Full wwPDB EM Validation Report ⓘ

Nov 6, 2022 – 01:51 PM EST

PDB ID	:	6MZL
EMDB ID	:	EMD-9305
Title	:	Human TFIID canonical state
Authors	:	Patel, A.B.; Louder, R.K.; Greber, B.J.; Grunberg, S.; Luo, J.; Fang, J.; Liu, Y.; Ranish, J.; Hahn, S.; Nogales, E.
Deposited on	:	2018-11-05
Resolution	:	23.00 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

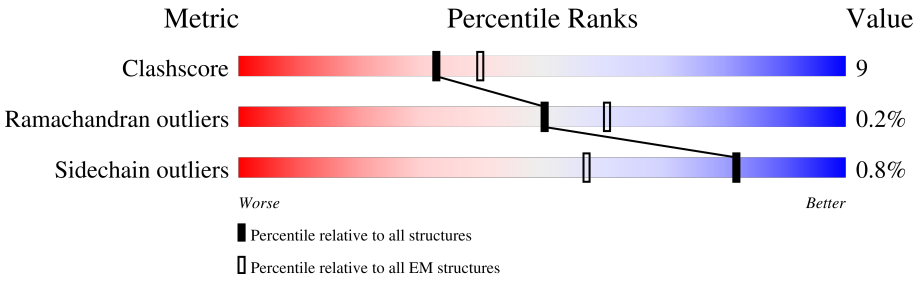
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 23.00 Å.

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



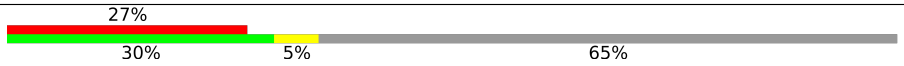
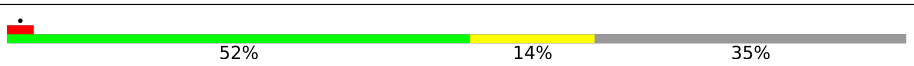
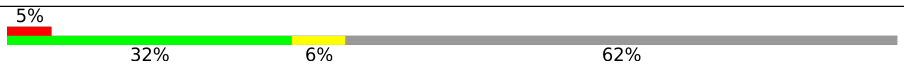
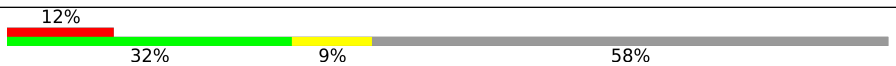
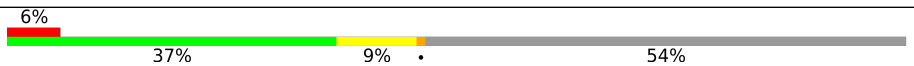
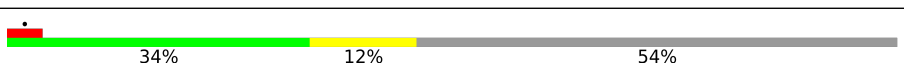
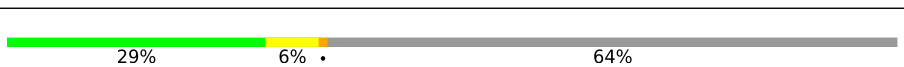
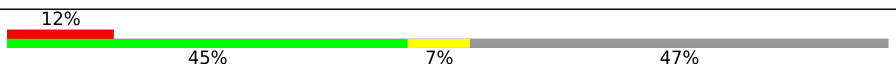
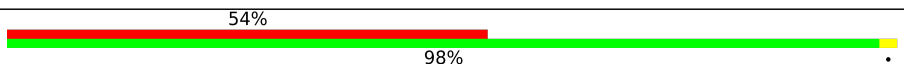
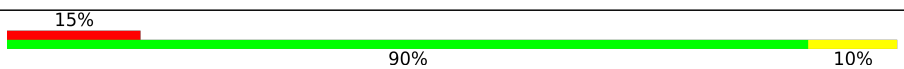
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	1872	14% 22% · 75%
2	B	1199	16% 52% 27% · 19%
3	C	929	· 9% · 90%
4	D	1085	· 9% · 91%
4	E	1085	· 8% · 91%
5	F	800	16% 48% 10% 41%
5	G	800	9% 42% 17% · 41%
6	H	677	7% 35% 13% 51%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
7	I	677	
8	J	349	
9	K	310	
10	L	264	
10	M	264	
11	N	218	
11	O	218	
12	P	211	
13	Q	161	
13	R	161	
14	S	124	
15	T	339	
16	Y	96	
17	Z	238	

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 36618 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 Transcription initiation factor TFIID subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	472	Total 3772	C 2397	N 659	O 693	S 23	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	968	Total 7832	C 5031	N 1322	O 1421	S 58	0	0

- Molecule 3 is a protein called Transcription initiation factor TFIID subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	93	Total 742	C 467	N 128	O 141	S 6	0	0

- Molecule 4 is a protein called Transcription initiation factor TFIID subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	102	Total 686	C 423	N 130	O 133	0	0
4	E	102	Total 686	C 423	N 130	O 133	0	0

- Molecule 5 is a protein called Transcription initiation factor TFIID subunit 5,TAF5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	473	Total 3646	C 2314	N 638	O 679	S 15	0	0
5	G	473	Total 3646	C 2314	N 638	O 679	S 15	0	0

- Molecule 6 is a protein called Transcription initiation factor TFIID subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	329	Total	C	N	O	S	0	0
			2494	1575	439	464	16		

- Molecule 7 is a protein called Transcription initiation factor TFIID subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	339	Total	C	N	O	S	0	0
			2520	1585	445	474	16		

- Molecule 8 is a protein called Transcription initiation factor TFIID subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	123	Total	C	N	O	S	0	0
			998	638	184	172	4		

- Molecule 9 is a protein called Transcription initiation factor TFIID subunit 8,TAF8.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	202	Total	C	N	O	S	0	0
			1449	906	260	278	5		

- Molecule 10 is a protein called Transcription initiation factor TFIID subunit 9, TAF9.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	104	Total	C	N	O	S	0	0
			732	456	129	142	5		
10	M	104	Total	C	N	O	S	0	0
			732	456	129	142	5		

- Molecule 11 is a protein called Transcription initiation factor TFIID subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	N	82	Total	C	N	O	S	0	0
			645	413	102	126	4		
11	O	82	Total	C	N	O	S	0	0
			645	413	102	126	4		

- Molecule 12 is a protein called Transcription initiation factor TFIID subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	P	89	Total	C	N	O	S	0	0
			707	447	127	128	5		

- Molecule 13 is a protein called Transcription initiation factor TFIID subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Q	74	Total	C	N	O	S	0	0
			611	381	107	120	3		
13	R	74	Total	C	N	O	S	0	0
			611	381	107	120	3		

- Molecule 14 is a protein called Transcription initiation factor TFIID subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	S	45	Total	C	N	O	S	0	0
			365	233	54	73	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	T	180	Total	C	N	O	S	0	0
			1429	927	252	243	7		

- Molecule 16 is a protein called poly(UNK).

Mol	Chain	Residues	Atoms				AltConf	Trace
16	Y	96	Total	C	N	O	0	0
			480	288	96	96		

- Molecule 17 is a protein called poly(UNK).

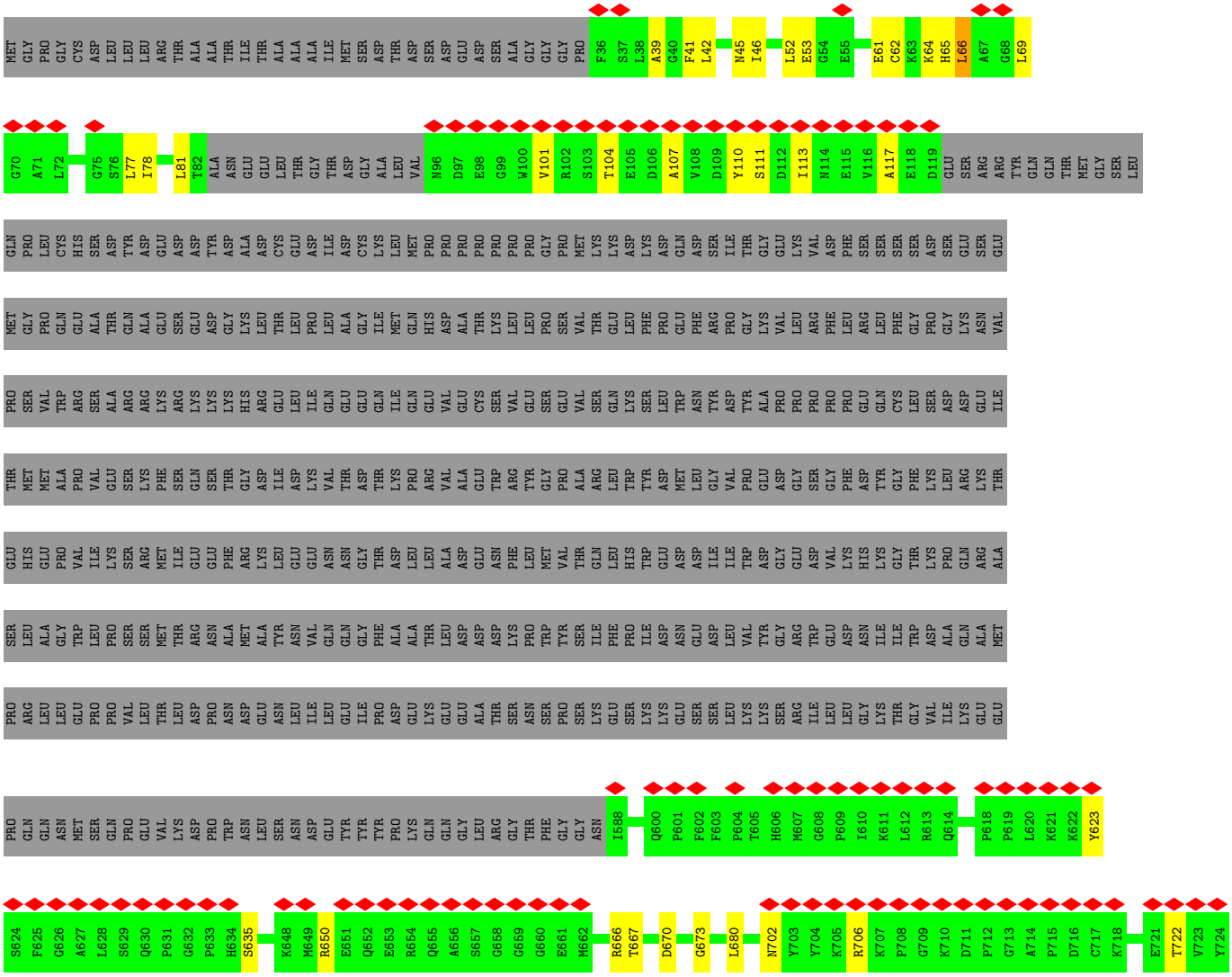
Mol	Chain	Residues	Atoms				AltConf	Trace
17	Z	238	Total	C	N	O	0	0
			1190	714	238	238		

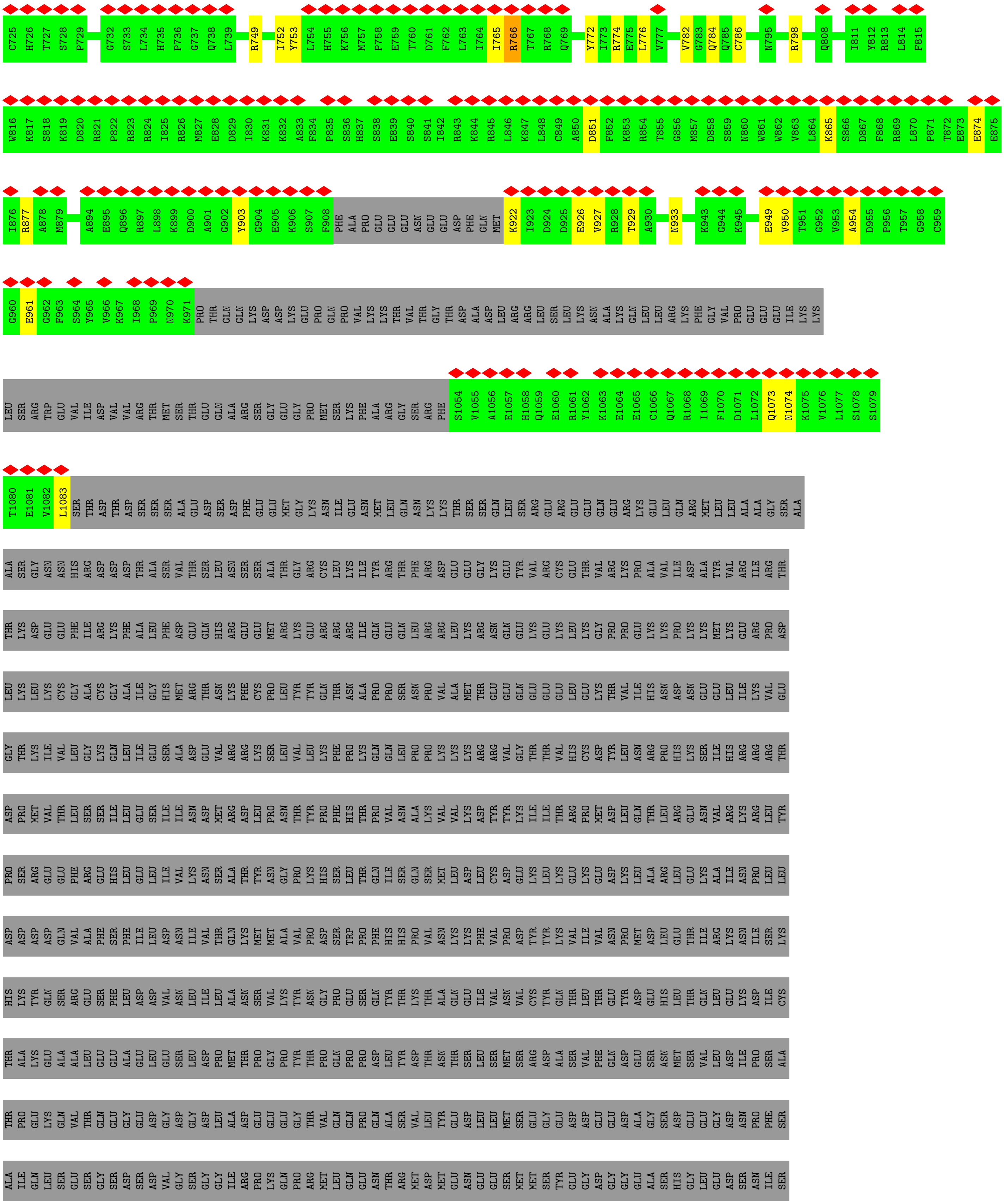
3 Residue-property plots (i)

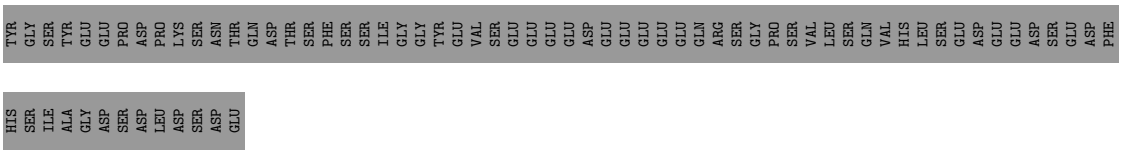
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: Transcription initiation factor TFIID subunit 1

Chain A:

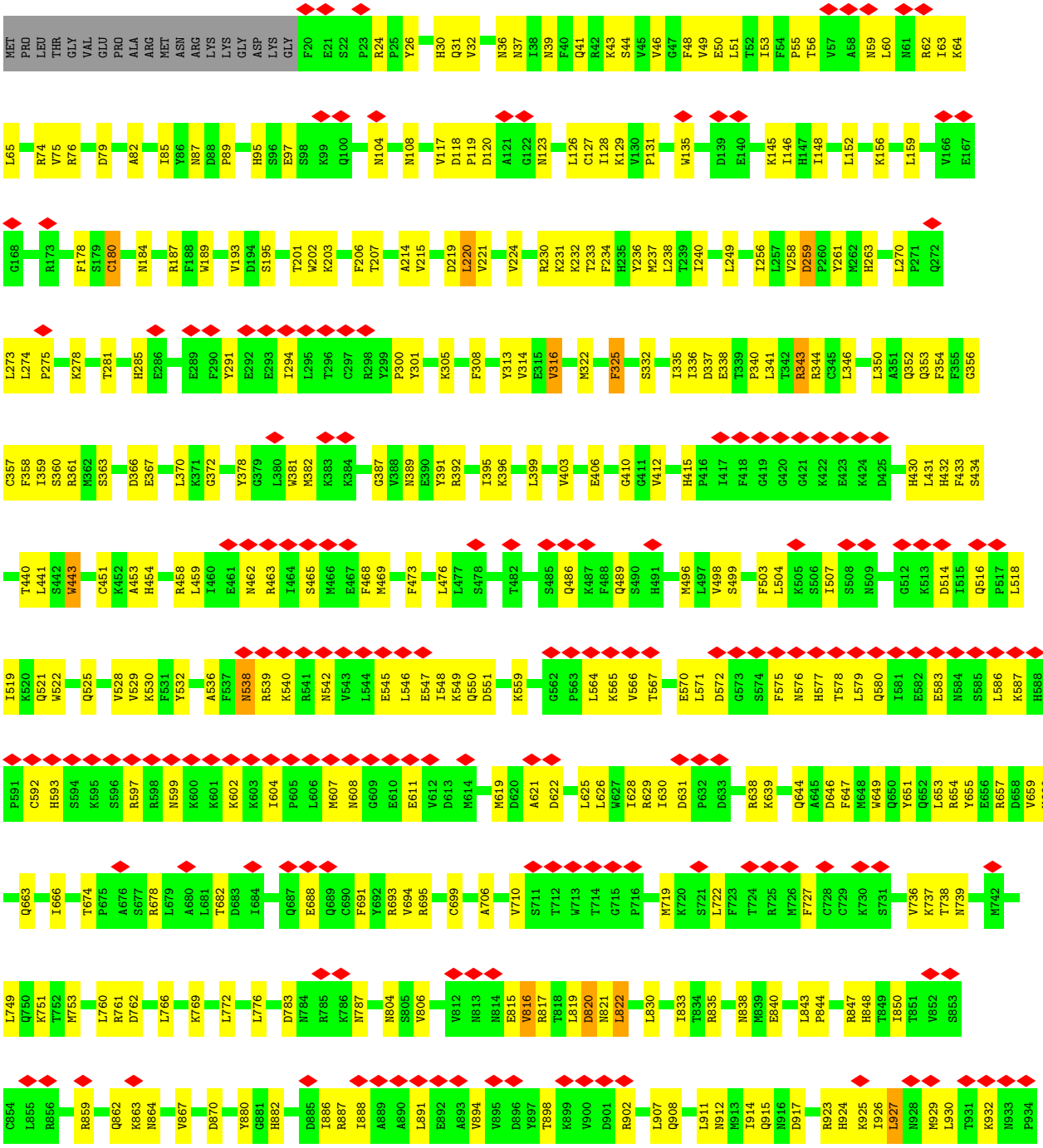


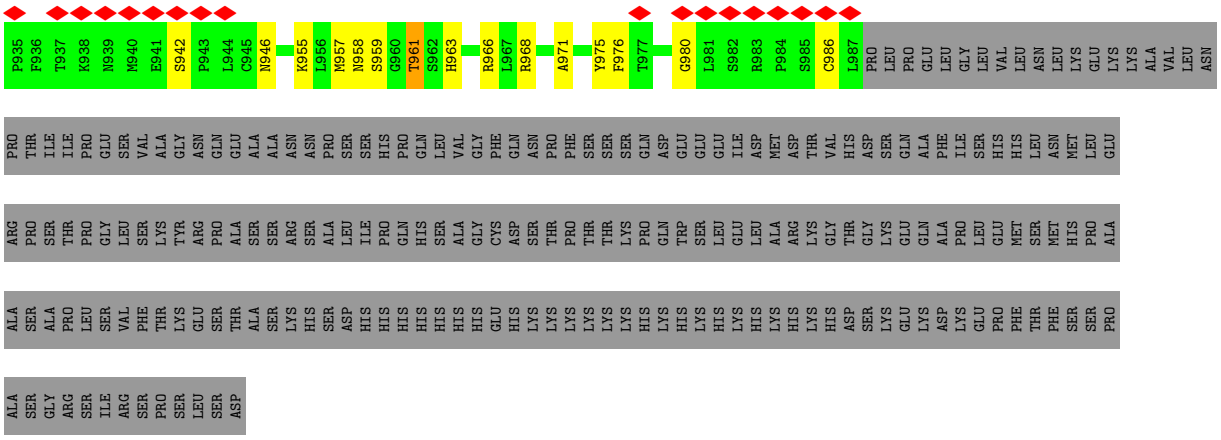

C725 H726 T727 S728 P729 G732 S733 L734 H735 P736 G737 Q738 L739 R749 I752 Y753 L754 H755 K756 M757 P758 E759 T760 D761 F762 L763 I764 I765 R766 T767 R768 Q769 Y772 I773 R774 E775 L776 V777 V782 G783 Q784 Q785 C786 N795 R798 Q808 I811 Y812 R813 L814 F815
W816 K817 S818 K819 D820 R821 P822 R823 R824 I825 R826 M827 E828 D829 I830 K831 K832 A833 F834 P835 S836 H837 S838 E839 S840 S841 I842 R843 K844 R845 L846 K847 L848 C849 A850 D851 F852 K853 R854 T855 G856 M857 D858 S859 N860 W861 W862 V863 L864 K865 S866 D867 F868 R869 L870 P871 T872 E873 E874 E875
I876 R877 A878 M879 A894 E895 Q896 R897 L898 K899 D900 A901 G902 Y903 G904 E905 K906 S907 F908 PHE ALA PRO GLU GLU GLU ASN GLU GLU ASP PHE GLN MET K922 I923 D924 D925 E926 V927 R928 T929 A930 N933 K943 G944 K945 E949 V950 T951 G952 V953 A954 D955 P956 T957 G958 C959
G960 E961 G962 F963 S964 Y965 V966 K967 I968 P969 N970 K971 PRO THR GLN GLN LYS ASP ASP LYS GLU PRO GLN PRO VAL LYS LYS THR VAL THR GLY THR ASP ALA ASP LEU ARG ARG LEU SER LEU LYS ASN ALA LYS GLN LEU LEU ARG LYS PHE GLY VAL PRO GLU GLU GLU ILE LYS LYS
LEU SER ARG TRP GLU VAL ILE ASP VAL VAL ARG THR MET SER THR GLU GLN ALA ARG SER GLY GLU GLY PRO MET SER LYS PHE ALA ARG GLY SER ARG PHE S1054 V1055 A1056 E1057 H1058 Q1059 E1060 R1061 Y1062 K1063 E1064 E1065 C1066 Q1067 R1068 I1069 F1070 D1071 L1072 Q1073 N1074 K1075 V1076 L1077 S1078 S1079
T1080 E1081 V1082 L1083 SER THR ASP THR ASP SER SER SER ALA GLU ASP SER ASP PHE GLU GLU MET GLY LYS ASN ILE GLU ASN MET LEU GLN ASN LYS LYS THR SER SER GLN LEU SER ARG GLU ARG GLU GLU GLN GLU ARG LYS GLU LEU GLN ARG MET LEU LEU ALA ALA GLY SER ALA
ALA SER GLY ASN ASN HIS ARG ASP ASP ASP THR ALA SER VAL THR SER LEU ASN SER SER ALA THR GLY ARG CYS LEU LYS ILE TYR ARG THR PHE ARG ASP GLU GLU GLY LYS GLU TYR VAL ARG CYS GLU THR VAL ARG LYS PRO ALA VAL ILE ASP ALA TYR VAL ARG ILE ARG THR
THR LYS ASP GLU GLU PHE ILE ARG LYS PHE ALA LEU PHE ASP GLU GLN HIS ARG GLU GLU MET ARG LYS GLU ARG ARG ARG ILE GLN GLU GLN LEU ARG ARG LEU LYS ARG ASN GLN GLU LYS GLU LYS LEU LYS GLY PRO PRO GLU LYS LYS PRO LYS LYS MET LYS GLU ARG PRO ASP
LEU LYS LEU LYS CYS GLY ALA CYS GLY ALA ILE GLY HIS MET ARG THR ASN LYS PHE CYS PRO LEU TYR TYR GLN THR ASN ALA PRO PRO SER ASN PRO VAL ALA MET THR GLU GLN GLN GLU GLU GLU LEU GLU LYS THR VAL ILE HIS ASN ASP ASN GLU GLU LEU ILE LYS VAL GLU
GLY THR LYS ILE VAL LEU GLY LYS GLN LEU ILE GLU SER ALA ASP GLU VAL ARG ARG LYS SER LEU VAL LEU LYS PHE PRO LYS GLN GLN LEU PRO PRO LYS LYS LYS ARG ARG VAL GLY THR THR VAL HIS CYS ASP TYR LEU ASN ARG PRO HIS LYS SER ILE HIS ARG ARG ARG THR
ASP PRO MET VAL THR LEU SER SER ILE LEU GLU SER ILE ILE ASN ASP MET ARG ASP LEU PRO ASN THR TYR PRO PHE HIS THR PRO VAL ASN ALA LYS VAL VAL LYS ASP TYR TYR LYS ILE ILE THR ARG PRO MET ASP LEU GLN THR LEU ARG GLU ASN VAL ARG LYS ARG LEU TYR
PRO SER ARG GLU GLU PHE ARG GLU HIS LEU GLU LEU ILE VAL LYS ASN SER ALA THR TYR ASN GLY PRO LYS HIS SER LEU THR GLN ILE SER GLN SER MET LEU ASP LEU CYS ASP GLU LYS LEU LYS GLU LYS GLU ASP LYS LEU ALA ARG LEU GLU LYS ALA ILE ASN PRO LEU LEU
ASP ASP ASP ASP GLN VAL ALA PHE SER PHE ILE LEU ASP ASN ILE VAL THR GLN LYS MET MET ALA VAL PRO ASP SER TRP PRO PHE HIS HIS PRO VAL ASN LYS LYS PHE VAL PRO ASP TYR TYR LYS VAL ILE VAL ASN PRO MET ASP LEU GLU THR ILE ARG LYS ASN ILE SER LYS
HIS LYS TYR GLN SER ARG GLU SER PHE LEU ASP ASP VAL ASN LEU ILE LEU ALA ASN SER VAL LYS TYR ASN GLY PRO GLU SER GLN TYR THR LYS THR ALA GLN GLU ILE VAL ASN VAL CYS TYR GLN THR LEU THR GLU TYR ASP GLU HIS LEU THR GLN LEU GLU LYS ASP ILE CYS
THR ALA LYS GLU ALA ALA LEU GLU GLU ALA GLU LEU GLU SER LEU ASP PRO MET THR PRO GLY PRO TYR THR PRO GLN PRO PRO ASP LEU TYR ASP THR ASN THR SER LEU SER MET SER ARG ASP ALA SER VAL PHE GLN ASP GLU SER ASN MET SER VAL LEU ASP ILE PRO SER ALA
THR PRO GLU LYS GLN VAL THR GLN GLU GLY GLU ASP GLY ASP GLY ASP LEU ALA ASP GLU GLU GLU GLY THR VAL GLN GLN PRO GLN ALA SER VAL LEU TYR GLU ASP LEU LEU MET SER GLU GLY GLU ASP ASP GLU GLU ASP ALA GLY SER ASP GLU GLU GLY ASP ASN PRO PHE SER
ALA ILE GLN LEU SER GLU SER GLY SER ASP SER ASP VAL GLY SER GLY GLY ILE ARG PRO LYS GLN PRO ARG MET LEU GLN GLU ASN THR ARG MET ASP MET GLU ASN GLU GLU SER MET MET SER TYR GLU GLY ASP GLY GLY GLU ALA SER HIS GLY LEU GLU ASP SER ASN ILE SER



• Molecule 2: Transcription initiation factor TFIID subunit 2

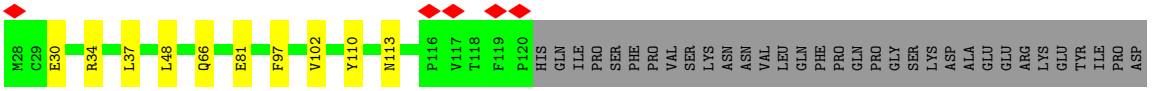
Chain B:





- Molecule 3: Transcription initiation factor TFIID subunit 3

Chain C:



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

TRP PHE CYS PRO LYS CYS ALA ASN LYS LYS LYS ASP LYS LYS HIS LYS LYS ARG LYS HIS ARG ALA HIS

- Molecule 4: Transcription initiation factor TFIID subunit 4

Chain D: 9% 91%

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

HIS VAL VAL SER GLY SER PRO ALA GLY ALA ALA GLY ALA GLY PRO ALA ALA PRO ALA GLU GLY ALA PRO GLY ALA ALA PRO GLU PRO PRO ALA GLY ARG ALA ARG PRO GLY GLY GLY GLY PRO GLN ARG PRO GLY PRO PRO SER PRO ARG ARG PRO LEU VAL PRO ALA GLY PRO ALA

PRO PRO ALA ALA LYS LEU ARG PRO PRO PRO GLU GLY SER ALA GLY SER CYS ALA PRO VAL PRO ALA ALA ALA ALA VAL ALA ALA GLY PRO GLU PRO ALA PRO ALA GLY PRO ALA LYS PRO ALA GLY PRO ALA ALA LEU ALA ALA ARG ALA GLY PRO GLY PRO GLY PRO GLY PRO GLY PRO

GLY PRO GLY PRO GLY PRO GLY LYS PRO ALA GLY PRO GLY ALA ALA GLN THR LEU ASN GLY SER ALA ALA LEU LEU ASN SER HIS HIS ALA ALA ALA PRO ALA VAL SER LEU VAL ASN ASN GLY PRO ALA ALA LEU LEU PRO LEU PRO LYS PRO ALA ALA PRO GLY THR VAL ILE GLN THR

PRO PRO PHE VAL GLY ALA ALA ALA PRO PRO ALA PRO ALA ALA PRO SER PRO PRO ALA ALA PRO ALA PRO ALA ALA PRO ALA ALA ALA PRO PRO PRO PRO PRO PRO ALA PRO ALA THR LEU ALA ARG PRO PRO GLY HIS PRO ALA GLY PRO PRO THR ALA ALA PRO ALA VAL PRO PRO PRO

ALA ALA ALA GLN ASN GLY GLY SER ALA GLY ALA ALA PRO ALA PRO ALA PRO ALA ALA GLY GLY PRO ALA GLY VAL SER GLY GLN PRO GLY PRO GLY ALA ALA ALA ALA ALA PRO ALA PRO GLY VAL LYS ALA GLU SER PRO LYS ARG VAL VAL GLN ALA ALA PRO PRO ALA ALA GLN THR

LEU ALA ALA SER GLY PRO ALA SER THR ALA ALA SER MET VAL ILE GLY PRO THR MET GLN GLY ALA LEU PRO SER PRO ALA ALA VAL PRO PRO PRO ALA PRO GLY THR PRO THR GLY LEU PRO LYS GLY ALA ALA GLY ALA VAL THR GLN SER LEU SER ARG THR PRO THR ALA THR THR

SER GLY ILE ARG ALA THR LEU THR PRO THR VAL LEU ALA PRO ARG LEU PRO GLN PRO PRO GLN ASN PRO THR ASN ILE GLN ASN PHE GLN LEU PRO PRO GLY MET VAL LEU VAL ARG SER GLU ASN GLY GLN LEU LEU MET ILE PRO GLN GLN ALA LEU ALA GLN MET GLN ALA GLN ALA

HIS ALA GLN PRO GLN THR THR MET ALA PRO ARG PRO ALA THR PRO THR SER ALA PRO PRO VAL GLN ILE SER THR VAL GLN ALA PRO GLY THR PRO ILE ILE ALA ARG GLN VAL THR PRO THR THR ILE ILE LYS GLN VAL SER GLN ALA GLN THR THR VAL GLN PRO SER ALA THR LEU

GLN ARG SER PRO GLY VAL GLN PRO GLN LEU VAL LEU GLY GLY ALA ALA GLN THR ALA SER LEU GLY THR ALA THR ALA VAL GLN THR GLY THR PRO GLN ARG THR VAL PRO GLY ALA THR THR THR SER SER ALA ALA THR GLU THR MET GLU ASN VAL LYS LYS CYS LYS ASN PHE LEU

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

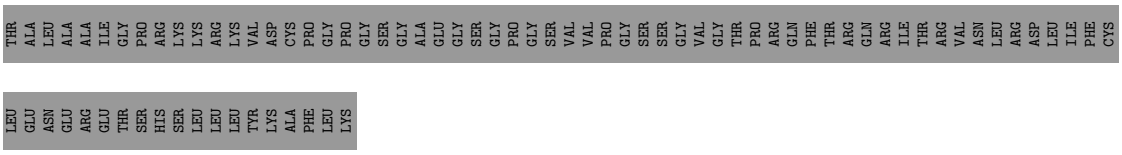
LEU PRO ALA LEU ARG GLN LEU THR PRO ASP SER ALA ALA PHE ILE GLN GLN SER GLN GLN GLN PRO PRO PRO PRO THR SER GLN ALA THR THR ALA LEU THR ALA VAL VAL LEU SER SER SER VAL GLN ARG THR ALA GLY LYS THR ALA ALA THR VAL THR SER ALA LEU GLN PRO PRO

VAL LEU SER LEU THR GLN PRO THR GLN VAL GLY VAL GLY LYS GLN GLY GLN PRO THR PRO LEU VAL ILE GLN GLN PRO PRO LYS PRO GLY ALA LEU ILE ARG PRO PRO GLN VAL THR LEU THR GLN THR PRO MET VAL ALA LEU ARG GLN PRO HIS ASN ARG ILE MET LEU THR THR PRO

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

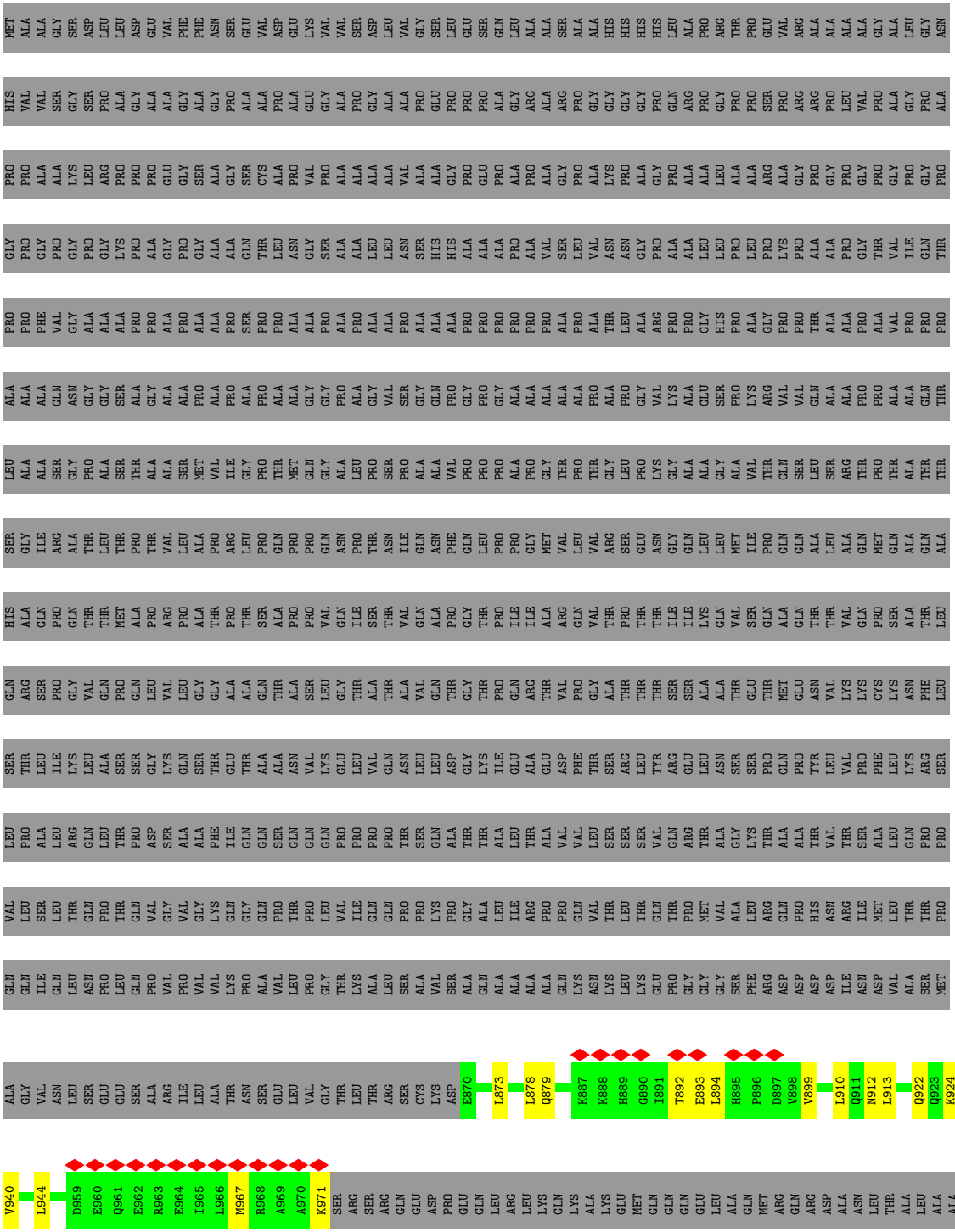
ALA GLY VAL ASN LEU SER GLU GLU SER ALA ARG ILE LEU ALA THR ASN SER GLU LEU VAL GLY THR LEU THR ARG SER CYS LYS ASP E870 L873 E884 I885 G886 K887 K888 H889 T892 E893 L894 V899 H904 Q908 Q911 V914 K929 D930 D931 D932 R933 Y934

E935 Q936 A937 S938 D939 I953 E954 K955 Q956 R957 K958 D959 E960 Q961 E962 R963 E964 I965 L966 M967 R968 A969 A970 K971 SER ARG SER ARG GLN GLU ASP PRO GLU GLN LEU ARG LEU LYS GLN LYS ALA LYS GLU MET GLN GLN GLN GLU LEU ALA GLN MET ARG GLN ARG ASP ALA ASN LEU



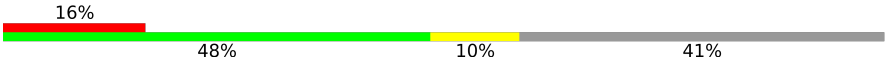
• Molecule 4: Transcription initiation factor TFIID subunit 4

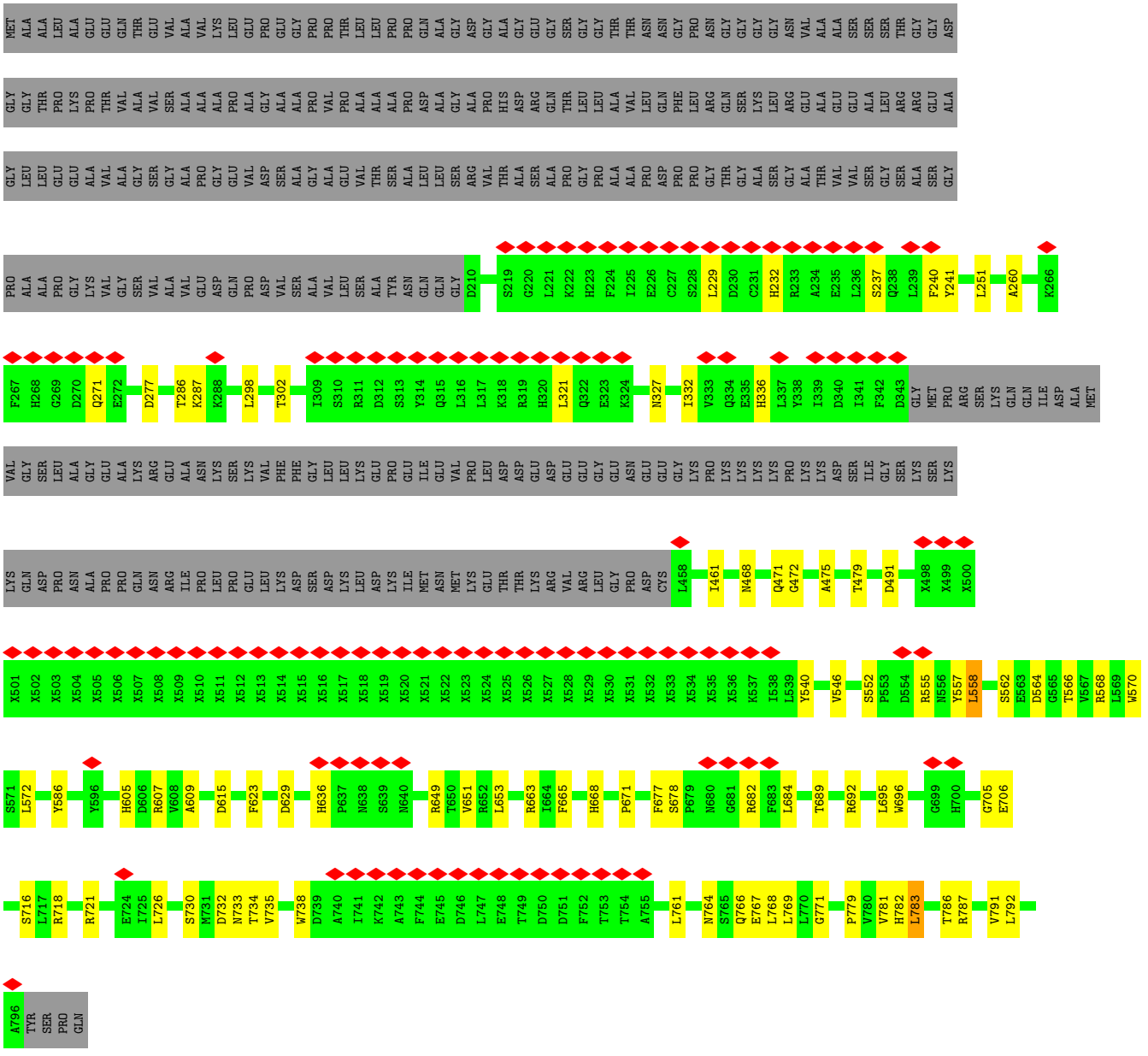
Chain E:



• Molecule 5: Transcription initiation factor TFIID subunit 5,TAF5

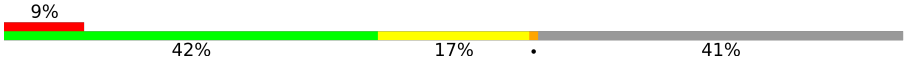
Chain F:

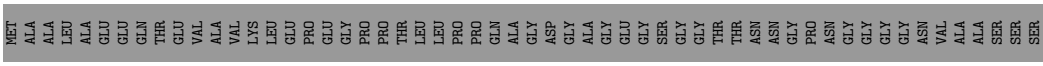


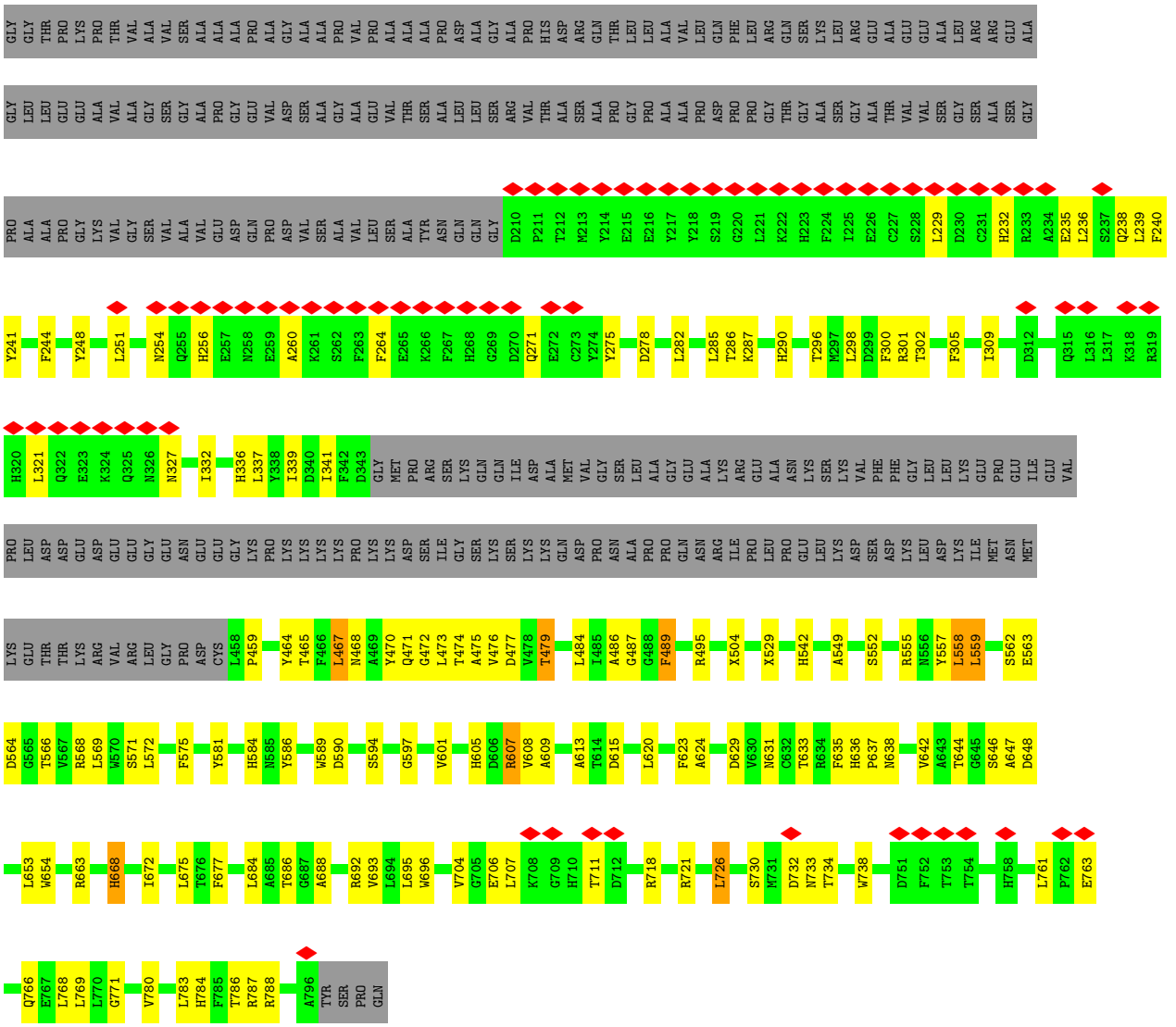


• Molecule 5: Transcription initiation factor TFIID subunit 5,TAF5

Chain G:

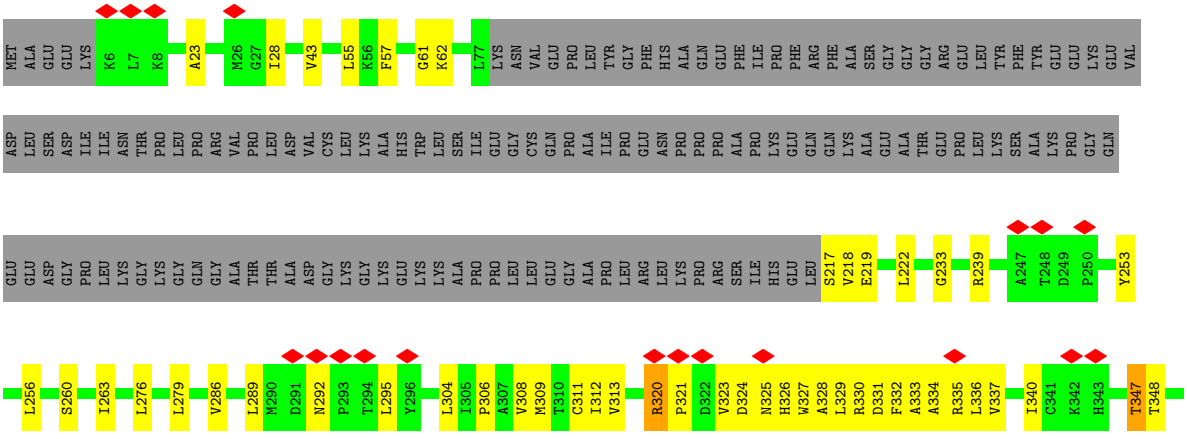


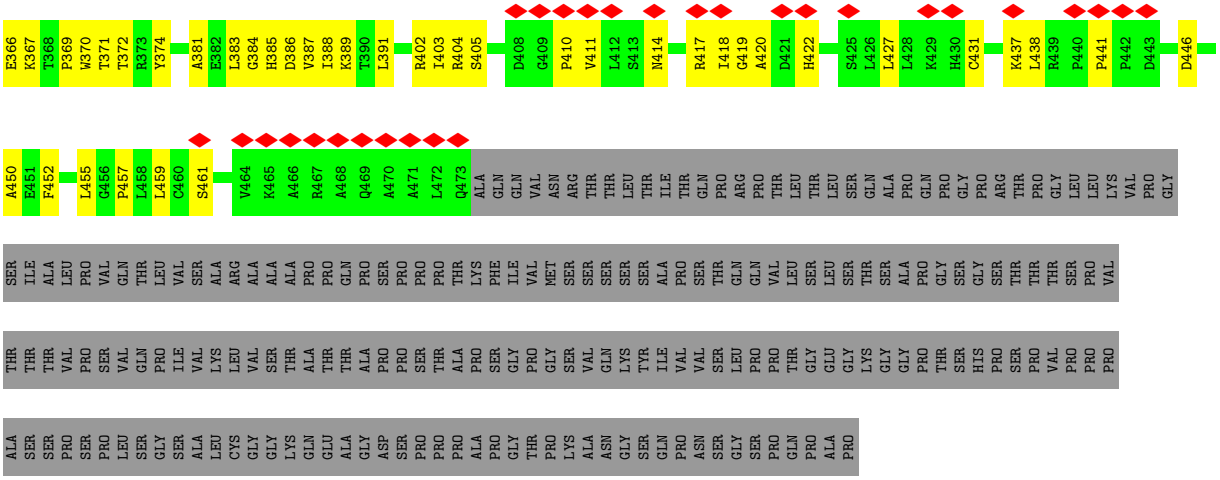




• Molecule 6: Transcription initiation factor TFIID subunit 6

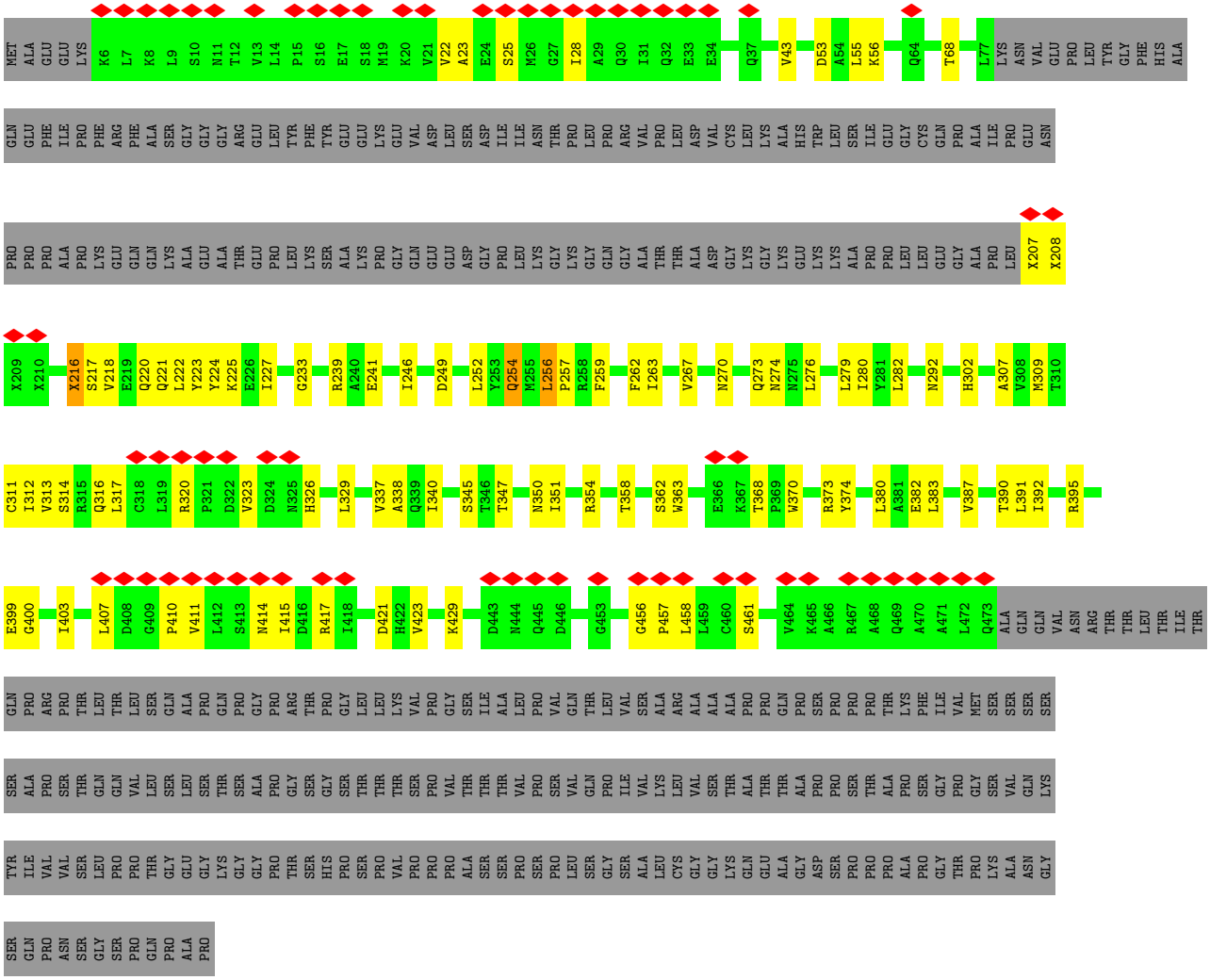
Chain H:





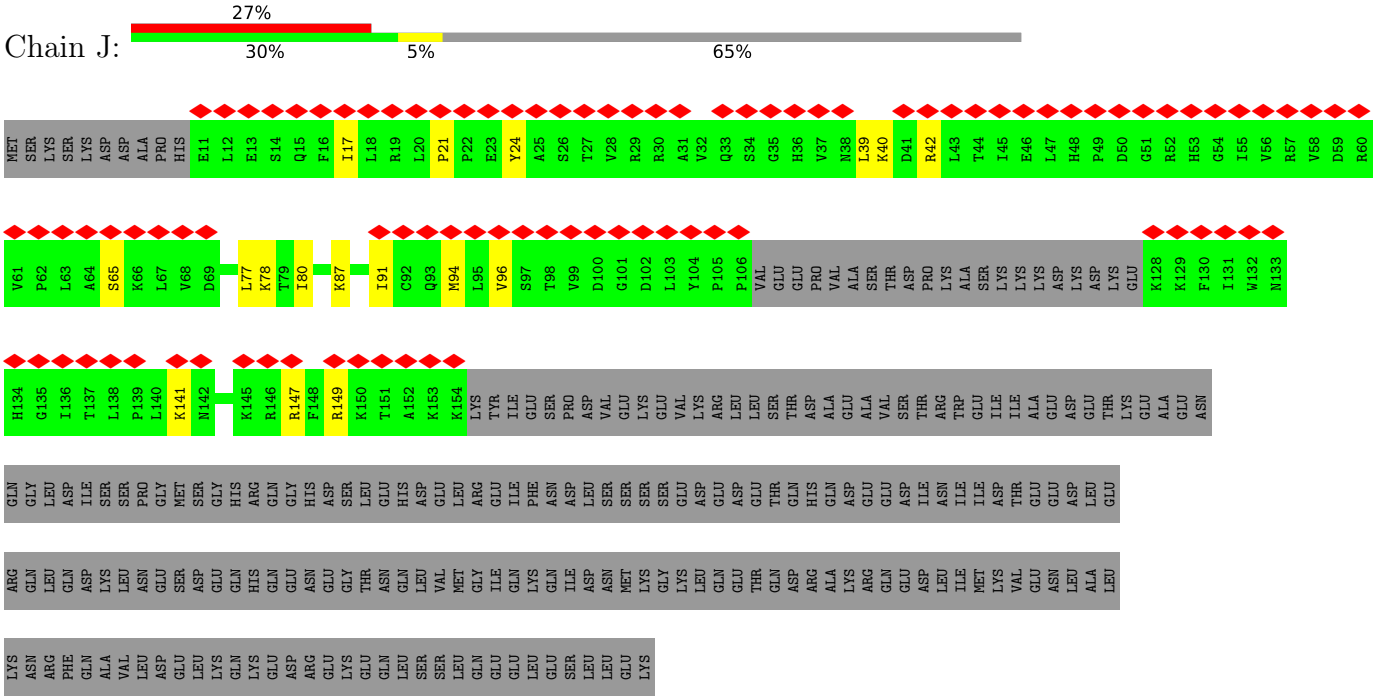
• Molecule 7: Transcription initiation factor TFIID subunit 6

Chain I:



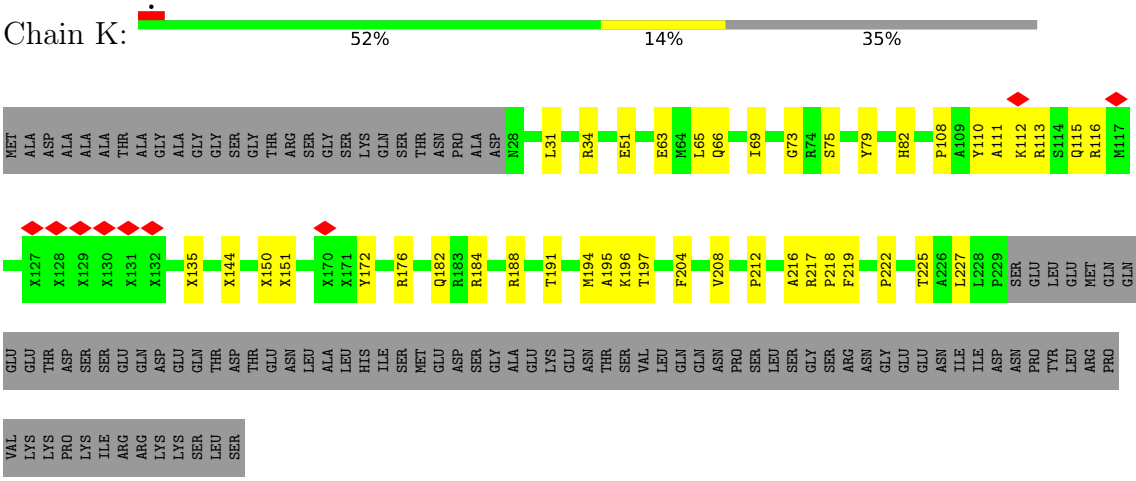
• Molecule 8: Transcription initiation factor TFIID subunit 7

Chain J:



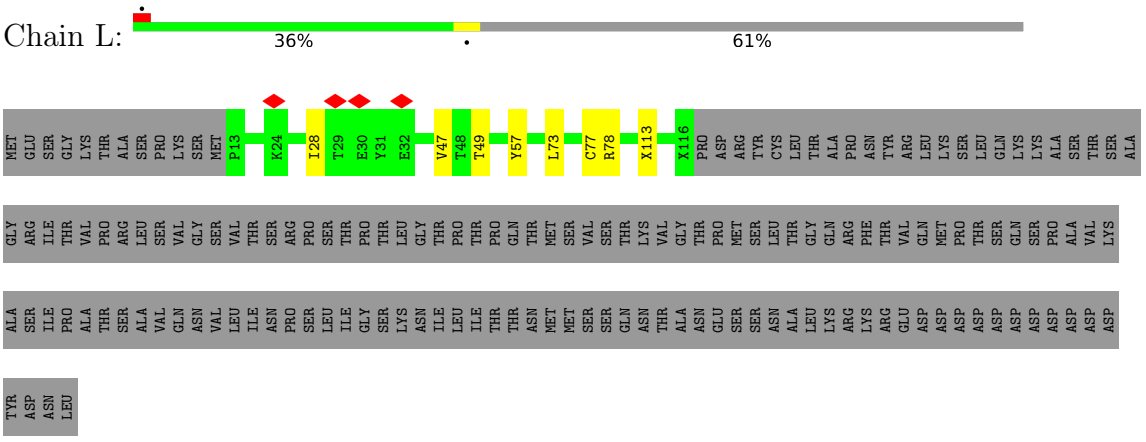
• Molecule 9: Transcription initiation factor TFIID subunit 8,TAF8

Chain K:



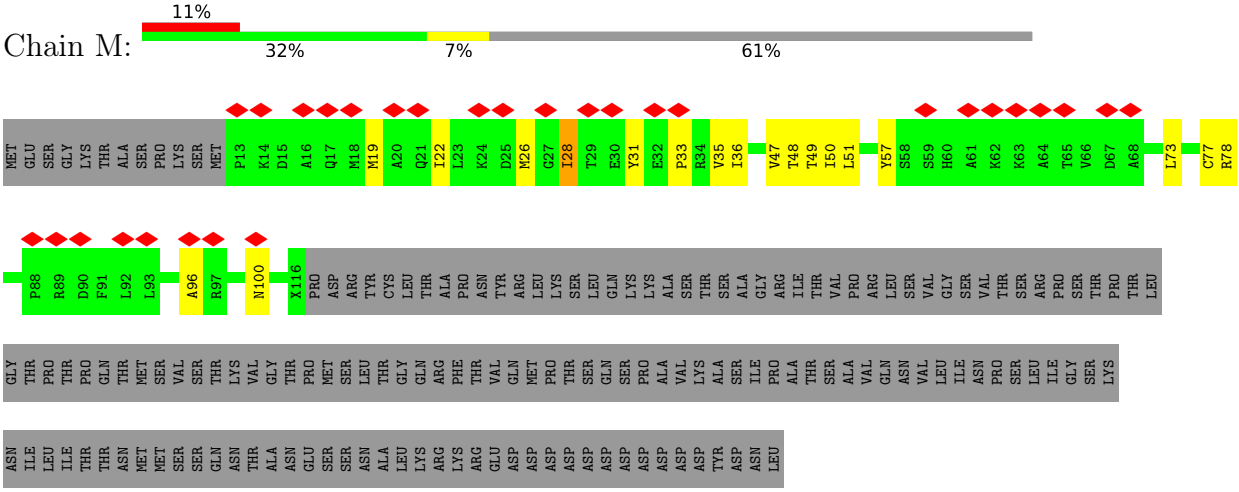
• Molecule 10: Transcription initiation factor TFIID subunit 9, TAF9

