6.42	109.97	119.60
5	H	149	DA	OP1-P-OP2	-6.41	109.98	119.60
9	T	20	DC	OP1-P-OP2	-6.41	109.99	119.60
5	H	47	DG	OP1-P-OP2	-6.40	109.99	119.60
9	T	169	DC	OP1-P-O3'	6.40	119.29	105.20
5	H	72	DA	OP1-P-OP2	-6.40	110.00	119.60
9	T	119	DC	OP1-P-OP2	-6.38	110.03	119.60
9	T	41	DC	OP1-P-OP2	-6.38	110.03	119.60
9	T	184	DC	OP1-P-OP2	-6.38	110.03	119.60
5	H	160	DA	OP1-P-OP2	-6.37	110.04	119.60
9	T	51	DC	OP1-P-O3'	6.37	119.22	105.20
5	H	153	DC	OP1-P-OP2	-6.37	110.05	119.60
5	H	120	DC	OP1-P-O3'	6.36	119.20	105.20
5	H	111	DC	OP1-P-OP2	-6.36	110.07	119.60
5	H	78	DG	OP1-P-OP2	-6.35	110.08	119.60
5	H	85	DC	OP1-P-OP2	-6.34	110.08	119.60
5	H	210	DG	OP1-P-OP2	-6.34	110.08	119.60
9	T	89	DA	OP1-P-OP2	-6.34	110.08	119.60
5	H	104	DC	OP1-P-OP2	-6.34	110.09	119.60
9	T	18	DG	OP1-P-O3'	6.34	119.14	105.20
5	H	154	DC	OP1-P-OP2	-6.34	110.09	119.60
9	T	38	DC	OP1-P-O3'	6.34	119.14	105.20
5	H	147	DC	OP1-P-OP2	-6.32	110.11	119.60
9	T	79	DA	OP1-P-O3'	6.32	119.09	105.20
5	H	71	DG	OP1-P-OP2	-6.30	110.14	119.60
5	H	60	DA	OP1-P-O3'	6.30	119.06	105.20
9	T	133	DC	OP1-P-OP2	-6.30	110.15	119.60
5	H	118	DT	OP1-P-O3'	6.30	119.06	105.20
9	T	74	DG	OP1-P-OP2	-6.29	110.16	119.60
9	T	146	DA	OP1-P-OP2	-6.29	110.16	119.60
9	T	164	DA	OP1-P-OP2	-6.29	110.17	119.60
5	H	93	DC	OP1-P-O3'	6.29	119.03	105.20
5	H	61	DC	OP1-P-O3'	6.27	119.00	105.20
9	T	172	DG	OP1-P-O3'	6.27	118.99	105.20
5	H	66	DC	OP1-P-OP2	-6.25	110.22	119.60
5	H	132	DC	OP1-P-O3'	6.24	118.92	105.20
9	T	65	DG	OP1-P-O3'	6.23	118.90	105.20
9	T	46	DG	OP1-P-OP2	-6.20	110.30	119.60
5	H	183	DC	OP1-P-OP2	-6.20	110.31	119.60
9	T	109	DA	OP1-P-OP2	-6.20	110.31	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	T	37	DG	OP1-P-O3'	6.19	118.83	105.20
5	H	33	DC	OP1-P-O3'	6.19	118.82	105.20
5	H	172	DA	OP1-P-O3'	6.18	118.80	105.20
9	T	90	DG	OP1-P-OP2	-6.17	110.34	119.60
9	T	42	DC	OP1-P-O3'	6.17	118.77	105.20
9	T	153	DA	OP1-P-O3'	6.16	118.74	105.20
5	H	141	DA	OP1-P-OP2	-6.15	110.37	119.60
5	H	75	DA	OP1-P-O3'	6.14	118.71	105.20
5	H	77	DG	OP1-P-O3'	6.13	118.70	105.20
5	H	120	DC	OP1-P-OP2	-6.13	110.41	119.60
9	T	122	DC	OP1-P-OP2	-6.11	110.44	119.60
9	T	21	DA	OP1-P-O3'	6.10	118.63	105.20
5	H	150	DC	OP1-P-O3'	6.09	118.61	105.20
5	H	174	DC	OP1-P-OP2	-6.08	110.48	119.60
9	T	132	DC	OP1-P-OP2	-6.08	110.48	119.60
9	T	34	DC	OP1-P-O3'	6.07	118.56	105.20
9	T	135	DC	OP1-P-O3'	6.07	118.56	105.20
5	H	32	DG	OP1-P-O3'	6.07	118.55	105.20
9	T	92	DA	OP1-P-O3'	6.07	118.55	105.20
5	H	45	DA	OP1-P-O3'	6.07	118.55	105.20
5	H	22	DC	OP1-P-O3'	6.06	118.52	105.20
5	H	44	DG	OP1-P-O3'	6.06	118.52	105.20
5	H	29	DC	OP1-P-OP2	-6.05	110.52	119.60
5	H	79	DA	OP1-P-O3'	6.05	118.52	105.20
5	H	99	DA	OP1-P-OP2	-6.05	110.53	119.60
9	T	159	DC	OP1-P-OP2	-6.04	110.55	119.60
9	T	139	DG	OP1-P-O3'	6.03	118.47	105.20
9	T	174	DT	OP1-P-O3'	6.03	118.46	105.20
5	H	202	DC	OP1-P-O3'	6.02	118.44	105.20
9	T	200	DC	OP1-P-O3'	6.02	118.44	105.20
9	T	95	DG	OP1-P-O3'	6.01	118.43	105.20
5	H	52	DT	OP1-P-O3'	6.01	118.42	105.20
9	T	36	DG	OP1-P-O3'	5.98	118.36	105.20
9	T	101	DA	OP1-P-OP2	-5.97	110.64	119.60
9	T	43	DG	OP1-P-O3'	5.97	118.33	105.20
9	T	47	DA	OP1-P-O3'	5.97	118.33	105.20
9	T	149	DC	OP1-P-O3'	5.96	118.32	105.20
5	H	100	DA	OP1-P-O3'	5.96	118.32	105.20
5	H	69	DG	OP1-P-OP2	-5.94	110.69	119.60
5	H	91	DG	OP1-P-O3'	5.93	118.25	105.20
5	H	67	DT	OP1-P-O3'	5.93	118.24	105.20
9	T	86	DC	OP1-P-O3'	5.93	118.24	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	T	190	DG	OP1-P-O3'	5.92	118.23	105.20
9	T	32	DC	OP1-P-O3'	5.91	118.21	105.20
5	H	167	DT	OP1-P-O3'	5.90	118.19	105.20
9	T	136	DC	OP1-P-O3'	5.90	118.19	105.20
5	H	110	DA	OP1-P-O3'	5.89	118.17	105.20
5	H	197	DC	OP1-P-O3'	5.88	118.13	105.20
9	T	25	DG	OP1-P-O3'	5.88	118.13	105.20
5	H	140	DG	OP1-P-OP2	-5.88	110.79	119.60
9	T	49	DT	OP1-P-O3'	5.87	118.12	105.20
5	H	152	DA	OP1-P-O3'	5.87	118.12	105.20
9	T	113	DG	OP1-P-O3'	5.87	118.11	105.20
5	H	113	DG	OP1-P-O3'	5.87	118.11	105.20
5	H	200	DA	OP1-P-O3'	5.87	118.11	105.20
9	T	197	DC	OP1-P-O3'	5.86	118.08	105.20
5	H	162	DC	OP1-P-OP2	-5.85	110.82	119.60
9	T	193	DC	OP1-P-O3'	5.85	118.07	105.20
5	H	54	DC	OP1-P-O3'	5.85	118.07	105.20
9	T	100	DA	OP1-P-OP2	-5.85	110.83	119.60
9	T	103	DG	OP1-P-O3'	5.84	118.05	105.20
5	H	142	DG	OP1-P-O3'	5.83	118.03	105.20
9	T	176	DT	OP1-P-O3'	5.83	118.03	105.20
9	T	27	DT	OP1-P-O3'	5.82	117.99	105.20
9	T	171	DA	OP2-P-O3'	5.82	117.99	105.20
9	T	84	DG	OP1-P-O3'	5.81	117.99	105.20
5	H	123	DG	OP1-P-OP2	-5.80	110.89	119.60
9	T	203	DT	OP1-P-O3'	5.79	117.94	105.20
5	H	124	DC	OP1-P-O3'	5.78	117.90	105.20
5	H	81	DT	OP1-P-O3'	5.76	117.88	105.20
9	T	28	DG	OP1-P-O3'	5.75	117.86	105.20
9	T	187	DT	OP1-P-O3'	5.75	117.86	105.20
9	T	179	DA	OP1-P-O3'	5.75	117.85	105.20
5	H	194	DC	OP1-P-O3'	5.74	117.84	105.20
9	T	41	DC	OP1-P-O3'	5.74	117.83	105.20
9	T	110	DC	OP1-P-O3'	5.74	117.83	105.20
5	H	141	DA	OP1-P-O3'	5.74	117.83	105.20
5	H	193	DG	OP1-P-O3'	5.74	117.83	105.20
5	H	161	DG	OP1-P-OP2	-5.73	111.00	119.60
5	H	138	DT	OP1-P-O3'	5.73	117.80	105.20
9	T	39	DG	OP1-P-O3'	5.73	117.80	105.20
5	H	162	DC	OP1-P-O3'	5.72	117.79	105.20
9	T	88	DC	OP1-P-O3'	5.72	117.79	105.20
5	H	43	DG	OP1-P-O3'	5.71	117.76	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	H	82	DA	OP1-P-O3'	5.71	117.76	105.20
5	H	185	DA	OP1-P-O3'	5.70	117.74	105.20
5	H	196	DG	OP1-P-O3'	5.69	117.72	105.20
5	H	176	DG	OP1-P-O3'	5.68	117.69	105.20
9	T	162	DG	OP1-P-OP2	-5.67	111.09	119.60
5	H	111	DC	OP1-P-O3'	5.67	117.68	105.20
5	H	180	DC	OP1-P-O3'	5.67	117.67	105.20
9	T	123	DG	OP1-P-OP2	-5.67	111.10	119.60
9	T	131	DA	OP1-P-OP2	-5.67	111.10	119.60
5	H	199	DC	OP1-P-O3'	5.67	117.67	105.20
5	H	209	DC	OP1-P-O3'	5.67	117.66	105.20
5	H	129	DA	OP1-P-O3'	5.66	117.65	105.20
5	H	94	DG	OP1-P-O3'	5.65	117.63	105.20
5	H	70	DA	OP1-P-O3'	5.65	117.62	105.20
5	H	168	DC	OP1-P-O3'	5.64	117.60	105.20
5	H	189	DG	OP1-P-O3'	5.63	117.59	105.20
5	H	78	DG	OP1-P-O3'	5.63	117.59	105.20
5	H	46	DT	OP1-P-O3'	5.63	117.59	105.20
5	H	76	DG	OP1-P-O3'	5.63	117.58	105.20
9	T	106	DC	OP1-P-O3'	5.62	117.58	105.20
5	H	112	DA	OP1-P-O3'	5.62	117.57	105.20
9	T	31	DC	OP1-P-O3'	5.62	117.57	105.20
9	T	81	DA	OP1-P-O3'	5.62	117.57	105.20
5	H	158	DG	OP1-P-O3'	5.61	117.55	105.20
9	T	53	DG	OP1-P-O3'	5.61	117.55	105.20
5	H	74	DT	OP1-P-O3'	5.61	117.54	105.20
5	H	36	DG	OP1-P-O3'	5.61	117.53	105.20
9	T	132	DC	OP1-P-O3'	5.60	117.51	105.20
5	H	56	DT	OP1-P-O3'	5.58	117.48	105.20
9	T	15	DC	OP1-P-O3'	5.58	117.48	105.20
5	H	190	DC	OP1-P-O3'	5.58	117.47	105.20
5	H	154	DC	OP1-P-O3'	5.57	117.46	105.20
9	T	121	DC	OP1-P-O3'	5.56	117.43	105.20
9	T	101	DA	OP1-P-O3'	5.56	117.42	105.20
5	H	186	DG	OP1-P-O3'	5.55	117.41	105.20
9	T	75	DT	OP1-P-O3'	5.55	117.41	105.20
9	T	17	DC	OP1-P-O3'	5.54	117.40	105.20
5	H	64	DG	OP1-P-O3'	5.52	117.34	105.20
9	T	134	DG	OP1-P-O3'	5.52	117.33	105.20
5	H	47	DG	OP1-P-O3'	5.51	117.33	105.20
5	H	188	DC	OP1-P-O3'	5.51	117.33	105.20
5	H	155	DA	OP1-P-O3'	5.51	117.32	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	H	201	DG	OP1-P-O3'	5.51	117.32	105.20
9	T	102	DC	OP1-P-O3'	5.49	117.28	105.20
9	T	195	DC	OP1-P-O3'	5.49	117.29	105.20
9	T	112	DC	OP1-P-O3'	5.49	117.28	105.20
5	H	135	DT	OP1-P-O3'	5.49	117.27	105.20
9	T	165	DC	OP1-P-O3'	5.49	117.27	105.20
9	T	115	DC	OP1-P-O3'	5.49	117.27	105.20
5	H	63	DT	OP1-P-O3'	5.48	117.25	105.20
5	H	123	DG	OP1-P-O3'	5.48	117.25	105.20
5	H	58	DA	OP1-P-O3'	5.47	117.24	105.20
9	T	142	DG	OP1-P-O3'	5.47	117.24	105.20
9	T	22	DG	OP1-P-O3'	5.47	117.24	105.20
5	H	40	DA	OP1-P-O3'	5.47	117.23	105.20
9	T	78	DT	OP2-P-O3'	5.46	117.21	105.20
9	T	40	DG	OP1-P-O3'	5.45	117.20	105.20
5	H	148	DT	OP1-P-O3'	5.45	117.18	105.20
9	T	64	DC	OP1-P-O3'	5.45	117.18	105.20
5	H	183	DC	OP1-P-O3'	5.44	117.17	105.20
9	T	26	DC	OP1-P-O3'	5.44	117.17	105.20
9	T	72	DT	OP1-P-O3'	5.44	117.17	105.20
9	T	16	DC	OP1-P-O3'	5.44	117.17	105.20
9	T	30	DG	OP1-P-O3'	5.44	117.17	105.20
5	H	103	DG	OP1-P-O3'	5.43	117.15	105.20
5	H	72	DA	OP1-P-O3'	5.43	117.14	105.20
9	T	118	DC	OP1-P-O3'	5.42	117.13	105.20
9	T	146	DA	OP1-P-O3'	5.42	117.13	105.20
9	T	105	DA	OP1-P-O3'	5.42	117.13	105.20
9	T	50	DC	OP1-P-O3'	5.42	117.12	105.20
9	T	191	DC	OP1-P-O3'	5.41	117.11	105.20
5	H	164	DG	OP1-P-O3'	5.39	117.06	105.20
9	T	23	DA	OP1-P-O3'	5.38	117.05	105.20
5	H	84	DC	OP1-P-O3'	5.38	117.04	105.20
5	H	49	DA	OP1-P-O3'	5.38	117.03	105.20
9	T	91	DC	OP1-P-OP2	-5.36	111.57	119.60
5	H	165	DC	OP1-P-O3'	5.35	116.97	105.20
5	H	151	DG	OP1-P-O3'	5.34	116.95	105.20
5	H	191	DC	OP1-P-O3'	5.34	116.95	105.20
9	T	178	DT	OP1-P-O3'	5.34	116.94	105.20
5	H	41	DC	OP1-P-O3'	5.33	116.94	105.20
9	T	194	DG	OP1-P-O3'	5.33	116.93	105.20
5	H	39	DT	OP1-P-O3'	5.33	116.92	105.20
9	T	140	DG	OP1-P-O3'	5.33	116.92	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	H	122	DT	OP1-P-O3'	5.31	116.88	105.20
9	T	155	DT	OP1-P-O3'	5.27	116.80	105.20
9	T	159	DC	OP1-P-O3'	5.26	116.77	105.20
9	T	145	DT	OP1-P-O3'	5.25	116.75	105.20
9	T	60	DA	OP1-P-O3'	5.24	116.72	105.20
5	H	144	DT	OP1-P-O3'	5.22	116.69	105.20
9	T	148	DC	OP1-P-O3'	5.22	116.69	105.20
5	H	31	DT	OP1-P-O3'	5.21	116.67	105.20
5	H	170	DG	OP1-P-O3'	5.21	116.67	105.20
5	H	195	DA	OP1-P-O3'	5.21	116.67	105.20
5	H	169	DG	OP1-P-O3'	5.21	116.65	105.20
9	T	91	DC	OP1-P-O3'	5.21	116.65	105.20
9	T	119	DC	OP1-P-O3'	5.20	116.64	105.20
5	H	37	DC	OP1-P-O3'	5.19	116.62	105.20
5	H	116	DC	OP1-P-O3'	5.18	116.60	105.20
9	T	20	DC	OP1-P-O3'	5.18	116.59	105.20
9	T	52	DC	OP1-P-O3'	5.17	116.56	105.20
5	H	26	DT	OP1-P-O3'	5.15	116.53	105.20
9	T	199	DT	OP1-P-O3'	5.14	116.51	105.20
9	T	44	DG	OP1-P-O3'	5.13	116.49	105.20
9	T	55	DT	OP1-P-O3'	5.12	116.46	105.20
9	T	122	DC	OP1-P-O3'	5.11	116.44	105.20
9	T	137	DA	OP1-P-O3'	5.10	116.42	105.20
9	T	35	DC	OP1-P-O3'	5.10	116.42	105.20
5	H	90	DT	OP1-P-O3'	5.08	116.39	105.20
9	T	183	DC	OP1-P-O3'	5.08	116.37	105.20
5	H	106	DG	OP1-P-O3'	5.08	116.37	105.20
9	T	164	DA	OP1-P-O3'	5.07	116.36	105.20
5	H	48	DT	OP1-P-O3'	5.06	116.33	105.20
5	H	65	DC	OP1-P-O3'	5.06	116.33	105.20
5	H	101	DA	OP1-P-O3'	5.05	116.32	105.20
5	H	160	DA	OP1-P-O3'	5.04	116.28	105.20
5	H	198	DG	OP1-P-O3'	5.03	116.27	105.20
9	T	157	DC	OP1-P-O3'	5.03	116.27	105.20
5	H	25	DA	OP1-P-O3'	5.02	116.25	105.20
9	T	152	DC	OP1-P-O3'	5.02	116.25	105.20
5	H	192	DG	OP1-P-O3'	5.02	116.24	105.20
9	T	182	DT	OP1-P-O3'	5.02	116.24	105.20
5	H	133	DG	OP1-P-O3'	5.01	116.21	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	D	3633	0	3628	94	0
2	E	4580	0	4483	168	0
3	G	2930	0	2839	147	0
4	I	917	0	971	44	0
4	W	817	0	858	36	0
5	H	3972	0	2154	133	0
6	J	661	0	709	29	0
6	X	666	0	679	20	0
7	R	829	0	887	39	0
7	U	825	0	876	39	0
8	S	742	0	753	22	0
8	V	737	0	751	30	0
9	T	3919	0	2153	133	0
10	O	3139	0	2986	97	0
11	Y	1047	0	1102	22	0
12	E	26	0	19	5	0
All	All	29440	0	25848	873	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 19.

