Full wwPDB EM Validation Report

Jun 24, 2024 – 08:47 PM EDT

PDB ID	:	8T1L
EMDB ID	:	EMD-40971
Title	:	Atomic model of the mammalian mouse Mediator complex with CKM module
Authors	:	Zhao, H.; Asturias, F.
Deposited on	:	2023-06-02
Resolution	:	4.83 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:

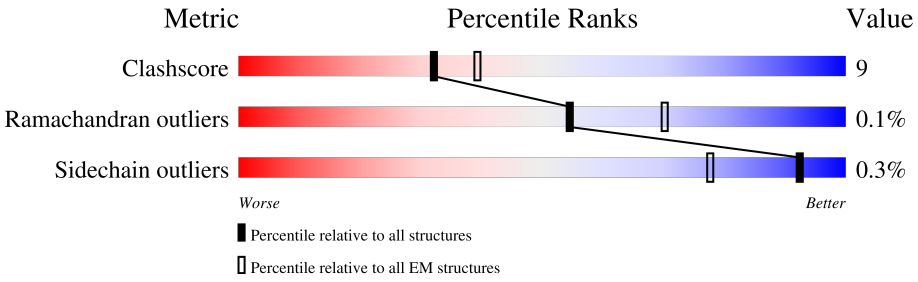
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.83 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.



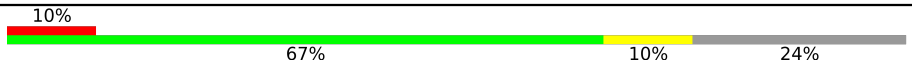
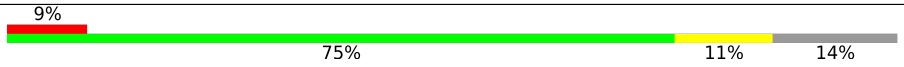
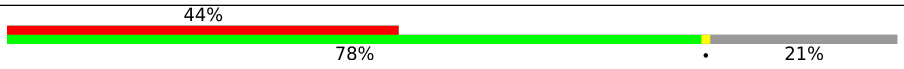
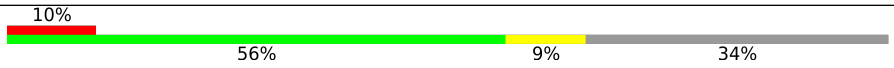
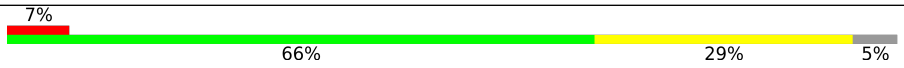
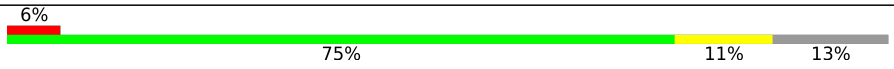
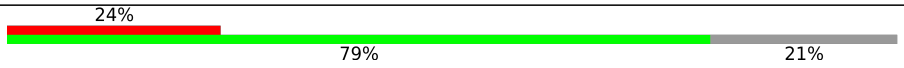
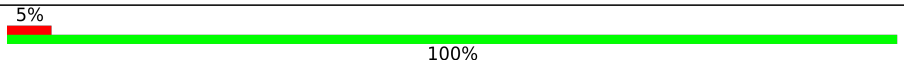
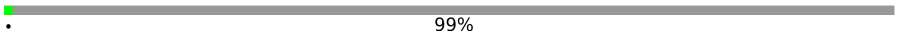
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	E	268	35% 66% · 33%
2	A	1575	· 29% · 70%
3	B	270	16% 59% 41%
4	C	246	43% 67% · 28%
5	D	233	41% 69% 31%
6	F	142	11% 51% 49%
7	G	135	87% 90% 10%
8	H	117	14% 79% 8% · 10%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	I	1459	
10	J	789	
11	K	828	
12	L	649	
13	M	208	
14	O	212	
15	P	144	
16	Q	200	
17	R	1367	
18	S	987	
19	T	745	
20	V	311	
21	W	178	
22	X	199	
23	Y	178	
24	Z	131	
25	a	20	
26	9	2171	

2 Entry composition

There are 26 unique types of molecules in this entry. The entry contains 49460 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 Mediator of RNA polymerase II transcription subunit 8.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	E	179	Total 888	C 530	N 179	O 179	0	0

- Molecule 2 is a protein called Mediator of RNA polymerase II transcription subunit 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	A	472	Total 2339	C 1395	N 472	O 472	0	0

- Molecule 3 is a protein called Mediator of RNA polymerase II transcription subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	B	158	Total 784	C 468	N 158	O 158	0	0

- Molecule 4 is a protein called Mediator of RNA polymerase II transcription subunit 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	C	176	Total 963	C 584	N 193	O 186	0	0

- Molecule 5 is a protein called Mediator of RNA polymerase II transcription subunit 7.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	D	161	Total 801	C 479	N 161	O 161	0	0

- Molecule 6 is a protein called Mediator of RNA polymerase II transcription subunit 9.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	F	73	Total 363	C 217	N 73	O 73	0	0

- Molecule 7 is a protein called Mediator of RNA polymerase II transcription subunit 10.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	G	122	Total	C	N	O	0	0
			605	361	122	122		

- Molecule 8 is a protein called Mediator of RNA polymerase II transcription subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	105	Total	C	N	O	S	0	0
			582	352	117	112	1		

- Molecule 9 is a protein called Mediator of RNA polymerase II transcription subunit 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	1111	Total	C	N	O	S	0	0
			6892	4356	1276	1240	20		

- Molecule 10 is a protein called Mediator of RNA polymerase II transcription subunit 15.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	167	Total	C	N	O	S	0	0
			1171	748	217	200	6		

- Molecule 11 is a protein called Mediator of RNA polymerase II transcription subunit 16.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	732	Total	C	N	O	S	0	0
			5051	3258	906	863	24		

- Molecule 12 is a protein called Mediator of RNA polymerase II transcription subunit 17.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	559	Total	C	N	O	S	0	0
			3424	2155	645	621	3		

- Molecule 13 is a protein called Mediator of RNA polymerase II transcription subunit 18.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	180	Total	C	N	O	S	0	0
			1140	725	217	197	1		

- Molecule 14 is a protein called Mediator of RNA polymerase II transcription subunit 20.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	174	Total	C	N	O	S	0	0
			1013	640	177	192	4		

- Molecule 15 is a protein called Mediator of RNA polymerase II transcription subunit 21.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	P	114	Total	C	N	O	0	0
			568	340	114	114		

- Molecule 16 is a protein called Mediator of RNA polymerase II transcription subunit 22.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	Q	131	Total	C	N	O	0	0
			754	463	145	146		

- Molecule 17 is a protein called Mediator of RNA polymerase II transcription subunit 23.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	1299	Total	C	N	O	S	0	0
			9771	6312	1684	1722	53		

