



## Full wwPDB EM Validation Report ⓘ

Nov 9, 2024 – 02:39 pm GMT

PDB ID : 6GMH  
EMDB ID : EMD-0031  
Title : Structure of activated transcription complex Pol II-DSIF-PAF-SPT6  
Authors : Vos, S.M.; Farnung, L.; Boehing, M.; Linden, A.; Wigge, C.; Urlaub, H.; Cramer, P.  
Deposited on : 2018-05-26  
Resolution : 3.10 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](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 : 1.8.4, CSD as541be (2020)  
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

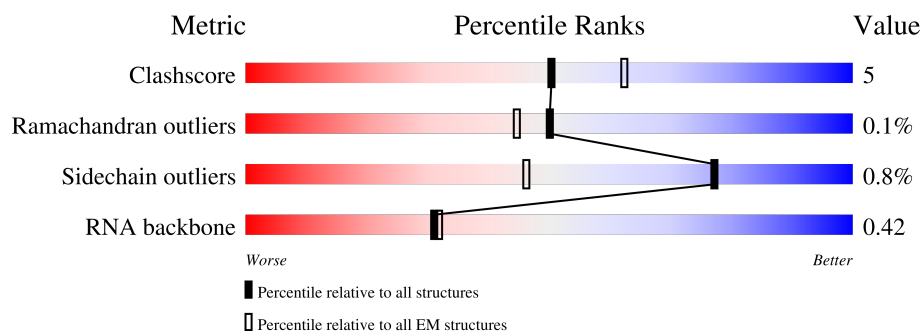
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.10 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
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	1970	
2	B	1174	
3	C	275	
4	D	142	
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	1726	
14	N	48	
15	P	46	
16	Q	1178	
17	T	48	
18	U	776	
19	V	613	
20	W	305	
21	X	16	
22	Y	121	
23	Z	1087	

## 2 Entry composition

There are 25 unique types of molecules in this entry. The entry contains 50239 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 RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1441	Total	C	N	O	P	S	
			11371	7151	2033	2115	2	70	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1132	Total	C	N	O	S		
			9052	5725	1592	1671	64	0	0

- Molecule 3 is a protein called RNA polymerase II subunit C.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	263	Total	C	N	O	S		
			2115	1324	365	420	6	0	0

- Molecule 4 is a protein called RNA polymerase II subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	126	Total	C	N	O	S		
			1004	630	170	200	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	209	Total	C	N	O	S		
			1720	1089	300	323	8	0	0

- Molecule 6 is a protein called RNA polymerase II subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	82	Total	C	N	O	S		
			657	418	113	121	5	0	0

- Molecule 7 is a protein called RNA polymerase II subunit G.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	171	Total	C	N	O	S	0	0
			1333	866	214	245	8		

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	148	Total	C	N	O	S	0	0
			1186	750	194	237	5		

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	117	Total	C	N	O	S	0	0
			949	587	169	182	11		

- Molecule 10 is a protein called RPB10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	67	Total	C	N	O	S	0	0
			533	345	90	92	6		

- Molecule 11 is a protein called RPB11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	115	Total	C	N	O	S	0	0
			920	593	152	173	2		

- Molecule 12 is a protein called RPB12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	46	Total	C	N	O	S	0	0
			388	241	75	66	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	1002	Total	C	N	O	S	0	0
			4737	2583	1071	1076	7		

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	37	Total	C	N	O	P	0	0
			773	361	158	217	37		

- Molecule 15 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	21	Total	C	N	O	P	0	0
			452	202	87	142	21		

- Molecule 16 is a protein called CTR9,RNA polymerase-associated protein CTR9 homolog,RNA polymerase-associated protein CTR9 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	884	Total	C	N	O	S	0	0
			4116	2199	953	961	3		

There are 5 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
Q	1178	GLN	-	expression tag	UNP Q6PD62

- Molecule 17 is a DNA chain called Template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	T	48	Total	C	N	O	P	0	0
			974	462	168	296	48		

- Molecule 18 is a protein called LEO1,LEO1,RNA polymerase-associated protein LEO1.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	U	110	Total	C	N	O	0	0
			440	220	110	110		

- Molecule 19 is a protein called PAF1,RNA polymerase II-associated factor 1 homolog,RNA polymerase II-associated factor 1 homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	V	81	Total	C	N	O	0	0
			324	162	81	81		

- Molecule 20 is a protein called WD repeat-containing protein 61.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	W	300	Total	C	N	O	S	0	0
			2333	1483	392	454	4		

- Molecule 21 is a protein called CDC73.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	X	16	Total	C	N	O	0	0
			63	32	16	15		

- Molecule 22 is a protein called Transcription elongation factor SPT4.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Y	116	Total	C	N	O	S	0	0
			911	570	159	173	9		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	-3	GLY	-	expression tag	UNP P63272
Y	-2	PRO	-	expression tag	UNP P63272
Y	-1	GLY	-	expression tag	UNP P63272
Y	0	SER	-	expression tag	UNP P63272

- Molecule 23 is a protein called Transcription elongation factor SPT5.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Z	486	Total	C	N	O	S	0	0
			3878	2465	684	712	17		

- Molecule 24 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
24	A	2	Total 2	Zn 2	0
24	B	1	Total 1	Zn 1	0
24	C	1	Total 1	Zn 1	0
24	I	2	Total 2	Zn 2	0
24	J	1	Total 1	Zn 1	0
24	L	1	Total 1	Zn 1	0
24	Y	1	Total 1	Zn 1	0

- Molecule 25 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

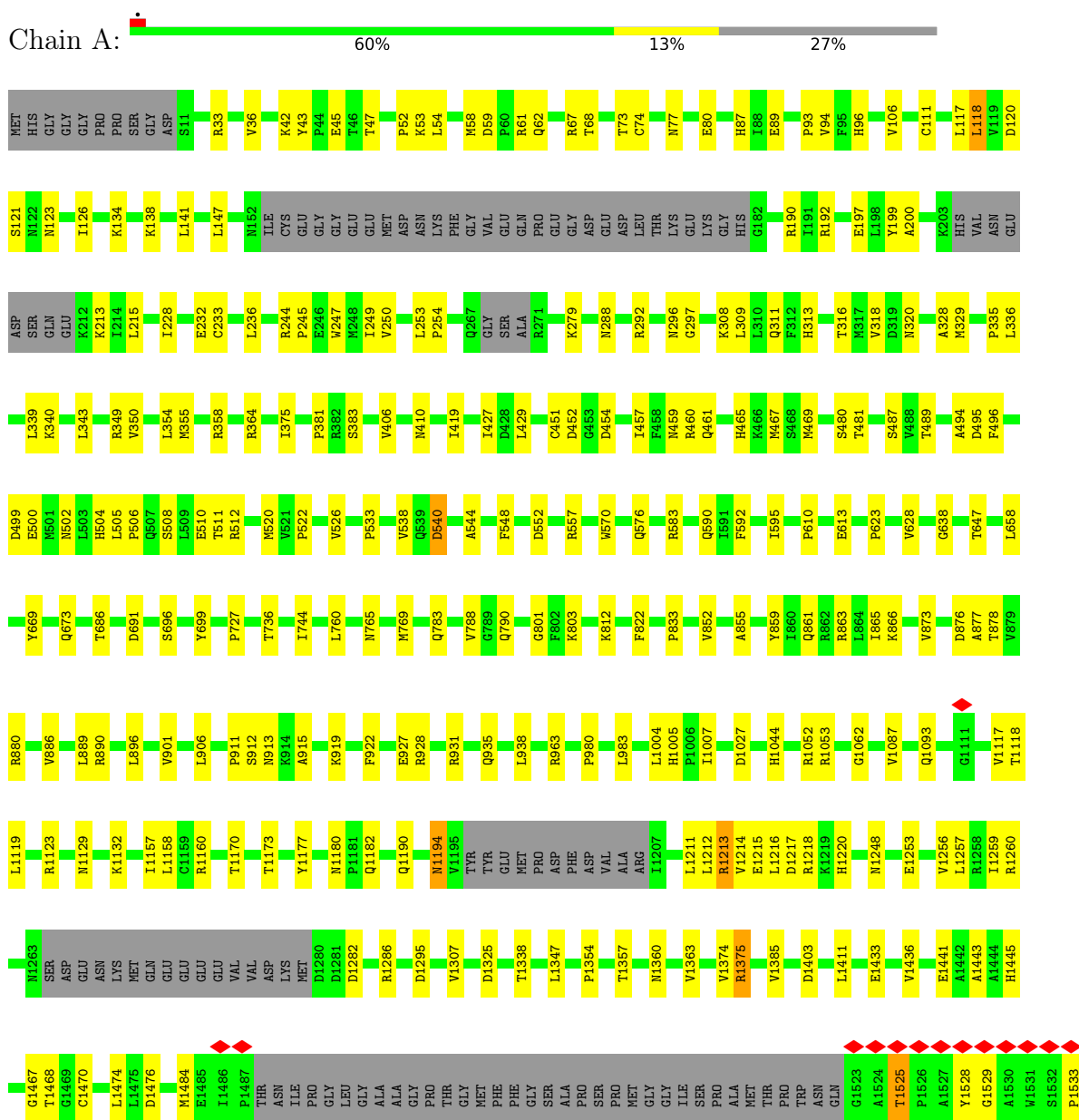
Mol	Chain	Residues	Atoms		AltConf
25	A	1	Total 1	Mg 1	0



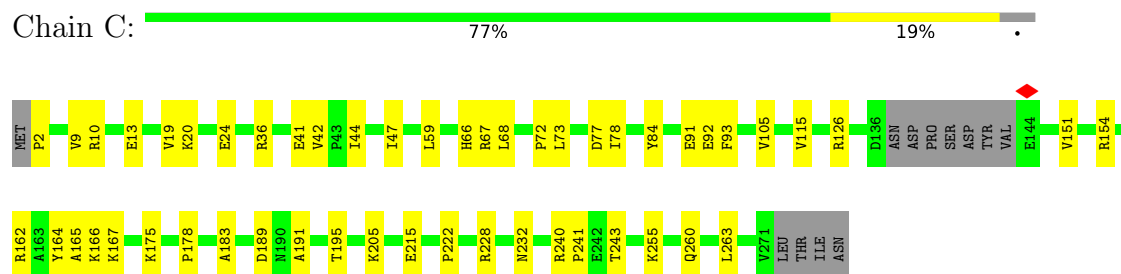
### 3 Residue-property plots

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.

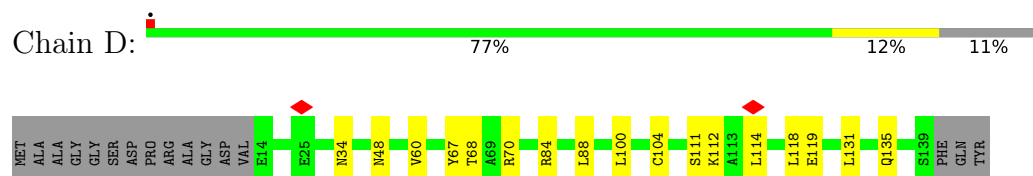
#### • Molecule 1: RPB1



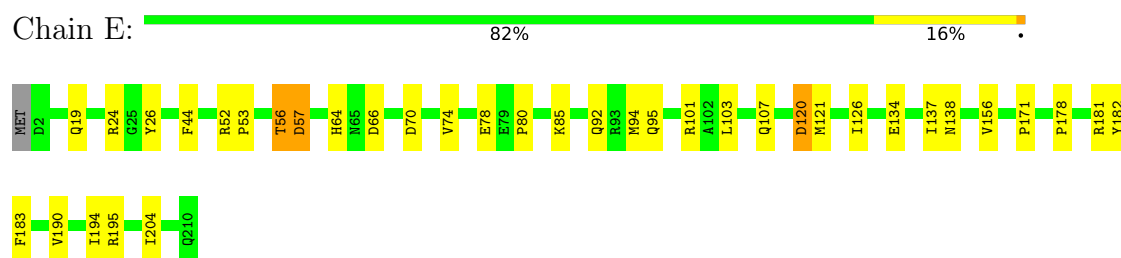




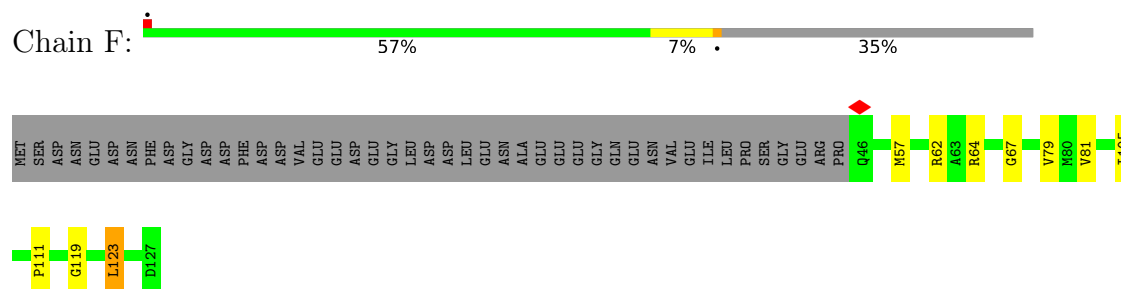
- Molecule 4: RNA polymerase II subunit D



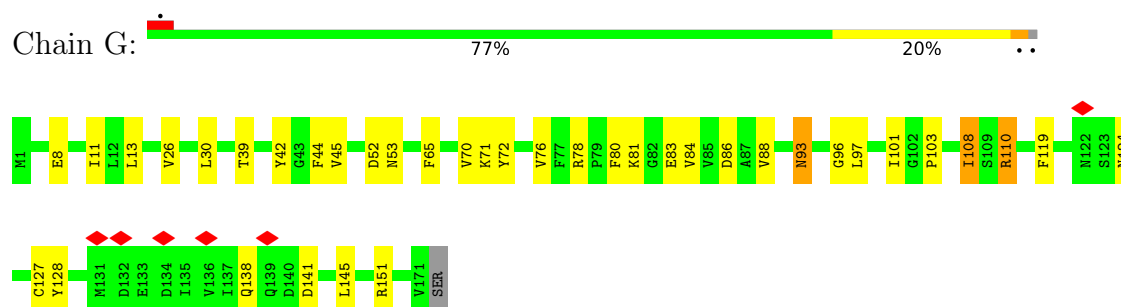
- Molecule 5: RNA polymerase II subunit E



- Molecule 6: RNA polymerase II subunit F



- Molecule 7: RNA polymerase II subunit G




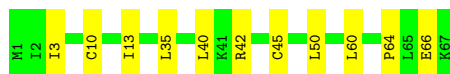
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

MET	A2	I15	D16	P17	V25	T63	L70	D71	D72	G73	E74	Y75	F88	E103	A109	L121	L144	A149	PHE
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- Chain I:  85% 9% 6%