All (873) 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)
3:G:191:ASN:HB3	3:G:211:LYS:HB3	1.50	0.92
3:G:175:ILE:HG13	3:G:182:CYS:HB2	1.54	0.90
7:U:84:GLN:HE21	7:U:88:ARG:HE	1.19	0.87
11:Y:243:TRP:HB2	11:Y:248:ILE:HG21	1.60	0.84
10:O:293:SER:HG	10:O:297:THR:HG1	1.28	0.80
5:H:169:DG:N2	9:T:58:DC:O2	2.15	0.79
4:W:61:LEU:HD12	6:X:36:ARG:HB3	1.64	0.79
7:R:78:ILE:HG22	8:S:51:ILE:HA	1.65	0.79
2:E:326:GLY:O	2:E:328:GLN:N	2.17	0.78
3:G:145:GLU:HB2	3:G:168:SER:HB2	1.66	0.77
10:O:180:GLY:HA3	10:O:197:SER:HA	1.65	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:205:DC:O2	9:T:22:DG:N2	2.14	0.77
3:G:330:CYS:H	3:G:354:GLY:HA3	1.48	0.76
2:E:682:ALA:O	2:E:690:ARG:NH1	2.19	0.75
5:H:182:DC:H42	9:T:45:DA:H61	1.32	0.75
7:R:25:PHE:HE2	7:R:56:GLU:HA	1.52	0.74
7:U:87:VAL:HG11	7:U:97:LEU:HD12	1.67	0.74
1:D:319:MET:HB2	1:D:353:PRO:HB2	1.69	0.74
2:E:512:GLN:HA	2:E:516:ASP:HB2	1.68	0.74
5:H:97:DT:H4'	5:H:98:DA:H5'	1.69	0.74
5:H:64:DG:O6	9:T:163:DC:N4	2.20	0.73
10:O:160:LYS:HD3	10:O:161:PRO:HD2	1.70	0.73
4:W:121:PRO:O	4:W:125:GLN:NE2	2.21	0.73
5:H:54:DC:H42	9:T:173:DA:H61	1.33	0.73
9:T:153:DA:OP2	7:U:35:ARG:NH2	2.22	0.73
2:E:448:LEU:HD13	2:E:459:ILE:HD12	1.69	0.72
7:U:42:ARG:HB2	8:V:85:THR:HG22	1.70	0.72
1:D:650:LYS:HB2	1:D:652:LEU:HD22	1.71	0.72
3:G:172:ILE:HB	3:G:186:TYR:HB2	1.72	0.71
5:H:80:DG:N2	9:T:148:DC:O2	2.24	0.71
2:E:60:TRP:HE1	3:G:105:SER:H	1.39	0.71
6:J:98:TYR:OH	8:S:65:ASP:OD2	2.07	0.71
2:E:181:TYR:HH	2:E:220:SER:HG	1.31	0.71
4:I:106:ASP:HA	4:I:109:LEU:HD12	1.73	0.70
5:H:194:DC:O2	9:T:33:DG:N2	2.17	0.70
1:D:613:VAL:HG12	1:D:652:LEU:HD12	1.74	0.69
2:E:575:GLN:NE2	9:T:44:DG:O3'	2.21	0.69
5:H:109:DG:N2	9:T:119:DC:O2	2.26	0.69
2:E:585:CYS:HB2	2:E:590:CYS:HB2	1.73	0.69
3:G:176:ASN:HB3	3:G:179:THR:HG22	1.75	0.69
9:T:152:DC:H5"	7:U:44:GLY:HA2	1.74	0.69
5:H:179:DT:H2"	5:H:180:DC:H5'	1.75	0.68
6:X:64:ASN:O	6:X:93:GLN:NE2	2.25	0.68
1:D:158:GLN:HE22	1:D:232:VAL:HG13	1.58	0.68
3:G:210:SER:OG	3:G:212:ASP:OD1	2.11	0.68
5:H:84:DC:H42	9:T:143:DA:H61	1.41	0.68
5:H:37:DC:O2	9:T:190:DG:N2	2.20	0.68
3:G:264:ARG:NH2	3:G:340:ILE:O	2.27	0.68
8:V:116:THR:HA	8:V:119:THR:HG22	1.74	0.68
10:O:386:GLU:HB3	10:O:389:VAL:HG12	1.76	0.67
7:R:62:ILE:HG13	7:R:93:LEU:HD21	1.76	0.67
10:O:318:ASP:OD2	10:O:338:THR:OG1	2.10	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:O:77:ASN:ND2	10:O:125:GLY:O	2.26	0.67
5:H:189:DG:N2	9:T:38:DC:O2	2.19	0.67
3:G:99:VAL:HG11	3:G:428:VAL:HG21	1.77	0.66
3:G:281:ASN:HB3	3:G:284:LYS:HG2	1.77	0.66
5:H:189:DG:N1	9:T:38:DC:N3	2.36	0.66
4:I:37:LYS:NZ	4:I:38:PRO:O	2.24	0.66
4:I:67:PHE:CD2	4:I:93:GLN:HG3	2.31	0.66
6:J:51:TYR:O	6:J:55:ARG:NH2	2.29	0.66
5:H:57:DG:O6	9:T:169:DC:N4	2.28	0.66
10:O:198:ASP:HA	10:O:229:VAL:HG13	1.76	0.66
2:E:586:ASP:HB3	2:E:589:LEU:HB2	1.78	0.66
6:J:39:ARG:NH1	6:J:44:LYS:O	2.28	0.66
3:G:86:ASN:ND2	3:G:130:GLY:O	2.28	0.66
4:I:123:ASP:OD1	4:W:113:HIS:NE2	2.28	0.66
5:H:51:DA:N6	9:T:176:DT:O4	2.20	0.66
10:O:204:LEU:O	10:O:220:LYS:N	2.26	0.66
3:G:211:LYS:HA	3:G:238:GLU:HG3	1.77	0.66
4:I:60:LEU:HD13	4:I:93:GLN:OE1	1.96	0.66
1:D:521:LYS:HD3	1:D:577:GLN:HG3	1.77	0.65
2:E:541:CYS:SG	2:E:560:ASN:ND2	2.68	0.65
5:H:192:DG:O6	9:T:34:DC:N4	2.29	0.65
2:E:236:THR:O	2:E:240:LEU:N	2.29	0.65
7:U:79:ILE:HG22	7:U:82:HIS:HD2	1.61	0.65
2:E:521:HIS:O	2:E:545:GLN:NE2	2.30	0.65
2:E:501:HIS:HA	2:E:504:TRP:CD1	2.32	0.65
7:R:25:PHE:HD2	7:R:56:GLU:HG2	1.61	0.65
8:V:106:HIS:O	8:V:109:SER:OG	2.12	0.65
10:O:93:PHE:HB2	11:Y:171:LYS:HD3	1.79	0.64
2:E:71:LEU:HB2	3:G:136:GLN:HG2	1.78	0.64
2:E:330:TYR:HE1	2:E:457:CYS:HB2	1.63	0.64
3:G:242:ALA:O	3:G:313:ARG:NH2	2.31	0.64
6:J:78:ARG:NH2	6:J:85:ASP:OD2	2.28	0.64
3:G:245:ASP:OD2	3:G:250:LYS:N	2.24	0.64
5:H:80:DG:OP2	8:V:83:ARG:NH2	2.29	0.64
7:U:20:ARG:NH1	8:V:121:ALA:O	2.30	0.64
4:W:102:ALA:O	4:W:131:ARG:NH2	2.29	0.64
2:E:620:LEU:HD11	2:E:634:LYS:HB3	1.80	0.64
2:E:624:SER:N	2:E:628:GLY:O	2.31	0.64
7:R:29:ARG:NH1	8:S:32:GLU:OE2	2.31	0.64
10:O:188:ASN:HB2	10:O:240:GLU:HB3	1.79	0.64
10:O:85:GLN:HB2	10:O:114:LYS:HB3	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:288:ARG:NH2	2:E:709:GLY:O	2.25	0.63
3:G:207:LEU:HB2	3:G:217:LEU:HD12	1.80	0.63
10:O:106:GLY:N	10:O:109:GLY:O	2.30	0.63
2:E:567:CYS:O	2:E:592:THR:OG1	2.10	0.63
7:R:64:GLU:HA	8:S:46:HIS:HE1	1.61	0.63
5:H:41:DC:H2"	5:H:42:DA:C8	2.34	0.63
11:Y:224:SER:OG	11:Y:259:ARG:NH1	2.31	0.63
6:J:44:LYS:HB2	7:R:115:LEU:HD13	1.81	0.62
1:D:586:GLU:HG2	1:D:588:ASP:H	1.64	0.62
1:D:125:THR:HB	10:O:410:ASN:HD21	1.65	0.62
10:O:292:GLY:HA2	10:O:298:VAL:HA	1.79	0.62
1:D:641:GLU:HA	1:D:680:LYS:HE2	1.82	0.62
6:X:29:ILE:O	6:X:55:ARG:NH1	2.33	0.62
3:G:89:LYS:HA	3:G:433:SER:HA	1.82	0.61
5:H:37:DC:N3	9:T:190:DG:N1	2.36	0.61
2:E:671:LEU:HD13	2:E:681:ASP:HB3	1.82	0.61
5:H:142:DG:N2	9:T:86:DC:O2	2.33	0.61
2:E:160:ASP:HA	3:G:306:ARG:HE	1.66	0.61
10:O:81:ILE:HB	10:O:119:ILE:HB	1.83	0.61
2:E:653:GLN:OE1	4:I:26:ARG:NE	2.33	0.61
2:E:664:ASP:OD1	2:E:741:TYR:OH	2.16	0.61
2:E:528:CYS:HB2	2:E:540:PRO:HD2	1.83	0.61
6:J:38:ALA:HB1	6:J:43:VAL:HB	1.83	0.61
1:D:556:THR:OG1	11:Y:173:ARG:NH2	2.34	0.61
2:E:529:ASP:HA	2:E:553:GLN:HB2	1.82	0.61
2:E:701:TYR:CZ	2:E:716:PHE:HB2	2.36	0.61
3:G:86:ASN:HB3	3:G:436:ARG:HB3	1.82	0.61
10:O:251:LYS:HE2	10:O:268:SER:HB3	1.83	0.61
2:E:502:ARG:NH1	4:I:39:HIS:O	2.33	0.61
9:T:32:DC:H2'	9:T:33:DG:C8	2.36	0.60
9:T:193:DC:H2'	9:T:194:DG:C8	2.36	0.60
10:O:281:PHE:CD1	10:O:289:LEU:HD13	2.36	0.60
2:E:86:THR:HA	2:E:93:THR:HG23	1.83	0.60
2:E:100:THR:HG23	3:G:141:ALA:HB3	1.83	0.60
2:E:554:CYS:HB3	2:E:558:CYS:HB2	1.84	0.60
3:G:201:ARG:NH1	3:G:247:LEU:O	2.34	0.60
5:H:182:DC:O2	9:T:46:DG:N2	2.35	0.60
9:T:98:DT:H2"	9:T:99:DA:C8	2.37	0.60
9:T:122:DC:H2'	9:T:123:DG:C8	2.38	0.59
10:O:79:LEU:HD21	10:O:140:ILE:HD11	1.83	0.59
2:E:556:SER:O	2:E:561:ARG:NH2	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:S:73:GLU:HG3	8:S:98:LEU:HD21	1.84	0.59
2:E:660:GLY:O	2:E:664:ASP:N	2.29	0.59
4:I:108:ASN:ND2	6:J:42:GLY:O	2.36	0.59
4:I:61:LEU:HD12	6:J:37:LEU:HD23	1.83	0.59
3:G:389:TRP:HE1	3:G:401:CYS:HG	1.51	0.59
5:H:40:DA:N6	9:T:186:DG:O6	2.36	0.59
2:E:587:PRO:HA	2:E:595:ALA:HB1	1.83	0.59
2:E:610:SER:O	2:E:614:GLY:N	2.35	0.59
2:E:693:ASN:OD1	12:E:801:SAH:N6	2.35	0.59
5:H:50:DT:H2'	5:H:51:DA:C8	2.37	0.59
7:R:97:LEU:HD22	7:R:100:VAL:HG11	1.84	0.59
6:J:29:ILE:O	6:J:55:ARG:NH1	2.36	0.59
2:E:336:ALA:HB1	2:E:472:TYR:HE2	1.68	0.58
1:D:247:SER:HB2	1:D:302:PHE:HB3	1.84	0.58
7:U:79:ILE:HG22	7:U:82:HIS:CD2	2.37	0.58
10:O:127:VAL:HG13	10:O:142:THR:HG23	1.84	0.58
1:D:189:VAL:HG23	1:D:205:GLN:HG3	1.84	0.58
10:O:61:PHE:HB2	10:O:85:GLN:HB3	1.83	0.58
10:O:65:ARG:HA	10:O:83:SER:HA	1.85	0.58
8:S:92:GLN:NE2	8:S:96:ARG:HH12	2.02	0.58
8:V:90:GLU:N	8:V:90:GLU:OE2	2.36	0.58
2:E:52:ARG:HD3	3:G:246:LEU:HB2	1.86	0.58
2:E:289:CYS:HB2	2:E:297:HIS:NE2	2.19	0.58
2:E:470:GLN:HA	2:E:473:GLU:HB2	1.86	0.58
2:E:647:CYS:SG	2:E:687:ASN:ND2	2.75	0.58
3:G:338:ASP:HA	3:G:342:LYS:HE2	1.84	0.58
1:D:157:LEU:HD11	1:D:359:LEU:HD11	1.85	0.58
3:G:240:LEU:O	3:G:367:ARG:NH2	2.37	0.58
7:U:84:GLN:NE2	7:U:88:ARG:HE	1.97	0.58
10:O:236:HIS:HA	10:O:281:PHE:CD2	2.38	0.58
1:D:632:MET:HE3	1:D:668:LEU:HB2	1.86	0.58
5:H:47:DG:H2'	5:H:48:DT:H71	1.86	0.58
7:U:34:LEU:HB3	7:U:43:VAL:HG21	1.84	0.58
1:D:103:ARG:NH1	11:Y:283:ASN:O	2.37	0.57
3:G:383:VAL:HG23	3:G:385:LYS:HG3	1.85	0.57
6:X:73:THR:HG23	6:X:78:ARG:HB2	1.86	0.57
1:D:572:LEU:HD11	3:G:225:LEU:HD22	1.86	0.57
2:E:624:SER:HB3	2:E:630:GLY:HA3	1.86	0.57
9:T:89:DA:H1'	9:T:90:DG:C8	2.39	0.57
5:H:29:DC:H42	9:T:197:DC:H42	1.50	0.57
9:T:163:DC:H2"	9:T:164:DA:H8	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:163:CYS:SG	2:E:167:ASN:ND2	2.77	0.57
7:R:25:PHE:CE2	7:R:56:GLU:HA	2.38	0.57
1:D:605:ASP:HA	2:E:257:PRO:HD3	1.85	0.57
10:O:36:MET:HB3	10:O:401:VAL:HB	1.87	0.57
1:D:570:THR:O	3:G:216:ARG:NH1	2.38	0.57
7:R:31:HIS:HD2	7:R:48:PRO:HG3	1.70	0.57
10:O:341:ARG:HE	10:O:371:GLY:HA3	1.69	0.57
1:D:569:ASP:N	1:D:584:GLU:OE1	2.37	0.57
5:H:168:DC:H2"	5:H:169:DG:C8	2.40	0.56
7:U:16:THR:HG22	7:U:18:SER:H	1.70	0.56
3:G:119:ASN:HB2	3:G:140:ASP:HB3	1.87	0.56
5:H:46:DT:O3'	4:W:41:TYR:OH	2.23	0.56
10:O:148:ASP:OD2	10:O:172:ARG:NH1	2.32	0.56
1:D:647:ILE:HA	1:D:652:LEU:HD21	1.87	0.56
3:G:160:HIS:HB3	3:G:178:ILE:HD13	1.87	0.56
5:H:207:DG:H2"	5:H:208:DA:C8	2.39	0.56
3:G:145:GLU:OE1	3:G:168:SER:N	2.38	0.56
2:E:228:SER:HB3	2:E:234:LYS:HB2	1.88	0.56
2:E:501:HIS:HA	2:E:504:TRP:HD1	1.69	0.56
2:E:675:ASN:OD1	2:E:678:PHE:N	2.31	0.56
3:G:406:HIS:HB2	3:G:437:TRP:CZ2	2.41	0.56
4:I:92:LEU:HD22	6:J:86:VAL:HG11	1.87	0.56
7:R:79:ILE:HB	7:R:82:HIS:HD1	1.71	0.56
3:G:193:ILE:HG12	3:G:210:SER:HB3	1.87	0.56
10:O:49:TRP:NE1	10:O:391:CYS:SG	2.79	0.56
2:E:433:GLU:H	2:E:470:GLN:HG2	1.70	0.56
9:T:88:DC:H2"	9:T:89:DA:C8	2.40	0.56
1:D:214:PRO:HD2	1:D:217:PRO:HG3	1.87	0.56
10:O:196:ALA:HB1	10:O:230:VAL:HG13	1.86	0.56
10:O:24:TRP:CE2	10:O:372:GLY:HA3	2.40	0.56
3:G:116:VAL:HG12	3:G:121:VAL:HG12	1.87	0.55
11:Y:243:TRP:HD1	11:Y:248:ILE:HD12	1.72	0.55
4:W:79:LYS:HD3	6:X:74:GLU:OE2	2.06	0.55
2:E:663:TYR:O	2:E:667:MET:N	2.40	0.55
3:G:311:CYS:HB2	3:G:322:LYS:HB2	1.88	0.55
1:D:184:LEU:HD22	1:D:211:LYS:HE2	1.88	0.55
1:D:431:GLN:HG2	1:D:441:GLN:HG3	1.89	0.55
3:G:423:SER:HA	3:G:439:ARG:HB3	1.89	0.55
9:T:50:DC:H2"	9:T:51:DC:H5"	1.87	0.55
6:X:59:LYS:NZ	6:X:63:GLU:OE2	2.38	0.55
10:O:382:TRP:HE3	10:O:390:ILE:HG12	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:T:153:DA:OP1	7:U:35:ARG:NH1	2.40	0.55
2:E:121:MET:HA	2:E:650:ILE:HB	1.88	0.55
5:H:56:DT:H2"	5:H:57:DG:N7	2.22	0.55
