



## Full wwPDB EM Validation Report ⓘ

Jun 25, 2025 – 04:56 am BST

PDB ID : 6GYL / pdb\_00006gyl  
EMDB ID : EMD-0091  
Title : Structure of a yeast closed complex with distorted DNA (core CCdist)  
Authors : Dienemann, C.; Schwalb, B.; Schilbach, S.; Cramer, P.  
Deposited on : 2018-06-30  
Resolution : 4.80 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.dev118  
MolProbity : 4-5-2 with Phenix2.0rc1  
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) : 2.44



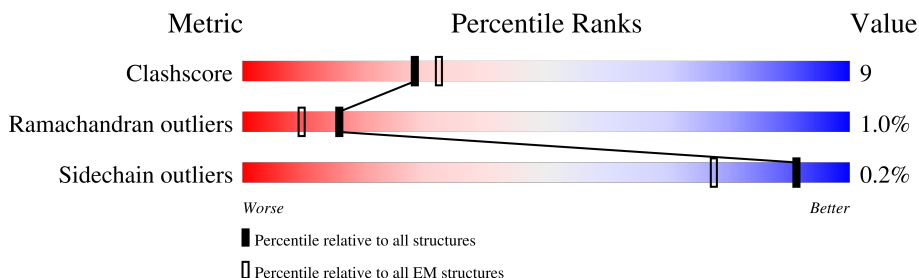
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.80 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	1733	<div> <div>44%</div> <div>66%</div> <div>14%</div> <div>19%</div> </div>
2	B	1224	<div> <div>53%</div> <div>73%</div> <div>21%</div> <div>6%</div> </div>
3	C	318	<div> <div>42%</div> <div>67%</div> <div>15%</div> <div>18%</div> </div>
4	D	221	<div> <div>56%</div> <div>62%</div> <div>9%</div> <div>29%</div> </div>
5	E	215	<div> <div>57%</div> <div>87%</div> <div>12%</div> <div>.</div> </div>
6	F	155	<div> <div>26%</div> <div>43%</div> <div>10%</div> <div>46%</div> </div>
7	G	171	<div> <div>57%</div> <div>66%</div> <div>34%</div> </div>
8	H	146	<div> <div>50%</div> <div>70%</div> <div>23%</div> <div>7%</div> </div>

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Mol	Chain	Length	Quality of chain
9	I	122	
10	J	70	
11	K	120	
12	L	70	
13	M	345	
14	N	56	
15	O	240	
16	Q	735	
17	R	400	
18	T	56	
19	U	171	
20	V	129	
21	W	586	
22	X	328	



## 2 Entry composition

There are 24 unique types of molecules in this entry. The entry contains 43409 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 DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1398	Total	C	N	O	S	0	0
			10997	6931	1927	2078	61		

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1152	Total	C	N	O	S	0	0
			9178	5807	1608	1708	55		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	262	Total	C	N	O	S	0	0
			2061	1299	343	406	13		

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	157	Total	C	N	O	S	0	0
			1253	779	220	252	2		

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	213	Total	C	N	O	S	0	0
			1744	1107	308	318	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	83	Total	C	N	O	S	0	0
			670	428	114	125	3		



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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	171	Total	C	N	O	S	0	0
			1340	861	222	249	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	136	Total	C	N	O	S	0	0
			1089	686	184	215	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	116	Total	C	N	O	S	0	0
			944	581	172	181	10		

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	65	Total	C	N	O	S	0	0
			532	339	93	94	6		

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	112	Total	C	N	O	S	0	0
			904	580	154	168	2		

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	45	Total	C	N	O	S	0	0
			358	221	71	62	4		

- Molecule 13 is a protein called Transcription initiation factor IIB.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	279	Total	C	N	O	S	0	0
			2175	1382	373	403	17		

- Molecule 14 is a DNA chain called GAT1 promoter DNA.



Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	56	Total	C	N	O	P	0	0
			1129	540	204	329	56		

- Molecule 15 is a protein called TATA-box-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	180	Total	C	N	O	S	0	0
			1416	921	242	247	6		

- Molecule 16 is a protein called Transcription initiation factor IIF subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	148	Total	C	N	O	S	0	0
			1144	733	195	212	4		

- Molecule 17 is a protein called Transcription initiation factor IIF subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	190	Total	C	N	O	S	0	0
			1303	812	238	246	7		

- Molecule 18 is a DNA chain called GAT1 promoter DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	T	56	Total	C	N	O	P	0	0
			1149	546	222	325	56		

- Molecule 19 is a protein called Transcription initiation factor IIA large subunit, Transcription initiation factor IIA large subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	U	92	Total	C	N	O	S	0	0
			757	474	130	150	3		

- Molecule 20 is a protein called Transcription initiation factor IIA subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	V	100	Total	C	N	O	S	0	0
			782	492	130	156	4		

There are 7 discrepancies between the modelled and reference sequences:



Chain	Residue	Modelled	Actual	Comment	Reference
V	123	LYS	-	expression tag	UNP P32774
V	124	HIS	-	expression tag	UNP P32774
V	125	HIS	-	expression tag	UNP P32774
V	126	HIS	-	expression tag	UNP P32774
V	127	HIS	-	expression tag	UNP P32774
V	128	HIS	-	expression tag	UNP P32774
V	129	HIS	-	expression tag	UNP P32774

- Molecule 21 is a protein called Transcription initiation factor IIE subunit alpha,Tfa1,Tfa1.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	W	191	Total	C	N	O	S	0	0
			1469	932	254	277	6		

- Molecule 22 is a protein called Transcription initiation factor IIE subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	X	160	Total	C	N	O	S	0	0
			1004	620	184	196	4		

- Molecule 23 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
23	A	2	Total	Zn	0
			2	2	
23	B	1	Total	Zn	0
			1	1	
23	C	1	Total	Zn	0
			1	1	
23	I	2	Total	Zn	0
			2	2	
23	J	1	Total	Zn	0
			1	1	
23	L	1	Total	Zn	0
			1	1	
23	M	1	Total	Zn	0
			1	1	
23	W	1	Total	Zn	0
			1	1	

- Molecule 24 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).



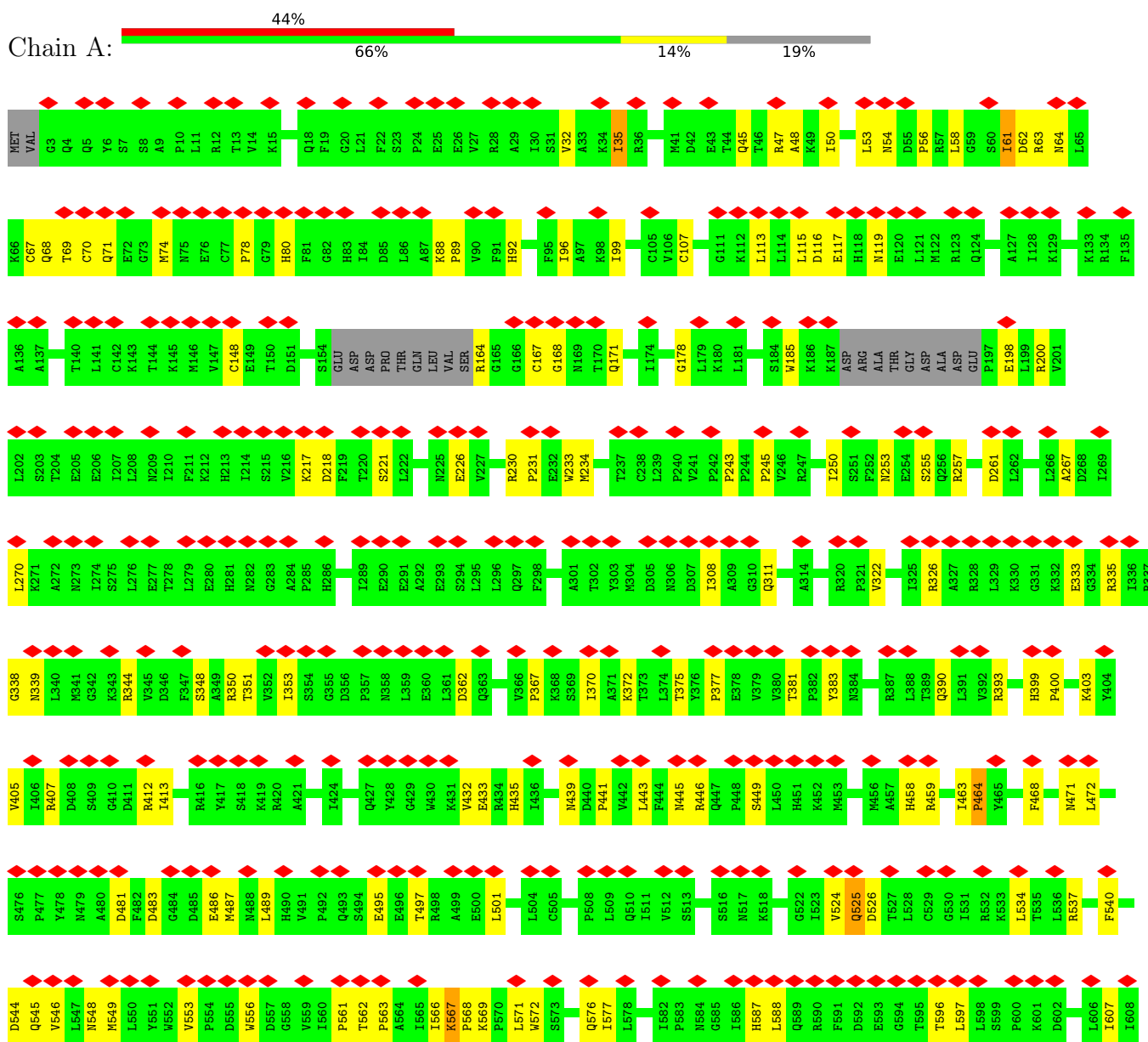
Mol	Chain	Residues	Atoms		AltConf
24	A	1	Total	Mg	0
			1	1	



### 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 II subunit RPB1



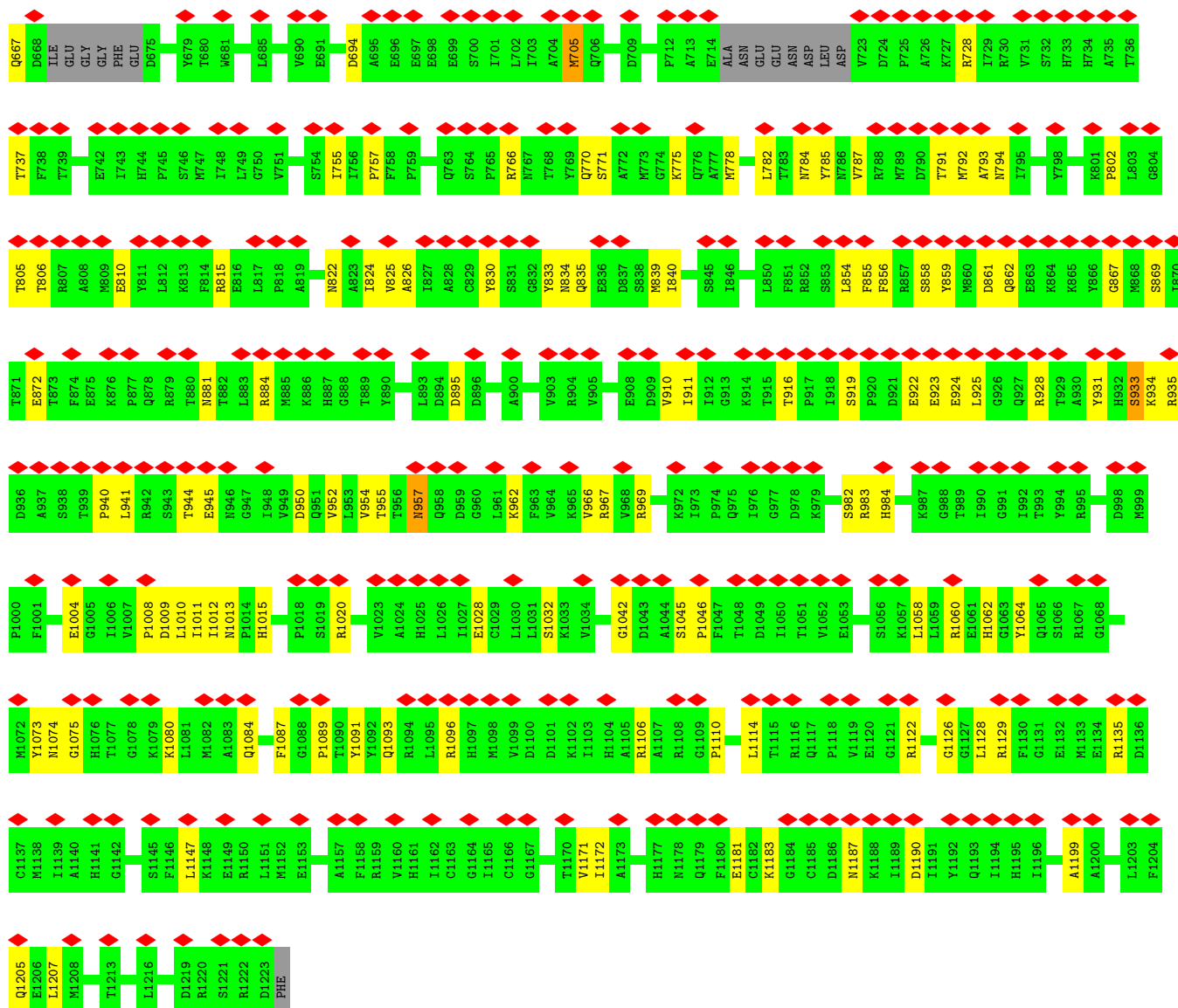


M1444	D1446	E1447	E1448	S1449	L1450	V1451	K1452	TYR	MET	PRO	GLU	GLN	LYS	ILE	THR	GLU	ILE	GLU	ASP	GLY	GLN	ASP	GLY	VAL	THR	PRO	TYR	SER	ASN	GLU	SER	GLY	VAL	ASN	ALA	ASP	LEU	ASP	LYS	GLU	LEU	MET	PHE	SER	PRO	LEU	VAL	ASP	SER	GLY	ASN	ASN	ASP			
V1372	D1373	V1374	T1377	G1380	L1381	T1385	R1386	H1387	G1388	F1389	N1390	R1391	S1392	N1393	T1394	G1395	A1396	R1399	E1404	T1405	V1406	I1407	I1408	L1409	F1410	E1411	A1412	G1413	A1414	S1415	A1416	E1417	L1418	D1419	D1420	G1421	R1422	G1423	V1424	S1425	E1426	L1430	G1431	Q1432	M1433	A1434	P1435	I1436	G1437	T1438	G1439	F1441				
E1307	T1308	D1309	G1310	V1311	S1314	E1315	V1316	M1317	T1318	V1319	G1320	G1321	I1322	D1323	P1324	T1325	L1326	I1327	Y1328	T1329	N1330	S1331	D1334	I1335	M1336	E1337	V1338	L1339	G1340	I1341	E1342	A1343	A1346	A1347	L1348	Y1349	K1350	E1351	V1352	Y1353	M1354	A1357	S1358	D1359	G1360	S1361	Y1362	V1363	R1366	H1367	M1368	A1369	L1370	L1371		
L1236	I1237	I1238	R1239	G1240	R1241	V1242	V1243	ARG	PRO	LYS	SER	LEU	ASP	ALA	THR	GLU	A1254	E1255	E1256	D1257	H1258	M1259	L1260	K1261	K1262	I1263	E1264	N1265	T1266	M1267	L1268	E1269	N1270	R1274	G1275	V1276	E1277	R1281	V1282	V1283	R1289	K1290	V1291	P1292	S1293	P1294	T1295	G1296	V1299	K1300	E1301	P1302	L1306			
F1174	S1175	LEU	LEU	ASP	GLU	GLU	ALA	GLN	SER	PHE	ASP	Q1187	Q1188	S1189	P1190	W1191	L1192	L1193	R1194	L1197	D1198	R1199	A1200	M1202	N1203	D1204	K1205	D1206	L1207	T1208	M1209	G1210	Q1211	V1212	G1213	R1214	I1215	I1216	K1217	Q1218	K1221	N1222	D1223	L1224	F1225	V1226	I1227	W1228	S1229	E1230	D1231	M1232	D1233	E1234	K1235	
E1103	I1104	L1105	N1106	V1107	A1108	K1109	N1110	M1111	L1116	T1117	V1118	E1121	P1122	G1123	H1124	A1125	A1126	Q1127	E1129	Q1130	A1131	K1132	L1133	I1134	R1135	S1136	A1137	I1138	T1141	S1145	V1146	T1147	Y1153	Y1154	D1155	P1156	D1157	P1158	R1159	S1160	T1161	V1162	I1163	P1164	E1165	D1166	E1167	I1169	Q1171	L1170	Q1171	L1172	H1173			
E1034	Y1035	R1036	L1037	K1039	Q1040	A1041	F1042	D1043	L1046	S1047	N1048	I1049	E1050	A1051	R1055	V1058	H1059	M1063	V1064	G1065	V1066	L1067	A1068	A1069	I1072	P1075	A1076	T1077	Q1078	THR	LEU	ASN	THR	PHE	HIS	PHE	ALA	GLY	VAL	ALA	SER	LYS	K1093	V1094	T1095	S1096	P1099	R1100	L1101	K1102						
T970	F971	H972	H973	D974	H975	T976	D980	L981	T982	K984	D985	I986	V987	L988	G989	K991	D992	L993	Q994	E995	N996	L997	L998	R1001	G1002	K1003	N1004	E1005	I1006	I1007	Q1008	N1009	R1012	D1013	A1014	V1015	T1016	L1017	F1018	G1019	C1020	N1021	L1022	R1023	S1024	R1025	L1026	A1027	T1028	R1029	L1032	Q1033				
N903	T904	D905	H906	T907	L908	D909	P910	S911	L912	L913	S917	E918	I919	L920	G921	D922	L923	K924	L925	Q926	V927	L928	L929	D930	E931	E932	Y933	K934	V937	K938	D939	R940	K941	F942	L943	R944	E945	V946	F947	V948	D949	G950	N953	Y954	P955	L956	F957	V958	N959	I960	R961	R962	I963	I964	Q965	N966
V829	K830	T831	A832	E833	T834	G835	Y836	I837	Q838	R839	R840	L841	A844	L845	E846	M849	Y852	D853	N854	T855	T856	R857	L860	V863	I864	Q865	F866	I867	Y868	G869	E870	D871	G872	M873	A876	S882	T885	I886	D890	A891	A892	F893	E894	K895	R898	Y899	D900	L901	L902							
S751	K752	G753	S754	F755	T756	N757	A759	Q760	M761	S762	G766	Q767	Q768	E771	G772	K773	A776	F777	G778	D781	K789	D790	D791	Q792	S793	P794	E795	E801	Y804	L805	R806	G807	L808	T809	P810	Q811	F814	F815	H816	G819	G820	R821	E822	G823	L824	I825	D826	T827	A828							
D609	I613	F614	G615	V616	V617	E618	K619	K620	T621	V622	G623	S624	G627	G628	L629	I630	H631	V632	V633	T634	R635	E636	K637	G638	P639	Q640	L645	F646	G647	N648	I649	V652	V653	N654	F655	W656	G661	F662	S663	T664	G665	I666	G667	D668	T669	I670	A671	D672	G673	P674	T675	M676	R677	E678		
E681	T682	E685	A686	K687	K688	K689	D692	V693	T694	K695	E696	A699	N700	L701	L702	T703	A704	K705	H706	G707	M708	T709	L710	F714	E715	D716	N717	R720	F721	L722	N723	E724	A725	R726	D727	K728	R731	L732	A733	E734	V735	K738	D739	V743	K744	V747	M748	A749	G750							

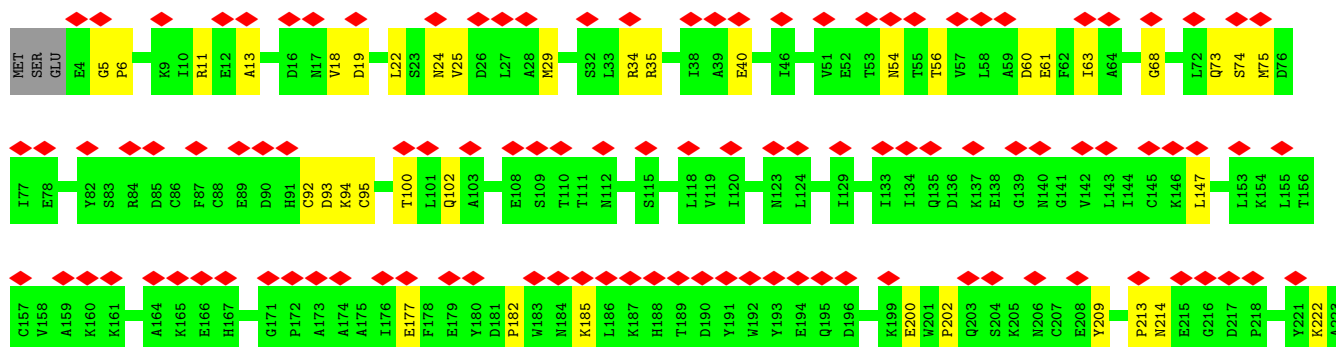
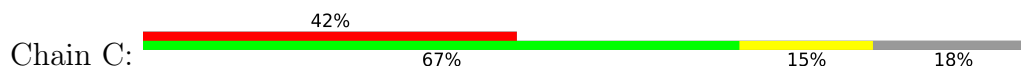