- Chain J:  84% 16%



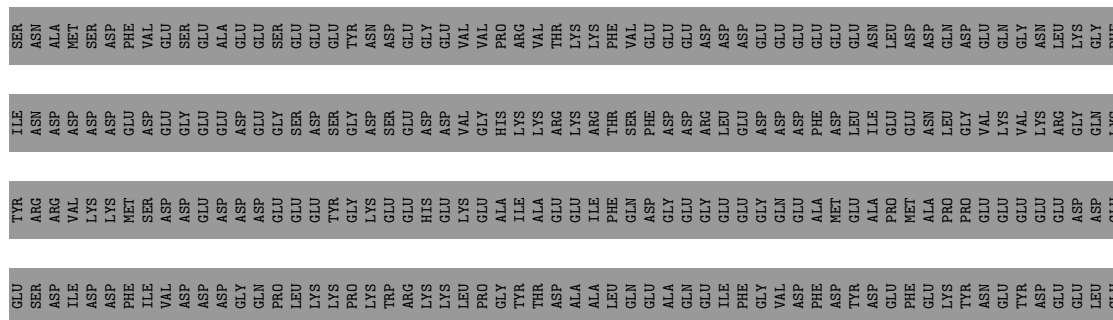
- Chain K:  83% 15%



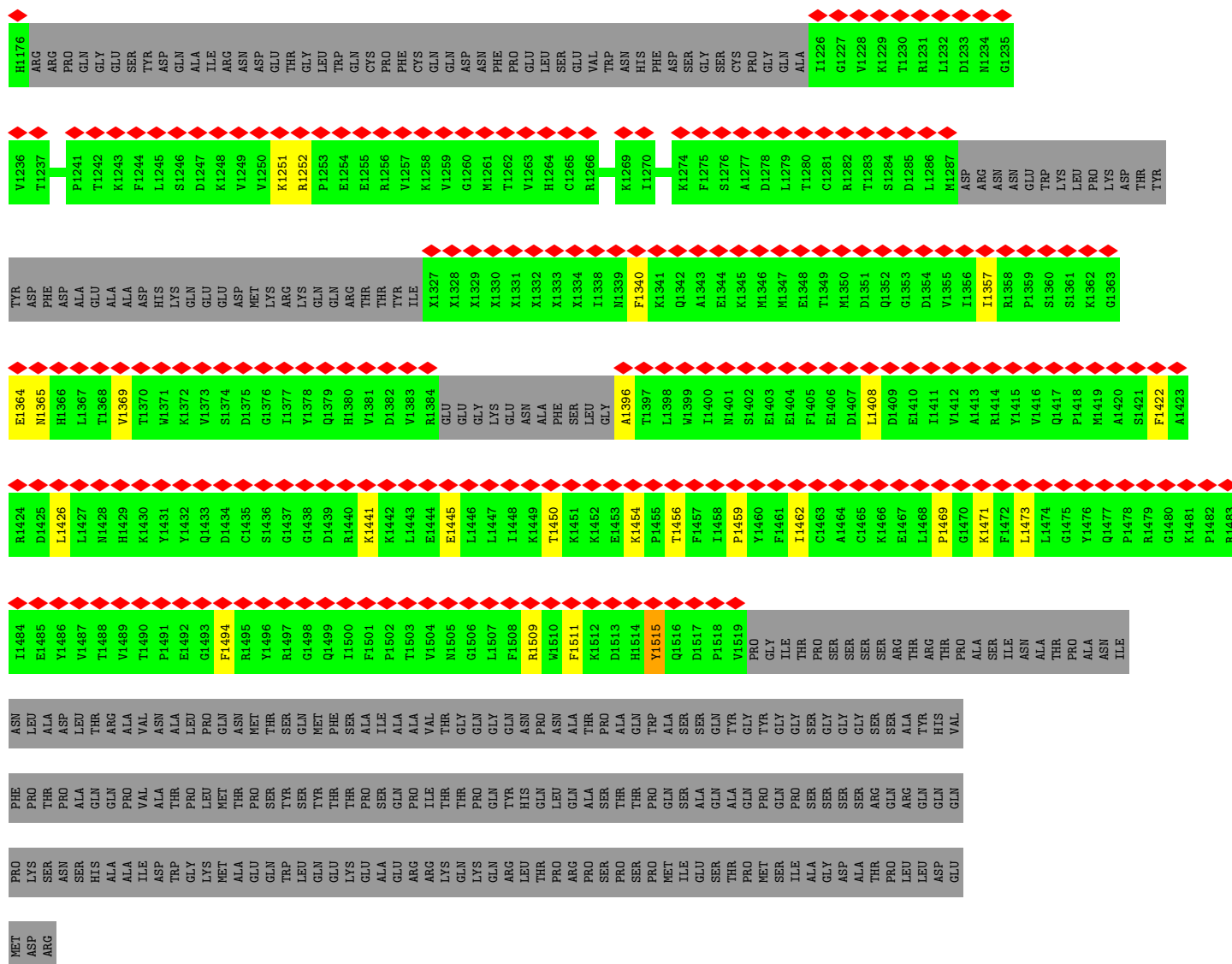
- Chain L:  71% 9% 21%



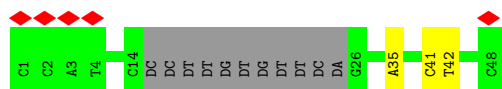
- Chain M:  44% 56% 42%



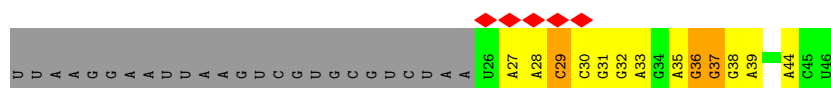
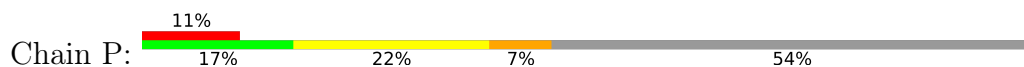
F1107	A1108	E1109	E1110	L1111	E1112	R1113	Q1114	G1115	Y1116	G1117	D1118	K1119	H1120	I1121	T1122	L1123	Y1124	D1125	I1126	R1127	A1128	E1129	L1130	S1131	C1132	R1133	Y1134	D1135	L1136	L1137	R1138	T1139	A1140	Y1141	R1142	S1143	P1144	N1145	T1146	E1147	E1148	I1149	T1157	T1160	I1163	L1166	I1167	I1168	C1169	N1170	V1171	T1172	G1173	I1174	A1175											
ASP	SER	TYR	ILE	E1051	V1052	L1053	D1054	G1055	S1056	R1057	V1058	H1059	P1060	E1061	T1062	Y1063	E1064	W1065	A1066	R1067	K1068	M1069	E1070	V1071	D1072	A1073	L1074	E1075	Y1076	D1077	E1078	S1079	T1080	E1081	D1082	A1083	N1084	P1085	A1086	G1087	A1088	L1089	E1090	E1091	I1092	L1093	E1094	M1095	P1096	E1097	R1098	L1099	K1100	D1101	L1102	D1103	L1104	D1105	A1106							
F298	Q299	L300	R301	S302	I303	P304	V305	K306	G307	A308	E309	D310	N391	D392	E314	E315	E316	A317	D318	Y321	R322	T327	P328	T329	I330	S331	L332	GLN	GLU	SER	CYS	ASP	LEU	THR	ASP	GLY	I440	R441	A442	L443	M448	K452	D453	V454	Q455	D462	G472	R473	I475	P476	K477	MET														
F378	Y379	R380	K381	E382	Y383	V384	E385	P386	ARG	E387	L388	H389	I390	N391	D392	T404	M412	A422	Y423	Q424	Y425	E426	Q427	I428	S429	A430	ASP	PRO	GLU	SER	LEU	LYS	ALA	VAL	GLY	PRO	ASP	GLY	T580	P581	E582	A583	V584	L585	Y590	L601	I618	T619	P620	T621	K622	G623	G624	R625	K626	D627	V628									
GLN	ASN	ALA	ALA	LYS	ALA	SER	ARG	LYS	LEU	LYS	ARG	GLU	GLY	ASP	GLU	GLY	GLY	ASP	GLU	ALA	ASP	GLU	GLN	ARG	GLY	PRO	GLU	LEU	LYS	ALA	SER	ARG	GLN	PHE	PRO	T580	P581	E582	A583	V584	L585	Y590	L601	I618	T619	P620	T621	K622	G623	G624	R625	K626	D627	V628												
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D284	Q285	D286	N287	E288	I289	R290	A291	T292	D293	L294	P295	E296	R297	F298	Q299	L300	R301	S302	I303	P304	V305	K306	G307	A308	E309	D310	N391	D392	E314	E315	E316	A317	D318	Y321	R322	T327	P328	T329	I330	S331	L332	GLN	GLU	SER	CYS	ASP	LEU	THR	ASP	GLY	I440	R441	A442	L443	M448	K452	D453	V454	Q455	D462	G472	R473	I475	P476	K477	MET
D284	Q285	D286	N287	E288	I289	R290	A291	T292	D293	L294	P295	E296	R297	F298	Q299	L300	R301	S302	I303	P304	V305	K306	G307	A308	E309	D310	N391	D392	E314	E315	E316	A317	D318	Y321	R322	T327	P328	T329	I330	S331	L332	GLN	GLU	SER	CYS	ASP	LEU	THR	ASP	GLY	I440	R441	A442	L443	M448	K452	D453	V454	Q455	D462	G472	R473	I475	P476	K477	MET
D284	Q285	D286	N287	E288	I289	R290	A291	T292	D293	L294	P295	E296	R297	F298	Q299	L300	R301	S302	I303	P304	V305	K306	G307	A308	E309	D310	N391	D392	E314	E315	E316	A317	D318	Y321	R322	T327	P328	T329	I330	S331	L332	GLN	GLU	SER	CYS	ASP	LEU	THR	ASP	GLY	I440	R441	A442	L443	M448	K452	D453	V454	Q455	D462	G472	R473	I475	P476	K477	MET
D284	Q285	D286	N287	E288	I289	R290	A291	T292	D293	L294	P295	E296	R297	F298	Q299	L300	R301	S302	I303	P304	V305	K306	G307	A308	E309	D310	N391	D392	E314	E315	E316	A317	D318	Y321	R322	T327	P328	T329	I330	S331	L332	GLN	GLU	SER	CYS	ASP	LEU	THR	ASP	GLY	I440	R441	A442	L443	M448	K452	D453	V454	Q455	D462	G472	R473	I475	P476	K477	MET
D284	Q285	D286	N287	E288	I289	R290	A291	T292	D293	L294	P295	E296	R297	F298	Q299	L300	R301	S302	I303	P304	V305	K306	G307	A308	E309	D310	N391	D392	E314	E315	E316	A317	D318	Y321	R322	T327	P328	T329	I330	S331	L332	GLN	GLU	SER	CYS	ASP	LEU	THR	ASP	GLY	I440	R441	A442	L443	M448	K452	D453	V454	Q455	D462	G472	R473	I475	P476	K477	MET
D284	Q285	D286	N287	E288	I289	R290	A291	T292	D293	L294	P295	E296	R297	F298	Q299	L300	R301	S302	I303	P304	V305	K306	G307	A308	E309	D310	N391	D392	E314	E315	E316	A317	D318	Y321	R322	T327	P328	T329	I330	S331	L332	GLN	GLU	SER	CYS	ASP	LEU	THR	ASP	GLY	I440	R441	A442	L443	M448	K452	D453	V454	Q455	D462	G472	R473	I475	P476	K477	MET
D284	Q285	D286	N287	E288	I289	R290	A291	T292	D293	L294	P295	E296	R297	F298	Q299	L300	R301	S302	I303	P304	V305	K306	G307	A308	E309	D310	N391	D392	E314	E315	E316	A317	D318	Y321	R322	T327	P328	T329	I330	S331	L332	GLN	GLU	SER	CYS	ASP	LEU	THR	ASP	GLY	I440	R441	A442	L443	M448	K452	D453	V454	Q455	D462	G472	R473	I475	P476	K477	MET
D284	Q285	D286	N287	E288	I289	R290	A291	T292	D293	L294	P295	E296	R297	F298	Q299	L300	R301	S302	I303	P304	V305	K306	G307	A308	E309	D310	N391	D392	E314	E315	E316	A317	D318	Y321	R322	T327	P328	T329	I330	S331	L332	GLN	GLU	SER	CYS	ASP	LEU	THR	ASP	GLY	I440	R441	A442	L443	M448	K452	D453	V454	Q455	D462	G472	R473	I475	P476	K477	MET
D284	Q285	D286	N287	E288	I289	R290	A291	T292	D293	L294	P295	E296	R297	F298	Q299	L300	R301	S302	I303	P304	V305	K306	G307	A308	E309	D310	N391	D392	E314	E315	E316	A317	D318	Y321	R322	T327	P328	T329	I330	S331	L332	GLN	GLU	SER	CYS	ASP	LEU	THR	ASP	GLY	I440	R441	A442	L443	M448	K452	D453	V454	Q455	D462	G472	R473	I475	P476	K477	MET
D284	Q285	D286	N287	E288</																																																														



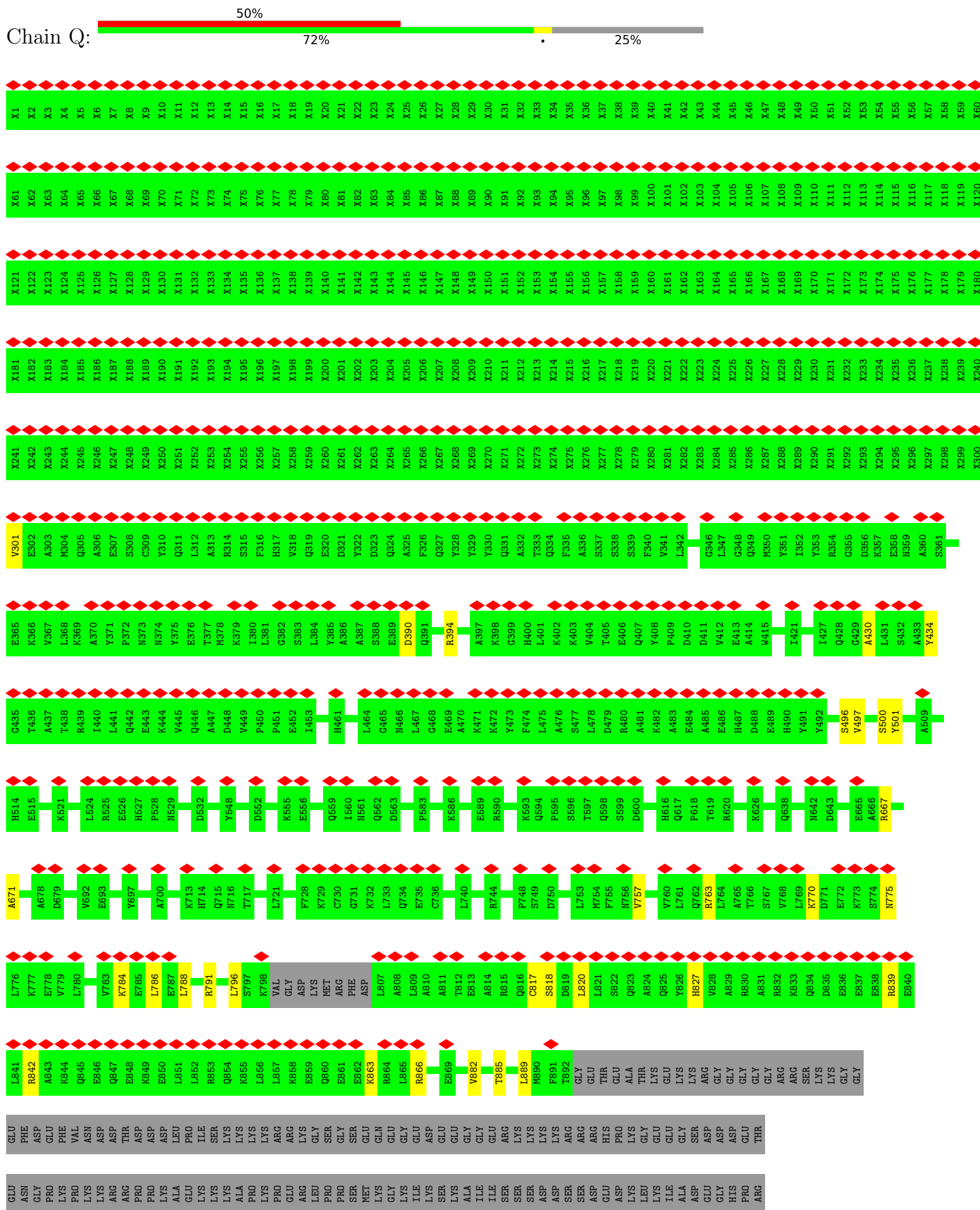
- Molecule 14: Non-template DNA



- Molecule 15: RNA

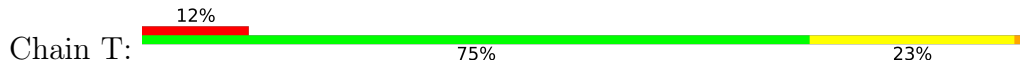


- Molecule 16: CTR9, RNA polymerase-associated protein CTR9 homolog, RNA polymerase-associated protein CTR9 homolog

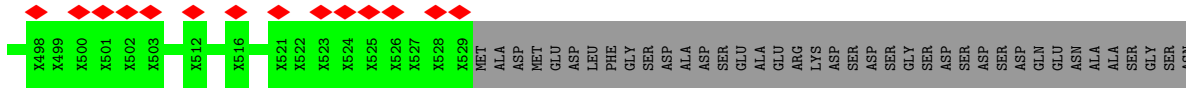
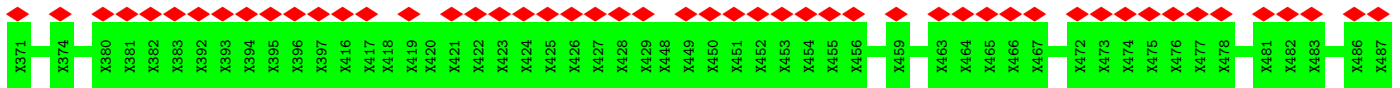


[illegible]

- Molecule 17: Template DNA



- Molecule 18: LEO1,LEO1,RNA polymerase-associated protein LEO1

[illegible]

ASP	PRO	SER	ASP	VAL	ASN	GLN	HIS	GLY	SER	GLU	ALA	PRO	ASN	ASP	ASP	GLU	ASP	GLY	GLY	ARG	SER	GLY	SER	HIS	SER	GLU	ALA	GLY	SER	LYS	GLU	LYS	TRP	GLY	ARG	GLU	ASP	LYS	LYS	ASP	GLU	LYS
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[illegible]

SER ASN ASP ASP GLU LYS GLN ASN SER ASP ASP GLU GLU PRO GLN LEU SER SER ASP ASP GLU LYS MET GLN ASN SER SER ASP ASP GLU LYS HIS ARG PRO GLN ALA SER SER SER ASP ASP GLU GLU HIS ARG HIS SER ASP ASP GLU GLU GLU GLN ASP ASP LYS SER GLU SER SER ARG ARG GLY SER ASP

