



## Full wwPDB EM Validation Report ⓘ

Oct 13, 2024 – 11:47 AM EDT

PDB ID : 7UNC  
EMDB ID : EMD-26620  
Title : Pol II-DSIF-SPT6-PAF1c-TFIIS complex with rewrapped nucleosome  
Authors : Filipovski, M.; Vos, S.M.; Farnung, L.  
Deposited on : 2022-04-10  
Resolution : 3.00 Å (reported)  
Based on initial models : 3LZ0, 6TED

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

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



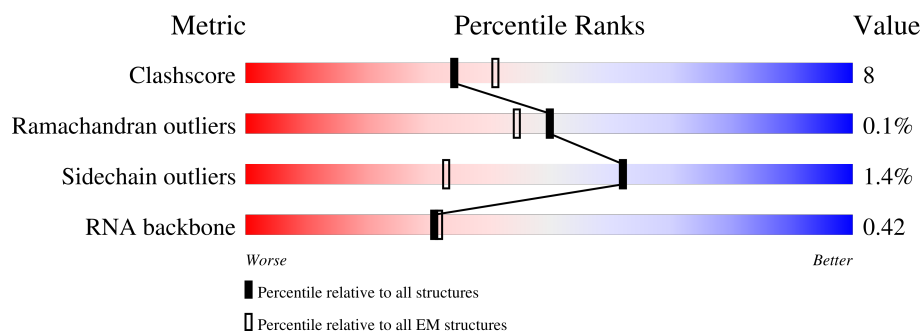
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191












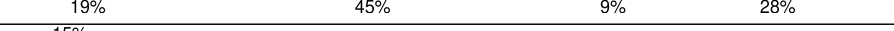


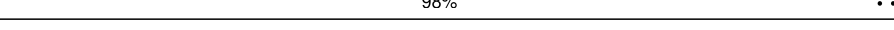




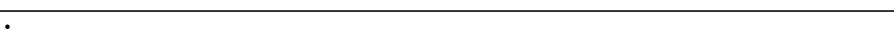

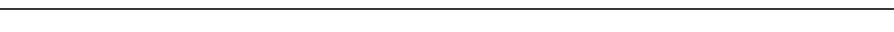
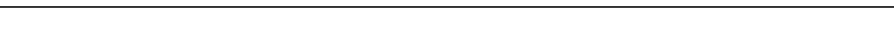


The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey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

Mol	Chain	Length	Quality of chain
1	A	1984	
2	B	1251	
3	C	275	
4	D	184	
5	E	210	
6	F	127	
7	G	172	

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Mol	Chain	Length	Quality of chain
8	H	150	
9	I	125	
10	J	67	
11	K	117	
12	L	58	
13	M	1729	
14	N	209	
15	O	304	
16	P	16	
17	Q	1179	
18	R	713	
19	T	215	
20	U	666	
21	V	531	
22	W	305	
23	X	531	
24	Z	1087	
25	a	136	
25	e	136	
26	b	103	
26	f	103	
27	c	130	
27	g	130	
28	d	123	
28	h	123	



## 2 Entry composition [i](#)

There are 30 unique types of molecules in this entry. The entry contains 105742 atoms, of which 48112 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 DNA-directed RNA polymerase subunit.

Mol	Chain	Residues	Atoms							AltConf	Trace
1	A	1426	Total	C	H	N	O	P	S	0	0
			22643	7074	11388	2014	2095	2	70		

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	1117	Total	C	H	N	O	S	0	0
			17949	5665	9002	1571	1647	64		

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	258	Total	C	H	N	O	S	0	0
			4096	1300	2024	356	410	6		

- Molecule 4 is a protein called RPOL4c domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	D	126	Total	C	H	N	O	S	0	0
			1985	630	981	170	200	4		

- Molecule 5 is a protein called DNA-directed RNA polymerase II subunit E.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	E	209	Total	C	H	N	O	S	0	0
			3458	1089	1738	300	323	8		

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	F	78	Total	C	H	N	O	S	0	0
			1284	401	658	106	114	5		



- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	G	171	Total	C	H	N	O	S	0	0
			2654	866	1321	214	245	8		

- Molecule 8 is a protein called RPB8.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	H	149	Total	C	H	N	O	S	0	0
			2354	759	1157	195	238	5		

- Molecule 9 is a protein called RPB9.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	I	116	Total	C	H	N	O	S	0	0
			1822	582	880	168	181	11		

- Molecule 10 is a protein called RPB10.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	J	66	Total	C	H	N	O	S	0	0
			1068	339	544	88	91	6		

- Molecule 11 is a protein called RPB11.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	K	115	Total	C	H	N	O	S	0	0
			1862	593	942	152	173	2		

- Molecule 12 is a protein called RNA polymerase II subunit K.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	L	47	Total	C	H	N	O	S	0	0
			803	246	406	77	68	6		

- Molecule 13 is a protein called Transcription elongation factor SPT6.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	M	1002	Total	C	H	N	O		0	0
			5267	2004	1259	1002	1002			

There are 3 discrepancies between the modelled and reference sequences:



Chain	Residue	Modelled	Actual	Comment	Reference
M	-2	SER	-	expression tag	UNP Q7KZ85
M	-1	ASN	-	expression tag	UNP Q7KZ85
M	0	ALA	-	expression tag	UNP Q7KZ85

- Molecule 14 is a DNA chain called Non-template DNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	N	140	Total	C	H	N	O	P	0	0
			4480	1376	1594	490	880	140		

- Molecule 15 is a protein called Transcription elongation factor A protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	O	161	Total	C	N	O	0	0
			645	322	161	162		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	-2	SER	-	expression tag	UNP P23193
O	-1	ASN	-	expression tag	UNP P23193
O	0	ALA	-	expression tag	UNP P23193

- Molecule 16 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	P	16	Total	C	H	N	O	P	0	0
			502	148	170	49	119	16		

- Molecule 17 is a protein called RNA polymerase-associated protein CTR9 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	890	Total	C	H	N	O	0	0
			5356	1780	1796	890	890		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	1174	GLU	-	expression tag	UNP Q6PD62
Q	1175	ASN	-	expression tag	UNP Q6PD62
Q	1176	LEU	-	expression tag	UNP Q6PD62
Q	1177	TYR	-	expression tag	UNP Q6PD62

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	1178	PHE	-	expression tag	UNP Q6PD62
Q	1179	GLN	-	expression tag	UNP Q6PD62

- Molecule 18 is a protein called RNA polymerase-associated protein RTF1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	244	Total	C	H	N	O	0	0
			1467	488	491	244	244		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	-2	SER	-	expression tag	UNP Q92541
R	-1	ASN	-	expression tag	UNP Q92541
R	0	ALA	-	expression tag	UNP Q92541

- Molecule 19 is a DNA chain called Template DNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	T	155	Total	C	H	N	O	P	0	0
			4885	1498	1719	629	884	155		

- Molecule 20 is a protein called RNA polymerase-associated protein LEO1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	U	104	Total	C	H	N	O	0	0
			626	208	210	104	104		

- Molecule 21 is a protein called RNA polymerase II-associated factor 1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V	244	Total	C	H	N	O	0	0
			1457	488	481	244	244		

- Molecule 22 is a protein called WDR61.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	300	Total	C	H	N	O	0	0
			1817	600	617	300	300		

- Molecule 23 is a protein called Parafibromin.



Mol	Chain	Residues	Atoms					AltConf	Trace
23	X	43	Total	C	H	N	O	0	0
			259	86	87	43	43		

- Molecule 24 is a protein called Transcription elongation factor SPT5.

Mol	Chain	Residues	Atoms							AltConf	Trace
24	Z	307	Total	C	H	N	O	P	S	0	0
			4751	1495	2363	430	450	1	12		

- Molecule 25 is a protein called Histone H3.2.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	a	97	Total	C	H	N	O	S	0	0
			1643	506	841	155	138	3		
25	e	97	Total	C	H	N	O	S	0	0
			1640	504	839	155	139	3		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	102	ALA	GLY	engineered mutation	UNP P84233
e	102	ALA	GLY	engineered mutation	UNP P84233

- Molecule 26 is a protein called Histone H4.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	b	83	Total	C	H	N	O	S	0	0
			1372	418	710	129	114	1		
26	f	78	Total	C	H	N	O	S	0	0
			1279	391	660	120	107	1		

- Molecule 27 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	c	103	Total	C	H	N	O	0	0
			1642	501	847	155	139		
27	g	105	Total	C	H	N	O	0	0
			1674	510	865	158	141		

- Molecule 28 is a protein called Histone H2B 1.1.



Mol	Chain	Residues	Atoms						AltConf	Trace
28	d	95	Total	C	H	N	O	S	0	0
			1519	469	774	134	140	2		
28	h	93	Total	C	H	N	O	S	0	0
			1474	457	748	130	137	2		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
d	0	MET	-	initiating methionine	UNP P02281
d	29	THR	SER	engineered mutation	UNP P02281
h	0	MET	-	initiating methionine	UNP P02281
h	29	THR	SER	engineered mutation	UNP P02281

- Molecule 29 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
29	A	2	Total	Zn	0
			2	2	
29	B	1	Total	Zn	0
			1	1	
29	C	1	Total	Zn	0
			1	1	
29	I	2	Total	Zn	0
			2	2	
29	J	1	Total	Zn	0
			1	1	
29	R	1	Total	Zn	0
			1	1	

- Molecule 30 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

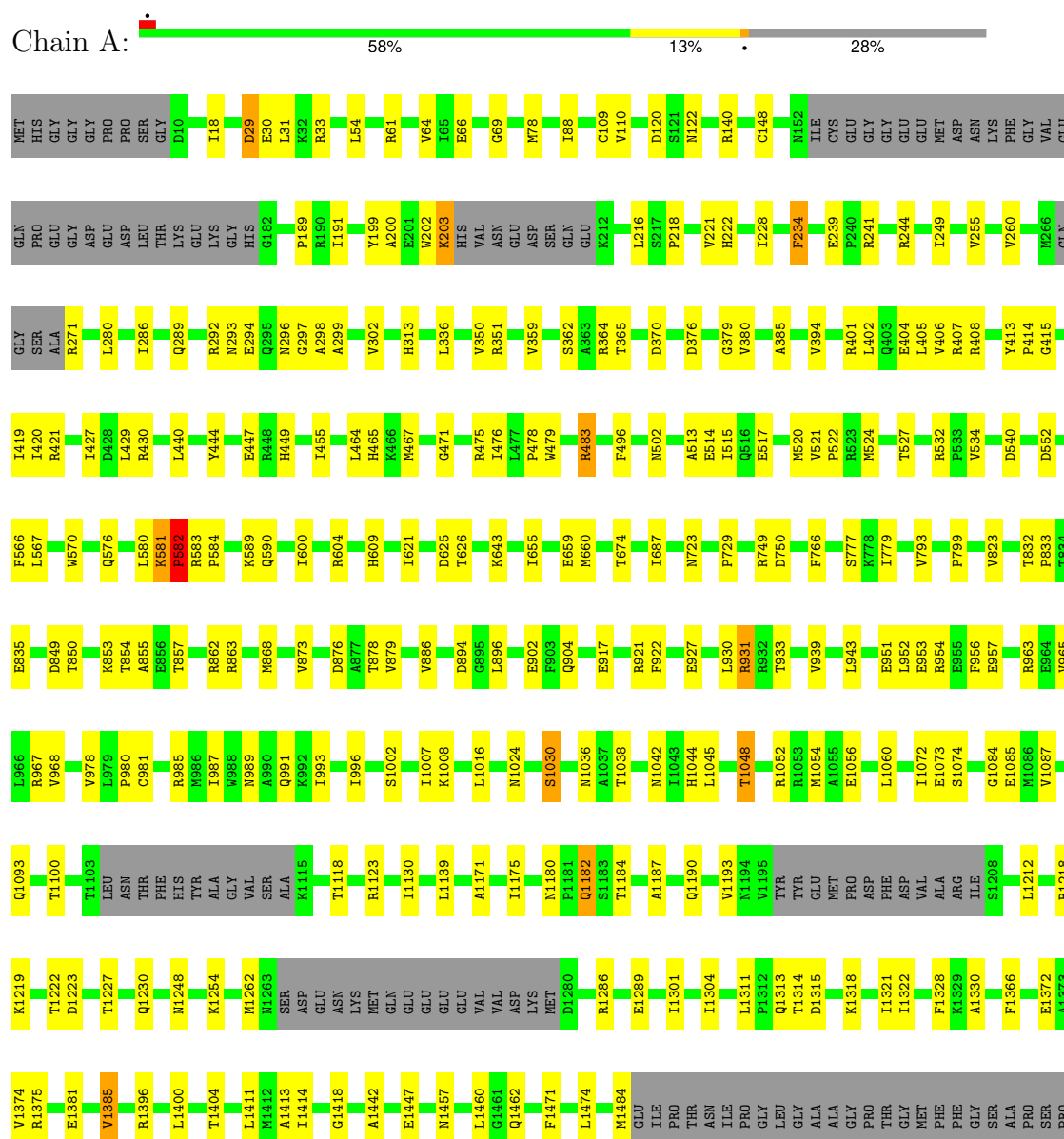
Mol	Chain	Residues	Atoms		AltConf
30	A	1	Total	Mg	0
			1	1	



### 3 Residue-property plots

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: DNA-directed RNA polymerase subunit

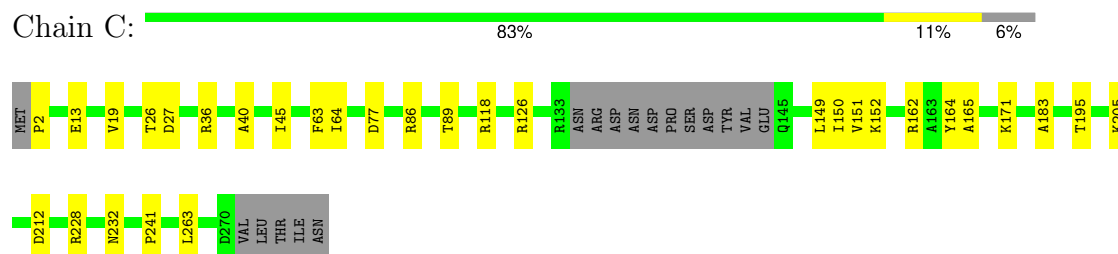




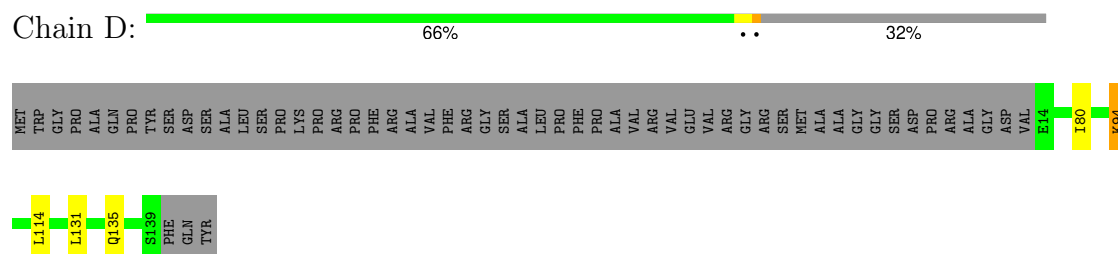




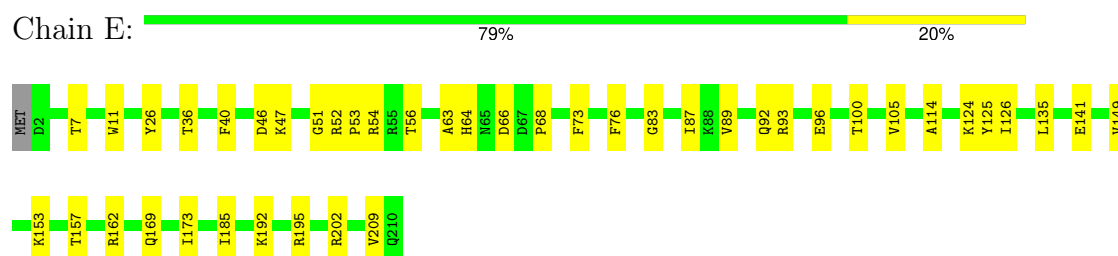
- Molecule 3: DNA-directed RNA polymerase II subunit RPB3



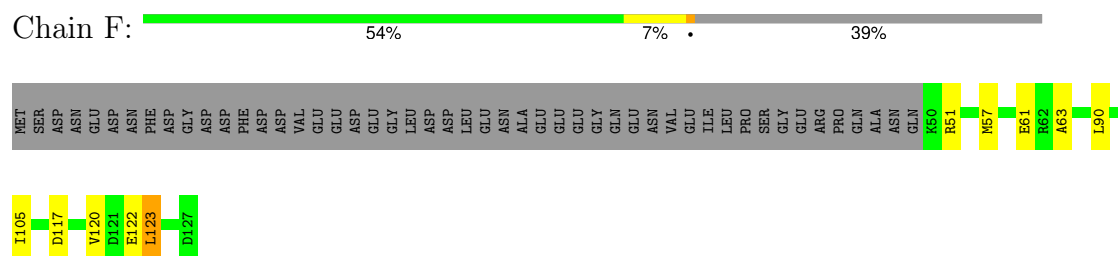
- Molecule 4: RPOL4c domain-containing protein



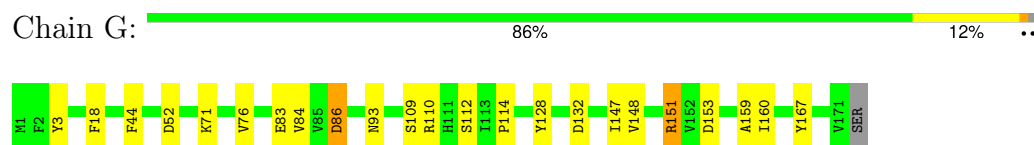
- Molecule 5: DNA-directed RNA polymerase II subunit E



- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2



- Molecule 7: DNA-directed RNA polymerase II subunit RPB7



- Molecule 8: RPB8



MET
A2
K20
D23
R24
R27
S32
K37
D38
L39
I40
L41
D42
T63
Y75
N76
P77
R84
A85
K95
M123
D128
F150

ME1	GLU	PRO	ASP	GLY	THR	TYR	GLU	PRO	GLI	F11	V12	N22	E31	C39	N41	C42	D43	Y44	N50	Y54	I58	E64	Q67	I68	A69	A70	D71	V72	T81	C86	H91	F96	H100	R109	L110	Y111	A116	H121	T124	F125
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M1	N2	K17	K18	I19	T20	I21	N36	L42	I46	D53	P54	Q55	V56	L57	V63	P64	H65	I71	Q76	T77	T78	D80	Y81	F87	D93	L94	G115	I1E	GU
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MET  
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 I16  
 Y17  
 E25  
 N26  
 R37  
 R58