- Molecule 2: DNA-directed RNA polymerase II subunit RPB2



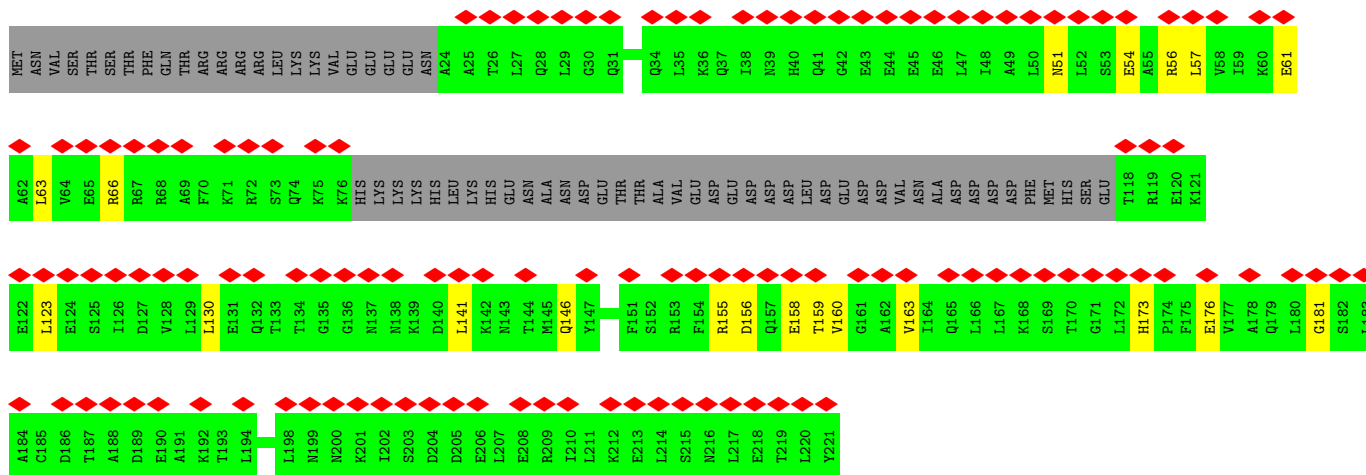


• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

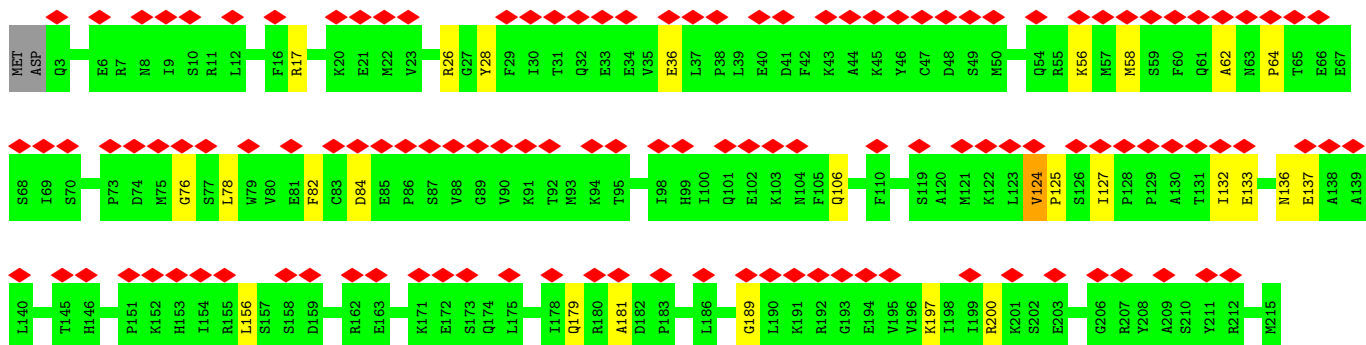
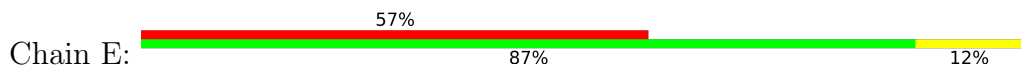




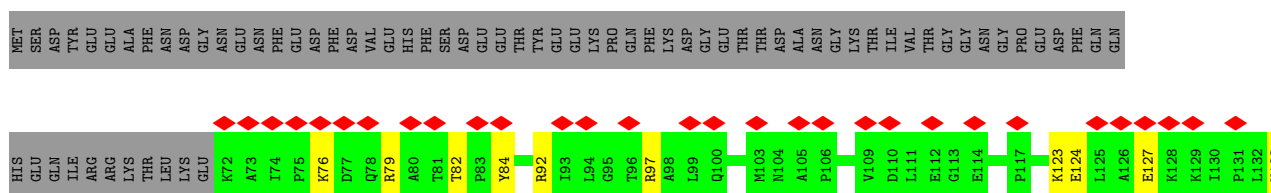
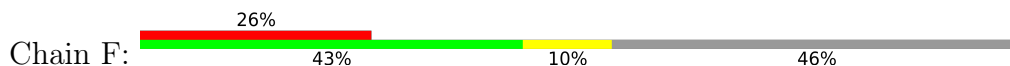
- Molecule 4: DNA-directed RNA polymerase II subunit RPB4



- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1



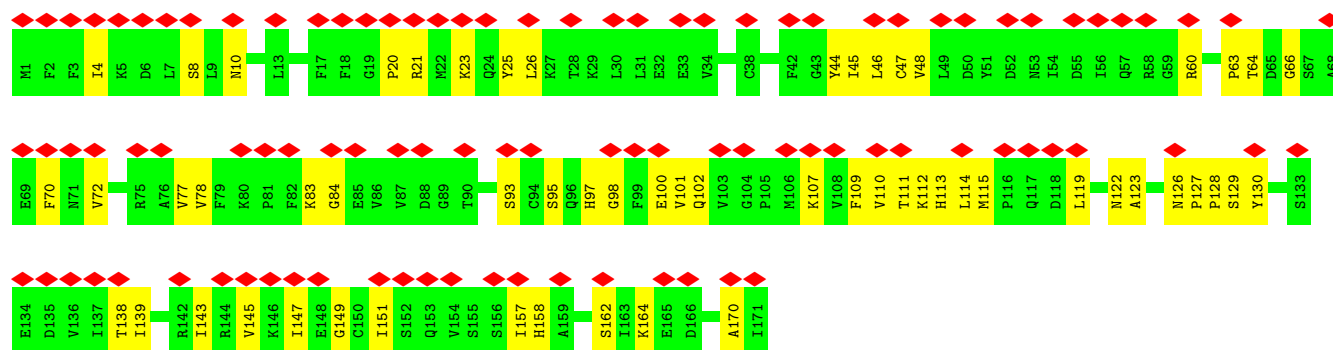
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2



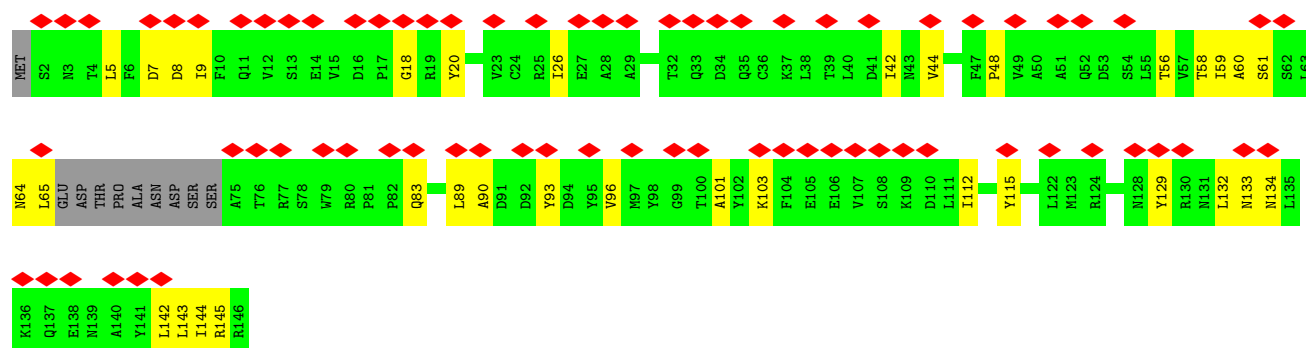




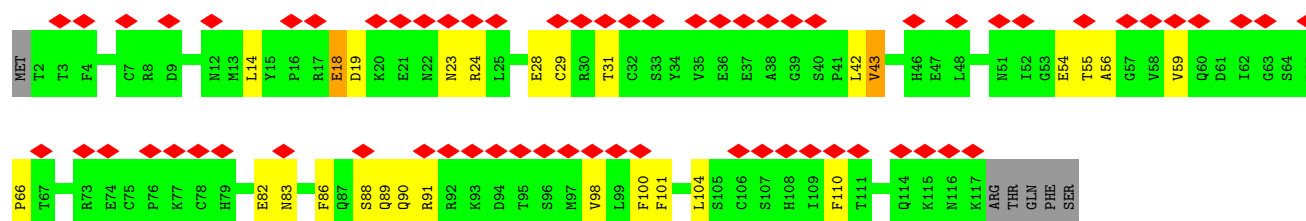
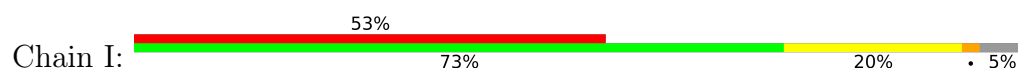
- Molecule 7: DNA-directed RNA polymerase II subunit RPB7



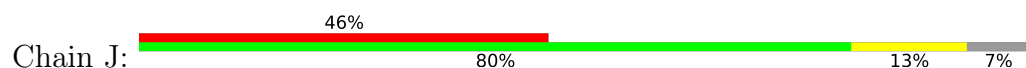
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



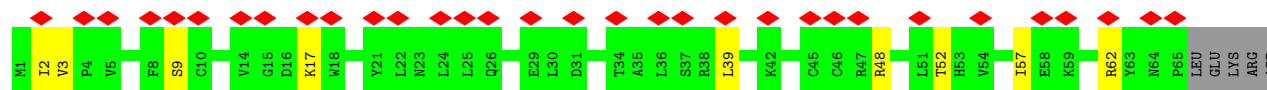
- Molecule 9: DNA-directed RNA polymerase II subunit RPB9



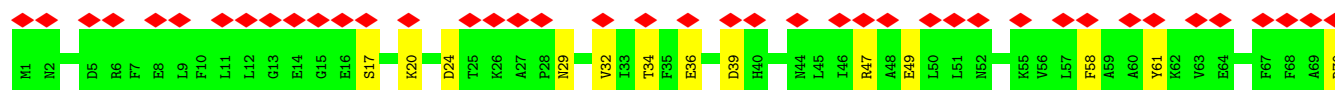
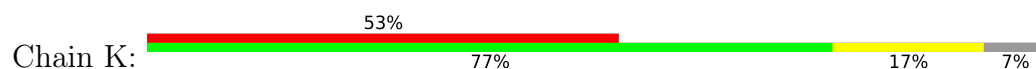
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5







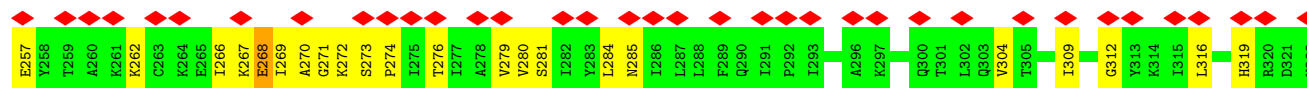
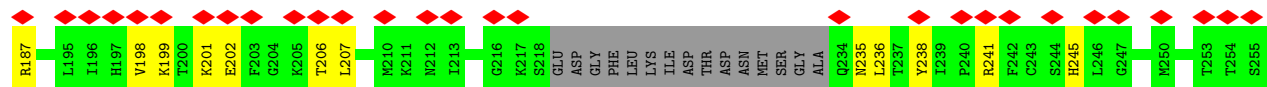
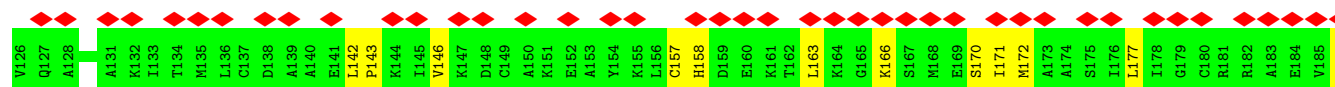
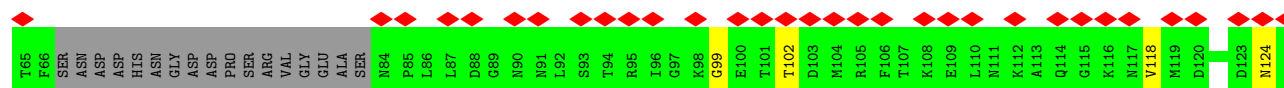
- Molecule 11: DNA-directed RNA polymerase II subunit RPB11



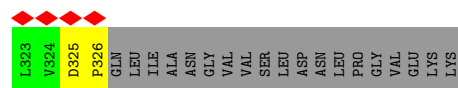
- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4



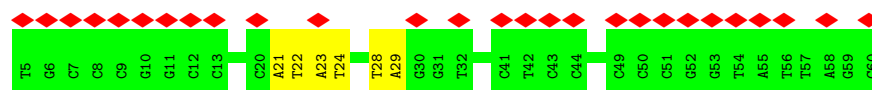
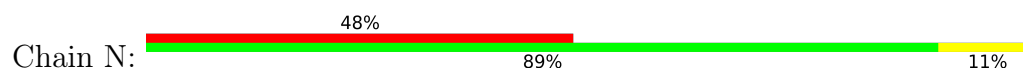
- Molecule 13: Transcription initiation factor IIB



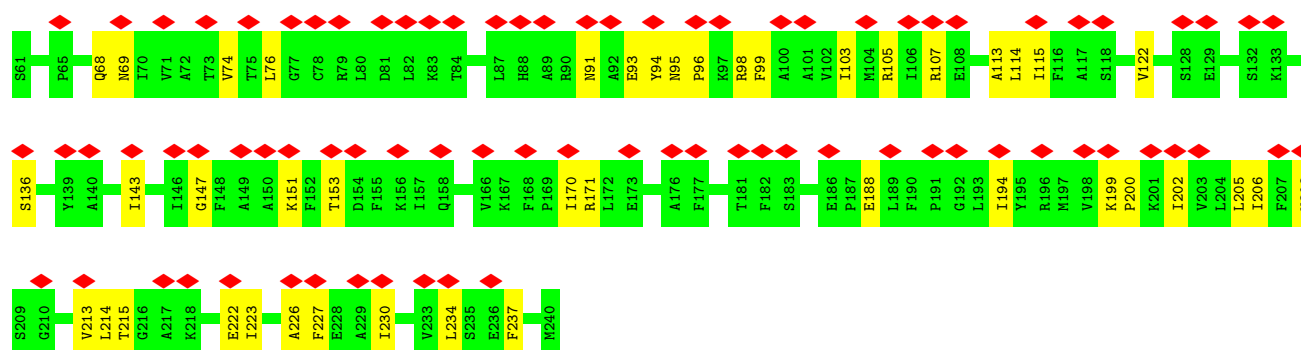
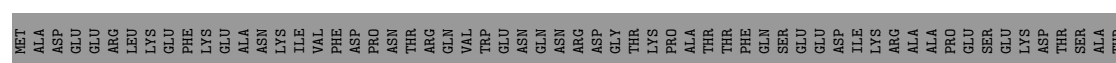




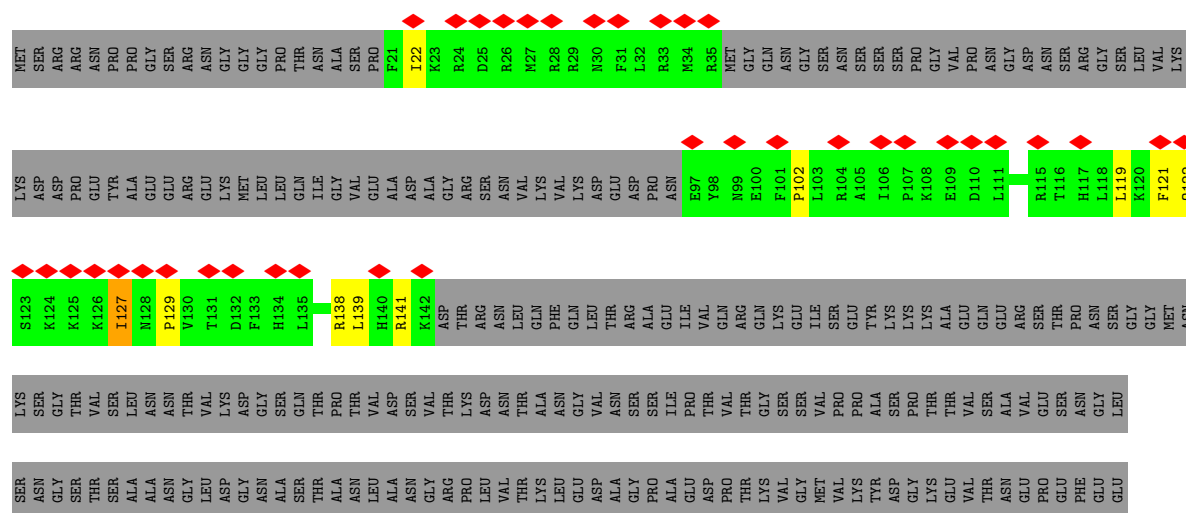
• Molecule 14: GAT1 promoter DNA



• Molecule 15: TATA-box-binding protein



• Molecule 16: Transcription initiation factor IIF subunit alpha



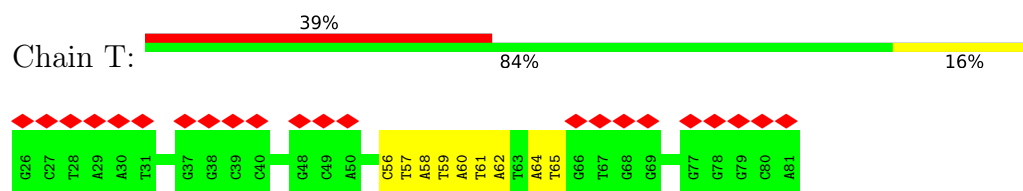






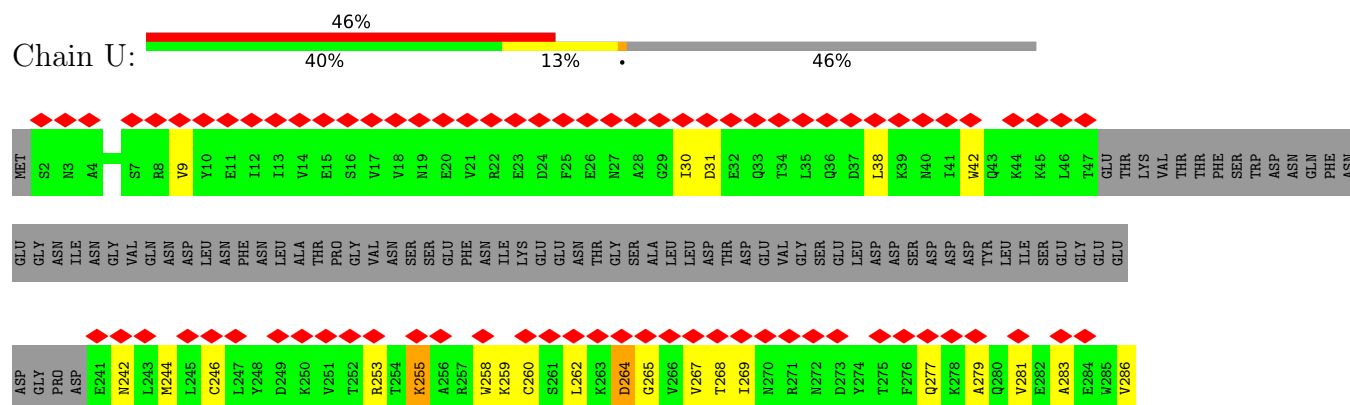
- Molecule 18: GAT1 promoter DNA

Chain T:



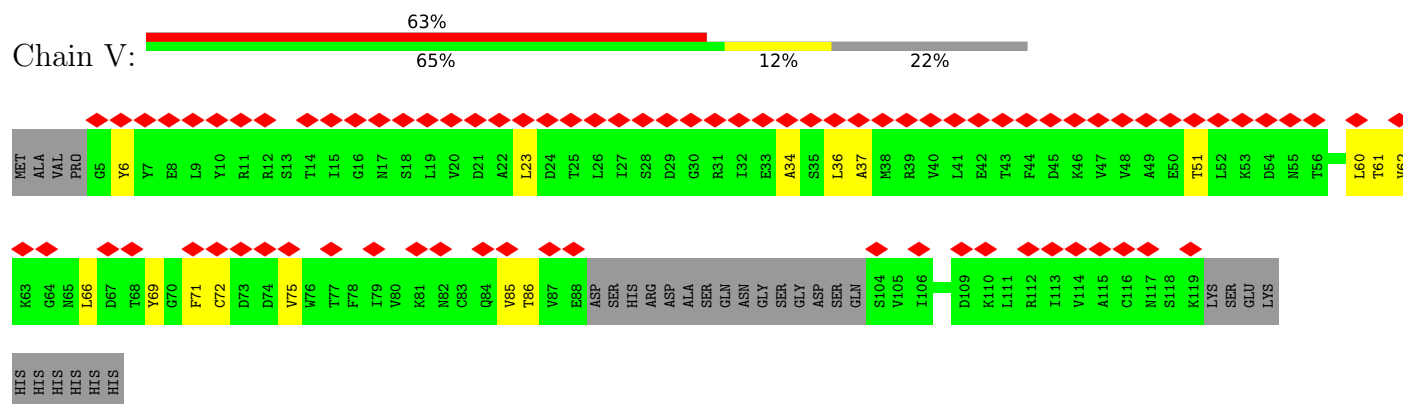
- Molecule 19: Transcription initiation factor IIA large subunit, Transcription initiation factor IIA large subunit

Chain U:



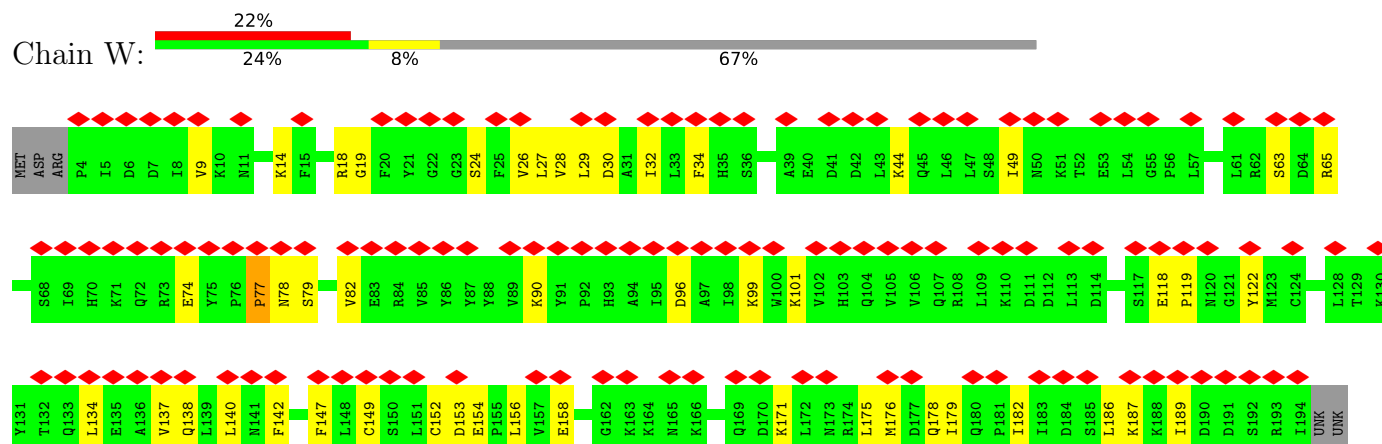
- Molecule 20: Transcription initiation factor IIA subunit 2

Chain V:



- Molecule 21: Transcription initiation factor IIE subunit alpha, Tfa1, Tfa1

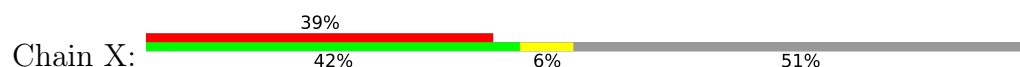
Chain W:





[illegible]

- Molecule 22: Transcription initiation factor IIE subunit beta



GLY	G249	◆	T183	LYS	◆
LYS	G250	◆	Y184	SER	◆
ILE	N251	◆	D185	ALA	◆
THR	L252	◆	Y186	LYS	◆
THR	K253	◆	H187	PRO	◆
MET	C254	◆	S188	VAL	◆
THR	T255	◆	P189	LEU	◆
GLY	D256	◆	S190	VAL	◆
THR	E257	◆	E191	ALA	◆
ILE	E258	◆	L192	ILE	◆
LEU	E259	◆	L193	ASN	◆
LYS	F260	◆	K194	LYS	◆
ASP	K261	◆	L195	GLU	◆
TYR	N262	◆	L196	ALA	◆
THR	N263	◆	R197	GLY	◆
HIS	E264	◆	S198	Y134	◆
SER	N265	◆	P199	T135	◆
HIS	V266	◆	V200	K138	◆
ARG	Q267	◆	T201	GLN	◆
VAL	L268	◆	F202	K140	◆
		◆	K203	P141	◆
		◆	G204	V142	◆
		◆	T205	L143	◆
		◆	S206	V144	◆
		◆	C207	E145	◆
		◆	K208	L147	◆
		◆	D209	L148	◆
		◆	L210	D149	◆
		◆	K211	Y150	◆
		◆	W214	L151	◆
		◆	P215	S152	◆
		◆	Q216	K155	◆
		◆	C217	D157	◆
		◆	D218	K158	◆
		◆	E219	V159	◆
		◆	T220	I160	◆
		◆	T221	E161	◆
		◆	N222	L162	◆
		◆	Q223	L163	◆
		◆	L224	K164	◆
		◆	E225	K165	◆
		◆	E226	L166	◆
		◆	D227	D167	◆
		◆	S228	R168	◆
		◆	K229	I169	◆
		◆	V232	E170	◆
		◆	L233	F171	◆
		◆	R234	D172	◆
		◆	D238	P173	◆
		◆	K239	K174	◆
		◆	T240	K175	◆
		◆	V244	G176	◆
		◆	W245	T177	◆
		◆	Y246	F178	◆
		◆	N247	K179	◆
		◆	S248	Y180	◆
		◆		L181	◆
		◆		SER	◆



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	38000	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 ( $e^-/\text{\AA}^2$ )	37	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.022	Depositor
Minimum map value	-0.011	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0028	Depositor
Map size (Å)	315.0, 315.0, 315.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 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	0.12	0/11192	0.30	2/15128 (0.0%)
2	B	0.11	0/9357	0.27	0/12618
3	C	0.09	0/2099	0.24	0/2845
4	D	0.08	0/1262	0.22	0/1693
5	E	0.11	0/1780	0.32	2/2395 (0.1%)
6	F	0.10	0/682	0.26	0/922
7	G	0.10	0/1368	0.24	0/1844
8	H	0.11	0/1107	0.28	0/1499
9	I	0.11	0/962	0.32	0/1295
10	J	0.14	0/541	0.33	0/727
11	K	0.08	0/922	0.21	0/1244
12	L	0.14	0/360	0.43	0/478
13	M	0.12	0/2204	0.30	0/2963
14	N	0.15	0/1264	0.30	0/1933
15	O	0.12	0/1443	0.28	0/1942
16	Q	0.22	0/1168	0.43	0/1579
17	R	0.13	0/1312	0.33	0/1777
18	T	0.16	0/1292	0.28	0/1981
19	U	0.09	0/766	0.25	0/1032
20	V	0.08	0/789	0.22	0/1066
21	W	0.10	0/1490	0.26	0/2014
22	X	0.12	0/1013	0.33	0/1385
All	All	0.12	0/44373	0.29	4/60360 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	127	ILE	CA-C-N	6.55	124.37	119.66
5	E	127	ILE	C-N-CA	6.55	124.37	119.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1146	VAL	CA-C-N	-6.33	114.35	122.77
1	A	1146	VAL	C-N-CA	-6.33	114.35	122.77

There are no chirality outliers.

There are no planarity outliers.

## 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	10997	0	11081	173	0
2	B	9178	0	9195	166	0
3	C	2061	0	2029	32	0
4	D	1253	0	1275	12	0
5	E	1744	0	1772	15	0
6	F	670	0	690	11	0
7	G	1340	0	1357	75	0
8	H	1089	0	1062	21	0
9	I	944	0	899	28	0
10	J	532	0	542	6	0
11	K	904	0	911	14	0
12	L	358	0	381	7	0
13	M	2175	0	2283	51	0
14	N	1129	0	629	8	0
15	O	1416	0	1493	77	0
16	Q	1144	0	1034	28	0
17	R	1303	0	1110	29	0
18	T	1149	0	627	51	0
19	U	757	0	747	23	0
20	V	782	0	790	15	0
21	W	1469	0	1431	97	0
22	X	1004	0	730	38	0
23	A	2	0	0	0	0
23	B	1	0	0	0	0
23	C	1	0	0	0	0
23	I	2	0	0	0	0
23	J	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	L	1	0	0	0	0
23	M	1	0	0	0	0
23	W	1	0	0	0	0
24	A	1	0	0	0	0
All	All	43409	0	42068	769	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 9.