9:T:133:DC:H2'	9:T:134:DG:C8	2.42	0.55
10:O:132:TYR:HB3	10:O:140:ILE:HG22	1.88	0.55
5:H:148:DT:H3	9:T:79:DA:H61	1.53	0.55
3:G:226:VAL:HG12	3:G:227:ALA:H	1.71	0.55
7:R:31:HIS:CD2	7:R:48:PRO:HG3	2.42	0.55
1:D:450:CYS:HB3	1:D:455:LEU:H	1.72	0.54
2:E:631:ILE:HG13	2:E:689:ILE:HA	1.90	0.54
3:G:118:SER:OG	3:G:146:ASN:ND2	2.41	0.54
2:E:673:ASN:N	4:I:27:LYS:O	2.32	0.54
9:T:126:DT:H2"	9:T:127:DT:H5'	1.89	0.54
10:O:281:PHE:CE1	10:O:289:LEU:HD13	2.42	0.54
1:D:481:HIS:ND1	1:D:486:ARG:HD3	2.23	0.54
2:E:46:ARG:NH1	3:G:391:LEU:O	2.40	0.54
2:E:562:PHE:CD1	2:E:583:ARG:HG3	2.43	0.54
7:R:22:GLY:HA3	8:S:117:LYS:NZ	2.23	0.54
3:G:389:TRP:NE1	3:G:401:CYS:SG	2.76	0.54
10:O:327:PRO:HD3	10:O:382:TRP:CD1	2.43	0.54
2:E:643:ILE:HG22	2:E:644:SER:H	1.72	0.54
3:G:412:ALA:O	3:G:430:ASP:N	2.34	0.54
4:W:100:LEU:HD11	6:X:58:LEU:HD13	1.89	0.54
1:D:631:GLN:HG2	2:E:599:TRP:CE2	2.43	0.54
2:E:39:LYS:NZ	3:G:393:VAL:O	2.40	0.54
2:E:105:ALA:O	3:G:169:ARG:NH2	2.41	0.54
2:E:331:GLN:O	2:E:469:ARG:NH2	2.41	0.54
3:G:379:LEU:O	3:G:387:TYR:N	2.33	0.54
2:E:296:LEU:HD23	2:E:296:LEU:H	1.73	0.53
1:D:562:ASN:OD1	1:D:563:ARG:N	2.41	0.53
3:G:90:GLU:HG3	3:G:92:HIS:H	1.73	0.53
3:G:127:HIS:HB2	3:G:131:GLU:HB3	1.90	0.53
3:G:384:GLY:HA2	3:G:413:ILE:HG12	1.91	0.53
5:H:54:DC:N4	9:T:173:DA:H61	2.05	0.53
6:J:75:HIS:HB2	8:V:93:THR:HG21	1.91	0.53
2:E:599:TRP:HA	2:E:613:ARG:NH2	2.23	0.53
5:H:77:DG:H1	9:T:150:DC:H42	1.57	0.53
4:I:39:HIS:NE2	5:H:183:DC:H4'	2.23	0.53
4:I:57:SER:O	6:J:40:ARG:NH2	2.38	0.53
9:T:17:DC:H1'	9:T:18:DG:H5'	1.89	0.53
3:G:406:HIS:HB2	3:G:437:TRP:HZ2	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:150:DC:H1'	5:H:151:DG:C8	2.44	0.53
2:E:659:ARG:NH1	2:E:681:ASP:OD2	2.42	0.53
2:E:700:CYS:HA	2:E:717:ALA:HA	1.90	0.53
1:D:607:ASN:HB2	1:D:610:GLU:HG2	1.91	0.53
2:E:570:GLN:HB2	2:E:606:CYS:HA	1.89	0.53
2:E:657:ASP:OD1	4:I:26:ARG:NH1	2.31	0.53
3:G:153:THR:HG21	3:G:174:ILE:HD11	1.91	0.53
3:G:169:ARG:NH1	3:G:171:ILE:HD12	2.24	0.53
10:O:271:ALA:HB3	10:O:276:VAL:HG21	1.90	0.53
3:G:80:TYR:HA	3:G:402:THR:HG21	1.91	0.53
3:G:164:ALA:HA	3:G:174:ILE:HA	1.91	0.53
9:T:76:DC:H2"	9:T:77:DG:C8	2.44	0.53
1:D:532:ARG:HH21	10:O:93:PHE:HZ	1.57	0.52
5:H:66:DC:H2"	5:H:67:DT:C5	2.44	0.52
5:H:139:DA:H2"	5:H:140:DG:C8	2.44	0.52
10:O:274:ALA:HB3	10:O:295:ASP:HB2	1.91	0.52
3:G:96:LEU:HG	3:G:432:ALA:HA	1.90	0.52
9:T:68:DC:H4'	9:T:69:DT:OP1	2.08	0.52
10:O:177:GLN:N	10:O:199:ASP:OD2	2.42	0.52
1:D:499:TYR:HB3	1:D:506:ILE:HD11	1.90	0.52
4:W:125:GLN:HA	4:W:134:ARG:NH1	2.24	0.52
10:O:316:HIS:NE2	10:O:335:SER:OG	2.43	0.52
1:D:643:TYR:O	1:D:647:ILE:HG12	2.09	0.52
7:R:57:TYR:HB2	8:S:110:GLU:HG3	1.90	0.52
10:O:170:ASP:HA	10:O:215:LYS:HE2	1.91	0.52
10:O:313:PHE:HB3	10:O:345:TRP:CZ2	2.44	0.52
1:D:575:ARG:NH1	1:D:578:GLU:OE1	2.41	0.52
2:E:221:ASP:HA	2:E:224:PHE:CD2	2.43	0.52
2:E:224:PHE:HB3	2:E:237:ALA:H	1.75	0.52
11:Y:225:THR:N	11:Y:242:HIS:O	2.42	0.52
5:H:101:DA:OP2	6:J:30:THR:OG1	2.28	0.52
2:E:507:HIS:ND1	2:E:559:GLN:O	2.41	0.52
5:H:166:DC:N3	9:T:60:DA:N6	2.58	0.52
1:D:607:ASN:ND2	2:E:261:THR:O	2.36	0.52
3:G:252:MET:SD	3:G:262:LEU:HB3	2.50	0.52
4:I:48:LEU:HB3	4:I:52:ARG:NH2	2.24	0.52
2:E:683:THR:O	2:E:690:ARG:NH1	2.43	0.51
2:E:704:VAL:HG22	2:E:713:ILE:HG22	1.92	0.51
5:H:35:DT:H2"	5:H:36:DG:C8	2.45	0.51
7:R:104:GLN:HE22	8:S:54:LYS:NZ	2.07	0.51
5:H:194:DC:H42	9:T:32:DC:H42	1.56	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:250:LEU:N	1:D:299:MET:O	2.36	0.51
4:I:46:VAL:HB	9:T:123:DG:OP2	2.10	0.51
10:O:43:PRO:O	10:O:71:HIS:N	2.43	0.51
6:J:35:ARG:HG3	6:J:46:ILE:HD12	1.90	0.51
9:T:69:DT:H2"	9:T:70:DA:C8	2.46	0.51
4:W:107:THR:HG21	4:W:124:ILE:HG12	1.92	0.51
10:O:68:LEU:HB2	10:O:80:VAL:HG13	1.93	0.51
1:D:311:LEU:HD12	1:D:313:GLY:H	1.75	0.51
1:D:629:ASP:HA	1:D:632:MET:HE1	1.93	0.51
2:E:273:GLN:HA	2:E:446:ARG:HD2	1.91	0.51
2:E:475:ARG:HA	2:E:478:GLU:HB2	1.93	0.51
7:U:100:VAL:HG12	6:X:96:THR:OG1	2.10	0.51
6:X:39:ARG:NH1	6:X:43:VAL:O	2.44	0.51
2:E:29:LEU:HA	2:E:32:PHE:CE2	2.46	0.51
2:E:500:LYS:HG3	2:E:502:ARG:H	1.75	0.51
2:E:503:LEU:O	2:E:507:HIS:N	2.33	0.51
9:T:66:DC:H2"	9:T:67:DC:C5	2.45	0.51
2:E:236:THR:HG23	2:E:239:GLU:H	1.75	0.51
2:E:628:GLY:HA3	12:E:801:SAH:C	2.40	0.51
3:G:406:HIS:NE2	3:G:408:LYS:HB2	2.25	0.51
5:H:191:DC:H2"	5:H:192:DG:C8	2.45	0.51
4:W:83:ARG:O	6:X:80:THR:HA	2.10	0.51
2:E:437:TRP:HE1	2:E:466:LYS:HG2	1.76	0.51
2:E:643:ILE:HG12	2:E:716:PHE:HA	1.92	0.51
4:I:37:LYS:HD2	4:I:38:PRO:HD2	1.92	0.51
7:R:25:PHE:CD2	7:R:56:GLU:HG2	2.45	0.51
9:T:172:DG:H4'	7:U:77:ARG:HH21	1.76	0.51
4:W:116:ARG:NH2	4:W:123:ASP:OD1	2.43	0.51
7:R:80:PRO:HD3	8:S:55:ALA:HB2	1.94	0.50
2:E:54:GLU:O	2:E:58:GLN:NE2	2.26	0.50
3:G:237:ASP:HB2	3:G:257:ASP:HB2	1.92	0.50
5:H:79:DA:OP1	8:V:84:SER:OG	2.23	0.50
7:U:79:ILE:HG13	7:U:80:PRO:HD2	1.92	0.50
10:O:118:GLU:O	10:O:159:SER:OG	2.29	0.50
3:G:82:PHE:HB2	3:G:404:LEU:HD21	1.92	0.50
3:G:90:GLU:HB3	3:G:432:ALA:HB1	1.94	0.50
3:G:222:THR:HG21	3:G:278:TYR:HA	1.93	0.50
3:G:386:LEU:HB2	3:G:404:LEU:HB2	1.93	0.50
3:G:387:TYR:HB3	3:G:389:TRP:CZ3	2.46	0.50
5:H:25:DA:N6	9:T:201:DA:N1	2.59	0.50
9:T:124:DC:H2"	9:T:125:DG:H8	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:31:HIS:HD1	7:U:48:PRO:HG3	1.75	0.50
1:D:652:LEU:H	1:D:652:LEU:HD23	1.75	0.50
9:T:77:DG:H4'	9:T:78:DT:H5'	1.94	0.50
3:G:230:GLY:O	3:G:295:HIS:ND1	2.27	0.50
5:H:166:DC:H1'	5:H:167:DT:C6	2.47	0.50
8:V:40:LYS:O	8:V:43:LYS:N	2.44	0.50
8:V:76:ARG:O	8:V:80:TYR:N	2.39	0.50
10:O:350:ILE:HA	10:O:365:GLU:HB3	1.94	0.50
3:G:239:VAL:HA	3:G:255:GLY:HA3	1.93	0.50
1:D:569:ASP:OD1	1:D:570:THR:N	2.45	0.50
3:G:206:LEU:HB3	3:G:220:ILE:HD11	1.94	0.50
3:G:311:CYS:O	3:G:322:LYS:N	2.43	0.50
3:G:332:LYS:HD3	3:G:336:MET:HA	1.93	0.50
7:R:79:ILE:HG22	7:R:81:ARG:H	1.76	0.50
7:U:58:LEU:HD23	8:V:66:VAL:HG11	1.94	0.50
4:W:109:LEU:O	4:W:113:HIS:N	2.40	0.50
2:E:108:PRO:HG2	2:E:629:TRP:CE2	2.46	0.50
3:G:169:ARG:HH12	3:G:171:ILE:HD12	1.76	0.50
4:I:40:ARG:HD2	9:T:124:DC:H5"	1.94	0.50
9:T:77:DG:H1'	9:T:78:DT:C6	2.47	0.50
9:T:108:DT:H2"	9:T:109:DA:C8	2.47	0.50
1:D:156:HIS:CE1	1:D:235:ASN:HB2	2.47	0.49
9:T:171:DA:H2"	9:T:172:DG:C8	2.47	0.49
10:O:404:MET:SD	10:O:404:MET:N	2.84	0.49
5:H:52:DT:H2'	5:H:53:DA:C8	2.48	0.49
5:H:106:DG:H2"	5:H:107:DG:N7	2.27	0.49
7:R:63:LEU:HA	7:R:66:ALA:HB3	1.94	0.49
1:D:295:PHE:HA	1:D:320:GLN:O	2.13	0.49
2:E:470:GLN:O	2:E:474:PHE:HB2	2.12	0.49
10:O:178:LYS:NZ	10:O:199:ASP:OD1	2.29	0.49
2:E:649:GLU:O	2:E:680:VAL:HA	2.13	0.49
5:H:161:DG:OP1	8:S:37:TYR:OH	2.24	0.49
5:H:185:DA:N6	9:T:42:DC:H42	2.10	0.49
11:Y:229:LYS:HG2	11:Y:239:LEU:HD22	1.94	0.49
1:D:249:SER:HA	1:D:300:THR:HA	1.94	0.49
2:E:99:LYS:HB3	3:G:138:TYR:CD1	2.47	0.49
2:E:437:TRP:NE1	2:E:466:LYS:HG2	2.27	0.49
2:E:619:LEU:HD13	2:E:631:ILE:HG21	1.93	0.49
3:G:99:VAL:O	3:G:417:SER:OG	2.20	0.49
3:G:207:LEU:HA	3:G:217:LEU:HA	1.94	0.49
10:O:173:LEU:HB3	10:O:205:TRP:CE2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:205:PHE:HE1	11:Y:280:LEU:HD12	1.78	0.49
3:G:114:ALA:HA	3:G:123:LEU:HA	1.95	0.49
3:G:171:ILE:HG12	3:G:187:VAL:HG23	1.94	0.49
1:D:481:HIS:CG	1:D:482:PRO:HD2	2.47	0.49
7:U:73:ASN:HB3	7:U:82:HIS:HE1	1.78	0.49
1:D:631:GLN:O	1:D:635:ALA:N	2.40	0.49
2:E:636:PRO:HB3	2:E:722:GLN:HA	1.94	0.49
5:H:56:DT:H1'	5:H:57:DG:C5	2.47	0.49
7:R:88:ARG:HB2	7:R:108:LEU:HD21	1.94	0.49
1:D:627:ILE:HD13	2:E:612:GLN:NE2	2.28	0.49
3:G:304:ILE:HD11	3:G:350:VAL:HG11	1.94	0.49
5:H:141:DA:H2"	5:H:142:DG:C8	2.48	0.49
4:W:120:MET:N	4:W:123:ASP:OD2	2.35	0.49
10:O:215:LYS:HD3	10:O:215:LYS:O	2.11	0.49
2:E:84:SER:HA	2:E:95:VAL:HA	1.95	0.49
3:G:113:PHE:CZ	3:G:124:TYR:HB2	2.48	0.49
7:R:88:ARG:NH2	7:R:100:VAL:O	2.46	0.49
1:D:565:TYR:HA	2:E:622:ALA:HB2	1.94	0.48
3:G:82:PHE:CE1	3:G:439:ARG:HB2	2.47	0.48
4:I:118:THR:N	5:H:110:DA:OP1	2.42	0.48
1:D:458:ARG:NE	10:O:357:GLU:OE2	2.43	0.48
5:H:73:DC:H2'	5:H:74:DT:C6	2.48	0.48
5:H:121:DG:H2'	5:H:122:DT:H71	1.95	0.48
9:T:127:DT:H1'	9:T:128:DT:C5	2.47	0.48
7:U:79:ILE:O	7:U:82:HIS:N	2.46	0.48
1:D:606:VAL:HG13	1:D:610:GLU:HG3	1.94	0.48
2:E:622:ALA:HB3	2:E:632:PHE:CE1	2.48	0.48
10:O:278:CYS:HB2	10:O:323:VAL:HG22	1.95	0.48
2:E:695:SER:HB3	2:E:698:PRO:HB3	1.95	0.48
3:G:86:ASN:HB3	3:G:436:ARG:HD3	1.94	0.48
4:I:67:PHE:HD2	4:I:93:GLN:HG3	1.75	0.48
5:H:185:DA:H61	9:T:42:DC:H42	1.61	0.48
9:T:191:DC:H2"	9:T:192:DA:C8	2.49	0.48
10:O:169:PRO:HG2	10:O:215:LYS:HZ3	1.78	0.48
1:D:627:ILE:HD13	2:E:612:GLN:HE21	1.78	0.48
1:D:666:PHE:HB2	1:D:668:LEU:HD23	1.95	0.48
2:E:180:GLN:HE22	2:E:223:ILE:HG21	1.79	0.48
3:G:199:HIS:CE1	3:G:201:ARG:HB2	2.49	0.48
4:I:68:GLN:HG2	4:I:72:ARG:HE	1.79	0.48
4:I:72:ARG:HH12	5:H:90:DT:P	2.36	0.48
10:O:120:LYS:HB2	10:O:161:PRO:HD3	1.93	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:O:253:MET:SD	10:O:268:SER:OG	2.70	0.48
10:O:302:ASP:OD1	10:O:303:LEU:N	2.47	0.48
10:O:380:PHE:HA	10:O:392:SER:HA	1.96	0.48
1:D:567:HIS:HB3	1:D:569:ASP:OD1	2.12	0.48
2:E:52:ARG:HD2	3:G:246:LEU:HD12	1.95	0.48
2:E:287:ARG:HA	2:E:290:PHE:HA	1.95	0.48
2:E:670:PHE:HD2	2:E:683:THR:HA	1.79	0.48
5:H:175:DG:O6	9:T:51:DC:N4	2.46	0.48
4:W:37:LYS:HB3	4:W:38:PRO:HD3	1.96	0.48
10:O:298:VAL:O	10:O:313:PHE:N	2.44	0.48
10:O:318:ASP:CG	10:O:319:GLU:H	2.17	0.48
3:G:219:ASN:O	3:G:223:ASP:N	2.46	0.48
3:G:260:LEU:O	3:G:300:SER:HA	2.13	0.48
6:J:78:ARG:HH22	6:J:85:ASP:CG	2.13	0.48
9:T:150:DC:H4'	9:T:151:DC:OP1	2.10	0.48
6:X:68:ASP:OD2	6:X:92:ARG:NH2	2.42	0.48
3:G:245:ASP:HB3	3:G:314:TRP:CD2	2.48	0.48
4:I:23:LYS:NZ	4:I:26:ARG:HD2	2.29	0.48
1:D:91:GLU:HB3	1:D:95:GLN:NE2	2.29	0.48
7:U:93:LEU:HD22	8:V:103:LEU:HD11	1.96	0.48
1:D:510:PRO:HG2	3:G:183:ILE:HG23	1.94	0.48