SER	ASN	ALA	ALA	MET	SER	ASP	PHE	VAL	GLU	SER	SER	GLU	ALA	ALA	GLU	GLU	SER	SER	GLU	GLU	GLY	GLY	TYR	ASN	ASN	ASP	ASP	GLU	GLY	GLU	VAL	VAL	PRO	ARG	VAL	THR	LYS	LYS	PHE	VAL	VAL	GLU	GLU	GLU	GLU	ASP	ASP	ASP	ASP	GLU	GLU	GLU	GLN	ASP	ASP	LEU	ASN	GLU	GLU	GLY	GLN	GLN	ASN	ASN	LEU	LYS	GLY	PHE
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TILE	ASN	ASP	ASP	ASP	ASP	GLU	GLY	GLY	GLY	GLY	GLU	GLU	GLU	GLY	GLY	GLY	SER	ASP	ASP	SER	SER	GLP	ASP	VAL	LYS	HIS	GLY	LYS	LYS	ARG	ARG	THR	SER	PHE	ASP	ASP	LEU	GLY	ASP	ASP	ASP	PHE	ASP	ASP	ASN	LEU	GLY	VAL	LYS	VAL	LYS	ARG	GLY	GLN	LYS
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TYR	ARG	ARG	VAL	LYS	LYS	MET	SER	ASP	ASP	GLU	ASP	ASP	ASP	GLU	GLU	TYR	GLY	LYS	GLU	GLU	HIS	GLU	LYS	ALA	ALA	ILE	GLN	ASP	GLY	GLU	GLY	GLU	GLN	GLU	ALA	ALA	MET	GLU	ALA	PRO	PRO	GLU	GLU	GLU	ASP	ASP	GLN
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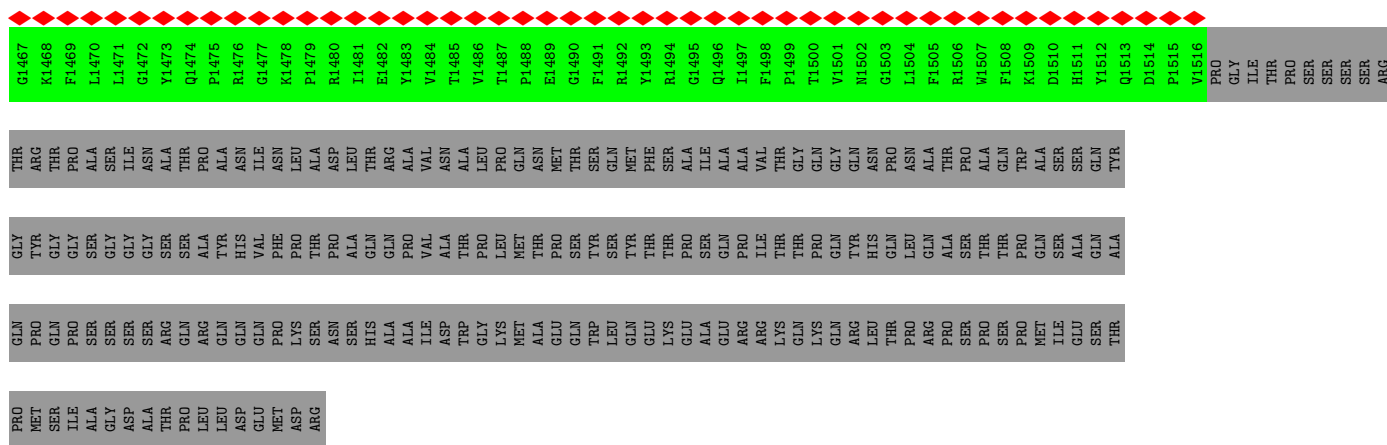
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GLU	GLU	TYR	GLU	TYR	GLU	ASP	ASP	GLU	ALA	GLU	GLY	GLU	ILE	ARG	VAL	ARG	PRO	LYS	LYS	THR	THR	LYS	LYS	ARG	VAL	SER	SER	ARG	ARG	SER	ILE	PHE	GLU	MET	TYR	GLU	GLU	PRO	SER	SER	GLU	LEU	GLU	GLU	SER	SER	HIS	LEU	LEU	THR	D284	Q285	D286	N287	E288	I289	R290	A291	T292	D293	L294	P295	E296	S297
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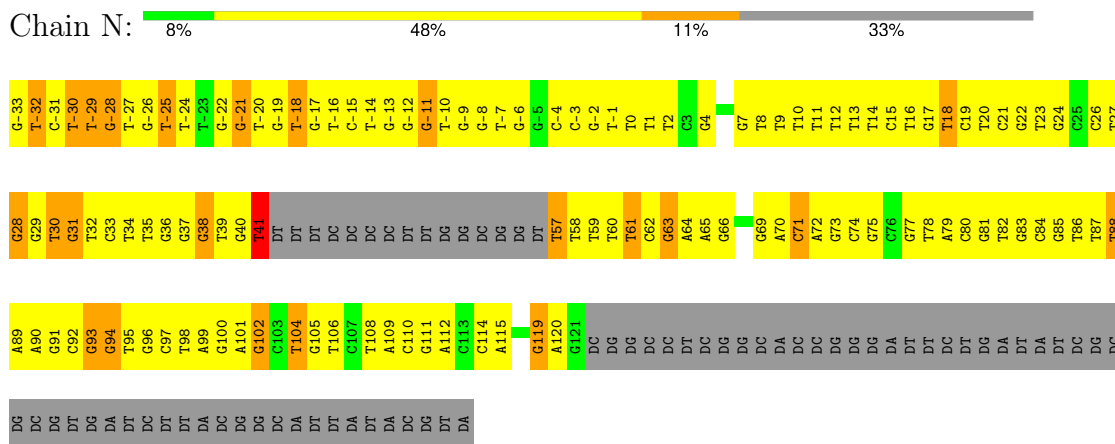




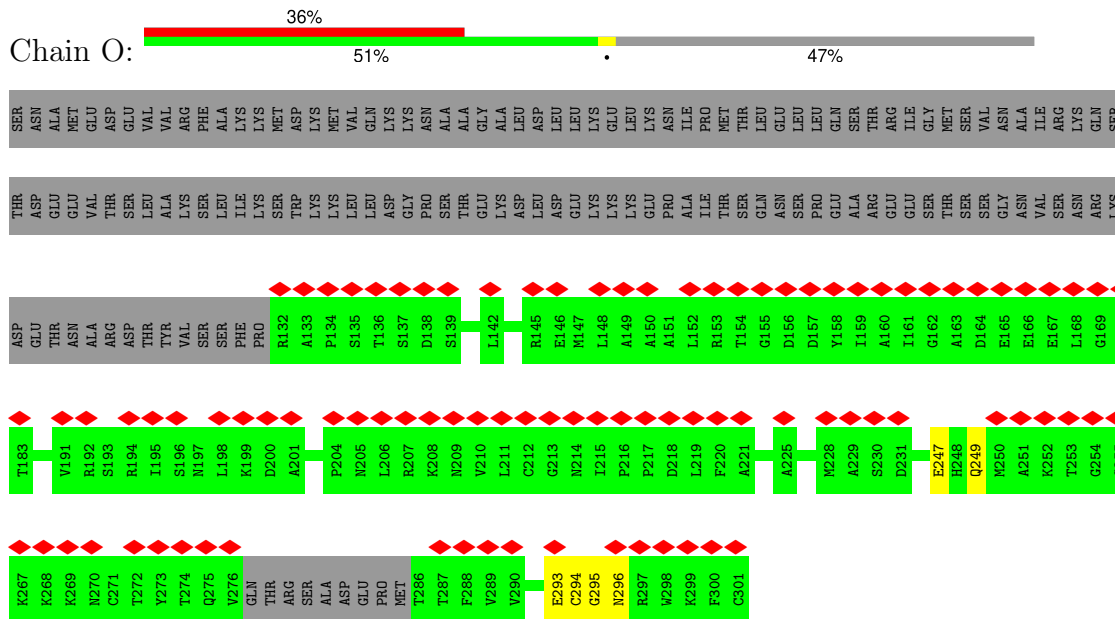




- Molecule 14: Non-template DNA

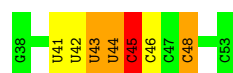


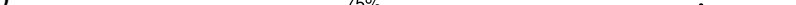
- Molecule 15: Transcription elongation factor A protein 1

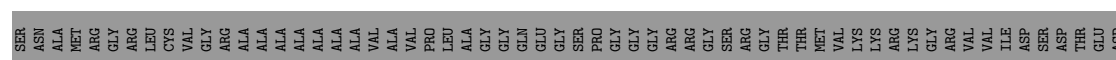


- Molecule 16: RNA

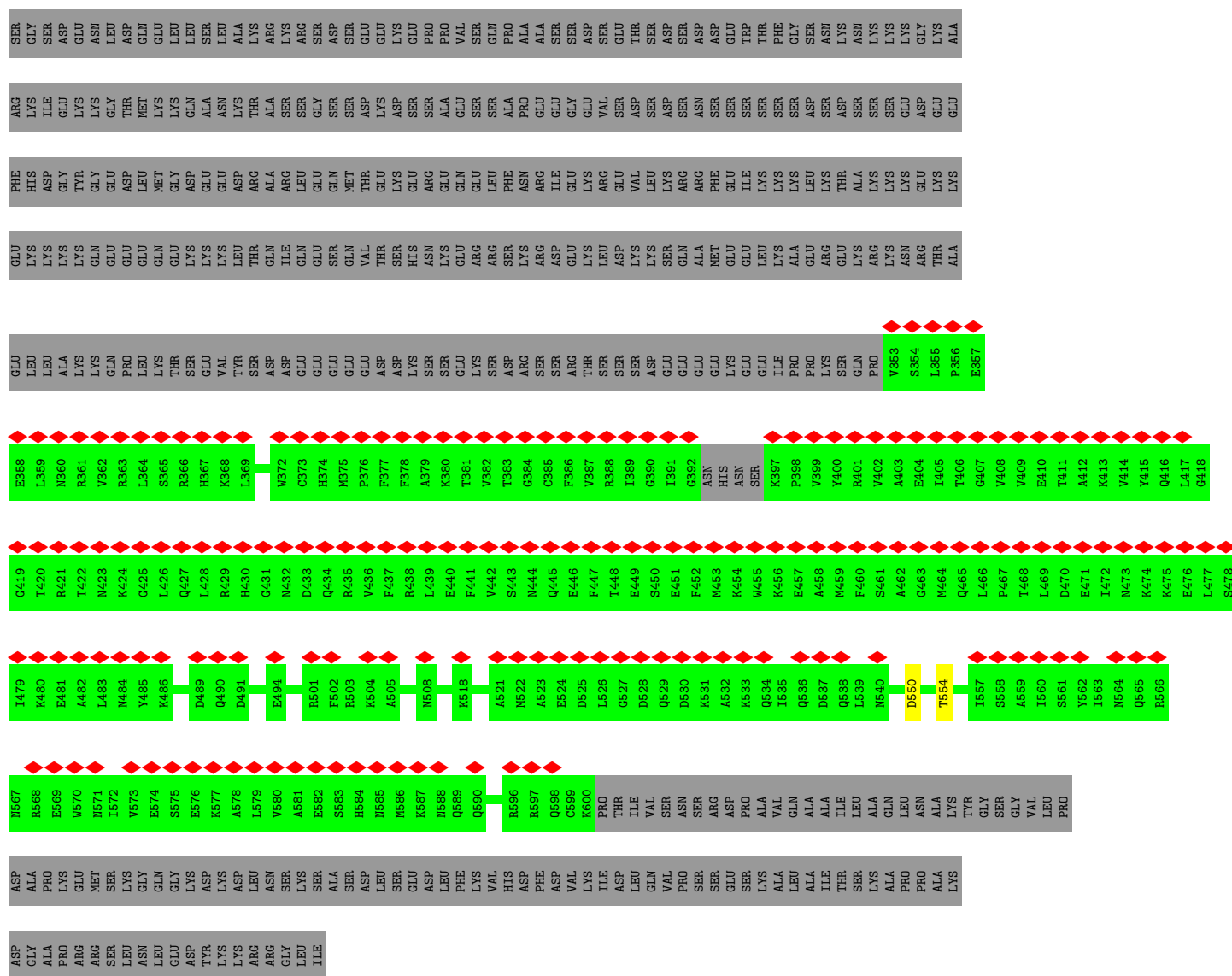




- Chain Q: 

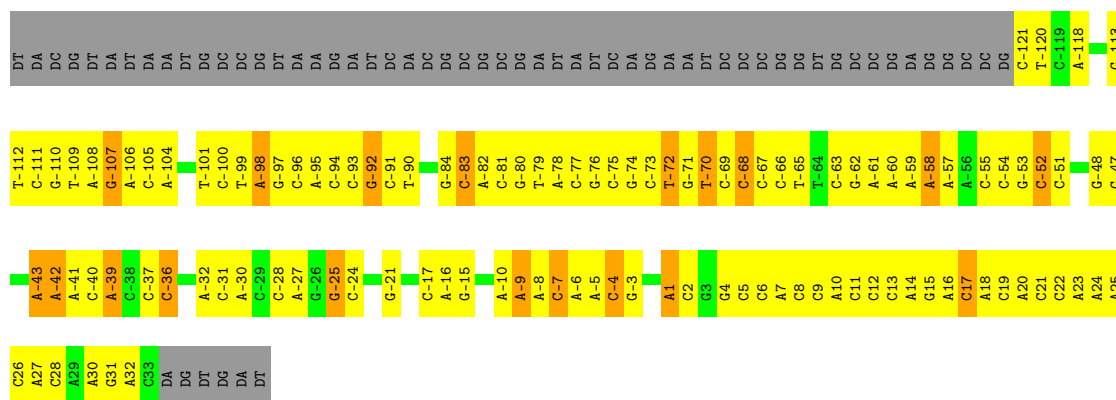






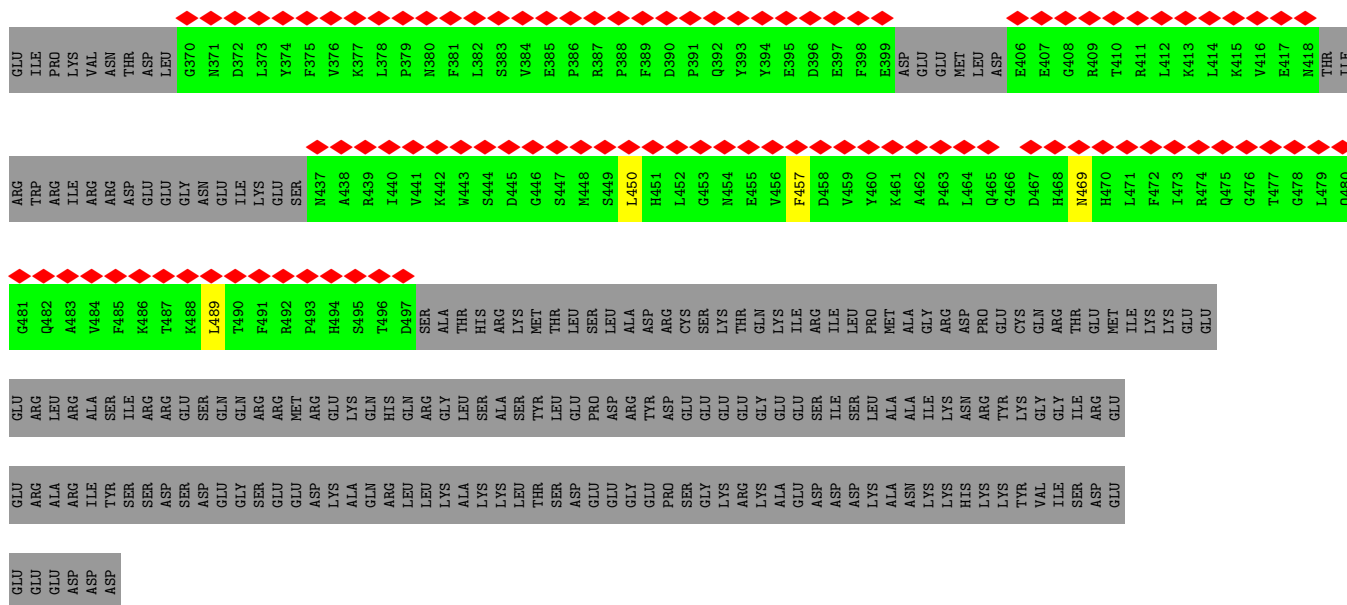
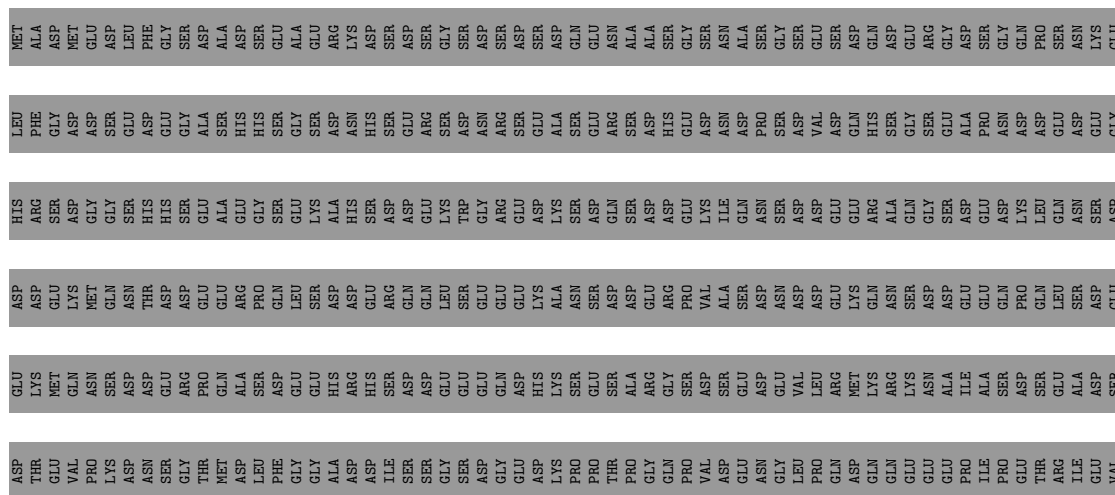
## • Molecule 19: Template DNA

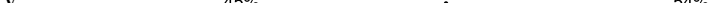
Chain T: 19% 45% 9% 28%

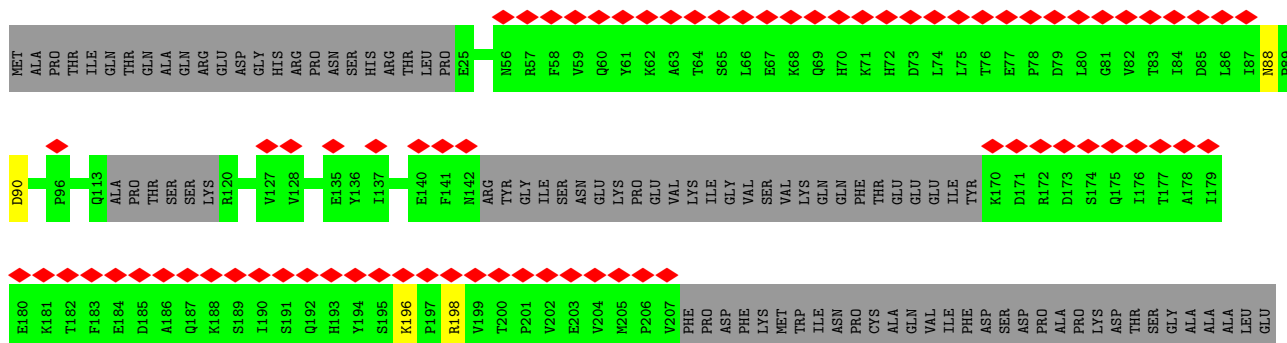


## • Molecule 20: RNA polymerase-associated protein LEO1





- Chain V: 