All (769) 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)
15:O:99:PHE:CD2	18:T:58:DA:H1'	1.23	1.65
15:O:98:ARG:HG2	18:T:58:DA:C5'	1.46	1.43
15:O:99:PHE:CG	18:T:58:DA:H1'	1.57	1.37
15:O:99:PHE:CZ	18:T:58:DA:N3	1.95	1.35
7:G:158:HIS:HB2	21:W:138:GLN:NE2	1.40	1.32
15:O:98:ARG:CD	18:T:58:DA:H5''	1.55	1.30
15:O:99:PHE:CB	18:T:58:DA:O4'	1.80	1.27
15:O:99:PHE:HB2	18:T:58:DA:O4'	1.10	1.26
15:O:99:PHE:CD2	18:T:58:DA:C1'	2.16	1.26
13:M:272:LYS:HE2	18:T:65:DT:O5'	1.36	1.25
7:G:97:HIS:CE1	21:W:122:TYR:HE2	1.54	1.24
7:G:158:HIS:CG	21:W:138:GLN:HE22	1.55	1.23
15:O:99:PHE:CG	18:T:58:DA:C1'	2.20	1.23
15:O:98:ARG:CG	18:T:58:DA:C5'	2.16	1.21
21:W:178:GLN:NE2	22:X:254:CYS:SG	2.12	1.21
7:G:113:HIS:HB3	21:W:118:GLU:OE2	1.06	1.20
15:O:98:ARG:CG	18:T:58:DA:H5'	1.73	1.19
7:G:113:HIS:CB	21:W:118:GLU:OE2	1.91	1.18
7:G:158:HIS:CB	21:W:138:GLN:HE22	1.55	1.16
15:O:103:ILE:HD13	18:T:59:DT:H5'	1.29	1.11
7:G:158:HIS:CB	21:W:138:GLN:NE2	2.09	1.10
21:W:65:ARG:NH2	22:X:274:LEU:HD23	1.67	1.09
15:O:98:ARG:O	18:T:57:DT:H2''	1.50	1.09
21:W:65:ARG:HH22	22:X:274:LEU:HB3	1.18	1.07
7:G:97:HIS:CE1	21:W:122:TYR:CE2	2.42	1.06
7:G:158:HIS:CD2	21:W:138:GLN:HE22	1.76	1.04
15:O:98:ARG:CD	18:T:58:DA:C5'	2.35	1.04
9:I:54:GLU:O	9:I:89:GLN:N	1.93	1.02
7:G:158:HIS:CG	21:W:138:GLN:NE2	2.28	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:U:242:ASN:HA	19:U:268:THR:O	1.62	0.99
21:W:65:ARG:NH2	22:X:274:LEU:CD2	2.25	0.99
15:O:99:PHE:CE1	18:T:58:DA:N3	2.31	0.99
14:N:24:DT:OP1	15:O:194:ILE:HD13	1.63	0.98
21:W:18:ARG:NE	22:X:250:GLY:H	1.60	0.97
15:O:103:ILE:CD1	18:T:59:DT:H5'	1.95	0.96
15:O:98:ARG:HD3	18:T:58:DA:H5''	1.47	0.95
1:A:70:CYS:SG	1:A:80:HIS:NE2	2.40	0.93
15:O:99:PHE:CZ	18:T:58:DA:C2	2.58	0.91
17:R:106:LEU:O	17:R:119:GLU:HA	1.72	0.90
9:I:54:GLU:HB3	9:I:88:SER:OG	1.71	0.90
1:A:1444:MET:SD	7:G:60:ARG:HG3	2.12	0.90
15:O:98:ARG:CG	18:T:58:DA:H5''	1.89	0.89
16:Q:138:ARG:O	16:Q:352:MET:HA	1.72	0.89
17:R:98:ASN:HB3	17:R:103:LYS:O	1.71	0.89
7:G:158:HIS:HB2	21:W:138:GLN:HE21	1.30	0.88
15:O:103:ILE:HD13	18:T:59:DT:C5'	2.05	0.87
13:M:274:PRO:HD2	15:O:188:GLU:HG2	1.57	0.87
7:G:158:HIS:CD2	21:W:138:GLN:NE2	2.40	0.87
15:O:99:PHE:CE2	18:T:58:DA:H1'	2.07	0.86
15:O:99:PHE:CE2	18:T:58:DA:N3	2.44	0.85
7:G:109:PHE:CZ	21:W:147:PHE:HZ	1.93	0.84
21:W:18:ARG:NH1	22:X:249:GLY:HA3	1.93	0.84
2:B:70:ILE:HD11	16:Q:333:LYS:HB2	1.59	0.83
21:W:65:ARG:HH22	22:X:274:LEU:CB	1.91	0.83
9:I:54:GLU:CB	9:I:88:SER:OG	2.27	0.83
3:C:11:ARG:NH1	3:C:209:TYR:OH	2.12	0.82
21:W:34:PHE:HB3	22:X:201:THR:HG22	1.58	0.82
21:W:14:LYS:O	21:W:18:ARG:HB2	1.79	0.82
9:I:54:GLU:HA	9:I:90:GLN:H	1.43	0.82
21:W:18:ARG:CZ	22:X:250:GLY:H	1.93	0.81
13:M:272:LYS:HE2	18:T:65:DT:C5'	2.10	0.80
18:T:60:DA:OP1	19:U:253:ARG:NH1	2.11	0.80
21:W:65:ARG:NH2	22:X:274:LEU:HB3	1.96	0.79
21:W:149:CYS:O	21:W:153:ASP:N	2.16	0.79
15:O:103:ILE:HD11	18:T:58:DA:H2''	1.65	0.79
7:G:158:HIS:CD2	21:W:138:GLN:OE1	2.37	0.78
21:W:101:LYS:HD3	22:X:263:TRP:CE2	2.18	0.78
2:B:835:GLN:HA	2:B:1013:ASN:ND2	1.99	0.78
1:A:78:PRO:O	2:B:1205:GLN:NE2	2.18	0.77
4:D:57:LEU:O	4:D:61:GLU:HB2	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:376:LEU:HD21	16:Q:386:MET:HE3	1.65	0.77
13:M:272:LYS:CE	18:T:65:DT:O5'	2.28	0.77
1:A:1141:THR:HG23	1:A:1205:LYS:HD3	1.67	0.76
15:O:98:ARG:HG3	18:T:57:DT:O3'	1.85	0.76
21:W:96:ASP:HB3	22:X:278:LEU:CD1	2.16	0.76
3:C:177:GLU:HB2	3:C:231:ASN:HB3	1.65	0.76
15:O:99:PHE:HB2	18:T:58:DA:C4'	2.16	0.76
2:B:839:MET:HG2	2:B:1012:ILE:HG22	1.66	0.76
21:W:65:ARG:NH2	22:X:274:LEU:CB	2.49	0.75
11:K:20:LYS:HB2	11:K:34:THR:HB	1.67	0.75
8:H:56:THR:O	8:H:144:ILE:HA	1.86	0.75
7:G:113:HIS:CE1	21:W:119:PRO:HG2	2.22	0.75
15:O:98:ARG:HG2	18:T:58:DA:H5'	0.78	0.75
21:W:65:ARG:CZ	22:X:274:LEU:HD23	2.17	0.75
3:C:75:MET:O	3:C:246:ARG:NH2	2.21	0.74
3:C:56:THR:HG22	3:C:147:LEU:HD21	1.70	0.74
21:W:149:CYS:HB2	21:W:156:LEU:HD21	1.70	0.74
15:O:91:ASN:OD1	20:V:69:TYR:CE2	2.40	0.73
21:W:18:ARG:HB3	22:X:252:LEU:HD12	1.70	0.73
1:A:1055:ARG:NH1	6:F:154:ASP:O	2.20	0.73
13:M:279:VAL:HG11	13:M:304:VAL:HG11	1.70	0.73
1:A:441:PRO:HA	1:A:458:HIS:O	1.88	0.73
9:I:101:PHE:HB2	9:I:110:PHE:O	1.89	0.73
16:Q:127:ILE:HG22	16:Q:129:PRO:HD3	1.70	0.72
21:W:65:ARG:HH21	22:X:274:LEU:CD2	2.02	0.72
7:G:113:HIS:HB3	21:W:118:GLU:CD	2.11	0.72
2:B:835:GLN:HA	2:B:1013:ASN:HD22	1.55	0.72
1:A:243:PRO:HB2	1:A:245:PRO:HD2	1.72	0.71
12:L:32:ALA:HB2	12:L:55:ILE:HB	1.70	0.71
7:G:101:VAL:HG21	7:G:145:VAL:HG21	1.73	0.70
16:Q:375:LEU:O	16:Q:386:MET:HA	1.91	0.70
9:I:19:ASP:HB3	9:I:24:ARG:O	1.92	0.70
7:G:158:HIS:CD2	21:W:138:GLN:CD	2.70	0.70
7:G:10:ASN:HA	7:G:70:PHE:O	1.92	0.69
15:O:91:ASN:OD1	20:V:69:TYR:CZ	2.44	0.69
13:M:34:ILE:HG22	13:M:45:CYS:HA	1.75	0.69
8:H:93:TYR:HA	8:H:145:ARG:HB3	1.73	0.69
13:M:236:LEU:HD11	13:M:257:GLU:HG3	1.74	0.69
13:M:274:PRO:HD2	15:O:188:GLU:CG	2.23	0.69
1:A:344:ARG:HA	2:B:1129:ARG:HA	1.75	0.69
8:H:96:VAL:HA	8:H:142:LEU:O	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:ILE:HG22	1:A:270:LEU:HD11	1.74	0.68
1:A:524:VAL:HG12	1:A:525:GLN:HG2	1.75	0.68
2:B:373:ARG:HG3	2:B:566:LEU:HD23	1.75	0.68
2:B:825:VAL:HA	2:B:1010:LEU:O	1.93	0.68
21:W:18:ARG:CB	22:X:252:LEU:HD12	2.23	0.68
7:G:97:HIS:ND1	21:W:122:TYR:HE2	1.90	0.68
13:M:99:GLY:H	13:M:102:THR:HG21	1.58	0.68
7:G:113:HIS:CE1	21:W:119:PRO:HB2	2.30	0.67
3:C:40:GLU:OE1	3:C:254:LYS:NZ	2.23	0.67
12:L:38:LEU:HD21	12:L:48:CYS:HA	1.77	0.67
13:M:157:CYS:SG	13:M:158:HIS:N	2.68	0.67
3:C:18:VAL:HG21	3:C:240:VAL:HG21	1.77	0.67
2:B:383:ASN:O	2:B:387:LEU:HB2	1.96	0.66
17:R:64:SER:HA	17:R:216:GLY:HA2	1.77	0.66
21:W:18:ARG:HG2	22:X:250:GLY:HA2	1.78	0.66
1:A:1146:VAL:HG23	1:A:1197:LEU:HD22	1.77	0.66
2:B:67:SER:HB2	2:B:92:PHE:H	1.61	0.66
15:O:98:ARG:O	18:T:57:DT:C2'	2.36	0.66
15:O:107:ARG:HG2	19:U:286:VAL:O	1.95	0.66
1:A:807:GLY:HA3	2:B:728:ARG:HH21	1.60	0.66
1:A:446:ARG:HD2	1:A:487:MET:HE2	1.77	0.65
2:B:770:GLN:NE2	2:B:982:SER:O	2.29	0.65
1:A:61:ILE:HG22	1:A:62:ASP:H	1.59	0.65
15:O:170:ILE:HD13	15:O:234:LEU:HD22	1.78	0.65
3:C:11:ARG:NH2	3:C:19:ASP:OD2	2.30	0.65
2:B:1171:VAL:HA	2:B:1181:GLU:O	1.97	0.65
1:A:69:THR:HG23	1:A:80:HIS:CD2	2.32	0.65
7:G:109:PHE:CZ	21:W:147:PHE:CZ	2.81	0.65
7:G:97:HIS:ND1	21:W:122:TYR:CE2	2.63	0.64
13:M:267:LYS:HE2	13:M:270:ALA:HB2	1.78	0.64
2:B:826:ALA:HB3	2:B:1011:ILE:HG12	1.79	0.64
2:B:822:ASN:O	10:J:48:ARG:NH1	2.30	0.64
16:Q:121:PHE:HB2	17:R:131:ASN:HB3	1.78	0.64
1:A:178:GLY:HA2	1:A:311:GLN:HE22	1.63	0.64
4:D:173:HIS:HB3	4:D:176:GLU:HG3	1.80	0.64
1:A:107:CYS:SG	1:A:171:GLN:NE2	2.70	0.64
1:A:860:LEU:HD11	1:A:1394:THR:HA	1.80	0.64
7:G:113:HIS:ND1	21:W:119:PRO:HD2	2.13	0.64
2:B:115:GLN:NE2	2:B:787:VAL:O	2.31	0.64
13:M:272:LYS:CE	18:T:65:DT:C5'	2.76	0.63
7:G:113:HIS:CA	21:W:118:GLU:OE2	2.46	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:267:LYS:HE2	15:O:208:VAL:HG11	1.79	0.63
1:A:32:VAL:HG12	2:B:1183:LYS:HE2	1.81	0.63
1:A:1329:THR:HG22	1:A:1331:SER:H	1.62	0.63
1:A:70:CYS:SG	1:A:80:HIS:CE1	2.91	0.63
17:R:126:LYS:HB3	17:R:221:GLU:HB2	1.79	0.63
3:C:13:ALA:HA	3:C:18:VAL:HG22	1.80	0.62
1:A:1192:LEU:HD11	1:A:1239:ARG:HB3	1.80	0.62
2:B:25:ILE:HA	2:B:655:LYS:HE3	1.82	0.62
2:B:249:ARG:HG2	2:B:415:GLN:HE22	1.64	0.62
1:A:68:GLN:O	1:A:71:GLN:NE2	2.33	0.62
2:B:944:THR:HG21	2:B:1122:ARG:HH12	1.63	0.62
7:G:113:HIS:C	21:W:118:GLU:OE2	2.43	0.62
2:B:490:SER:O	2:B:494:HIS:HB2	2.00	0.62
13:M:163:LEU:O	13:M:166:LYS:NZ	2.33	0.62
1:A:1444:MET:HE2	6:F:135:ARG:HH21	1.65	0.61
7:G:114:LEU:HD23	7:G:162:SER:HB3	1.81	0.61
1:A:1451:VAL:HG12	7:G:20:PRO:HB3	1.82	0.61
2:B:785:TYR:O	2:B:967:ARG:NH1	2.32	0.61
2:B:911:ILE:HD11	2:B:941:LEU:HD12	1.81	0.61
1:A:1199:ARG:O	1:A:1203:ASN:ND2	2.33	0.61
15:O:99:PHE:CE1	18:T:58:DA:C2	2.87	0.61
21:W:101:LYS:HD2	22:X:263:TRP:CZ2	2.36	0.61
13:M:118:VAL:HG22	13:M:124:ASN:HD21	1.65	0.61
7:G:113:HIS:CE1	21:W:119:PRO:CG	2.82	0.61
3:C:25:VAL:HG13	3:C:29:MET:HB3	1.83	0.60
15:O:91:ASN:ND2	20:V:69:TYR:OH	2.32	0.60
13:M:22:LEU:HB3	13:M:52:LEU:HD23	1.83	0.60
7:G:113:HIS:O	21:W:118:GLU:OE2	2.20	0.60
16:Q:373:TYR:OH	17:R:72:ARG:NH2	2.34	0.60
19:U:259:LYS:HA	19:U:281:VAL:O	2.00	0.60
1:A:562:THR:O	1:A:576:GLN:NE2	2.34	0.60
2:B:1106:ARG:NH2	2:B:1110:PRO:O	2.34	0.60
16:Q:139:LEU:HA	16:Q:351:VAL:O	2.02	0.60
1:A:481:ASP:O	1:A:483:ASP:OD1	2.20	0.60
1:A:483:ASP:OD1	1:A:483:ASP:N	2.35	0.60
1:A:544:ASP:HB2	11:K:47:ARG:HH12	1.65	0.60
1:A:185:TRP:HB2	1:A:198:GLU:O	2.02	0.60
1:A:671:ALA:HB3	1:A:676:MET:HE2	1.83	0.60
1:A:1257:ASP:OD1	1:A:1258:HIS:N	2.35	0.60
2:B:298:LEU:HD23	2:B:311:LEU:HD22	1.84	0.60
8:H:101:ALA:HA	8:H:115:TYR:O	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:W:65:ARG:HH21	22:X:274:LEU:HD22	1.66	0.60
1:A:537:ARG:HD2	8:H:20:TYR:CZ	2.37	0.59
1:A:115:LEU:O	1:A:164:ARG:NH1	2.35	0.59
4:D:66:ARG:NH2	7:G:47:CYS:SG	2.75	0.59
4:D:57:LEU:O	4:D:61:GLU:CB	2.50	0.59
2:B:287:ARG:NH2	2:B:294:ASP:OD1	2.36	0.59
2:B:364:ILE:HG12	2:B:585:VAL:HG13	1.83	0.59
13:M:281:SER:O	13:M:285:ASN:ND2	2.31	0.59
15:O:105:ARG:NE	19:U:253:ARG:NH2	2.50	0.59
2:B:193:LYS:HB3	2:B:787:VAL:HG21	1.83	0.59
22:X:200:VAL:HG12	22:X:201:THR:HG23	1.85	0.59
3:C:5:GLY:O	3:C:24:ASN:ND2	2.36	0.59
7:G:109:PHE:CE1	21:W:147:PHE:HZ	2.20	0.59
21:W:96:ASP:HB3	22:X:278:LEU:HD11	1.85	0.59
9:I:82:GLU:HG2	9:I:104:LEU:HD12	1.85	0.58
3:C:73:GLN:HE21	3:C:74:SER:H	1.50	0.58
16:Q:141:ARG:HA	16:Q:350:TRP:HA	1.85	0.58
2:B:802:PRO:HG2	2:B:805:THR:HG22	1.84	0.58
13:M:284:LEU:HD22	13:M:316:LEU:HG	1.86	0.58
19:U:244:MET:HG3	19:U:267:VAL:HG22	1.86	0.58
1:A:1189:SER:N	1:A:1242:VAL:O	2.31	0.58
7:G:4:ILE:HG12	7:G:77:VAL:HG22	1.84	0.58
2:B:919:SER:HB2	2:B:922:GLU:HB2	1.84	0.58
1:A:326:ARG:HG2	1:A:1406:VAL:HG11	1.86	0.58
2:B:969:ARG:NH2	3:C:60:ASP:OD2	2.36	0.58
7:G:84:GLY:CA	7:G:147:ILE:O	2.52	0.58
8:H:129:TYR:O	8:H:133:ASN:ND2	2.35	0.58
15:O:99:PHE:CB	18:T:58:DA:C4'	2.77	0.58
8:H:65:LEU:HD21	8:H:89:LEU:HD13	1.86	0.58
1:A:250:ILE:HD13	13:M:62:GLU:HG3	1.85	0.58
3:C:22:LEU:O	3:C:228:PHE:HB2	2.03	0.58
1:A:549:MET:HE1	1:A:656:TRP:HD1	1.68	0.58
1:A:1146:VAL:HG12	1:A:1201:ALA:HB1	1.85	0.58
2:B:445:LYS:NZ	17:R:267:GLY:O	2.36	0.58
14:N:24:DT:P	15:O:194:ILE:HD13	2.44	0.58
15:O:68:GLN:OE1	18:T:62:DA:H5'	2.04	0.58
1:A:335:ARG:HH22	2:B:1114:LEU:HD11	1.69	0.57
3:C:54:ASN:HD21	3:C:63:ILE:HD12	1.68	0.57
1:A:333:GLU:OE1	2:B:1129:ARG:NH2	2.37	0.57
1:A:390:GLN:OE1	1:A:393:ARG:NH2	2.37	0.57
2:B:872:GLU:HG2	2:B:916:THR:HG22	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:97:HIS:CE1	21:W:158:GLU:HG2	2.38	0.57
9:I:19:ASP:O	9:I:23:ASN:HA	2.04	0.57
11:K:49:GLU:OE2	11:K:97:LYS:NZ	2.36	0.57
1:A:443:LEU:HG	1:A:501:LEU:HD21	1.87	0.57
7:G:8:SER:HA	7:G:72:VAL:O	2.05	0.57
17:R:104:ILE:HD11	17:R:122:LEU:HD22	1.86	0.57
1:A:62:ASP:O	1:A:64:ASN:N	2.35	0.57
2:B:881:ASN:O	2:B:933:SER:OG	2.23	0.57
11:K:29:ASN:ND2	11:K:78:THR:O	2.37	0.57
16:Q:122:GLN:HB2	16:Q:394:LYS:HE3	1.87	0.57
17:R:104:ILE:HD11	17:R:122:LEU:HB3	1.86	0.56
19:U:262:LEU:HB2	19:U:279:ALA:HB3	1.87	0.56
5:E:28:TYR:HA	5:E:64:PRO:HA	1.86	0.56
21:W:175:LEU:HB2	22:X:259:PHE:CZ	2.39	0.56
1:A:348:SER:HA	1:A:489:LEU:O	2.04	0.56
2:B:118:ARG:NH2	2:B:202:TYR:OH	2.38	0.56
2:B:858:SER:HA	2:B:966:VAL:O	2.04	0.56
2:B:969:ARG:NH1	3:C:61:GLU:OE1	2.38	0.56
2:B:1009:ASP:OD2	10:J:48:ARG:NH2	2.38	0.56
3:C:73:GLN:NE2	3:C:237:SER:O	2.38	0.56
7:G:138:THR:HG22	7:G:139:ILE:H	1.70	0.56
9:I:55:THR:HG22	9:I:100:PHE:CD2	2.40	0.56
13:M:34:ILE:HG21	13:M:52:LEU:HD22	1.87	0.56
2:B:834:ASN:O	2:B:1013:ASN:HB2	2.05	0.56
17:R:67:GLN:HB3	17:R:219:CYS:HB2	1.87	0.56
2:B:483:LEU:HD11	2:B:491:THR:HG23	1.86	0.56
5:E:17:ARG:HH12	5:E:36:GLU:HA	1.71	0.56
7:G:107:LYS:NZ	21:W:142:PHE:CE1	2.73	0.56
13:M:177:LEU:HD22	13:M:207:LEU:HD11	1.87	0.56
7:G:84:GLY:HA2	7:G:147:ILE:O	2.05	0.56
2:B:794:ASN:HA	2:B:854:LEU:O	2.06	0.56
5:E:76:GLY:N	5:E:106:GLN:OE1	2.39	0.56
2:B:71:LEU:HD21	2:B:436:VAL:HG11	1.88	0.56
7:G:84:GLY:N	7:G:147:ILE:O	2.39	0.55
15:O:99:PHE:CB	18:T:58:DA:C1'	2.56	0.55
1:A:544:ASP:O	1:A:548:ASN:ND2	2.38	0.55
1:A:545:GLN:HG2	1:A:549:MET:HE3	1.88	0.55
2:B:278:GLN:HB2	2:B:337:ARG:HD2	1.88	0.55
4:D:141:LEU:HD13	7:G:46:LEU:HB3	1.88	0.55
19:U:30:ILE:HG23	19:U:31:ASP:H	1.71	0.55
1:A:687:LYS:NZ	1:A:801:GLU:OE1	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:97:HIS:HE1	21:W:158:GLU:HG2	1.72	0.55
15:O:74:VAL:HG21	15:O:136:SER:HB3	1.88	0.55
1:A:335:ARG:HA	1:A:339:ASN:HD22	1.72	0.55
2:B:984:HIS:NE2	2:B:1028:GLU:OE1	2.32	0.55
3:C:242:GLN:O	3:C:246:ARG:HB2	2.06	0.55
11:K:36:GLU:OE1	11:K:70:ARG:NH1	2.39	0.55
19:U:246:CYS:HB3	19:U:265:GLY:HA3	1.89	0.55
21:W:101:LYS:HB3	22:X:263:TRP:CZ3	2.42	0.55
1:A:845:LEU:HD11	1:A:1371:LEU:HD23	1.89	0.55
12:L:30:ILE:HB	12:L:57:LEU:HB2	1.88	0.55
2:B:211:VAL:O	2:B:480:SER:HA	2.07	0.54
1:A:908:LEU:HA	1:A:1029:ARG:HH22	1.72	0.54
1:A:1342:GLU:OE1	5:E:200:ARG:NH2	2.36	0.54
2:B:347:LYS:O	2:B:351:TYR:HB2	2.07	0.54
21:W:19:GLY:HA2	22:X:252:LEU:HB3	1.88	0.54
1:A:1441:PHE:O	6:F:92:ARG:NH1	2.41	0.54
15:O:69:ASN:HB2	18:T:61:DT:H1'	1.89	0.54
1:A:185:TRP:HZ3	1:A:200:ARG:HB2	1.72	0.54
2:B:298:LEU:HG	2:B:314:LEU:HD13	1.89	0.54
13:M:43:VAL:HG12	13:M:53:SER:HB3	1.90	0.54
15:O:205:LEU:HB2	15:O:213:VAL:HB	1.90	0.54
1:A:261:ASP:HB3	1:A:322:VAL:HG13	1.88	0.54
2:B:429:PHE:CZ	16:Q:332:LEU:HB2	2.43	0.54
5:E:62:ALA:HB3	5:E:78:LEU:HB3	1.90	0.54
5:E:124:VAL:HG13	5:E:132:ILE:HB	1.90	0.54
17:R:127:LYS:HA	17:R:220:HIS:CE1	2.43	0.54
21:W:101:LYS:CD	22:X:263:TRP:CE2	2.89	0.54
1:A:588:LEU:HD13	1:A:632:VAL:HG21	1.89	0.54
1:A:778:GLY:HA3	2:B:516:ASN:HB2	1.88	0.54
8:H:112:ILE:HG23	8:H:132:LEU:HD12	1.89	0.54
9:I:56:ALA:O	9:I:89:GLN:HG3	2.08	0.54
9:I:54:GLU:HG2	9:I:90:GLN:HB3	1.89	0.54
14:N:28:DT:H3	14:N:29:DA:H62	1.55	0.54
2:B:55:VAL:HA	2:B:59:LEU:HD13	1.90	0.53
2:B:303:TYR:HD1	2:B:571:PRO:HB3	1.73	0.53
11:K:17:SER:H	11:K:20:LYS:HZ1	1.55	0.53
15:O:91:ASN:ND2	20:V:69:TYR:CZ	2.76	0.53
21:W:18:ARG:NE	22:X:250:GLY:N	2.43	0.53
7:G:158:HIS:HD2	21:W:138:GLN:OE1	1.88	0.53
21:W:178:GLN:CD	22:X:254:CYS:SG	2.90	0.53
2:B:833:TYR:HB2	2:B:840:ILE:HD11	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:95:SER:OG	7:G:98:GLY:O	2.23	0.53
1:A:899:VAL:H	1:A:929:LEU:HD11	1.72	0.53
2:B:549:THR:HG1	2:B:628:THR:HG1	1.51	0.53
10:J:2:ILE:HD13	10:J:57:ILE:HG21	1.90	0.53
13:M:241:ARG:O	13:M:245:HIS:ND1	2.34	0.53
9:I:29:CYS:SG	9:I:31:THR:OG1	2.66	0.53
21:W:14:LYS:NZ	21:W:30:ASP:OD1	2.41	0.53
21:W:96:ASP:HB3	22:X:278:LEU:HD12	1.90	0.53
2:B:1187:ASN:ND2	2:B:1190:ASP:O	2.39	0.53
17:R:98:ASN:CB	17:R:103:LYS:O	2.50	0.53
2:B:128:LEU:HB2	2:B:168:GLY:O	2.09	0.53
2:B:1042:GLY:HA2	16:Q:22:ILE:HA	1.90	0.53
7:G:47:CYS:SG	7:G:48:VAL:N	2.81	0.53
15:O:99:PHE:CE1	18:T:58:DA:C4	2.97	0.53
2:B:43:LEU:O	2:B:496:ARG:NH1	2.41	0.53
3:C:6:PRO:HB3	3:C:25:VAL:HG23	1.90	0.53
1:A:226:GLU:HA	1:A:230:ARG:HE	1.74	0.53
1:A:353:ILE:HG22	1:A:468:PHE:HB2	1.90	0.52
1:A:700:ASN:HB2	9:I:98:VAL:HG22	1.90	0.52
2:B:458:LYS:O	2:B:462:ALA:HB2	2.09	0.52
2:B:806:THR:HG23	2:B:1045:SER:HA	1.91	0.52
2:B:923:GLU:HB3	2:B:925:LEU:HG	1.91	0.52
2:B:1106:ARG:HH11	2:B:1126:GLY:HA2	1.73	0.52
21:W:175:LEU:HD23	22:X:259:PHE:CG	2.44	0.52
20:V:72:CYS:O	20:V:75:VAL:HB	2.10	0.52
1:A:115:LEU:HD22	1:A:119:ASN:HD22	1.73	0.52
3:C:100:THR:OG1	3:C:102:GLN:NE2	2.43	0.52
13:M:276:THR:HA	13:M:279:VAL:HG12	1.91	0.52
20:V:71:PHE:HA	20:V:75:VAL:O	2.09	0.52
15:O:93:GLU:OE2	15:O:105:ARG:NH1	2.41	0.52
1:A:445:ASN:OD1	1:A:449:SER:OG	2.21	0.52
1:A:752:LYS:HG3	2:B:1015:HIS:HB3	1.92	0.52
2:B:345:LYS:HA	2:B:348:ARG:HG2	1.91	0.52
3:C:34:ARG:HB3	3:C:230:MET:HE1	1.92	0.52
7:G:107:LYS:HZ2	21:W:142:PHE:HE1	1.56	0.52
1:A:48:ALA:HB3	1:A:56:PRO:HD3	1.90	0.52
2:B:757:PRO:HD3	2:B:983:ARG:HE	1.75	0.52
16:Q:366:GLU:O	16:Q:368:GLY:N	2.43	0.52
1:A:63:ARG:HA	1:A:74:MET:HG2	1.92	0.52
1:A:553:VAL:HB	1:A:556:TRP:HB2	1.92	0.52
2:B:791:THR:HG22	2:B:792:MET:HG3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:111:THR:HB	7:G:114:LEU:HD13	1.92	0.52
15:O:113:ALA:HA	15:O:122:VAL:O	2.09	0.52
21:W:101:LYS:CD	22:X:263:TRP:CZ2	2.91	0.52
2:B:826:ALA:O	2:B:1011:ILE:HA	2.10	0.52
8:H:142:LEU:HG	8:H:144:ILE:HD11	1.92	0.52
10:J:48:ARG:O	10:J:52:THR:OG1	2.14	0.52
16:Q:366:GLU:HB3	16:Q:392:VAL:HG13	1.90	0.52
17:R:73:LEU:HD23	17:R:78:ALA:HA	1.92	0.52
2:B:862:GLN:OE1	2:B:957:ASN:ND2	2.42	0.52
2:B:1060:ARG:NH1	3:C:200:GLU:O	2.42	0.52
13:M:199:LYS:O	13:M:201:LYS:N	2.42	0.52
17:R:105:THR:HA	17:R:120:TYR:O	2.09	0.52
2:B:1060:ARG:HH12	3:C:202:PRO:HD3	1.75	0.51
4:D:51:ASN:HD22	4:D:181:GLY:HA3	1.74	0.51
20:V:62:VAL:HG22	20:V:85:VAL:HG22	1.92	0.51
2:B:641:GLU:HB2	2:B:652:LYS:HE2	1.93	0.51
13:M:202:GLU:OE2	13:M:206:THR:OG1	2.24	0.51
2:B:342:GLY:O	2:B:344:LYS:N	2.41	0.51
11:K:61:TYR:HA	11:K:72:LYS:O	2.11	0.51
13:M:280:VAL:HG12	13:M:309:ILE:HA	1.92	0.51
15:O:99:PHE:CG	18:T:58:DA:O4'	2.34	0.51
22:X:193:LEU:HA	22:X:196:LEU:HD12	1.92	0.51
1:A:864:ILE:HG22	1:A:865:GLN:HG3	1.93	0.51
1:A:1154:TYR:HE2	9:I:18:GLU:HB2	1.75	0.51
1:A:1155:ASP:OD2	1:A:1241:ARG:NH2	2.39	0.51
2:B:22:SER:O	2:B:654:ARG:NH2	2.44	0.51
7:G:97:HIS:HE1	21:W:122:TYR:HE2	1.37	0.51
15:O:115:ILE:HD13	15:O:143:ILE:HD11	1.92	0.51
3:C:185:LYS:HE2	3:C:213:PRO:HB3	1.93	0.51
5:E:26:ARG:HH12	5:E:189:GLY:HA3	1.74	0.51
7:G:44:TYR:OH	7:G:157:ILE:O	2.28	0.51
8:H:8:ASP:OD1	8:H:9:ILE:N	2.44	0.51
16:Q:334:VAL:HG12	16:Q:335:LEU:H	1.75	0.51
1:A:88:LYS:HD3	1:A:89:PRO:HD2	1.92	0.51
3:C:222:LYS:H	3:C:222:LYS:HD3	1.76	0.51
6:F:82:THR:HG22	6:F:84:TYR:H	1.76	0.51
15:O:91:ASN:CG	20:V:69:TYR:CZ	2.89	0.51
1:A:966:ASN:O	1:A:970:THR:OG1	2.25	0.51
2:B:771:SER:O	2:B:775:LYS:NZ	2.43	0.51
3:C:35:ARG:NH2	11:K:39:ASP:OD2	2.41	0.51