Chain L:



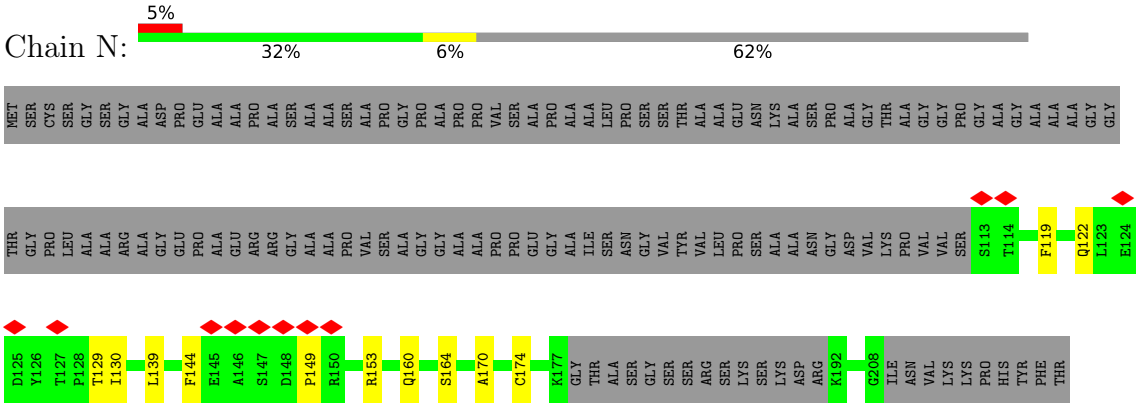
• Molecule 10: Transcription initiation factor TFIID subunit 9, TAF9

Chain M:



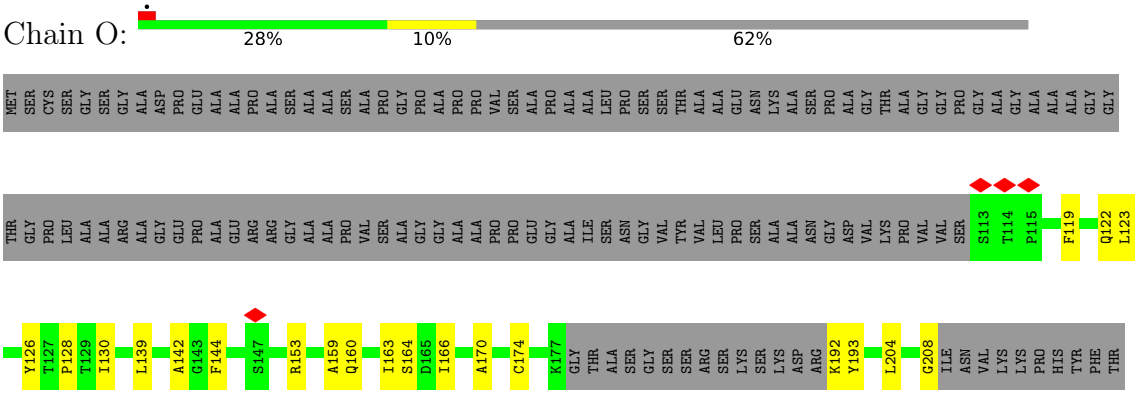
• Molecule 11: Transcription initiation factor TFIID subunit 10

Chain N:



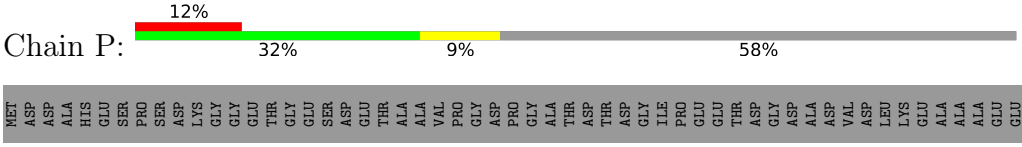
• Molecule 11: Transcription initiation factor TFIID subunit 10

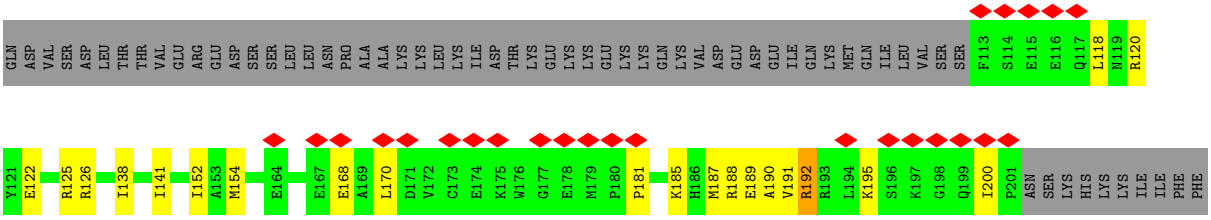
Chain O:

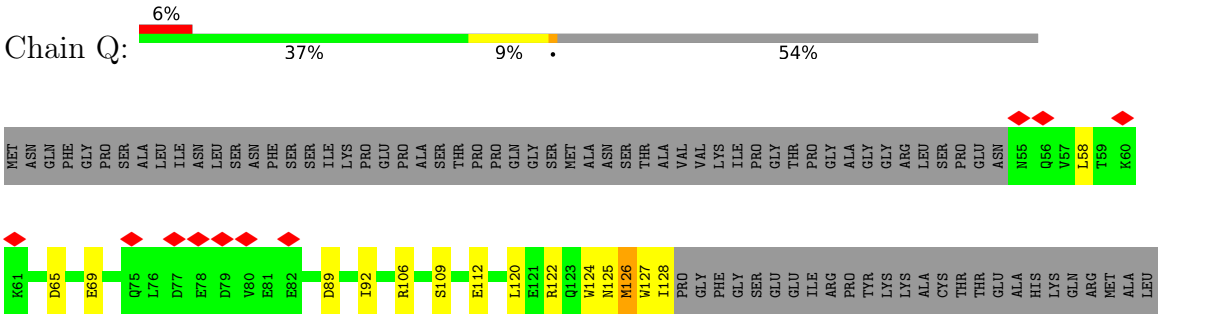


• Molecule 12: Transcription initiation factor TFIID subunit 11

Chain P:





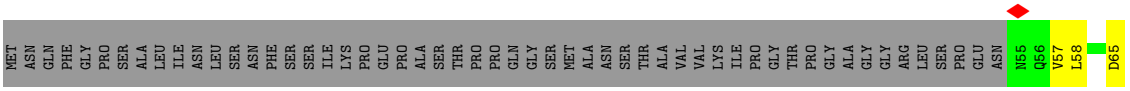


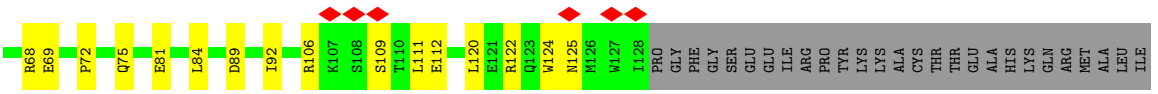
• Molecule 13: Transcription initiation factor TFIID subunit 12

Chain Q:

• Molecule 13: Transcription initiation factor TFIID subunit 12

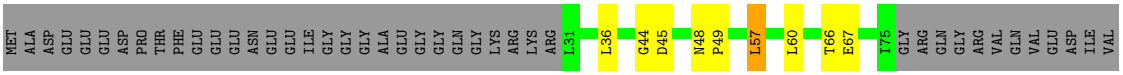
Chain R:





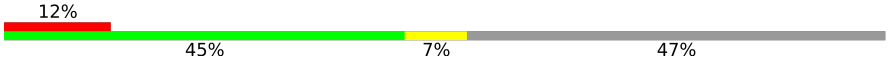
• Molecule 14: Transcription initiation factor TFIID subunit 13

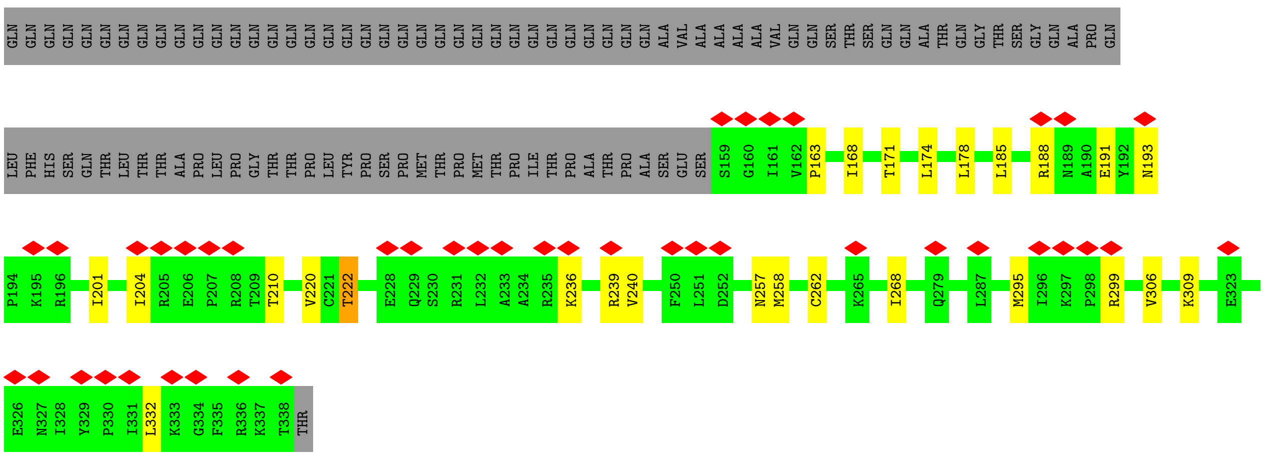
Chain S:



• Molecule 15: TATA-box-binding protein

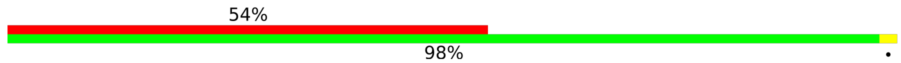
Chain T:

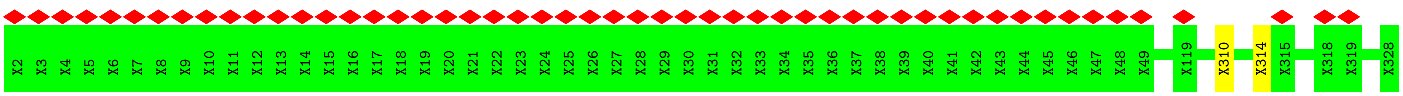




• Molecule 16: poly(UNK)

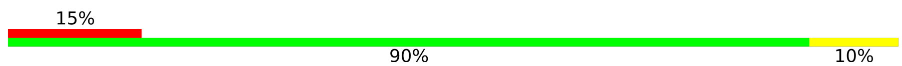
Chain Y:

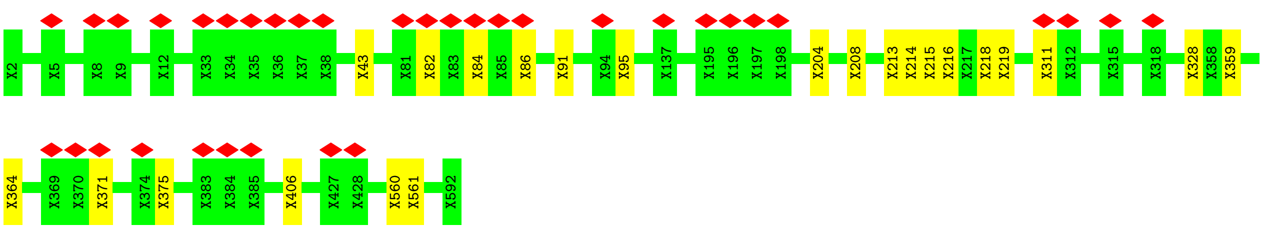




• Molecule 17: poly(UNK)

Chain Z:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	107900	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.065	Depositor
Minimum map value	-0.017	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.026	Depositor
Map size (Å)	380.16, 380.16, 380.16	wwPDB
Map dimensions	144, 144, 144	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.64, 2.64, 2.64	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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	0.27	0/3858	0.53	2/5193 (0.0%)
2	B	0.57	2/8029 (0.0%)	0.74	3/10882 (0.0%)
3	C	0.28	0/757	0.52	0/1027
4	D	0.34	0/692	0.61	1/945 (0.1%)
4	E	0.31	0/692	0.50	0/945
5	F	0.27	0/3537	0.58	0/4802
5	G	0.52	0/3537	0.72	2/4802 (0.0%)
6	H	0.46	0/2533	0.66	0/3439
7	I	0.44	0/2506	0.64	0/3402
8	J	0.26	0/1017	0.53	0/1370
9	K	0.43	0/1212	0.59	0/1640
10	L	0.25	0/705	0.48	0/955
10	M	0.37	0/705	0.59	0/955
11	N	0.27	0/657	0.47	0/891
11	O	0.38	0/657	0.51	0/891
12	P	0.37	0/719	0.72	4/965 (0.4%)
13	Q	0.31	0/618	0.62	1/835 (0.1%)
13	R	0.33	0/618	0.55	0/835
14	S	0.28	0/371	0.52	0/498
15	T	0.31	0/1455	0.55	0/1958
All	All	0.42	2/34875 (0.0%)	0.64	13/47230 (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	1
2	B	0	17
5	F	0	3
5	G	0	8
6	H	0	6

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
7	I	0	4
9	K	0	2
10	M	0	1
17	Z	0	1
All	All	0	43

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	443	TRP	CB-CG	-7.44	1.36	1.50
2	B	381	TRP	CB-CG	-5.07	1.41	1.50

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	220	LEU	CA-CB-CG	7.67	132.93	115.30
12	P	192	ARG	CG-CD-NE	6.62	125.71	111.80
2	B	927	LEU	CA-CB-CG	-6.32	100.76	115.30
1	A	69	LEU	CA-CB-CG	6.27	129.72	115.30
5	G	726	LEU	CB-CG-CD2	-6.05	100.72	111.00
12	P	192	ARG	CB-CG-CD	-5.65	96.92	111.60
12	P	192	ARG	CA-CB-CG	5.64	125.81	113.40
4	D	908	GLN	CB-CG-CD	5.42	125.69	111.60
12	P	118	LEU	CA-CB-CG	5.32	127.53	115.30
1	A	66	LEU	CA-CB-CG	5.25	127.37	115.30
13	Q	126	MET	CB-CG-SD	5.23	128.08	112.40
5	G	607	ARG	CA-CB-CG	5.18	124.79	113.40
2	B	443	TRP	CA-CB-CG	-5.04	104.12	113.70

There are no chirality outliers.