2:E:160:ASP:HA	3:G:306:ARG:HH21	1.79	0.48
5:H:45:DA:H2'	5:H:46:DT:H71	1.95	0.48
5:H:86:DC:H2"	5:H:87:DC:C5	2.49	0.48
7:R:64:GLU:HA	8:S:46:HIS:CE1	2.47	0.48
9:T:48:DA:H2'	9:T:49:DT:C6	2.49	0.48
9:T:168:DG:H2"	9:T:169:DC:C6	2.49	0.48
10:O:49:TRP:CG	10:O:383:ASN:HB3	2.48	0.47
2:E:224:PHE:HB3	2:E:236:THR:HA	1.96	0.47
2:E:598:HIS:ND1	2:E:601:SER:HB2	2.28	0.47
4:W:92:LEU:O	4:W:96:SER:N	2.46	0.47
11:Y:293:LEU:HG	11:Y:294:LYS:HG2	1.96	0.47
7:R:71:ARG:O	7:R:74:LYS:HD2	2.14	0.47
3:G:320:LEU:HA	3:G:330:CYS:HA	1.95	0.47
3:G:358:TYR:HE2	3:G:361:CYS:HB3	1.78	0.47
5:H:79:DA:H2"	5:H:80:DG:C8	2.49	0.47
8:V:61:SER:OG	6:X:101:GLY:O	2.21	0.47
10:O:393:VAL:HG13	10:O:399:MET:HE3	1.97	0.47
2:E:171:PHE:HE2	2:E:243:LYS:HZ3	1.62	0.47
4:I:86:SER:OG	5:H:89:DT:OP2	2.23	0.47
5:H:40:DA:H61	9:T:187:DT:H3	1.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:O:175:GLY:HA3	10:O:219:ALA:HB2	1.97	0.47
5:H:165:DC:H2"	5:H:166:DC:H5'	1.96	0.47
5:H:194:DC:N3	9:T:33:DG:N1	2.55	0.47
9:T:163:DC:H2"	9:T:164:DA:C8	2.48	0.47
4:W:126:LEU:O	4:W:130:ILE:HD12	2.14	0.47
3:G:193:ILE:HA	3:G:210:SER:HA	1.97	0.47
3:G:195:GLU:HB3	3:G:209:VAL:HB	1.97	0.47
5:H:176:DG:H2"	5:H:177:DG:C8	2.50	0.47
7:R:62:ILE:O	7:R:66:ALA:N	2.45	0.47
7:R:82:HIS:O	7:R:86:ALA:N	2.46	0.47
8:S:93:THR:HG21	6:X:75:HIS:HB2	1.97	0.47
9:T:16:DC:C2	9:T:17:DC:C4	3.03	0.47
9:T:90:DG:C4	9:T:91:DC:C5	3.03	0.47
9:T:122:DC:H4'	9:T:123:DG:OP1	2.14	0.47
7:U:77:ARG:HA	8:V:50:GLY:O	2.15	0.47
2:E:681:ASP:OD1	2:E:681:ASP:N	2.46	0.47
6:J:73:THR:HG21	6:J:81:VAL:HA	1.96	0.47
9:T:149:DC:H2"	9:T:150:DC:C6	2.49	0.47
4:W:121:PRO:HG2	6:X:49:LEU:HD23	1.95	0.47
10:O:194:LEU:HD13	10:O:233:VAL:HG22	1.96	0.47
3:G:197:LYS:HE2	3:G:243:ASP:HA	1.97	0.47
10:O:343:ASN:HD22	10:O:369:ILE:HG12	1.79	0.47
3:G:90:GLU:N	3:G:432:ALA:O	2.41	0.47
4:I:129:ARG:HD2	4:W:109:LEU:HD11	1.96	0.47
9:T:152:DC:H2"	9:T:153:DA:H8	1.80	0.47
10:O:327:PRO:HD3	10:O:382:TRP:NE1	2.30	0.47
2:E:696:VAL:HG22	2:E:745:GLU:HG3	1.98	0.46
2:E:704:VAL:HG23	4:I:29:ALA:HB3	1.95	0.46
9:T:17:DC:C4	9:T:18:DG:C6	3.03	0.46
8:V:73:GLU:OE2	8:V:76:ARG:NH2	2.48	0.46
1:D:431:GLN:NE2	1:D:439:ARG:HH12	2.13	0.46
2:E:333:LEU:HD12	2:E:469:ARG:NH1	2.30	0.46
5:H:79:DA:H61	9:T:148:DC:H42	1.63	0.46
5:H:98:DA:C6	5:H:99:DA:C6	3.03	0.46
5:H:108:DG:N2	9:T:120:DC:O2	2.48	0.46
9:T:104:DC:H4'	9:T:105:DA:OP1	2.14	0.46
1:D:478:TYR:OH	1:D:484:GLY:O	2.27	0.46
1:D:582:ASP:OD1	1:D:582:ASP:N	2.44	0.46
1:D:589:PRO:HG2	2:E:116:LEU:HA	1.96	0.46
2:E:673:ASN:HB2	4:I:26:ARG:HB3	1.97	0.46
2:E:734:SER:O	2:E:738:ALA:N	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:206:DT:O2	9:T:22:DG:N2	2.48	0.46
9:T:133:DC:H2"	9:T:134:DG:O5'	2.15	0.46
9:T:170:DC:H2"	9:T:171:DA:N9	2.30	0.46
11:Y:191:ASP:OD1	11:Y:192:ALA:N	2.48	0.46
2:E:524:ASN:HA	2:E:711:HIS:CD2	2.51	0.46
2:E:635:ASP:N	2:E:635:ASP:OD1	2.47	0.46
2:E:700:CYS:SG	2:E:715:ILE:HG22	2.56	0.46
3:G:371:ASP:OD1	3:G:375:LYS:N	2.39	0.46
2:E:98:LEU:HD23	3:G:139:VAL:HB	1.97	0.46
1:D:492:ASN:HB3	1:D:495:TYR:HB2	1.96	0.46
2:E:249:GLU:O	2:E:251:GLN:N	2.48	0.46
3:G:387:TYR:HB3	3:G:389:TRP:CH2	2.51	0.46
5:H:164:DG:N2	9:T:64:DC:O2	2.49	0.46
5:H:206:DT:O2	9:T:21:DA:H2	1.98	0.46
7:U:55:LEU:HD22	8:V:63:VAL:HG13	1.98	0.46
10:O:237:LEU:HG	10:O:281:PHE:HB2	1.98	0.46
1:D:218:ASP:OD1	1:D:218:ASP:N	2.49	0.46
2:E:701:TYR:CE1	2:E:703:LYS:HG3	2.51	0.46
5:H:162:DC:H2"	5:H:163:DG:C8	2.51	0.46
2:E:713:ILE:O	2:E:713:ILE:HG13	2.15	0.46
3:G:213:HIS:CD2	3:G:238:GLU:HA	2.51	0.46
3:G:261:LYS:HA	3:G:299:PHE:O	2.16	0.46
8:V:42:LEU:O	8:V:46:HIS:N	2.45	0.46
10:O:138:CYS:HA	10:O:154:TYR:CZ	2.51	0.46
5:H:54:DC:H42	9:T:173:DA:N6	2.09	0.46
9:T:168:DG:H2"	9:T:169:DC:N1	2.31	0.46
10:O:346:ASP:N	10:O:365:GLU:O	2.34	0.46
11:Y:214:LEU:HD12	11:Y:221:VAL:HG21	1.97	0.46
7:U:70:ALA:HA	7:U:82:HIS:CE1	2.51	0.46
1:D:528:ILE:HB	1:D:557:TYR:HB3	1.97	0.45
2:E:329:CYS:HA	2:E:468:CYS:HB3	1.98	0.45
2:E:625:ASP:HB2	2:E:746:ARG:NH1	2.31	0.45
5:H:52:DT:H2'	5:H:53:DA:H8	1.80	0.45
5:H:103:DG:H5'	5:H:103:DG:H8	1.81	0.45
7:R:97:LEU:HB3	7:R:100:VAL:CG1	2.46	0.45
3:G:83:LYS:HD3	3:G:440:LEU:HD21	1.98	0.45
5:H:118:DT:H2"	5:H:119:DA:N7	2.32	0.45
10:O:43:PRO:HG2	10:O:71:HIS:HB3	1.97	0.45
1:D:488:ASP:OD1	1:D:488:ASP:N	2.48	0.45
3:G:153:THR:HB	3:G:162:LEU:HB2	1.98	0.45
7:U:26:PRO:HD3	8:V:37:TYR:CG	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:122:DT:H3'	4:W:46:VAL:HG21	1.98	0.45
10:O:375:ALA:HB1	10:O:395:GLU:HB2	1.98	0.45
1:D:161:PHE:HZ	1:D:231:ALA:HB2	1.82	0.45
3:G:311:CYS:SG	3:G:367:ARG:HA	2.56	0.45
8:S:94:ALA:O	8:S:98:LEU:HG	2.16	0.45
9:T:20:DC:C4	9:T:21:DA:C6	3.04	0.45
10:O:300:LEU:HG	10:O:310:LEU:HB2	1.99	0.45
5:H:76:DG:H1'	5:H:77:DG:C4	2.52	0.45
9:T:134:DG:C5	9:T:135:DC:C4	3.04	0.45
10:O:318:ASP:HB3	10:O:339:ASP:HB3	1.99	0.45
1:D:565:TYR:CG	2:E:620:LEU:HD23	2.52	0.45
2:E:646:TYR:HB3	2:E:713:ILE:HD11	1.99	0.45
3:G:267:SER:O	3:G:270:MET:HG3	2.17	0.45
5:H:211:DG:N2	9:T:17:DC:N3	2.65	0.45
6:J:30:THR:OG1	6:J:32:PRO:HD2	2.17	0.45
1:D:161:PHE:CZ	1:D:231:ALA:HB2	2.52	0.45
1:D:311:LEU:HD12	1:D:313:GLY:N	2.31	0.45
1:D:632:MET:CE	1:D:668:LEU:HB2	2.47	0.45
2:E:737:ASP:HA	2:E:740:LYS:HB3	1.99	0.45
3:G:379:LEU:N	3:G:387:TYR:O	2.50	0.45
4:W:51:ILE:HD11	6:X:39:ARG:HD2	1.98	0.45
7:U:92:GLU:OE2	8:V:102:GLU:N	2.48	0.45
4:W:47:ALA:O	4:W:51:ILE:HG12	2.17	0.45
1:D:494:CYS:SG	11:Y:180:ARG:NH2	2.90	0.45
5:H:48:DT:H2"	5:H:49:DA:C8	2.51	0.45
5:H:71:DG:C8	5:H:71:DG:H5'	2.52	0.45
5:H:98:DA:H61	9:T:129:DT:H3	1.65	0.45
5:H:99:DA:H2"	5:H:100:DA:H8	1.82	0.45
5:H:208:DA:H2	9:T:19:DT:H3	1.65	0.45
8:V:53:SER:O	8:V:57:SER:N	2.46	0.45
1:D:163:GLY:HA2	1:D:217:PRO:HG2	1.99	0.44
2:E:565:CYS:HB3	2:E:590:CYS:CB	2.47	0.44
2:E:670:PHE:HB2	2:E:683:THR:OG1	2.17	0.44
5:H:39:DT:H2"	5:H:40:DA:C8	2.51	0.44
5:H:174:DC:H2'	5:H:175:DG:C8	2.52	0.44
9:T:162:DG:OP1	8:V:37:TYR:OH	2.19	0.44
9:T:176:DT:O4	9:T:177:DA:N6	2.50	0.44
1:D:101:ARG:HD3	1:D:452:TRP:O	2.17	0.44
6:J:98:TYR:CZ	7:R:100:VAL:HG21	2.52	0.44
8:S:38:VAL:HG11	8:S:59:MET:HG3	2.00	0.44
1:D:86:PHE:CE1	1:D:434:TYR:HB2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:21:SER:O	2:E:25:ARG:HG2	2.16	0.44
5:H:105:DG:C2	5:H:106:DG:C2	3.05	0.44
6:J:31:LYS:HG3	6:J:51:TYR:CE1	2.52	0.44
6:J:73:THR:HG21	6:J:81:VAL:HG22	1.98	0.44
7:U:103:ALA:HB1	4:W:94:GLU:OE1	2.17	0.44
4:W:88:ALA:HB2	6:X:83:ALA:N	2.33	0.44
1:D:597:ILE:HA	1:D:600:ILE:HD12	2.00	0.44
3:G:429:CYS:HB3	3:G:433:SER:OG	2.18	0.44
9:T:67:DC:H4'	9:T:68:DC:OP1	2.16	0.44
9:T:143:DA:H2'	9:T:144:DT:H71	1.99	0.44
7:U:29:ARG:CZ	8:V:32:GLU:HG2	2.48	0.44
2:E:289:CYS:O	2:E:291:LYS:HG3	2.17	0.44
2:E:616:LYS:HG3	2:E:617:LYS:O	2.17	0.44
3:G:360:GLN:HG2	3:G:381:ASN:HD21	1.83	0.44
4:I:121:PRO:HG2	6:J:49:LEU:HB3	2.00	0.44
5:H:71:DG:H5'	5:H:71:DG:H8	1.82	0.44
5:H:171:DC:OP1	7:R:76:THR:N	2.50	0.44
9:T:97:DC:H2'	9:T:98:DT:C6	2.53	0.44
9:T:206:DA:H2"	9:T:207:DT:C6	2.52	0.44
4:W:42:ARG:O	4:W:45:THR:HG22	2.17	0.44
2:E:120:PHE:O	2:E:650:ILE:N	2.24	0.44
9:T:92:DA:C5	9:T:93:DC:C4	3.06	0.44
9:T:133:DC:H2'	9:T:134:DG:H8	1.82	0.44
9:T:197:DC:H2'	9:T:198:DA:C8	2.53	0.44
7:U:29:ARG:NH2	8:V:32:GLU:HG2	2.32	0.44
11:Y:259:ARG:HG3	11:Y:260:HIS:ND1	2.32	0.44
1:D:663:MET:O	1:D:668:LEU:HG	2.17	0.44
2:E:626:VAL:HG22	2:E:746:ARG:HD3	2.00	0.44
3:G:147:PHE:HA	3:G:167:GLY:HA3	1.99	0.44
4:W:54:TYR:HE2	6:X:36:ARG:HD2	1.82	0.44
10:O:126:GLU:O	10:O:145:PRO:HD3	2.18	0.44
10:O:147:SER:HB3	10:O:176:HIS:O	2.17	0.44
11:Y:225:THR:O	11:Y:242:HIS:N	2.44	0.44
1:D:83:HIS:HA	1:D:86:PHE:HB3	1.99	0.44
1:D:607:ASN:O	1:D:611:LYS:N	2.51	0.44
1:D:647:ILE:HG22	1:D:653:CYS:SG	2.58	0.44
2:E:701:TYR:CD1	2:E:703:LYS:HG3	2.53	0.44
3:G:384:GLY:HA3	3:G:410:GLY:HA2	1.99	0.44
9:T:142:DG:C2	9:T:143:DA:C4	3.06	0.44
1:D:659:HIS:O	1:D:663:MET:HG2	2.17	0.44
2:E:565:CYS:HB3	2:E:590:CYS:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:573:THR:HG23	2:E:575:GLN:HG2	1.99	0.44
4:I:44:GLY:N	9:T:123:DG:OP1	2.43	0.44
5:H:59:DC:H2'	5:H:60:DA:C8	2.52	0.44
9:T:119:DC:H2"	9:T:120:DC:C6	2.53	0.44
10:O:287:PHE:HB3	10:O:302:ASP:OD1	2.18	0.44
1:D:632:MET:HA	1:D:635:ALA:HB3	2.00	0.43
4:I:83:ARG:O	6:J:80:THR:HA	2.18	0.43
5:H:79:DA:H61	9:T:148:DC:N4	2.16	0.43
3:G:97:PHE:C	3:G:415:GLN:HG3	2.38	0.43
3:G:189:HIS:CE1	3:G:216:ARG:HB2	2.53	0.43
4:W:82:LEU:HD23	4:W:82:LEU:HA	1.72	0.43
6:X:35:ARG:O	6:X:39:ARG:HG2	2.18	0.43
2:E:584:GLU:HG2	2:E:608:ASN:O	2.18	0.43
5:H:94:DG:H2"	5:H:95:DG:H8	1.83	0.43
5:H:171:DC:H3'	7:R:75:LYS:NZ	2.32	0.43
9:T:161:DG:C6	9:T:162:DG:C6	3.07	0.43
1:D:316:GLU:HB2	1:D:356:GLN:NE2	2.33	0.43
2:E:336:ALA:O	2:E:472:TYR:OH	2.18	0.43
2:E:660:GLY:HA2	2:E:663:TYR:CD1	2.54	0.43
3:G:264:ARG:HH22	3:G:343:ILE:HG22	1.84	0.43
3:G:371:ASP:CG	3:G:375:LYS:H	2.19	0.43
4:I:63:ARG:HB2	4:I:66:PRO:HG2	2.00	0.43
5:H:61:DC:C2	5:H:62:DG:C8	3.06	0.43
5:H:76:DG:N2	9:T:152:DC:N3	2.63	0.43
7:R:65:LEU:HD23	7:R:65:LEU:HA	1.82	0.43
9:T:75:DT:H2"	9:T:76:DC:C6	2.53	0.43
7:U:76:THR:O	8:V:49:THR:HG23	2.19	0.43
10:O:232:ASP:OD1	10:O:233:VAL:N	2.51	0.43
2:E:102:ASN:O	3:G:173:ARG:NH1	2.48	0.43
2:E:575:GLN:NE2	9:T:44:DG:H4'	2.33	0.43
3:G:380:GLY:HA3	3:G:413:ILE:HG21	2.00	0.43
4:I:108:ASN:ND2	6:J:43:VAL:HA	2.33	0.43
6:J:102:GLY:O	8:S:64:ASN:ND2	2.23	0.43
9:T:80:DG:H2"	9:T:81:DA:H8	1.83	0.43
2:E:85:VAL:N	2:E:94:GLN:O	2.51	0.43
3:G:271:MET:HA	3:G:274:ILE:HB	2.00	0.43
3:G:326:ASN:HA	3:G:358:TYR:CZ	2.53	0.43
6:J:31:LYS:HE3	6:J:51:TYR:CE2	2.54	0.43
9:T:118:DC:H2"	9:T:119:DC:C5	2.54	0.43
11:Y:288:MET:HG2	11:Y:289:PRO:HD3	1.99	0.43
1:D:310:LEU:HD23	1:D:315:TYR:CE2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:616:LEU:HG	1:D:639:PHE:HZ	1.84	0.43