13:M:187:ARG:HH11	13:M:241:ARG:HH21	1.59	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:R:63:ARG:C	17:R:65:ASN:H	2.19	0.51
1:A:840:ARG:O	1:A:844:ALA:HB2	2.11	0.50
2:B:413:LEU:HD21	2:B:461:LEU:HD11	1.93	0.50
7:G:113:HIS:NE2	21:W:119:PRO:HB2	2.24	0.50
13:M:267:LYS:HE2	15:O:208:VAL:CG1	2.41	0.50
1:A:869:GLY:HA3	1:A:1366:ARG:HD2	1.93	0.50
2:B:952:VAL:HG22	2:B:966:VAL:HG13	1.93	0.50
19:U:283:ALA:HB1	20:V:66:LEU:HB2	1.94	0.50
2:B:102:VAL:O	2:B:109:THR:HA	2.12	0.50
2:B:376:PHE:HD2	2:B:566:LEU:HG	1.75	0.50
9:I:55:THR:HG22	9:I:100:PHE:CE2	2.47	0.50
9:I:86:PHE:O	9:I:100:PHE:HB2	2.12	0.50
1:A:961:ARG:NH1	1:A:1035:TYR:OH	2.44	0.50
2:B:269:ILE:HD11	2:B:386:LEU:HD21	1.94	0.50
2:B:521:LEU:HD22	2:B:633:VAL:HG12	1.93	0.50
15:O:202:ILE:HD11	15:O:222:GLU:HB3	1.94	0.50
1:A:534:LEU:HD11	1:A:577:ILE:HD11	1.93	0.50
2:B:755:ILE:O	2:B:983:ARG:NE	2.45	0.50
1:A:882:SER:O	1:A:1025:ARG:NH2	2.43	0.49
2:B:766:ARG:HE	2:B:1020:ARG:HB3	1.77	0.49
2:B:1091:TYR:HE2	2:B:1093:GLN:HE21	1.58	0.49
7:G:107:LYS:NZ	21:W:142:PHE:HE1	2.08	0.49
15:O:206:ILE:HD13	15:O:234:LEU:HD21	1.93	0.49
19:U:38:LEU:O	19:U:42:TRP:HB2	2.12	0.49
21:W:99:LYS:HG2	21:W:186:LEU:HD13	1.93	0.49
22:X:273:GLU:HG2	22:X:276:ARG:HH11	1.76	0.49
1:A:1029:ARG:O	1:A:1033:GLN:HB3	2.12	0.49
1:A:1118:VAL:HB	1:A:1306:LEU:HB2	1.93	0.49
1:A:1373:ASP:O	1:A:1377:THR:HG23	2.12	0.49
2:B:226:PHE:HD1	2:B:395:GLN:HE21	1.60	0.49
21:W:24:SER:HA	21:W:27:LEU:HD22	1.94	0.49
1:A:597:LEU:HD13	8:H:103:LYS:HD3	1.94	0.49
1:A:984:LYS:O	1:A:988:LEU:HB2	2.12	0.49
1:A:1020:CYS:SG	1:A:1023:ARG:NH2	2.85	0.49
2:B:87:LYS:HB2	2:B:137:TYR:HB2	1.93	0.49
16:Q:119:LEU:HD12	17:R:133:TYR:HB2	1.93	0.49
2:B:793:ALA:O	2:B:855:PHE:HA	2.13	0.49
9:I:54:GLU:HA	9:I:90:GLN:N	2.21	0.49
1:A:69:THR:HG23	1:A:80:HIS:NE2	2.28	0.49
21:W:175:LEU:HD23	22:X:259:PHE:CD2	2.47	0.49
1:A:63:ARG:HH11	13:M:57:VAL:HG22	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:19:ASP:HB2	3:C:231:ASN:HD22	1.76	0.49
4:D:54:GLU:HB2	4:D:160:VAL:HG11	1.95	0.49
7:G:113:HIS:CE1	21:W:119:PRO:CB	2.94	0.49
15:O:105:ARG:NE	19:U:253:ARG:CZ	2.76	0.49
1:A:1191:TRP:CZ3	9:I:43:VAL:HG21	2.48	0.49
16:Q:381:ASP:OD1	16:Q:382:GLY:N	2.42	0.49
1:A:446:ARG:O	1:A:449:SER:OG	2.31	0.49
6:F:133:VAL:HA	6:F:147:SER:HA	1.95	0.49
1:A:495:GLU:OE1	1:A:495:GLU:N	2.46	0.49
1:A:526:ASP:OD1	2:B:1015:HIS:ND1	2.46	0.49
1:A:1199:ARG:NH1	1:A:1233:ASP:O	2.45	0.49
2:B:402:GLY:O	2:B:405:ARG:NH1	2.41	0.49
8:H:26:ILE:HG13	8:H:42:ILE:HD12	1.95	0.49
9:I:14:LEU:HA	9:I:28:GLU:O	2.13	0.49
15:O:98:ARG:CG	18:T:57:DT:O3'	2.59	0.49
1:A:381:THR:HG23	1:A:383:TYR:H	1.78	0.48
18:T:56:DC:OP2	18:T:56:DC:H2'	2.12	0.48
1:A:1116:LEU:HD11	1:A:1311:VAL:HG23	1.94	0.48
2:B:120:ARG:HG2	2:B:955:THR:HG21	1.96	0.48
2:B:810:GLU:HB2	2:B:815:ARG:HH12	1.79	0.48
13:M:267:LYS:HG3	13:M:268:GLU:H	1.78	0.48
16:Q:352:MET:HG3	16:Q:361:TRP:HB2	1.94	0.48
17:R:73:LEU:HD23	17:R:78:ALA:CA	2.43	0.48
1:A:481:ASP:C	1:A:483:ASP:OD1	2.56	0.48
5:E:179:GLN:HG2	5:E:181:ALA:H	1.78	0.48
13:M:118:VAL:HG22	13:M:124:ASN:ND2	2.28	0.48
15:O:68:GLN:HB3	18:T:61:DT:H2''	1.94	0.48
9:I:19:ASP:CB	9:I:24:ARG:O	2.60	0.48
15:O:105:ARG:HE	19:U:253:ARG:NH2	2.10	0.48
15:O:105:ARG:CZ	19:U:253:ARG:CZ	2.92	0.48
21:W:77:PRO:O	21:W:79:SER:N	2.46	0.48
1:A:1336:MET:HE2	1:A:1380:GLY:HA2	1.96	0.48
2:B:364:ILE:HG22	2:B:365:THR:HG22	1.96	0.48
16:Q:363:GLY:HA2	16:Q:395:PHE:HA	1.95	0.48
1:A:99:ILE:HG12	1:A:234:MET:HE3	1.94	0.48
1:A:338:GLY:HA2	2:B:1129:ARG:HH22	1.79	0.48
1:A:540:PHE:HB3	1:A:571:LEU:HD23	1.94	0.48
2:B:63:ILE:O	2:B:67:SER:HB3	2.13	0.48
2:B:282:ILE:HD12	2:B:382:ILE:HD13	1.96	0.48
6:F:76:LYS:HA	6:F:79:ARG:HE	1.79	0.48
1:A:481:ASP:OD2	1:A:483:ASP:OD2	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1012:ARG:O	1:A:1016:THR:OG1	2.30	0.48
11:K:32:VAL:HG22	11:K:74:ARG:HG2	1.94	0.48
1:A:1002:GLY:HA3	1:A:1007:ILE:HG21	1.95	0.47
9:I:54:GLU:CG	9:I:88:SER:OG	2.62	0.47
2:B:363:HIS:CD2	2:B:364:ILE:HG13	2.49	0.47
17:R:69:TRP:CD1	17:R:219:CYS:HB3	2.49	0.47
2:B:249:ARG:HG2	2:B:415:GLN:NE2	2.29	0.47
2:B:1004:GLU:OE1	2:B:1064:TYR:OH	2.27	0.47
14:N:24:DT:H1'	15:O:215:THR:HG21	1.97	0.47
21:W:18:ARG:NH1	22:X:249:GLY:CA	2.70	0.47
1:A:308:ILE:HG23	1:A:311:GLN:HB2	1.97	0.47
2:B:398:ARG:H	2:B:398:ARG:HD2	1.80	0.47
2:B:737:THR:OG1	9:I:66:PRO:O	2.27	0.47
2:B:861:ASP:OD1	2:B:862:GLN:N	2.48	0.47
21:W:74:GLU:CB	21:W:82:VAL:O	2.63	0.47
1:A:630:ILE:O	1:A:634:THR:OG1	2.27	0.47
1:A:810:PRO:HG2	2:B:705:MET:HE2	1.95	0.47
2:B:924:GLU:H	2:B:928:ARG:HD2	1.80	0.47
13:M:268:GLU:C	13:M:270:ALA:H	2.23	0.47
1:A:58:LEU:HA	1:A:80:HIS:HB2	1.96	0.47
2:B:70:ILE:HG22	2:B:89:GLU:HG3	1.97	0.47
2:B:114:PRO:HG2	2:B:181:LEU:HD11	1.95	0.47
2:B:810:GLU:HG3	2:B:815:ARG:HH22	1.80	0.47
3:C:29:MET:HE1	11:K:97:LYS:HE3	1.97	0.47
7:G:119:LEU:HD11	7:G:130:TYR:HB3	1.95	0.47
8:H:89:LEU:HG	8:H:90:ALA:H	1.78	0.47
13:M:272:LYS:CE	18:T:65:DT:H5''	2.44	0.47
21:W:179:ILE:HD12	21:W:182:ILE:HD12	1.97	0.47
21:W:187:LYS:HD3	21:W:187:LYS:HA	1.69	0.47
15:O:214:LEU:HD22	15:O:223:ILE:HG23	1.96	0.47
17:R:97:ILE:HA	17:R:104:ILE:HG22	1.97	0.47
17:R:122:LEU:HD21	17:R:222:CYS:HB3	1.97	0.47
11:K:24:ASP:HB2	11:K:32:VAL:HG23	1.95	0.47
13:M:312:GLY:O	13:M:316:LEU:HB2	2.14	0.47
15:O:171:ARG:HB2	15:O:237:PHE:HB3	1.96	0.47
16:Q:102:PRO:HA	17:R:94:LYS:HA	1.97	0.47
18:T:56:DC:H2''	18:T:57:DT:C5	2.50	0.47
2:B:458:LYS:O	2:B:462:ALA:CB	2.63	0.47
5:E:156:LEU:HD11	5:E:197:LYS:HB2	1.96	0.47
2:B:336:ARG:HD2	2:B:348:ARG:NH1	2.30	0.46
15:O:99:PHE:CD2	18:T:58:DA:C2'	2.93	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:W:176:MET:HA	21:W:179:ILE:HG22	1.96	0.46
22:X:218:ASP:HA	22:X:221:ILE:HD12	1.97	0.46
1:A:1012:ARG:HH21	1:A:1015:VAL:HG11	1.81	0.46
2:B:931:TYR:O	2:B:933:SER:N	2.43	0.46
10:J:17:LYS:HB3	10:J:39:LEU:HD13	1.96	0.46
1:A:806:ARG:HD2	2:B:728:ARG:HA	1.97	0.46
20:V:60:LEU:HA	20:V:86:THR:O	2.15	0.46
1:A:1161:THR:HG22	1:A:1163:ILE:H	1.81	0.46
2:B:194:GLU:HA	2:B:784:ASN:HD22	1.80	0.46
1:A:1444:MET:HE1	7:G:60:ARG:HB2	1.96	0.46
7:G:97:HIS:HE1	21:W:158:GLU:CG	2.29	0.46
15:O:95:ASN:N	15:O:95:ASN:OD1	2.47	0.46
1:A:471:ASN:OD1	1:A:472:LEU:N	2.48	0.46
2:B:393:LYS:NZ	2:B:621:GLU:OE1	2.46	0.46
5:E:58:MET:HE2	5:E:82:PHE:HE2	1.80	0.46
1:A:561:PRO:HB2	1:A:576:GLN:HE21	1.80	0.46
1:A:855:THR:HG21	1:A:857:ARG:HH21	1.81	0.46
9:I:88:SER:O	9:I:91:ARG:NH1	2.47	0.46
4:D:123:LEU:HD21	4:D:146:GLN:HA	1.97	0.46
2:B:824:ILE:HD13	2:B:1089:PRO:HB3	1.98	0.46
6:F:135:ARG:HA	6:F:144:GLU:O	2.16	0.46
15:O:202:ILE:HG13	15:O:226:ALA:HB2	1.98	0.46
1:A:481:ASP:CG	1:A:483:ASP:OD1	2.59	0.45
17:R:263:MET:O	17:R:266:THR:OG1	2.28	0.45
18:T:61:DT:P	19:U:255:LYS:HZ2	2.38	0.45
1:A:116:ASP:OD1	1:A:117:GLU:N	2.43	0.45
1:A:993:LEU:HD13	1:A:1046:LEU:HD22	1.98	0.45
2:B:314:LEU:O	2:B:318:VAL:HG23	2.16	0.45
18:T:61:DT:H2'	18:T:62:DA:C8	2.51	0.45
2:B:290:GLY:HA2	2:B:327:ARG:HD2	1.98	0.45
2:B:663:ALA:O	2:B:667:GLN:HB2	2.17	0.45
13:M:262:LYS:O	13:M:266:ILE:HG13	2.17	0.45
20:V:61:THR:HB	20:V:86:THR:HB	1.99	0.45
1:A:563:PRO:HG2	1:A:566:ILE:HG13	1.98	0.45
1:A:990:VAL:HG12	1:A:994:GLN:HE21	1.80	0.45
2:B:737:THR:HB	9:I:66:PRO:CB	2.47	0.45
7:G:64:THR:C	7:G:66:GLY:H	2.25	0.45
7:G:123:ALA:HA	7:G:128:PRO:HB3	1.97	0.45
8:H:5:LEU:HD22	8:H:134:ASN:HB3	1.99	0.45
15:O:227:PHE:HA	15:O:230:ILE:HG22	1.99	0.45
21:W:77:PRO:C	21:W:79:SER:H	2.23	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:596:THR:HG22	1:A:597:LEU:H	1.80	0.45
1:A:864:ILE:HG12	1:A:1374:VAL:HG22	1.97	0.45
2:B:301:ILE:O	2:B:383:ASN:ND2	2.49	0.45
4:D:63:LEU:HD13	4:D:130:LEU:HD13	1.99	0.45
1:A:45:GLN:O	1:A:257:ARG:NH1	2.41	0.45
1:A:1191:TRP:CD1	1:A:1256:GLU:HB2	2.52	0.45
2:B:867:GLY:C	2:B:869:SER:H	2.25	0.45
16:Q:379:GLU:OE2	16:Q:383:SER:OG	2.35	0.45
20:V:23:LEU:HD13	20:V:37:ALA:HB1	1.99	0.45
1:A:463:ILE:HD12	1:A:464:PRO:O	2.17	0.45
2:B:933:SER:OG	2:B:934:LYS:N	2.49	0.45
7:G:97:HIS:CE1	21:W:158:GLU:CG	2.99	0.45
2:B:276:ILE:HA	2:B:338:GLY:HA3	1.99	0.45
1:A:231:PRO:HA	1:A:234:MET:HE2	1.99	0.45
2:B:859:TYR:OH	2:B:945:GLU:OE1	2.35	0.45
13:M:268:GLU:OE1	13:M:319:HIS:NE2	2.38	0.45
15:O:199:LYS:HA	15:O:200:PRO:HA	1.84	0.45
16:Q:402:ALA:O	16:Q:403:THR:HG23	2.16	0.45
1:A:367:PRO:HD2	1:A:370:ILE:HD12	1.98	0.45
1:A:1146:VAL:HG11	1:A:1207:LEU:HD12	2.00	0.45
18:T:64:DA:H2''	18:T:65:DT:C5	2.52	0.45
21:W:152:CYS:O	21:W:154:GLU:HG3	2.17	0.45
1:A:92:HIS:O	1:A:96:ILE:HG13	2.17	0.44
2:B:954:VAL:HG11	2:B:962:LYS:HE3	1.98	0.44
7:G:23:LYS:O	7:G:26:LEU:HB2	2.16	0.44
12:L:43:THR:HG22	12:L:43:THR:O	2.16	0.44
2:B:634:TYR:HA	2:B:694:ASP:HA	1.98	0.44
21:W:18:ARG:CG	22:X:250:GLY:HA2	2.47	0.44
1:A:350:ARG:HA	1:A:487:MET:O	2.17	0.44
1:A:587:HIS:HA	1:A:607:ILE:O	2.16	0.44
2:B:1172:ILE:HD11	2:B:1183:LYS:HD2	1.98	0.44
21:W:171:LYS:O	21:W:175:LEU:HB2	2.16	0.44
15:O:76:LEU:HD13	15:O:143:ILE:HG21	2.00	0.44
1:A:567:LYS:HA	1:A:568:PRO:HA	1.82	0.44
2:B:226:PHE:HA	2:B:395:GLN:HG3	1.99	0.44
2:B:238:ALA:HB2	2:B:385:LEU:HD13	1.99	0.44
7:G:21:ARG:HG3	7:G:25:TYR:HE2	1.81	0.44
16:Q:352:MET:CG	16:Q:361:TRP:HB2	2.47	0.44
1:A:53:LEU:HD21	1:A:267:ALA:HB2	1.99	0.44
9:I:83:ASN:HA	9:I:104:LEU:HG	1.98	0.44
13:M:198:VAL:HG12	13:M:198:VAL:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:W:24:SER:HA	21:W:27:LEU:HB2	1.98	0.44
1:A:443:LEU:HD21	1:A:501:LEU:HD11	2.00	0.44
2:B:499:ASN:OD1	2:B:500:THR:N	2.50	0.44
8:H:5:LEU:HD11	8:H:61:SER:HB3	2.00	0.44
13:M:44:VAL:HG22	13:M:51:VAL:HA	2.00	0.44
13:M:166:LYS:HB3	13:M:170:SER:HB3	2.00	0.44
1:A:253:ASN:C	1:A:255:SER:H	2.25	0.44
1:A:849:MET:HE3	1:A:1063:MET:HE1	1.98	0.44
1:A:1051:ALA:O	1:A:1055:ARG:HG2	2.18	0.44
1:A:1409:LEU:HD13	2:B:1207:LEU:HD21	1.99	0.44
2:B:281:PRO:HD2	2:B:284:ILE:HD12	2.00	0.44
8:H:44:VAL:HG13	8:H:48:PRO:HA	1.99	0.44
19:U:260:CYS:HB2	19:U:281:VAL:HB	1.99	0.44
1:A:882:SER:OG	1:A:953:ASN:ND2	2.51	0.43
2:B:195:CYS:HB3	2:B:782:LEU:HD22	2.00	0.43
3:C:92:CYS:C	3:C:94:LYS:H	2.26	0.43
9:I:54:GLU:HB3	9:I:88:SER:CB	2.46	0.43
19:U:9:VAL:HG13	20:V:51:THR:HG21	2.00	0.43
1:A:351:THR:O	1:A:486:GLU:HA	2.18	0.43
2:B:1073:TYR:CE1	2:B:1080:LYS:HG2	2.53	0.43
7:G:102:GLN:HE22	7:G:107:LYS:HE2	1.83	0.43
13:M:325:ASP:HB3	13:M:326:PRO:HD3	2.00	0.43
1:A:439:ASN:HA	1:A:459:ARG:HG3	1.99	0.43
1:A:1146:VAL:HG11	1:A:1207:LEU:CD1	2.47	0.43
7:G:113:HIS:HE1	21:W:119:PRO:HG2	1.78	0.43
9:I:54:GLU:CA	9:I:88:SER:OG	2.66	0.43
1:A:362:ASP:OD2	1:A:459:ARG:NH1	2.52	0.43
3:C:19:ASP:HA	3:C:231:ASN:HA	2.00	0.43
7:G:97:HIS:O	7:G:112:LYS:N	2.51	0.43
1:A:339:ASN:HB3	2:B:1199:ALA:HB1	2.01	0.43
1:A:405:VAL:HG13	1:A:432:VAL:HG22	2.01	0.43
6:F:123:LYS:NZ	6:F:127:GLU:OE2	2.51	0.43
8:H:64:ASN:OD1	8:H:65:LEU:N	2.52	0.43
19:U:267:VAL:HG12	19:U:269:ILE:HG13	2.00	0.43
2:B:279:ASP:OD1	2:B:279:ASP:N	2.50	0.43
2:B:412:LEU:HB3	2:B:466:TRP:CE2	2.53	0.43
17:R:133:TYR:CD1	17:R:217:THR:HG22	2.52	0.43
1:A:407:ARG:HH11	1:A:413:ILE:HD11	1.83	0.43
1:A:546:VAL:HG21	1:A:572:TRP:HB2	1.99	0.43
2:B:273:LEU:HD12	2:B:280:ILE:HD12	2.00	0.43
12:L:38:LEU:HD23	12:L:40:LEU:HD23	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:388:PRO:HB2	17:R:82:ARG:NH1	2.34	0.43
1:A:348:SER:HB2	2:B:1128:LEU:HD12	2.01	0.43
1:A:399:HIS:HB3	1:A:400:PRO:HD3	2.00	0.43
1:A:663:SER:OG	2:B:1084:GLN:O	2.25	0.43
2:B:884:ARG:HG3	2:B:935:ARG:HE	1.84	0.43
16:Q:376:LEU:HB2	17:R:69:TRP:HB2	2.01	0.43
1:A:412:ARG:NH2	13:M:54:ASP:OD1	2.36	0.43
2:B:223:VAL:HG22	2:B:240:ILE:HD12	2.00	0.43
7:G:143:ILE:HG13	7:G:170:ALA:HA	2.01	0.43
1:A:148:CYS:O	1:A:168:GLY:HA2	2.19	0.43
1:A:375:THR:HB	1:A:403:LYS:HD3	2.01	0.43
1:A:377:PRO:HB3	1:A:433:GLU:HG2	2.00	0.43
1:A:1260:LEU:O	1:A:1264:GLU:HG3	2.19	0.43
2:B:376:PHE:HE2	2:B:567:GLU:HA	1.84	0.43
2:B:1074:ASN:OD1	2:B:1075:GLY:N	2.52	0.43
5:E:56:LYS:NZ	5:E:84:ASP:OD2	2.43	0.43
13:M:235:ASN:CG	13:M:274:PRO:HB2	2.44	0.43
1:A:849:MET:SD	1:A:849:MET:N	2.92	0.42
17:R:105:THR:OG1	17:R:106:LEU:N	2.52	0.42
1:A:362:ASP:O	1:A:458:HIS:ND1	2.51	0.42
11:K:58:PHE:HB3	11:K:76:GLN:HB3	2.01	0.42
17:R:258:THR:O	17:R:260:GLY:N	2.42	0.42
17:R:262:THR:O	17:R:266:THR:HG23	2.19	0.42
2:B:283:VAL:O	2:B:287:ARG:HG2	2.19	0.42
8:H:7:ASP:OD1	8:H:58:THR:OG1	2.37	0.42
8:H:18:GLY:C	8:H:20:TYR:H	2.27	0.42
14:N:22:DT:H2'	14:N:23:DA:C8	2.55	0.42
21:W:63:SER:O	22:X:268:LEU:HD12	2.19	0.42
1:A:113:LEU:HD11	1:A:218:ASP:HA	2.01	0.42
1:A:372:LYS:HA	1:A:435:HIS:HD2	1.84	0.42
2:B:1008:PRO:HB3	2:B:1087:PHE:HE1	1.84	0.42
13:M:201:LYS:HG3	14:N:23:DA:P	2.60	0.42
1:A:54:ASN:OD1	1:A:54:ASN:N	2.52	0.42
1:A:217:LYS:O	1:A:221:SER:OG	2.33	0.42
2:B:910:VAL:HA	2:B:940:PRO:HA	2.01	0.42
21:W:9:VAL:HG22	21:W:189:ILE:HD13	2.01	0.42
13:M:187:ARG:NH1	13:M:241:ARG:HH21	2.17	0.42
18:T:61:DT:P	19:U:255:LYS:NZ	2.92	0.42
21:W:26:VAL:HA	21:W:29:LEU:HB3	2.00	0.42
4:D:158:GLU:OE1	4:D:158:GLU:N	2.41	0.42
13:M:142:LEU:HD23	13:M:146:VAL:HG11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:U:253:ARG:HD2	19:U:258:TRP:CZ2	2.54	0.42
21:W:44:LYS:NZ	21:W:49:ILE:O	2.50	0.42
1:A:481:ASP:N	1:A:481:ASP:OD1	2.52	0.42
1:A:1035:TYR:HB3	1:A:1037:LEU:HG	2.01	0.42
7:G:83:LYS:HG2	7:G:149:GLY:HA2	2.01	0.42
1:A:913:LEU:HD11	1:A:919:ILE:HG13	2.02	0.42
7:G:98:GLY:HA3	7:G:110:VAL:O	2.20	0.42
9:I:55:THR:CG2	9:I:100:PHE:CE2	3.03	0.42
1:A:925:LEU:HD22	1:A:983:ILE:HB	2.00	0.41
1:A:1191:TRP:CZ3	1:A:1257:ASP:HB3	2.55	0.41
2:B:487:THR:HG23	2:B:490:SER:H	1.85	0.41
3:C:68:GLY:HA3	12:L:69:ALA:HB1	2.01	0.41
3:C:262:LEU:HD22	11:K:87:LEU:HD23	2.01	0.41
13:M:267:LYS:CE	15:O:208:VAL:CG1	2.98	0.41
15:O:68:GLN:HG3	18:T:62:DA:H4'	2.01	0.41
1:A:1012:ARG:HA	1:A:1015:VAL:HG12	2.02	0.41
7:G:126:ASN:HA	7:G:127:PRO:HA	1.96	0.41
7:G:151:ILE:HD11	21:W:134:LEU:HD23	2.02	0.41
13:M:267:LYS:CG	13:M:268:GLU:H	2.31	0.41
1:A:230:ARG:HB2	1:A:233:TRP:CG	2.55	0.41
15:O:94:TYR:CZ	15:O:96:PRO:HG3	2.54	0.41
1:A:497:THR:O	1:A:501:LEU:HB2	2.20	0.41
1:A:1022:LEU:O	1:A:1026:LEU:HB2	2.20	0.41
2:B:778:MET:HA	2:B:1096:ARG:HH12	1.86	0.41
2:B:895:ASP:OD2	12:L:42:ARG:NH2	2.54	0.41
5:E:124:VAL:H	5:E:125:PRO:HD2	1.85	0.41
6:F:76:LYS:HB3	6:F:79:ARG:HH21	1.85	0.41
1:A:167:CYS:SG	1:A:168:GLY:N	2.92	0.41
2:B:451:LYS:O	2:B:455:SER:HB2	2.20	0.41
2:B:950:ASP:HB2	2:B:969:ARG:HG2	2.02	0.41
2:B:1058:LEU:O	2:B:1062:HIS:ND1	2.50	0.41
4:D:56:ARG:HH22	4:D:155:ARG:HE	1.68	0.41
7:G:109:PHE:CD2	21:W:137:VAL:HG12	2.56	0.41
15:O:114:LEU:HD11	18:T:59:DT:O2	2.20	0.41
21:W:90:LYS:HD2	21:W:90:LYS:HA	1.95	0.41
21:W:140:LEU:HD22	21:W:147:PHE:HE1	1.85	0.41
2:B:70:ILE:HG21	16:Q:335:LEU:HD21	2.01	0.41
2:B:24:PRO:HA	2:B:654:ARG:HH12	1.86	0.41
2:B:474:SER:O	2:B:476:ARG:N	2.53	0.41
4:D:159:THR:O	4:D:163:VAL:HG23	2.21	0.41
14:N:21:DA:H2'	14:N:22:DT:C6	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:28:DT:H3	14:N:29:DA:N6	2.18	0.41
2:B:26:THR:OG1	2:B:27:ALA:N	2.54	0.41
2:B:1135:ARG:HG3	2:B:1147:LEU:HD11	2.03	0.41
7:G:115:MET:O	7:G:164:LYS:NZ	2.49	0.41
13:M:143:PRO:HG2	13:M:146:VAL:HG23	2.03	0.41
15:O:105:ARG:NH2	19:U:253:ARG:NH1	2.68	0.41
1:A:1242:VAL:HG12	1:A:1243:VAL:N	2.36	0.41
5:E:58:MET:HE2	5:E:82:PHE:CE2	2.55	0.41
5:E:136:ASN:OD1	5:E:137:GLU:N	2.54	0.41
6:F:97:ARG:NE	6:F:124:GLU:OE1	2.38	0.41
8:H:93:TYR:CG	8:H:143:LEU:HB3	2.56	0.41
13:M:186:ALA:HB1	13:M:238:TYR:CZ	2.56	0.41
16:Q:378:VAL:HG22	16:Q:384:PHE:CD1	2.56	0.41
19:U:264:ASP:OD1	19:U:277:GLN:NE2	2.54	0.41
1:A:635:ARG:NH2	1:A:876:ALA:O	2.54	0.41
1:A:1194:ARG:HA	1:A:1238:ILE:O	2.20	0.41
7:G:45:ILE:HA	7:G:78:VAL:HG12	2.02	0.41
15:O:107:ARG:HD3	19:U:286:VAL:HB	2.03	0.41
2:B:443:ASN:HD22	2:B:446:LEU:HG	1.86	0.40
7:G:122:ASN:HB3	7:G:129:SER:O	2.21	0.40
1:A:885:THR:HB	1:A:943:LEU:HD12	2.03	0.40
1:A:1165:GLU:O	1:A:1167:GLU:N	2.55	0.40
2:B:26:THR:HG23	2:B:29:ASP:H	1.86	0.40
2:B:54:PHE:O	2:B:58:THR:HB	2.21	0.40
2:B:657:HIS:HA	2:B:660:LYS:HZ3	1.86	0.40
2:B:1183:LYS:HB3	2:B:1183:LYS:HE3	1.83	0.40
3:C:255:VAL:HG21	11:K:94:ILE:HG21	2.04	0.40
7:G:93:SER:OG	7:G:100:GLU:OE1	2.39	0.40
7:G:97:HIS:ND1	21:W:122:TYR:OH	2.49	0.40
16:Q:139:LEU:HD23	17:R:212:THR:HG21	2.03	0.40
20:V:34:ALA:C	20:V:36:LEU:H	2.29	0.40
2:B:259:TYR:HE1	2:B:270:LYS:HB2	1.85	0.40
5:E:26:ARG:NH2	5:E:133:GLU:OE1	2.54	0.40
8:H:56:THR:HB	8:H:145:ARG:HG2	2.03	0.40
6:F:146:TRP:HB3	6:F:151:LEU:HD21	2.03	0.40
13:M:171:ILE:HD12	13:M:172:MET:HG3	2.03	0.40
15:O:91:ASN:OD1	20:V:69:TYR:CD2	2.74	0.40
21:W:28:VAL:O	21:W:32:ILE:HG13	2.22	0.40
2:B:186:GLU:OE2	10:J:62:ARG:NH1	2.52	0.40
2:B:247:GLY:C	2:B:249:ARG:H	2.29	0.40
2:B:793:ALA:HB3	2:B:856:PHE:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1028:GLU:O	2:B:1032:SER:OG	2.26	0.40
15:O:151:LYS:HG2	15:O:153:THR:HG23	2.02	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	1386/1733 (80%)	1298 (94%)	77 (6%)	11 (1%)	16	53
2	B	1136/1224 (93%)	1064 (94%)	62 (6%)	10 (1%)	14	50
3	C	260/318 (82%)	236 (91%)	20 (8%)	4 (2%)	8	39
4	D	153/221 (69%)	145 (95%)	7 (5%)	1 (1%)	19	56
5	E	211/215 (98%)	202 (96%)	8 (4%)	1 (0%)	25	64
6	F	81/155 (52%)	79 (98%)	2 (2%)	0	100	100
7	G	169/171 (99%)	156 (92%)	12 (7%)	1 (1%)	22	59
8	H	132/146 (90%)	117 (89%)	12 (9%)	3 (2%)	5	28
9	I	114/122 (93%)	99 (87%)	15 (13%)	0	100	100
10	J	63/70 (90%)	58 (92%)	3 (5%)	2 (3%)	3	21
11	K	110/120 (92%)	109 (99%)	1 (1%)	0	100	100
12	L	43/70 (61%)	37 (86%)	6 (14%)	0	100	100
13	M	273/345 (79%)	252 (92%)	16 (6%)	5 (2%)	7	34
15	O	178/240 (74%)	164 (92%)	13 (7%)	1 (1%)	22	59
16	Q	140/735 (19%)	119 (85%)	17 (12%)	4 (3%)	3	23
17	R	176/400 (44%)	160 (91%)	15 (8%)	1 (1%)	22	59
19	U	88/171 (52%)	82 (93%)	4 (4%)	2 (2%)	5	28
20	V	96/129 (74%)	92 (96%)	3 (3%)	1 (1%)	13	48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	W	189/586 (32%)	183 (97%)	4 (2%)	2 (1%)	12	46
22	X	156/328 (48%)	129 (83%)	23 (15%)	4 (3%)	4	25
All	All	5154/7499 (69%)	4781 (93%)	320 (6%)	53 (1%)	16	48