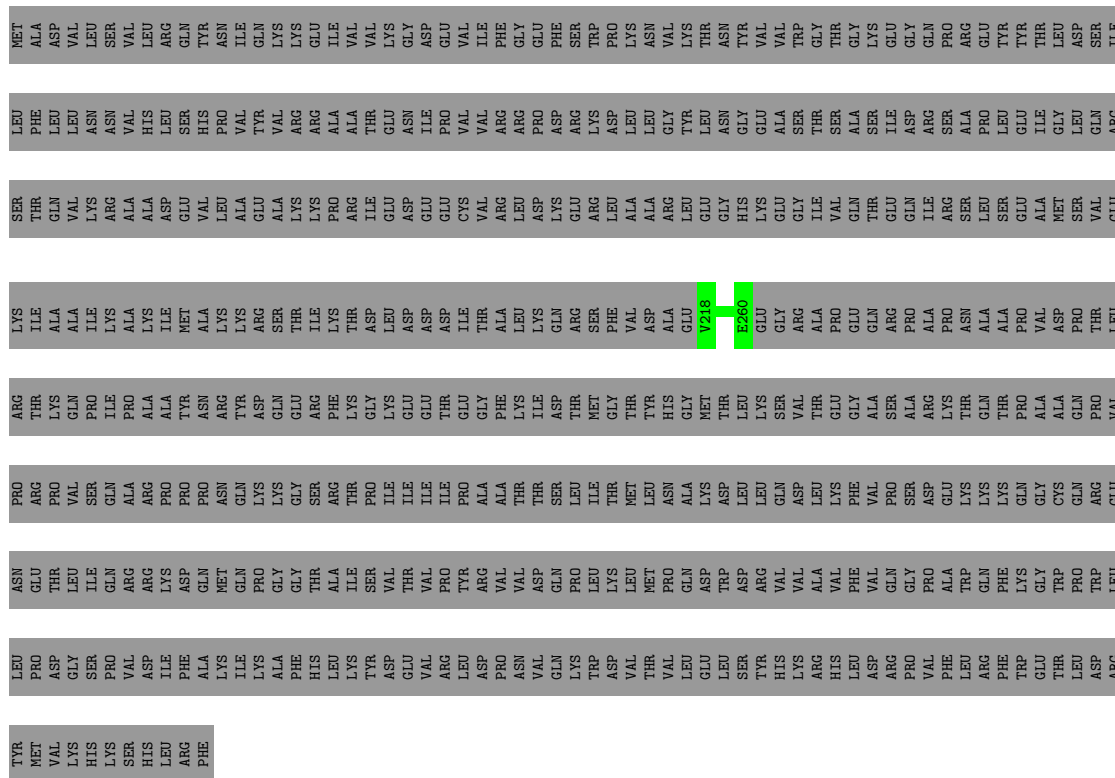




- Molecule 22: WDR61

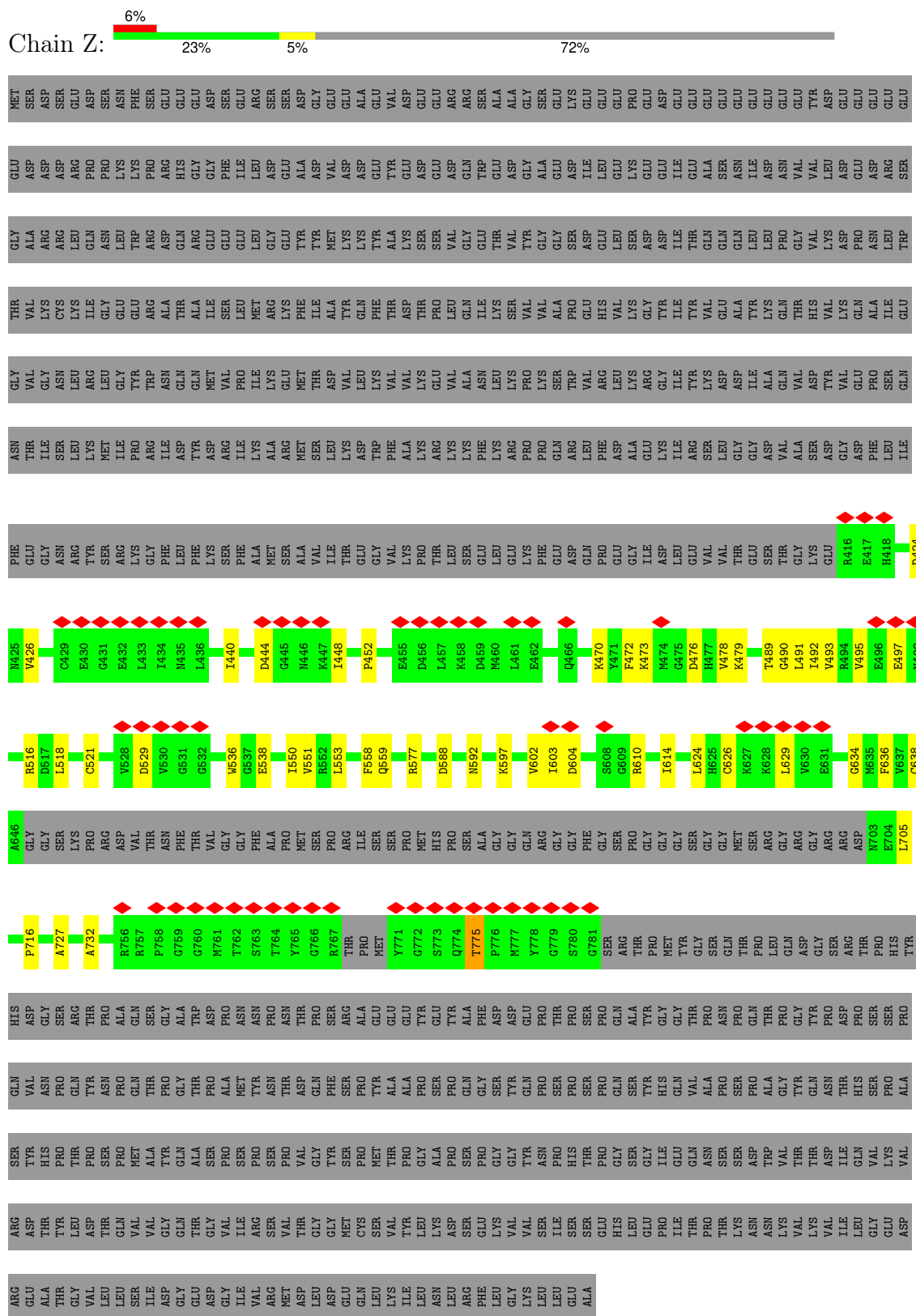


- Molecule 23: Parafibromin



- Molecule 24: Transcription elongation factor SPT5

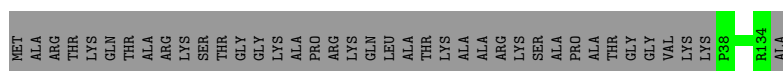




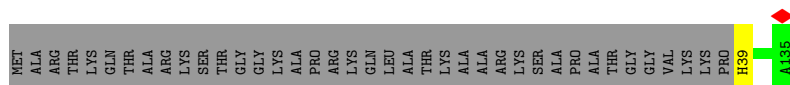
# - Molecule 25: Histone H3.2



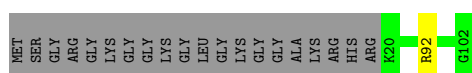
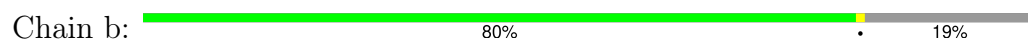




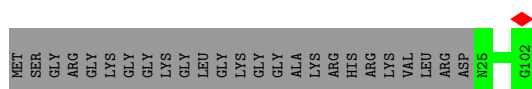
- Molecule 25: Histone H3.2



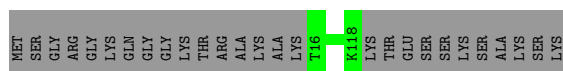
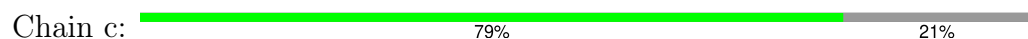
- Molecule 26: Histone H4



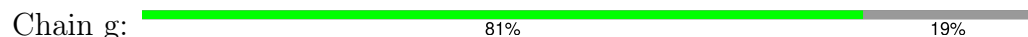
- Molecule 26: Histone H4



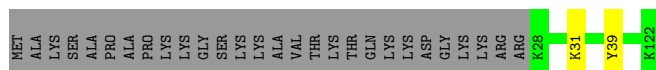
- Molecule 27: Histone H2A



- Molecule 27: Histone H2A



- Molecule 28: Histone H2B 1.1



- Molecule 28: Histone H2B 1.1





MET	ALA	LYS	SER	ALA	PRO	PRO	LYS	LYS	GLY	SER	LYS	LYS	ALA	VAL	THR	LYS	LYS	LYS	ASP	GLY	GLY	LYS	LYS	ARG	ARG	LYS	T29	RE3	A121	LYS
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	-----





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	105420	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	52	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.466	Depositor
Minimum map value	-0.485	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.044	Depositor
Recommended contour level	0.106	Depositor
Map size ( $\text{\AA}$ )	373.5, 373.5, 373.5	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.83, 0.83, 0.83	Depositor



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.39	0/11437	0.61	2/15433 (0.0%)
2	B	0.42	0/9124	0.58	0/12313
3	C	0.42	0/2115	0.54	0/2873
4	D	0.26	0/1017	0.48	0/1368
5	E	0.33	0/1751	0.57	0/2366
6	F	0.45	0/636	0.57	0/859
7	G	0.29	0/1364	0.51	0/1853
8	H	0.38	0/1219	0.55	0/1644
9	I	0.33	0/964	0.54	0/1305
10	J	0.51	0/533	0.57	0/719
11	K	0.41	0/939	0.54	0/1271
12	L	0.41	0/403	0.66	0/536
13	M	0.26	0/3995	0.50	1/4971 (0.0%)
14	N	0.77	1/3226 (0.0%)	1.33	29/4986 (0.6%)
15	O	0.36	0/643	0.62	0/799
16	P	0.63	0/367	1.13	2/568 (0.4%)
17	Q	0.23	0/3559	0.47	0/4447
18	R	0.23	0/974	0.48	0/1214
19	T	0.80	1/3564 (0.0%)	1.19	22/5487 (0.4%)
20	U	0.25	0/413	0.48	0/511
21	V	0.27	0/972	0.53	0/1208
22	W	0.24	0/1199	0.55	0/1497
23	X	0.24	0/171	0.46	0/212
24	Z	0.26	0/2414	0.53	0/3250
25	a	0.30	0/814	0.62	0/1092
25	e	0.28	0/812	0.57	0/1088
26	b	0.33	0/669	0.60	0/894
26	f	0.32	0/626	0.59	0/837
27	c	0.28	0/805	0.56	0/1088
27	g	0.29	0/819	0.56	0/1106
28	d	0.29	0/756	0.50	0/1015
28	h	0.32	0/737	0.50	0/993



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
All	All	0.42	2/59037 (0.0%)	0.70	56/79803 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
2	B	0	3
7	G	0	1
10	J	0	1
13	M	0	1
14	N	0	1
21	V	0	1
All	All	0	10

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	N	41	DT	C4'-O4'	5.26	1.50	1.45
19	T	-51	DC	C3'-O3'	-5.19	1.37	1.44

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	581	LYS	C-N-CD	-28.87	57.08	120.60
19	T	-42	DA	O4'-C1'-N9	10.77	115.54	108.00
14	N	28	DG	O4'-C1'-N9	10.03	115.02	108.00
14	N	38	DG	O4'-C1'-N9	9.74	114.82	108.00
19	T	1	DA	O4'-C1'-N9	9.66	114.76	108.00
14	N	93	DG	O4'-C1'-N9	9.51	114.66	108.00
14	N	24	DG	O4'-C1'-N9	8.59	114.01	108.00
14	N	-28	DG	O4'-C1'-N9	8.52	113.96	108.00
14	N	63	DG	O4'-C1'-N9	7.92	113.55	108.00
19	T	-43	DA	O4'-C4'-C3'	-7.88	101.27	106.00
14	N	18	DT	O4'-C1'-N1	7.69	113.38	108.00
14	N	95	DT	O4'-C1'-N1	7.49	113.24	108.00
1	A	582	PRO	CA-N-CD	-7.44	101.09	111.50
14	N	-32	DT	O4'-C1'-N1	7.42	113.19	108.00
13	M	1333	HIS	CA-C-N	-7.33	101.08	117.20
19	T	-107	DG	O4'-C1'-N9	7.31	113.12	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	74	DC	O4'-C1'-N1	7.19	113.03	108.00
19	T	-40	DC	O4'-C1'-N1	7.08	112.96	108.00
19	T	-7	DC	O4'-C1'-N1	6.88	112.81	108.00
19	T	-52	DC	O4'-C1'-N1	6.88	112.81	108.00
19	T	-70	DT	O4'-C1'-N1	6.54	112.58	108.00
19	T	-39	DA	OP1-P-OP2	-6.53	109.81	119.60
14	N	30	DT	OP1-P-OP2	-6.40	110.00	119.60
19	T	-72	DT	O4'-C1'-N1	6.33	112.43	108.00
14	N	-29	DT	O4'-C1'-N1	-6.32	103.58	108.00
14	N	57	DT	O4'-C1'-N1	6.19	112.33	108.00
19	T	-25	DG	O4'-C1'-N9	6.14	112.30	108.00
19	T	-40	DC	OP1-P-O3'	5.99	118.38	105.20
19	T	-58	DA	O4'-C1'-N9	5.99	112.19	108.00
14	N	88	DT	O4'-C1'-N1	-5.94	103.84	108.00
14	N	102	DG	O4'-C1'-N9	5.93	112.15	108.00
19	T	-92	DG	O4'-C1'-N9	5.91	112.14	108.00
19	T	-36	DC	O4'-C1'-N1	-5.90	103.87	108.00
14	N	31	DG	C1'-O4'-C4'	-5.64	104.46	110.10
14	N	71	DC	C1'-O4'-C4'	-5.59	104.51	110.10
14	N	24	DG	C1'-O4'-C4'	-5.58	104.52	110.10
14	N	94	DG	C1'-O4'-C4'	-5.51	104.59	110.10
19	T	-9	DA	O4'-C1'-N9	5.45	111.82	108.00
16	P	48	C	C5'-C4'-O4'	5.43	115.61	109.10
14	N	-21	DG	O4'-C1'-N9	-5.42	104.21	108.00
19	T	-98	DA	O4'-C1'-N9	5.32	111.72	108.00
14	N	-25	DT	O4'-C1'-N1	5.25	111.67	108.00
14	N	41	DT	O4'-C1'-N1	-5.23	104.34	108.00
14	N	-30	DT	O4'-C1'-N1	-5.19	104.36	108.00
14	N	104	DT	O4'-C1'-N1	5.19	111.64	108.00
19	T	-17	DC	O4'-C1'-N1	5.17	111.62	108.00
19	T	17	DC	C1'-O4'-C4'	-5.16	104.94	110.10
14	N	119	DG	O4'-C1'-N9	5.13	111.59	108.00
14	N	-18	DT	O4'-C1'-N1	5.12	111.59	108.00
14	N	28	DG	C1'-O4'-C4'	-5.10	105.00	110.10
14	N	61	DT	O4'-C1'-N1	5.09	111.56	108.00
19	T	-83	DC	C1'-O4'-C4'	-5.07	105.03	110.10
19	T	-68	DC	O4'-C1'-C2'	5.04	109.93	105.90
16	P	45	C	C5'-C4'-O4'	5.04	115.14	109.10
19	T	-4	DC	C1'-O4'-C4'	-5.02	105.08	110.10
14	N	-11	DG	O4'-C1'-N9	-5.02	104.49	108.00

There are no chirality outliers.



All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	244	ARG	Sidechain
1	A	430	ARG	Sidechain
2	B	491	ARG	Sidechain
2	B	743	ARG	Sidechain
2	B	859	ARG	Sidechain
7	G	151	ARG	Sidechain
10	J	6	ARG	Sidechain
13	M	1333	HIS	Mainchain
14	N	41	DT	Sidechain
21	V	299	GLU	Peptide

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11255	11388	11374	221	0
2	B	8947	9002	8994	118	0
3	C	2072	2024	2019	21	0
4	D	1004	981	980	4	0
5	E	1720	1738	1737	29	0
6	F	626	658	657	8	0
7	G	1333	1321	1321	17	0
8	H	1197	1157	1156	9	0
9	I	942	880	872	17	0
10	J	524	544	540	11	0
11	K	920	942	942	17	0
12	L	397	406	405	4	0
13	M	4008	1259	1035	8	0
14	N	2886	1594	1596	160	0
15	O	645	0	171	30	0
16	P	332	170	169	3	0
17	Q	3560	1796	940	4	0
18	R	976	491	255	1	0
19	T	3166	1719	1720	133	0
20	U	416	210	111	2	0
21	V	976	481	240	2	0
22	W	1200	617	341	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	X	172	87	44	0	0
24	Z	2388	2363	2360	43	0
25	a	802	841	841	0	0
25	e	801	839	838	0	0
26	b	662	710	709	0	0
26	f	619	660	659	0	0
27	c	795	847	846	0	0
27	g	809	865	864	0	0
28	d	745	774	773	0	0
28	h	726	748	747	0	0
29	A	2	0	0	0	0
29	B	1	0	0	0	0
29	C	1	0	0	0	0
29	I	2	0	0	0	0
29	J	1	0	0	0	0
29	R	1	0	0	0	0
30	A	1	0	0	0	0
All	All	57630	48112	46256	753	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 8.