2:E:502:ARG:HH21	9:T:47:DA:H5"	1.84	0.43
2:E:699:ASN:HB3	2:E:721:ILE:HD11	2.01	0.43
4:I:61:LEU:HD11	6:J:40:ARG:HD2	2.00	0.43
5:H:70:DA:H61	9:T:157:DC:H42	1.67	0.43
5:H:130:DA:OP1	4:W:66:PRO:HG3	2.18	0.43
8:S:84:SER:O	8:S:84:SER:OG	2.30	0.43
9:T:83:DA:C6	9:T:84:DG:C6	3.06	0.43
11:Y:230:ARG:NE	11:Y:232:GLU:OE2	2.51	0.43
2:E:731:TYR:OH	12:E:801:SAH:H8	2.18	0.43
2:E:732:ARG:HD2	4:I:30:PRO:HD3	1.99	0.43
3:G:85:VAL:HG21	3:G:438:ASP:HB2	1.99	0.43
3:G:404:LEU:HD23	3:G:437:TRP:CZ3	2.54	0.43
5:H:85:DC:H2'	5:H:86:DC:C2	2.53	0.43
5:H:101:DA:H1'	5:H:102:DC:H5'	2.01	0.43
7:U:64:GLU:HG2	8:V:46:HIS:HE1	1.82	0.43
4:W:39:HIS:HE1	4:W:41:TYR:CD1	2.36	0.43
2:E:458:ALA:O	2:E:461:ARG:HG3	2.19	0.43
2:E:470:GLN:N	2:E:473:GLU:OE1	2.46	0.43
4:I:58:THR:OG1	7:R:104:GLN:O	2.33	0.43
5:H:119:DA:H2"	5:H:120:DC:C5	2.53	0.43
10:O:24:TRP:O	10:O:28:THR:OG1	2.24	0.43
1:D:628:ALA:HB2	2:E:587:PRO:HB2	2.00	0.43
5:H:97:DT:H1'	5:H:98:DA:C8	2.54	0.43
5:H:128:DT:H2"	5:H:129:DA:C8	2.53	0.43
5:H:149:DA:H2"	5:H:150:DC:C5	2.54	0.43
8:S:30:ARG:NH2	9:T:69:DT:OP1	2.34	0.43
9:T:61:DG:H4'	9:T:62:DG:OP1	2.19	0.43
10:O:236:HIS:HA	10:O:281:PHE:HD2	1.83	0.43
1:D:183:THR:OG1	1:D:211:LYS:O	2.35	0.42
3:G:216:ARG:HE	3:G:228:ILE:HD12	1.84	0.42
3:G:333:PRO:HG2	3:G:340:ILE:HG22	2.01	0.42
4:I:131:ARG:HG3	4:W:130:ILE:HG22	2.01	0.42
5:H:157:DT:H2"	5:H:158:DG:C8	2.53	0.42
5:H:168:DC:H42	9:T:59:DG:H1	1.67	0.42
7:U:115:LEU:HD11	4:W:108:ASN:HD21	1.84	0.42
1:D:600:ILE:HD13	1:D:615:LYS:HG2	2.00	0.42
5:H:144:DT:H2"	5:H:145:DG:H5'	2.01	0.42
9:T:119:DC:H2"	9:T:120:DC:C5	2.54	0.42
10:O:279:LEU:HD12	10:O:291:THR:HG22	2.01	0.42
2:E:60:TRP:HA	2:E:63:ARG:HD3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:612:GLN:OE1	2:E:613:ARG:NH1	2.46	0.42
2:E:704:VAL:HA	2:E:713:ILE:HA	2.01	0.42
3:G:103:TRP:CH2	3:G:372:PHE:HA	2.54	0.42
3:G:235:HIS:CD2	3:G:259:SER:HB2	2.53	0.42
4:W:39:HIS:HE1	4:W:41:TYR:CE1	2.37	0.42
4:W:68:GLN:NE2	4:W:72:ARG:HH21	2.17	0.42
1:D:252:PHE:HB2	1:D:297:ALA:HB3	2.00	0.42
2:E:456:PHE:HA	2:E:459:ILE:HG12	2.02	0.42
2:E:699:ASN:O	2:E:718:LYS:N	2.47	0.42
3:G:150:CYS:HB2	3:G:163:LEU:HD21	2.01	0.42
7:R:37:GLY:HA3	7:R:39:TYR:CE2	2.55	0.42
7:R:92:GLU:HG3	8:S:103:LEU:CD1	2.49	0.42
6:X:66:ILE:HA	6:X:69:ALA:HB3	2.01	0.42
10:O:49:TRP:HZ2	10:O:391:CYS:HB3	1.85	0.42
10:O:232:ASP:OD2	10:O:279:LEU:N	2.52	0.42
1:D:557:TYR:CZ	10:O:106:GLY:HA3	2.55	0.42
2:E:108:PRO:HG2	2:E:629:TRP:CD2	2.55	0.42
2:E:502:ARG:NH2	4:I:39:HIS:HB3	2.34	0.42
3:G:191:ASN:OD1	3:G:192:ALA:N	2.51	0.42
4:I:129:ARG:HB2	4:I:134:ARG:HD2	2.02	0.42
5:H:207:DG:N2	9:T:21:DA:O4'	2.53	0.42
6:J:35:ARG:HH11	6:J:39:ARG:NH2	2.17	0.42
8:V:116:THR:O	8:V:120:SER:N	2.51	0.42
3:G:151:ALA:O	3:G:163:LEU:HG	2.20	0.42
3:G:201:ARG:NH2	3:G:247:LEU:HD22	2.35	0.42
5:H:120:DC:N4	9:T:107:DG:H1	2.17	0.42
7:R:84:GLN:HE21	7:R:88:ARG:HG3	1.84	0.42
7:R:84:GLN:HG2	7:R:105:GLY:O	2.19	0.42
9:T:82:DC:H2"	9:T:83:DA:C8	2.55	0.42
7:U:63:LEU:HD11	8:V:38:VAL:HG13	2.01	0.42
10:O:49:TRP:CZ2	10:O:391:CYS:HB3	2.54	0.42
10:O:178:LYS:HE2	10:O:198:ASP:HB2	2.01	0.42
5:H:210:DG:C2	5:H:211:DG:C4	3.07	0.42
10:O:174:ARG:HG2	10:O:175:GLY:N	2.35	0.42
10:O:294:ALA:HA	10:O:319:GLU:HG2	2.01	0.42
2:E:110:MET:HB3	2:E:629:TRP:HE1	1.84	0.42
3:G:340:ILE:HG13	3:G:341:ASP:N	2.35	0.42
1:D:603:PHE:HE2	1:D:605:ASP:HB2	1.85	0.42
2:E:318:THR:HG23	2:E:320:LEU:HG	2.02	0.42
5:H:191:DC:O2	9:T:37:DG:N2	2.53	0.42
9:T:180:DC:H2"	9:T:181:DA:H8	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:55:LEU:O	7:U:59:THR:HG22	2.20	0.42
10:O:393:VAL:HA	10:O:399:MET:HE1	2.01	0.42
2:E:25:ARG:O	2:E:28:GLN:N	2.53	0.42
2:E:620:LEU:N	2:E:632:PHE:O	2.44	0.42
4:I:50:GLU:OE1	6:J:39:ARG:NE	2.50	0.42
4:I:75:ALA:HB1	4:I:82:LEU:HD12	2.02	0.42
5:H:43:DG:C6	5:H:44:DG:C6	3.08	0.42
5:H:80:DG:H2"	5:H:81:DT:C6	2.55	0.42
5:H:163:DG:OP1	8:S:31:LYS:N	2.51	0.42
5:H:208:DA:C5	5:H:209:DC:C4	3.08	0.42
6:J:26:ILE:HD11	6:J:55:ARG:O	2.19	0.42
9:T:93:DC:H2"	9:T:94:DC:H6	1.85	0.42
8:V:113:LYS:HA	8:V:116:THR:HG22	2.01	0.42
1:D:130:LYS:HB3	10:O:348:SER:HB2	2.02	0.41
2:E:273:GLN:HE21	2:E:276:GLN:HG3	1.85	0.41
5:H:159:DG:H1'	5:H:160:DA:C8	2.54	0.41
9:T:45:DA:H2'	9:T:46:DG:C8	2.55	0.41
6:X:33:ALA:HA	6:X:36:ARG:NH2	2.35	0.41
11:Y:287:THR:HG22	11:Y:289:PRO:HD2	2.02	0.41
1:D:198:ASP:N	1:D:198:ASP:OD1	2.53	0.41
1:D:595:LYS:O	1:D:598:THR:OG1	2.35	0.41
1:D:663:MET:SD	1:D:668:LEU:HD21	2.60	0.41
3:G:102:ASN:HB2	3:G:152:TRP:CH2	2.55	0.41
3:G:226:VAL:HG12	3:G:227:ALA:N	2.33	0.41
3:G:311:CYS:HB3	3:G:368:PHE:CE1	2.55	0.41
7:R:62:ILE:HD12	7:R:62:ILE:H	1.85	0.41
9:T:17:DC:H2"	9:T:18:DG:H8	1.85	0.41
7:U:26:PRO:HB3	8:V:37:TYR:CZ	2.55	0.41
2:E:584:GLU:OE2	2:E:609:CYS:HA	2.19	0.41
5:H:91:DG:C4	5:H:92:DG:C8	3.08	0.41
9:T:118:DC:H4'	9:T:119:DC:H5'	2.01	0.41
7:U:112:GLN:H	7:U:115:LEU:HD12	1.85	0.41
10:O:150:LEU:HB3	10:O:169:PRO:HB3	2.03	0.41
10:O:373:HIS:HD2	10:O:375:ALA:O	2.03	0.41
11:Y:243:TRP:H	11:Y:248:ILE:HD13	1.84	0.41
1:D:166:HIS:CD2	1:D:353:PRO:HG3	2.56	0.41
3:G:228:ILE:HG23	3:G:293:LYS:HA	2.02	0.41
3:G:269:ARG:HD3	3:G:292:GLN:OE1	2.20	0.41
4:I:95:ALA:O	4:I:99:TYR:N	2.43	0.41
5:H:122:DT:P	4:W:46:VAL:HB	2.60	0.41
5:H:185:DA:H61	9:T:42:DC:N4	2.17	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:T:170:DC:H2”	9:T:171:DA:O4’	2.21	0.41
4:W:80:THR:OG1	4:W:81:ASP:OD1	2.35	0.41
1:D:575:ARG:NH1	3:G:286:ASN:O	2.53	0.41
2:E:558:CYS:HB3	2:E:561:ARG:NE	2.36	0.41
3:G:115:THR:HB	3:G:122:THR:HG23	2.02	0.41
7:U:85:LEU:O	7:U:89:ASN:HB2	2.20	0.41
10:O:56:PRO:HD2	10:O:62:SER:HA	2.02	0.41
5:H:61:DC:H2”	5:H:62:DG:H8	1.85	0.41
10:O:246:VAL:HG11	10:O:276:VAL:HG12	2.01	0.41
1:D:613:VAL:HG23	1:D:614:MET:SD	2.60	0.41
2:E:104:VAL:HG21	3:G:171:ILE:HG21	2.01	0.41
3:G:179:THR:HG23	3:G:181:GLN:H	1.86	0.41
3:G:229:PHE:HE2	3:G:251:ILE:HD12	1.86	0.41
5:H:160:DA:C6	5:H:161:DG:C6	3.08	0.41
10:O:257:THR:O	10:O:258:ARG:HG2	2.20	0.41
2:E:629:TRP:N	12:E:801:SAH:OXT	2.43	0.41
3:G:95:PRO:HA	3:G:430:ASP:O	2.20	0.41
3:G:219:ASN:HB3	3:G:224:THR:HG22	2.01	0.41
3:G:240:LEU:HD23	3:G:255:GLY:HA2	2.01	0.41
5:H:89:DT:H6	5:H:89:DT:H2’	1.72	0.41
5:H:189:DG:C2	9:T:39:DG:C2	3.09	0.41
5:H:205:DC:N4	9:T:21:DA:H61	2.19	0.41
5:H:205:DC:H42	9:T:21:DA:H61	1.67	0.41
7:R:92:GLU:OE2	8:S:100:PRO:HG2	2.20	0.41
11:Y:244:MET:O	11:Y:246:GLU:HG3	2.21	0.41
1:D:650:LYS:HB2	1:D:652:LEU:CD2	2.44	0.41
2:E:624:SER:OG	2:E:627:ALA:O	2.38	0.41
2:E:636:PRO:HD3	2:E:723:THR:OG1	2.20	0.41
3:G:324:CYS:SG	3:G:364:TRP:HB3	2.61	0.41
3:G:326:ASN:HA	3:G:358:TYR:CE2	2.56	0.41
3:G:374:GLN:O	3:G:391:LEU:HD12	2.21	0.41
5:H:139:DA:H2”	5:H:140:DG:H8	1.84	0.41
5:H:197:DC:H42	9:T:29:DC:N4	2.19	0.41
7:R:53:ALA:O	7:R:56:GLU:HB2	2.20	0.41
9:T:93:DC:H4’	9:T:94:DC:OP1	2.19	0.41
9:T:122:DC:H2”	9:T:123:DG:O5’	2.21	0.41
7:U:50:TYR:OH	8:V:108:VAL:HA	2.21	0.41
10:O:183:LEU:HG	10:O:193:LEU:HD11	2.02	0.41
10:O:281:PHE:HD1	10:O:289:LEU:HD13	1.83	0.41
10:O:379:ASP:HB3	10:O:393:VAL:HB	2.03	0.41
11:Y:190:PHE:CE2	11:Y:195:LEU:HB2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:580:GLU:N	1:D:580:GLU:OE1	2.54	0.41
1:D:663:MET:SD	1:D:668:LEU:HD11	2.61	0.41
2:E:539:CYS:HB3	2:E:542:VAL:HG23	2.02	0.41
3:G:373:TRP:CZ3	3:G:421:ASP:HA	2.56	0.41
3:G:411:ALA:HB3	3:G:429:CYS:SG	2.60	0.41
4:I:63:ARG:O	4:I:66:PRO:HD2	2.21	0.41
5:H:69:DG:H2"	5:H:70:DA:H8	1.85	0.41
8:S:111:GLY:O	8:S:114:ALA:N	2.54	0.41
9:T:78:DT:H2"	9:T:79:DA:C8	2.56	0.41
4:W:65:LEU:HB3	4:W:66:PRO:HD3	2.03	0.41
2:E:659:ARG:HB3	2:E:663:TYR:CZ	2.56	0.40
3:G:220:ILE:HD12	3:G:220:ILE:H	1.85	0.40
5:H:96:DT:H4'	5:H:97:DT:OP1	2.21	0.40
5:H:128:DT:H6	5:H:128:DT:H2'	1.72	0.40
5:H:204:DC:H2"	5:H:205:DC:C6	2.56	0.40
9:T:172:DG:H4'	7:U:77:ARG:HE	1.86	0.40
10:O:10:ASP:O	10:O:14:GLU:HG2	2.21	0.40
2:E:600:ASP:OD1	2:E:600:ASP:N	2.53	0.40
5:H:105:DG:C5	5:H:106:DG:C6	3.09	0.40
5:H:169:DG:H1'	5:H:170:DG:C8	2.56	0.40
4:W:61:LEU:HD13	4:W:61:LEU:HA	1.95	0.40
10:O:79:LEU:N	10:O:121:ILE:O	2.34	0.40
2:E:634:LYS:O	2:E:723:THR:HG23	2.21	0.40
3:G:250:LYS:HG2	3:G:264:ARG:HG2	2.03	0.40
3:G:275:LYS:HD3	3:G:275:LYS:HA	1.73	0.40
4:I:84:PHE:HD1	4:I:89:VAL:HG22	1.86	0.40
5:H:206:DT:H1'	5:H:207:DG:C8	2.55	0.40
9:T:100:DA:C2	9:T:101:DA:C4	3.09	0.40
9:T:158:DC:H6	9:T:158:DC:H2'	1.74	0.40
7:U:63:LEU:HA	7:U:63:LEU:HD23	1.84	0.40
2:E:83:CYS:HB3	2:E:98:LEU:HD11	2.04	0.40
3:G:230:GLY:N	3:G:294:ILE:O	2.54	0.40
3:G:409:CYS:HB2	3:G:435:TRP:CD2	2.57	0.40
4:I:99:TYR:OH	4:I:133:GLU:OE1	2.30	0.40
7:R:58:LEU:HD23	7:R:58:LEU:HA	1.92	0.40
9:T:65:DG:C5	9:T:66:DC:C4	3.09	0.40
11:Y:240:LEU:HD13	11:Y:253:TRP:CE2	2.56	0.40
2:E:472:TYR:O	2:E:476:VAL:HG23	2.21	0.40
2:E:629:TRP:H	12:E:801:SAH:C	2.33	0.40
3:G:308:TYR:HB2	3:G:324:CYS:SG	2.62	0.40
10:O:129:ARG:N	10:O:143:LYS:HB2	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:O:224:THR:O	10:O:224:THR:HG22	2.22	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	D	423/619 (68%)	403 (95%)	20 (5%)	0	100	100
2	E	560/753 (74%)	511 (91%)	47 (8%)	2 (0%)	30	67
3	G	360/441 (82%)	329 (91%)	31 (9%)	0	100	100
4	I	112/136 (82%)	107 (96%)	5 (4%)	0	100	100
4	W	97/136 (71%)	92 (95%)	5 (5%)	0	100	100
6	J	81/106 (76%)	76 (94%)	5 (6%)	0	100	100
6	X	85/106 (80%)	78 (92%)	7 (8%)	0	100	100
7	R	106/133 (80%)	101 (95%)	5 (5%)	0	100	100
7	U	106/133 (80%)	103 (97%)	3 (3%)	0	100	100
8	S	94/123 (76%)	84 (89%)	10 (11%)	0	100	100
8	V	93/123 (76%)	85 (91%)	8 (9%)	0	100	100
10	O	391/425 (92%)	376 (96%)	15 (4%)	0	100	100
11	Y	124/303 (41%)	114 (92%)	9 (7%)	1 (1%)	16	53
All	All	2632/3537 (74%)	2459 (93%)	170 (6%)	3 (0%)	50	82