All (53) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	Q	127	ILE
21	W	77	PRO
2	B	830	TYR
2	B	933	SER
7	G	63	PRO
13	M	269	ILE
16	Q	405	THR
21	W	78	ASN
22	X	251	ASN
2	B	277	LYS
2	B	475	SER
3	C	214	ASN
8	H	60	ALA
8	H	83	GLN
13	M	268	GLU
16	Q	406	ILE
19	U	255	LYS
22	X	152	SER
1	A	47	ARG
1	A	67	CYS
1	A	567	LYS
1	A	958	VAL
2	B	364	ILE
2	B	957	ASN
3	C	93	ASP
4	D	156	ASP
10	J	9	SER
19	U	264	ASP
20	V	6	TYR
1	A	35	ILE
1	A	50	ILE
1	A	525	GLN
1	A	569	LYS
2	B	339	THR

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Mol	Chain	Res	Type
2	B	705	MET
3	C	236	GLY
5	E	124	VAL
10	J	3	VAL
13	M	271	GLY
22	X	240	THR
1	A	464	PRO
2	B	1046	PRO
13	M	273	SER
16	Q	367	ALA
15	O	147	GLY
22	X	205	ILE
2	B	343	ILE
1	A	61	ILE
3	C	182	PRO
8	H	59	ILE
17	R	215	VAL
1	A	1327	ILE
13	M	32	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	1221/1520 (80%)	1221 (100%)	0	100	100
2	B	1000/1061 (94%)	999 (100%)	1 (0%)	92	94
3	C	230/274 (84%)	229 (100%)	1 (0%)	89	91
4	D	139/200 (70%)	139 (100%)	0	100	100
5	E	195/197 (99%)	195 (100%)	0	100	100
6	F	73/137 (53%)	73 (100%)	0	100	100
7	G	152/152 (100%)	152 (100%)	0	100	100
8	H	119/128 (93%)	119 (100%)	0	100	100
9	I	110/116 (95%)	106 (96%)	4 (4%)	30	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	J	60/65 (92%)	60 (100%)	0	100	100
11	K	97/102 (95%)	97 (100%)	0	100	100
12	L	40/57 (70%)	40 (100%)	0	100	100
13	M	245/299 (82%)	245 (100%)	0	100	100
15	O	152/205 (74%)	152 (100%)	0	100	100
16	Q	109/641 (17%)	108 (99%)	1 (1%)	75	83
17	R	107/363 (30%)	107 (100%)	0	100	100
19	U	84/154 (54%)	84 (100%)	0	100	100
20	V	90/115 (78%)	90 (100%)	0	100	100
21	W	155/244 (64%)	155 (100%)	0	100	100
22	X	62/295 (21%)	62 (100%)	0	100	100
All	All	4440/6325 (70%)	4433 (100%)	7 (0%)	91	94

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

Mol	Chain	Res	Type
2	B	70	ILE
3	C	95	CYS
9	I	18	GLU
9	I	42	LEU
9	I	43	VAL
9	I	59	VAL
16	Q	334	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (91) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	68	GLN
1	A	253	ASN
1	A	256	GLN
1	A	311	GLN
1	A	313	GLN
1	A	339	ASN
1	A	363	GLN
1	A	488	ASN
1	A	517	ASN

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Mol	Chain	Res	Type
1	A	525	GLN
1	A	576	GLN
1	A	589	GLN
1	A	640	GLN
1	A	698	GLN
1	A	723	ASN
1	A	745	GLN
1	A	760	GLN
1	A	767	GLN
1	A	881	GLN
1	A	953	ASN
1	A	965	GLN
1	A	968	GLN
1	A	994	GLN
1	A	1040	GLN
1	A	1130	GLN
1	A	1140	HIS
1	A	1265	ASN
1	A	1330	ASN
1	A	1367	HIS
1	A	1427	ASN
2	B	47	GLN
2	B	73	GLN
2	B	103	ASN
2	B	224	GLN
2	B	415	GLN
2	B	433	GLN
2	B	516	ASN
2	B	573	GLN
2	B	587	HIS
2	B	657	HIS
2	B	667	GLN
2	B	763	GLN
2	B	784	ASN
2	B	800	GLN
2	B	958	GLN
2	B	1093	GLN
2	B	1193	GLN
2	B	1211	ASN
3	C	73	GLN
3	C	79	GLN
3	C	102	GLN

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Mol	Chain	Res	Type
3	C	184	ASN
3	C	206	ASN
3	C	224	GLN
3	C	231	ASN
3	C	242	GLN
3	C	264	GLN
4	D	165	GLN
4	D	179	GLN
4	D	216	ASN
5	E	54	GLN
7	G	102	GLN
7	G	153	GLN
7	G	158	HIS
8	H	35	GLN
8	H	83	GLN
9	I	60	GLN
9	I	89	GLN
9	I	108	HIS
10	J	53	HIS
11	K	112	GLN
13	M	90	ASN
13	M	114	GLN
13	M	193	GLN
15	O	91	ASN
15	O	158	GLN
16	Q	117	HIS
17	R	138	GLN
19	U	33	GLN
19	U	280	GLN
20	V	55	ASN
20	V	84	GLN
21	W	11	ASN
21	W	107	GLN
21	W	138	GLN
21	W	178	GLN
22	X	216	GLN
22	X	223	GLN
22	X	267	GLN
22	X	279	GLN



### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 11 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.



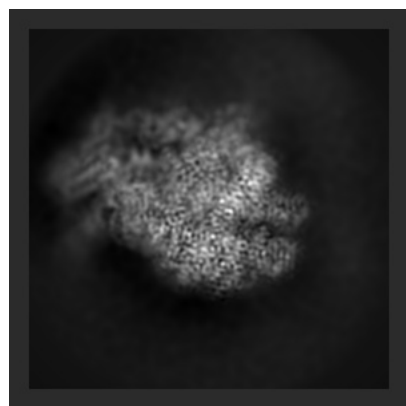
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0091. These allow visual inspection of the internal detail of the map and identification of artifacts.