All (753) 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)
1:A:729:PRO:CG	15:O:249:GLN:O	1.79	1.27
1:A:1314:THR:C	15:O:295:GLY:HA3	1.56	1.23
1:A:729:PRO:HB3	15:O:247:GLU:O	1.38	1.21
1:A:203:LYS:NZ	19:T:-67:DC:OP1	1.75	1.20
1:A:729:PRO:CB	15:O:247:GLU:O	1.90	1.17
1:A:1314:THR:O	15:O:295:GLY:HA3	1.40	1.16
1:A:203:LYS:NZ	19:T:-67:DC:P	2.17	1.16
1:A:729:PRO:HG3	15:O:249:GLN:O	1.44	1.05
1:A:1315:ASP:CG	15:O:296:ASN:N	2.03	1.00
1:A:203:LYS:HZ3	19:T:-67:DC:P	1.84	0.97
1:A:729:PRO:CA	15:O:247:GLU:O	2.13	0.97
11:K:77:THR:OG1	11:K:81:TYR:O	1.83	0.96
1:A:1314:THR:C	15:O:295:GLY:CA	2.32	0.96
1:A:904:GLN:NE2	1:A:981:CYS:O	1.98	0.95
10:J:47:ARG:NH1	10:J:48:MET:SD	2.42	0.93
1:A:582:PRO:HG2	1:A:583:ARG:H	1.36	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:894:ASP:OD2	1:A:1396:ARG:NH2	2.05	0.89
1:A:729:PRO:HG2	15:O:249:GLN:O	1.72	0.89
1:A:1313:GLN:O	15:O:295:GLY:HA2	1.74	0.86
1:A:729:PRO:HA	15:O:247:GLU:O	1.75	0.85
1:A:552:ASP:OD2	8:H:24:ARG:NH1	2.10	0.85
1:A:1130:ILE:O	1:A:1130:ILE:HD12	1.77	0.84
1:A:917:GLU:OE2	1:A:921:ARG:NH1	2.12	0.83
1:A:54:LEU:O	1:A:61:ARG:NH2	2.14	0.80
1:A:1330:ALA:HB3	15:O:294:CYS:CA	2.11	0.80
1:A:440:LEU:O	1:A:440:LEU:HD12	1.83	0.79
1:A:729:PRO:HB3	15:O:247:GLU:C	2.04	0.79
1:A:1024:ASN:O	5:E:162:ARG:NH2	2.17	0.78
1:A:296:ASN:OD1	1:A:297:GLY:N	2.17	0.77
1:A:1315:ASP:OD2	15:O:296:ASN:N	2.16	0.77
1:A:394:VAL:HG23	1:A:444:TYR:O	1.84	0.77
11:K:78:THR:OG1	11:K:80:ASP:OD1	2.02	0.77
1:A:66:GLU:OE1	1:A:271:ARG:NH2	2.18	0.76
1:A:1314:THR:HA	15:O:295:GLY:O	1.85	0.76
24:Z:602:VAL:HG21	24:Z:636:PHE:HE2	1.50	0.76
3:C:26:THR:HG22	3:C:27:ASP:H	1.49	0.76
1:A:1315:ASP:CG	15:O:296:ASN:H	1.88	0.75
14:N:-15:DC:H2'	14:N:-14:DT:H71	1.70	0.74
1:A:729:PRO:CB	15:O:249:GLN:O	2.36	0.73
2:B:953:ASP:OD1	3:C:36:ARG:NH2	2.21	0.73
1:A:239:GLU:OE2	1:A:241:ARG:NH1	2.21	0.73
1:A:1016:LEU:HD23	1:A:1045:LEU:HD21	1.71	0.73
1:A:203:LYS:HZ2	19:T:-67:DC:P	2.11	0.72
1:A:1218:ARG:O	1:A:1222:THR:HG23	1.88	0.72
5:E:153:LYS:O	5:E:157:THR:HG23	1.88	0.72
1:A:1248:ASN:ND2	1:A:1254:LYS:O	2.22	0.72
18:R:550:ASP:O	18:R:554:THR:N	2.23	0.71
14:N:57:DT:O2	19:T:-55:DC:N4	2.23	0.70
3:C:86:ARG:NH1	24:Z:716:PRO:O	2.24	0.70
11:K:93:ASP:OD1	11:K:94:LEU:N	2.25	0.70
1:A:447:GLU:OE2	2:B:1064:ARG:NH1	2.24	0.70
1:A:876:ASP:HB3	1:A:878:THR:HG22	1.73	0.70
2:B:851:ASP:OD2	12:L:17:TYR:OH	2.09	0.70
2:B:565:THR:HG21	2:B:580:PRO:HB3	1.73	0.69
1:A:66:GLU:O	1:A:69:GLY:N	2.26	0.69
1:A:902:GLU:OE1	1:A:985:ARG:NH2	2.27	0.68
1:A:1315:ASP:N	15:O:295:GLY:HA3	2.09	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:423:ILE:HD12	2:B:428:ASP:HA	1.76	0.68
9:I:109:ARG:HD3	9:I:124:THR:HG21	1.76	0.68
14:N:9:DT:H2''	14:N:10:DT:H71	1.75	0.68
14:N:-28:DG:H2''	14:N:-27:DT:H72	1.75	0.67
24:Z:602:VAL:HG21	24:Z:636:PHE:CE2	2.29	0.67
1:A:581:LYS:NZ	8:H:85:ALA:O	2.27	0.67
1:A:1038:THR:O	1:A:1042:ASN:ND2	2.28	0.67
1:A:1314:THR:O	15:O:295:GLY:CA	2.31	0.67
2:B:939:HIS:NE2	2:B:983:GLU:OE1	2.25	0.67
14:N:98:DT:O2	19:T:-97:DG:N2	2.28	0.66
17:Q:506:LEU:O	17:Q:510:MET:N	2.28	0.66
24:Z:478:VAL:HG11	24:Z:492:ILE:HG23	1.77	0.66
14:N:86:DT:H2'	14:N:87:DT:H72	1.77	0.66
1:A:832:THR:HG22	1:A:833:PRO:HD2	1.78	0.65
1:A:823:VAL:HG22	1:A:835:GLU:HB2	1.78	0.65
1:A:896:LEU:HD13	1:A:980:PRO:HG3	1.78	0.65
24:Z:550:ILE:HD13	24:Z:558:PHE:HB3	1.78	0.64
1:A:1400:LEU:O	1:A:1404:THR:HG23	1.98	0.64
14:N:59:DT:H2'	14:N:60:DT:H72	1.79	0.64
7:G:110:ARG:NH1	7:G:114:PRO:O	2.30	0.64
1:A:659:GLU:OE2	1:A:985:ARG:NH1	2.25	0.63
9:I:81:THR:HG23	9:I:96:PHE:CD2	2.33	0.63
2:B:824:ASP:O	2:B:872:THR:HG23	1.98	0.63
14:N:41:DT:H5'	14:N:41:DT:C6	2.33	0.63
14:N:63:DG:H1'	14:N:64:DA:N7	2.14	0.63
1:A:582:PRO:HG2	1:A:583:ARG:N	2.09	0.63
19:T:11:DC:H2''	19:T:12:DC:C5	2.34	0.63
1:A:203:LYS:HZ1	19:T:-67:DC:P	2.20	0.63
14:N:32:DT:H2''	14:N:33:DC:C6	2.34	0.62
1:A:455:ILE:HG23	1:A:520:MET:HE1	1.80	0.62
1:A:1007:ILE:HD12	1:A:1008:LYS:N	2.14	0.62
1:A:421:ARG:NE	1:A:427:ILE:HD11	2.14	0.62
2:B:266:GLU:OE1	2:B:266:GLU:O	2.18	0.62
24:Z:473:LYS:O	24:Z:492:ILE:HD11	1.99	0.62
1:A:933:THR:O	1:A:1002:SER:N	2.33	0.61
1:A:1318:LYS:HZ3	15:O:293:GLU:C	2.03	0.61
2:B:931:ILE:HD12	2:B:931:ILE:H	1.65	0.61
11:K:1:MET:SD	11:K:2:ASN:N	2.73	0.61
19:T:-72:DT:H1'	19:T:-71:DG:C8	2.35	0.61
1:A:886:VAL:HG12	5:E:169:GLN:O	2.00	0.61
2:B:845:TYR:HA	2:B:865:VAL:HG11	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:T:-107:DG:H1'	19:T:-106:DA:C8	2.36	0.61
1:A:582:PRO:CG	1:A:583:ARG:N	2.64	0.61
14:N:-8:DG:N2	19:T:9:DC:O2	2.33	0.61
19:T:-37:DC:H2'	19:T:-36:DC:C5	2.36	0.61
1:A:1314:THR:CA	15:O:295:GLY:O	2.49	0.61
5:E:96:GLU:OE1	5:E:96:GLU:N	2.27	0.60
14:N:87:DT:H2'	14:N:88:DT:H72	1.83	0.60
19:T:16:DA:H2''	19:T:17:DC:C6	2.36	0.60
1:A:873:VAL:HG22	1:A:879:VAL:HG22	1.83	0.60
1:A:1315:ASP:N	15:O:295:GLY:O	2.35	0.60
9:I:31:GLU:N	9:I:31:GLU:OE1	2.34	0.60
14:N:97:DC:H2''	14:N:98:DT:C6	2.37	0.60
6:F:120:VAL:HG12	6:F:120:VAL:O	2.02	0.60
6:F:105:ILE:HD12	6:F:117:ASP:HB3	1.83	0.60
1:A:965:VAL:O	1:A:968:VAL:HG22	2.01	0.60
2:B:423:ILE:HD13	2:B:429:PHE:CD1	2.37	0.60
3:C:183:ALA:HB3	3:C:232:ASN:HB3	1.83	0.60
11:K:63:VAL:HG22	11:K:71:ILE:HG22	1.84	0.59
13:M:1230:THR:O	13:M:1238:GLY:N	2.35	0.59
14:N:33:DC:H2''	14:N:34:DT:H71	1.84	0.59
14:N:61:DT:H2''	14:N:62:DC:C5	2.36	0.59
8:H:63:THR:O	8:H:84:ARG:NH1	2.35	0.59
14:N:99:DA:H2''	14:N:100:DG:C8	2.37	0.59
1:A:479:TRP:O	1:A:483:ARG:NH2	2.36	0.59
14:N:26:DC:O2	19:T:-25:DG:N2	2.35	0.59
14:N:69:DG:H2''	14:N:70:DA:C8	2.38	0.59
2:B:198:GLU:OE2	2:B:391:LYS:NZ	2.20	0.59
6:F:51:ARG:NH1	6:F:122:GLU:OE1	2.33	0.59
24:Z:626:CYS:HB3	24:Z:629:LEU:HD12	1.84	0.59
10:J:10:CYS:SG	10:J:11:GLY:N	2.76	0.59
24:Z:610:ARG:HD2	24:Z:629:LEU:HD21	1.85	0.58
14:N:57:DT:C6	14:N:57:DT:O5'	2.56	0.58
14:N:13:DT:H2'	14:N:14:DT:H71	1.84	0.58
14:N:58:DT:H2'	14:N:59:DT:H71	1.84	0.58
19:T:-61:DA:H2'	19:T:-60:DA:C8	2.39	0.58
24:Z:492:ILE:HG22	24:Z:502:LEU:HB3	1.85	0.58
1:A:413:TYR:O	1:A:415:GLY:N	2.37	0.58
1:A:1315:ASP:N	15:O:295:GLY:C	2.57	0.58
7:G:147:ILE:HG23	7:G:159:ALA:HB1	1.86	0.58
14:N:31:DG:C2	19:T:-30:DA:C2	2.91	0.58
2:B:631:GLN:O	2:B:683:GLN:NE2	2.32	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:850:THR:O	1:A:854:THR:HG23	2.03	0.57
19:T:-67:DC:H2'	19:T:-66:DC:C6	2.38	0.57
2:B:275:ALA:O	2:B:314:GLN:NE2	2.36	0.57
14:N:9:DT:H2''	14:N:10:DT:C7	2.33	0.57
14:N:93:DG:H1'	14:N:94:DG:C8	2.39	0.57
1:A:189:PRO:CB	1:A:200:ALA:HB1	2.35	0.57
24:Z:492:ILE:HD12	24:Z:495:VAL:CG1	2.34	0.57
19:T:-92:DG:H1'	19:T:-91:DC:C6	2.40	0.57
19:T:21:DC:H2''	19:T:22:DC:C5	2.39	0.57
2:B:867:ILE:HD12	2:B:894:THR:HG21	1.87	0.57
1:A:1045:LEU:HD11	1:A:1072:ILE:HD13	1.86	0.56
1:A:1190:GLN:O	1:A:1193:VAL:HG12	2.04	0.56
1:A:404:GLU:OE2	1:A:407:ARG:NH1	2.38	0.56
19:T:8:DC:H2''	19:T:9:DC:C6	2.41	0.56
14:N:-25:DT:C6	14:N:-24:DT:H72	2.40	0.56
14:N:77:DG:H2''	14:N:78:DT:C5	2.41	0.56
1:A:1087:VAL:HG23	1:A:1400:LEU:HD21	1.87	0.56
8:H:32:SER:OG	8:H:37:MET:N	2.39	0.56
14:N:-28:DG:H1'	14:N:-27:DT:C6	2.40	0.56
19:T:-105:DC:H1'	19:T:-104:DA:C8	2.41	0.56
14:N:81:DG:H2'	14:N:82:DT:H72	1.87	0.56
19:T:-80:DG:H2''	19:T:-79:DT:C5	2.40	0.56
19:T:-78:DA:H2''	19:T:-77:DC:C5	2.41	0.56
19:T:1:DA:H2''	19:T:2:DC:C5	2.40	0.56
1:A:402:LEU:O	1:A:406:VAL:HG23	2.06	0.56
14:N:104:DT:H2''	14:N:105:DG:C8	2.41	0.56
1:A:1318:LYS:NZ	15:O:293:GLU:C	2.60	0.56
7:G:151:ARG:NE	7:G:153:ASP:OD1	2.39	0.55
24:Z:478:VAL:HG21	24:Z:502:LEU:HD22	1.87	0.55
1:A:582:PRO:CG	1:A:583:ARG:H	2.12	0.55
14:N:22:DG:H2'	14:N:23:DT:H71	1.87	0.55
1:A:359:VAL:HG23	1:A:362:SER:OG	2.06	0.55
21:V:196:LYS:O	21:V:198:ARG:N	2.38	0.55
2:B:227:ASN:OD1	2:B:405:ARG:NH2	2.36	0.55
10:J:53:VAL:O	10:J:53:VAL:HG13	2.06	0.55
14:N:-2:DG:H2''	14:N:-1:DT:C5	2.41	0.55
22:W:163:LEU:O	22:W:175:PHE:N	2.33	0.55
3:C:19:VAL:HG23	3:C:241:PRO:HB2	1.88	0.55
7:G:147:ILE:HD12	7:G:147:ILE:H	1.72	0.55
14:N:81:DG:C2	19:T:-80:DG:N2	2.75	0.55
14:N:38:DG:H2''	14:N:39:DT:C5	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:18:DT:H1'	14:N:19:DC:C6	2.42	0.54
5:E:126:ILE:HG23	5:E:126:ILE:O	2.07	0.54
24:Z:492:ILE:HD12	24:Z:495:VAL:HG13	1.89	0.54
11:K:17:LYS:O	11:K:36:ASN:ND2	2.32	0.54
14:N:10:DT:H2'	14:N:11:DT:H72	1.89	0.54
14:N:15:DC:H2'	14:N:16:DT:H72	1.89	0.54
1:A:1227:THR:N	1:A:1230:GLN:OE1	2.38	0.54
14:N:11:DT:H2'	14:N:12:DT:H72	1.89	0.54
3:C:149:LEU:HG	10:J:2:ILE:HD11	1.90	0.54
13:M:1173:GLY:O	13:M:1229:LYS:N	2.41	0.54
24:Z:588:ASP:OD1	24:Z:592:ASN:N	2.35	0.54
9:I:81:THR:HG23	9:I:96:PHE:HD2	1.73	0.54
19:T:-91:DC:H2'	19:T:-90:DT:H71	1.90	0.54
19:T:-68:DC:H2'	19:T:-67:DC:C5	2.43	0.54
2:B:907:VAL:HG13	2:B:921:ILE:HG12	1.90	0.54
9:I:22:ASN:ND2	9:I:41:ASN:OD1	2.41	0.53
19:T:27:DA:H2''	19:T:28:DC:C6	2.44	0.53
24:Z:638:CYS:SG	24:Z:643:LEU:HD21	2.48	0.53
3:C:77:ASP:OD2	3:C:126:ARG:NH2	2.40	0.53
14:N:-1:DT:H2''	14:N:0:DT:C7	2.39	0.53
2:B:515:PRO:O	2:B:520:VAL:HA	2.09	0.53
2:B:534:VAL:N	2:B:600:GLU:OE1	2.40	0.53
1:A:413:TYR:O	1:A:449:HIS:ND1	2.42	0.53
1:A:200:ALA:HB2	1:A:216:LEU:HD21	1.91	0.53
2:B:343:LEU:O	2:B:361:LYS:NZ	2.30	0.53
14:N:-17:DG:C2	19:T:18:DA:C2	2.97	0.53
19:T:-113:DG:H2'	19:T:-112:DT:H72	1.91	0.53
14:N:32:DT:H2''	14:N:33:DC:C5	2.44	0.52
1:A:922:PHE:H	1:A:1052:ARG:HD2	1.74	0.52
1:A:1322:ILE:HD12	1:A:1322:ILE:H	1.75	0.52
14:N:108:DT:O3'	14:N:109:DA:C8	2.62	0.52
2:B:179:LEU:HD22	2:B:768:ARG:HD3	1.91	0.52
9:I:42:CYS:SG	9:I:43:ASP:N	2.83	0.52
1:A:951:GLU:OE1	1:A:954:ARG:NH1	2.41	0.52
12:L:37:ARG:H	12:L:37:ARG:HD3	1.75	0.52
13:M:783:GLY:N	13:M:797:ALA:O	2.42	0.52
14:N:7:DG:C2	19:T:-6:DA:C2	2.98	0.52
1:A:406:VAL:HG21	1:A:440:LEU:HD23	1.92	0.52
1:A:514:GLU:HA	6:F:63:ALA:HB1	1.91	0.52
1:A:853:LYS:O	1:A:857:THR:HG23	2.10	0.52
2:B:848:LEU:HD23	2:B:865:VAL:HG13	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:2:ASN:OD1	11:K:2:ASN:O	2.26	0.52
1:A:1052:ARG:NE	1:A:1056:GLU:OE2	2.42	0.52
2:B:139:GLN:OE1	2:B:139:GLN:N	2.42	0.52
14:N:29:DG:N2	19:T:-28:DC:O2	2.43	0.52
24:Z:516:ARG:HG2	24:Z:516:ARG:HH11	1.75	0.52
1:A:621:ILE:HG23	1:A:621:ILE:O	2.10	0.52
1:A:1315:ASP:N	15:O:295:GLY:CA	2.72	0.52
2:B:897:ARG:HB2	2:B:900:GLU:HG3	1.92	0.52
14:N:39:DT:C4	14:N:40:DG:C6	2.98	0.52
2:B:591:ARG:NH2	2:B:663:GLU:OE2	2.42	0.52
14:N:-1:DT:H2''	14:N:0:DT:C5	2.45	0.51
14:N:78:DT:H1'	14:N:79:DA:C5	2.45	0.51
14:N:105:DG:C2	19:T:-104:DA:C2	2.98	0.51
19:T:-42:DA:H1'	19:T:-41:DA:C8	2.44	0.51
24:Z:424:ASP:HB2	24:Z:440:ILE:HD12	1.92	0.51
14:N:-20:DT:H2''	14:N:-19:DG:C8	2.46	0.51
1:A:989:ASN:O	1:A:993:ILE:HG13	2.11	0.51
14:N:-16:DT:H2''	14:N:-15:DC:C6	2.45	0.51
19:T:30:DA:H4'	19:T:31:DG:OP1	2.10	0.51
7:G:84:VAL:HG23	7:G:84:VAL:O	2.11	0.51
13:M:973:VAL:N	13:M:1036:LYS:O	2.44	0.51
1:A:567:LEU:HD23	1:A:570:TRP:HB2	1.91	0.51
2:B:595:ASP:OD1	2:B:596:ILE:N	2.38	0.51
16:P:48:C:O2	19:T:-47:DG:N2	2.43	0.51
13:M:717:LEU:O	13:M:722:TYR:N	2.36	0.51
1:A:1414:ILE:O	1:A:1414:ILE:HG22	2.10	0.51
19:T:-55:DC:C2'	19:T:-55:DC:O2	2.58	0.51
1:A:1044:HIS:O	1:A:1048:THR:HG23	2.12	0.50
2:B:257:VAL:HB	2:B:266:GLU:OE1	2.11	0.50
2:B:758:LEU:HD11	10:J:47:ARG:HB2	1.93	0.50
14:N:98:DT:H2''	14:N:99:DA:N7	2.26	0.50
19:T:20:DA:H2''	19:T:21:DC:C5	2.46	0.50
1:A:600:ILE:HG23	1:A:655:ILE:HG22	1.93	0.50
1:A:1311:LEU:O	1:A:1313:GLN:NE2	2.45	0.50
2:B:818:GLU:OE1	2:B:828:VAL:HA	2.11	0.50
14:N:84:DC:H2''	14:N:85:DG:C8	2.46	0.50
1:A:465:HIS:CE1	1:A:467:MET:HB2	2.47	0.50
1:A:902:GLU:O	1:A:978:VAL:HA	2.12	0.50
1:A:930:LEU:HB3	1:A:939:VAL:HG12	1.93	0.50
3:C:45:ILE:HG22	3:C:165:ALA:HB1	1.93	0.50
3:C:162:ARG:NH1	3:C:164:TYR:OH	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:728:MET:HA	2:B:731:GLN:OE1	2.12	0.50
7:G:86:ASP:OD1	7:G:86:ASP:N	2.40	0.50
14:N:75:DG:C2	19:T:-74:DG:C2	3.00	0.50
14:N:79:DA:H2''	14:N:80:DC:C6	2.47	0.50
24:Z:629:LEU:HB2	24:Z:634:GLY:HA2	1.94	0.50
13:M:781:VAL:O	13:M:799:VAL:N	2.43	0.50
17:Q:291:LEU:O	17:Q:295:ALA:N	2.42	0.50
19:T:13:DC:H2''	19:T:14:DA:C8	2.47	0.50
1:A:1366:PHE:HA	1:A:1374:VAL:CG2	2.42	0.50
3:C:263:LEU:HD13	11:K:19:ILE:HD13	1.94	0.49
21:V:88:ASN:O	21:V:90:ASP:N	2.45	0.49
14:N:102:DG:N2	19:T:-101:DT:O2	2.45	0.49
19:T:-9:DA:H1'	19:T:-8:DA:C8	2.47	0.49
24:Z:626:CYS:CB	24:Z:629:LEU:HD12	2.41	0.49
2:B:786:THR:O	2:B:786:THR:HG22	2.13	0.49
1:A:401:ARG:O	1:A:405:LEU:HD13	2.12	0.49
5:E:54:ARG:NH1	5:E:56:THR:OG1	2.45	0.49
14:N:35:DT:H1'	14:N:36:DG:N7	2.26	0.49
24:Z:602:VAL:HG22	24:Z:643:LEU:CD2	2.42	0.49
1:A:406:VAL:HG13	1:A:429:LEU:HD11	1.95	0.49
1:A:576:GLN:O	1:A:590:GLN:NE2	2.45	0.49
1:A:1381:GLU:O	1:A:1385:VAL:HG13	2.12	0.49
2:B:854:ILE:HG22	2:B:921:ILE:HD13	1.93	0.49
7:G:52:ASP:N	7:G:71:LYS:O	2.44	0.49
19:T:-94:DC:H1'	19:T:-93:DC:C6	2.48	0.49
19:T:-53:DG:C6	19:T:-52:DC:N4	2.81	0.49
19:T:15:DG:H2''	19:T:16:DA:C8	2.47	0.49
1:A:30:GLU:HA	1:A:33:ARG:HE	1.77	0.49
2:B:207:VAL:HG11	2:B:375:ALA:CB	2.43	0.49
2:B:395:LEU:HD11	2:B:532:ILE:HB	1.93	0.49
2:B:867:ILE:HB	2:B:894:THR:HG22	1.95	0.49
14:N:98:DT:H2''	14:N:99:DA:C8	2.48	0.49
2:B:553:LEU:HA	2:B:556:ILE:HD12	1.94	0.49
1:A:140:ARG:NH2	1:A:234:PHE:O	2.44	0.49
1:A:1372:GLU:OE2	5:E:195:ARG:NH1	2.36	0.49
3:C:205:LYS:NZ	3:C:212:ASP:O	2.46	0.49
14:N:28:DG:C2	19:T:-27:DA:C2	3.01	0.49
24:Z:603:ILE:HG23	24:Z:604:ASP:N	2.27	0.49
1:A:868:MET:HG2	1:A:1404:THR:HG21	1.94	0.49
2:B:421:LYS:HD3	2:B:425:ARG:HE	1.78	0.49
3:C:150:ILE:O	3:C:151:VAL:HG13	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:89:DA:H1'	14:N:90:DA:N7	2.27	0.49
7:G:3:TYR:N	7:G:76:VAL:O	2.46	0.48
19:T:-84:DG:H2''	19:T:-83:DC:C6	2.48	0.48
2:B:607:ILE:HG21	9:I:72:VAL:HA	1.95	0.48
14:N:12:DT:C2'	14:N:13:DT:H71	2.42	0.48
19:T:22:DC:H2''	19:T:23:DA:C8	2.49	0.48
1:A:1318:LYS:HD2	15:O:294:CYS:C	2.33	0.48
2:B:501:LEU:HD12	2:B:505:LEU:HD12	1.95	0.48
1:A:1054:MET:SD	1:A:1060:LEU:HD12	2.53	0.48
14:N:-33:DG:H2'	14:N:-32:DT:H72	1.96	0.48
14:N:21:DC:H1'	14:N:22:DG:C8	2.48	0.48
19:T:-98:DA:H1'	19:T:-97:DG:C8	2.47	0.48
24:Z:479:LYS:NZ	24:Z:521:CYS:O	2.25	0.48
2:B:446:TYR:CE1	2:B:450:THR:HG21	2.48	0.48
1:A:18:ILE:HD11	2:B:1149:VAL:HG21	1.95	0.48
14:N:12:DT:H2''	14:N:13:DT:H71	1.96	0.48
20:U:450:LEU:N	20:U:457:PHE:O	2.47	0.48
1:A:370:ASP:OD2	11:K:65:HIS:NE2	2.36	0.48
2:B:565:THR:HG22	2:B:577:HIS:O	2.13	0.48
14:N:4:DG:C2	19:T:-3:DG:C2	3.02	0.48
1:A:576:GLN:HA	8:H:75:TYR:HB2	1.95	0.48
1:A:286:ILE:HD12	1:A:313:HIS:CD2	2.48	0.48
1:A:1314:THR:C	15:O:295:GLY:C	2.72	0.48
1:A:1330:ALA:CB	15:O:294:CYS:CA	2.88	0.48
14:N:-8:DG:H2'	14:N:-7:DT:H71	1.96	0.48
24:Z:504:SER:OG	24:Z:507:THR:O	2.28	0.48
2:B:423:ILE:HD13	2:B:429:PHE:HD1	1.79	0.48
19:T:-68:DC:H2'	19:T:-67:DC:C6	2.49	0.48
1:A:1093:GLN:HE22	2:B:1093:CYS:HA	1.78	0.47
8:H:128:ASP:N	8:H:128:ASP:OD1	2.44	0.47
19:T:-70:DT:H1'	19:T:-69:DC:C6	2.48	0.47
1:A:421:ARG:HE	1:A:427:ILE:HD11	1.79	0.47
1:A:1314:THR:C	15:O:295:GLY:O	2.53	0.47
2:B:491:ARG:H	2:B:491:ARG:HD2	1.79	0.47
2:B:992:ASN:O	10:J:46:ARG:NH1	2.47	0.47
11:K:80:ASP:OD1	11:K:80:ASP:N	2.47	0.47
14:N:38:DG:H2''	14:N:39:DT:C7	2.44	0.47
1:A:1322:ILE:HD12	1:A:1322:ILE:N	2.28	0.47
2:B:311:ILE:HG23	2:B:316:VAL:HG13	1.96	0.47
19:T:-121:DC:H2''	19:T:-120:DT:C6	2.49	0.47
1:A:793:VAL:HG23	1:A:793:VAL:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:17:TYR:O	12:L:26:ASN:N	2.40	0.47
13:M:1176:HIS:C	13:M:1226:ILE:N	2.68	0.47
14:N:-30:DT:C2'	14:N:-29:DT:H71	2.44	0.47
14:N:33:DC:H1'	14:N:34:DT:C5	2.49	0.47
1:A:18:ILE:HD12	2:B:1171:MET:HB3	1.96	0.47
1:A:364:ARG:NH1	1:A:502:ASN:OD1	2.47	0.47
2:B:818:GLU:HB2	2:B:916:TYR:HB3	1.97	0.47
14:N:-22:DG:O3'	14:N:-21:DG:C8	2.67	0.47
14:N:63:DG:N2	19:T:-62:DG:N2	2.62	0.47
1:A:1130:ILE:O	1:A:1130:ILE:CD1	2.57	0.47
14:N:15:DC:H2'	14:N:16:DT:C7	2.45	0.47
5:E:76:PHE:CE2	5:E:105:VAL:HG11	2.50	0.47
14:N:-26:DG:C5	14:N:-25:DT:C4	3.01	0.47
14:N:29:DG:C2'	14:N:30:DT:H71	2.45	0.47
19:T:-101:DT:H2''	19:T:-100:DC:C6	2.50	0.47
19:T:10:DA:H2''	19:T:11:DC:C5	2.49	0.47
1:A:376:ASP:HB3	1:A:522:PRO:HD3	1.97	0.47
3:C:212:ASP:OD1	3:C:212:ASP:N	2.46	0.47
19:T:-62:DG:C2	19:T:-61:DA:C2	3.02	0.47
4:D:114:LEU:HD21	7:G:167:TYR:HB2	1.97	0.47
14:N:72:DA:H1'	14:N:73:DG:C5	2.50	0.47
1:A:222:HIS:ND1	1:A:249:ILE:HD11	2.30	0.47
2:B:765:GLU:OE1	2:B:770:ARG:NE	2.40	0.47
14:N:-4:DC:H2'	14:N:-3:DC:C6	2.49	0.47
1:A:31:LEU:O	1:A:31:LEU:HD23	2.15	0.46
2:B:220:GLU:OE2	2:B:222:ARG:NE	2.36	0.46
9:I:12:VAL:HG22	9:I:50:ASN:HD22	1.80	0.46
14:N:114:DC:H2'	14:N:115:DA:C8	2.49	0.46
1:A:527:THR:HG22	1:A:532:ARG:O	2.15	0.46
1:A:1374:VAL:HG11	1:A:1411:LEU:HD21	1.97	0.46