- Molecule 18 is a protein called Mediator of RNA polymerase II transcription subunit 24.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	913	Total	C	N	O	S	0	0
			5934	3785	1074	1048	27		

- Molecule 19 is a protein called Mediator of RNA polymerase II transcription subunit 25.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	197	Total	C	N	O	S	0	0
			1287	814	226	241	6		

- Molecule 20 is a protein called Mediator of RNA polymerase II transcription subunit 27.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	V	278	Total	C	N	O	S	0	0
			1726	1097	313	313	3		

- Molecule 21 is a protein called Mediator of RNA polymerase II transcription subunit 28.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	W	119	Total	C	N	O	S	0	0
			778	489	146	141	2		

- Molecule 22 is a protein called Mediator of RNA polymerase II transcription subunit 29.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	X	127	Total	C	N	O	S	0	0
			859	540	154	162	3		

- Molecule 23 is a protein called Mediator of RNA polymerase II transcription subunit 30.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Y	154	Total	C	N	O	S	0	0
			994	616	198	177	3		

- Molecule 24 is a protein called Mediator of RNA polymerase II transcription subunit 31.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	Z	103	Total	C	N	O	0	0
			513	307	103	103		

- Molecule 25 is a protein called Unknown.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	a	20	Total	C	N	O	0	0
			100	60	20	20		

- Molecule 26 is a protein called Mediator of RNA polymerase II transcription subunit 13.

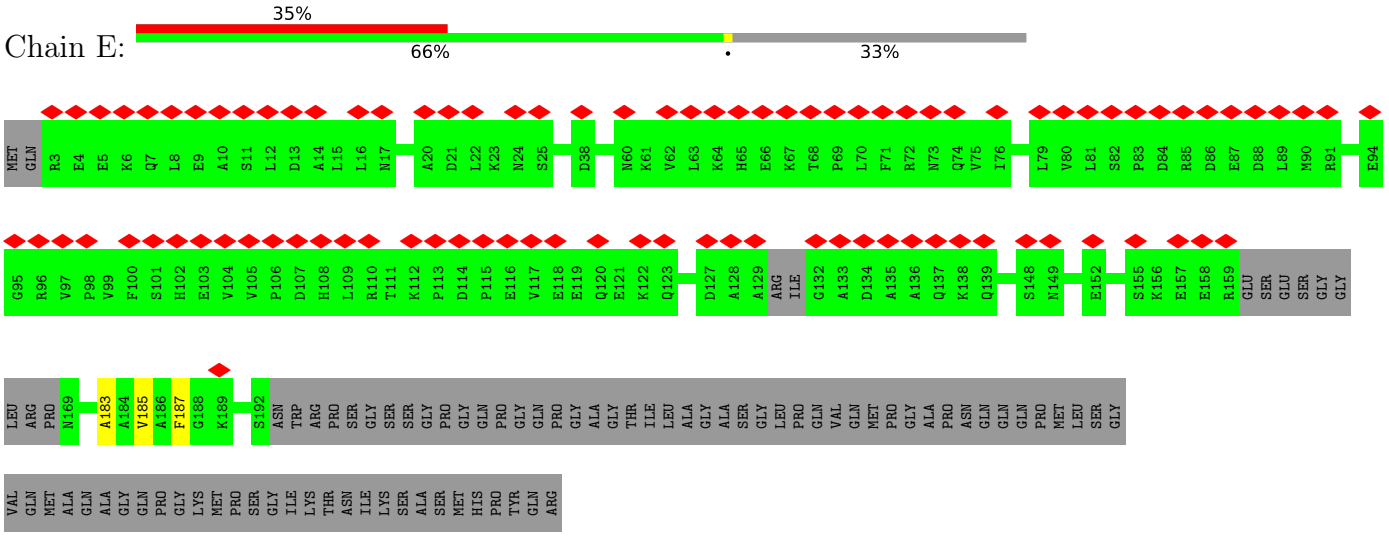
Mol	Chain	Residues	Atoms				AltConf	Trace
26	9	19	Total	C	N	O	0	0
			160	107	26	27		

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.

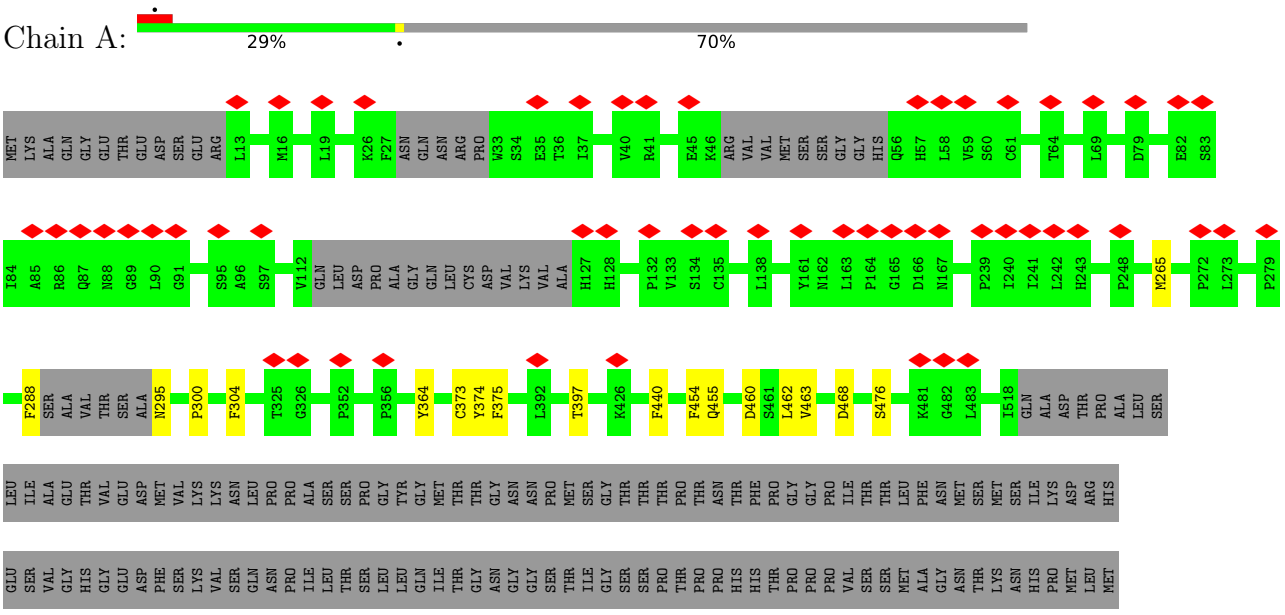
• Molecule 1: Mediator of RNA polymerase II transcription subunit 8