All (43) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	949	GLU	Peptide
2	B	193	VAL	Peptide
2	B	259	ASP	Peptide
2	B	316	VAL	Peptide
2	B	325	PHE	Peptide
2	B	340	PRO	Peptide
2	B	415	HIS	Peptide
2	B	434	SER	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
2	B	538	ASN	Peptide
2	B	540	LYS	Peptide
2	B	583	GLU	Peptide
2	B	674	THR	Peptide
2	B	737	LYS	Peptide
2	B	816	VAL	Peptide
2	B	820	ASP	Peptide
2	B	821	ASN	Peptide
2	B	822	LEU	Peptide
2	B	843	LEU	Peptide
5	F	668	HIS	Peptide
5	F	721	ARG	Peptide
5	F	783	LEU	Peptide
5	G	275	TYR	Peptide
5	G	467	LEU	Peptide
5	G	479	THR	Peptide
5	G	489	PHE	Peptide
5	G	615	ASP	Peptide
5	G	668	HIS	Peptide
5	G	711	THR	Peptide
5	G	721	ARG	Peptide
6	H	313	VAL	Peptide
6	H	320	ARG	Peptide
6	H	347	THR	Peptide
6	H	348	THR	Peptide
6	H	384	GLY	Peptide
6	H	441	PRO	Peptide
7	I	216	UNK	Peptide
7	I	254	GLN	Peptide
7	I	256	LEU	Peptide
7	I	262	PHE	Peptide
9	K	144	UNK	Peptide
9	K	217	ARG	Peptide
10	M	28	ILE	Peptide
17	Z	364	UNK	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3772	0	3742	43	0
2	B	7832	0	7789	217	0
3	C	742	0	719	8	0
4	D	686	0	572	8	0
4	E	686	0	572	13	0
5	F	3646	0	3312	48	0
5	G	3646	0	3312	95	0
6	H	2494	0	2474	58	0
7	I	2520	0	2422	61	0
8	J	998	0	1055	12	0
9	K	1449	0	1281	33	0
10	L	732	0	624	6	0
10	M	732	0	623	13	0
11	N	645	0	640	7	0
11	O	645	0	640	15	0
12	P	707	0	730	24	0
13	Q	611	0	610	16	0
13	R	611	0	610	16	0
14	S	365	0	351	10	0
15	T	1429	0	1521	18	0
16	Y	480	0	112	1	0
17	Z	1190	0	280	16	0
All	All	36618	0	33991	655	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 (655) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:874:GLU:HG2	2:B:468:PHE:HZ	1.27	0.99
2:B:566:VAL:O	2:B:577:HIS:HA	1.64	0.97
2:B:532:TYR:O	2:B:551:ASP:HB2	1.67	0.94
2:B:50:GLU:HA	2:B:146:ILE:O	1.70	0.92
1:A:874:GLU:HG2	2:B:468:PHE:CZ	2.04	0.91
5:G:309:ILE:O	5:G:341:ILE:HA	1.73	0.88
2:B:567:THR:O	2:B:629:ARG:HB3	1.73	0.87
2:B:350:LEU:O	2:B:353:GLN:HB3	1.77	0.84
4:D:908:GLN:HG2	12:P:192:ARG:HD3	1.61	0.83
6:H:329:LEU:O	6:H:332:PHE:HB3	1.79	0.80
12:P:195:LYS:HE2	13:Q:127:TRP:H	1.45	0.80
7:I:350:ASN:O	7:I:354:ARG:HB2	1.82	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:904:HIS:HA	12:P:192:ARG:HH21	1.50	0.76
1:A:62:CYS:O	1:A:66:LEU:HB2	1.84	0.76
3:C:34:ARG:HG2	3:C:66:GLN:HE22	1.53	0.73
2:B:538:ASN:HA	2:B:542:ASN:HD22	1.51	0.73
2:B:39:ASN:HB3	2:B:44:SER:H	1.52	0.73
2:B:835:ARG:HH22	9:K:184:ARG:HE	1.36	0.73
5:G:474:THR:O	5:G:486:ALA:HB3	1.89	0.72
7:I:392:ILE:HA	7:I:395:ARG:HB2	1.71	0.71
2:B:305:LYS:O	2:B:322:MET:HA	1.91	0.70
5:G:726:LEU:HB2	5:G:738:TRP:HB2	1.73	0.70
9:K:112:LYS:HA	9:K:116:ARG:HD2	1.74	0.70
2:B:564:LEU:H	2:B:580:GLN:HB2	1.57	0.69
11:N:139:LEU:HB3	11:N:144:PHE:HB3	1.73	0.69
5:F:718:ARG:HG2	5:F:771:GLY:H	1.58	0.68
5:G:475:ALA:HA	5:G:484:LEU:O	1.93	0.68
9:K:195:ALA:HB1	9:K:212:PRO:HG2	1.76	0.68
5:F:586:TYR:HB3	5:F:605:HIS:HB3	1.75	0.68
7:I:338:ALA:HB2	7:I:382:GLU:HB3	1.76	0.67
2:B:463:ARG:NH1	2:B:514:ASP:O	2.27	0.67
11:O:130:ILE:HG13	11:O:160:GLN:HE21	1.59	0.66
2:B:64:LYS:HA	2:B:126:LEU:O	1.96	0.66
6:H:330:ARG:O	6:H:333:ALA:HB3	1.95	0.66
6:H:333:ALA:O	6:H:336:LEU:HB2	1.94	0.66
6:H:325:ASN:O	6:H:328:ALA:HB3	1.95	0.66
7:I:323:VAL:HA	7:I:326:HIS:HD2	1.60	0.66
1:A:101:VAL:HG21	15:T:191:GLU:HA	1.78	0.66
1:A:666:ARG:HG3	1:A:667:THR:HG23	1.77	0.66
2:B:62:ARG:HG2	2:B:129:LYS:HG2	1.76	0.66
2:B:815:GLU:HA	2:B:819:LEU:HD12	1.79	0.65
2:B:835:ARG:HH21	9:K:188:ARG:HD2	1.61	0.65
2:B:354:PHE:O	2:B:357:CYS:HB2	1.97	0.65
5:F:321:LEU:HD22	5:F:327:ASN:HD21	1.61	0.65
6:H:323:VAL:O	6:H:327:TRP:N	2.29	0.65
2:B:359:ILE:HG23	2:B:498:VAL:HB	1.78	0.64
2:B:888:ILE:HD11	2:B:925:LYS:HG3	1.79	0.64
5:G:733:ASN:HB3	5:G:761:LEU:HB2	1.80	0.64
4:E:892:THR:H	13:R:109:SER:HB2	1.63	0.64
12:P:185:LYS:O	12:P:189:GLU:HB2	1.97	0.63
5:G:586:TYR:HB3	5:G:605:HIS:HB3	1.79	0.63
10:L:77:CYS:SG	13:Q:122:ARG:NH2	2.71	0.63
2:B:396:LYS:HD2	2:B:660:VAL:HA	1.80	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:630:ILE:O	2:B:638:ARG:NH1	2.31	0.63
5:F:472:GLY:HA3	5:F:783:LEU:HD13	1.80	0.63
5:F:726:LEU:HB2	5:F:738:TRP:HB2	1.81	0.63
9:K:108:PRO:O	9:K:111:ALA:HB3	1.99	0.63
12:P:122:GLU:OE2	12:P:125:ARG:NH2	2.32	0.63
2:B:118:ASP:O	2:B:123:ASN:ND2	2.32	0.63
1:A:874:GLU:CG	2:B:468:PHE:HZ	2.06	0.62
2:B:32:VAL:HA	2:B:203:LYS:O	1.99	0.62
2:B:459:LEU:HD23	2:B:462:ASN:HD22	1.63	0.62
15:T:191:GLU:HB2	15:T:201:ILE:HB	1.81	0.62
2:B:63:ILE:O	2:B:127:CYS:HA	2.00	0.62
2:B:646:ASP:HA	2:B:649:TRP:HD1	1.65	0.62
5:G:229:LEU:HB2	5:G:232:HIS:HD2	1.64	0.62
5:G:684:LEU:HB2	5:G:696:TRP:HB2	1.80	0.62
2:B:338:GLU:OE2	2:B:847:ARG:NH2	2.32	0.62
2:B:651:TYR:OH	2:B:654:ARG:NH2	2.33	0.62
5:F:286:THR:HG22	5:F:287:LYS:HG3	1.82	0.61
10:M:57:TYR:OH	13:R:122:ARG:NH2	2.33	0.61
1:A:77:LEU:HD23	15:T:257:ASN:HD21	1.64	0.61
2:B:206:PHE:O	2:B:233:THR:HA	2.00	0.61
2:B:550:GLN:HB2	2:B:586:LEU:HB2	1.83	0.61
5:F:546:VAL:HA	5:F:562:SER:HA	1.83	0.61
2:B:955:LYS:O	2:B:959:SER:N	2.31	0.61
5:G:464:TYR:HE1	9:K:151:UNK:HA	1.66	0.61
13:R:65:ASP:O	13:R:69:GLU:HB2	2.01	0.61
5:G:718:ARG:HG2	5:G:771:GLY:H	1.64	0.61
6:H:427:LEU:O	6:H:431:CYS:HB3	2.01	0.61
9:K:65:LEU:HD11	11:O:159:ALA:HB1	1.83	0.60
11:N:130:ILE:HG13	11:N:160:GLN:HE21	1.65	0.60
15:T:236:LYS:HG2	15:T:239:ARG:HH12	1.66	0.60
2:B:433:PHE:HB3	2:B:440:THR:HG21	1.84	0.60
6:H:55:LEU:HD13	10:L:28:ILE:HD12	1.83	0.60
2:B:911:LEU:HA	2:B:914:ILE:HD12	1.82	0.60
5:F:229:LEU:HB2	5:F:232:HIS:HD2	1.67	0.60
13:R:120:LEU:O	13:R:124:TRP:N	2.32	0.60
2:B:691:PHE:HD2	2:B:694:VAL:H	1.48	0.60
6:H:292:ASN:HD22	6:H:295:LEU:HG	1.67	0.60
2:B:41:GLN:O	2:B:43:LYS:NZ	2.35	0.60
5:F:651:VAL:HB	5:F:665:PHE:HB2	1.84	0.60
9:K:31:LEU:HD11	9:K:34:ARG:HH21	1.67	0.59
1:A:927:VAL:O	1:A:933:ASN:ND2	2.35	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Q:106:ARG:HH22	13:Q:112:GLU:HB2	1.66	0.59
7:I:55:LEU:HD13	10:M:28:ILE:HD12	1.84	0.59
2:B:24:ARG:NH1	2:B:120:ASP:OD1	2.33	0.59
5:G:787:ARG:NH2	17:Z:328:UNK:O	2.35	0.59
2:B:538:ASN:HD22	2:B:547:GLU:HB2	1.68	0.59
2:B:219:ASP:O	2:B:236:TYR:HA	2.02	0.59
1:A:117:ALA:H	15:T:239:ARG:HH21	1.50	0.59
2:B:352:GLN:O	2:B:356:GLY:N	2.35	0.59
6:H:233:GLY:O	6:H:239:ARG:NH1	2.35	0.59
10:M:77:CYS:SG	13:R:122:ARG:NH2	2.76	0.59
5:F:733:ASN:HB3	5:F:761:LEU:HB2	1.84	0.58
2:B:230:ARG:HG3	2:B:231:LYS:HG3	1.84	0.58
2:B:915:GLN:O	2:B:923:ARG:NH2	2.37	0.58
5:G:287:LYS:H	5:G:290:HIS:HD2	1.49	0.58
5:G:321:LEU:HD22	5:G:327:ASN:HD21	1.69	0.58
9:K:115:GLN:HE22	11:O:126:TYR:HB3	1.67	0.58
1:A:635:SER:HB3	8:J:40:LYS:HB2	1.84	0.58
5:F:609:ALA:HB3	5:F:623:PHE:HB2	1.86	0.58
7:I:414:ASN:HA	7:I:417:ARG:HB2	1.85	0.58
5:G:472:GLY:HA3	5:G:783:LEU:HD13	1.85	0.58
17:Z:82:UNK:O	17:Z:86:UNK:N	2.37	0.58
2:B:917:ASP:OD1	2:B:923:ARG:NE	2.33	0.58
5:G:562:SER:OG	5:G:563:GLU:N	2.37	0.58
12:P:126:ARG:HG3	15:T:306:VAL:HB	1.84	0.58
2:B:391:TYR:OH	2:B:458:ARG:NH1	2.33	0.58
2:B:608:ASN:O	2:B:657:ARG:NH2	2.37	0.58
2:B:341:LEU:O	2:B:344:ARG:HB3	2.04	0.57
5:G:552:SER:HB3	5:G:557:TYR:HB2	1.86	0.57
5:G:465:THR:HA	5:G:788:ARG:HG2	1.86	0.57
5:G:646:SER:OG	5:G:647:ALA:N	2.36	0.57
12:P:191:VAL:HG12	12:P:195:LYS:HE3	1.85	0.57
5:G:635:PHE:HA	5:G:642:VAL:HG12	1.85	0.57
9:K:73:GLY:HA3	11:O:142:ALA:HB1	1.86	0.57
2:B:550:GLN:HE22	2:B:580:GLN:HA	1.69	0.57
2:B:929:MET:HG2	2:B:932:LYS:HD2	1.87	0.57
5:G:278:ASP:O	5:G:282:LEU:HB2	2.04	0.57
6:H:324:ASP:O	6:H:327:TRP:HB2	2.04	0.57
2:B:184:ASN:OD1	2:B:195:SER:OG	2.23	0.57
2:B:599:ASN:HA	2:B:602:LYS:HB2	1.87	0.57
2:B:367:GLU:HG3	2:B:370:LEU:HD12	1.86	0.57
5:F:277:ASP:OD1	5:F:649:ARG:NH2	2.38	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:337:ASP:OD2	2:B:751:LYS:NZ	2.33	0.57
2:B:917:ASP:H	2:B:923:ARG:HH21	1.53	0.57
9:K:51:GLU:OE1	11:O:192:LYS:N	2.38	0.57
2:B:783:ASP:OD2	2:B:787:ASN:ND2	2.38	0.57
5:F:240:PHE:HB3	5:F:271:GLN:HE22	1.70	0.57
2:B:51:LEU:HB2	2:B:146:ILE:HB	1.86	0.56
5:G:564:ASP:HB2	5:G:566:THR:HG22	1.86	0.56
12:P:200:ILE:HD12	13:Q:127:TRP:HD1	1.70	0.56
15:T:168:ILE:HG12	15:T:258:MET:HG2	1.87	0.56
6:H:404:ARG:NH2	6:H:452:PHE:O	2.38	0.56
2:B:530:LYS:HE2	2:B:639:LYS:HD3	1.88	0.56
5:G:332:ILE:HA	5:G:336:HIS:HD2	1.71	0.56
5:G:476:VAL:HG22	5:G:768:LEU:HD22	1.87	0.56
7:I:363:TRP:NE1	7:I:399:GLU:OE2	2.38	0.56
9:K:75:SER:O	9:K:79:TYR:HB2	2.04	0.56
5:G:235:GLU:O	5:G:238:GLN:NE2	2.38	0.56
6:H:253:TYR:O	9:K:182:GLN:NE2	2.39	0.56
2:B:678:ARG:NH1	2:B:682:THR:OG1	2.39	0.56
5:F:237:SER:HA	5:F:240:PHE:HD2	1.71	0.56
6:H:306:PRO:HB3	17:Z:406:UNK:HA	1.86	0.56
2:B:631:ASP:O	2:B:638:ARG:NH1	2.38	0.56
9:K:191:THR:O	9:K:195:ALA:HB2	2.06	0.56
2:B:344:ARG:NH1	2:B:382:MET:SD	2.79	0.55
5:G:594:SER:HB2	5:G:597:GLY:H	1.71	0.55
2:B:946:ASN:ND2	2:B:986:CYS:SG	2.76	0.55
5:F:692:ARG:NH2	5:F:706:GLU:OE1	2.39	0.55
7:I:246:ILE:O	7:I:292:ASN:ND2	2.39	0.55
4:E:894:LEU:HA	13:R:111:LEU:H	1.71	0.55
5:G:613:ALA:HB2	5:G:620:LEU:HD11	1.89	0.55
6:H:57:PHE:O	6:H:61:GLY:N	2.38	0.55
9:K:196:LYS:HE2	9:K:208:VAL:HG12	1.87	0.55
11:O:139:LEU:HB3	11:O:144:PHE:HB3	1.88	0.55
3:C:30:GLU:OE2	5:F:471:GLN:NE2	2.37	0.55
2:B:597:ARG:NH1	2:B:621:ALA:O	2.37	0.55
1:A:903:TYR:HE2	1:A:926:GLU:HB3	1.72	0.55
2:B:806:VAL:HG13	2:B:864:ASN:HD21	1.70	0.55
3:C:81:GLU:OE2	5:F:568:ARG:NH2	2.39	0.55
4:D:873:LEU:HD23	13:Q:58:LEU:HD13	1.88	0.55
1:A:961:GLU:OE1	8:J:147:ARG:NH1	2.40	0.55
2:B:820:ASP:HB2	2:B:822:LEU:HA	1.88	0.55
4:E:924:LYS:NZ	13:R:75:GLN:O	2.40	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:468:ASN:HA	5:F:786:THR:HG23	1.87	0.55
5:G:286:THR:HG22	5:G:287:LYS:HG3	1.87	0.55
7:I:337:VAL:HA	7:I:340:ILE:HD12	1.88	0.55
2:B:840:GLU:HG3	2:B:850:ILE:HB	1.87	0.55
4:E:873:LEU:HD23	13:R:58:LEU:HD13	1.87	0.55
1:A:61:GLU:O	1:A:65:HIS:HB2	2.06	0.55
7:I:233:GLY:O	7:I:239:ARG:NH1	2.37	0.55
10:L:57:TYR:OH	13:Q:122:ARG:NH2	2.33	0.54
12:P:120:ARG:NH1	14:S:45:ASP:O	2.39	0.54
17:Z:204:UNK:O	17:Z:208:UNK:N	2.40	0.54
6:H:217:SER:OG	6:H:218:VAL:N	2.41	0.54
9:K:172:TYR:OH	9:K:176:ARG:NH1	2.40	0.54
2:B:504:LEU:HA	2:B:507:ILE:HD12	1.89	0.54
2:B:536:ALA:H	2:B:548:ILE:HG12	1.72	0.54
2:B:32:VAL:HG22	2:B:203:LYS:HB3	1.87	0.54
5:G:609:ALA:HB3	5:G:623:PHE:HB2	1.88	0.54
7:I:345:SER:HB3	7:I:351:ILE:HB	1.90	0.54
5:F:684:LEU:HB2	5:F:696:TRP:HB2	1.88	0.54
7:I:208:UNK:HA	17:Z:560:UNK:HA	1.89	0.54
5:G:309:ILE:HD11	5:G:339:ILE:HG12	1.90	0.54
7:I:429:LYS:NZ	7:I:458:LEU:O	2.33	0.54
5:G:549:ALA:HA	5:G:559:LEU:O	2.07	0.54
15:T:163:PRO:HA	15:T:262:CYS:HB3	1.90	0.54
4:E:940:VAL:O	4:E:944:LEU:N	2.40	0.53
15:T:268:ILE:HD13	15:T:332:LEU:HD22	1.90	0.53
2:B:82:ALA:HB3	2:B:128:ILE:HD11	1.88	0.53
5:G:240:PHE:HB3	5:G:271:GLN:HE22	1.73	0.53
7:I:224:TYR:HA	7:I:227:ILE:HD12	1.91	0.53
2:B:902:ARG:NH2	2:B:942:SER:O	2.42	0.53
5:G:468:ASN:HA	5:G:786:THR:HG23	1.91	0.53
12:P:185:LYS:O	12:P:189:GLU:CB	2.57	0.53
2:B:406:GLU:OE2	2:B:412:VAL:N	2.42	0.53
2:B:663:GLN:HA	2:B:666:ILE:HB	1.91	0.53
5:F:491:ASP:HA	5:F:540:TYR:HB3	1.90	0.53
2:B:761:ARG:NH2	2:B:804:ASN:O	2.41	0.53
5:G:653:LEU:HD12	5:G:663:ARG:HB2	1.90	0.53
1:A:680:LEU:HD11	8:J:91:ILE:HD12	1.91	0.53
2:B:206:PHE:HB2	2:B:234:PHE:HB2	1.91	0.53
7:I:368:THR:OG1	7:I:373:ARG:NE	2.42	0.53
13:Q:65:ASP:O	13:Q:69:GLU:HB2	2.09	0.53
13:R:106:ARG:HH22	13:R:112:GLU:HB2	1.74	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:THR:HG23	15:T:185:LEU:HB3	1.91	0.52
2:B:392:ARG:HD3	2:B:395:ILE:HD12	1.91	0.52
2:B:486:GLN:OE1	2:B:489:GLN:NE2	2.41	0.52
5:G:692:ARG:NH2	5:G:706:GLU:OE1	2.41	0.52
11:N:170:ALA:O	11:N:174:CYS:HB2	2.10	0.52
14:S:57:LEU:HA	14:S:60:LEU:HD12	1.91	0.52
5:F:332:ILE:HA	5:F:336:HIS:HD2	1.74	0.52
13:Q:120:LEU:HD13	13:Q:126:MET:HG3	1.90	0.52
1:A:753:TYR:OH	1:A:1074:ASN:OD1	2.27	0.52
7:I:276:LEU:HA	7:I:279:LEU:HD12	1.91	0.52
5:F:671:PRO:O	5:F:689:THR:OG1	2.27	0.52
6:H:410:PRO:O	6:H:417:ARG:NH2	2.43	0.52
13:R:89:ASP:HA	13:R:92:ILE:HD12	1.91	0.52
1:A:706:ARG:CZ	2:B:263:HIS:NE2	2.72	0.52
5:F:767:GLU:O	6:H:62:LYS:NZ	2.41	0.52
5:G:300:PHE:HB3	5:G:301:ARG:HH11	1.75	0.52
2:B:859:ARG:HE	2:B:863:LYS:HE3	1.75	0.52
7:I:311:CYS:O	7:I:316:GLN:NE2	2.42	0.52
2:B:224:VAL:O	2:B:232:LYS:NZ	2.43	0.52
5:G:459:PRO:O	17:Z:359:UNK:N	2.43	0.52
9:K:110:TYR:HH	11:O:164:SER:HG	1.57	0.52
2:B:270:LEU:HB2	2:B:273:LEU:HD12	1.91	0.52
5:G:608:VAL:HG12	5:G:624:ALA:HB2	1.91	0.52
7:I:23:ALA:HB1	7:I:28:ILE:HD12	1.91	0.52
2:B:525:GLN:O	2:B:559:LYS:NZ	2.34	0.51
2:B:530:LYS:HG2	2:B:639:LYS:HB3	1.93	0.51
1:A:784:GLN:H	1:A:1073:GLN:HE22	1.58	0.51
2:B:76:ARG:NH1	2:B:79:ASP:OD1	2.43	0.51
2:B:232:LYS:HE3	2:B:234:PHE:HE1	1.76	0.51
5:G:693:VAL:HB	5:G:707:LEU:HB2	1.93	0.51
6:H:256:LEU:HD22	6:H:295:LEU:HD22	1.92	0.51
17:Z:371:UNK:O	17:Z:375:UNK:N	2.44	0.51
1:A:702:ASN:HB2	1:A:722:THR:HA	1.92	0.51
2:B:353:GLN:O	2:B:357:CYS:N	2.44	0.51
4:D:894:LEU:HD22	4:D:899:VAL:HG21	1.92	0.51
6:H:328:ALA:O	6:H:331:ASP:HB2	2.10	0.51
2:B:392:ARG:HA	2:B:395:ILE:HD12	1.92	0.51
3:C:37:LEU:HD12	3:C:66:GLN:HE21	1.76	0.51
9:K:63:GLU:OE1	9:K:66:GLN:NE2	2.44	0.51
5:F:730:SER:OG	5:F:732:ASP:OD1	2.29	0.51
2:B:118:ASP:OD1	2:B:187:ARG:NH2	2.44	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:472:GLY:HA2	5:G:487:GLY:HA2	1.93	0.50
7:I:410:PRO:HG2	7:I:417:ARG:HE	1.76	0.50
12:P:170:LEU:HD11	14:S:44:GLY:HA3	1.93	0.50
1:A:111:SER:HA	15:T:204:ILE:HG22	1.93	0.50
2:B:366:ASP:HB3	2:B:499:SER:HB2	1.92	0.50
2:B:539:ARG:HG3	2:B:545:GLU:HA	1.92	0.50
2:B:565:LYS:HA	2:B:578:THR:O	2.12	0.50
9:K:66:GLN:HA	9:K:69:ILE:HD12	1.93	0.50
12:P:189:GLU:HA	12:P:192:ARG:HD2	1.94	0.50
2:B:48:PHE:HA	2:B:148:ILE:O	2.11	0.50
2:B:688:GLU:H	2:B:695:ARG:HH12	1.60	0.50
5:F:298:LEU:O	5:F:302:THR:OG1	2.25	0.50
7:I:207:UNK:O	17:Z:561:UNK:N	2.44	0.50
14:S:57:LEU:HG	14:S:60:LEU:HD12	1.92	0.50
6:H:387:VAL:O	6:H:391:LEU:HB2	2.11	0.50
6:H:457:PRO:O	6:H:461:SER:N	2.42	0.50
7:I:223:TYR:OH	7:I:249:ASP:OD2	2.28	0.50
2:B:156:LYS:O	2:B:963:HIS:ND1	2.34	0.50
2:B:360:SER:OG	2:B:496:MET:O	2.26	0.50
7:I:43:VAL:HG21	10:M:47:VAL:HG22	1.92	0.50
1:A:46:ILE:HG22	1:A:52:LEU:HA	1.94	0.50
7:I:410:PRO:O	7:I:417:ARG:NH2	2.44	0.50
17:Z:91:UNK:O	17:Z:95:UNK:N	2.45	0.50
2:B:24:ARG:HD3	2:B:120:ASP:HA	1.93	0.50
2:B:387:GLY:O	2:B:391:TYR:N	2.38	0.50
2:B:958:ASN:O	2:B:968:ARG:NH2	2.43	0.50
5:F:783:LEU:HD21	5:F:787:ARG:HG3	1.93	0.50
5:G:769:LEU:HD13	5:G:780:VAL:HG13	1.94	0.50
10:M:48:THR:HA	10:M:51:LEU:HD12	1.92	0.50
5:G:298:LEU:O	5:G:302:THR:OG1	2.28	0.50
7:I:217:SER:H	7:I:220:GLN:HG2	1.77	0.49
13:Q:120:LEU:O	13:Q:124:TRP:N	2.38	0.49
2:B:55:PRO:HB3	2:B:60:LEU:HD23	1.93	0.49
2:B:104:ASN:O	2:B:108:ASN:ND2	2.45	0.49
2:B:256:ILE:HD11	2:B:274:LEU:HB3	1.93	0.49
13:Q:128:ILE:HA	14:S:60:LEU:HD23	1.95	0.49
2:B:44:SER:OG	2:B:152:LEU:O	2.23	0.49
5:G:244:PHE:HZ	5:G:264:PHE:HA	1.78	0.49
6:H:419:GLY:HA2	6:H:422:HIS:CE1	2.47	0.49
7:I:267:VAL:HG11	7:I:307:ALA:HB1	1.95	0.49
1:A:62:CYS:O	1:A:66:LEU:CB	2.56	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:752:ILE:HG22	1:A:782:VAL:HG22	1.92	0.49
2:B:313:TYR:O	2:B:966:ARG:NH2	2.45	0.49
5:G:644:THR:HB	5:G:654:TRP:HE1	1.78	0.49
2:B:314:VAL:HG12	2:B:316:VAL:H	1.77	0.49
5:G:558:LEU:O	5:G:569:LEU:HA	2.13	0.49
12:P:120:ARG:HD3	14:S:44:GLY:HA2	1.95	0.49
12:P:200:ILE:HB	13:Q:127:TRP:HE1	1.77	0.49
1:A:41:PHE:HB3	1:A:81:LEU:HD23	1.95	0.49
2:B:215:VAL:HA	2:B:236:TYR:HE2	1.78	0.49
6:H:260:SER:HA	6:H:263:ILE:HD12	1.94	0.49
7:I:216:UNK:HA	7:I:220:GLN:HE21	1.78	0.49
13:R:106:ARG:NH1	13:R:112:GLU:OE1	2.41	0.49
2:B:451:CYS:HA	2:B:454:HIS:HD2	1.78	0.49
2:B:546:LEU:HB3	2:B:590:ILE:HB	1.93	0.49
2:B:727:PHE:HB3	2:B:736:VAL:HG11	1.94	0.49
3:C:110:TYR:HH	11:N:164:SER:HG	1.60	0.49
5:G:601:VAL:HG11	5:G:642:VAL:HG11	1.95	0.49
1:A:110:TYR:HD1	1:A:113:ILE:HD11	1.78	0.49
2:B:220:LEU:HD23	2:B:236:TYR:HE1	1.78	0.49
2:B:570:GLU:OE1	2:B:593:HIS:ND1	2.38	0.49
2:B:291:TYR:HA	2:B:294:ILE:HD12	1.95	0.48
2:B:431:LEU:HD13	2:B:976:PHE:HB2	1.95	0.48