GLU	ASP	GLU	GLU	VAL	LEU	ARG	MET	LYS	ARG	LYS	ASN	ALA	ALA	ALA	SER	ASP	SER	GLU	ALA	ASP	SER	THR	GLU	VAL	PRO	LYS	ASP	ASP	ASN	SER	GLY	GLY	ASP	ASP	ILE	SER	SER	SER	GLY	ASP	GLY	GLU	ASP	LYS	PRO	THR	PRO	GLN	PRO	VAL	ASP
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ASN	GLN	GLY	LEU	PRO	GLN	ASP	GLN	GLN	GLU	GLU	GLU	PRO	PRO	ILE	ILE	GLU	VAL	VAL	GLU	ILE	PRO	LYS	VAL	ASN	ASP	LEU	TYR	THR	ASP	LEU	GLY	ASN	ASP	ASN	PHE	VAL	LYS	LEU	LEU	PRO	PRO	ASN	PHE	LEU	LEU	SER	LEU	VAL	VAL	GLU	PRO	PRO	ARG	ASP	PRO	PRO	PHE	ASP	GLU	GLU	PHE	GLU
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ASP GLU MET ASP GLU GLY GLY ARG THR ARG ARG LYS LYS VAL GLU ASN THR THR LYS ASP ASP GLU GLY GLY ASN GLU LYS LYS ASP ASN ALA ARG ARG LYS LYS VAL VAL TRP TRP SER SER ASP GLY SER SER MET SER SER LEU HIS LEU GLY ASN GLU VAL PHE ASP VAL

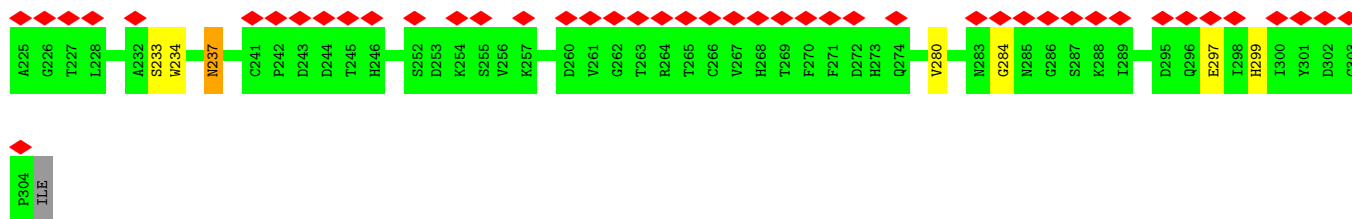
TVR	LYS	ALA	PRO	LEU	GLN	GLY	ASP	HIS	ASN	HIS	LEU	PHE	ARG	ILE	GLN	GLY	THR	GLY	LEU	GLN	GLY	GLN	ALA	VAL	PHE	ARG	THR	LYS	LYS	LEU	THR	THR	ASP	ASP	SER	ALA	ALA	THR	HIS	ARG	LYS	MET	THR	LEU	LEU	LEU	ASP	ALA	ARG	CYS	SER	SER	LYS	THR	GLN	LYS	ILE	ARG
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TLE	LEU	PRO	MET	ALA	GLY	ARG	ASP	PRO	GLU	CYS	GLN	ARG	THR	GLU	MET	TLE	LYS	LYS	GLU	GLU	GLU	ARG	LEU	ARG	ALA	SER	ILE	ARG	ARG	GLU	SER	GLN	GLN	ARG	ARG	MET	ARG	GLU	LYS	GLN	HIS	GLN	GLN	GLY	LEU	SER	ALA	SER	TYR	LEU	PRO	ASP	ARG	TYR	GLU	GLU
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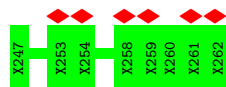
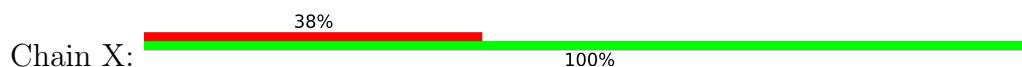
GLY GLU GLU GLU SER ILE SER LEU ALA ALA ILE LYS ASN ARG TYR LYS GLY GLY ILE ARG ARG GLU GLU ARG ALA ILE TYR SER SER ASP SER ASP GLU GLY SER GLU GLU ASP LYS ALA ALA GLN ARG ARG LEU LEU LYS ALA LYS LYS LYS LEU LEU THR SER ASP GLU GLU GLY PRO GLY GLY



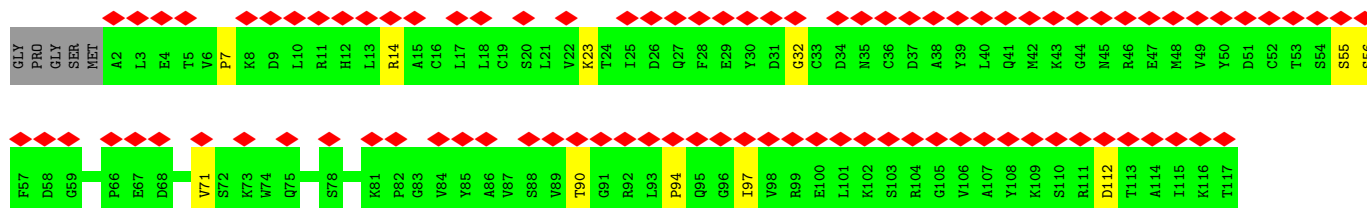
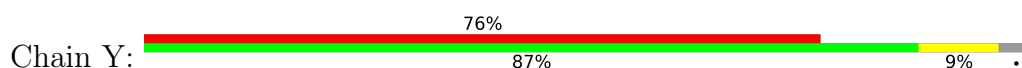




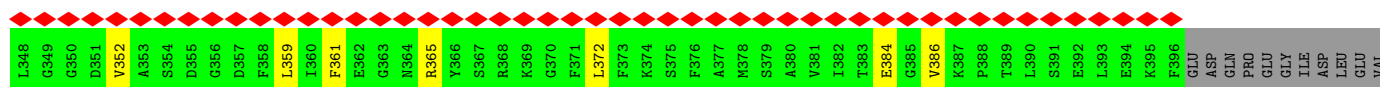
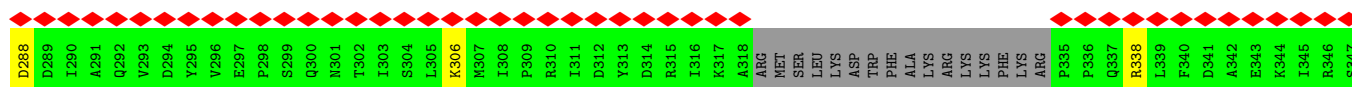
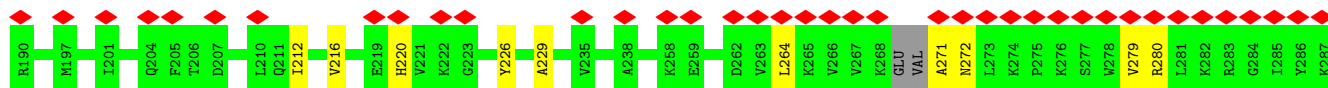
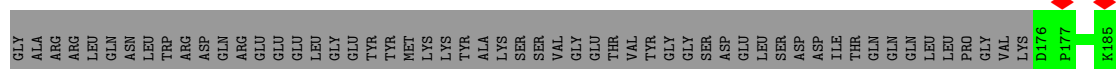
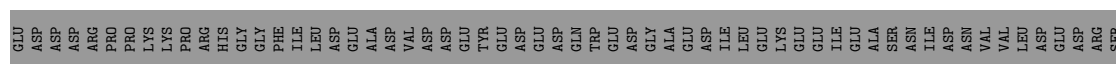
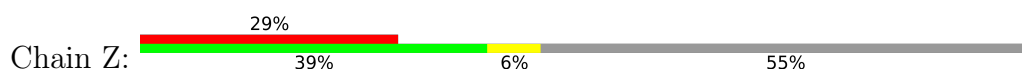
• Molecule 21: CDC73



• Molecule 22: Transcription elongation factor SPT4



• Molecule 23: Transcription elongation factor SPT5



WORLDWIDE  
**PDB**  
PROTEIN DATA BANK

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	374964	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 ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.155	Depositor
Minimum map value	-0.057	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0157	Depositor
Map size ( $\text{\AA}$ )	377.64, 377.64, 377.64	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.049, 1.049, 1.049	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

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	0.38	0/11558	0.63	3/15601 (0.0%)
2	B	0.41	0/9232	0.61	2/12462 (0.0%)
3	C	0.42	0/2158	0.58	0/2931
4	D	0.31	0/1017	0.55	0/1368
5	E	0.36	0/1751	0.65	1/2366 (0.0%)
6	F	0.35	0/667	0.55	0/901
7	G	0.34	0/1364	0.64	0/1853
8	H	0.41	0/1207	0.65	0/1628
9	I	0.35	0/972	0.56	0/1316
10	J	0.42	0/542	0.56	0/730
11	K	0.40	0/939	0.60	2/1271 (0.2%)
12	L	0.41	0/394	0.65	0/524
13	M	0.26	0/4724	0.49	0/6031
14	N	0.59	0/870	0.88	0/1341
15	P	0.44	0/506	1.08	5/787 (0.6%)
16	Q	0.25	0/2923	0.44	0/3746
17	T	0.64	0/1087	0.96	1/1674 (0.1%)
20	W	0.27	0/2392	0.55	0/3257
22	Y	0.26	0/927	0.48	0/1250
23	Z	0.28	0/3946	0.53	0/5314
All	All	0.37	0/49176	0.61	14/66351 (0.0%)

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
3	C	0	1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	#Chirality outliers	#Planarity outliers
5	E	0	2
7	G	0	1
13	M	0	3
All	All	0	12

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	120	ASP	CB-CG-OD1	8.67	126.11	118.30
11	K	80	ASP	CB-CG-OD1	7.44	124.99	118.30
15	P	36	G	P-O3'-C3'	6.96	128.05	119.70
15	P	32	G	C4-N9-C1'	6.88	135.44	126.50
1	A	118	LEU	CA-CB-CG	6.87	131.09	115.30
2	B	492	ASP	CB-CG-OD1	6.35	124.02	118.30
15	P	32	G	C8-N9-C1'	-5.81	119.44	127.00
1	A	1158	LEU	CA-CB-CG	5.76	128.56	115.30
2	B	556	ILE	C-N-CA	5.53	135.52	121.70
1	A	1257	LEU	CA-CB-CG	5.50	127.94	115.30
17	T	33	DC	OP1-P-O3'	5.29	116.84	105.20
15	P	32	G	N3-C4-C5	-5.28	125.96	128.60
15	P	32	G	N3-C4-N9	5.21	129.13	126.00
11	K	79	PRO	C-N-CA	5.06	134.36	121.70

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	460	ARG	Peptide
1	A	538	VAL	Peptide
2	B	629	GLU	Peptide
2	B	71	ALA	Peptide
2	B	98	HIS	Peptide
3	C	91	GLU	Peptide
5	E	56	THR	Peptide
5	E	57	ASP	Peptide
7	G	124	ASN	Peptide
13	M	1145	ASN	Peptide
13	M	1251	LYS	Peptide
13	M	1252	ARG	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11371	0	11488	183	0
2	B	9052	0	9081	130	0
3	C	2115	0	2057	36	0
4	D	1004	0	980	12	0
5	E	1720	0	1737	25	0
6	F	657	0	684	8	0
7	G	1333	0	1321	26	0
8	H	1186	0	1147	11	0
9	I	949	0	879	9	0
10	J	533	0	554	9	0
11	K	920	0	942	12	0
12	L	388	0	393	6	0
13	M	4737	0	2252	21	0
14	N	773	0	412	3	0
15	P	452	0	229	5	0
16	Q	4116	0	1657	20	0
17	T	974	0	541	9	0
18	U	440	0	18	0	0
19	V	324	0	15	1	0
20	W	2333	0	2246	21	0
21	X	63	0	2	0	0
22	Y	911	0	904	8	0
23	Z	3878	0	3941	38	0
24	A	2	0	0	0	0
24	B	1	0	0	0	0
24	C	1	0	0	0	0
24	I	2	0	0	0	0
24	J	1	0	0	0	0
24	L	1	0	0	0	0
24	Y	1	0	0	0	0
25	A	1	0	0	0	0
All	All	50239	0	43480	495	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 5.