24:Z:478:VAL:HB	24:Z:518:LEU:HD21	1.97	0.46
24:Z:597:LYS:N	24:Z:614:ILE:O	2.47	0.46
17:Q:663:PHE:O	17:Q:667:ARG:N	2.42	0.46
14:N:-1:DT:H2''	14:N:0:DT:H71	1.96	0.46
14:N:78:DT:O3'	14:N:79:DA:C8	2.69	0.46
14:N:111:DG:C2	19:T:-110:DG:N2	2.84	0.46
24:Z:426:VAL:HG13	24:Z:440:ILE:HD11	1.97	0.46
1:A:540:ASP:C	1:A:540:ASP:OD1	2.54	0.46
1:A:749:ARG:NH1	1:A:750:ASP:OD1	2.48	0.46
1:A:963:ARG:O	1:A:967:ARG:HG3	2.16	0.46
2:B:706:VAL:HG13	2:B:767:LEU:HD22	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:755:GLN:HB3	10:J:51:ALA:HB1	1.97	0.46
14:N:36:DG:C6	14:N:37:DG:C6	3.03	0.46
19:T:-63:DC:H2''	19:T:-62:DG:N7	2.31	0.46
1:A:218:PRO:O	1:A:221:VAL:HG22	2.15	0.46
1:A:464:LEU:HD22	1:A:1100:THR:HG21	1.97	0.46
5:E:105:VAL:HG13	5:E:135:LEU:HD12	1.97	0.46
14:N:33:DC:H2''	14:N:34:DT:C7	2.46	0.46
14:N:65:DA:H2'	14:N:66:DG:C8	2.50	0.46
1:A:191:ILE:HA	1:A:199:TYR:O	2.15	0.46
1:A:471:GLY:O	1:A:521:VAL:HG23	2.16	0.46
1:A:1471:PHE:CZ	6:F:61:GLU:HA	2.51	0.46
2:B:606:ASP:O	2:B:609:GLU:O	2.34	0.46
4:D:80:ILE:HD12	4:D:80:ILE:N	2.31	0.46
14:N:-6:DG:C2	19:T:7:DA:C2	3.04	0.46
7:G:109:SER:HB3	24:Z:493:VAL:HG21	1.97	0.46
10:J:41:LYS:HA	10:J:41:LYS:HE2	1.97	0.46
14:N:-12:DG:H1'	14:N:-11:DG:N7	2.31	0.46
14:N:41:DT:C6	14:N:41:DT:C3'	2.99	0.46
1:A:1321:ILE:O	1:A:1321:ILE:HG23	2.15	0.46
14:N:77:DG:N2	19:T:-76:DG:C2	2.84	0.46
14:N:114:DC:C2	19:T:-113:DG:N2	2.84	0.46
1:A:687:ILE:HD11	1:A:766:PHE:CE1	2.51	0.45
2:B:61:ASP:OD1	2:B:61:ASP:C	2.54	0.45
5:E:149:VAL:O	5:E:192:LYS:N	2.47	0.45
7:G:93:ASN:O	7:G:128:TYR:OH	2.26	0.45
12:L:16:ILE:HD11	12:L:25:GLU:HB3	1.97	0.45
14:N:-28:DG:H2''	14:N:-27:DT:C7	2.43	0.45
14:N:104:DT:H2''	14:N:105:DG:H8	1.81	0.45
19:T:-58:DA:H1'	19:T:-57:DA:C8	2.51	0.45
1:A:189:PRO:HB3	1:A:202:TRP:CE2	2.51	0.45
1:A:793:VAL:CG2	1:A:799:PRO:HD3	2.46	0.45
1:A:854:THR:OG1	1:A:855:ALA:N	2.49	0.45
2:B:853:LEU:HD23	2:B:867:ILE:HG23	1.98	0.45
19:T:-79:DT:H2''	19:T:-78:DA:N7	2.31	0.45
19:T:-62:DG:H1'	19:T:-61:DA:C8	2.52	0.45
19:T:-53:DG:O6	19:T:-52:DC:N4	2.49	0.45
7:G:160:ILE:HB	24:Z:491:LEU:HD13	1.98	0.45
14:N:61:DT:O3'	14:N:62:DC:C6	2.69	0.45
19:T:-101:DT:H2''	19:T:-100:DC:C5	2.51	0.45
24:Z:478:VAL:HG23	24:Z:478:VAL:O	2.16	0.45
1:A:222:HIS:HB2	1:A:249:ILE:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:142:THR:O	2:B:142:THR:HG23	2.17	0.45
2:B:387:HIS:NE2	2:B:671:GLU:OE2	2.49	0.45
5:E:52:ARG:N	5:E:53:PRO:HD3	2.32	0.45
5:E:185:ILE:HD12	5:E:209:VAL:CG2	2.46	0.45
14:N:-30:DT:H2'	14:N:-29:DT:H71	1.99	0.45
14:N:1:DT:H2''	14:N:2:DT:C6	2.51	0.45
14:N:20:DT:H2''	14:N:21:DC:C5	2.50	0.45
14:N:26:DC:H2'	14:N:27:DT:H71	1.96	0.45
1:A:566:PHE:HB3	1:A:674:THR:HG22	1.99	0.45
1:A:1087:VAL:HG23	1:A:1400:LEU:CD2	2.47	0.45
14:N:-9:DG:H1'	14:N:-8:DG:C8	2.52	0.45
19:T:-96:DC:H2'	19:T:-95:DA:C8	2.51	0.45
19:T:-10:DA:H2''	19:T:-9:DA:C8	2.52	0.45
24:Z:536:TRP:NE1	24:Z:551:VAL:O	2.48	0.45
1:A:404:GLU:O	1:A:408:ARG:HG3	2.16	0.45
1:A:467:MET:HG2	1:A:534:VAL:HG21	1.99	0.45
19:T:18:DA:H2'	19:T:19:DC:C5	2.51	0.45
1:A:987:ILE:O	1:A:991:GLN:HG3	2.17	0.45
2:B:666:ASP:O	2:B:669:GLU:N	2.50	0.45
2:B:873:LEU:HD12	2:B:888:THR:N	2.32	0.45
14:N:72:DA:C2	19:T:-71:DG:C2	3.05	0.45
1:A:515:ILE:HD11	2:B:1102:PHE:CD1	2.52	0.45
2:B:1105:GLU:HG3	2:B:1106:ARG:N	2.32	0.45
14:N:100:DG:H1'	14:N:101:DA:N7	2.32	0.45
14:N:109:DA:H1'	14:N:110:DC:O4'	2.17	0.45
2:B:743:ARG:NH1	2:B:745:ASP:OD1	2.50	0.45
14:N:33:DC:C2'	14:N:34:DT:H71	2.46	0.45
14:N:93:DG:N1	19:T:-92:DG:N1	2.64	0.45
14:N:119:DG:O3'	14:N:120:DA:C8	2.70	0.45
1:A:293:ASN:O	1:A:298:ALA:N	2.44	0.44
1:A:419:ILE:CD1	1:A:440:LEU:HB3	2.47	0.44
5:E:93:ARG:HA	5:E:96:GLU:OE1	2.17	0.44
14:N:13:DT:H5'	14:N:13:DT:C6	2.52	0.44
14:N:83:DG:C2	19:T:-82:DA:C2	3.06	0.44
2:B:84:TYR:HA	2:B:132:VAL:HA	1.98	0.44
2:B:669:GLU:O	2:B:672:THR:HG22	2.18	0.44
2:B:905:ASP:OD2	2:B:922:ARG:NH2	2.47	0.44
2:B:928:ILE:HD12	2:B:928:ILE:H	1.83	0.44
19:T:23:DA:C2'	19:T:24:DA:C8	3.01	0.44
1:A:832:THR:HG22	1:A:833:PRO:CD	2.45	0.44
1:A:1052:ARG:HE	1:A:1056:GLU:CD	2.20	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:203:ASN:N	2:B:222:ARG:O	2.35	0.44
2:B:553:LEU:HD12	2:B:556:ILE:HD12	1.98	0.44
19:T:-112:DT:H2''	19:T:-111:DC:C6	2.53	0.44
14:N:105:DG:C8	14:N:106:DT:H72	2.52	0.44
1:A:64:VAL:HG11	1:A:78:MET:HA	1.99	0.44
1:A:583:ARG:HG3	1:A:584:PRO:HD2	1.99	0.44
1:A:921:ARG:HD2	1:A:956:PHE:CG	2.53	0.44
5:E:83:GLY:HA2	5:E:114:ALA:HB2	1.99	0.44
14:N:-33:DG:H2'	14:N:-32:DT:C7	2.48	0.44
14:N:29:DG:N2	19:T:-28:DC:C2	2.86	0.44
14:N:90:DA:C6	14:N:91:DG:C6	3.05	0.44
19:T:-100:DC:H1'	19:T:-99:DT:C4	2.53	0.44
1:A:203:LYS:NZ	19:T:-67:DC:OP2	2.32	0.44
5:E:11:TRP:HA	5:E:40:PHE:CE2	2.53	0.44
5:E:26:TYR:HA	5:E:64:HIS:HA	2.00	0.44
14:N:-32:DT:O2	19:T:32:DA:C2	2.71	0.44
19:T:-5:DA:H2''	19:T:-4:DC:C6	2.53	0.44
1:A:289:GLN:O	1:A:292:ARG:HG2	2.18	0.44
2:B:166:LEU:HG	2:B:170:ASP:HB2	2.00	0.44
2:B:818:GLU:OE2	2:B:829:PHE:CE1	2.70	0.44
6:F:120:VAL:O	6:F:120:VAL:CG1	2.64	0.44
14:N:-18:DT:H2''	14:N:-17:DG:H8	1.82	0.44
19:T:-80:DG:H2''	19:T:-79:DT:C6	2.53	0.44
19:T:-32:DA:H2''	19:T:-31:DC:C6	2.52	0.44
19:T:21:DC:H2''	19:T:22:DC:C6	2.53	0.44
1:A:385:ALA:HB2	1:A:476:ILE:HD12	2.00	0.44
14:N:35:DT:C2	14:N:36:DG:O6	2.70	0.44
1:A:1413:ALA:O	1:A:1418:GLY:HA3	2.18	0.44
9:I:69:ILE:HD13	9:I:71:ASP:HB2	1.99	0.44
14:N:-26:DG:C2	19:T:27:DA:C2	3.05	0.44
14:N:29:DG:H2''	14:N:30:DT:H71	2.00	0.44
19:T:-25:DG:H1'	19:T:-24:DC:C6	2.53	0.44
1:A:862:ARG:HG3	1:A:863:ARG:N	2.33	0.43
24:Z:476:ASP:O	24:Z:478:VAL:HG13	2.18	0.43
1:A:1474:LEU:HD12	6:F:105:ILE:HD11	2.00	0.43
5:E:173:ILE:O	5:E:209:VAL:HA	2.18	0.43
14:N:-13:DG:H2''	14:N:-12:DG:N7	2.33	0.43
1:A:927:GLU:HG2	1:A:931:ARG:NE	2.33	0.43
2:B:193:VAL:HG11	2:B:470:LEU:HD13	2.01	0.43
2:B:499:ARG:NH1	2:B:518:HIS:O	2.46	0.43
2:B:711:ILE:HG12	2:B:725:GLN:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:94:LYS:NZ	7:G:3:TYR:OH	2.47	0.43
14:N:10:DT:H2'	14:N:11:DT:C7	2.48	0.43
14:N:57:DT:C6	14:N:57:DT:P	3.12	0.43
19:T:1:DA:H2''	19:T:2:DC:C6	2.53	0.43
2:B:331:THR:HG23	2:B:334:LYS:H	1.84	0.43
17:Q:723:LEU:O	17:Q:725:ARG:N	2.51	0.43
19:T:25:DA:H2''	19:T:26:DC:C6	2.53	0.43
1:A:88:ILE:HD12	1:A:88:ILE:N	2.34	0.43
1:A:991:GLN:HA	1:A:996:ILE:CG1	2.49	0.43
1:A:1085:GLU:O	1:A:1087:VAL:HG13	2.17	0.43
2:B:741:HIS:CE1	2:B:742:VAL:HG23	2.53	0.43
2:B:854:ILE:O	2:B:907:VAL:HG21	2.19	0.43
14:N:-15:DC:H2'	14:N:-14:DT:C7	2.44	0.43
14:N:8:DT:H2''	14:N:9:DT:C5	2.53	0.43
19:T:-113:DG:H2'	19:T:-112:DT:C7	2.48	0.43
1:A:855:ALA:HA	19:T:-54:DC:O4'	2.19	0.43
1:A:1182:GLN:C	1:A:1182:GLN:OE1	2.57	0.43
2:B:423:ILE:CG2	2:B:424:ASP:N	2.81	0.43
2:B:698:ILE:HG23	2:B:699:HIS:H	1.84	0.43
2:B:859:ARG:NH1	2:B:901:THR:HG23	2.33	0.43
5:E:66:ASP:C	5:E:66:ASP:OD1	2.56	0.43
14:N:7:DG:H8	14:N:7:DG:OP2	2.01	0.43
14:N:34:DT:C5	14:N:35:DT:C4	3.06	0.43
1:A:255:VAL:HG23	1:A:280:LEU:HD13	1.99	0.43
2:B:652:SER:N	2:B:655:ASP:OD2	2.50	0.43
14:N:26:DC:H2'	14:N:27:DT:C7	2.49	0.43
14:N:40:DG:N2	19:T:-39:DA:C4	2.86	0.43
19:T:-81:DC:H2''	19:T:-80:DG:C8	2.53	0.43
24:Z:550:ILE:HD12	24:Z:559:GLN:O	2.19	0.43
1:A:260:VAL:HG12	1:A:260:VAL:O	2.18	0.43
1:A:849:ASP:OD1	1:A:849:ASP:N	2.52	0.43
1:A:1374:VAL:CG1	1:A:1411:LEU:HD21	2.49	0.43
2:B:497:LYS:HG2	2:B:498:PRO:HD3	2.01	0.43
14:N:22:DG:H2'	14:N:23:DT:C7	2.47	0.43
14:N:111:DG:H1'	14:N:112:DA:C8	2.54	0.43
19:T:-80:DG:OP2	19:T:-80:DG:H2'	2.18	0.43
19:T:6:DC:H2'	19:T:7:DA:C8	2.54	0.43
24:Z:529:ASP:HB3	24:Z:553:LEU:HD23	1.99	0.43
1:A:991:GLN:HA	1:A:996:ILE:HG12	2.01	0.43
2:B:520:VAL:HG13	2:B:520:VAL:O	2.18	0.43
9:I:39:CYS:SG	9:I:40:ARG:N	2.92	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:T:-66:DC:H2'	19:T:-65:DT:C6	2.54	0.43
1:A:1301:ILE:HG13	1:A:1304:ILE:HG12	2.01	0.43
2:B:491:ARG:H	2:B:491:ARG:CD	2.32	0.43
3:C:263:LEU:HD22	11:K:87:PHE:CD1	2.54	0.43
5:E:89:VAL:O	5:E:93:ARG:HD2	2.19	0.43
7:G:148:VAL:HG22	7:G:160:ILE:HG23	2.01	0.43
8:H:20:LYS:HE2	8:H:23:ASP:HA	1.99	0.43
11:K:57:LEU:N	11:K:76:GLN:O	2.52	0.43
14:N:85:DG:C8	14:N:86:DT:H72	2.54	0.43
19:T:-75:DC:H2'	19:T:-74:DG:C8	2.53	0.43
19:T:14:DA:H8	19:T:14:DA:OP2	2.01	0.43
1:A:427:ILE:N	1:A:427:ILE:HD12	2.34	0.42
1:A:580:LEU:O	1:A:582:PRO:HD2	2.19	0.42
2:B:545:LEU:O	2:B:550:MET:CB	2.67	0.42
3:C:26:THR:HG22	3:C:27:ASP:N	2.26	0.42
14:N:11:DT:H2''	14:N:12:DT:C6	2.54	0.42
14:N:91:DG:H2''	14:N:92:DC:C6	2.54	0.42
1:A:413:TYR:CD1	1:A:413:TYR:C	2.91	0.42
2:B:786:THR:HG21	2:B:949:TYR:OH	2.19	0.42
3:C:40:ALA:O	3:C:171:LYS:N	2.52	0.42
11:K:93:ASP:OD1	11:K:93:ASP:C	2.56	0.42
14:N:1:DT:H2'	14:N:2:DT:H71	2.00	0.42
14:N:99:DA:H2''	14:N:100:DG:N7	2.34	0.42
19:T:-73:DC:H2''	19:T:-72:DT:C6	2.55	0.42
19:T:-8:DA:C5	19:T:-7:DC:C4	3.08	0.42
24:Z:775:TPO:O2P	24:Z:775:TPO:N	2.52	0.42
1:A:1171:ALA:O	9:I:58:ILE:N	2.53	0.42
2:B:284:ILE:HG22	2:B:285:LEU:H	1.84	0.42
2:B:291:ASP:OD1	2:B:291:ASP:N	2.52	0.42
19:T:-108:DA:C5	19:T:-107:DG:C6	3.07	0.42
19:T:-28:DC:H2'	19:T:-27:DA:C8	2.53	0.42
19:T:4:DG:C4	19:T:5:DC:C5	3.08	0.42
2:B:622:CYS:HB3	2:B:666:ASP:HB3	2.02	0.42
3:C:152:LYS:HB2	10:J:60:LEU:HD11	2.02	0.42
19:T:9:DC:OP2	19:T:9:DC:H6	2.02	0.42
2:B:545:LEU:O	2:B:550:MET:HB3	2.20	0.42
14:N:91:DG:N2	19:T:-90:DT:O2	2.52	0.42
19:T:14:DA:C6	19:T:15:DG:C6	3.07	0.42
1:A:996:ILE:HD13	1:A:996:ILE:HA	1.94	0.42
11:K:53:ASP:HB3	11:K:56:VAL:HG23	2.00	0.42
19:T:-53:DG:C6	19:T:-52:DC:C4	3.08	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:T:-48:DG:H4'	19:T:-48:DG:OP1	2.19	0.42
24:Z:538:GLU:OE2	24:Z:577:ARG:NE	2.48	0.42
1:A:420:ILE:HD11	1:A:447:GLU:OE2	2.20	0.42
1:A:1073:GLU:HG3	1:A:1074:SER:N	2.35	0.42
1:A:1442:ALA:HA	1:A:1447:GLU:HG3	2.01	0.42
3:C:89:THR:HG23	3:C:89:THR:O	2.19	0.42
5:E:93:ARG:HD2	5:E:93:ARG:N	2.34	0.42
14:N:-31:DC:H1'	14:N:-30:DT:C5	2.54	0.42
14:N:9:DT:H1'	14:N:10:DT:C6	2.55	0.42
19:T:-43:DA:H3'	19:T:-42:DA:O4'	2.20	0.42
19:T:23:DA:H2'	19:T:24:DA:C8	2.53	0.42
1:A:413:TYR:HB3	1:A:414:PRO:HD3	2.02	0.42
1:A:1286:ARG:O	1:A:1289:GLU:HG3	2.19	0.42
1:A:1322:ILE:H	1:A:1322:ILE:CD1	2.32	0.42
16:P:44:U:H2'	16:P:45:C:C6	2.54	0.42
1:A:1184:THR:O	1:A:1187:ALA:N	2.48	0.42
7:G:83:GLU:O	7:G:147:ILE:HD12	2.19	0.42
14:N:105:DG:H2'	14:N:106:DT:H72	2.00	0.42
19:T:8:DC:H2''	19:T:9:DC:C5	2.54	0.42
24:Z:603:ILE:HG23	24:Z:604:ASP:H	1.85	0.42
1:A:29:ASP:O	1:A:33:ARG:HG2	2.19	0.41
1:A:589:LYS:HZ3	1:A:625:ASP:CG	2.22	0.41
3:C:64:ILE:CD1	3:C:151:VAL:HG11	2.50	0.41
8:H:27:ARG:HD3	8:H:42:ASP:OD1	2.20	0.41
14:N:-11:DG:H2'	14:N:-10:DT:H71	2.02	0.41
14:N:57:DT:H2'	14:N:58:DT:H71	2.01	0.41
19:T:-73:DC:H2''	19:T:-72:DT:C2	2.54	0.41
24:Z:470:LYS:HB3	24:Z:472:PHE:CE2	2.54	0.41
1:A:120:ASP:OD2	1:A:122:ASN:ND2	2.50	0.41
1:A:379:GLY:HA2	1:A:475:ARG:O	2.20	0.41
1:A:513:ALA:O	1:A:517:GLU:HG2	2.20	0.41
1:A:873:VAL:O	1:A:1084:GLY:N	2.50	0.41
2:B:528:LEU:HD21	2:B:767:LEU:HD21	2.02	0.41
2:B:956:PHE:CZ	2:B:1029:TYR:HB2	2.56	0.41
6:F:57:MET:HB2	6:F:123:LEU:HD13	2.01	0.41
11:K:21:ILE:HD12	11:K:21:ILE:H	1.85	0.41
14:N:-3:DC:H2''	14:N:-2:DG:C8	2.55	0.41
19:T:25:DA:H1'	19:T:26:DC:C6	2.55	0.41
1:A:299:ALA:HB3	1:A:302:VAL:HG12	2.03	0.41
1:A:1262:MET:SD	1:A:1262:MET:N	2.93	0.41
1:A:1484:MET:SD	1:A:1484:MET:N	2.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:63:ALA:HB1	5:E:68:PRO:HA	2.02	0.41
5:E:83:GLY:O	5:E:87:ILE:HG23	2.19	0.41
16:P:43:U:O2'	16:P:44:U:OP2	2.23	0.41
24:Z:489:THR:HG22	24:Z:490:GLY:N	2.34	0.41
24:Z:727:ALA:HA	24:Z:732:ALA:HA	2.02	0.41
1:A:109:CYS:HA	1:A:148:CYS:SG	2.61	0.41
1:A:1030:SER:HB2	5:E:162:ARG:HE	1.86	0.41
1:A:1036:ASN:OD1	5:E:202:ARG:NH1	2.41	0.41
2:B:193:VAL:CG1	2:B:470:LEU:HD13	2.51	0.41
2:B:813:SER:HA	2:B:922:ARG:HA	2.02	0.41
5:E:100:THR:HB	5:E:125:TYR:HA	2.02	0.41
14:N:-19:DG:C2'	14:N:-18:DT:C6	3.03	0.41
14:N:17:DG:C2	19:T:-16:DA:C2	3.08	0.41
19:T:-97:DG:C4	19:T:-96:DC:C5	3.08	0.41
1:A:286:ILE:CD1	1:A:313:HIS:CD2	3.04	0.41
1:A:1321:ILE:O	1:A:1328:PHE:O	2.38	0.41
2:B:1060:HIS:NE2	2:B:1082:GLY:O	2.50	0.41
5:E:7:THR:OG1	5:E:46:ASP:OD1	2.39	0.41
5:E:47:LYS:HB3	5:E:51:GLY:HA3	2.02	0.41
9:I:69:ILE:HD12	9:I:69:ILE:O	2.20	0.41
10:J:44:CYS:O	10:J:47:ARG:CD	2.68	0.41
11:K:42:LEU:O	11:K:46:ILE:HG13	2.20	0.41
19:T:-25:DG:H2''	19:T:-24:DC:C5	2.54	0.41
24:Z:603:ILE:CG2	24:Z:604:ASP:H	2.33	0.41
1:A:110:VAL:HG11	1:A:228:ILE:HD11	2.01	0.41
2:B:357:CYS:SG	2:B:361:LYS:HE2	2.60	0.41
2:B:581:GLU:O	2:B:585:ASN:OD1	2.38	0.41
14:N:36:DG:C5	14:N:37:DG:C5	3.08	0.41
14:N:71:DC:H4'	14:N:72:DA:OP1	2.21	0.41
19:T:24:DA:H2''	19:T:25:DA:H5'	2.02	0.41
1:A:832:THR:CG2	1:A:833:PRO:HD2	2.48	0.41
1:A:1457:ASN:O	1:A:1462:GLN:N	2.53	0.41
2:B:756:LYS:HD2	2:B:996:ILE:HD11	2.03	0.41
2:B:818:GLU:OE2	2:B:829:PHE:CD1	2.74	0.41
5:E:124:LYS:HD3	5:E:125:TYR:CE2	2.56	0.41
14:N:31:DG:C2	14:N:32:DT:C2	3.08	0.41
2:B:407:MET:O	2:B:410:ASN:HB2	2.21	0.41
8:H:40:ILE:O	8:H:123:MET:HA	2.21	0.41
9:I:91:HIS:CD2	9:I:116:ALA:HB2	2.55	0.41
14:N:11:DT:H2'	14:N:12:DT:C7	2.49	0.41
24:Z:603:ILE:CG2	24:Z:604:ASP:N	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:PRO:HB2	1:A:200:ALA:HB1	2.03	0.41
1:A:350:VAL:HG23	1:A:351:ARG:N	2.36	0.41
1:A:527:THR:HB	1:A:534:VAL:HG13	2.03	0.41
1:A:600:ILE:HG12	1:A:660:MET:HE1	2.02	0.41
1:A:604:ARG:NH2	1:A:643:LYS:O	2.52	0.41
1:A:927:GLU:HG3	1:A:943:LEU:HD11	2.03	0.41
1:A:1175:ILE:HD13	9:I:54:TYR:HB3	2.03	0.41
1:A:1180:ASN:OD1	1:A:1182:GLN:HG3	2.21	0.41
1:A:1460:LEU:HD22	1:A:1460:LEU:N	2.35	0.41
2:B:185:PHE:O	2:B:191:GLU:HA	2.21	0.41
2:B:190:SER:HB3	2:B:192:LYS:HE2	2.03	0.41
2:B:190:SER:CB	2:B:192:LYS:HE2	2.51	0.41
2:B:425:ARG:CB	2:B:427:LYS:HG3	2.50	0.41
2:B:597:ILE:CG2	2:B:601:VAL:HB	2.51	0.41
2:B:749:HIS:CE1	2:B:810:PHE:CD1	3.09	0.41
2:B:781:ALA:O	2:B:966:ILE:HA	2.21	0.41
2:B:833:THR:HG22	2:B:835:GLU:OE1	2.21	0.41
2:B:1102:PHE:HA	2:B:1105:GLU:HG2	2.02	0.41
3:C:2:PRO:HB3	11:K:54:PRO:HD2	2.02	0.41
4:D:131:LEU:O	4:D:135:GLN:HG2	2.21	0.41
9:I:42:CYS:SG	9:I:44:TYR:HB2	2.61	0.41
9:I:64:GLU:HB2	9:I:111:TYR:CE2	2.55	0.41
9:I:86:CYS:SG	9:I:121:HIS:HB3	2.60	0.41
14:N:-21:DG:H2''	14:N:-20:DT:C6	2.55	0.41
14:N:-11:DG:H2''	14:N:-10:DT:C6	2.56	0.41
14:N:0:DT:H2'	14:N:1:DT:C6	2.56	0.41
14:N:13:DT:H2''	14:N:14:DT:C6	2.56	0.41
14:N:93:DG:C4	14:N:94:DG:C5	3.08	0.41
14:N:96:DG:N1	19:T:-95:DA:C6	2.89	0.41
14:N:105:DG:H8	14:N:105:DG:OP2	2.03	0.41
14:N:119:DG:N2	19:T:-118:DA:C2	2.89	0.41
19:T:-110:DG:H2''	19:T:-109:DT:C5	2.56	0.41
19:T:-78:DA:H2''	19:T:-77:DC:C6	2.56	0.41
19:T:-70:DT:H2''	19:T:-69:DC:C5	2.56	0.41
19:T:10:DA:H2''	19:T:11:DC:C6	2.55	0.41
24:Z:497:GLU:OE1	24:Z:497:GLU:N	2.49	0.41
1:A:419:ILE:HD11	1:A:440:LEU:HB3	2.01	0.41
1:A:467:MET:HG3	1:A:524:MET:HB3	2.03	0.41
1:A:1219:LYS:O	1:A:1223:ASP:OD2	2.39	0.41
2:B:237:VAL:O	2:B:372:LEU:HD22	2.20	0.41
2:B:266:GLU:O	2:B:266:GLU:CD	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:848:VAL:O	13:M:883:GLU:N	2.54	0.41
14:N:22:DG:N2	19:T:-21:DG:C2	2.89	0.41
14:N:33:DC:H1'	14:N:34:DT:C7	2.51	0.41
14:N:40:DG:N2	19:T:-39:DA:C5	2.89	0.41
19:T:-76:DG:C4	19:T:-75:DC:C5	3.09	0.41
24:Z:705:LEU:O	24:Z:705:LEU:HG	2.20	0.41
1:A:854:THR:HB	19:T:-54:DC:C4	2.56	0.40
1:A:1118:THR:O	1:A:1123:ARG:HB2	2.22	0.40
14:N:-29:DT:C4	14:N:-28:DG:O6	2.74	0.40
14:N:-26:DG:N1	19:T:27:DA:N1	2.68	0.40
14:N:-20:DT:H2''	14:N:-19:DG:N7	2.36	0.40
14:N:57:DT:P	14:N:57:DT:H72	2.61	0.40
19:T:-59:DA:C6	19:T:-58:DA:C6	3.08	0.40
19:T:-16:DA:C6	19:T:-15:DG:C6	3.09	0.40
1:A:609:HIS:HA	1:A:626:THR:HG21	2.02	0.40
1:A:777:SER:OG	1:A:779:ILE:HG22	2.21	0.40
5:E:92:GLN:O	5:E:96:GLU:OE1	2.40	0.40
19:T:-69:DC:H2'	19:T:-68:DC:C6	2.56	0.40
19:T:-7:DC:H1'	19:T:-6:DA:C8	2.57	0.40
19:T:24:DA:C6	19:T:25:DA:C6	3.09	0.40
20:U:469:ASN:O	20:U:489:LEU:N	2.53	0.40
24:Z:444:ASP:HB3	24:Z:448:ILE:HA	2.02	0.40
7:G:18:PHE:CD1	7:G:18:PHE:N	2.88	0.40
14:N:-18:DT:C2	14:N:-17:DG:N7	2.89	0.40
1:A:496:PHE:CD2	2:B:791:GLU:HB2	2.57	0.40
1:A:527:THR:HB	1:A:534:VAL:CG1	2.52	0.40
2:B:29:VAL:HG12	2:B:30:ILE:H	1.87	0.40
2:B:225:LEU:HA	2:B:350:HIS:HA	2.03	0.40
2:B:403:LEU:HD13	2:B:447:SER:OG	2.22	0.40
2:B:565:THR:HA	2:B:610:ARG:HB3	2.03	0.40
2:B:847:LYS:HG2	2:B:858:VAL:HG11	2.03	0.40
2:B:1038:THR:HA	3:C:195:THR:HA	2.04	0.40
10:J:53:VAL:O	10:J:53:VAL:CG1	2.69	0.40
14:N:-33:DG:H2'	14:N:-32:DT:C5	2.57	0.40
14:N:114:DC:H2'	14:N:115:DA:N7	2.36	0.40
1:A:953:GLU:O	1:A:957:GLU:HG3	2.21	0.40
7:G:109:SER:O	7:G:112:SER:OG	2.34	0.40
14:N:-17:DG:H2'	14:N:-16:DT:H72	2.03	0.40
14:N:85:DG:C2	19:T:-84:DG:C2	3.10	0.40
19:T:13:DC:H1'	19:T:14:DA:C8	2.56	0.40