2:B:76:ARG:HD2	2:B:79:ASP:HA	1.95	0.48
6:H:371:THR:HG23	6:H:372:THR:HG23	1.95	0.48
7:I:270:ASN:HA	7:I:273:GLN:HB2	1.95	0.48
1:A:64:LYS:HD3	12:P:152:ILE:HD11	1.95	0.48
2:B:410:GLY:HA3	2:B:430:HIS:CD2	2.48	0.48
2:B:521:GLN:O	2:B:559:LYS:NZ	2.40	0.48
6:H:427:LEU:O	6:H:431:CYS:CB	2.61	0.48
10:M:96:ALA:O	10:M:100:ASN:CB	2.61	0.48
5:G:296:THR:O	5:G:300:PHE:HB3	2.13	0.48
6:H:337:VAL:HA	6:H:340:ILE:HD12	1.95	0.48
4:E:878:LEU:HD13	13:R:57:VAL:HG21	1.94	0.48
4:E:967:MET:O	4:E:971:LYS:N	2.44	0.48
7:I:374:TYR:HD1	7:I:423:VAL:HG13	1.79	0.48
1:A:45:ASN:HB3	1:A:53:GLU:HB2	1.95	0.48
2:B:26:TYR:HB2	2:B:53:ILE:HD11	1.96	0.48
6:H:336:LEU:O	6:H:340:ILE:N	2.47	0.48
10:L:49:THR:OG1	10:L:78:ARG:NH1	2.45	0.48
13:R:81:GLU:HA	13:R:84:LEU:HD12	1.95	0.48
15:T:295:MET:O	15:T:299:ARG:HA	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:258:VAL:HG11	2:B:281:THR:HB	1.95	0.48
2:B:259:ASP:O	2:B:261:TYR:N	2.47	0.48
2:B:655:TYR:OH	17:Z:84:UNK:O	2.28	0.48
7:I:222:LEU:HD23	7:I:225:LYS:HD2	1.95	0.48
2:B:830:LEU:HD23	2:B:833:ILE:HD11	1.95	0.48
11:O:170:ALA:O	11:O:174:CYS:N	2.47	0.48
4:E:894:LEU:HD22	4:E:899:VAL:HG21	1.95	0.48
10:M:33:PRO:HA	10:M:36:ILE:HD12	1.96	0.48
15:T:174:LEU:HD12	15:T:178:LEU:HD11	1.96	0.48
5:F:735:VAL:HG22	5:F:766:GLN:HE22	1.79	0.47
11:O:128:PRO:HG3	11:O:153:ARG:HG2	1.95	0.47
6:H:324:ASP:HA	6:H:327:TRP:HD1	1.78	0.47
2:B:275:PRO:O	2:B:278:LYS:HB2	2.13	0.47
6:H:323:VAL:HA	6:H:326:HIS:HB2	1.94	0.47
6:H:332:PHE:O	6:H:335:ARG:HB3	2.14	0.47
2:B:403:VAL:HG22	2:B:528:VAL:HG11	1.96	0.47
2:B:607:MET:HG3	2:B:611:GLU:HB2	1.97	0.47
2:B:769:LYS:HA	2:B:772:LEU:HD12	1.95	0.47
5:F:695:LEU:HB3	5:F:705:GLY:H	1.79	0.47
6:H:370:TRP:O	6:H:374:TYR:CB	2.63	0.47
5:G:542:HIS:CD2	5:G:562:SER:HB2	2.50	0.47
6:H:455:LEU:O	6:H:459:LEU:N	2.43	0.47
10:M:28:ILE:O	10:M:31:TYR:OH	2.21	0.47
1:A:765:ILE:HB	1:A:772:TYR:HB2	1.96	0.47
5:G:287:LYS:H	5:G:290:HIS:CD2	2.30	0.47
1:A:670:ASP:O	8:J:78:LYS:NZ	2.37	0.47
2:B:346:LEU:HD23	2:B:346:LEU:HA	1.76	0.47
2:B:389:ASN:HB3	2:B:659:VAL:HG21	1.97	0.47
2:B:565:LYS:HG2	2:B:579:LEU:HA	1.96	0.47
2:B:738:THR:HG22	2:B:739:ASN:HB2	1.97	0.47
2:B:820:ASP:HB2	2:B:822:LEU:HD23	1.96	0.47
5:G:786:THR:HG22	5:G:788:ARG:HG3	1.97	0.47
10:M:49:THR:OG1	10:M:78:ARG:NH1	2.40	0.47
1:A:110:TYR:HB3	15:T:240:VAL:HG22	1.95	0.47
2:B:37:ASN:HB2	2:B:46:VAL:HG22	1.97	0.47
2:B:89:PRO:HG2	2:B:117:VAL:HG22	1.96	0.47
2:B:529:VAL:HG22	2:B:559:LYS:HB3	1.96	0.47
4:E:879:GLN:HG3	4:E:894:LEU:HD21	1.96	0.47
11:O:119:PHE:HA	11:O:122:GLN:HG2	1.97	0.47
1:A:107:ALA:O	15:T:188:ARG:NE	2.41	0.47
1:A:929:THR:HG22	1:A:954:ALA:HA	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:119:PRO:HA	2:B:123:ASN:HD22	1.80	0.47
2:B:459:LEU:HA	2:B:462:ASN:HD22	1.80	0.47
6:H:276:LEU:HA	6:H:279:LEU:HD12	1.97	0.47
5:F:552:SER:HB3	5:F:557:TYR:HB2	1.97	0.47
14:S:36:LEU:HD11	14:S:57:LEU:HD22	1.96	0.47
5:F:653:LEU:HD12	5:F:663:ARG:HB2	1.97	0.46
4:D:892:THR:H	13:Q:109:SER:HB2	1.80	0.46
5:G:636:HIS:HA	5:G:677:PHE:HD2	1.79	0.46
6:H:292:ASN:HB3	6:H:295:LEU:HB2	1.97	0.46
8:J:21:PRO:HB2	8:J:24:TYR:HD2	1.80	0.46
2:B:880:TYR:HD1	2:B:887:ARG:HH22	1.63	0.46
7:I:387:VAL:O	7:I:390:THR:OG1	2.28	0.46
2:B:473:PHE:HA	2:B:476:LEU:HD12	1.97	0.46
7:I:370:TRP:HA	7:I:373:ARG:HD3	1.97	0.46
1:A:1083:LEU:O	8:J:141:LYS:NZ	2.49	0.46
2:B:961:THR:HB	2:B:968:ARG:HE	1.80	0.46
5:G:590:ASP:HB3	5:G:633:THR:HG22	1.97	0.46
5:G:631:ASN:ND2	5:G:672:ILE:O	2.49	0.46
6:H:381:ALA:HA	6:H:388:ILE:HD11	1.98	0.46
6:H:414:ASN:HA	6:H:417:ARG:HB3	1.97	0.46
5:G:684:LEU:O	5:G:695:LEU:HA	2.16	0.46
2:B:59:ASN:H	2:B:135:TRP:HE1	1.64	0.46
5:F:475:ALA:HB3	5:F:781:VAL:HG11	1.98	0.46
5:G:631:ASN:H	5:G:646:SER:HA	1.81	0.46
5:G:636:HIS:HD2	5:G:638:ASN:H	1.63	0.46
4:D:904:HIS:NE2	12:P:188:ARG:HB3	2.31	0.46
5:F:779:PRO:HA	5:F:791:VAL:HA	1.98	0.46
6:H:383:LEU:HB3	6:H:387:VAL:HG21	1.98	0.46
7:I:263:ILE:HG23	7:I:282:LEU:HD22	1.97	0.46
11:O:126:TYR:O	11:O:153:ARG:NE	2.45	0.46
12:P:141:ILE:HD13	14:S:66:THR:HA	1.98	0.46
2:B:221:VAL:HG11	2:B:237:MET:HB3	1.98	0.46
5:G:636:HIS:HA	5:G:677:PHE:CD2	2.51	0.46
7:I:326:HIS:HA	7:I:329:LEU:HD12	1.98	0.46
7:I:395:ARG:O	7:I:399:GLU:HB2	2.16	0.46
9:K:222:PRO:O	9:K:225:THR:OG1	2.33	0.46
10:M:47:VAL:HA	10:M:50:ILE:HD12	1.97	0.46
11:O:123:LEU:HA	11:O:126:TYR:HD2	1.81	0.46
1:A:673:GLY:O	1:A:774:ARG:NH1	2.49	0.46
2:B:539:ARG:HH11	2:B:592:CYS:HB3	1.80	0.46
11:N:129:THR:HB	11:N:160:GLN:HE22	1.81	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:300:PRO:HB2	2:B:358:PHE:HE2	1.81	0.45
6:H:370:TRP:O	6:H:374:TYR:HB2	2.16	0.45
9:K:219:PHE:HE2	9:K:222:PRO:HA	1.80	0.45
2:B:64:LYS:HD3	2:B:119:PRO:HB3	1.97	0.45
5:G:467:LEU:H	5:G:495:ARG:HH12	1.65	0.45
5:G:470:TYR:CD2	5:G:471:GLN:HG3	2.52	0.45
6:H:402:ARG:O	6:H:405:SER:OG	2.28	0.45
1:A:39:ALA:HB2	1:A:78:ILE:HD11	1.99	0.45
2:B:85:ILE:HD11	2:B:129:LYS:HE3	1.97	0.45
2:B:518:LEU:HD12	2:B:522:TRP:HD1	1.82	0.45
12:P:192:ARG:HA	12:P:195:LYS:HD2	1.98	0.45
2:B:159:LEU:HD21	2:B:189:TRP:CD1	2.51	0.45
5:F:461:ILE:HG12	5:F:792:LEU:HB3	1.99	0.45
7:I:456:GLY:HA2	7:I:457:PRO:HA	1.78	0.45
2:B:908:GLN:HE21	2:B:912:ASN:HD21	1.63	0.45
5:G:783:LEU:HD21	5:G:787:ARG:HG3	1.98	0.45
2:B:26:TYR:N	2:B:56:THR:OG1	2.46	0.45
4:E:912:ASN:HB2	13:R:124:TRP:HH2	1.81	0.45
1:A:706:ARG:NH1	2:B:263:HIS:NE2	2.63	0.45
2:B:343:ARG:HA	2:B:346:LEU:HB2	1.99	0.45
2:B:880:TYR:HA	2:B:887:ARG:CZ	2.47	0.45
2:B:570:GLU:OE2	2:B:576:ASN:ND2	2.47	0.45
2:B:95:HIS:CE1	2:B:97:GLU:HB2	2.52	0.44
4:D:908:GLN:HG2	12:P:192:ARG:HB3	1.99	0.44
6:H:389:LYS:HG3	6:H:438:LEU:HD11	1.98	0.44
11:O:204:LEU:HB3	11:O:208:GLY:HA3	1.99	0.44
5:F:558:LEU:HB3	5:F:570:TRP:HB2	2.00	0.44
9:K:194:MET:HA	9:K:197:THR:HB	2.00	0.44
2:B:572:ASP:HA	2:B:607:MET:HA	1.99	0.44
4:E:910:LEU:HD23	4:E:913:LEU:HD12	2.00	0.44
5:G:668:HIS:HD2	5:G:688:ALA:HB3	1.81	0.44
2:B:848:HIS:CD2	2:B:886:ILE:HD11	2.53	0.44
5:G:251:LEU:HB3	5:G:260:ALA:HB2	1.98	0.44
5:G:254:ASN:HB3	5:G:256:HIS:HD2	1.82	0.44
7:I:55:LEU:HD23	7:I:55:LEU:HA	1.83	0.44
5:F:241:TYR:HD1	5:F:271:GLN:HG3	1.83	0.44
5:F:716:SER:HB2	5:F:769:LEU:HB2	2.00	0.44
5:G:504:UNK:HA	5:G:529:UNK:HA	1.99	0.44
6:H:334:ALA:O	6:H:337:VAL:HB	2.17	0.44
10:M:22:ILE:O	10:M:26:MET:N	2.50	0.44
1:A:851:ASP:OD1	1:A:865:LYS:NZ	2.41	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:65:LEU:O	2:B:126:LEU:HB2	2.17	0.44
5:G:768:LEU:HB3	5:G:769:LEU:H	1.49	0.44
2:B:26:TYR:HA	2:B:55:PRO:HA	2.00	0.44
2:B:31:GLN:HB3	2:B:202:TRP:CD1	2.52	0.44
2:B:201:THR:OG1	2:B:238:LEU:O	2.26	0.44
5:G:638:ASN:HD22	17:Z:43:UNK:HA	1.83	0.44
7:I:68:THR:HG23	10:M:35:VAL:HG22	2.00	0.44
11:N:119:PHE:HA	11:N:122:GLN:HG2	1.99	0.44
2:B:95:HIS:HE1	2:B:97:GLU:HB2	1.82	0.44
2:B:372:GLY:HA2	2:B:453:ALA:HB1	2.00	0.44
2:B:626:LEU:HD23	2:B:626:LEU:HA	1.84	0.44
5:G:236:LEU:HD22	5:G:239:LEU:HD11	2.00	0.44
5:G:542:HIS:CE1	5:G:568:ARG:HD2	2.53	0.44
7:I:457:PRO:O	7:I:461:SER:N	2.43	0.44
1:A:623:TYR:HE2	1:A:766:ARG:HE	1.66	0.43
1:A:926:GLU:OE1	8:J:149:ARG:NH1	2.39	0.43
2:B:51:LEU:O	2:B:145:LYS:HA	2.18	0.43
2:B:332:SER:H	2:B:335:ILE:HD12	1.83	0.43
2:B:597:ARG:NH2	2:B:622:ASP:OD1	2.51	0.43
5:F:636:HIS:HA	5:F:677:PHE:HD2	1.83	0.43
5:F:764:ASN:HB2	5:F:782:HIS:HB3	1.99	0.43
6:H:333:ALA:HA	6:H:336:LEU:HD12	1.98	0.43
7:I:417:ARG:O	7:I:421:ASP:HB2	2.18	0.43
13:Q:89:ASP:HA	13:Q:92:ILE:HD12	2.00	0.43
2:B:214:ALA:HB1	2:B:249:LEU:HD11	1.98	0.43
2:B:628:ILE:H	2:B:644:GLN:NE2	2.16	0.43
5:F:615:ASP:HB3	10:L:113:UNK:HA	1.99	0.43
5:G:479:THR:O	5:G:555:ARG:NH2	2.48	0.43
5:G:542:HIS:HD2	5:G:562:SER:HB2	1.83	0.43
2:B:862:GLN:NE2	2:B:870:ASP:H	2.16	0.43
2:B:891:LEU:HA	2:B:894:VAL:HG12	1.99	0.43
3:C:110:TYR:HA	3:C:113:ASN:HD22	1.82	0.43
5:F:605:HIS:ND1	5:F:629:ASP:OD1	2.51	0.43
5:G:571:SER:HB2	5:G:575:PHE:N	2.33	0.43
5:G:648:ASP:N	5:G:648:ASP:OD1	2.50	0.43
8:J:65:SER:HA	8:J:96:VAL:O	2.18	0.43
2:B:36:ASN:OD1	2:B:207:THR:OG1	2.36	0.43
2:B:549:LYS:HG2	2:B:587:LYS:HG2	2.01	0.43
2:B:914:ILE:HD13	2:B:927:LEU:HD21	2.00	0.43
5:G:464:TYR:OH	9:K:150:UNK:O	2.25	0.43
8:J:77:LEU:HG	8:J:87:LYS:HA	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:835:ARG:NH2	9:K:184:ARG:HE	2.12	0.43
5:G:590:ASP:OD2	5:G:633:THR:N	2.40	0.43
5:G:732:ASP:N	5:G:732:ASP:OD1	2.49	0.43
7:I:22:VAL:O	7:I:25:SER:OG	2.28	0.43
4:E:892:THR:HG22	4:E:893:GLU:HG3	2.00	0.43
5:F:768:LEU:HB3	5:F:769:LEU:H	1.65	0.43
6:H:403:ILE:HG23	6:H:420:ALA:HB1	2.01	0.43
7:I:358:THR:O	7:I:362:SER:OG	2.30	0.43
2:B:308:PHE:HA	2:B:325:PHE:O	2.18	0.43
2:B:503:PHE:CE2	2:B:507:ILE:HD11	2.54	0.43
7:I:313:VAL:HG12	7:I:314:SER:HB3	2.00	0.43
12:P:187:MET:O	12:P:191:VAL:HG23	2.19	0.43
17:Z:213:UNK:O	17:Z:216:UNK:CB	2.67	0.43
1:A:874:GLU:HA	1:A:877:ARG:HD2	2.01	0.43
2:B:567:THR:HG23	2:B:577:HIS:HE1	1.83	0.43
2:B:611:GLU:OE2	2:B:657:ARG:NE	2.51	0.43
2:B:957:MET:HG2	2:B:971:ALA:HB1	2.01	0.43
2:B:975:TYR:O	2:B:980:GLY:HA2	2.19	0.43
5:G:566:THR:HA	5:G:581:TYR:O	2.18	0.43
1:A:650:ARG:HH11	8:J:80:ILE:HD11	1.84	0.43
2:B:180:CYS:HB3	2:B:313:TYR:HB2	2.01	0.43
2:B:443:TRP:CG	2:B:924:HIS:HE1	2.37	0.43
2:B:699:CYS:SG	2:B:753:MET:HG2	2.59	0.43
15:T:262:CYS:O	15:T:309:LYS:HA	2.18	0.43
2:B:516:GLN:HA	2:B:519:ILE:HD12	1.99	0.42
5:G:594:SER:HB2	5:G:597:GLY:N	2.32	0.42
6:H:411:VAL:HA	6:H:417:ARG:HH21	1.84	0.42
8:J:39:LEU:HA	8:J:42:ARG:HB2	2.00	0.42
2:B:706:ALA:HB3	2:B:760:LEU:HD22	2.01	0.42
6:H:43:VAL:HG21	10:L:47:VAL:HG22	2.01	0.42
6:H:385:HIS:HE1	6:H:437:LYS:HD2	1.84	0.42
6:H:418:ILE:O	6:H:422:HIS:ND1	2.38	0.42
2:B:30:HIS:ND1	2:B:201:THR:HG23	2.35	0.42
2:B:75:VAL:HG13	2:B:148:ILE:HG12	2.00	0.42
2:B:575:PHE:HB3	2:B:577:HIS:CE1	2.55	0.42
9:K:51:GLU:O	17:Z:311:UNK:N	2.51	0.42
2:B:363:SER:H	2:B:366:ASP:HB2	1.85	0.42
5:G:605:HIS:ND1	5:G:629:ASP:OD1	2.52	0.42
15:T:171:THR:HG22	15:T:220:VAL:HG22	2.00	0.42
5:F:564:ASP:HB2	5:F:566:THR:HG22	2.01	0.42
5:G:241:TYR:HD1	5:G:271:GLN:HG3	1.83	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:467:LEU:O	5:G:787:ARG:NE	2.41	0.42
6:H:23:ALA:HB1	6:H:28:ILE:HD12	2.02	0.42
6:H:308:VAL:O	6:H:311:CYS:HB2	2.19	0.42
6:H:320:ARG:O	6:H:323:VAL:HB	2.18	0.42
7:I:309:MET:HA	7:I:312:ILE:HD12	2.02	0.42
7:I:400:GLY:HA2	7:I:403:ILE:HD12	2.00	0.42
2:B:688:GLU:H	2:B:695:ARG:NH1	2.18	0.42
2:B:749:LEU:HD12	2:B:749:LEU:HA	1.87	0.42
5:G:730:SER:OG	5:G:734:THR:OG1	2.34	0.42
9:K:79:TYR:HA	9:K:82:HIS:HD2	1.85	0.42
17:Z:214:UNK:O	17:Z:218:UNK:N	2.52	0.42
2:B:87:ASN:HB3	2:B:89:PRO:HD3	2.02	0.42
2:B:261:TYR:HB2	2:B:285:HIS:CG	2.55	0.42
5:G:695:LEU:O	5:G:704:VAL:N	2.53	0.42
6:H:446:ASP:O	6:H:450:ALA:N	2.50	0.42
7:I:276:LEU:HB3	7:I:326:HIS:CE1	2.55	0.42
11:O:163:ILE:HD13	11:O:166:ILE:HD12	2.01	0.42
13:R:68:ARG:NH1	13:R:72:PRO:O	2.53	0.42
2:B:238:LEU:HD11	2:B:240:ILE:HB	2.01	0.42
2:B:571:LEU:HD23	2:B:626:LEU:HG	2.02	0.42
2:B:772:LEU:O	2:B:776:LEU:HG	2.20	0.42
4:D:911:GLN:HA	4:D:914:VAL:HB	2.01	0.42
5:F:251:LEU:HB3	5:F:260:ALA:HB2	2.02	0.42
5:F:783:LEU:HD23	5:F:783:LEU:HA	1.84	0.42
5:G:623:PHE:HB3	5:G:654:TRP:CE2	2.55	0.42
5:G:730:SER:OG	5:G:732:ASP:OD1	2.37	0.42
2:B:51:LEU:HD21	2:B:65:LEU:HD21	2.01	0.42
2:B:867:VAL:HA	9:K:204:PHE:HE1	1.85	0.42
4:E:922:GLN:HA	4:E:925:ASN:HD22	1.85	0.42
6:H:369:PRO:O	6:H:372:THR:OG1	2.30	0.42
7:I:252:LEU:O	7:I:254:GLN:N	2.53	0.42
1:A:680:LEU:HD23	1:A:776:LEU:HD22	2.01	0.41
1:A:749:ARG:HB3	1:A:786:CYS:HB2	2.02	0.41
2:B:653:LEU:HA	2:B:653:LEU:HD23	1.83	0.41
13:R:65:ASP:O	13:R:69:GLU:CB	2.68	0.41
3:C:48:LEU:HD23	3:C:48:LEU:HA	1.94	0.41
7:I:53:ASP:HA	7:I:56:LYS:HE3	2.01	0.41
7:I:403:ILE:O	7:I:407:LEU:N	2.37	0.41
12:P:168:GLU:HB3	12:P:190:ALA:HB1	2.02	0.41
13:Q:120:LEU:HB3	13:Q:126:MET:HG2	2.02	0.41
2:B:838:ASN:HD22	9:K:191:THR:HG23	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:366:GLU:HG2	6:H:367:LYS:H	1.84	0.41
7:I:224:TYR:HE1	7:I:259:PHE:HD1	1.67	0.41
7:I:320:ARG:HD3	7:I:415:ILE:HD13	2.02	0.41
9:K:51:GLU:N	11:O:193:TYR:O	2.53	0.41
5:G:584:HIS:HB3	5:G:586:TYR:HB2	2.03	0.41
8:J:17:ILE:O	8:J:94:MET:HA	2.20	0.41
12:P:181:PRO:HB3	14:S:49:PRO:HA	2.01	0.41
2:B:26:TYR:HB3	2:B:60:LEU:HD21	2.02	0.41
2:B:49:VAL:HG12	2:B:148:ILE:HB	2.01	0.41
2:B:926:ILE:O	2:B:930:LEU:HB2	2.20	0.41
5:G:286:THR:H	5:G:290:HIS:CD2	2.39	0.41
7:I:274:ASN:HD21	7:I:317:LEU:H	1.67	0.41
7:I:302:HIS:CD2	17:Z:213:UNK:HA	2.55	0.41
9:K:227:LEU:HA	9:K:227:LEU:HD12	1.84	0.41
13:Q:127:TRP:CZ3	14:S:67:GLU:HB3	2.55	0.41
2:B:178:PHE:HA	2:B:249:LEU:O	2.21	0.41
5:G:761:LEU:HD11	5:G:766:GLN:HE21	1.85	0.41
15:T:210:THR:O	15:T:222:THR:OG1	2.35	0.41
2:B:816:VAL:HB	2:B:817:ARG:HG3	2.02	0.41
2:B:882:HIS:CE1	9:K:216:ALA:HB1	2.56	0.41
5:F:678:SER:HG	5:F:682:ARG:H	1.66	0.41
6:H:286:VAL:HA	6:H:289:LEU:HD12	2.03	0.41
9:K:110:TYR:CD1	9:K:113:ARG:HD2	2.56	0.41
10:M:19:MET:HA	10:M:22:ILE:HD12	2.02	0.41
11:N:149:PRO:HG2	11:N:153:ARG:HH12	1.86	0.41
12:P:200:ILE:HB	13:Q:127:TRP:NE1	2.35	0.41
2:B:465:SER:O	2:B:469:MET:HG3	2.21	0.41
2:B:604:ILE:HG12	2:B:607:MET:HE3	2.02	0.41
2:B:619:MET:HG3	2:B:647:PHE:CE2	2.56	0.41
5:F:730:SER:OG	5:F:734:THR:OG1	2.37	0.41
5:G:477:ASP:OD1	5:G:477:ASP:N	2.51	0.41
5:G:675:LEU:HG	5:G:686:THR:HG22	2.03	0.41
6:H:219:GLU:HA	6:H:222:LEU:HD12	2.03	0.41
6:H:304:LEU:O	6:H:308:VAL:N	2.41	0.41
7:I:411:VAL:O	7:I:417:ARG:NH2	2.53	0.41
12:P:138:ILE:HD11	12:P:154:MET:HG2	2.03	0.41
16:Y:310:UNK:O	16:Y:314:UNK:N	2.54	0.41
2:B:31:GLN:HE21	2:B:49:VAL:HG21	1.86	0.41
2:B:432:HIS:NE2	2:B:441:LEU:HA	2.35	0.41
2:B:691:PHE:HE2	2:B:693:ARG:HB2	1.85	0.41
5:F:479:THR:O	5:F:555:ARG:NH2	2.53	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:473:LEU:HD21	5:G:489:PHE:HE1	1.86	0.41
5:G:763:GLU:O	5:G:784:HIS:HB3	2.21	0.41
7:I:383:LEU:HB2	7:I:387:VAL:HG11	2.01	0.41
2:B:131:PRO:O	2:B:135:TRP:N	2.50	0.40
2:B:719:MET:HA	2:B:722:LEU:HG	2.02	0.40
7:I:218:VAL:HA	7:I:221:GLN:HG2	2.03	0.40
7:I:241:GLU:OE2	9:K:135:UNK:N	2.54	0.40
7:I:270:ASN:O	7:I:274:ASN:N	2.49	0.40
2:B:898:THR:HG21	2:B:907:LEU:HB2	2.03	0.40
3:C:97:PHE:HB3	3:C:102:VAL:HB	2.04	0.40
5:F:558:LEU:HD23	5:F:572:LEU:HD21	2.03	0.40
6:H:386:ASP:HA	6:H:389:LYS:HB3	2.02	0.40
17:Z:215:UNK:O	17:Z:219:UNK:N	2.55	0.40
2:B:546:LEU:HD22	2:B:625:LEU:HD21	2.02	0.40
2:B:710:VAL:HG22	2:B:762:ASP:HA	2.04	0.40
2:B:761:ARG:HB3	2:B:766:LEU:HB3	2.03	0.40
7:I:252:LEU:HD12	7:I:252:LEU:HA	1.90	0.40
7:I:380:LEU:HD13	7:I:391:LEU:HD13	2.02	0.40
7:I:383:LEU:HB3	7:I:387:VAL:HG21	2.02	0.40
5:G:305:PHE:HD2	5:G:337:LEU:HD23	1.85	0.40
5:G:572:LEU:HD13	5:G:575:PHE:HE1	1.87	0.40
5:G:783:LEU:HA	5:G:783:LEU:HD23	1.77	0.40
7:I:280:ILE:HB	7:I:329:LEU:HD21	2.04	0.40
2:B:341:LEU:HA	2:B:341:LEU:HD23	1.90	0.40
2:B:399:LEU:HD23	2:B:399:LEU:HA	1.83	0.40
5:G:248:TYR:HE2	5:G:285:LEU:HD12	1.85	0.40
5:G:474:THR:O	5:G:486:ALA:CB	2.65	0.40
6:H:309:MET:HA	6:H:312:ILE:HD12	2.04	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	462/1872 (25%)	454 (98%)	7 (2%)	1 (0%)	47 81
2	B	966/1199 (81%)	781 (81%)	183 (19%)	2 (0%)	47 81
3	C	91/929 (10%)	89 (98%)	2 (2%)	0	100 100
4	D	100/1085 (9%)	93 (93%)	7 (7%)	0	100 100
4	E	100/1085 (9%)	94 (94%)	6 (6%)	0	100 100
5	F	429/800 (54%)	382 (89%)	47 (11%)	0	100 100
5	G	429/800 (54%)	352 (82%)	77 (18%)	0	100 100
6	H	325/677 (48%)	293 (90%)	31 (10%)	1 (0%)	41 77
7	I	326/677 (48%)	292 (90%)	32 (10%)	2 (1%)	25 66
8	J	119/349 (34%)	117 (98%)	2 (2%)	0	100 100
9	K	149/310 (48%)	133 (89%)	15 (10%)	1 (1%)	22 63
10	L	96/264 (36%)	93 (97%)	3 (3%)	0	100 100
10	M	96/264 (36%)	89 (93%)	7 (7%)	0	100 100
11	N	78/218 (36%)	75 (96%)	3 (4%)	0	100 100
11	O	78/218 (36%)	74 (95%)	4 (5%)	0	100 100
12	P	87/211 (41%)	86 (99%)	1 (1%)	0	100 100
13	Q	72/161 (45%)	71 (99%)	1 (1%)	0	100 100
13	R	72/161 (45%)	68 (94%)	4 (6%)	0	100 100
14	S	43/124 (35%)	43 (100%)	0	0	100 100
15	T	178/339 (52%)	177 (99%)	1 (1%)	0	100 100
All	All	4296/11743 (37%)	3856 (90%)	433 (10%)	7 (0%)	50 81