All (495) 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)
5:E:85:LYS:NZ	14:N:41:DC:OP2	1.92	1.03
2:B:816:GLU:OE2	2:B:869:LYS:NZ	2.00	0.95
9:I:65:LEU:O	9:I:122:ARG:NH1	2.06	0.88
1:A:803:LYS:O	1:A:812:LYS:NZ	2.12	0.83
1:A:355:MET:SD	2:B:1091:ARG:NH1	2.50	0.82
2:B:387:HIS:NE2	2:B:671:GLU:OE2	2.13	0.81
13:M:1454:LYS:NZ	13:M:1456:THR:OG1	2.15	0.79
1:A:358:ARG:NH1	17:T:27:DT:OP1	2.17	0.78
3:C:93:PHE:HE1	3:C:166:LYS:HZ3	1.32	0.78
1:A:1375:ARG:NH1	1:A:1403:ASP:OD1	2.18	0.77
2:B:1131:ARG:NH1	23:Z:535:GLU:OE1	2.18	0.77
2:B:859:ARG:NH1	2:B:860:VAL:O	2.19	0.76
1:A:927:GLU:OE2	1:A:931:ARG:NH2	2.14	0.75
16:Q:885:THR:O	16:Q:889:LEU:HB2	1.87	0.75
1:A:340:LYS:HG3	1:A:1436:VAL:HG21	1.72	0.71
3:C:19:VAL:HG23	3:C:241:PRO:HB2	1.72	0.71
1:A:686:THR:HG21	2:B:1041:ILE:HA	1.74	0.70
1:A:33:ARG:HH21	2:B:1141:ARG:HE	1.40	0.69
16:Q:784:LYS:NZ	20:W:64:GLN:OE1	2.26	0.68
1:A:87:HIS:NE2	1:A:89:GLU:OE2	2.27	0.68
2:B:592:ARG:NE	2:B:663:GLU:OE2	2.18	0.68
2:B:274:ARG:NH1	2:B:311:ILE:O	2.26	0.67
7:G:97:LEU:HB3	7:G:108:ILE:HG23	1.76	0.67
22:Y:23:LYS:NZ	22:Y:32:GLY:O	2.26	0.66
4:D:114:LEU:HD22	7:G:84:VAL:HG11	1.78	0.66
2:B:473:LEU:HD11	2:B:1052:LYS:HD3	1.76	0.65
2:B:819:SER:H	2:B:827:GLU:HB2	1.61	0.65
23:Z:529:ASP:HB2	23:Z:553:LEU:HD13	1.78	0.65
6:F:57:MET:HB2	6:F:123:LEU:HD13	1.79	0.65
3:C:92:GLU:OE1	23:Z:711:ARG:NH1	2.30	0.65
1:A:861:GLN:HE21	1:A:865:ILE:HD11	1.61	0.65
1:A:54:LEU:HB3	1:A:61:ARG:HH12	1.62	0.64
4:D:60:VAL:HG13	7:G:103:PRO:HB3	1.79	0.64
1:A:199:TYR:HB3	1:A:215:LEU:HD23	1.80	0.64
2:B:282:ARG:HH11	9:I:16:PHE:HD2	1.45	0.64
1:A:461:GLN:NE2	2:B:1090:GLU:OE2	2.30	0.64
23:Z:417:GLU:OE2	23:Z:516:ARG:NH1	2.31	0.64
2:B:91:ILE:HD11	2:B:124:LEU:HD12	1.80	0.63
2:B:310:VAL:HG23	2:B:311:ILE:HD12	1.80	0.63
3:C:47:ILE:HD11	3:C:68:LEU:HB3	1.80	0.63
1:A:459:ASN:HB3	1:A:469:MET:HG2	1.81	0.63
1:A:865:ILE:HD13	2:B:1092:ASP:OD2	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:11:ILE:HD11	7:G:26:VAL:HG13	1.81	0.63
13:M:1441:LYS:NZ	13:M:1445:GLU:OE2	2.31	0.63
1:A:381:PRO:HB3	1:A:480:SER:HA	1.81	0.62
3:C:47:ILE:HA	3:C:165:ALA:HA	1.81	0.62
1:A:576:GLN:O	1:A:590:GLN:NE2	2.32	0.62
1:A:865:ILE:HG21	2:B:1092:ASP:OD2	2.00	0.62
2:B:458:LYS:HB2	2:B:461:GLN:HB2	1.81	0.62
3:C:41:GLU:OE1	3:C:255:LYS:NZ	2.27	0.62
23:Z:306:LYS:HA	23:Z:372:LEU:O	2.01	0.61
2:B:98:HIS:HB2	2:B:108:MET:HB2	1.83	0.61
1:A:200:ALA:O	1:A:213:LYS:HA	2.01	0.60
23:Z:479:LYS:HD3	23:Z:521:CYS:HB2	1.83	0.60
2:B:354:SER:HG	2:B:357:CYS:HG	1.48	0.60
23:Z:220:HIS:NE2	23:Z:384:GLU:OE1	2.34	0.60
1:A:457:ILE:HG22	1:A:504:HIS:HB2	1.84	0.60
23:Z:450:ILE:HG23	23:Z:452:PRO:HD3	1.84	0.59
20:W:35:VAL:HB	20:W:47:TRP:HB2	1.83	0.59
23:Z:639:LYS:HB2	23:Z:642:HIS:HD2	1.68	0.59
2:B:344:GLN:NE2	2:B:354:SER:O	2.36	0.59
2:B:565:THR:HG22	2:B:610:ARG:HB3	1.85	0.59
2:B:32:SER:HB3	2:B:643:LEU:HD21	1.83	0.59
3:C:154:ARG:NH1	10:J:60:LEU:O	2.36	0.59
16:Q:763:ARG:HH12	20:W:65:LEU:HD11	1.68	0.59
13:M:1357:ILE:HG21	13:M:1408:LEU:HD13	1.85	0.59
23:Z:439:LYS:O	23:Z:452:PRO:HA	2.03	0.59
2:B:179:LEU:HD22	2:B:768:ARG:HD3	1.84	0.59
1:A:318:VAL:HG12	1:A:339:LEU:HD12	1.85	0.58
1:A:727:PRO:HA	1:A:736:THR:HG21	1.84	0.58
1:A:1190:GLN:O	1:A:1194:ASN:HB2	2.03	0.58
7:G:8:GLU:HA	7:G:70:VAL:O	2.03	0.58
1:A:94:VAL:HG13	1:A:311:GLN:HG2	1.83	0.58
1:A:47:THR:HA	1:A:52:PRO:HA	1.85	0.58
1:A:1218:ARG:NH1	1:A:1253:GLU:HA	2.18	0.58
20:W:36:VAL:HG22	20:W:46:VAL:HG22	1.86	0.58
1:A:520:MET:HG3	1:A:522:PRO:HD2	1.85	0.58
1:A:783:GLN:HG3	1:A:788:VAL:HA	1.86	0.58
1:A:919:LYS:HE2	1:A:1053:ARG:HH12	1.67	0.58
1:A:320:ASN:ND2	1:A:336:LEU:O	2.37	0.58
9:I:73:SER:HA	9:I:95:VAL:HG11	1.86	0.57
2:B:953:ASP:OD1	3:C:36:ARG:NH2	2.33	0.57
23:Z:595:HIS:N	23:Z:598:ASP:OD2	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:175:LYS:NZ	12:L:57:ALA:HB3	2.19	0.57
1:A:45:GLU:HB2	1:A:53:LYS:NZ	2.19	0.57
1:A:576:GLN:HA	8:H:75:TYR:HB2	1.87	0.57
1:A:886:VAL:HG13	5:E:171:PRO:HD3	1.86	0.57
2:B:483:ARG:NH2	2:B:527:ALA:O	2.38	0.57
2:B:725:GLN:NE2	2:B:937:SER:O	2.38	0.57
1:A:138:LYS:NZ	1:A:1441:GLU:OE2	2.26	0.57
23:Z:279:VAL:HA	23:Z:386:VAL:HG21	1.87	0.56
2:B:748:ALA:HB3	2:B:811:TYR:HB2	1.86	0.56
4:D:67:TYR:OH	7:G:86:ASP:O	2.22	0.56
23:Z:444:ASP:H	23:Z:448:ILE:HG23	1.70	0.56
2:B:549:SER:HG	2:B:577:HIS:HE2	1.53	0.56
2:B:718:GLN:HG2	2:B:720:PRO:HD2	1.88	0.56
4:D:100:LEU:HD21	4:D:118:LEU:HD11	1.87	0.56
16:Q:763:ARG:HH22	16:Q:788:LEU:HD23	1.70	0.56
20:W:206:VAL:HG22	20:W:216:ILE:HG12	1.88	0.56
23:Z:272:ASN:HD21	23:Z:384:GLU:HB2	1.70	0.56
1:A:1552:SER:HB3	13:M:1509:ARG:HH12	1.70	0.56
3:C:59:LEU:HD12	3:C:151:VAL:HG23	1.88	0.56
2:B:191:GLU:OE2	2:B:743:ARG:NH2	2.39	0.56
2:B:692:THR:OG1	9:I:80:ARG:NH1	2.39	0.56
1:A:922:PHE:HA	1:A:1052:ARG:HD3	1.87	0.55
16:Q:885:THR:O	16:Q:889:LEU:CB	2.53	0.55
2:B:806:PHE:O	2:B:1050:ARG:NH1	2.39	0.55
9:I:29:ASP:O	9:I:33:ARG:HA	2.05	0.55
5:E:64:HIS:ND1	5:E:66:ASP:OD1	2.38	0.55
1:A:866:LYS:NZ	2:B:1091:ARG:HH22	2.05	0.55
2:B:1062:ARG:NH2	2:B:1066:PRO:O	2.37	0.55
1:A:42:LYS:O	1:A:288:ASN:ND2	2.40	0.54
23:Z:552:ARG:HB3	23:Z:559:GLN:HB2	1.89	0.54
1:A:855:ALA:HB3	2:B:494:LYS:NZ	2.23	0.54
1:A:919:LYS:HE2	1:A:1053:ARG:NH1	2.22	0.54
3:C:9:VAL:HG11	11:K:105:PHE:HD1	1.72	0.54
16:Q:763:ARG:NH1	20:W:65:LEU:HD21	2.23	0.54
20:W:75:THR:OG1	20:W:116:PRO:O	2.26	0.54
1:A:1552:SER:HB3	13:M:1509:ARG:NH1	2.21	0.53
1:A:358:ARG:NH2	2:B:1076:GLU:OE1	2.41	0.53
1:A:111:CYS:HB2	1:A:118:LEU:HB3	1.90	0.53
1:A:279:LYS:HZ1	1:A:328:ALA:HB1	1.73	0.53
2:B:193:VAL:HG21	2:B:470:LEU:HD13	1.90	0.53
2:B:770:ARG:HH11	2:B:771:GLU:HG3	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:877:ALA:HB3	1:A:890:ARG:NH1	2.23	0.53
1:A:1123:ARG:NH2	1:A:1360:ASN:OD1	2.42	0.53
10:J:10:CYS:SG	10:J:42:ARG:NH2	2.78	0.53
1:A:43:TYR:HB3	1:A:53:LYS:NZ	2.24	0.53
1:A:138:LYS:HG3	1:A:1441:GLU:OE2	2.09	0.53
5:E:134:GLU:OE2	5:E:181:ARG:NH2	2.42	0.53
1:A:1347:LEU:HD22	1:A:1354:PRO:HA	1.90	0.53
2:B:280:SER:OG	2:B:281:ASP:N	2.42	0.53
1:A:1212:LEU:HD22	1:A:1259:ILE:HD12	1.91	0.52
2:B:603:MET:HG3	2:B:614:ILE:HG12	1.91	0.52
7:G:138:GLN:N	7:G:141:ASP:OD2	2.29	0.52
1:A:1375:ARG:NH1	5:E:195:ARG:HH22	2.07	0.52
2:B:92:TYR:HB2	2:B:125:TYR:HB2	1.90	0.52
3:C:205:LYS:NZ	3:C:215:GLU:O	2.35	0.52
3:C:260:GLN:HB2	11:K:91:ILE:HG21	1.92	0.52
1:A:343:LEU:HA	1:A:349:ARG:H	1.74	0.52
2:B:872:THR:HA	2:B:889:LYS:HG2	1.89	0.52
2:B:225:LEU:HD22	2:B:228:SER:HB2	1.91	0.52
6:F:105:ILE:HG22	6:F:119:GLY:HA2	1.92	0.52
7:G:81:LYS:HD3	23:Z:473:LYS:NZ	2.24	0.52
20:W:297:GLU:OE1	20:W:299:HIS:NE2	2.43	0.52
23:Z:441:LEU:HB3	23:Z:451:MET:HB2	1.92	0.52
1:A:1005:HIS:HD2	1:A:1007:ILE:HG22	1.74	0.52
2:B:790:GLN:O	2:B:968:ASN:ND2	2.43	0.52
1:A:1546:PHE:HB3	13:M:1515:TYR:CZ	2.45	0.51
2:B:760:THR:OG1	2:B:764:MET:SD	2.62	0.51
1:A:106:VAL:HG22	1:A:236:LEU:HD11	1.93	0.51
1:A:508:SER:HB2	1:A:511:THR:HG22	1.92	0.51
1:A:866:LYS:HZ3	2:B:1091:ARG:HH22	1.58	0.51
1:A:1286:ARG:HH22	2:B:252:ILE:HA	1.75	0.51
3:C:67:ARG:NH1	10:J:3:ILE:O	2.40	0.51
1:A:1173:THR:HG22	1:A:1214:VAL:HG12	1.93	0.51
20:W:43:LEU:HD22	20:W:61:GLU:HG2	1.93	0.51
1:A:67:ARG:NE	15:P:35:A:OP1	2.44	0.51
3:C:10:ARG:HH22	3:C:228:ARG:HH22	1.59	0.51
2:B:939:HIS:NE2	2:B:983:GLU:OE1	2.38	0.50
22:Y:71:VAL:HG13	23:Z:264:LEU:HD11	1.93	0.50
1:A:197:GLU:OE2	1:A:308:LYS:NZ	2.45	0.50
5:E:80:PRO:HA	5:E:107:GLN:HB3	1.94	0.50
20:W:24:TRP:HE1	20:W:284:GLY:H	1.60	0.50
22:Y:14:ARG:HA	22:Y:55:SER:HA	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:592:PHE:HA	1:A:595:ILE:HD12	1.92	0.50
2:B:624:PRO:HA	2:B:663:GLU:O	2.11	0.50
7:G:101:ILE:HD11	7:G:145:LEU:HD11	1.94	0.50
1:A:190:ARG:HH12	1:A:192:ARG:HH22	1.59	0.50
2:B:1029:TYR:HA	2:B:1036:LYS:HA	1.94	0.50
1:A:489:THR:HG23	1:A:494:ALA:HB3	1.93	0.50
22:Y:7:PRO:HG3	22:Y:23:LYS:HA	1.94	0.50
1:A:583:ARG:NH1	3:C:222:PRO:O	2.45	0.50
1:A:1177:TYR:OH	1:A:1282:ASP:OD2	2.27	0.50
2:B:627:ILE:HD11	2:B:663:GLU:HG3	1.93	0.50
13:M:1462:ILE:HA	13:M:1473:LEU:O	2.12	0.50
1:A:228:ILE:O	1:A:244:ARG:NH2	2.34	0.49
3:C:47:ILE:HG22	3:C:165:ALA:HB2	1.94	0.49
1:A:613:GLU:OE2	1:A:623:PRO:HD2	2.12	0.49
1:A:913:ASN:N	1:A:1325:ASP:O	2.38	0.49
1:A:1347:LEU:HD21	1:A:1357:THR:HB	1.94	0.49
2:B:505:LEU:HD22	2:B:509:VAL:HB	1.94	0.49
2:B:626:LEU:HD23	2:B:662:VAL:HG12	1.95	0.49
23:Z:361:PHE:O	23:Z:365:ARG:HB2	2.12	0.49
1:A:67:ARG:HD3	1:A:68:THR:HG23	1.94	0.49
1:A:880:ARG:HG2	1:A:886:VAL:HA	1.95	0.49
2:B:1038:THR:HA	3:C:195:THR:HA	1.93	0.49
7:G:80:PHE:HD2	7:G:83:GLU:OE2	1.96	0.49
11:K:61:TYR:HA	11:K:72:ILE:O	2.13	0.49
5:E:74:VAL:HG12	5:E:103:LEU:HB2	1.95	0.49
23:Z:280:ARG:HH21	23:Z:288:ASP:HB3	1.78	0.49
8:H:72:ASP:HB3	8:H:74:GLU:H	1.77	0.49
11:K:85:GLU:HA	11:K:88:THR:HG22	1.94	0.49
1:A:244:ARG:HD2	1:A:245:PRO:HD2	1.94	0.49
1:A:1375:ARG:HH11	5:E:195:ARG:HH12	1.60	0.49
8:H:103:GLU:HB3	8:H:109:ALA:HB2	1.94	0.49
1:A:495:ASP:N	1:A:499:ASP:OD2	2.42	0.49
1:A:1533:PRO:HD3	13:M:1471:LYS:NZ	2.28	0.49
2:B:133:ILE:HB	2:B:139:GLN:HB3	1.94	0.49
2:B:1060:HIS:HB3	2:B:1078:ARG:HG3	1.94	0.49
3:C:72:PRO:HG3	10:J:13:ILE:HD11	1.95	0.49
5:E:19:GLN:OE1	5:E:138:ASN:ND2	2.41	0.49
7:G:8:GLU:HG2	7:G:71:LYS:HG2	1.95	0.49
9:I:97:PHE:HB2	9:I:100:HIS:HE2	1.76	0.49
20:W:165:SER:O	20:W:172:ILE:HA	2.12	0.49
1:A:790:GLN:HA	1:A:822:PHE:HA	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1374:VAL:HG11	1:A:1411:LEU:HD21	1.95	0.48
2:B:124:LEU:HD13	2:B:152:ILE:HD11	1.95	0.48
4:D:112:LYS:HD2	4:D:119:GLU:HG2	1.95	0.48
9:I:29:ASP:O	9:I:33:ARG:CA	2.61	0.48
1:A:296:ASN:OD1	1:A:297:GLY:N	2.46	0.48
2:B:130:LYS:O	2:B:141:GLN:HA	2.13	0.48
3:C:2:PRO:HB3	11:K:54:PRO:HD2	1.95	0.48
2:B:677:MET:H	2:B:682:LEU:HD22	1.79	0.48
2:B:733:MET:HE2	2:B:1052:LYS:HA	1.95	0.48
3:C:24:GLU:OE2	3:C:228:ARG:HG2	2.13	0.48
8:H:88:PHE:HD2	8:H:144:LEU:HD12	1.78	0.48
9:I:113:VAL:HG22	9:I:122:ARG:HG2	1.95	0.48
1:A:801:GLY:HA3	2:B:503:ASN:HB2	1.96	0.48
5:E:92:GLN:HG2	5:E:95:GLN:HE21	1.78	0.48
16:Q:863:LYS:HG2	16:Q:866:ARG:HH22	1.77	0.48
22:Y:90:THR:HG23	22:Y:112:ASP:OD2	2.13	0.48
1:A:500:GLU:OE2	2:B:1058:LYS:HD3	2.14	0.48
5:E:178:PRO:O	5:E:182:TYR:HB2	2.13	0.48
16:Q:791:ARG:HB3	20:W:106:PRO:HB3	1.96	0.48
7:G:30:LEU:HD22	7:G:70:VAL:HG11	1.95	0.48
23:Z:479:LYS:HG3	23:Z:489:THR:HG22	1.94	0.48
1:A:487:SER:OG	1:A:673:GLN:NE2	2.47	0.48
1:A:45:GLU:HB2	1:A:53:LYS:HZ3	1.78	0.48
3:C:183:ALA:HB3	3:C:232:ASN:HB3	1.95	0.48
4:D:34:ASN:O	4:D:68:THR:OG1	2.31	0.48
16:Q:786:LEU:HD21	16:Q:820:LEU:HB3	1.96	0.48
1:A:383:SER:H	11:K:2:ASN:HD21	1.61	0.48
2:B:864:ASP:OD1	23:Z:725:LYS:NZ	2.47	0.48
1:A:419:ILE:HG23	1:A:427:ILE:HB	1.94	0.48
2:B:272:VAL:O	2:B:276:LEU:HB2	2.14	0.48
20:W:126:HIS:HA	20:W:150:PHE:HD1	1.79	0.48
1:A:540:ASP:OD2	2:B:790:GLN:HG2	2.14	0.47
1:A:1528:TYR:CG	13:M:1469:PRO:HD2	2.49	0.47
1:A:1476:ASP:HB2	6:F:105:ILE:HG23	1.96	0.47
2:B:744:MET:SD	2:B:906:GLN:NE2	2.79	0.47
1:A:36:VAL:HG23	2:B:1138:ARG:NH1	2.29	0.47
22:Y:56:SER:HB3	23:Z:271:ALA:HA	1.96	0.47
1:A:451:CYS:SG	1:A:452:ASP:N	2.87	0.47
2:B:341:GLU:HG3	2:B:345:LYS:NZ	2.29	0.47
14:N:42:DT:O4	17:T:6:DC:N4	2.47	0.47
1:A:855:ALA:HB3	2:B:494:LYS:HZ1	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:88:PHE:HZ	2:B:412:LEU:HD21	1.80	0.47
10:J:35:LEU:HD11	10:J:50:LEU:HD12	1.95	0.47
5:E:194:ILE:HG13	5:E:204:ILE:HG22	1.95	0.47
11:K:82:SER:HB3	11:K:85:GLU:HG2	1.97	0.47
23:Z:490:GLY:HA3	23:Z:502:LEU:HD13	1.97	0.47
1:A:233:CYS:HA	1:A:236:LEU:HB3	1.95	0.47
1:A:861:GLN:HE22	1:A:1093:GLN:HA	1.80	0.47
1:A:1027:ASP:OD1	1:A:1027:ASP:N	2.46	0.47
2:B:949:TYR:HB3	2:B:953:ASP:HB2	1.96	0.47
6:F:79:VAL:HG22	6:F:81:VAL:H	1.78	0.47