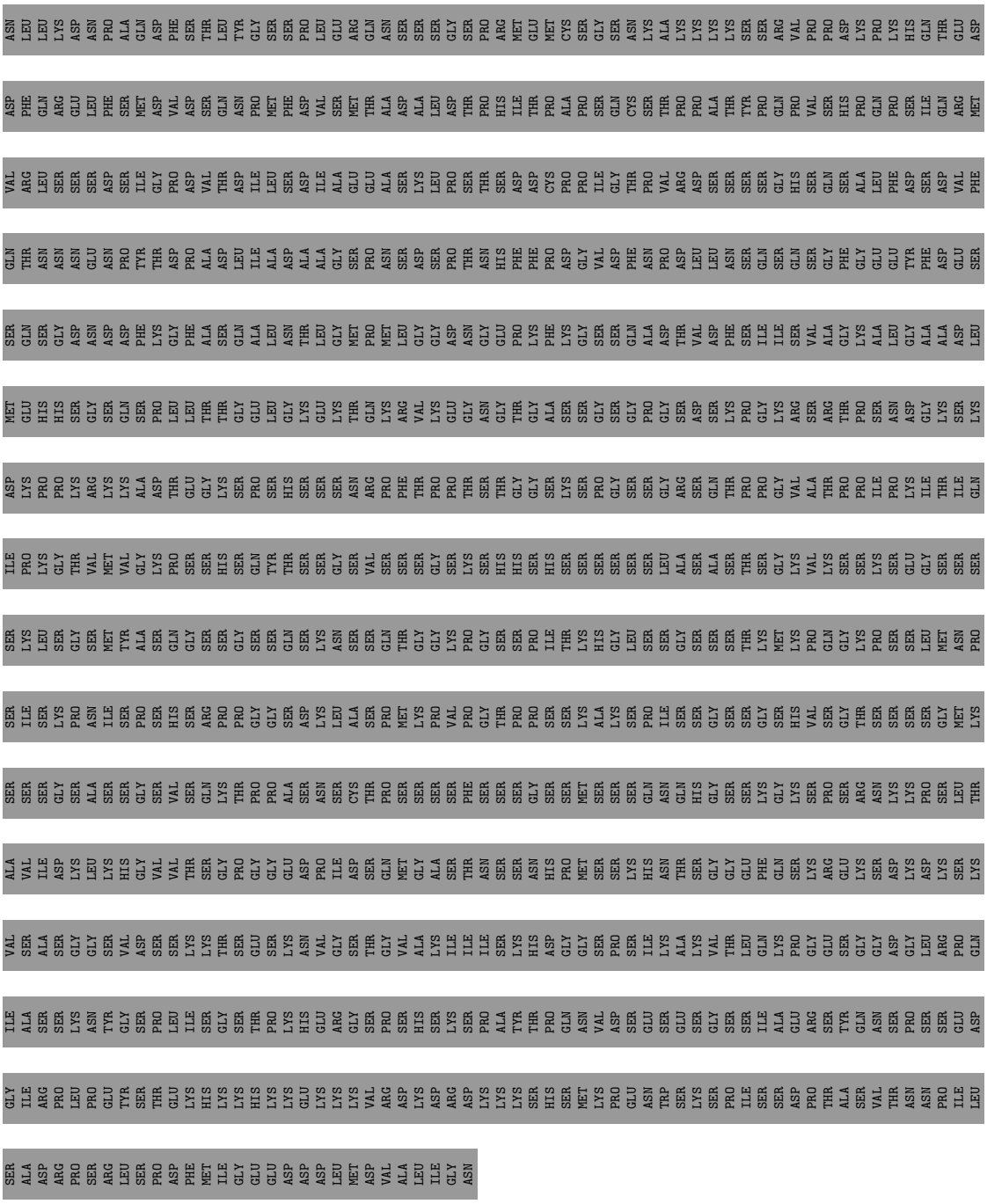
Chain E:



• Molecule 2: Mediator of RNA polymerase II transcription subunit 1

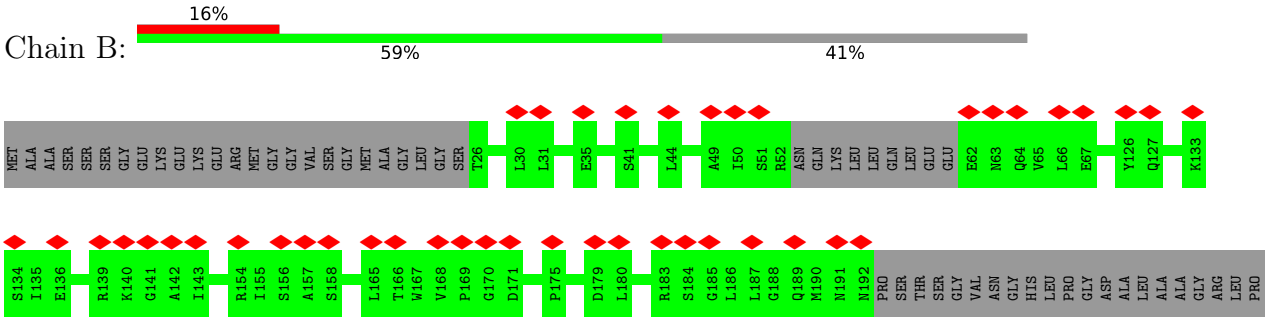
Chain A:



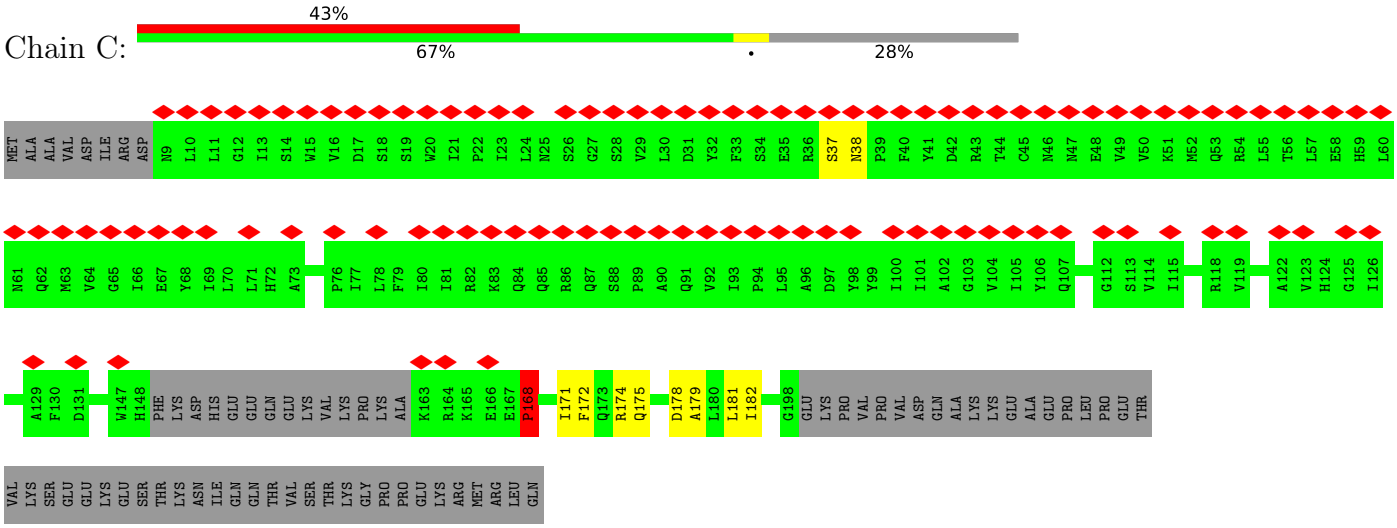


• Molecule 3: Mediator of RNA polymerase II transcription subunit 4

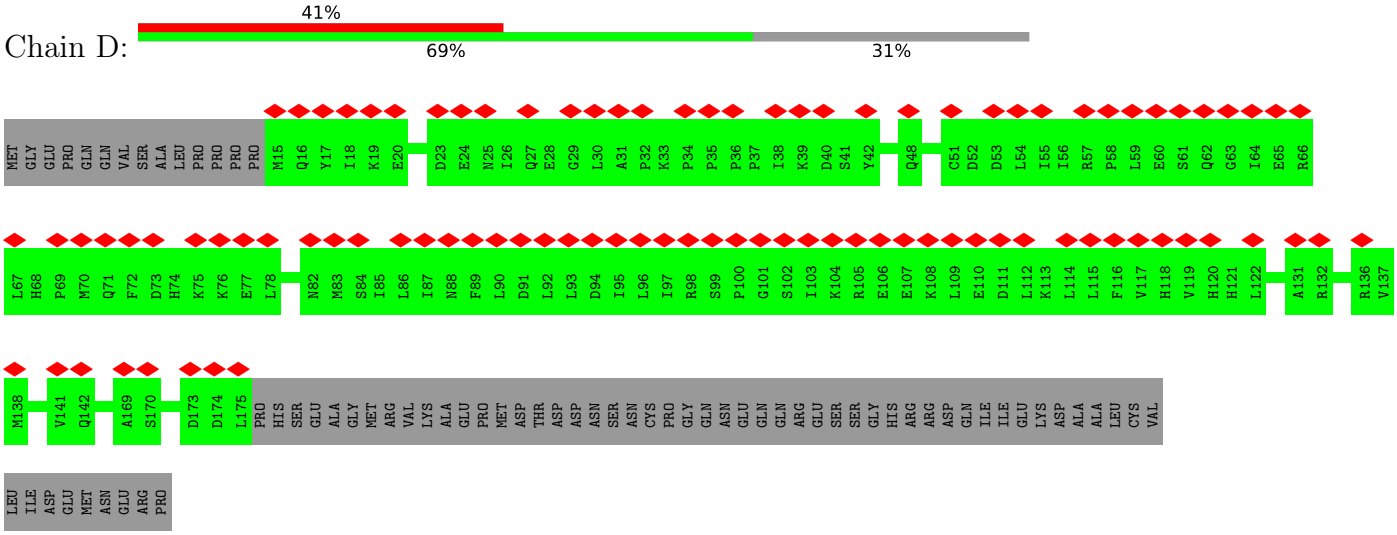
Chain B:



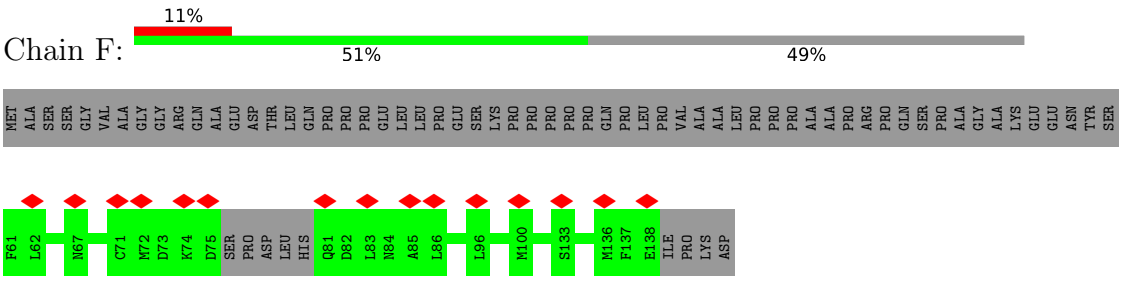
• Molecule 4: Mediator of RNA polymerase II transcription subunit 6



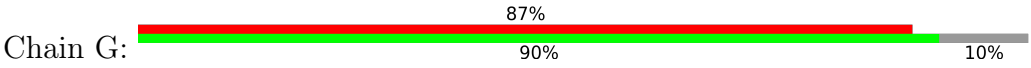
• Molecule 5: Mediator of RNA polymerase II transcription subunit 7

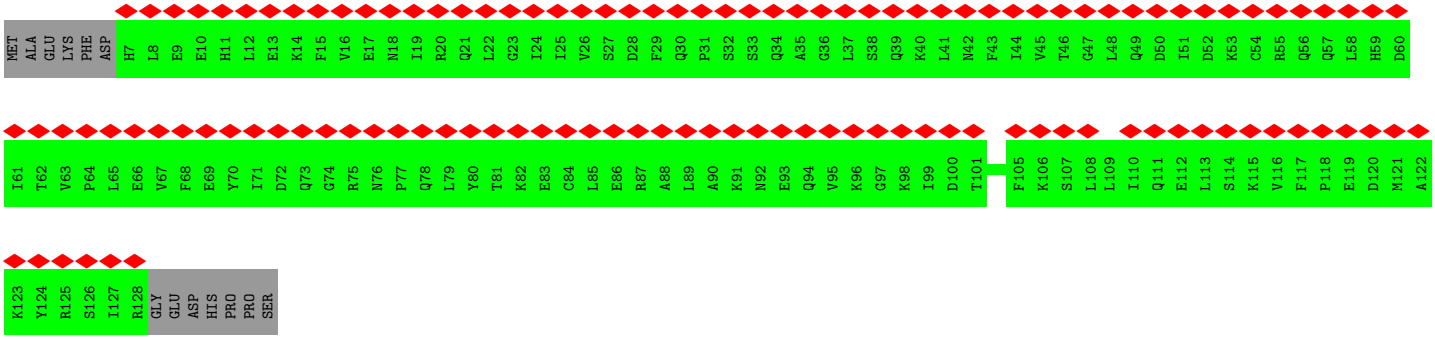


• Molecule 6: Mediator of RNA polymerase II transcription subunit 9



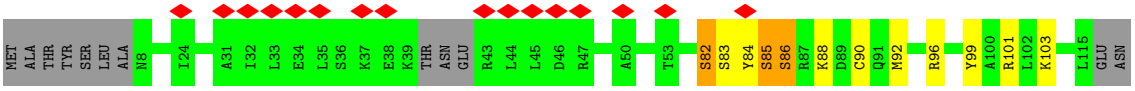
• Molecule 7: Mediator of RNA polymerase II transcription subunit 10