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	950	VAL
7	I	256	LEU
6	H	321	PRO
7	I	257	PRO
9	K	218	PRO
2	B	336	ILE
2	B	844	PRO

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	407/1665 (24%)	403 (99%)	4 (1%)	76 86
2	B	879/1083 (81%)	872 (99%)	7 (1%)	81 89
3	C	83/833 (10%)	83 (100%)	0	100 100
4	D	52/815 (6%)	51 (98%)	1 (2%)	57 75
4	E	52/815 (6%)	52 (100%)	0	100 100
5	F	367/619 (59%)	365 (100%)	2 (0%)	88 93
5	G	367/619 (59%)	362 (99%)	5 (1%)	67 80
6	H	260/574 (45%)	259 (100%)	1 (0%)	91 94
7	I	252/564 (45%)	251 (100%)	1 (0%)	91 94
8	J	113/322 (35%)	113 (100%)	0	100 100
9	K	132/223 (59%)	132 (100%)	0	100 100
10	L	61/229 (27%)	60 (98%)	1 (2%)	62 79
10	M	61/229 (27%)	60 (98%)	1 (2%)	62 79
11	N	71/154 (46%)	71 (100%)	0	100 100
11	O	71/154 (46%)	71 (100%)	0	100 100
12	P	78/182 (43%)	78 (100%)	0	100 100
13	Q	70/141 (50%)	69 (99%)	1 (1%)	67 80
13	R	70/141 (50%)	69 (99%)	1 (1%)	67 80
14	S	42/106 (40%)	40 (95%)	2 (5%)	25 51
15	T	155/293 (53%)	153 (99%)	2 (1%)	69 81
All	All	3643/9761 (37%)	3614 (99%)	29 (1%)	82 89

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	LEU
1	A	766	ARG
1	A	798	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	922	LYS
2	B	74	ARG
2	B	180	CYS
2	B	301	TYR
2	B	343	ARG
2	B	361	ARG
2	B	378	TYR
2	B	961	THR
4	D	908	GLN
5	F	558	LEU
5	F	607	ARG
5	G	558	LEU
5	G	559	LEU
5	G	589	TRP
5	G	607	ARG
5	G	637	PRO
6	H	347	THR
7	I	347	THR
10	L	73	LEU
10	M	73	LEU
13	Q	125	ASN
13	R	125	ASN
14	S	48	ASN
14	S	57	LEU
15	T	193	ASN
15	T	222	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (67) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1073	GLN
1	A	1074	ASN
2	B	36	ASN
2	B	108	ASN
2	B	123	ASN
2	B	137	HIS
2	B	147	HIS
2	B	160	HIS
2	B	430	HIS
2	B	437	HIS
2	B	454	HIS
2	B	462	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	486	GLN
2	B	489	GLN
2	B	509	ASN
2	B	538	ASN
2	B	542	ASN
2	B	550	GLN
2	B	644	GLN
2	B	740	ASN
2	B	838	ASN
2	B	864	ASN
2	B	908	GLN
2	B	912	ASN
2	B	924	HIS
3	C	66	GLN
3	C	113	ASN
4	D	925	ASN
4	E	925	ASN
5	F	232	HIS
5	F	271	GLN
5	F	290	HIS
5	F	327	ASN
5	F	336	HIS
5	F	626	HIS
5	F	710	HIS
5	F	766	GLN
5	G	232	HIS
5	G	246	HIS
5	G	256	HIS
5	G	290	HIS
5	G	327	ASN
5	G	336	HIS
5	G	542	HIS
5	G	636	HIS
5	G	638	ASN
5	G	784	HIS
6	H	274	ASN
6	H	343	HIS
6	H	385	HIS
7	I	220	GLN
7	I	244	GLN
7	I	326	HIS
7	I	385	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	I	397	GLN
8	J	48	HIS
9	K	82	HIS
11	N	122	GLN
11	N	160	GLN
11	O	122	GLN
11	O	160	GLN
11	O	168	ASN
13	Q	125	ASN
13	R	125	ASN
14	S	48	ASN
15	T	193	ASN
15	T	327	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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
17	Z	8
16	Y	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Z	95:UNK	C	119:UNK	N	129.81
1	Z	52:UNK	C	81:UNK	N	116.40
1	Z	143:UNK	C	195:UNK	N	95.92
1	Z	223:UNK	C	309:UNK	N	54.56
1	Y	143:UNK	C	309:UNK	N	54.12
1	Y	52:UNK	C	119:UNK	N	47.22
1	Z	386:UNK	C	401:UNK	N	34.09
1	Z	328:UNK	C	358:UNK	N	33.32
1	Z	428:UNK	C	551:UNK	N	24.82
1	Z	571:UNK	C	573:UNK	N	4.23

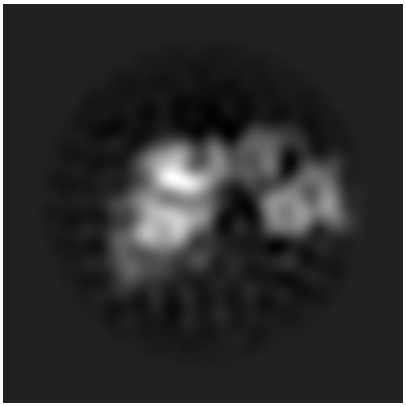
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-9305. These allow visual inspection of the internal detail of the map and identification of artifacts.

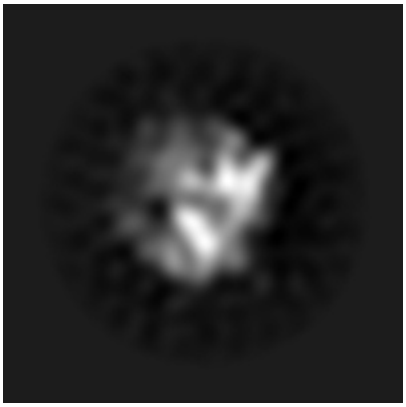
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

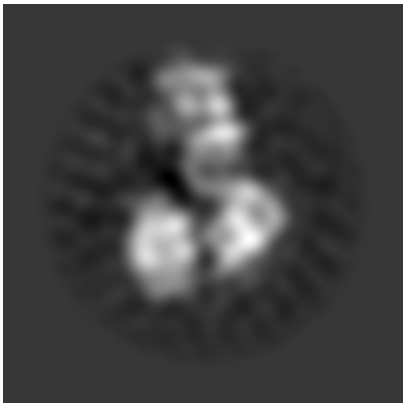
6.1.1 Primary map



X



Y



Z

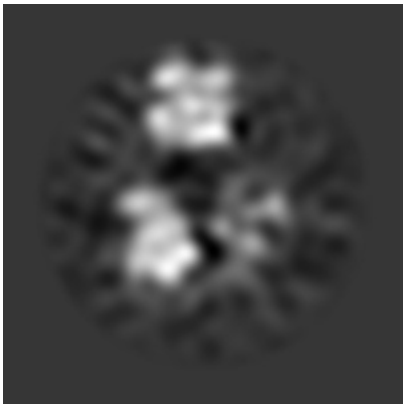
The images above show the map projected in three orthogonal directions.