7:G:151:ARG:HE	23:Z:491:LEU:HG	1.80	0.47
20:W:83:SER:OG	20:W:85:ASP:OD1	2.24	0.47
1:A:77:ASN:H	1:A:80:GLU:HB3	1.79	0.47
1:A:1467:GLY:H	1:A:1470:CYS:HB2	1.80	0.47
5:E:56:THR:OG1	5:E:78:GLU:OE2	2.21	0.47
14:N:35:DA:OP2	14:N:35:DA:H2'	2.15	0.47
1:A:190:ARG:NH1	1:A:192:ARG:HH22	2.12	0.47
2:B:117:ASN:ND2	2:B:188:ASN:O	2.39	0.47
4:D:84:ARG:O	4:D:88:LEU:HB2	2.15	0.47
23:Z:216:VAL:HB	23:Z:226:TYR:HB2	1.97	0.47
23:Z:588:ASP:OD1	23:Z:592:ASN:N	2.42	0.47
23:Z:714:GLN:HB2	23:Z:749:ARG:HG2	1.97	0.47
1:A:1123:ARG:HG2	1:A:1385:VAL:HG11	1.98	0.46
2:B:570:ASN:HD21	2:B:616:THR:HB	1.80	0.46
16:Q:430:ALA:O	16:Q:434:TYR:N	2.47	0.46
2:B:819:SER:HG	2:B:821:LYS:N	2.13	0.46
17:T:24:DG:H2'	17:T:25:DA:C8	2.50	0.46
2:B:994:GLY:HA2	10:J:50:LEU:HD11	1.96	0.46
9:I:29:ASP:O	9:I:33:ARG:N	2.48	0.46
17:T:33:DC:H2''	17:T:34:DT:H5''	1.96	0.46
1:A:880:ARG:NH1	6:F:111:PRO:HB2	2.31	0.46
2:B:157:ARG:NH2	2:B:177:CYS:O	2.46	0.46
1:A:96:HIS:HB2	1:A:250:VAL:HG23	1.98	0.46
2:B:934:LYS:HG2	2:B:1051:LEU:HD12	1.96	0.46
7:G:127:CYS:SG	7:G:128:TYR:N	2.89	0.46
1:A:329:MET:HA	1:A:335:PRO:HA	1.96	0.46
1:A:1375:ARG:NH1	5:E:195:ARG:HH12	2.13	0.46
2:B:905:ASP:HB2	2:B:924:ARG:HG3	1.97	0.46
2:B:1069:ILE:HD11	15:P:37:G:OP1	2.16	0.46
1:A:43:TYR:HB3	1:A:53:LYS:HZ2	1.81	0.46
1:A:866:LYS:HZ3	2:B:1091:ARG:NH2	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1066:PRO:HB3	15:P:35:A:H62	1.80	0.46
3:C:42:VAL:HB	3:C:178:PRO:HG3	1.98	0.46
5:E:44:PHE:HB3	5:E:53:PRO:HB3	1.97	0.46
13:M:1357:ILE:HG12	13:M:1369:VAL:HG22	1.98	0.46
1:A:358:ARG:HH12	17:T:27:DT:P	2.38	0.46
2:B:252:ILE:HG22	2:B:303:PRO:HB3	1.98	0.46
23:Z:472:PHE:HE1	23:Z:520:LEU:HB2	1.81	0.46
8:H:16:ASP:HA	8:H:17:PRO:HD3	1.80	0.46
13:M:1511:PHE:O	13:M:1515:TYR:N	2.48	0.46
17:T:39:DC:H2"	17:T:40:DT:H72	1.98	0.46
7:G:80:PHE:HB2	7:G:83:GLU:HG3	1.98	0.45
1:A:1004:LEU:HD13	1:A:1062:GLY:HA2	1.98	0.45
1:A:1170:THR:HA	1:A:1216:LEU:HA	1.99	0.45
2:B:274:ARG:NH1	2:B:312:GLN:HA	2.31	0.45
1:A:375:ILE:HD13	1:A:669:TYR:HD2	1.81	0.45
3:C:44:ILE:HD12	3:C:178:PRO:HB3	1.97	0.45
8:H:63:THR:HB	8:H:70:LEU:HD23	1.97	0.45
10:J:40:LEU:HD22	10:J:45:CYS:HB3	1.98	0.45
23:Z:352:VAL:HG23	23:Z:359:LEU:HD21	1.98	0.45
1:A:93:PRO:HB3	1:A:249:ILE:HD13	1.98	0.45
23:Z:479:LYS:NZ	23:Z:521:CYS:O	2.50	0.45
1:A:228:ILE:HG23	1:A:232:GLU:HG2	1.99	0.45
1:A:1529:GLY:H	13:M:1396:ALA:HB2	1.81	0.45
8:H:25:VAL:HG21	8:H:121:LEU:HD22	1.96	0.45
2:B:54:SER:HA	2:B:57:ARG:HG2	1.99	0.45
7:G:138:GLN:HG2	7:G:141:ASP:OD2	2.16	0.45
1:A:889:LEU:O	1:A:890:ARG:NE	2.48	0.45
1:A:1282:ASP:N	1:A:1282:ASP:OD1	2.47	0.45
20:W:193:ILE:HA	20:W:209:SER:HA	1.99	0.45
22:Y:94:PRO:HD2	22:Y:97:ILE:HD12	1.98	0.45
1:A:244:ARG:HB3	1:A:247:TRP:CD2	2.52	0.45
1:A:502:ASN:OD1	1:A:502:ASN:N	2.46	0.45
2:B:1062:ARG:NH1	2:B:1081:ASP:O	2.49	0.45
13:M:1426:LEU:HD22	13:M:1462:ILE:HD13	1.99	0.45
23:Z:433:LEU:HD13	23:Z:461:LEU:HD13	1.97	0.45
2:B:1062:ARG:HH12	2:B:1066:PRO:HD2	1.82	0.45
11:K:89:ASN:HA	11:K:92:THR:HG22	1.99	0.45
1:A:480:SER:HB3	11:K:2:ASN:HB2	1.99	0.44
1:A:628:VAL:HA	1:A:638:GLY:HA3	1.99	0.44
16:Q:882:VAL:HA	16:Q:885:THR:HG22	1.98	0.44
16:Q:839:ARG:HA	16:Q:842:ARG:HG2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:Z:554:GLU:OE1	23:Z:557:THR:OG1	2.36	0.44
1:A:906:LEU:HD23	1:A:1044:HIS:HD2	1.82	0.44
5:E:70:ASP:OD1	5:E:70:ASP:N	2.49	0.44
16:Q:817:CYS:SG	16:Q:818:SER:N	2.91	0.44
7:G:39:THR:HG23	7:G:42:TYR:H	1.82	0.44
1:A:526:VAL:HA	1:A:533:PRO:HA	1.99	0.44
2:B:98:HIS:CE1	2:B:116:ARG:NH1	2.85	0.44
17:T:30:DG:H2'	17:T:31:DT:C6	2.53	0.44
1:A:696:SER:HA	1:A:699:TYR:HB2	1.98	0.44
1:A:1217:ASP:OD2	1:A:1220:HIS:HD2	2.01	0.44
2:B:907:VAL:HG22	2:B:921:ILE:HG12	1.99	0.44
2:B:1112:ASP:OD1	2:B:1112:ASP:N	2.48	0.44
2:B:206:TYR:HA	2:B:383:ASP:OD2	2.17	0.44
7:G:81:LYS:HD3	23:Z:473:LYS:HZ1	1.81	0.44
16:Q:667:ARG:O	16:Q:671:ALA:N	2.51	0.44
1:A:1093:GLN:HE22	2:B:1093:CYS:HA	1.83	0.44
3:C:78:ILE:HD11	3:C:126:ARG:HD2	1.99	0.44
1:A:454:ASP:HA	1:A:512:ARG:HH22	1.83	0.44
1:A:510:GLU:HG3	6:F:67:GLY:HA3	2.00	0.44
1:A:552:ASP:HB3	8:H:25:VAL:HG12	2.00	0.44
1:A:896:LEU:HD13	1:A:980:PRO:HG3	1.98	0.44
1:A:912:SER:HB3	1:A:915:ALA:H	1.83	0.44
1:A:912:SER:O	1:A:963:ARG:NH2	2.51	0.43
2:B:778:SER:O	2:B:1045:PRO:HA	2.18	0.43
3:C:175:LYS:HZ3	12:L:57:ALA:HB3	1.83	0.43
1:A:120:ASP:O	1:A:123:ASN:N	2.52	0.43
7:G:45:VAL:HG22	7:G:76:VAL:HG12	2.00	0.43
13:M:1422:PHE:HB3	13:M:1494:PHE:CE1	2.54	0.43
1:A:852:VAL:HG13	2:B:494:LYS:HD3	2.00	0.43
1:A:533:PRO:O	1:A:647:THR:OG1	2.29	0.43
1:A:253:LEU:HD12	1:A:254:PRO:HD2	2.00	0.43
1:A:1211:LEU:HB3	1:A:1260:ARG:NH1	2.33	0.43
2:B:330:VAL:HG13	2:B:331:THR:HG23	2.00	0.43
13:M:1450:THR:HB	13:M:1459:PRO:HG3	2.00	0.43
16:Q:770:LYS:O	16:Q:827:HIS:NE2	2.52	0.43
2:B:212:ASP:OD1	2:B:212:ASP:N	2.51	0.43
1:A:350:VAL:HA	1:A:354:LEU:HD12	2.00	0.43
1:A:496:PHE:HB2	2:B:791:GLU:O	2.19	0.43
1:A:833:PRO:HG3	2:B:1002:PHE:CG	2.53	0.43
1:A:1295:ASP:OD1	1:A:1295:ASP:N	2.51	0.43
1:A:364:ARG:NE	1:A:500:GLU:OE1	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:ARG:HD2	2:B:1084:LEU:HD11	2.00	0.43
1:A:1468:THR:HG23	6:F:64:ARG:HB2	1.99	0.43
1:A:1474:LEU:HB2	6:F:105:ILE:HG13	2.00	0.43
5:E:24:ARG:NH2	5:E:182:TYR:O	2.42	0.43
13:M:1364:GLU:OE1	13:M:1365:ASN:ND2	2.52	0.43
19:V:204:UNK:O	19:V:332:UNK:N	2.52	0.43
1:A:1118:THR:O	1:A:1123:ARG:HB2	2.19	0.43
3:C:105:VAL:HG11	3:C:115:VAL:HG22	2.01	0.43
7:G:13:LEU:O	7:G:65:PHE:HA	2.19	0.43
7:G:52:ASP:H	7:G:72:TYR:HA	1.84	0.43
22:Y:14:ARG:HG2	22:Y:55:SER:HB3	2.01	0.43
2:B:388:TYR:HE1	2:B:391:LYS:HZ2	1.65	0.42
3:C:162:ARG:NH1	3:C:164:TYR:HE2	2.17	0.42
5:E:120:ASP:OD1	5:E:121:MET:N	2.52	0.42
8:H:16:ASP:OD1	8:H:16:ASP:N	2.52	0.42
2:B:132:VAL:O	2:B:139:GLN:HA	2.18	0.42
2:B:591:ARG:HE	2:B:603:MET:HE2	1.84	0.42
2:B:937:SER:OG	2:B:938:ARG:N	2.52	0.42
4:D:60:VAL:HG11	7:G:44:PHE:CE2	2.54	0.42
16:Q:497:VAL:O	16:Q:501:TYR:N	2.51	0.42
3:C:77:ASP:N	3:C:77:ASP:OD1	2.52	0.42
10:J:64:PRO:O	12:L:23:HIS:NE2	2.48	0.42
11:K:4:PRO:HA	11:K:5:PRO:HD3	1.91	0.42
1:A:1375:ARG:HD2	5:E:195:ARG:NH1	2.34	0.42
2:B:124:LEU:HD22	2:B:152:ILE:HG13	2.01	0.42
2:B:789:ASN:HB3	2:B:795:ILE:HG13	2.01	0.42
2:B:830:GLU:OE2	2:B:889:LYS:NZ	2.36	0.42
2:B:873:LEU:HD12	2:B:874:PRO:HD2	2.00	0.42
3:C:240:ARG:HB2	3:C:243:THR:HG22	2.02	0.42
11:K:58:PHE:HB3	11:K:76:GLN:HB3	2.01	0.42
13:M:824:GLU:N	15:P:29:C:OP2	2.53	0.42
16:Q:496:SER:O	16:Q:500:SER:N	2.43	0.42
1:A:873:VAL:HG23	1:A:1087:VAL:HG21	2.02	0.42
1:A:901:VAL:HA	1:A:980:PRO:HA	2.02	0.42
1:A:1525:TPO:O1P	13:M:1340:PHE:HB2	2.20	0.42
2:B:731:GLN:NE2	15:P:44:A:O3'	2.53	0.42
4:D:70:ARG:HH12	7:G:88:VAL:HG11	1.82	0.42
4:D:70:ARG:NH1	7:G:88:VAL:HG11	2.34	0.42
5:E:26:TYR:HA	5:E:64:HIS:HA	2.01	0.42
8:H:15:ILE:HD12	8:H:15:ILE:HA	1.97	0.42
20:W:189:HIS:CE1	20:W:215:LYS:HD2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:HIS:HA	1:A:316:THR:HG22	2.01	0.42
2:B:581:GLU:OE2	2:B:585:ASN:ND2	2.52	0.42
20:W:65:LEU:HD12	20:W:85:ASP:HB3	2.02	0.42
1:A:769:MET:SD	2:B:973:PRO:HG3	2.60	0.42
1:A:1215:GLU:OE2	1:A:1256:VAL:HG22	2.20	0.42
2:B:770:ARG:NH1	2:B:771:GLU:HG3	2.34	0.42
23:Z:639:LYS:HB2	23:Z:642:HIS:CD2	2.52	0.42
1:A:406:VAL:HG13	1:A:429:LEU:HD21	2.02	0.42
3:C:47:ILE:HG23	3:C:73:LEU:HD11	2.00	0.42
7:G:110:ARG:HG3	7:G:119:PHE:CZ	2.55	0.42
1:A:544:ALA:O	1:A:548:PHE:HB2	2.20	0.42
1:A:1180:ASN:ND2	1:A:1182:GLN:HE21	2.18	0.42
2:B:785:TYR:CZ	2:B:955:PRO:HD3	2.55	0.42
8:H:71:ASP:N	8:H:71:ASP:OD1	2.53	0.42
1:A:658:LEU:HD23	1:A:658:LEU:HA	1.88	0.42
5:E:24:ARG:NE	5:E:183:PHE:O	2.53	0.42
10:J:66:GLU:HG2	12:L:18:ILE:HD13	2.02	0.42
20:W:237:ASN:HB3	20:W:280:VAL:HG22	2.01	0.42
23:Z:212:ILE:HG22	23:Z:229:ALA:HB2	2.02	0.42
1:A:481:THR:HG22	2:B:1055:VAL:HG21	2.01	0.41
2:B:796:MET:HB2	2:B:948:GLN:HG2	2.02	0.41
2:B:801:VAL:HG13	2:B:929:PRO:HD2	2.02	0.41
2:B:870:THR:HA	2:B:891:ASP:HA	2.01	0.41
5:E:101:ARG:HD3	5:E:126:ILE:HG13	2.01	0.41
5:E:156:VAL:HG22	5:E:190:VAL:HG12	2.01	0.41
1:A:279:LYS:HZ1	1:A:328:ALA:CB	2.34	0.41
1:A:461:GLN:HG2	17:T:26:DG:H1'	2.02	0.41
1:A:1213:ARG:NE	1:A:1215:GLU:OE2	2.52	0.41
2:B:513:GLU:HG2	2:B:525:ASN:HD22	1.85	0.41
2:B:735:VAL:HG23	2:B:754:PRO:HG2	2.01	0.41
1:A:691:ASP:OD2	1:A:765:ASN:HB2	2.20	0.41
2:B:474:THR:OG1	2:B:732:ALA:O	2.33	0.41
1:A:1547:SEP:O	1:A:1547:SEP:OG	2.39	0.41
2:B:513:GLU:HG3	2:B:726:SER:HB3	2.03	0.41
2:B:601:VAL:HG22	2:B:616:THR:HG23	2.01	0.41
1:A:59:ASP:HB3	1:A:62:GLN:HB2	2.02	0.41
1:A:570:TRP:O	11:K:26:LYS:NZ	2.41	0.41
17:T:27:DT:H2'	17:T:28:DG:H8	1.85	0.41
1:A:876:ASP:HB2	1:A:878:THR:HG22	2.02	0.41
1:A:1117:VAL:HG23	1:A:1119:LEU:HG	2.03	0.41
13:M:749:LEU:O	13:M:753:LEU:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:757:VAL:HA	16:Q:796:LEU:HD12	2.01	0.41
20:W:146:THR:HG22	20:W:182:LEU:HD22	2.03	0.41
1:A:505:LEU:HD12	1:A:506:PRO:HD2	2.03	0.41
1:A:1157:ILE:HD12	1:A:1160:ARG:HH11	1.85	0.41
1:A:1347:LEU:HB3	5:E:137:ILE:HD12	2.03	0.41
1:A:1547:SEP:HA	1:A:1548:PRO:HD3	1.74	0.41
2:B:67:LEU:HD11	2:B:416:ARG:HG3	2.02	0.41
16:Q:763:ARG:NH1	20:W:65:LEU:HD11	2.34	0.41
1:A:126:ILE:HD11	1:A:147:LEU:HD22	2.02	0.41
1:A:935:GLN:HB2	1:A:938:LEU:HD13	2.03	0.41
1:A:1132:LYS:HE3	1:A:1363:VAL:HG11	2.03	0.41
1:A:1307:VAL:HG13	1:A:1338:THR:HG22	2.02	0.41
2:B:903:ILE:O	2:B:924:ARG:N	2.54	0.41
7:G:93:ASN:HB3	7:G:96:GLY:H	1.85	0.41
23:Z:420:PHE:CD1	23:Z:470:LYS:HE3	2.56	0.41
1:A:610:PRO:HG2	1:A:613:GLU:HB2	2.03	0.41
2:B:807:ARG:NH1	3:C:66:HIS:CD2	2.89	0.41
3:C:84:TYR:CZ	3:C:167:LYS:HE3	2.56	0.41
4:D:111:SER:HB2	4:D:131:LEU:HD21	2.02	0.41
1:A:983:LEU:HD23	1:A:983:LEU:HA	1.89	0.41
1:A:1443:ALA:HB2	2:B:1167:ILE:HG23	2.02	0.41
2:B:956:PHE:HB3	2:B:962:THR:HG22	2.03	0.41
4:D:104:CYS:SG	4:D:135:GLN:NE2	2.93	0.41
1:A:141:LEU:HD13	1:A:1445:HIS:HE1	1.86	0.40
1:A:465:HIS:CD2	1:A:467:MET:HB2	2.57	0.40
1:A:1546:PHE:HB3	13:M:1515:TYR:CE1	2.56	0.40
2:B:556:ILE:H	2:B:556:ILE:HG13	1.61	0.40
2:B:561:ILE:HD11	2:B:573:TRP:HH2	1.86	0.40
3:C:13:GLU:HB3	3:C:20:LYS:HB3	2.02	0.40
1:A:1533:PRO:HD3	13:M:1471:LYS:HZ3	1.86	0.40
2:B:86:LEU:HD23	2:B:130:LYS:HB3	2.03	0.40
3:C:189:ASP:O	3:C:191:ALA:N	2.55	0.40
16:Q:390:ASP:O	16:Q:394:ARG:N	2.53	0.40
1:A:859:TYR:OH	1:A:1433:GLU:OE2	2.30	0.40
12:L:16:ILE:HG12	12:L:27:GLU:HG2	2.03	0.40
20:W:233:SER:OG	20:W:234:TRP:N	2.52	0.40
1:A:73:THR:OG1	1:A:74:CYS:N	2.52	0.40
2:B:998:ASP:OD2	2:B:1000:THR:HG22	2.21	0.40
3:C:175:LYS:HZ2	12:L:57:ALA:HB3	1.86	0.40
1:A:54:LEU:CB	1:A:61:ARG:HH12	2.31	0.40
1:A:863:ARG:NH1	1:A:1129:ASN:HD21	2.19	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1375:ARG:HH12	5:E:195:ARG:HH22	1.69	0.40
23:Z:427:GLU:OE2	23:Z:469:ARG:NH2	2.55	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1425/1970 (72%)	1340 (94%)	82 (6%)	3 (0%)	44	74
2	B	1122/1174 (96%)	1062 (95%)	59 (5%)	1 (0%)	48	79
3	C	259/275 (94%)	245 (95%)	14 (5%)	0	100	100
4	D	124/142 (87%)	122 (98%)	2 (2%)	0	100	100
5	E	207/210 (99%)	199 (96%)	7 (3%)	1 (0%)	25	58
6	F	80/127 (63%)	78 (98%)	2 (2%)	0	100	100
7	G	169/172 (98%)	165 (98%)	4 (2%)	0	100	100
8	H	146/150 (97%)	135 (92%)	11 (8%)	0	100	100
9	I	115/125 (92%)	107 (93%)	8 (7%)	0	100	100
10	J	65/67 (97%)	64 (98%)	1 (2%)	0	100	100
11	K	113/117 (97%)	109 (96%)	4 (4%)	0	100	100
12	L	44/58 (76%)	38 (86%)	6 (14%)	0	100	100
13	M	970/1726 (56%)	918 (95%)	52 (5%)	0	100	100
16	Q	581/1178 (49%)	555 (96%)	25 (4%)	1 (0%)	44	74
20	W	298/305 (98%)	278 (93%)	20 (7%)	0	100	100
22	Y	114/121 (94%)	114 (100%)	0	0	100	100
23	Z	476/1087 (44%)	466 (98%)	9 (2%)	1 (0%)	44	74
All	All	6308/9004 (70%)	5995 (95%)	306 (5%)	7 (0%)	50	79