There are no symmetry-related clashes.



## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1408/1984 (71%)	1297 (92%)	109 (8%)	2 (0%)	48	81
2	B	1107/1251 (88%)	1022 (92%)	85 (8%)	0	100	100
3	C	254/275 (92%)	241 (95%)	13 (5%)	0	100	100
4	D	124/184 (67%)	118 (95%)	6 (5%)	0	100	100
5	E	207/210 (99%)	199 (96%)	8 (4%)	0	100	100
6	F	76/127 (60%)	71 (93%)	5 (7%)	0	100	100
7	G	169/172 (98%)	160 (95%)	9 (5%)	0	100	100
8	H	147/150 (98%)	138 (94%)	8 (5%)	1 (1%)	19	54
9	I	114/125 (91%)	100 (88%)	14 (12%)	0	100	100
10	J	64/67 (96%)	60 (94%)	3 (5%)	1 (2%)	8	34
11	K	113/117 (97%)	106 (94%)	7 (6%)	0	100	100
12	L	45/58 (78%)	39 (87%)	6 (13%)	0	100	100
13	M	976/1729 (56%)	903 (92%)	72 (7%)	1 (0%)	48	81
15	O	157/304 (52%)	154 (98%)	3 (2%)	0	100	100
17	Q	888/1179 (75%)	832 (94%)	56 (6%)	0	100	100
18	R	240/713 (34%)	227 (95%)	13 (5%)	0	100	100
20	U	98/666 (15%)	87 (89%)	11 (11%)	0	100	100
21	V	236/531 (44%)	200 (85%)	34 (14%)	2 (1%)	16	51
22	W	298/305 (98%)	271 (91%)	27 (9%)	0	100	100
23	X	41/531 (8%)	38 (93%)	3 (7%)	0	100	100
24	Z	300/1087 (28%)	274 (91%)	25 (8%)	1 (0%)	37	70
25	a	95/136 (70%)	90 (95%)	5 (5%)	0	100	100
25	e	95/136 (70%)	92 (97%)	3 (3%)	0	100	100
26	b	81/103 (79%)	80 (99%)	1 (1%)	0	100	100
26	f	76/103 (74%)	72 (95%)	4 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	c	101/130 (78%)	97 (96%)	4 (4%)	0	100	100
27	g	103/130 (79%)	99 (96%)	4 (4%)	0	100	100
28	d	93/123 (76%)	88 (95%)	5 (5%)	0	100	100
28	h	91/123 (74%)	87 (96%)	4 (4%)	0	100	100
All	All	7797/12749 (61%)	7242 (93%)	547 (7%)	8 (0%)	50	81

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	582	PRO
13	M	1334	ASN
21	V	300	ASN
8	H	77	PRO
1	A	478	PRO
10	J	64	PRO
21	V	301	TYR
24	Z	452	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1245/1761 (71%)	1226 (98%)	19 (2%)	60	83
2	B	983/1084 (91%)	968 (98%)	15 (2%)	60	83
3	C	235/252 (93%)	231 (98%)	4 (2%)	56	81
4	D	109/160 (68%)	108 (99%)	1 (1%)	75	89
5	E	191/192 (100%)	188 (98%)	3 (2%)	58	82
6	F	68/111 (61%)	66 (97%)	2 (3%)	37	70
7	G	146/153 (95%)	143 (98%)	3 (2%)	48	77
8	H	130/131 (99%)	128 (98%)	2 (2%)	60	83
9	I	104/112 (93%)	102 (98%)	2 (2%)	52	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	J	55/56 (98%)	54 (98%)	1 (2%)	54	80
11	K	104/106 (98%)	103 (99%)	1 (1%)	73	88
12	L	44/55 (80%)	42 (96%)	2 (4%)	23	57
24	Z	257/939 (27%)	256 (100%)	1 (0%)	89	95
25	a	85/111 (77%)	85 (100%)	0	100	100
25	e	84/111 (76%)	83 (99%)	1 (1%)	67	86
26	b	68/79 (86%)	67 (98%)	1 (2%)	60	83
26	f	63/79 (80%)	63 (100%)	0	100	100
27	c	82/102 (80%)	82 (100%)	0	100	100
27	g	83/102 (81%)	83 (100%)	0	100	100
28	d	81/103 (79%)	79 (98%)	2 (2%)	42	73
28	h	79/103 (77%)	78 (99%)	1 (1%)	65	85
All	All	4296/5902 (73%)	4235 (99%)	61 (1%)	62	83