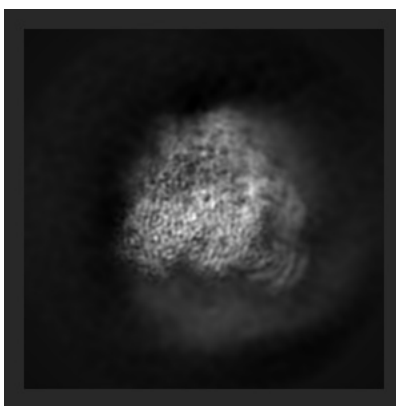
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

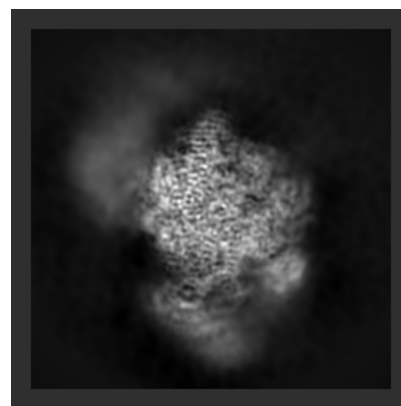
#### 6.1.1 Primary map



X

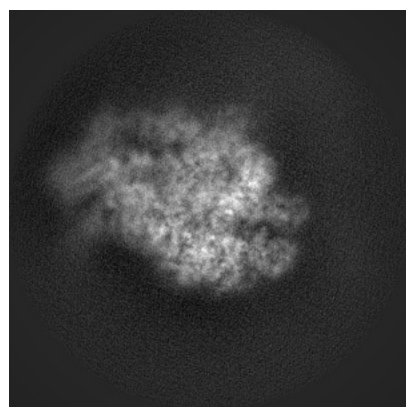


Y

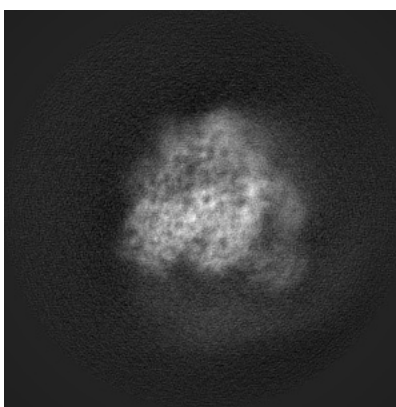


Z

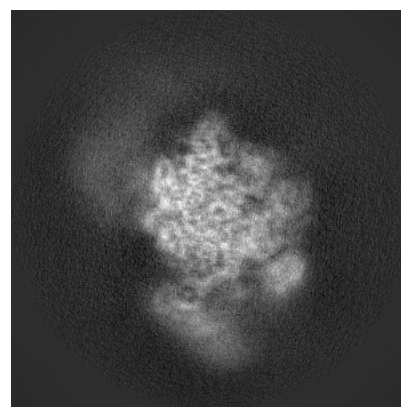
#### 6.1.2 Raw map



X



Y



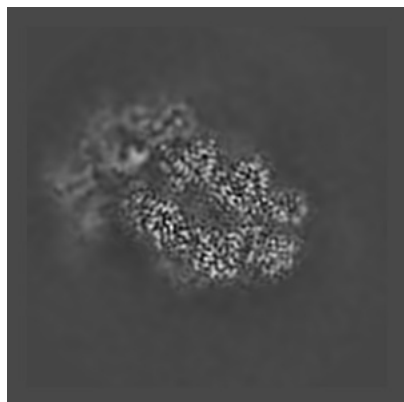
Z

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

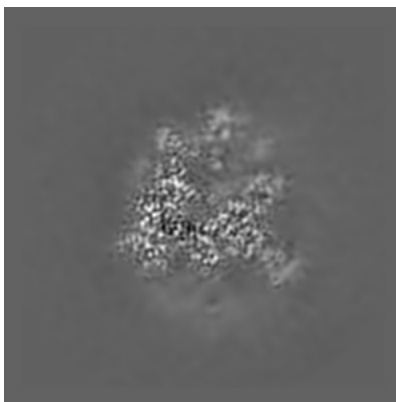


## 6.2 Central slices [i](#)

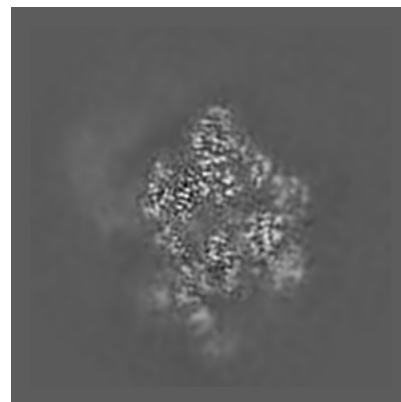
### 6.2.1 Primary map



X Index: 150

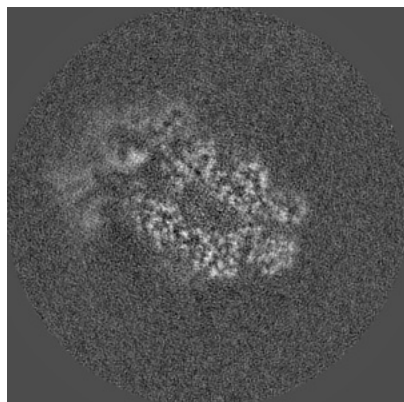


Y Index: 150

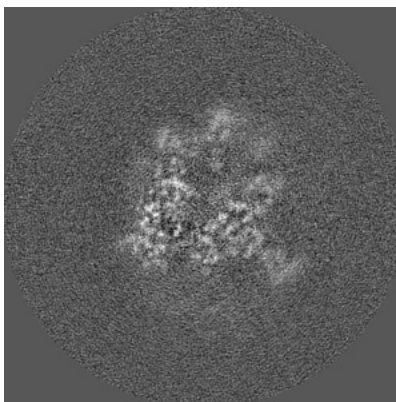


Z Index: 150

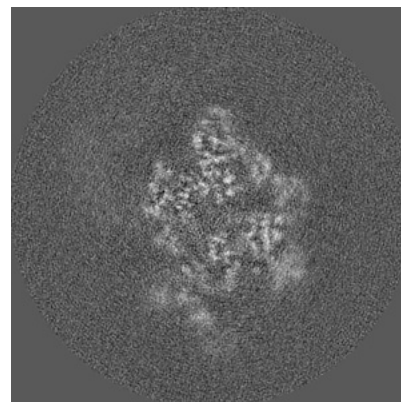
### 6.2.2 Raw map



X Index: 150



Y Index: 150



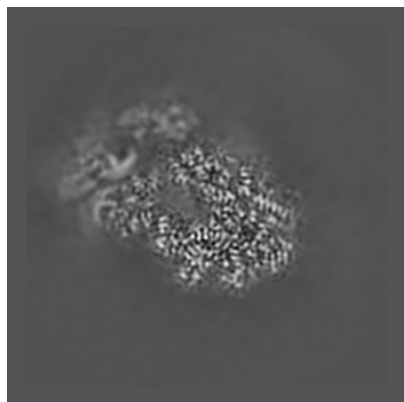
Z Index: 150

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

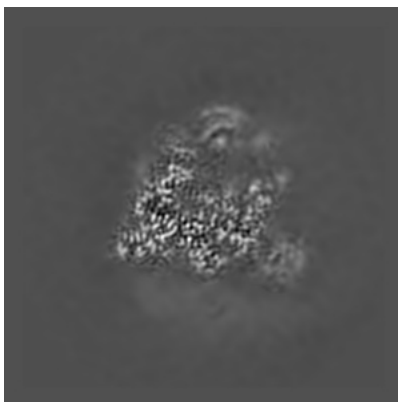


## 6.3 Largest variance slices [i](#)

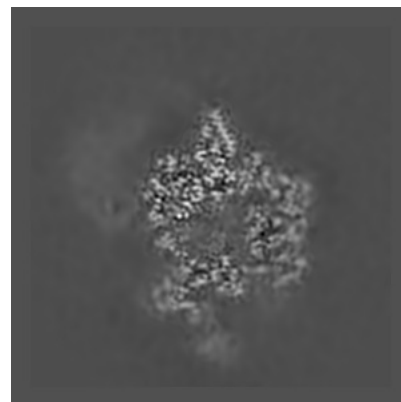
### 6.3.1 Primary map



X Index: 140

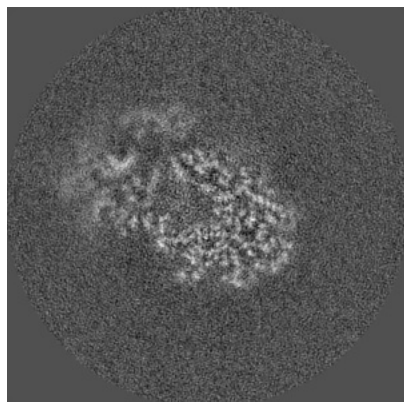


Y Index: 156

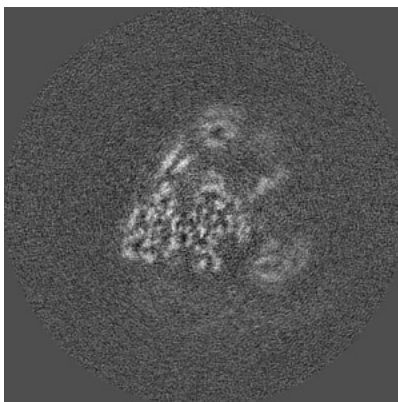


Z Index: 156

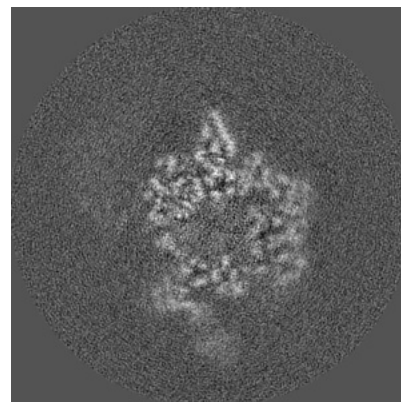
### 6.3.2 Raw map



X Index: 141



Y Index: 162



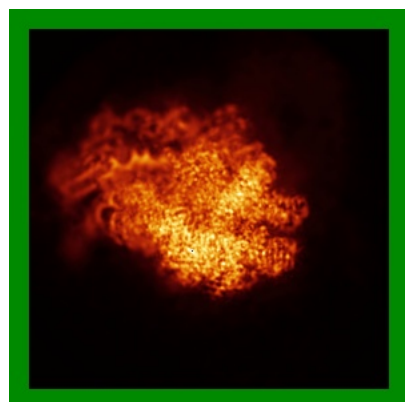
Z Index: 156

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

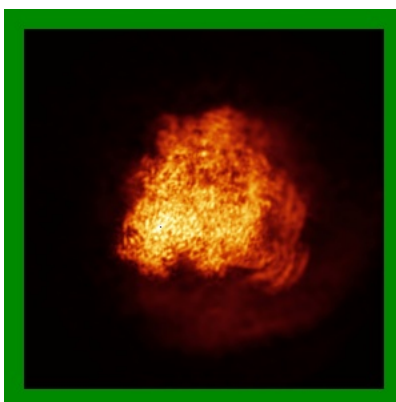


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

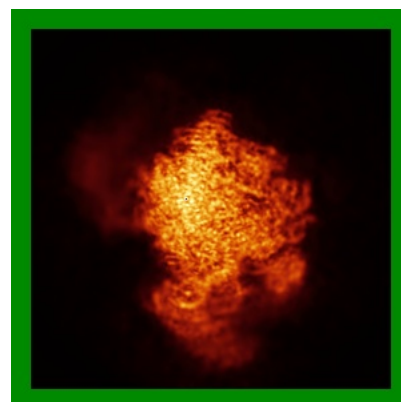
### 6.4.1 Primary map



X

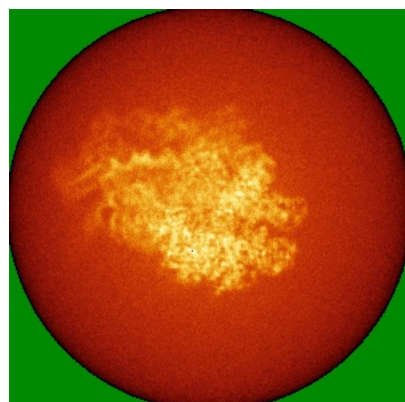


Y

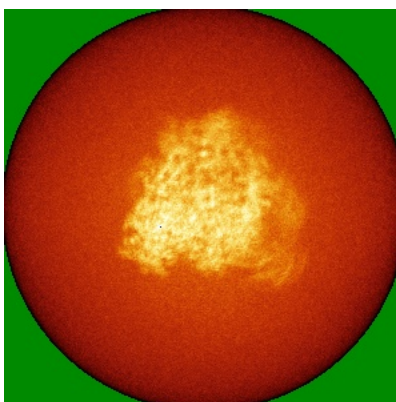


Z

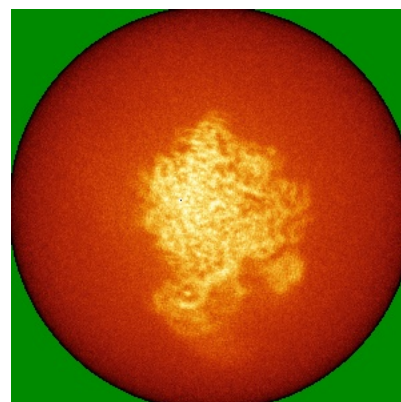
### 6.4.2 Raw map



X



Y



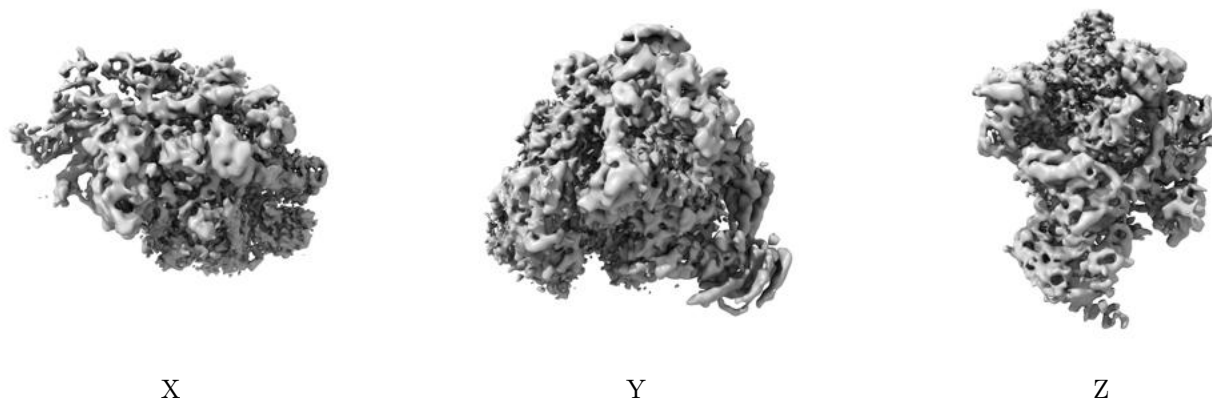
Z

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



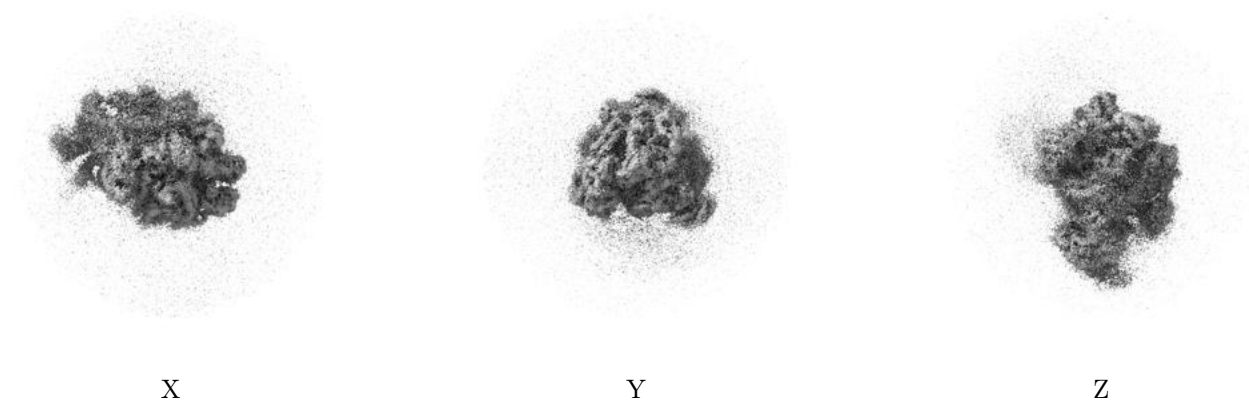
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0028. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

## 6.6 Mask visualisation [i](#)

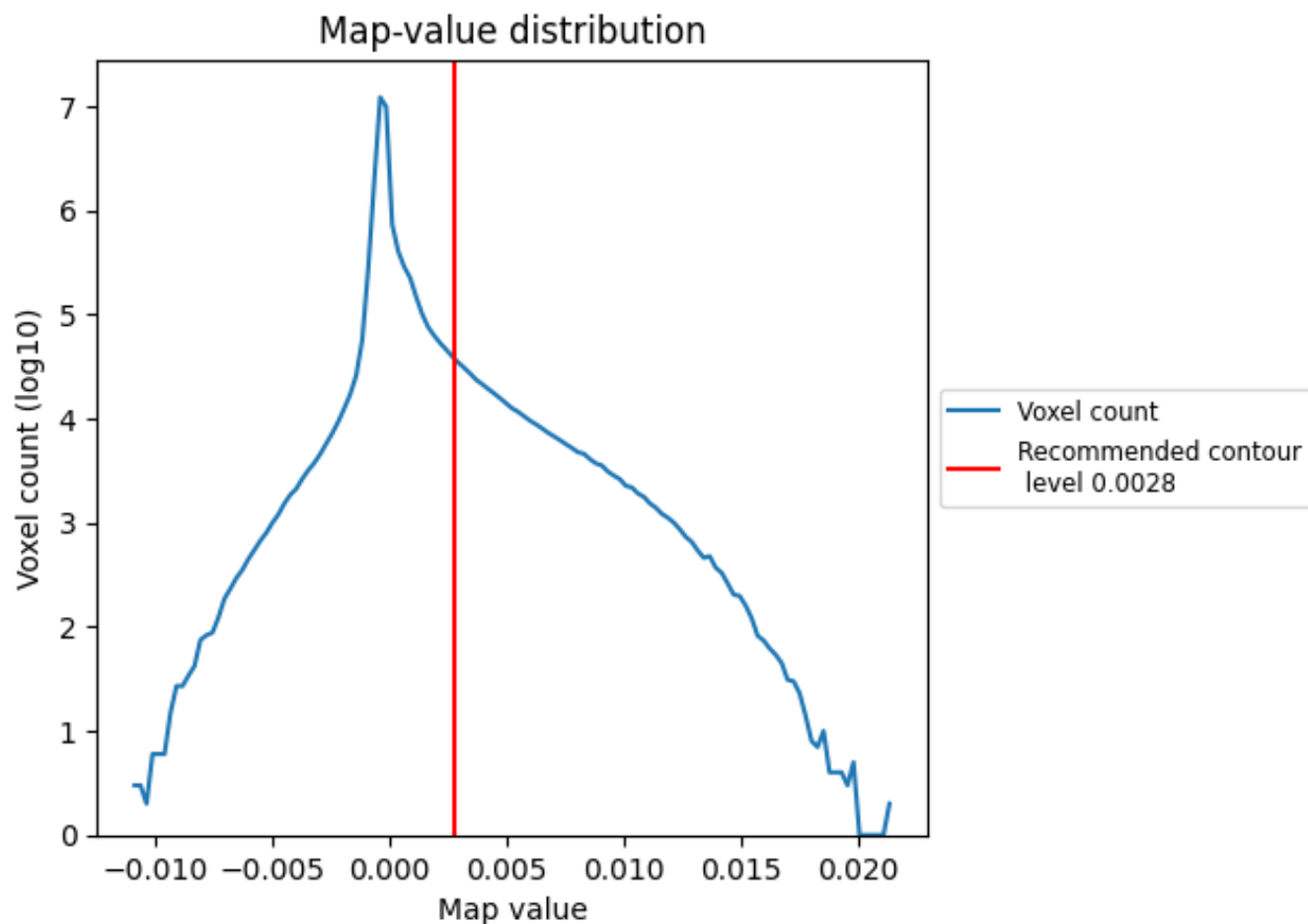
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