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	57	ASP
1	A	911	PRO
2	B	492	ASP
1	A	540	ASP
23	Z	506	LEU
1	A	121	SER
16	Q	301	VAL

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1257/1747 (72%)	1242 (99%)	15 (1%)	67	83
2	B	992/1027 (97%)	985 (99%)	7 (1%)	81	90
3	C	240/252 (95%)	239 (100%)	1 (0%)	89	94
4	D	109/126 (86%)	108 (99%)	1 (1%)	75	88
5	E	191/192 (100%)	189 (99%)	2 (1%)	73	86
6	F	71/111 (64%)	69 (97%)	2 (3%)	38	66
7	G	146/153 (95%)	141 (97%)	5 (3%)	32	62
8	H	129/131 (98%)	129 (100%)	0	100	100
9	I	105/112 (94%)	105 (100%)	0	100	100
10	J	56/56 (100%)	56 (100%)	0	100	100
11	K	104/106 (98%)	104 (100%)	0	100	100
12	L	43/55 (78%)	43 (100%)	0	100	100
13	M	154/1514 (10%)	153 (99%)	1 (1%)	84	91
16	Q	121/752 (16%)	120 (99%)	1 (1%)	79	89
20	W	255/260 (98%)	254 (100%)	1 (0%)	89	94
22	Y	102/105 (97%)	102 (100%)	0	100	100
23	Z	427/940 (45%)	426 (100%)	1 (0%)	92	96

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	4502/7639 (59%)	4465 (99%)	37 (1%)	77	89

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	MET
1	A	117	LEU
1	A	134	LYS
1	A	292	ARG
1	A	309	LEU
1	A	410	ASN
1	A	557	ARG
1	A	744	ILE
1	A	760	LEU
1	A	928	ARG
1	A	1194	ASN
1	A	1213	ARG
1	A	1248	ASN
1	A	1375	ARG
1	A	1484	MET
2	B	83	ARG
2	B	638	ARG
2	B	770	ARG
2	B	1080	ARG
2	B	1091	ARG
2	B	1104	ARG
2	B	1120	ASN
3	C	263	LEU
4	D	48	ASN
5	E	52	ARG
5	E	94	MET
6	F	62	ARG
6	F	123	LEU
7	G	53	ASN
7	G	78	ARG
7	G	93	ASN
7	G	108	ILE
7	G	110	ARG
13	M	1515	TYR
16	Q	775	ASN
20	W	237	ASN
23	Z	338	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	313	HIS
1	A	678	ASN
1	A	757	GLN
1	A	861	GLN
1	A	884	ASN
1	A	1005	HIS
1	A	1082	HIS
1	A	1108	HIS
1	A	1182	GLN
1	A	1194	ASN
1	A	1220	HIS
1	A	1248	ASN
2	B	23	GLN
2	B	98	HIS
2	B	344	GLN
2	B	725	GLN
2	B	1053	HIS
2	B	1120	ASN
3	C	66	HIS
3	C	145	GLN
4	D	135	GLN
5	E	95	GLN
7	G	53	ASN
7	G	93	ASN
9	I	22	ASN
9	I	41	ASN
13	M	1365	ASN
13	M	1514	HIS
16	Q	756	ASN
16	Q	775	ASN
20	W	126	HIS
20	W	189	HIS
20	W	221	HIS
20	W	273	HIS
22	Y	12	HIS
23	Z	272	ASN
23	Z	519	GLN

### 5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
15	P	20/46 (43%)	8 (40%)	3 (15%)

All (8) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
15	P	27	A
15	P	29	C
15	P	30	C
15	P	31	G
15	P	33	A
15	P	36	G
15	P	37	G
15	P	39	A

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
15	P	28	A
15	P	36	G
15	P	38	G

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

2 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	1,13	8,9,10	1.69	2 (25%)	8,12,14	2.36	2 (25%)
1	TPO	A	1525	1	8,10,11	1.52	1 (12%)	10,14,16	2.02	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	1,13	-	1/5/8/10	-
1	TPO	A	1525	1	-	0/9/11/13	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1547	SEP	P-O1P	3.57	1.62	1.50
1	A	1525	TPO	P-O1P	3.24	1.61	1.50
1	A	1547	SEP	P-O2P	2.00	1.62	1.54

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1525	TPO	P-OG1-CB	-5.99	105.11	123.21
1	A	1547	SEP	P-OG-CB	-5.94	101.94	118.30
1	A	1547	SEP	OG-CB-CA	2.46	110.53	108.14

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1547	SEP	N-CA-CB-OG

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1547	SEP	2	0
1	A	1525	TPO	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 10 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

There are no such residues in this entry.

## 5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
18	U	3
19	V	3
13	M	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	U	492:UNK	C	498:UNK	N	29.01
1	V	293:UNK	C	307:UNK	N	14.62
1	U	429:UNK	C	448:UNK	N	12.83
1	V	227:UNK	C	250:UNK	N	9.56
1	V	260:UNK	C	285:UNK	N	6.58
1	M	1334:UNK	C	1338:ILE	N	6.19
1	U	397:UNK	C	416:UNK	N	3.22

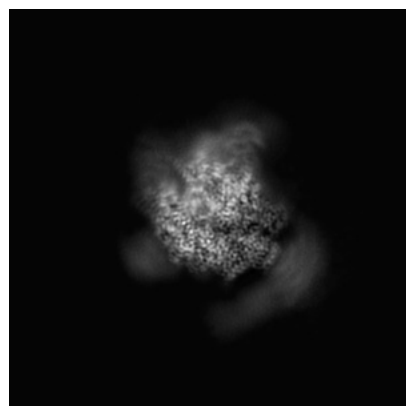
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0031. These allow visual inspection of the internal detail of the map and identification of artifacts.

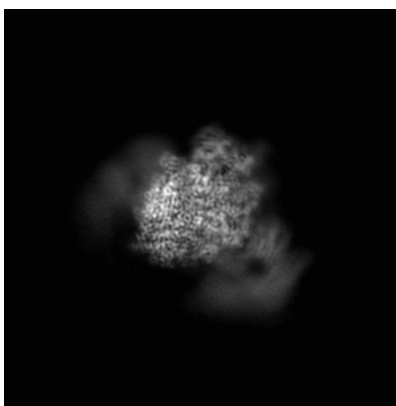
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

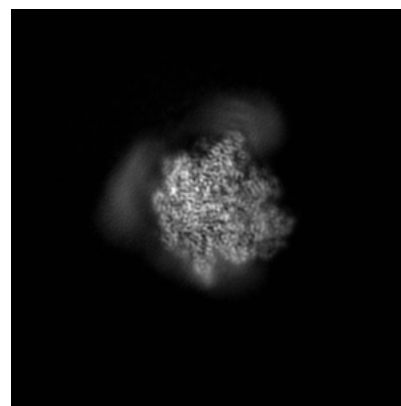
#### 6.1.1 Primary map



X

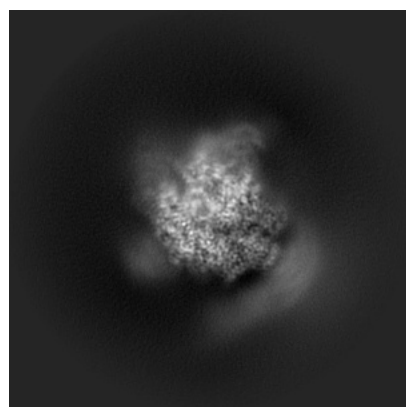


Y

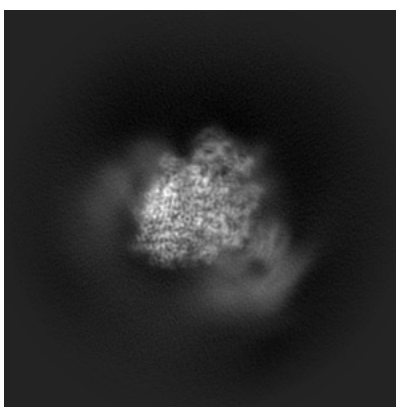


Z

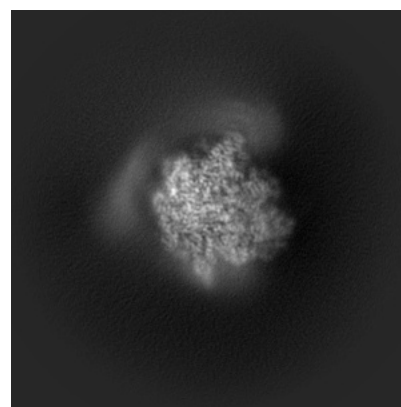
#### 6.1.2 Raw map



X



Y

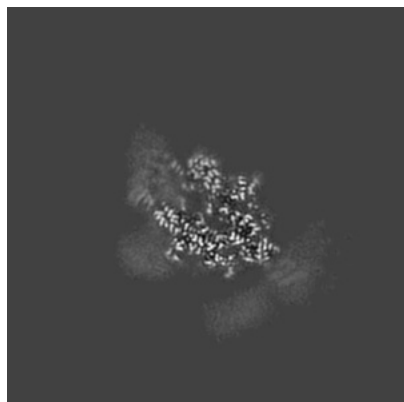


Z

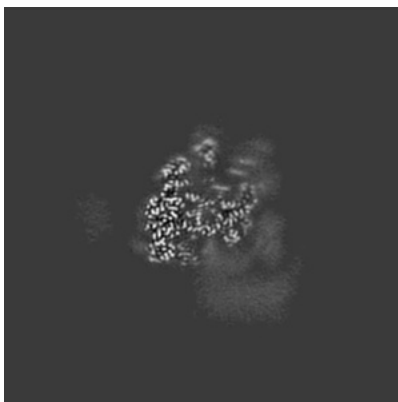
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

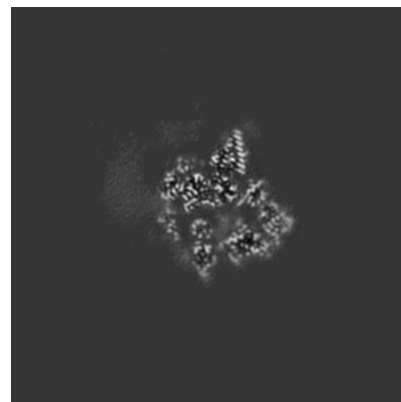
### 6.2.1 Primary map



X Index: 180

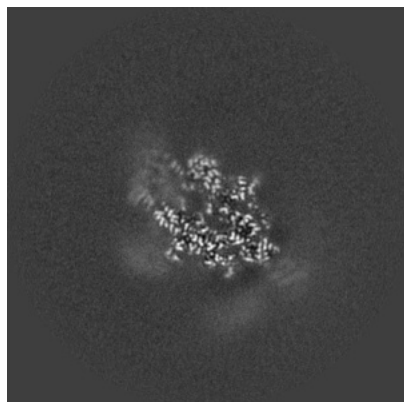


Y Index: 180

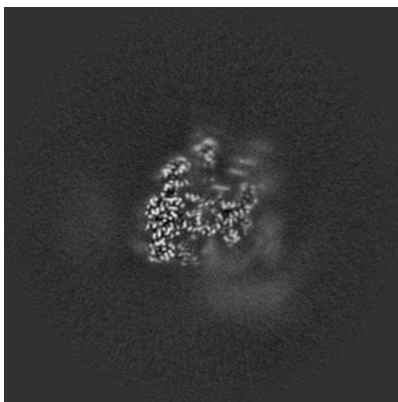


Z Index: 180

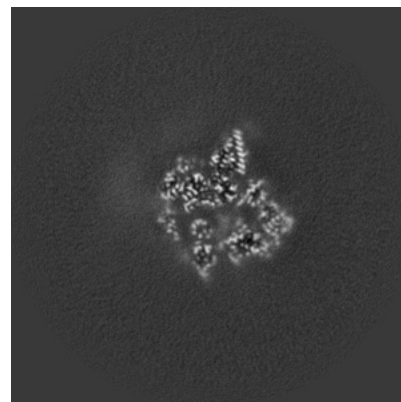
### 6.2.2 Raw map



X Index: 180



Y Index: 180

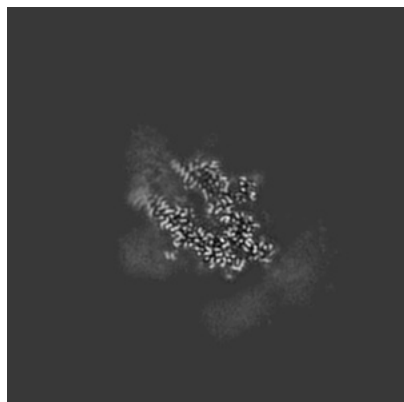


Z Index: 180

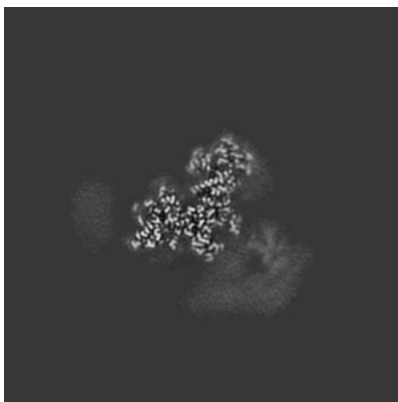
The images above show central slices of the map in three orthogonal directions.