6.2 Central slices

6.2.1 Primary map

X Index: 72

Y Index: 72

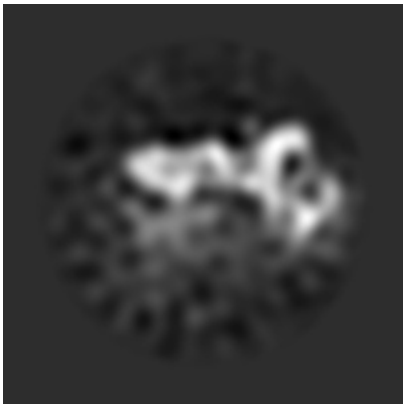


Z Index: 72

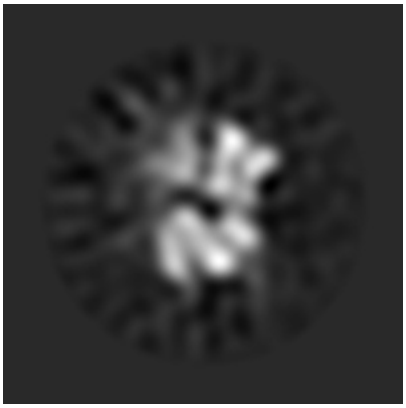
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 79



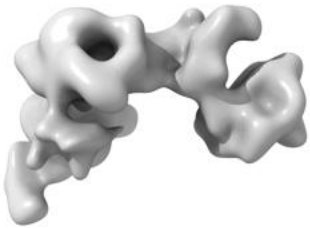
Y Index: 62

Z Index: 80

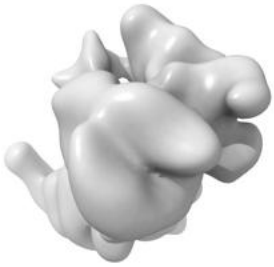
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

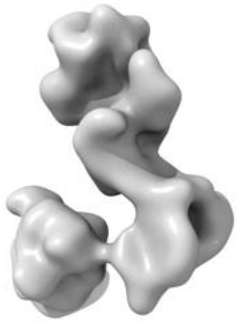
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.026. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

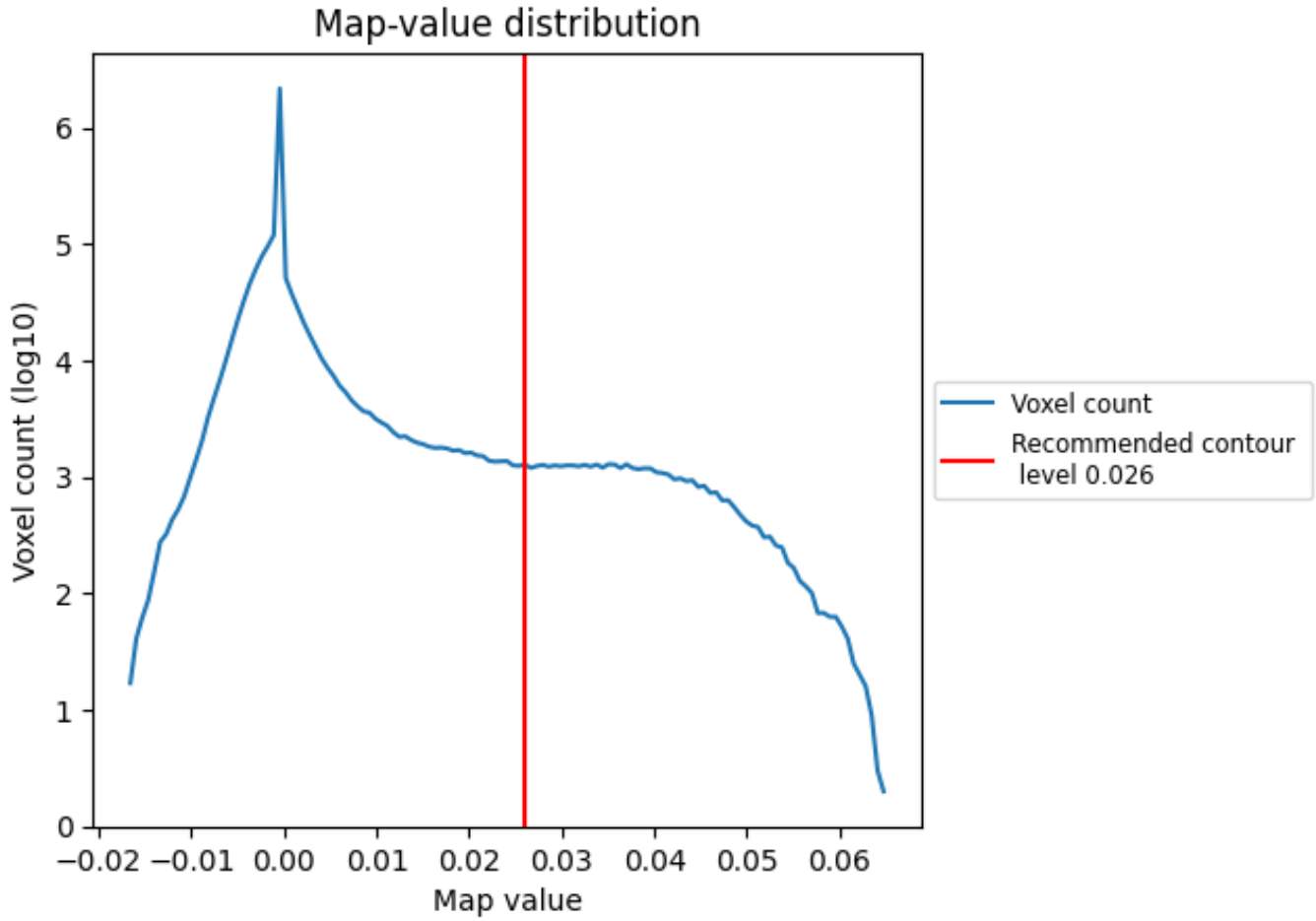
6.5 Mask visualisation (i)

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

7 Map analysis

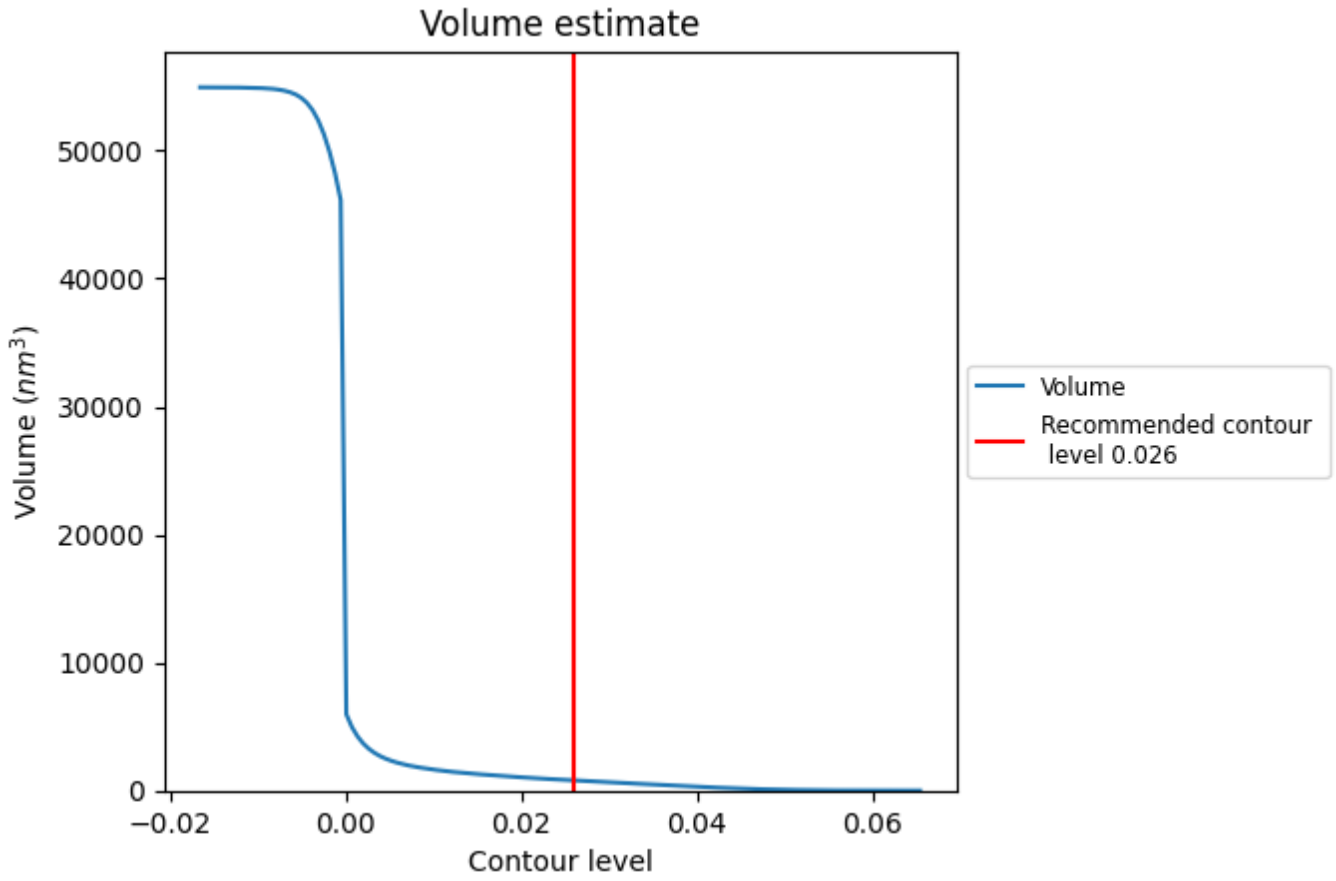
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

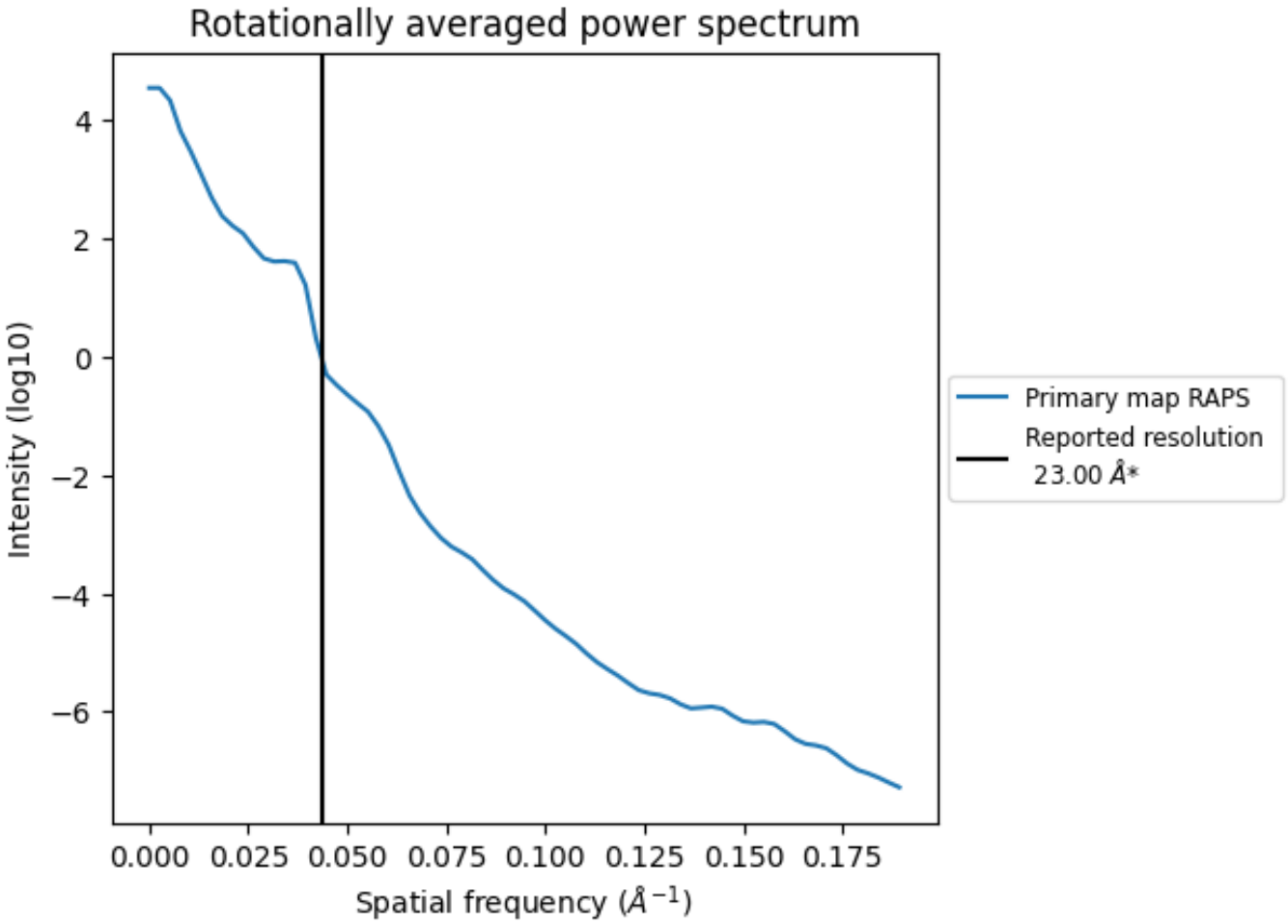
7.2 Volume estimate



The volume at the recommended contour level is 794 nm^3; this corresponds to an approximate mass of 717 kDa.

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

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.043 Å^{-1}

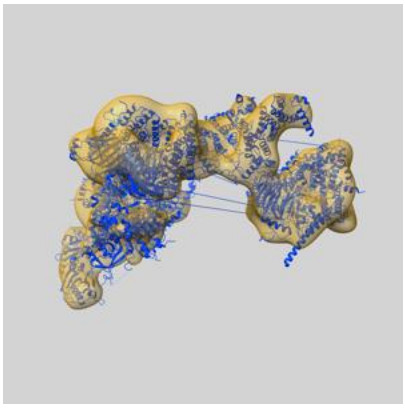
8 Fourier-Shell correlation

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

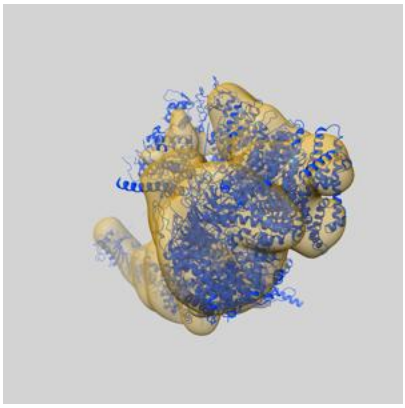
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-9305 and PDB model 6MZL. Per-residue inclusion information can be found in section 3 on page 7.

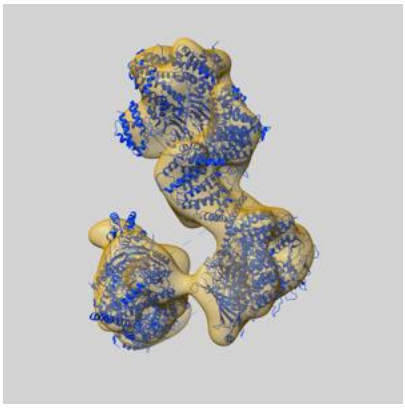
9.1 Map-model overlay



X



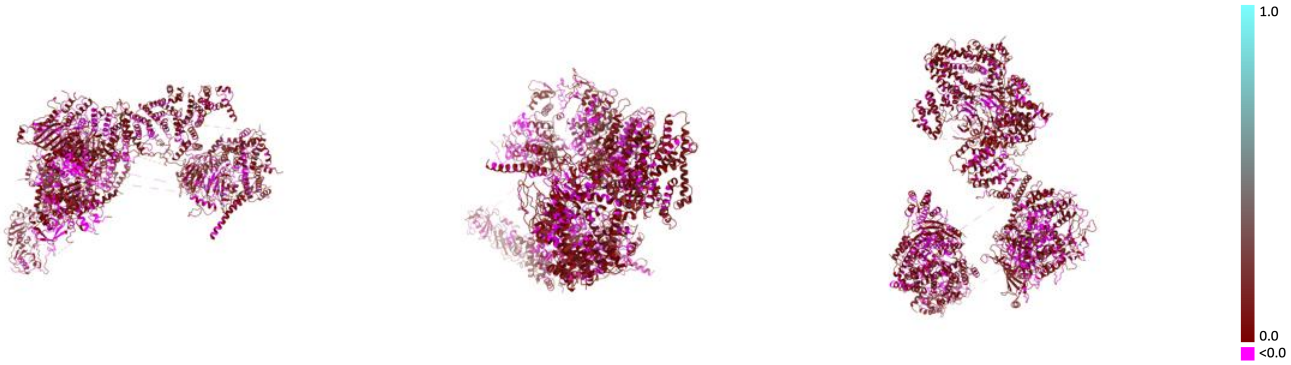
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.026 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

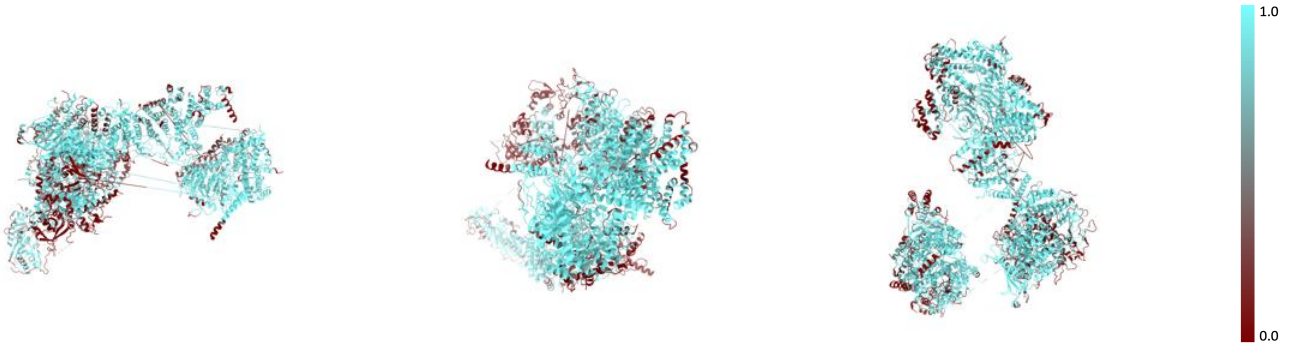
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

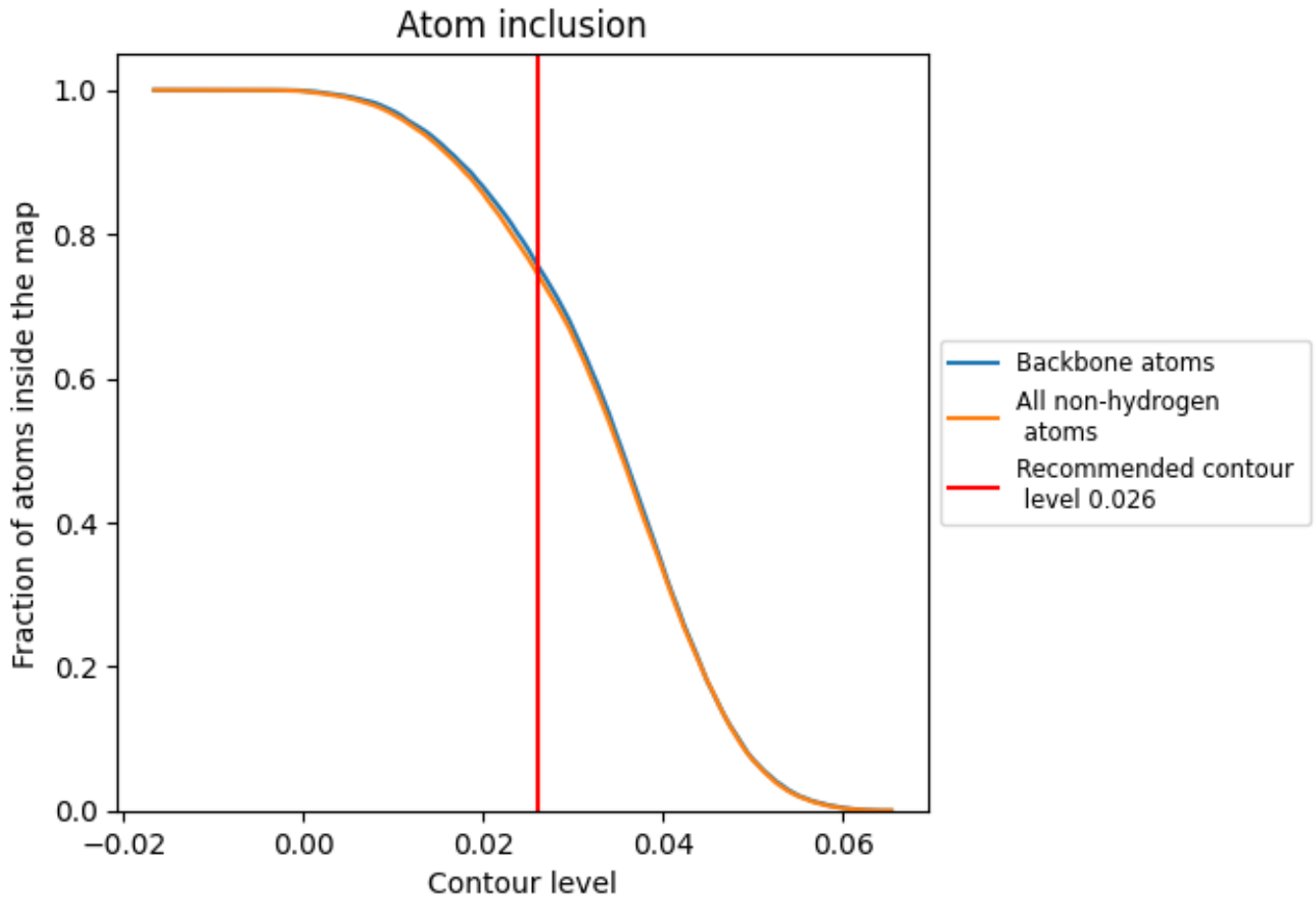
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.026).

9.4 Atom inclusion (i)



At the recommended contour level, 76% of all backbone atoms, 75% 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 (0.026) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7460	0.0510
A	0.4127	0.0390
B	0.7835	0.0480
C	0.9420	0.0820
D	0.6922	0.0730
E	0.7923	0.0700
F	0.7465	0.0340
G	0.8162	0.0530
H	0.8452	0.0500
I	0.8021	0.0650
J	0.2058	0.0100
K	0.9386	0.0760
L	0.9362	0.0420
M	0.7171	0.0580
N	0.8628	0.0590
O	0.9432	0.0750
P	0.6942	0.0320
Q	0.8170	0.0450
R	0.8403	0.0710
S	0.9668	0.0990
T	0.7176	0.0690
Y	0.4792	0.0320
Z	0.8571	0.0550