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	ASP
1	A	203	LYS
1	A	234	PHE
1	A	294	GLU
1	A	336	LEU
1	A	365	THR
1	A	380	VAL
1	A	483	ARG
1	A	582	PRO
1	A	723	ASN
1	A	931	ARG
1	A	952	LEU
1	A	1030	SER
1	A	1048	THR
1	A	1139	LEU
1	A	1182	GLN
1	A	1212	LEU
1	A	1375	ARG
1	A	1385	VAL
2	B	83	ARG
2	B	332	LYS

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Mol	Chain	Res	Type
2	B	388	TYR
2	B	424	ASP
2	B	453	TRP
2	B	491	ARG
2	B	550	MET
2	B	610	ARG
2	B	650	ASN
2	B	808	SER
2	B	841	ARG
2	B	995	GLU
2	B	1006	VAL
2	B	1150	ARG
2	B	1156	LYS
3	C	13	GLU
3	C	63	PHE
3	C	118	ARG
3	C	228	ARG
4	D	94	LYS
5	E	36	THR
5	E	73	PHE
5	E	141	GLU
6	F	90	LEU
6	F	123	LEU
7	G	44	PHE
7	G	86	ASP
7	G	132	ASP
8	H	38	ASP
8	H	95	LYS
9	I	67	GLN
9	I	100	HIS
10	J	47	ARG
11	K	1	MET
12	L	37	ARG
12	L	58	ARG
24	Z	624	LEU
26	b	92	ARG
28	d	31	LYS
28	d	39	TYR
25	e	39	HIS
28	h	83	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:



Mol	Chain	Res	Type
1	A	143	HIS
1	A	562	ASN
1	A	673	GLN
2	B	111	ASN
2	B	452	ASN
2	B	585	ASN
2	B	749	HIS
2	B	1040	GLN
3	C	260	GLN
7	G	4	HIS
9	I	32	ASN
11	K	2	ASN
24	Z	519	GLN
24	Z	642	HIS
26	f	64	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
16	P	15/16 (93%)	4 (26%)	2 (13%)

All (4) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
16	P	41	U
16	P	42	U
16	P	44	U
16	P	46	C

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
16	P	43	U
16	P	45	C

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

3 non-standard protein/DNA/RNA residues are 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
1	SEP	A	1547	1	8,9,10	1.62	1 (12%)	7,12,14	1.35	1 (14%)
1	TPO	A	1525	1	8,10,11	1.64	1 (12%)	10,14,16	2.08	1 (10%)
24	TPO	Z	775	24	8,10,11	1.66	1 (12%)	10,14,16	1.70	1 (10%)

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
1	SEP	A	1547	1	-	0/6/8/10	-
1	TPO	A	1525	1	-	2/9/11/13	-
24	TPO	Z	775	24	-	4/9/11/13	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1547	SEP	P-O1P	3.54	1.61	1.50
24	Z	775	TPO	P-O1P	3.53	1.61	1.50
1	A	1525	TPO	P-O1P	3.51	1.61	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1525	TPO	P-OG1-CB	-5.80	107.56	123.33
24	Z	775	TPO	P-OG1-CB	-4.44	111.27	123.33
1	A	1547	SEP	OG-CB-CA	2.94	111.00	108.14

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1525	TPO	C-CA-CB-CG2
24	Z	775	TPO	CB-OG1-P-O2P
1	A	1525	TPO	N-CA-CB-CG2

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Mol	Chain	Res	Type	Atoms
24	Z	775	TPO	CB-OG1-P-O1P
24	Z	775	TPO	CB-OG1-P-O3P
24	Z	775	TPO	C-CA-CB-CG2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	Z	775	TPO	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



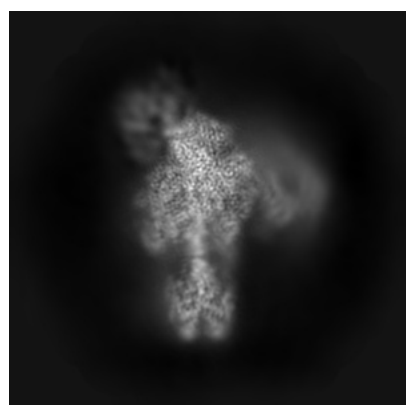
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26620. These allow visual inspection of the internal detail of the map and identification of artifacts.

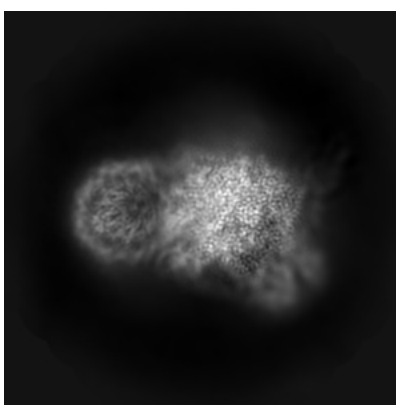
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

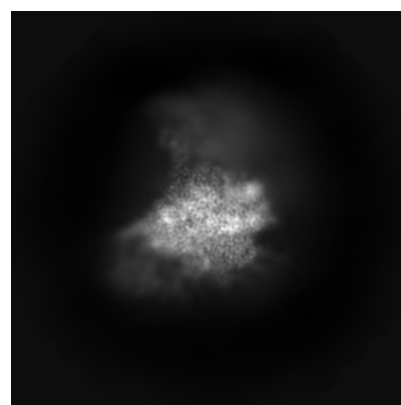
#### 6.1.1 Primary map



X



Y

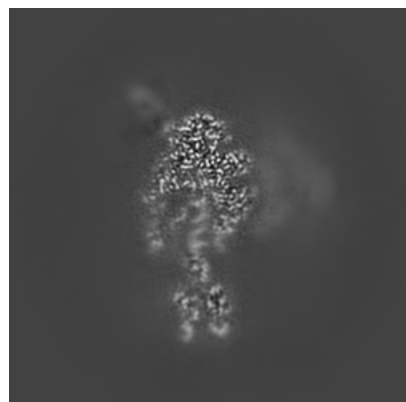


Z

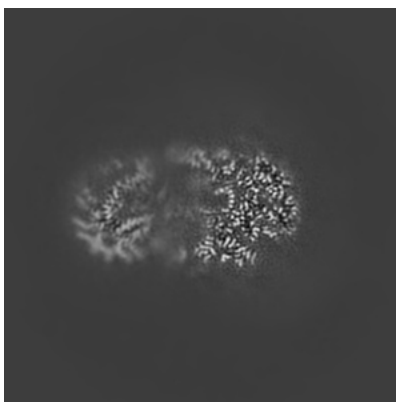
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

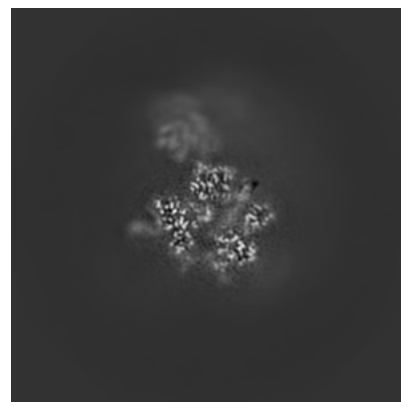
#### 6.2.1 Primary map



X Index: 225



Y Index: 225



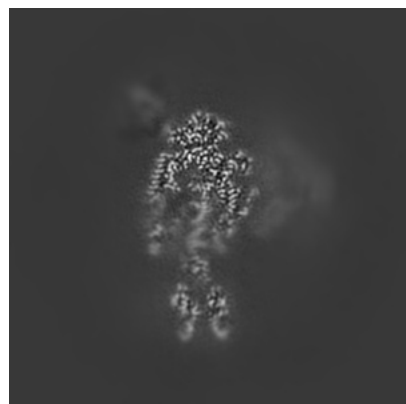
Z Index: 225



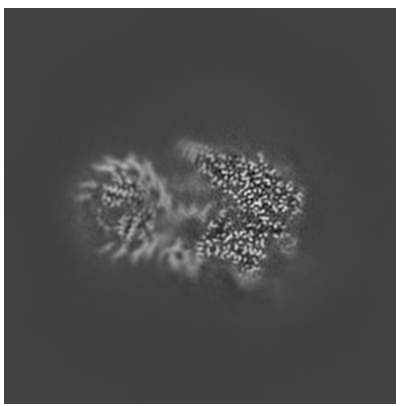
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

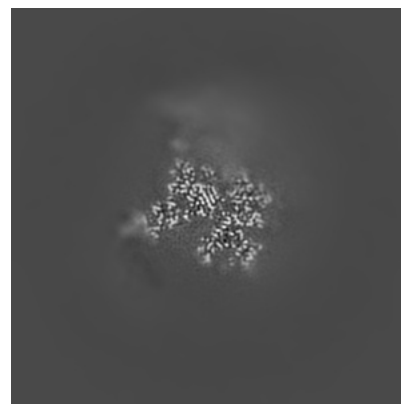
### 6.3.1 Primary map



X Index: 222



Y Index: 214

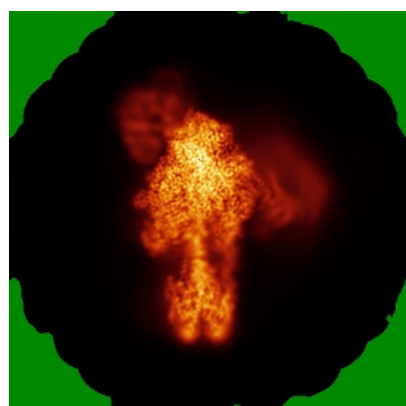


Z Index: 266

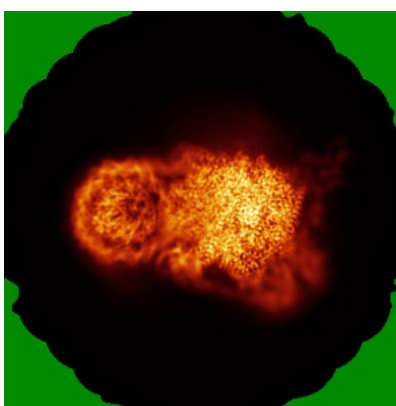
The images above show the largest variance slices of the map in three orthogonal directions.

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

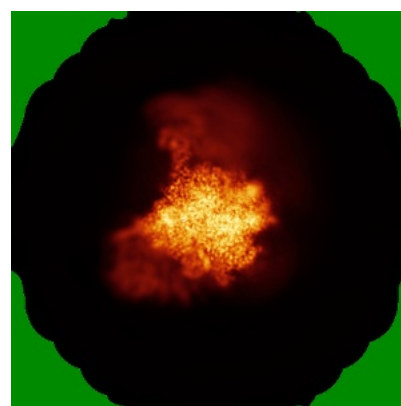
### 6.4.1 Primary map



X



Y



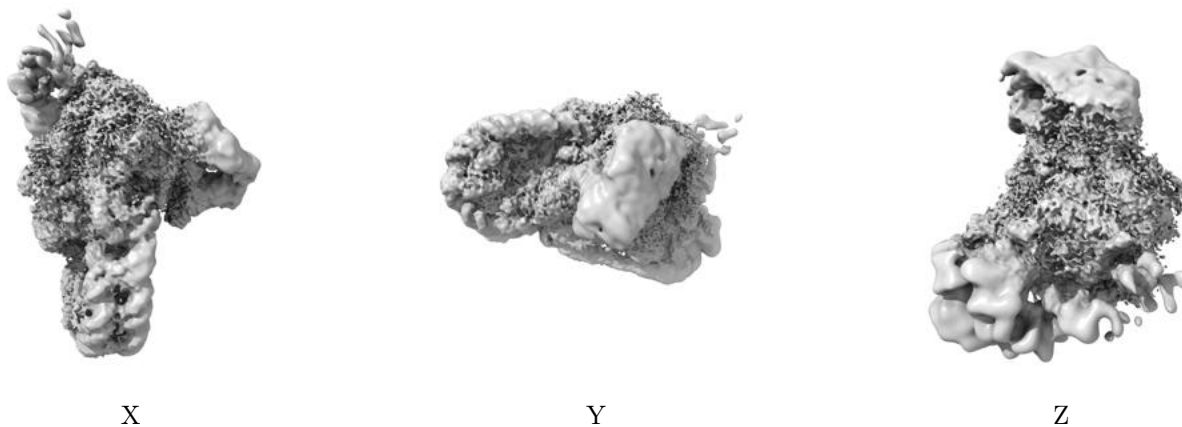
Z

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



## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.106. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.



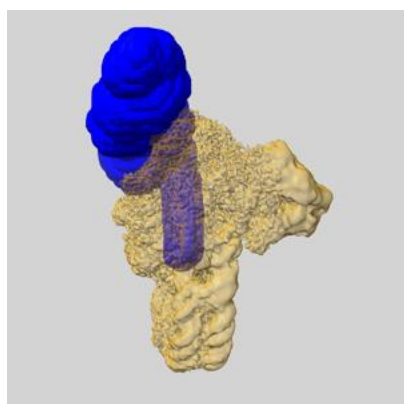
## 6.6 Mask visualisation [i](#)

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

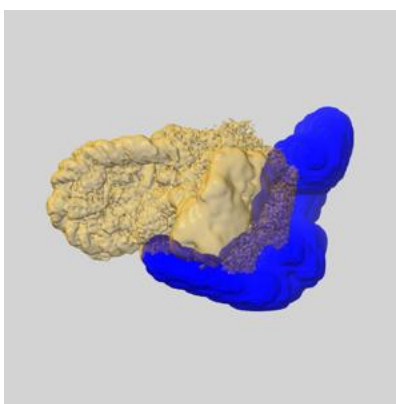
A mask typically either:

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

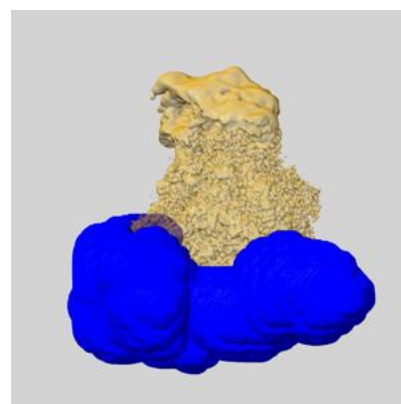
### 6.6.1 emd\_26620\_msk\_1.map [i](#)



X

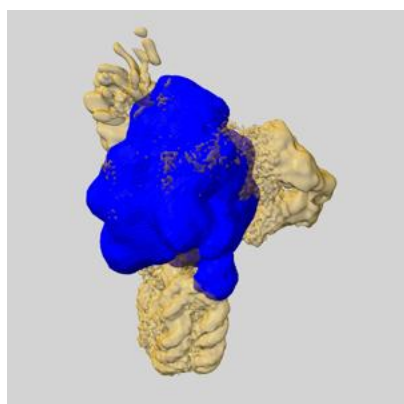


Y

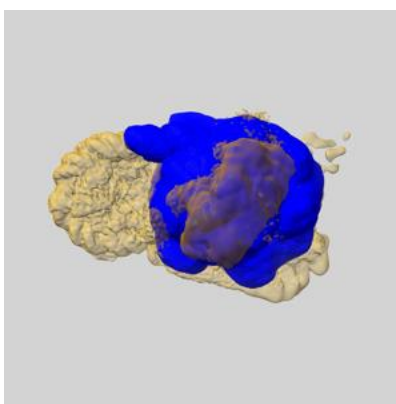


Z

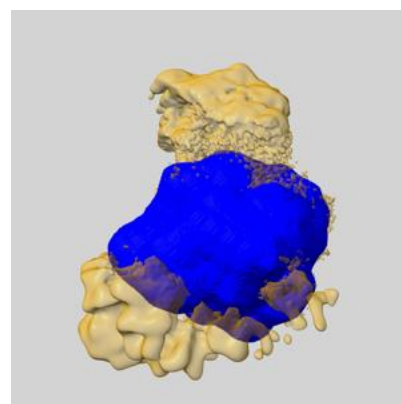
### 6.6.2 emd\_26620\_msk\_2.map [i](#)



X



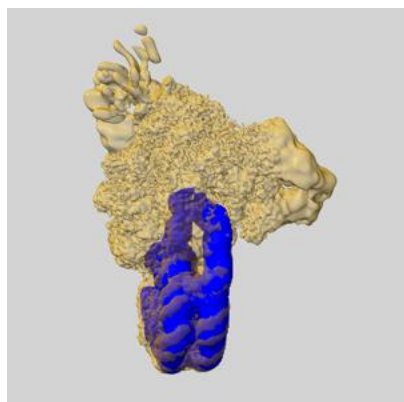
Y



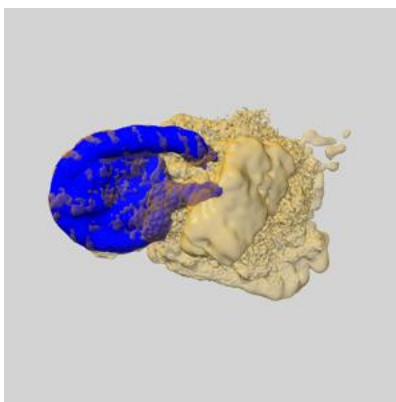
Z



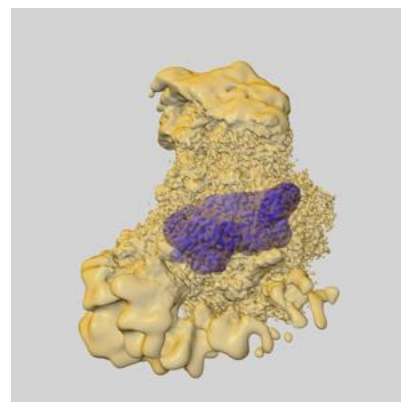
### 6.6.3 emd\_26620\_msk\_3.map [i](#)