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

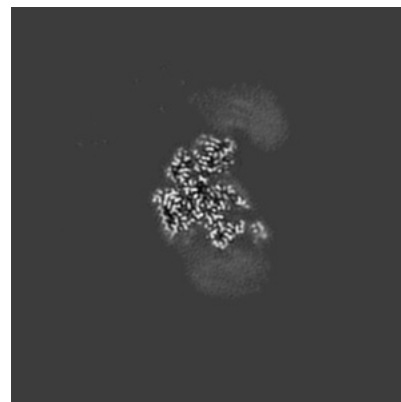
### 6.3.1 Primary map



X Index: 177

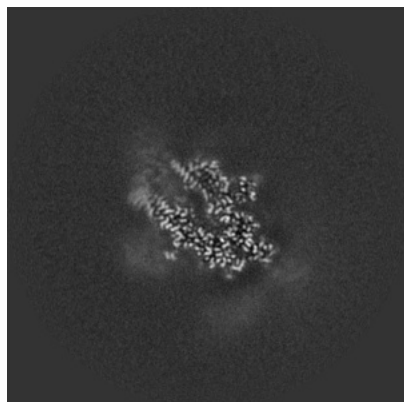


Y Index: 198

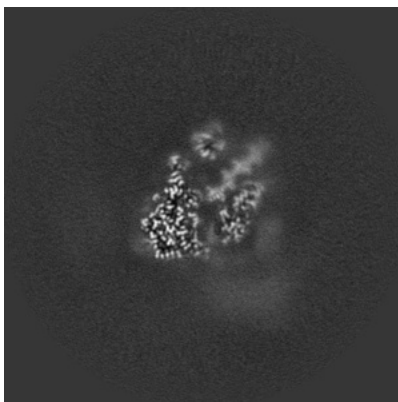


Z Index: 143

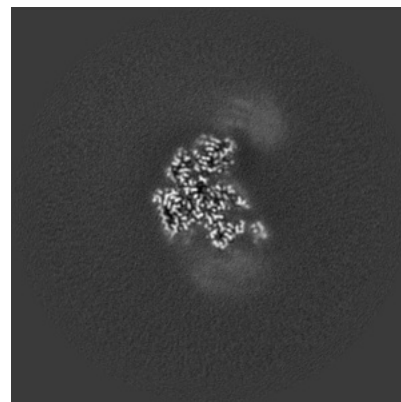
### 6.3.2 Raw map



X Index: 177



Y Index: 173

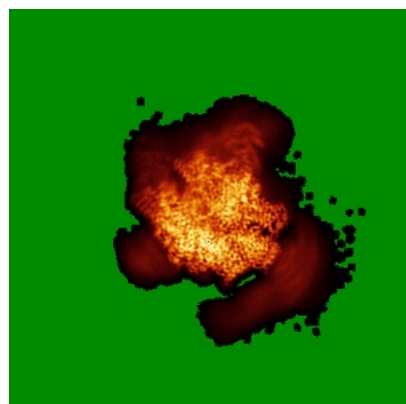


Z Index: 143

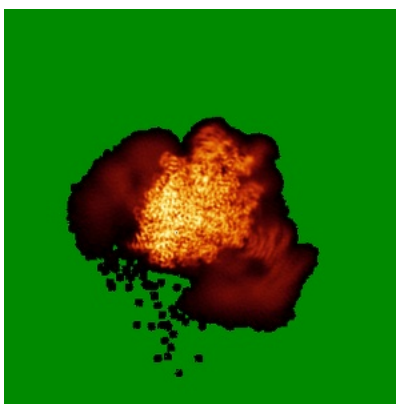
The images above show the largest variance slices of the map in three orthogonal directions.

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

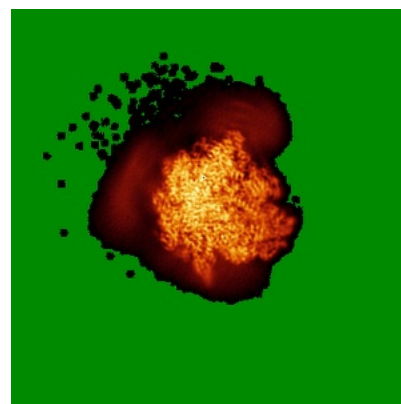
### 6.4.1 Primary map



X

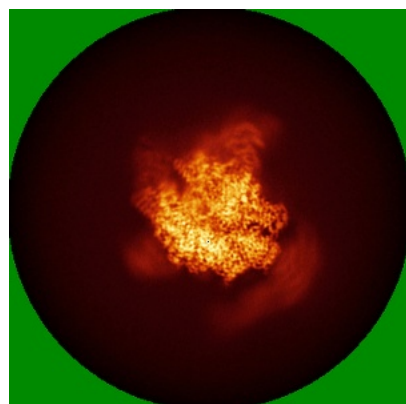


Y

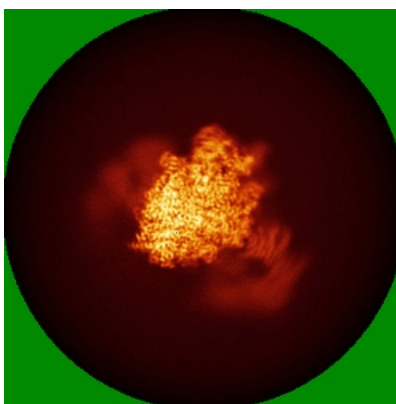


Z

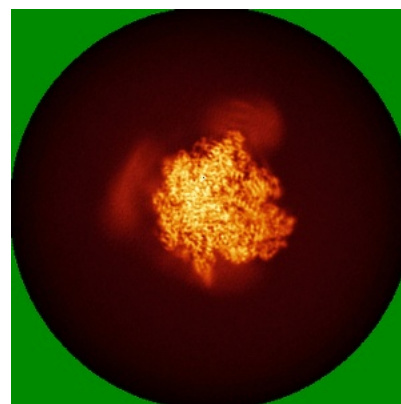
### 6.4.2 Raw map



X



Y

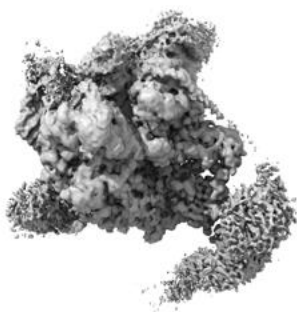


Z

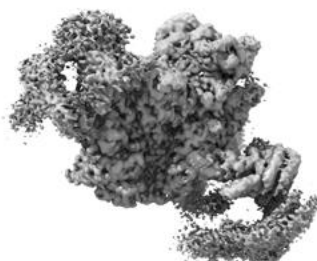
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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

### 6.5.1 Primary map



X



Y



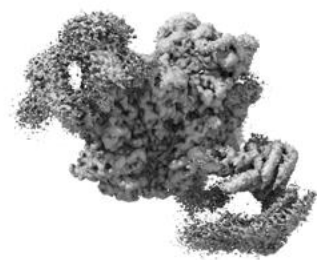
Z

The images above show the 3D surface view of the map at the recommended contour level 0.0157. 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.

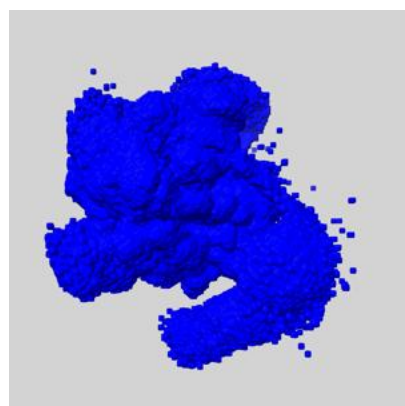
## 6.6 Mask visualisation [i](#)

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

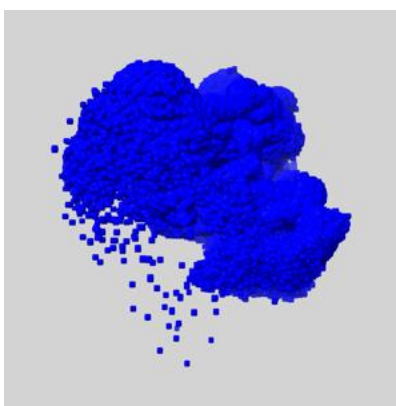
A mask typically either:

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

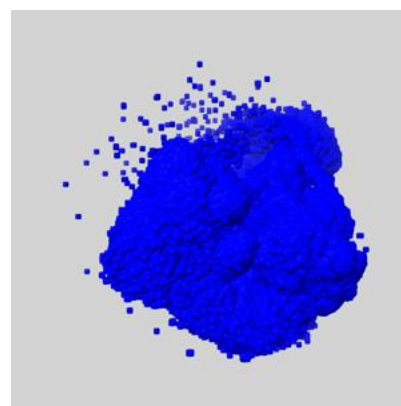
### 6.6.1 emd\_0031\_msk\_1.map [i](#)



X



Y



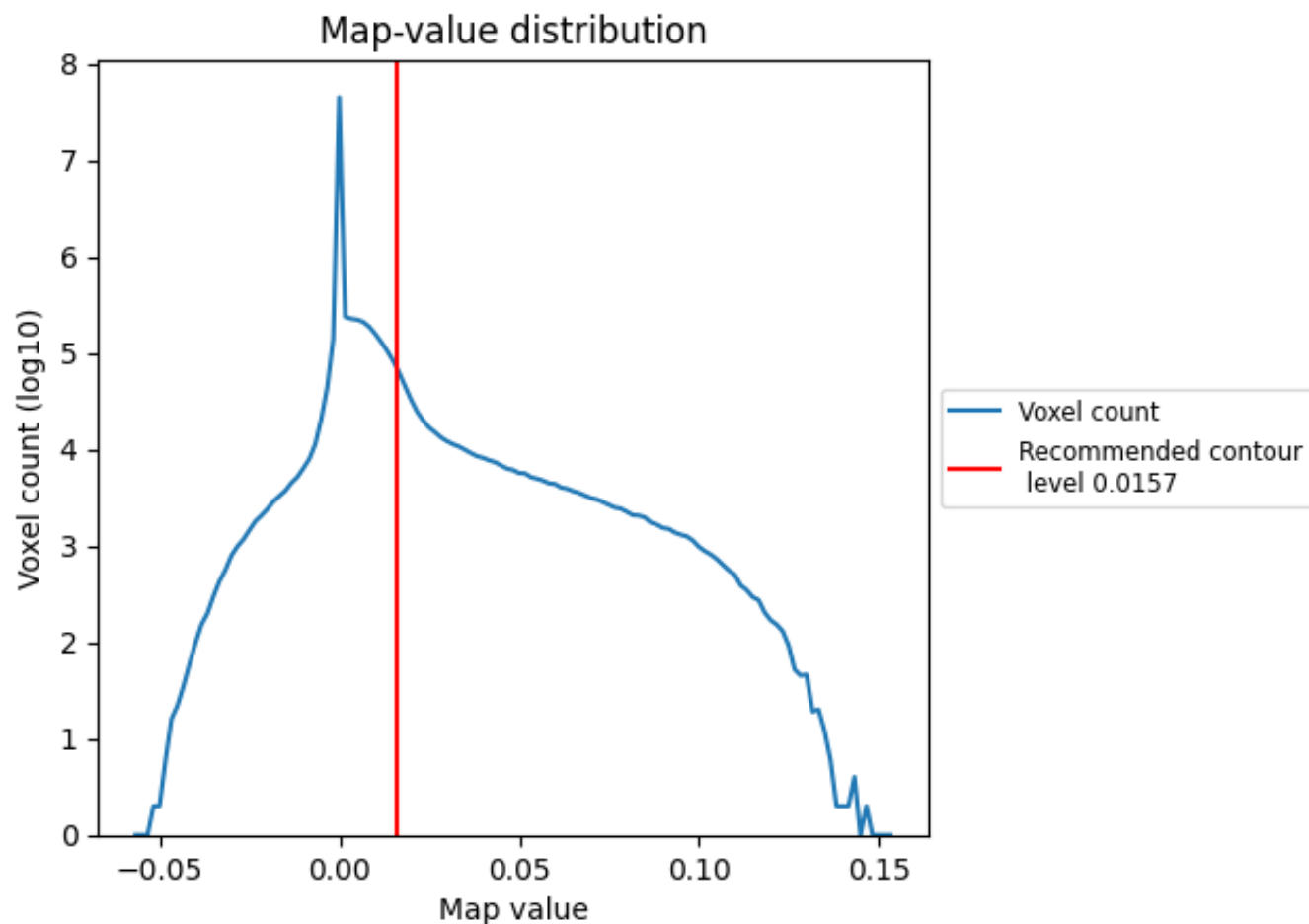
Z



## 7 Map analysis [i](#)

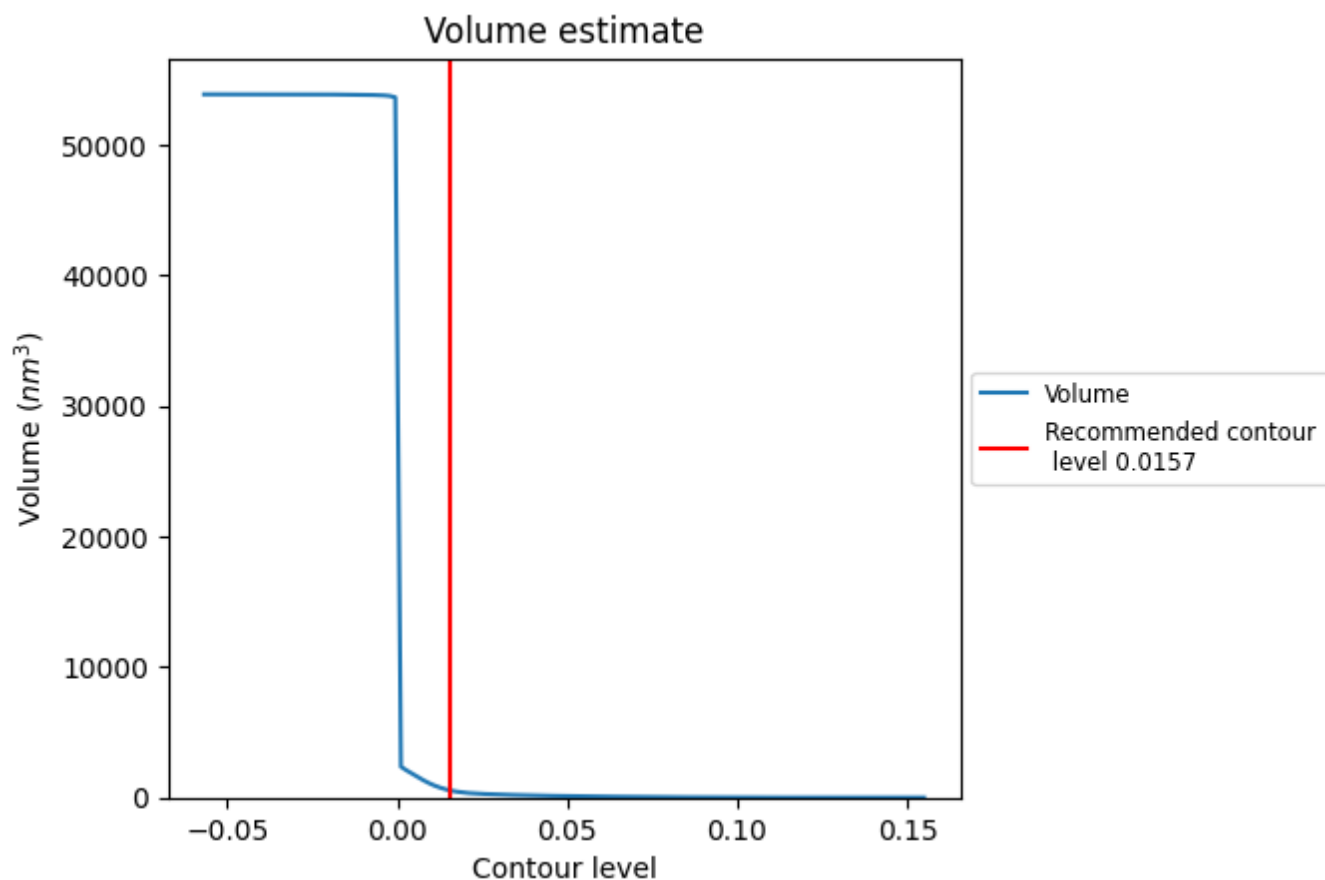
This section contains the results of statistical analysis of the map.