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	327	PRO
11	Y	187	HIS

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Mol	Chain	Res	Type
2	E	492	THR

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	D	411/575 (72%)	408 (99%)	3 (1%)	81 86
2	E	507/672 (75%)	507 (100%)	0	100 100
3	G	324/392 (83%)	324 (100%)	0	100 100
4	I	95/111 (86%)	95 (100%)	0	100 100
4	W	86/111 (78%)	86 (100%)	0	100 100
6	J	68/81 (84%)	68 (100%)	0	100 100
6	X	64/81 (79%)	64 (100%)	0	100 100
7	R	85/104 (82%)	85 (100%)	0	100 100
7	U	84/104 (81%)	84 (100%)	0	100 100
8	S	79/103 (77%)	79 (100%)	0	100 100
8	V	79/103 (77%)	79 (100%)	0	100 100
10	O	351/375 (94%)	350 (100%)	1 (0%)	91 92
11	Y	117/271 (43%)	116 (99%)	1 (1%)	75 83
All	All	2350/3083 (76%)	2345 (100%)	5 (0%)	91 94

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	124	ARG
1	D	129	ARG
1	D	672	MET
10	O	264	LYS
11	Y	180	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	156	HIS
1	D	166	HIS
1	D	356	GLN
1	D	449	HIS
1	D	517	ASN
2	E	45	ASN
2	E	102	ASN
2	E	119	ASN
2	E	180	GLN
2	E	273	GLN
2	E	520	ASN
2	E	560	ASN
3	G	146	ASN
3	G	185	HIS
3	G	272	ASN
3	G	283	ASN
3	G	360	GLN
4	I	108	ASN
7	R	31	HIS
7	R	84	GLN
7	R	104	GLN
8	S	92	GLN
8	S	106	HIS
7	U	82	HIS
7	U	84	GLN
8	V	46	HIS
8	V	92	GLN
4	W	39	HIS
4	W	125	GLN
10	O	48	GLN
10	O	329	ASN
10	O	383	ASN
10	O	403	GLN
10	O	410	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

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	$\#\|Z\| > 2$
12	SAH	E	801	-	23,28,28	1.27	3 (13%)	22,40,40	1.86	3 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	SAH	E	801	-	-	4/11/31/31	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	E	801	SAH	C2-N3	4.11	1.38	1.32
12	E	801	SAH	C2-N1	2.51	1.38	1.33
12	E	801	SAH	OXT-C	-2.32	1.23	1.30

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	E	801	SAH	N3-C2-N1	-6.18	120.28	128.67
12	E	801	SAH	C5'-SD-CG	-4.16	89.91	102.26
12	E	801	SAH	OXT-C-O	-2.61	118.17	124.08

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	E	801	SAH	C3'-C4'-C5'-SD
12	E	801	SAH	O4'-C4'-C5'-SD
12	E	801	SAH	C-CA-CB-CG
12	E	801	SAH	CA-CB-CG-SD

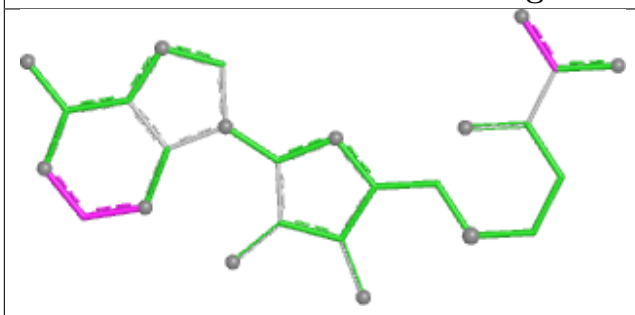
There are no ring outliers.

1 monomer is involved in 5 short contacts:

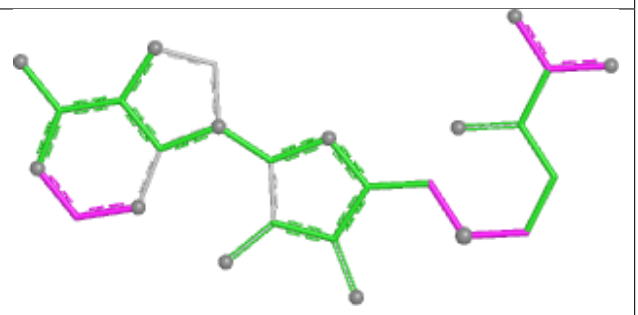
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	E	801	SAH	5	0

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

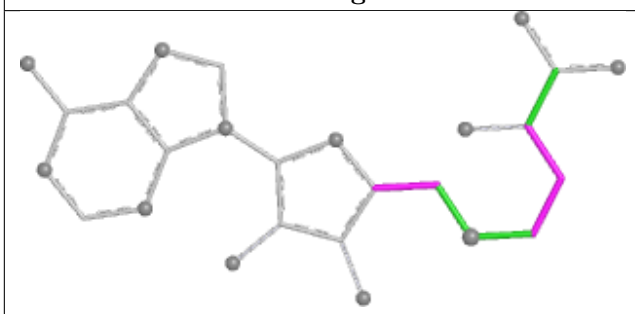
Ligand SAH E 801



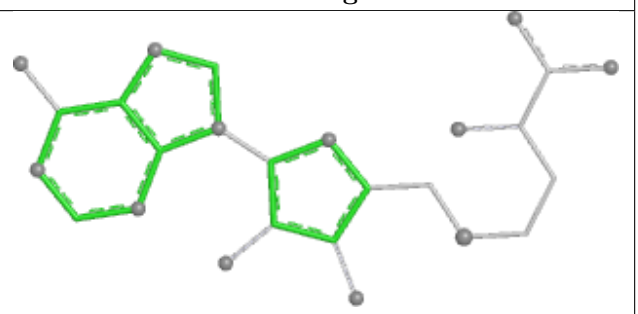
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

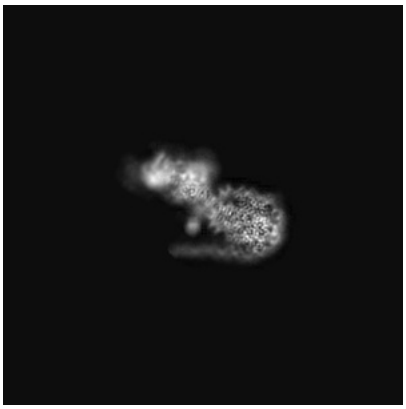
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-41141. These allow visual inspection of the internal detail of the map and identification of artifacts.

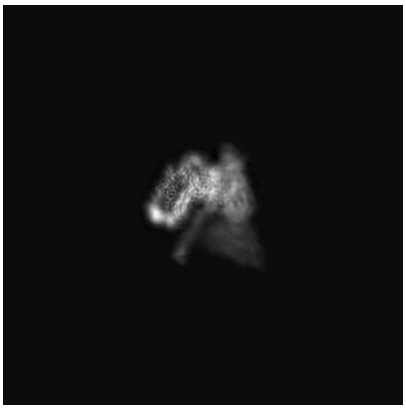
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

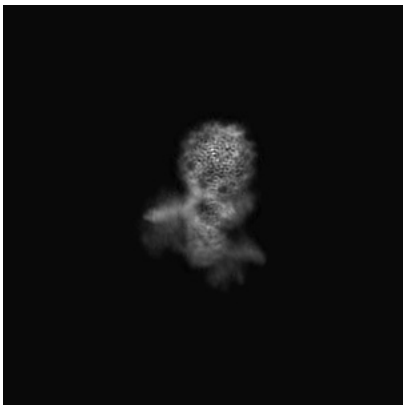
6.1.1 Primary map



X

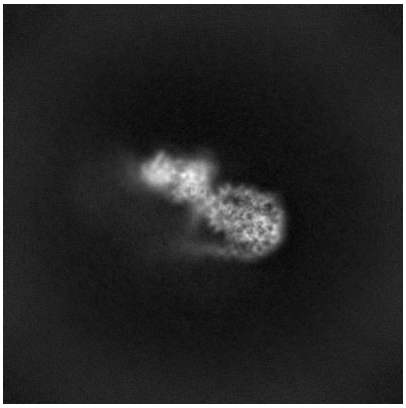


Y

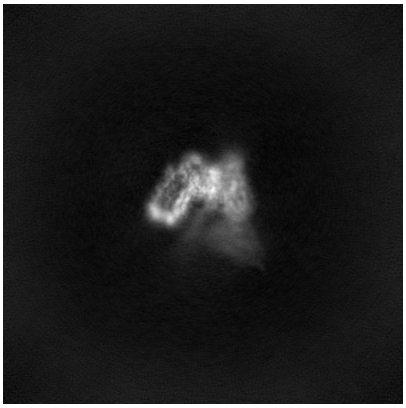


Z

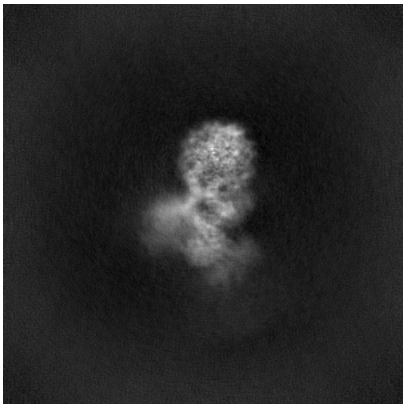
6.1.2 Raw map



X



Y

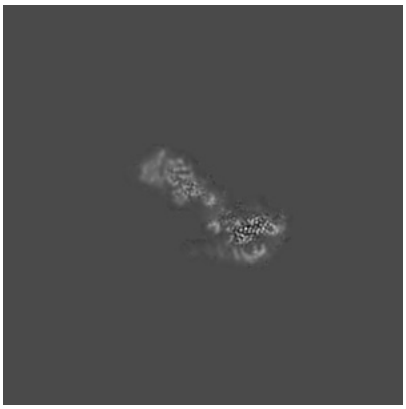


Z

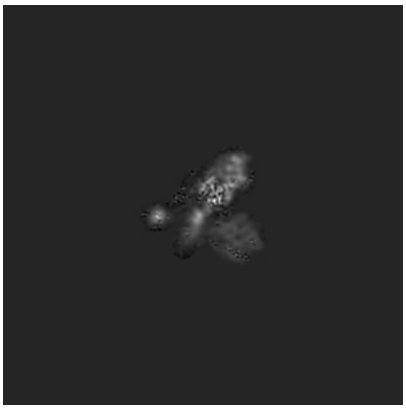
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map