X



Y



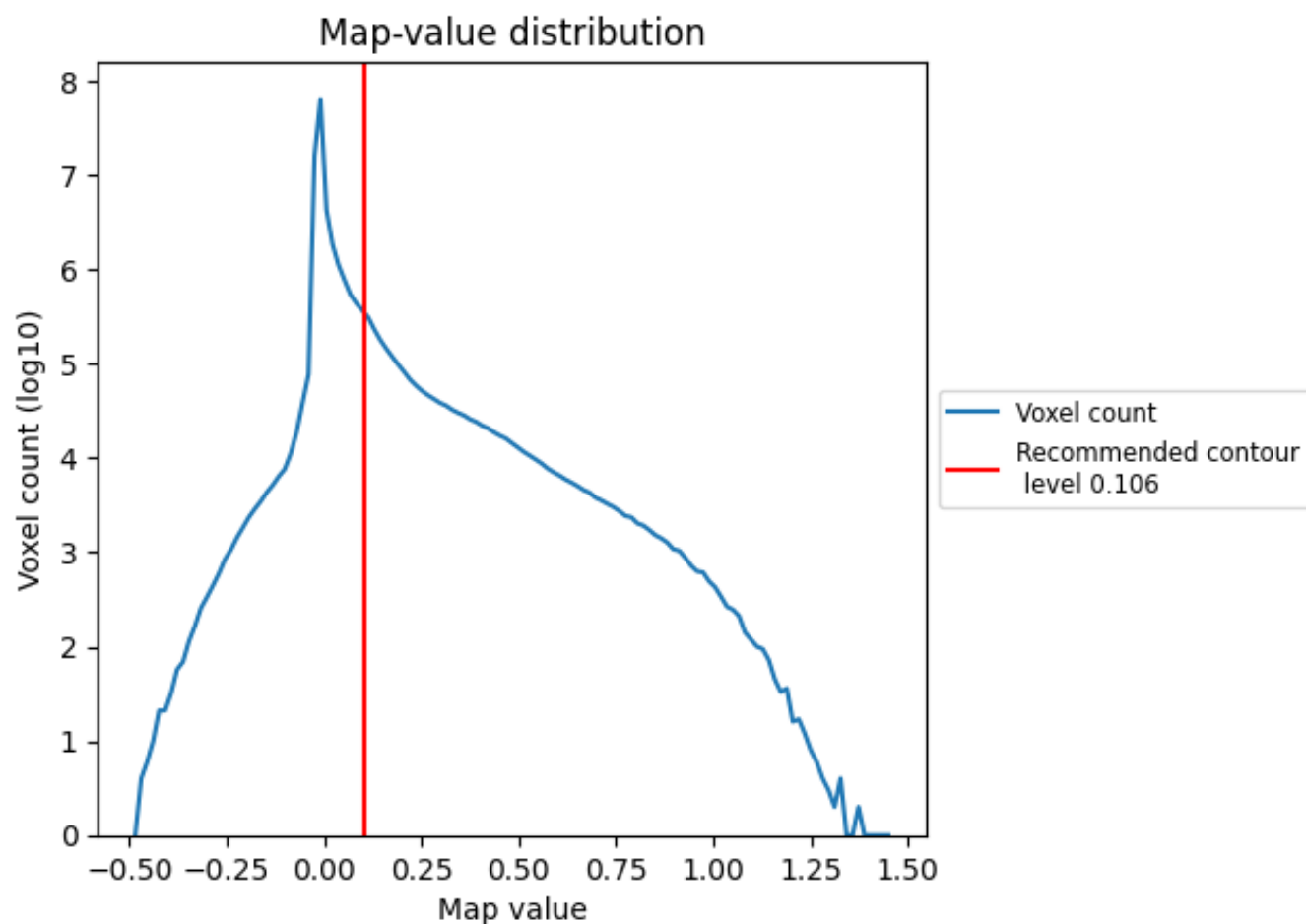
Z



## 7 Map analysis [i](#)

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

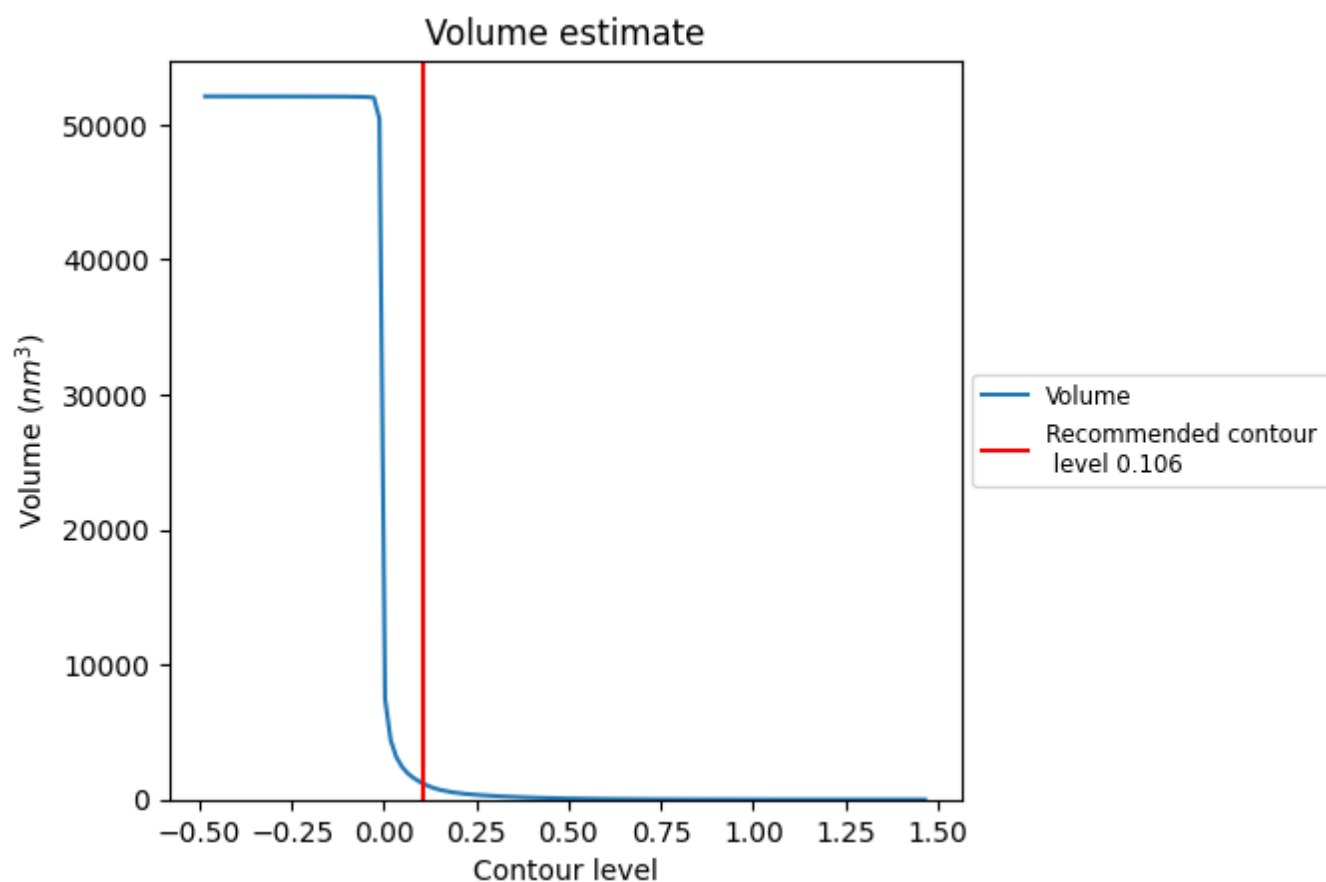
### 7.1 Map-value distribution [i](#)



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



## 7.2 Volume estimate [i](#)

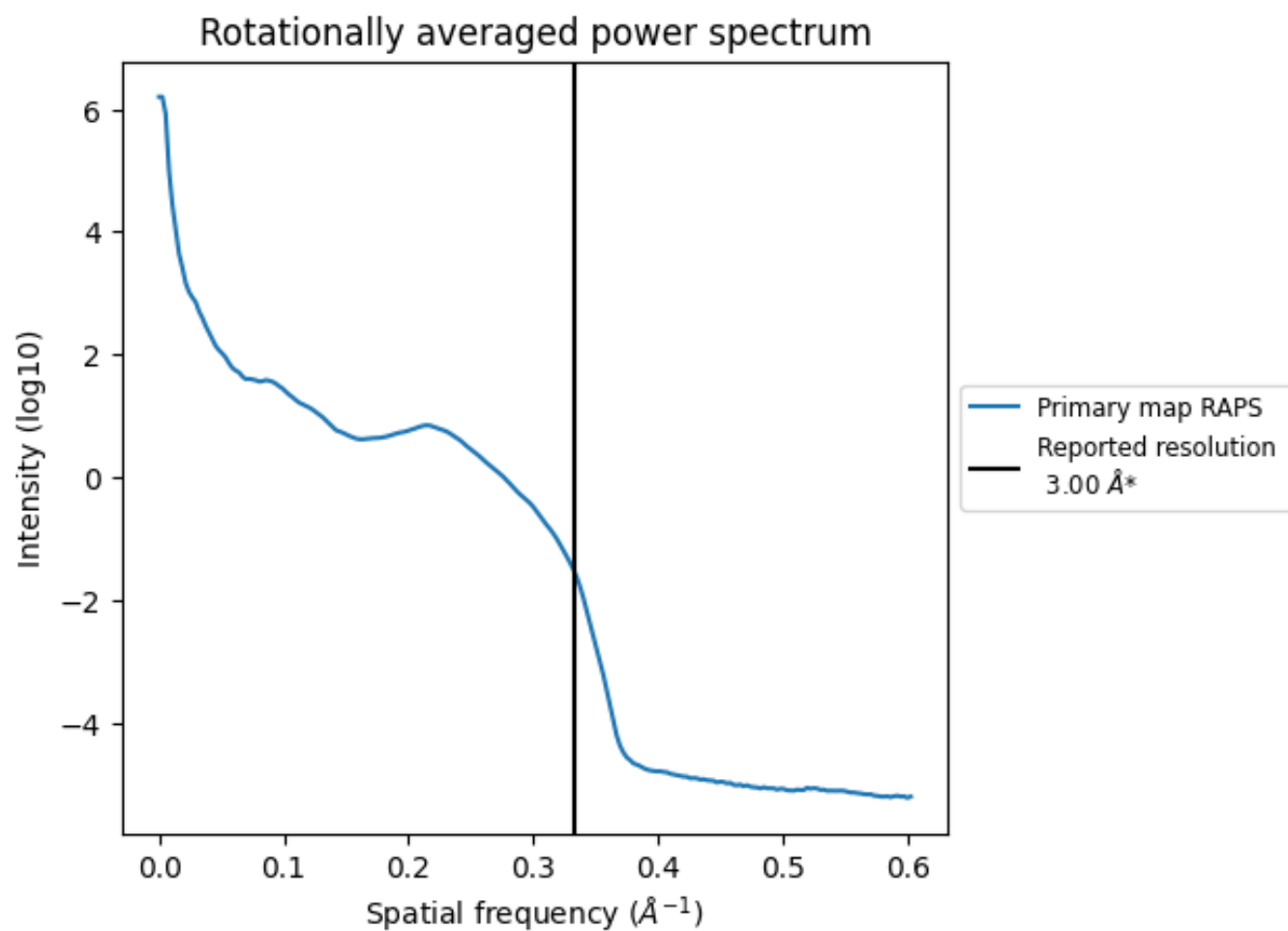


The volume at the recommended contour level is 1190 nm<sup>3</sup>; this corresponds to an approximate mass of 1075 kDa.

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



### 7.3 Rotationally averaged power spectrum ⓘ



\*Reported resolution corresponds to spatial frequency of 0.333 Å<sup>-1</sup>



## 8 Fourier-Shell correlation

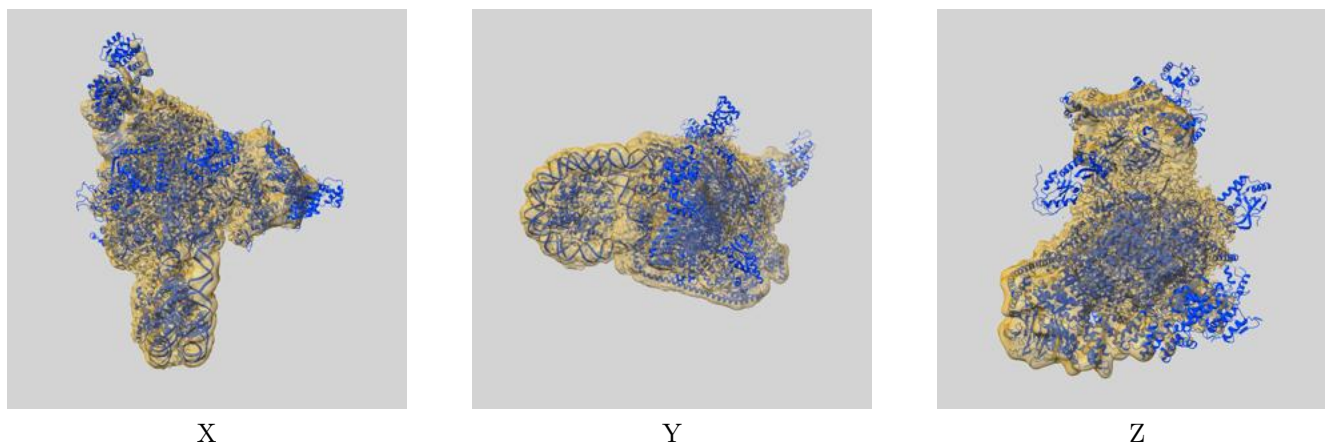
This section was not generated. No FSC curve or half-maps provided.



## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-26620 and PDB model 7UNC. Per-residue inclusion information can be found in section [3](#) on page [10](#).

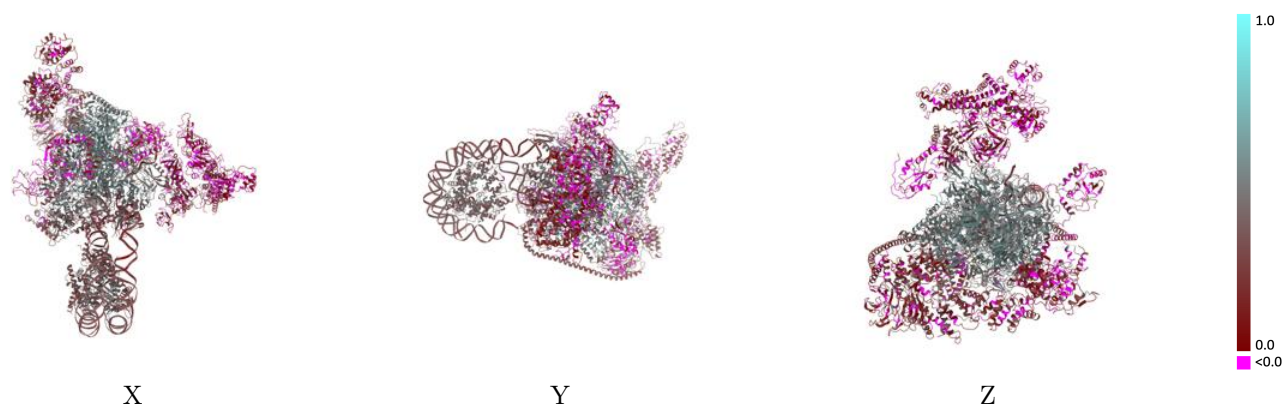
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.106 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

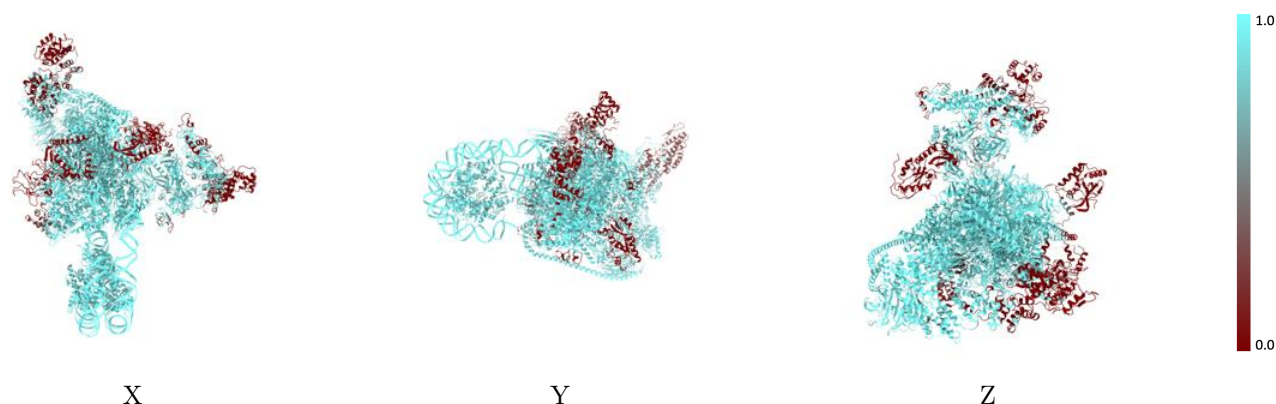


## 9.2 Q-score mapped to coordinate model [i](#)



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

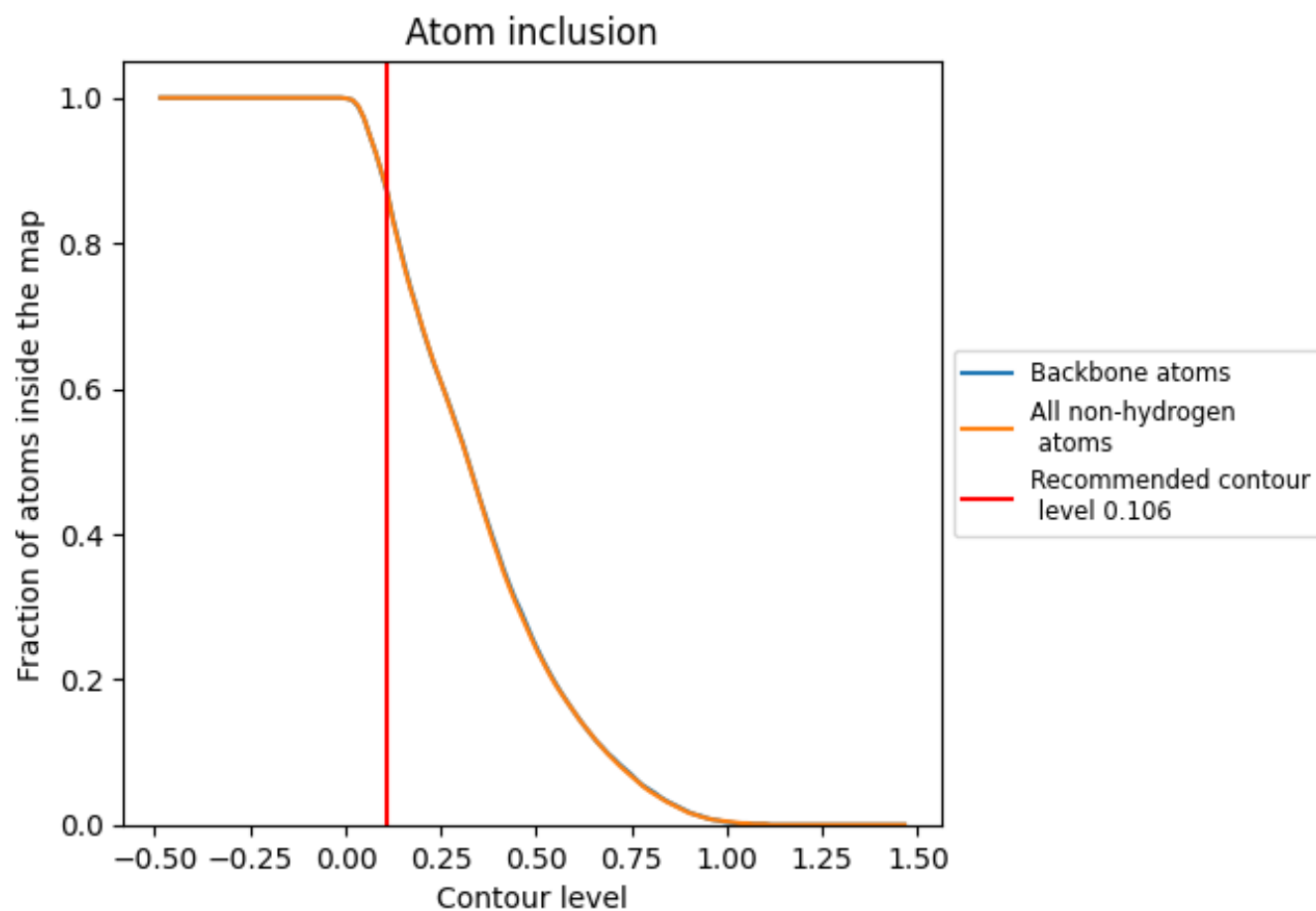
## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.106).



## 9.4 Atom inclusion ⓘ





































































At the recommended contour level, 88% of all backbone atoms, 88% 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 (0.106) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8780	 0.3440
A	 0.9760	 0.4790
B	 0.9910	 0.4950
C	 0.9950	 0.5280
D	 0.9570	 0.1580
E	 0.9910	 0.3560
F	 0.9920	 0.5280
G	 0.9770	 0.2300
H	 0.9830	 0.4160
I	 0.9970	 0.3840
J	 0.9820	 0.5340
K	 0.9920	 0.5250
L	 0.9760	 0.4380
M	 0.4380	 0.0470
N	 0.9980	 0.2890
O	 0.2820	 0.1330
P	 1.0000	 0.4100
Q	 0.6660	 0.1610
R	 0.1910	 0.0900
T	 1.0000	 0.3130
U	 0.0050	 0.0230
V	 0.2770	 0.1000
W	 0.9510	 0.1380
X	 0.9830	 0.2460
Z	 0.7620	 0.1280
a	 0.9870	 0.3510
b	 0.9890	 0.3960
c	 0.9700	 0.3650
d	 0.9740	 0.3460
e	 0.9730	 0.3290
f	 0.9830	 0.3670
g	 0.9750	 0.3930
h	 0.9890	 0.3890