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



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

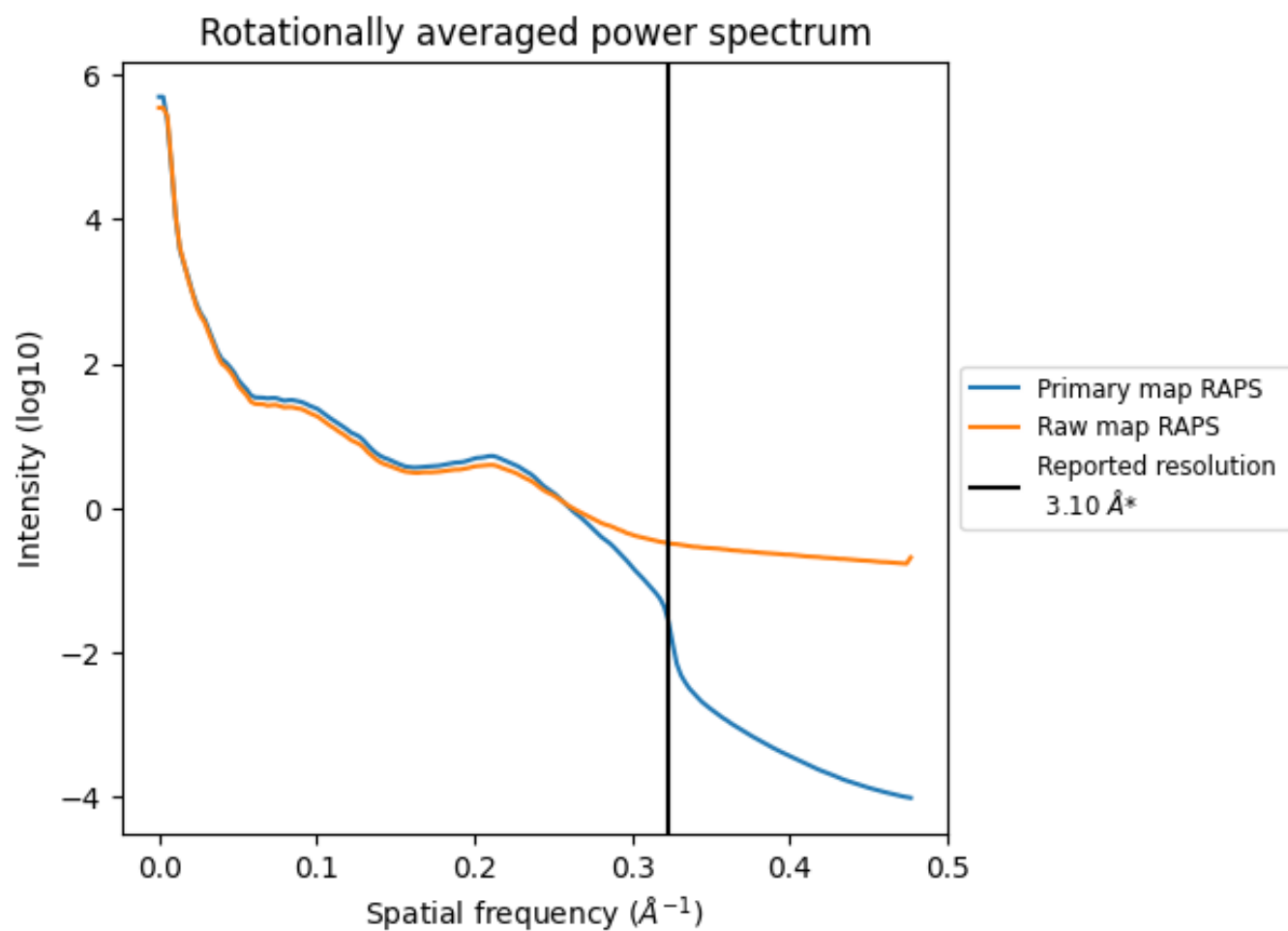
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 541 nm<sup>3</sup>; this corresponds to an approximate mass of 489 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 ⓘ

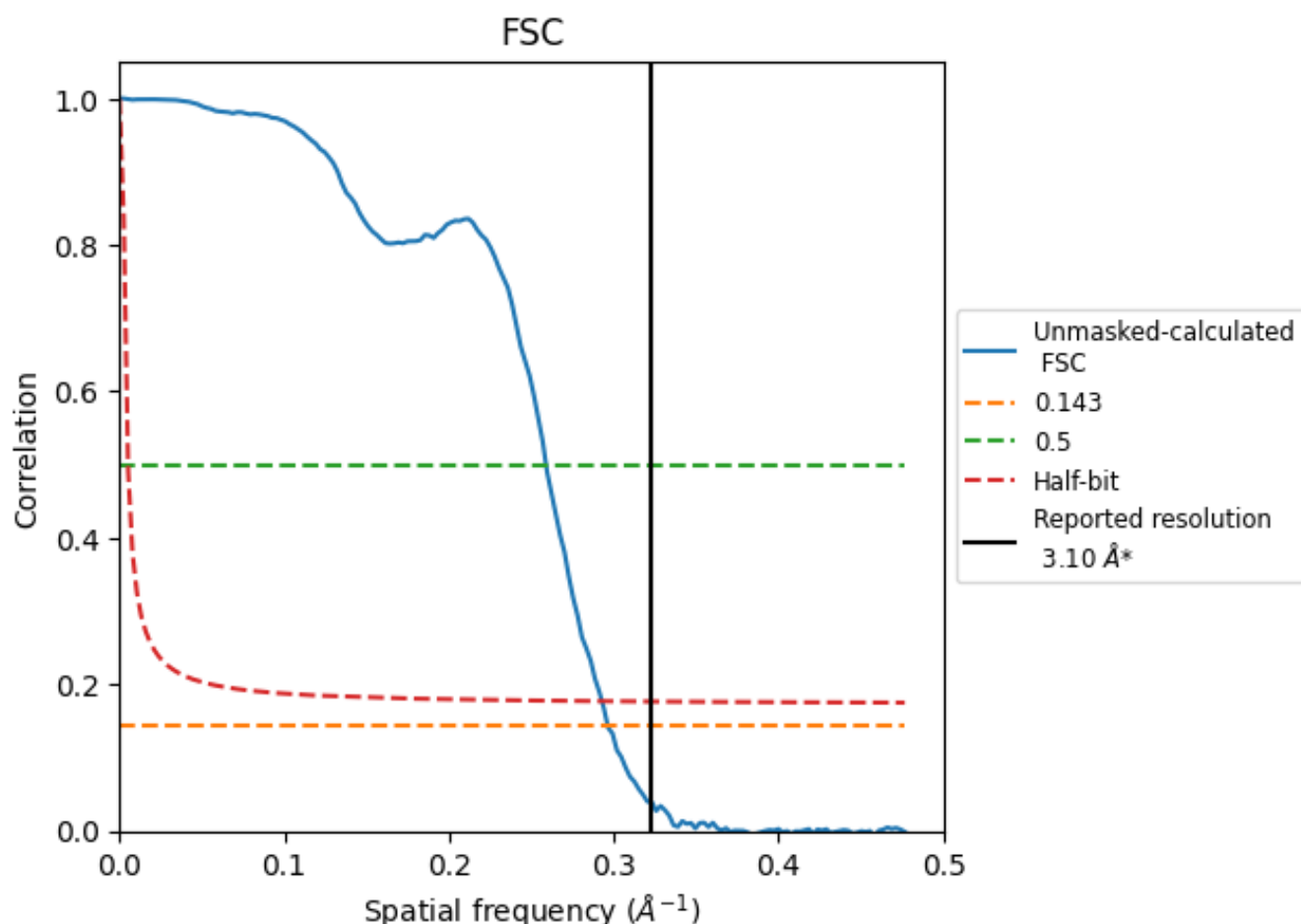


\*Reported resolution corresponds to spatial frequency of  $0.323 \text{ \AA}^{-1}$

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.323  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

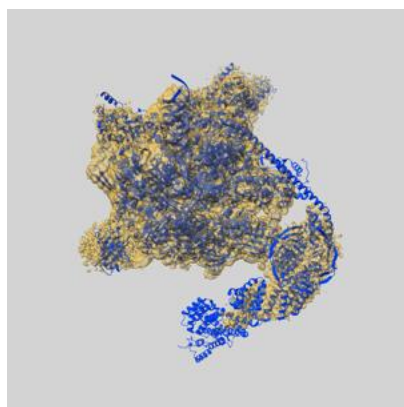
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.37	3.86	3.42

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

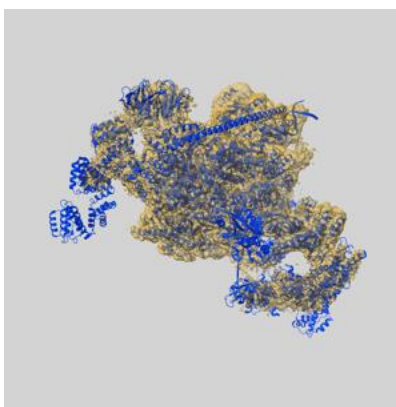
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-0031 and PDB model 6GMH. Per-residue inclusion information can be found in section [3](#) on page [9](#).

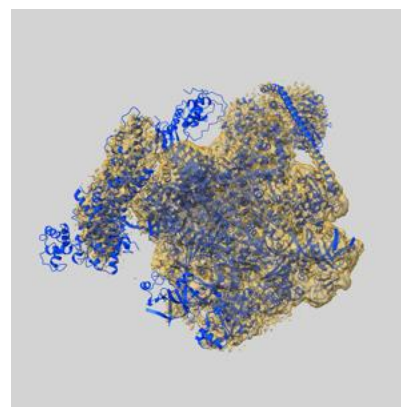
### 9.1 Map-model overlay [i](#)



X



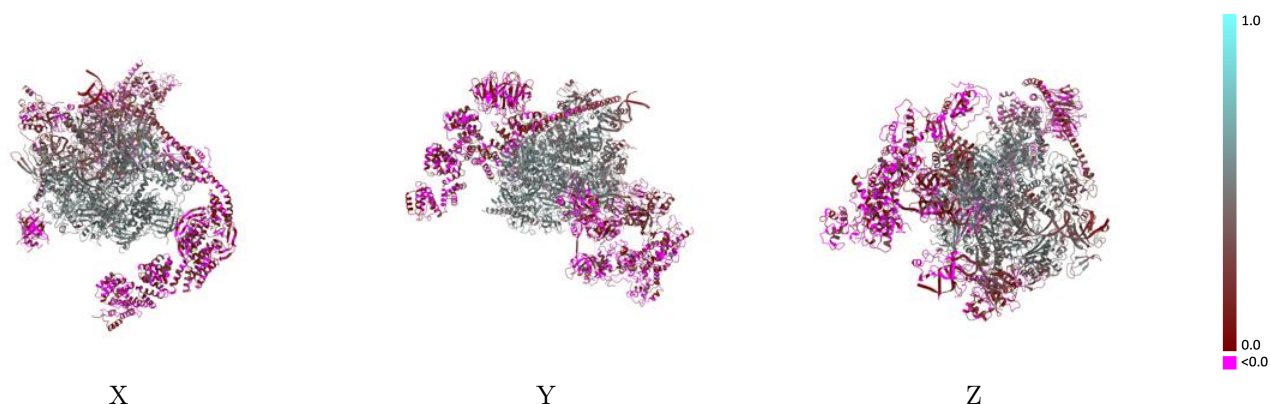
Y



Z

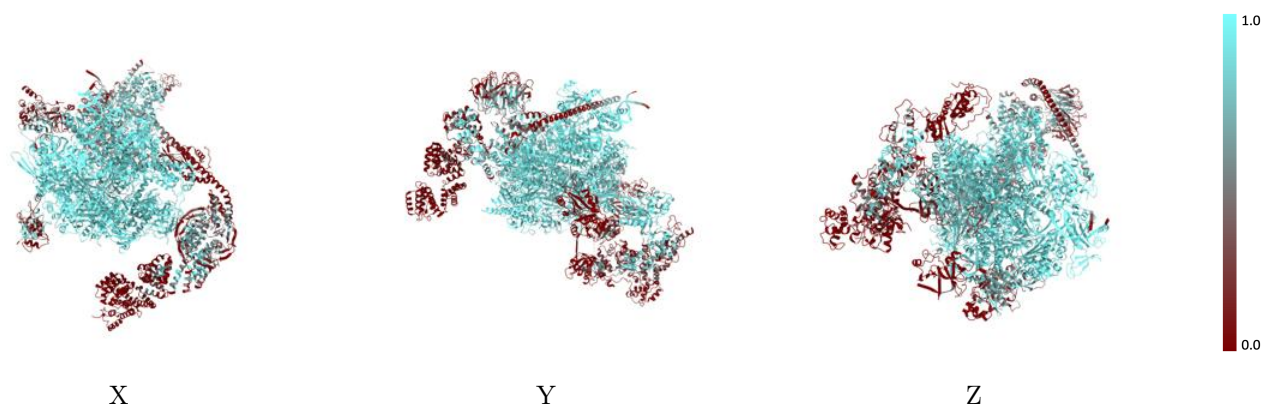
The images above show the 3D surface view of the map at the recommended contour level 0.0157 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



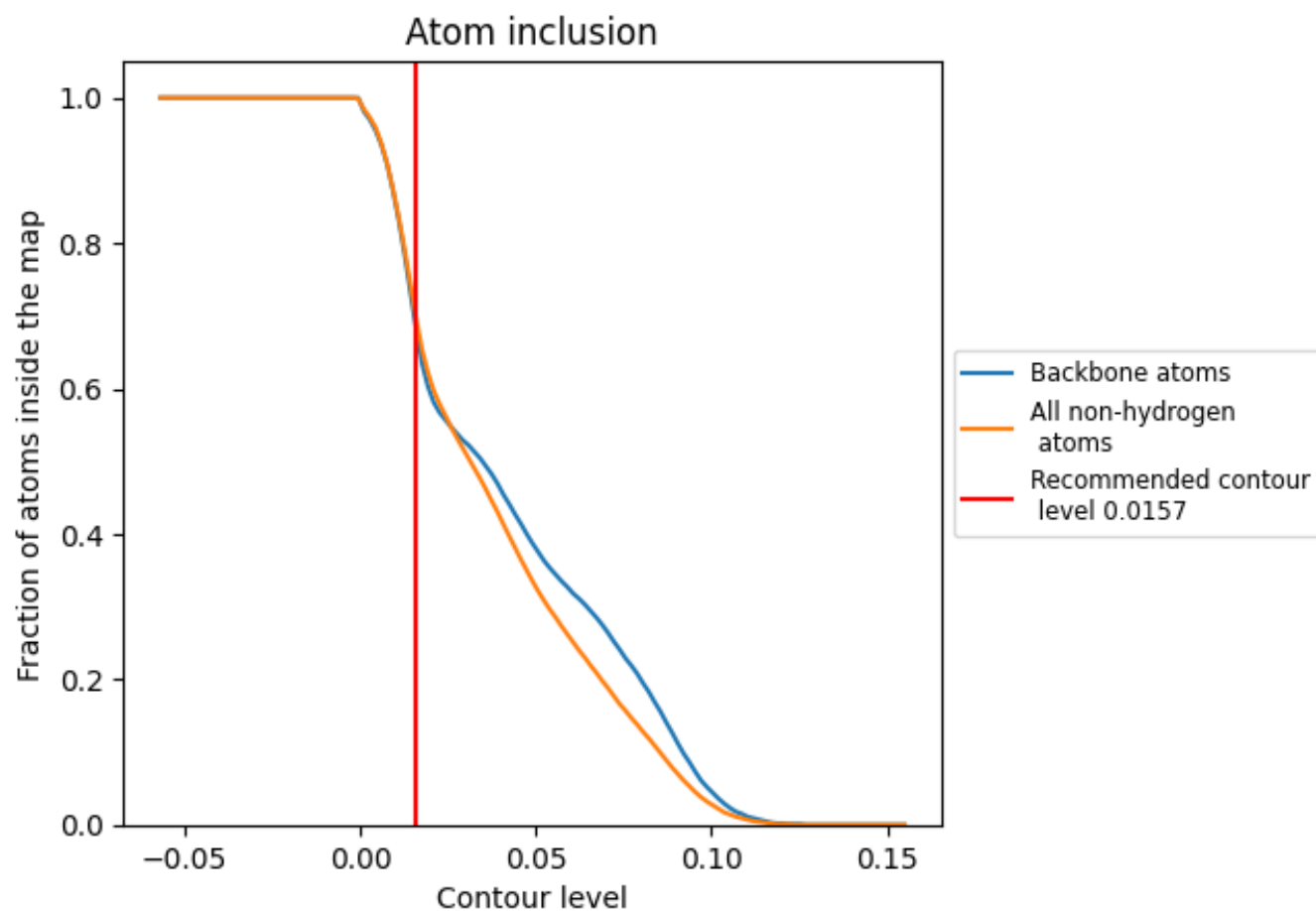
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0157).

## 9.4 Atom inclusion [i](#)



















































At the recommended contour level, 69% of all backbone atoms, 70% 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 (0.0157) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7030	 0.3240
A	 0.9290	 0.4710
B	 0.9540	 0.4950
C	 0.9460	 0.5090
D	 0.8230	 0.2100
E	 0.9540	 0.4400
F	 0.9330	 0.5000
G	 0.8430	 0.2540
H	 0.9280	 0.4960
I	 0.9400	 0.4270
J	 0.9600	 0.5360
K	 0.9620	 0.5230
L	 0.9410	 0.4820
M	 0.1680	 0.0280
N	 0.8370	 0.2560
P	 0.7010	 0.2670
Q	 0.2770	 0.0810
T	 0.8400	 0.3330
U	 0.3480	 0.0230
V	 0.4380	 0.0630
W	 0.3520	 0.0410
X	 0.5710	 0.1690
Y	 0.2040	 0.1250
Z	 0.3030	 0.1100