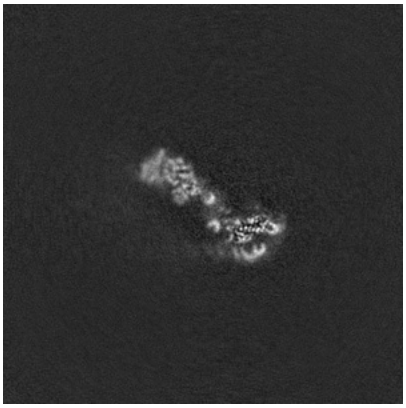
X Index: 165



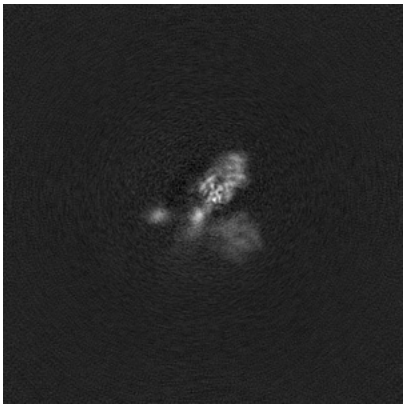
Y Index: 165

Z Index: 165

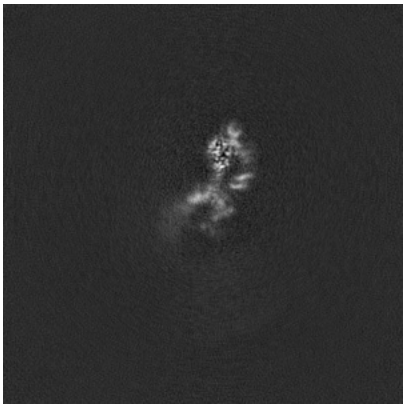
6.2.2 Raw map



X Index: 165



Y Index: 165

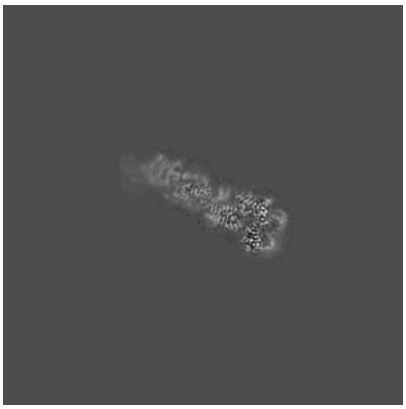


Z Index: 165

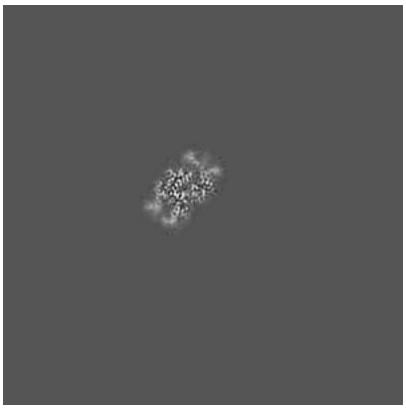
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

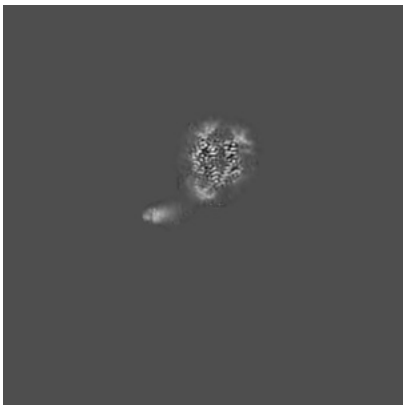
6.3.1 Primary map



X Index: 175

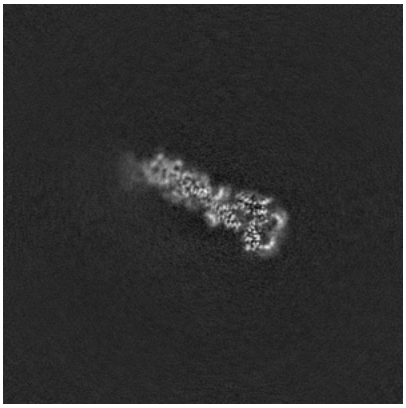


Y Index: 207

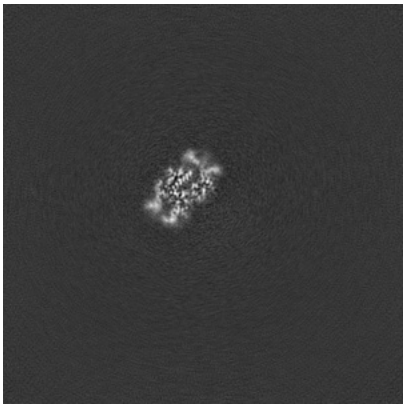


Z Index: 148

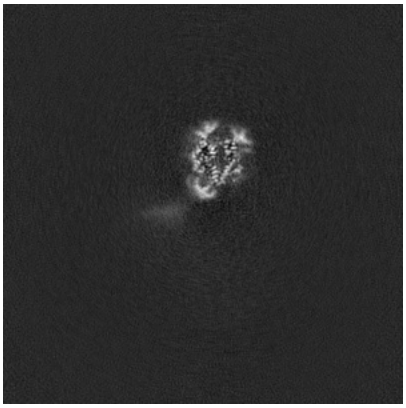
6.3.2 Raw map



X Index: 174



Y Index: 207

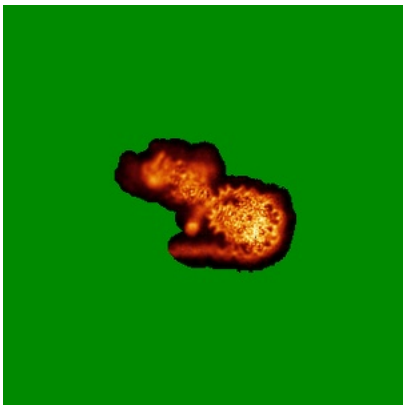


Z Index: 148

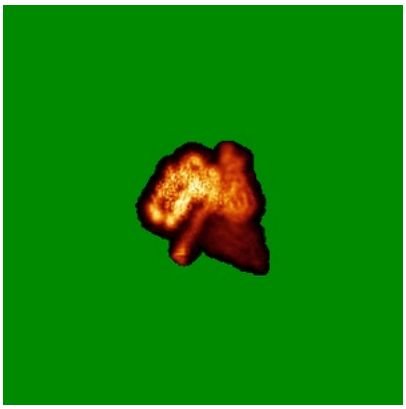
The images above show the largest variance slices of the map in three orthogonal directions.

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

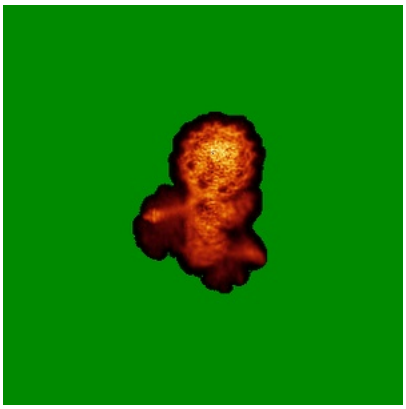
6.4.1 Primary map



X

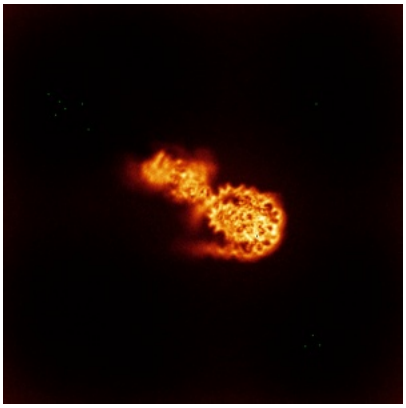


Y

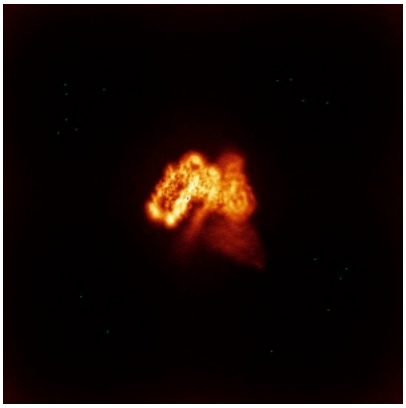


Z

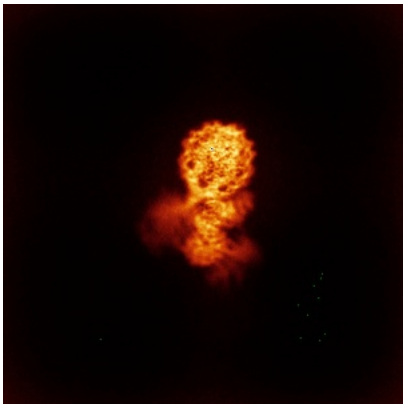
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

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

6.5.2 Raw map

X Y Z

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

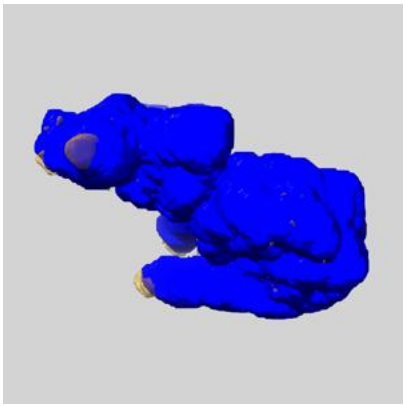
6.6 Mask visualisation (i)

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

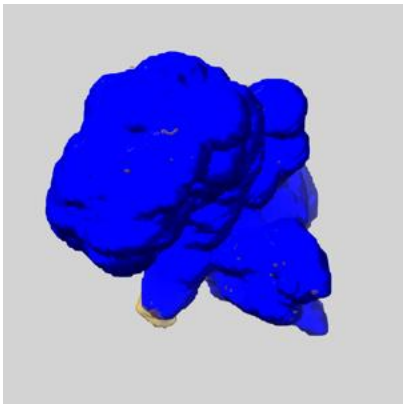
A mask typically either:

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

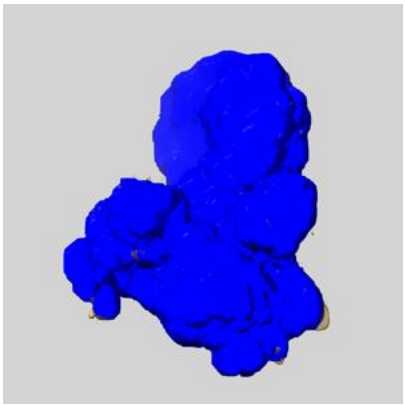
6.6.1 emd_41141_msk_1.map (i)



X



Y

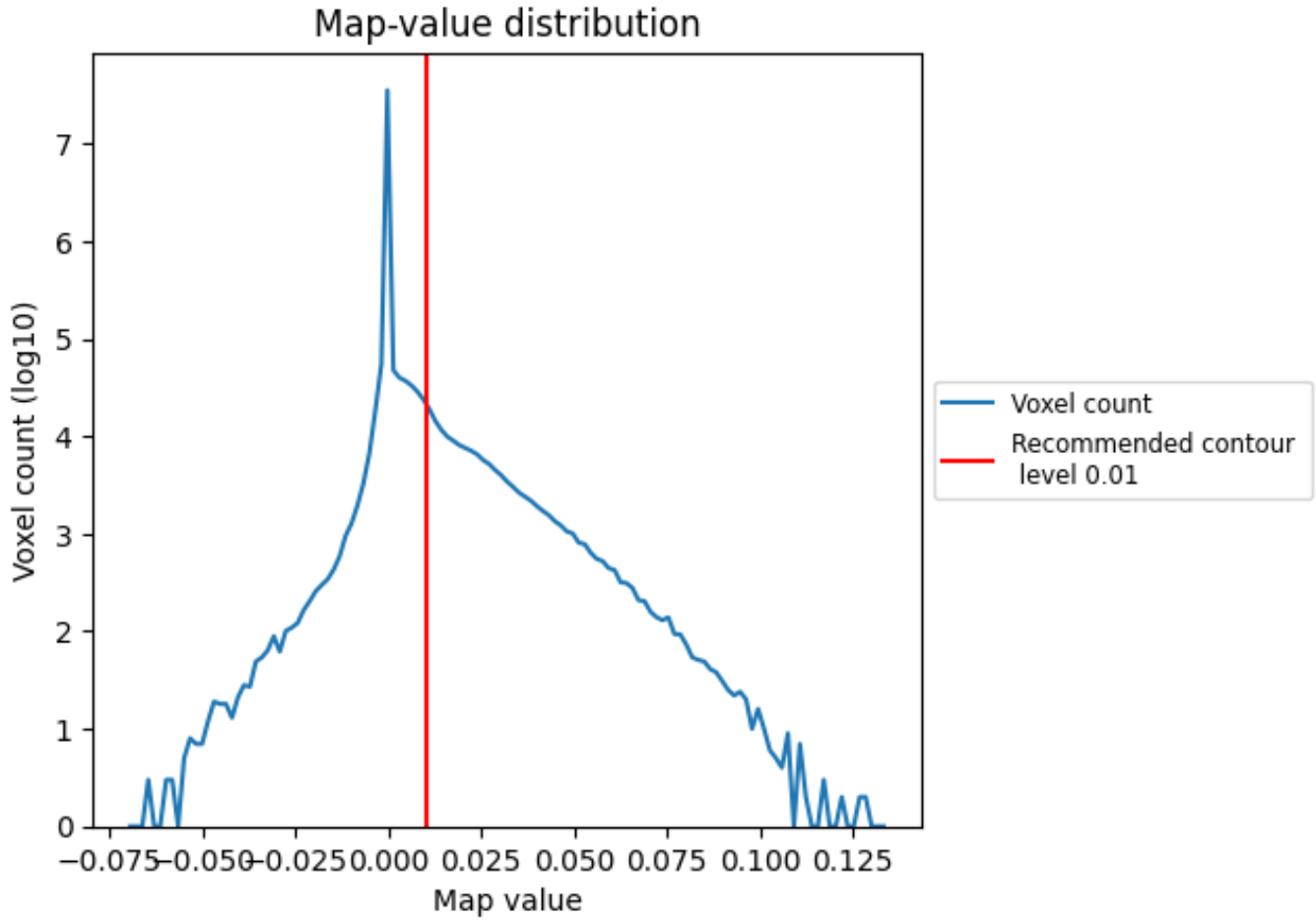


Z

7 Map analysis

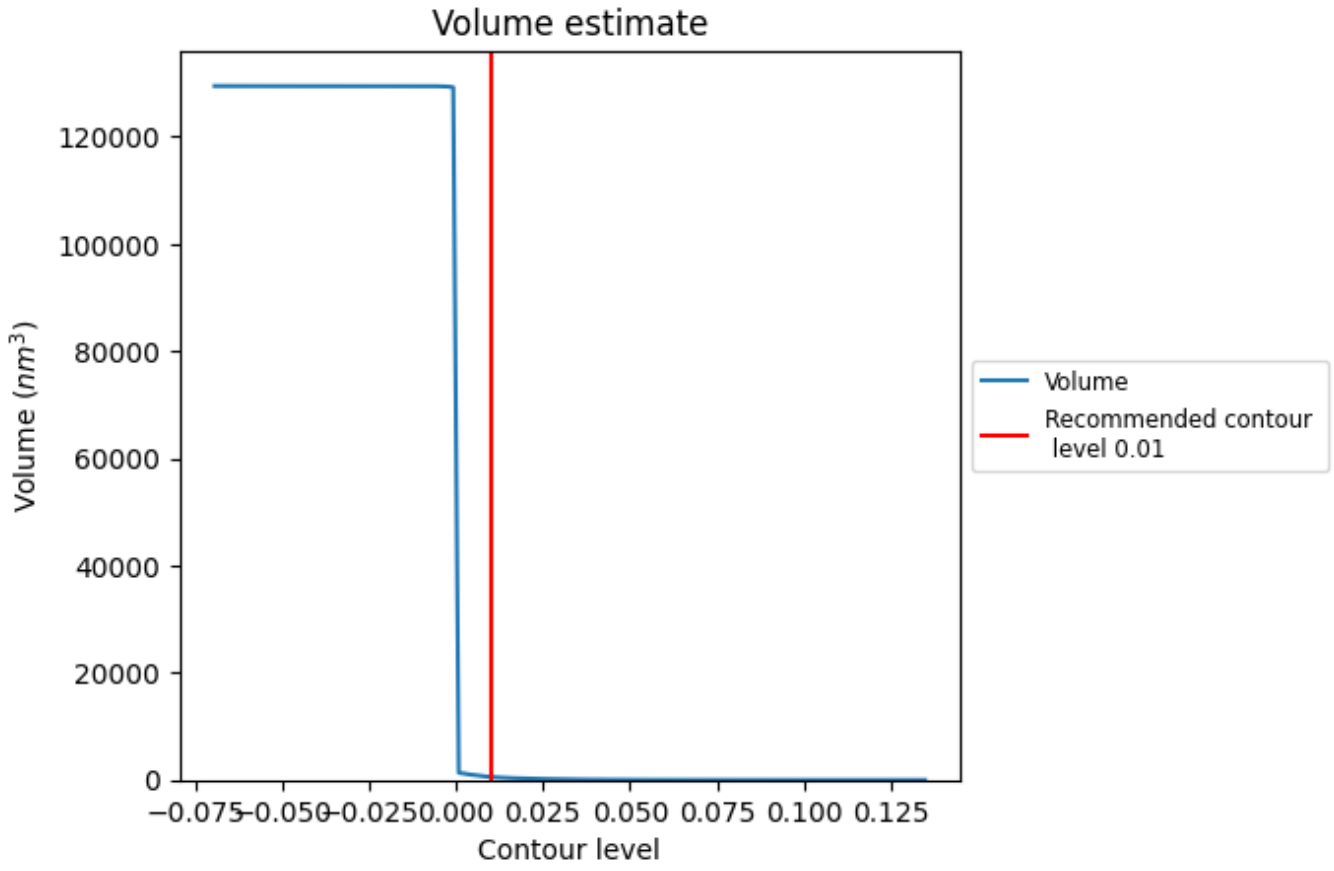
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