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

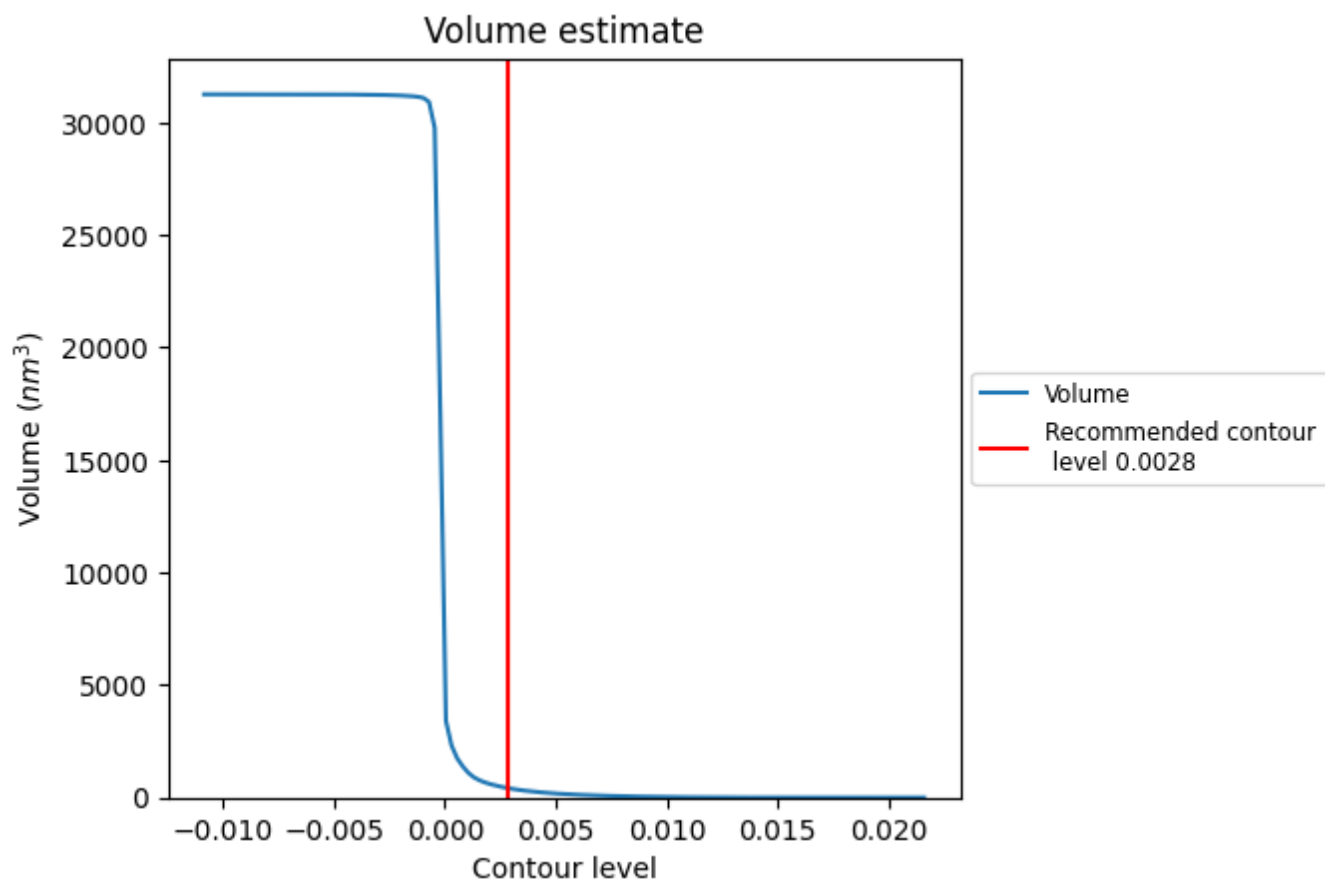
### 7.1 Map-value distribution [i](#)



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](#)

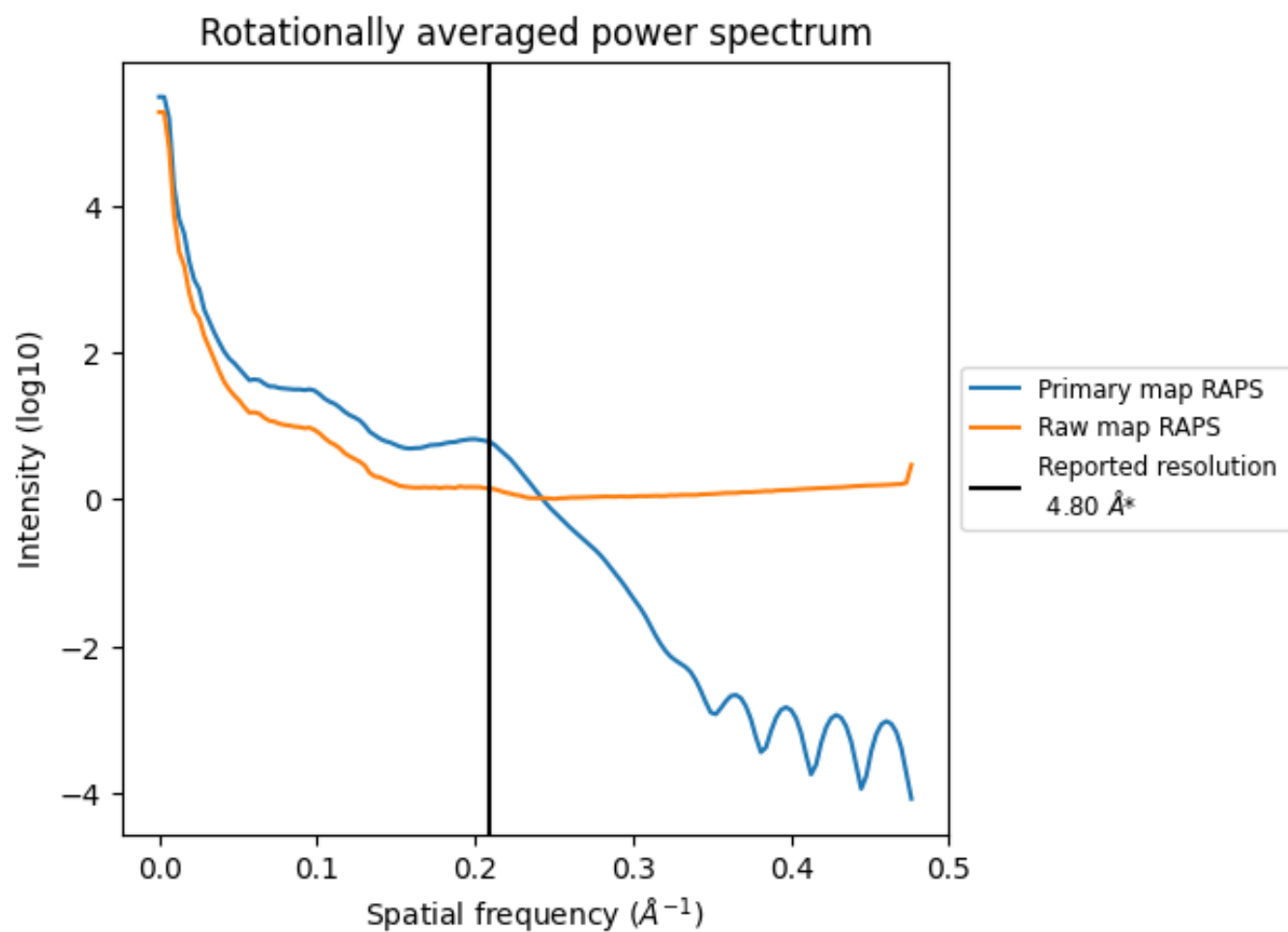


The volume at the recommended contour level is 426  $\text{nm}^3$ ; this corresponds to an approximate mass of 385 kDa.

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 ⓘ



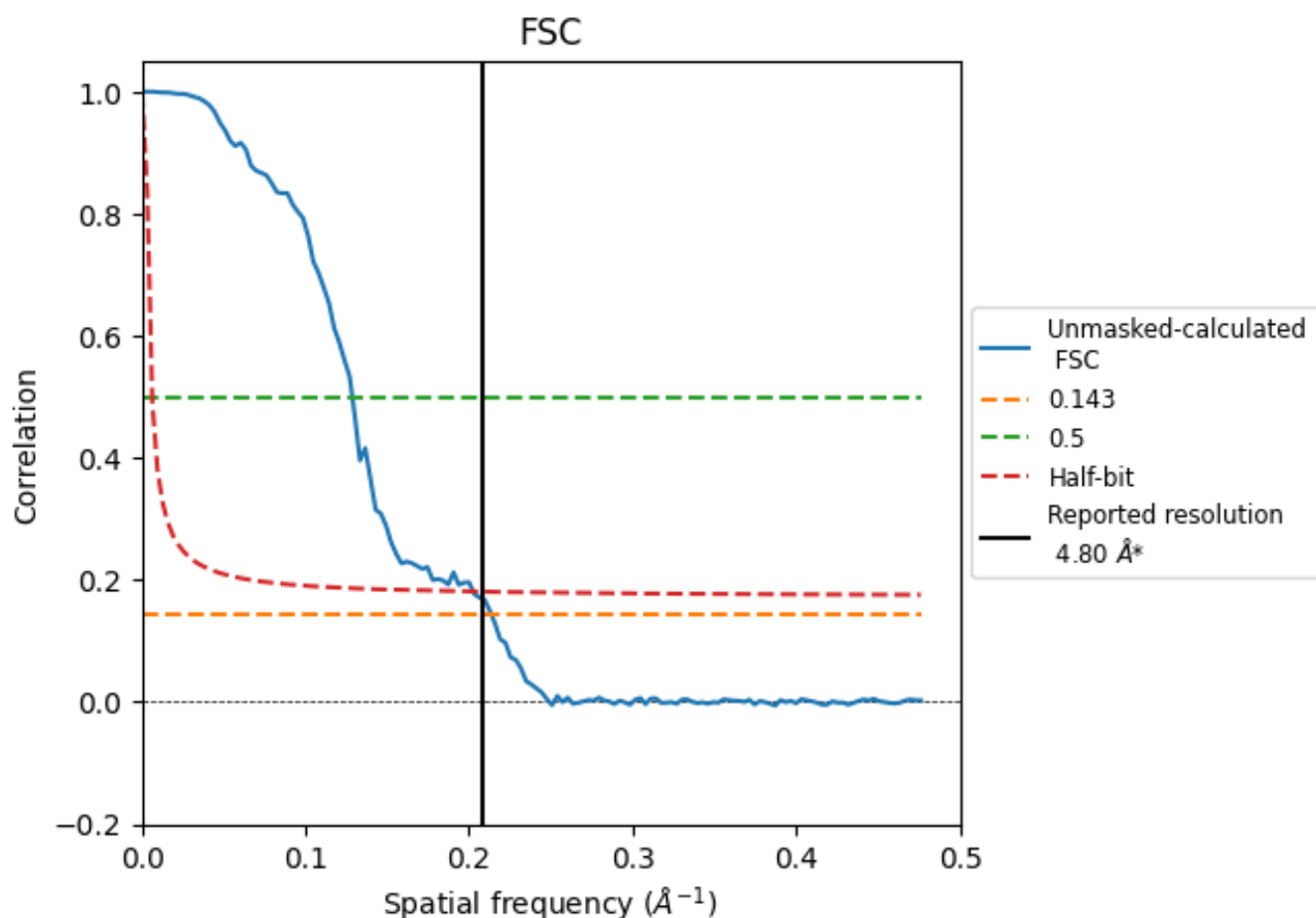
\*Reported resolution corresponds to spatial frequency of 0.208  $\text{\AA}^{-1}$



## 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 0.208  $\text{\AA}^{-1}$



## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.68	7.78	4.94

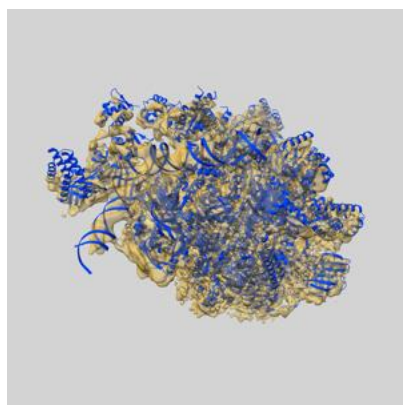
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.



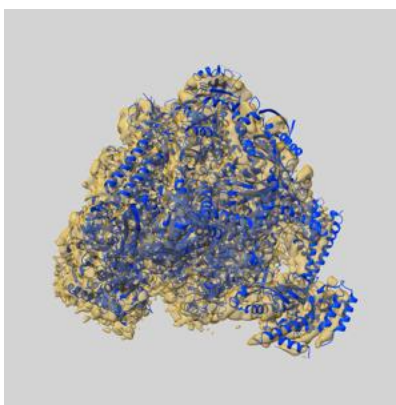
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-0091 and PDB model 6GYL. Per-residue inclusion information can be found in section 3 on page 9.

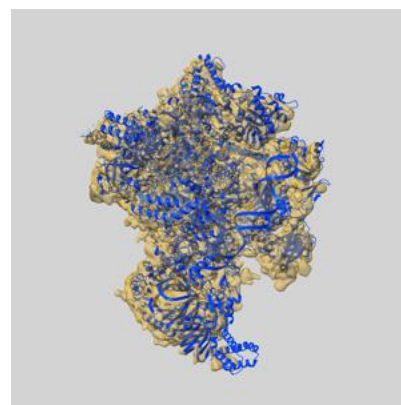
### 9.1 Map-model overlay [i](#)



X



Y

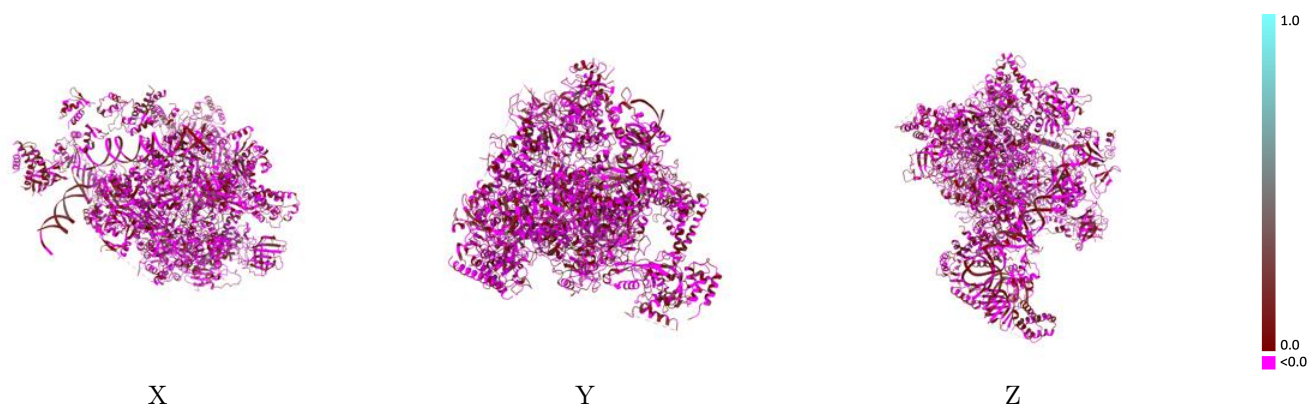


Z

The images above show the 3D surface view of the map at the recommended contour level 0.0028 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.

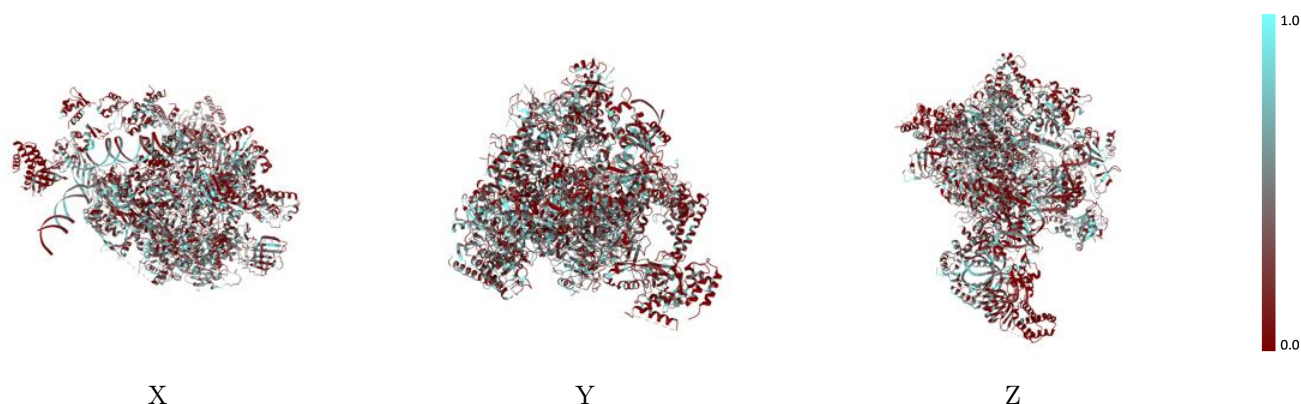


## 9.2 Q-score mapped to coordinate model [i](#)



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.

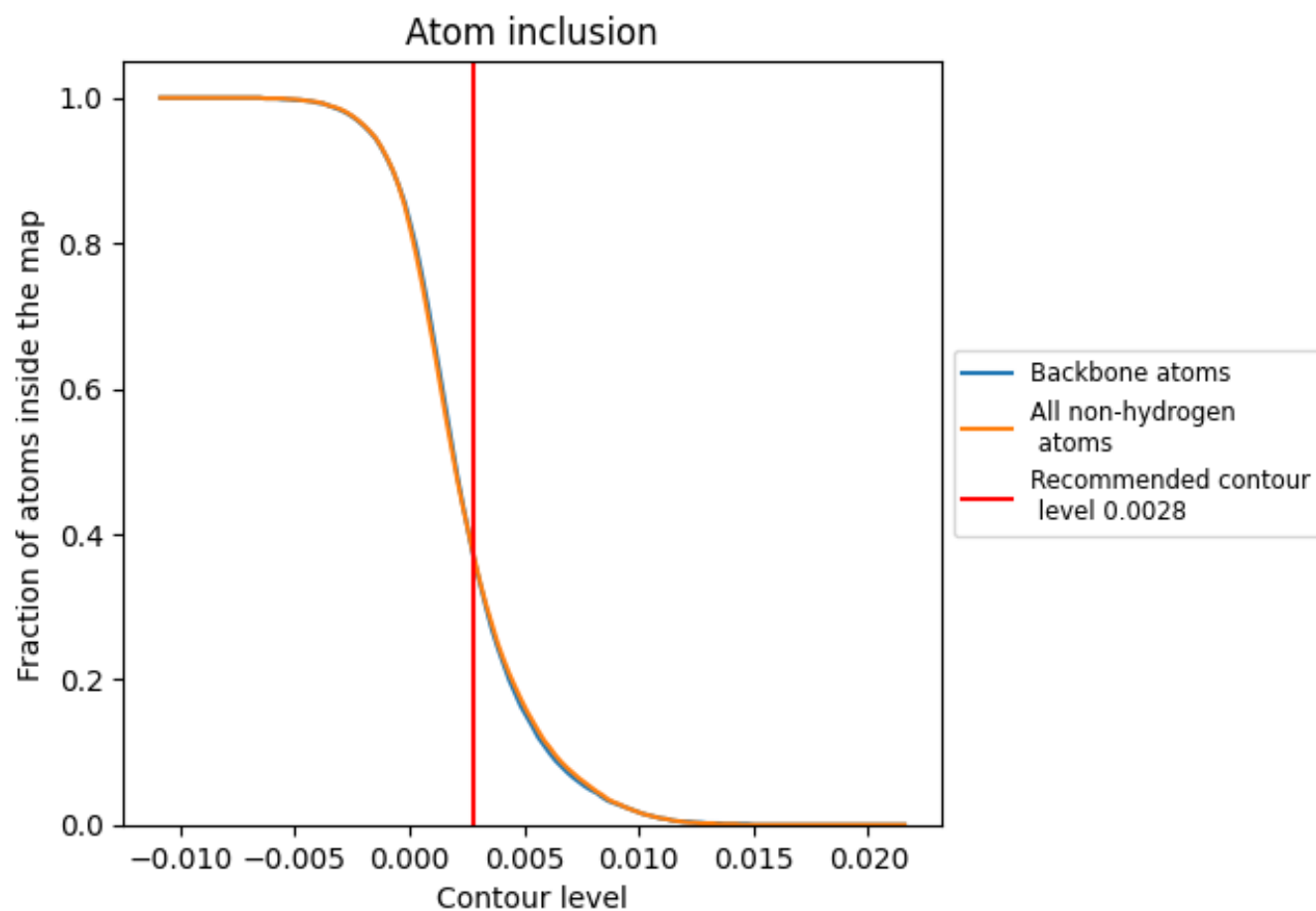
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.0028).



## 9.4 Atom inclusion [i](#)

















































At the recommended contour level, 37% of all backbone atoms, 37% 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 (0.0028) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.3700	 -0.0040
A	 0.3840	 -0.0110
B	 0.3770	 -0.0240
C	 0.4250	 -0.0310
D	 0.1990	 0.0040
E	 0.3740	 0.0120
F	 0.4200	 0.0230
G	 0.3480	 -0.0030
H	 0.3780	 -0.0040
I	 0.3820	 0.0160
J	 0.4330	 -0.0570
K	 0.3850	 -0.0410
L	 0.3640	 -0.0550
M	 0.3360	 -0.0170
N	 0.4180	 0.0710
O	 0.4780	 0.0280
Q	 0.3800	 0.0050
R	 0.4090	 -0.0100
T	 0.5000	 0.0660
U	 0.1610	 0.0330
V	 0.1630	 0.0540
W	 0.3140	 0.0240
X	 0.2140	 0.0330