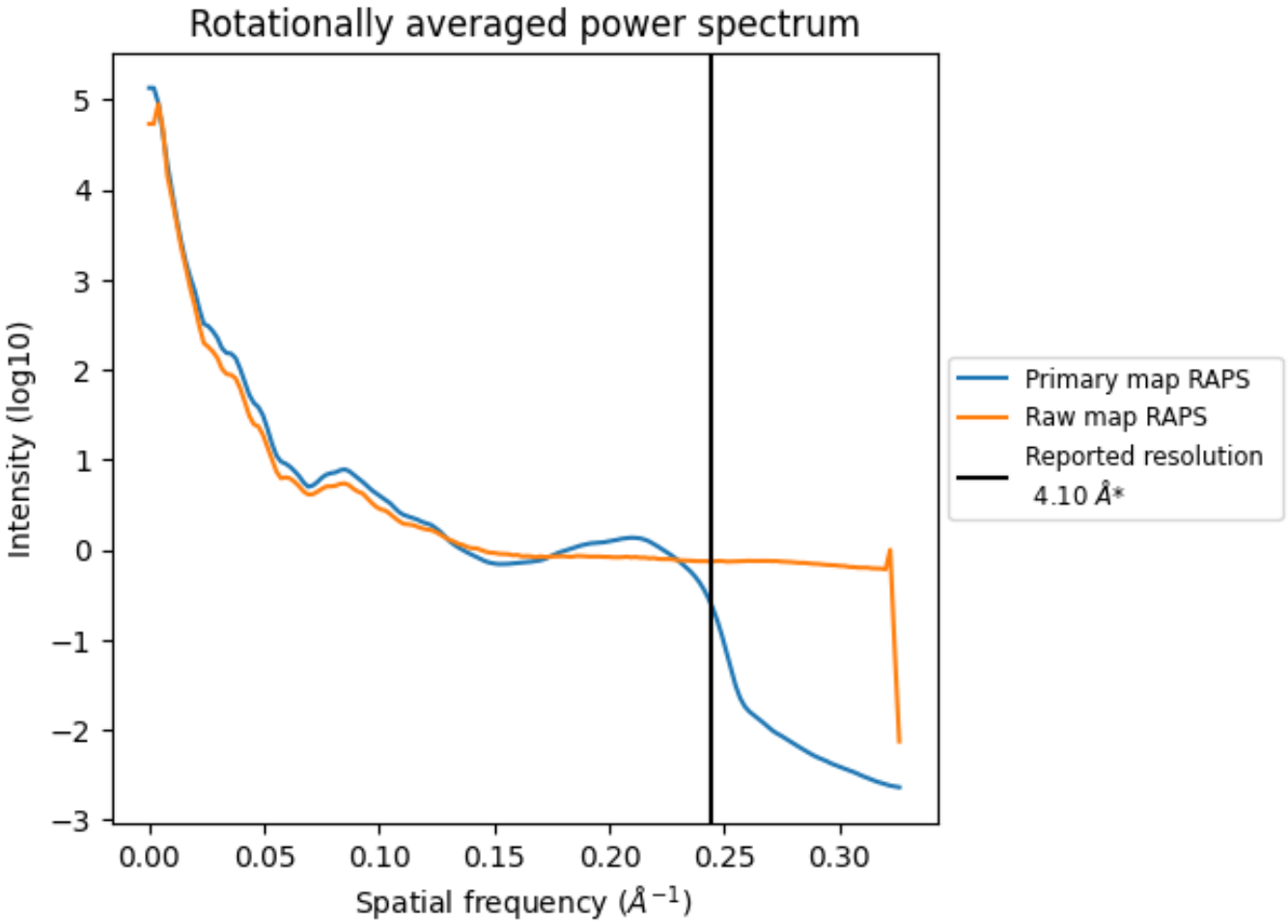
7.2 Volume estimate



The volume at the recommended contour level is 570 nm^3; this corresponds to an approximate mass of 515 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)

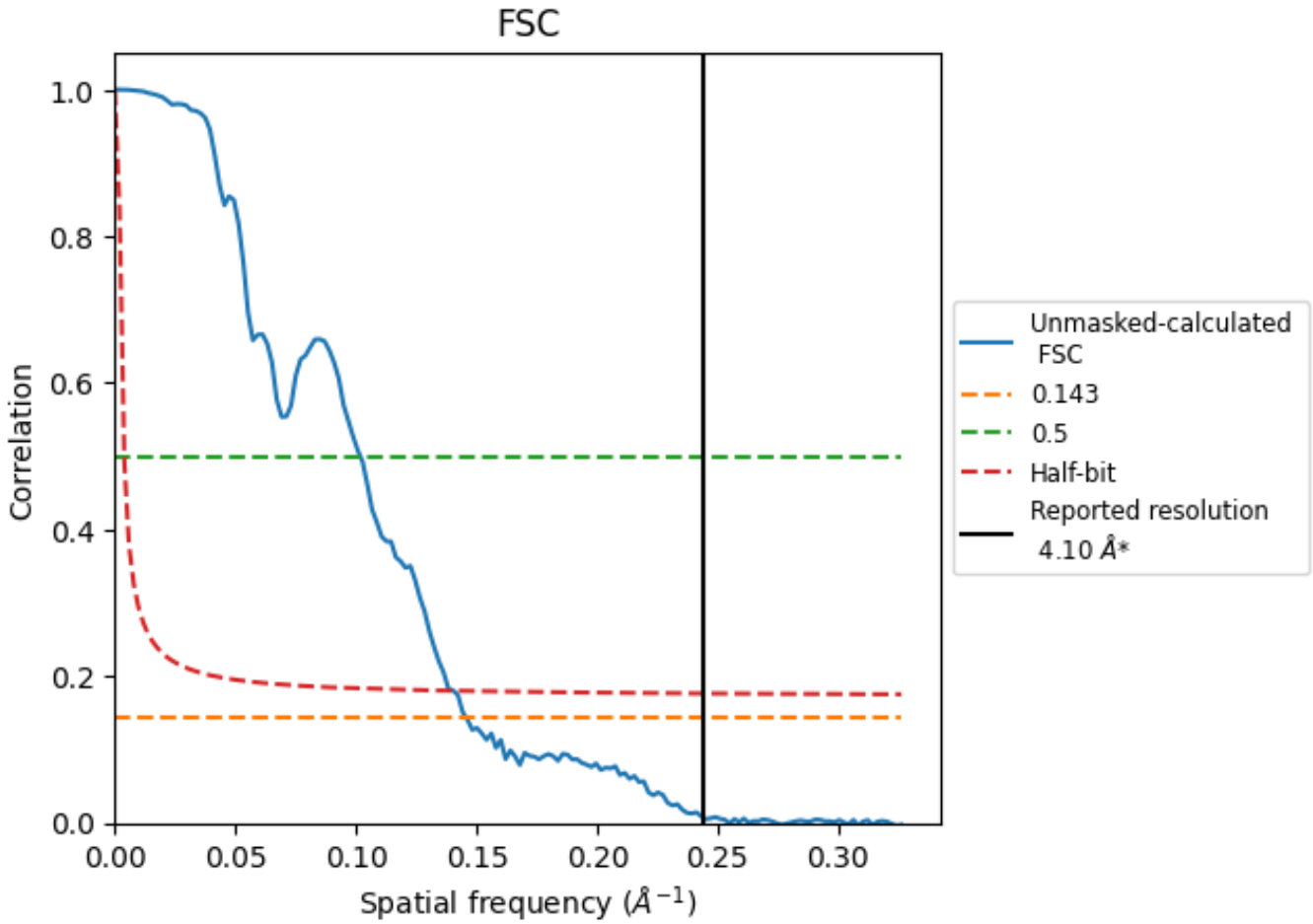


*Reported resolution corresponds to spatial frequency of 0.244 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.244 Å^{-1}

8.2 Resolution estimates (i)

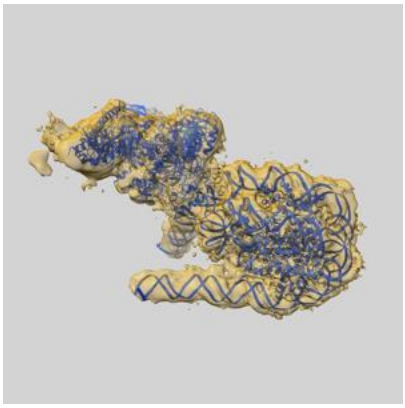
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.86	9.82	7.12

*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 6.86 differs from the reported value 4.1 by more than 10 %

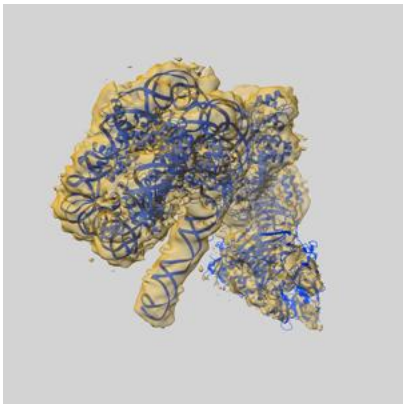
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-41141 and PDB model 8TAS. Per-residue inclusion information can be found in section 3 on page 8.

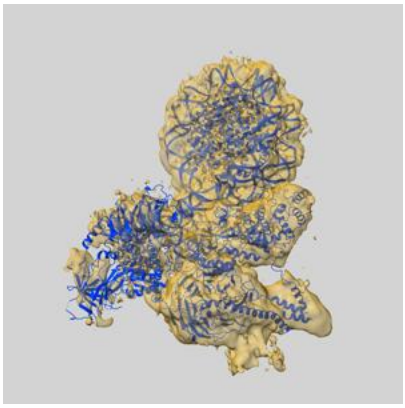
9.1 Map-model overlay



X



Y



Z

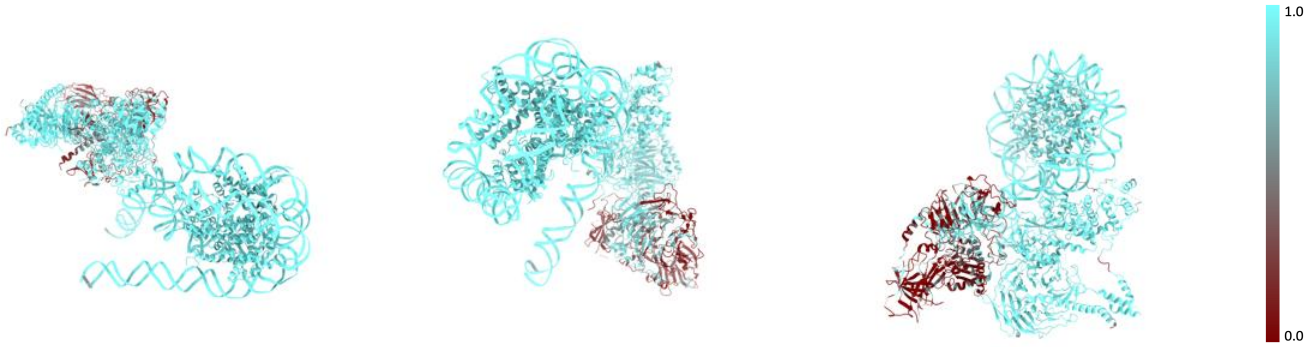
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)

X Y Z

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

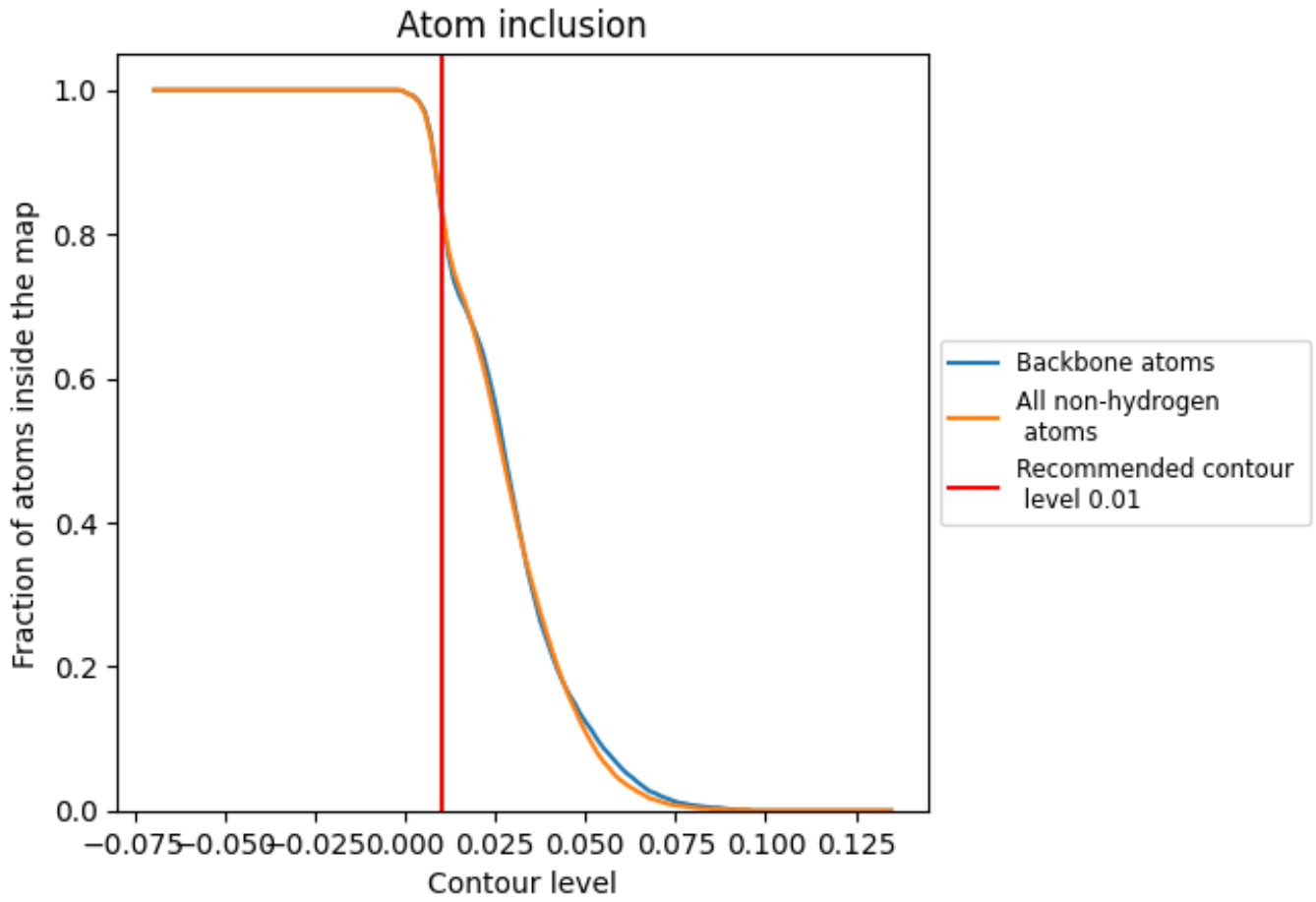
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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

9.4 Atom inclusion (i)



At the recommended contour level, 84% of all backbone atoms, 84% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8410	0.2590
D	0.4870	0.1280
E	0.9630	0.2310
G	0.9910	0.2000
H	0.9900	0.2930
I	0.9920	0.4530
J	0.9780	0.4400
O	0.4800	0.0920
R	0.9910	0.4540
S	0.9960	0.4590
T	0.9940	0.2910
U	0.9880	0.4640
V	0.9890	0.4610
W	0.9920	0.4520
X	0.9920	0.4630
Y	0.1680	0.1000