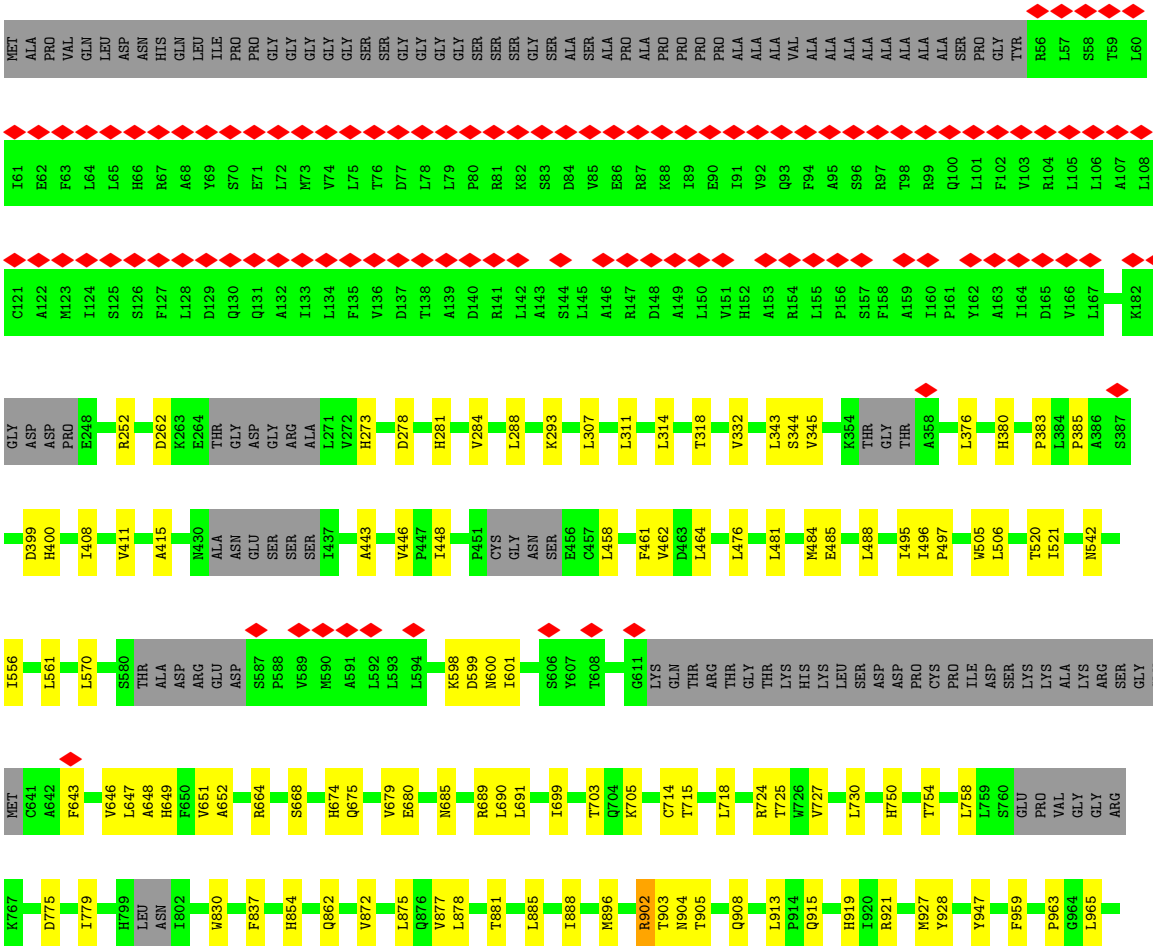
• Molecule 8: Mediator of RNA polymerase II transcription subunit 11

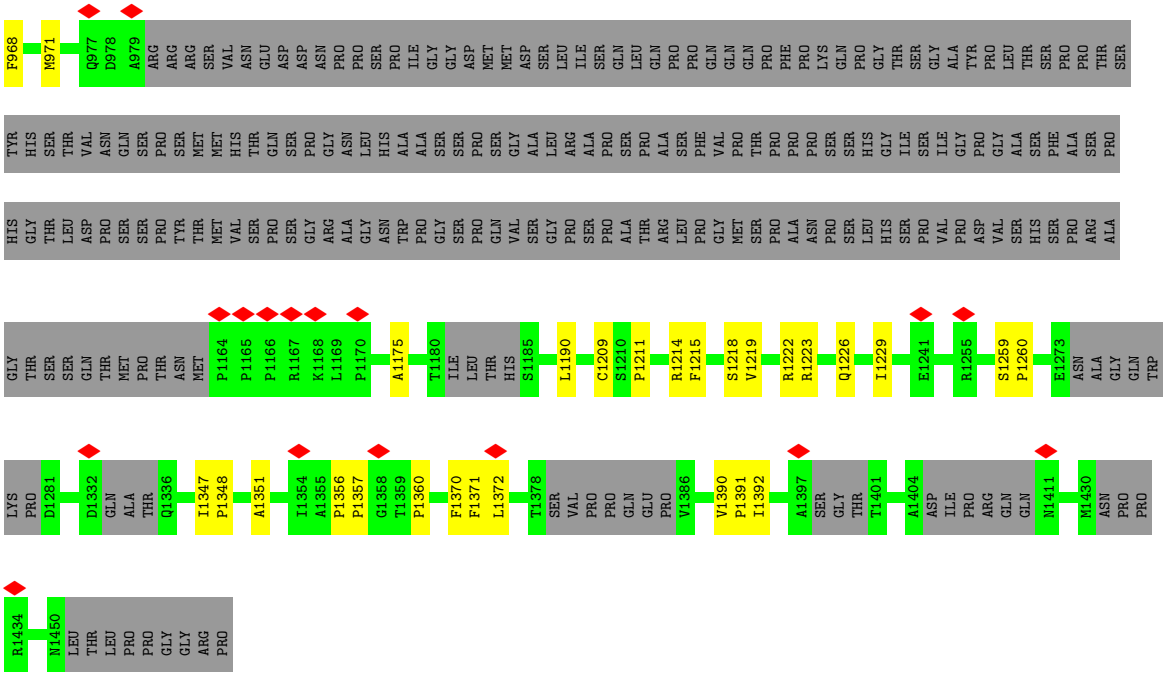
Chain H:



• Molecule 9: Mediator of RNA polymerase II transcription subunit 14

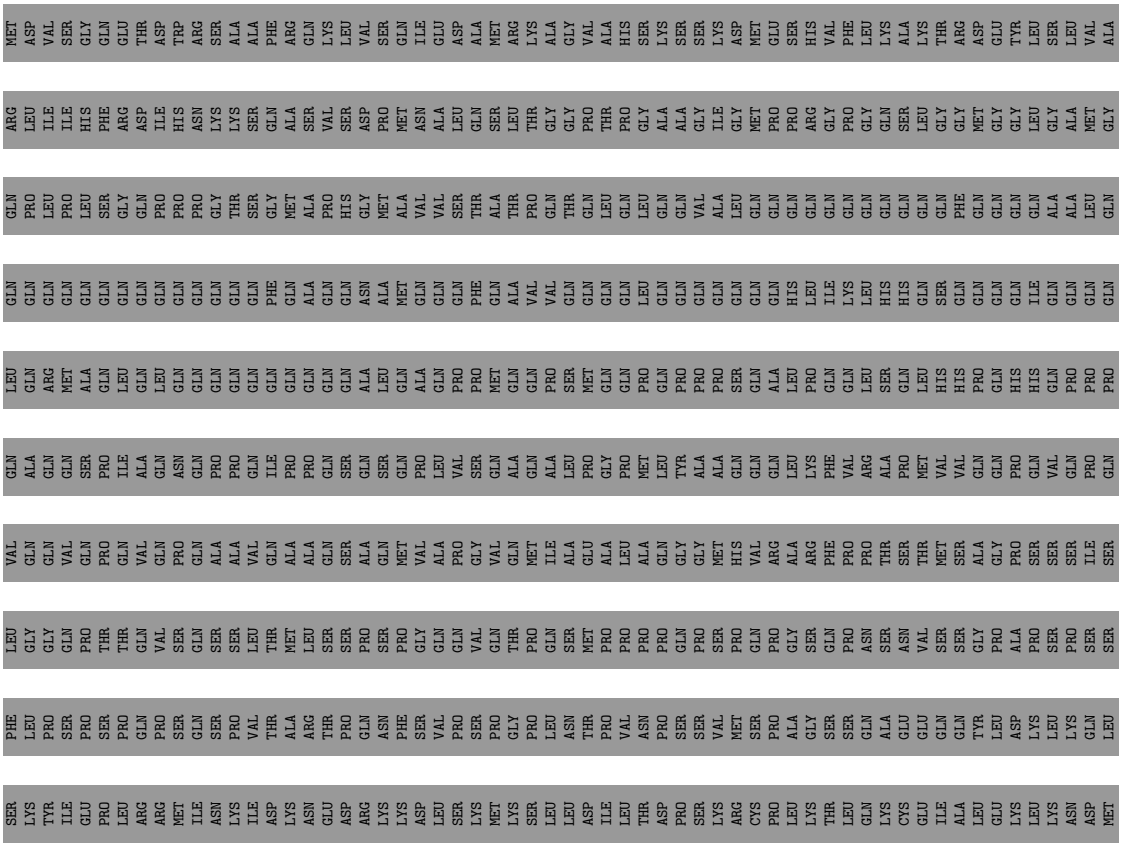
Chain I:

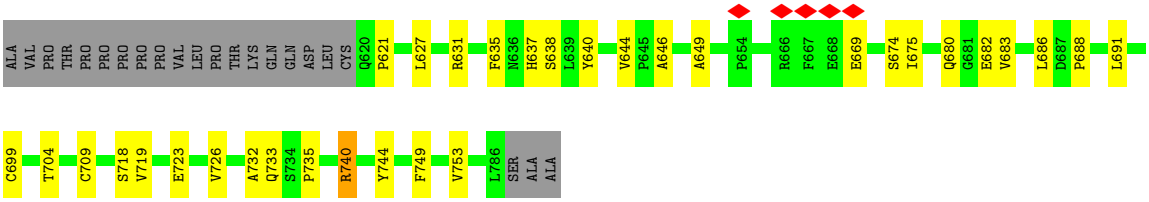




• Molecule 10: Mediator of RNA polymerase II transcription subunit 15

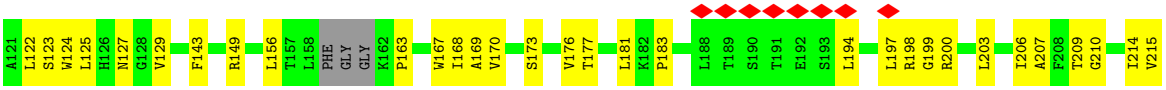
Chain J: 17% 79%

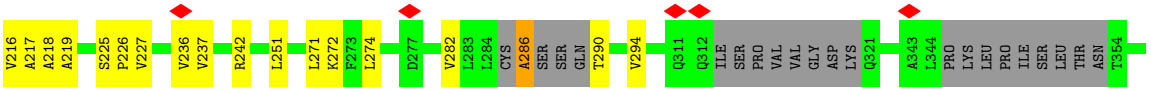


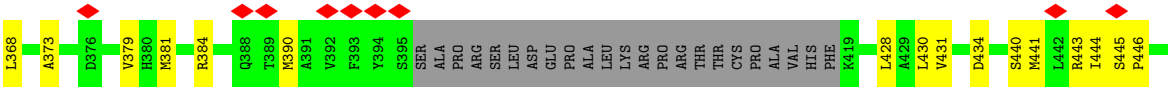


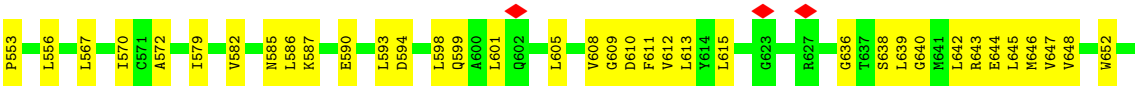
• Molecule 11: Mediator of RNA polymerase II transcription subunit 16

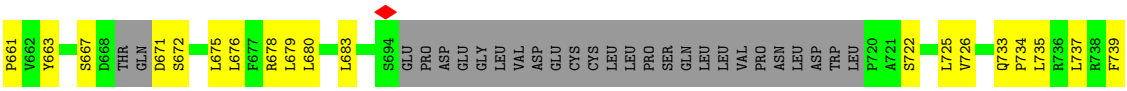
Chain K:

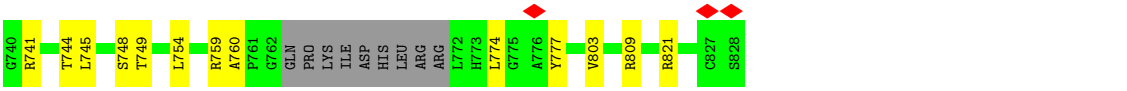


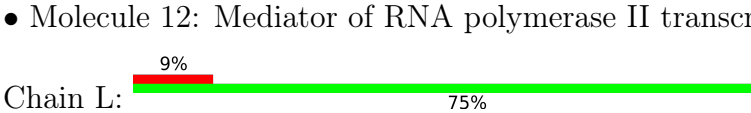






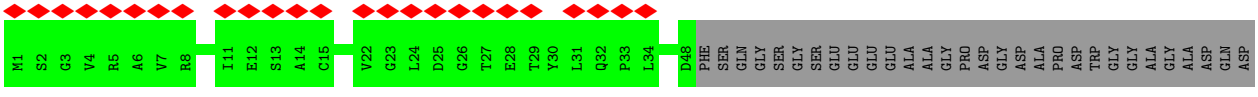


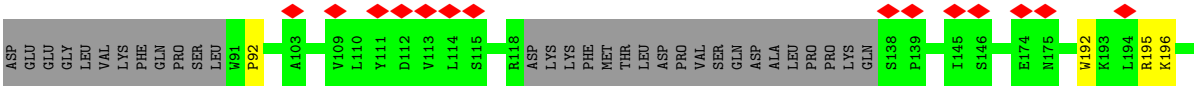


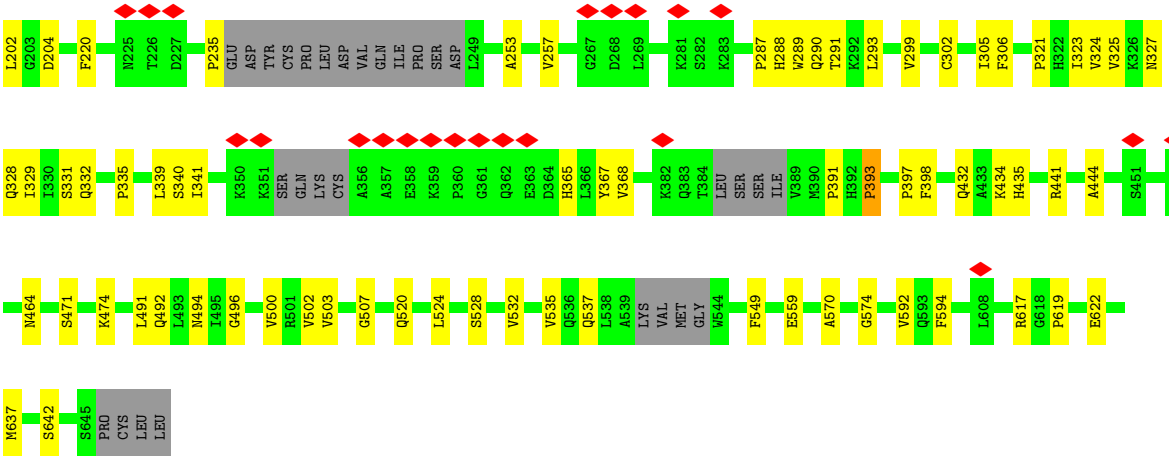


• Molecule 12: Mediator of RNA polymerase II transcription subunit 17

Chain L:





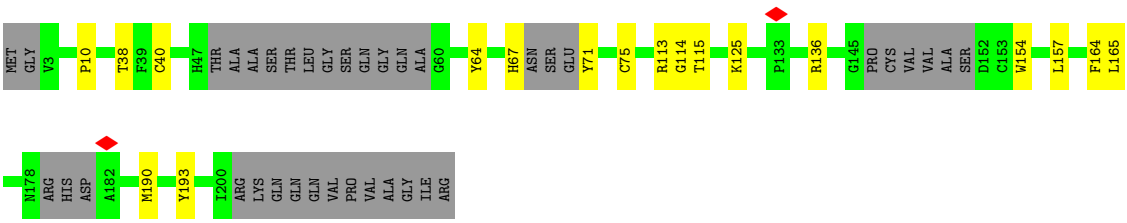


• Molecule 13: Mediator of RNA polymerase II transcription subunit 18

Chain M:

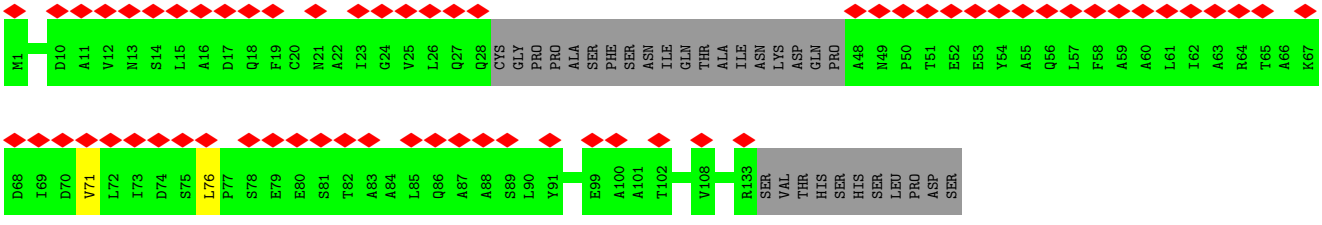
• Molecule 14: Mediator of RNA polymerase II transcription subunit 20

Chain O:



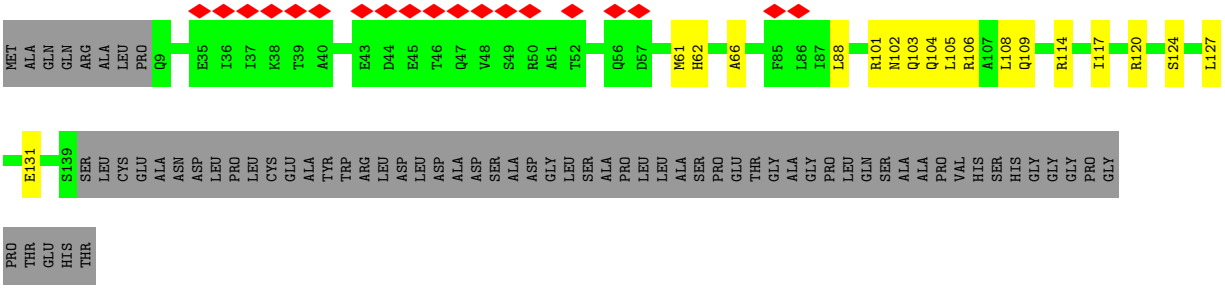
• Molecule 15: Mediator of RNA polymerase II transcription subunit 21

Chain P:



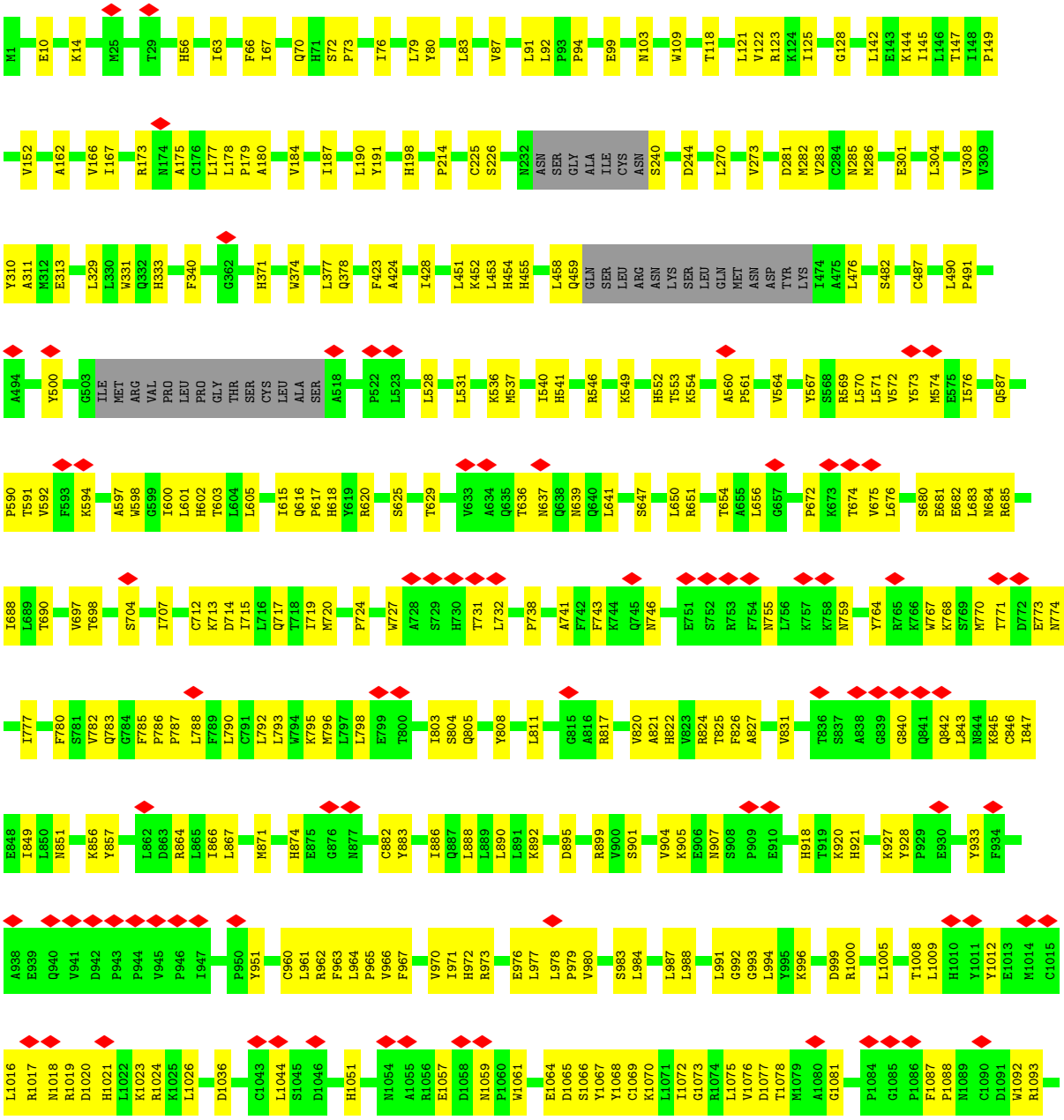
• Molecule 16: Mediator of RNA polymerase II transcription subunit 22

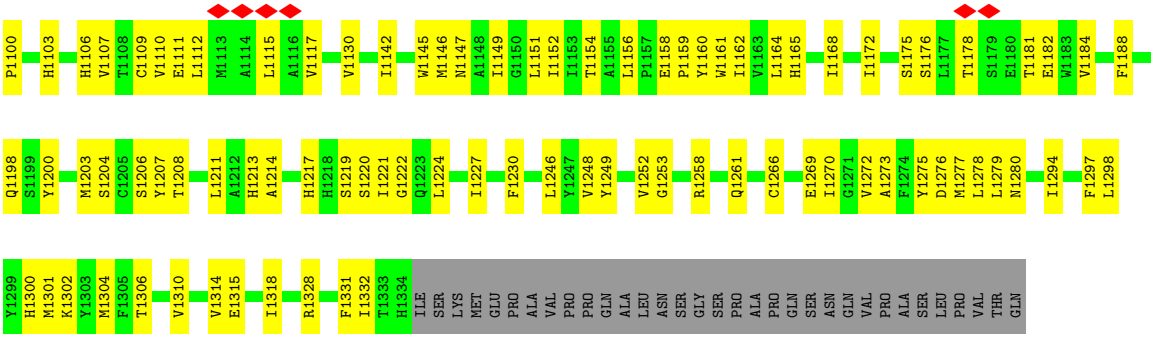
Chain Q:



• Molecule 17: Mediator of RNA polymerase II transcription subunit 23

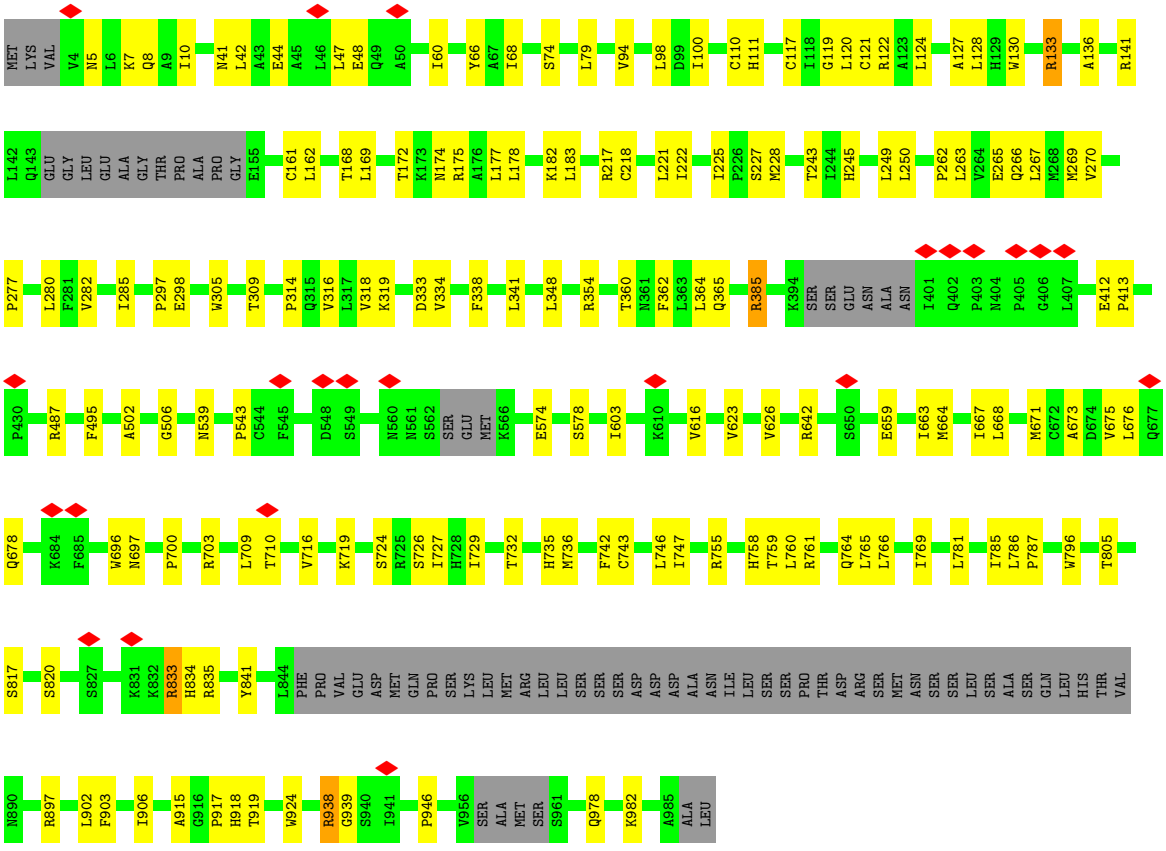
Chain R:





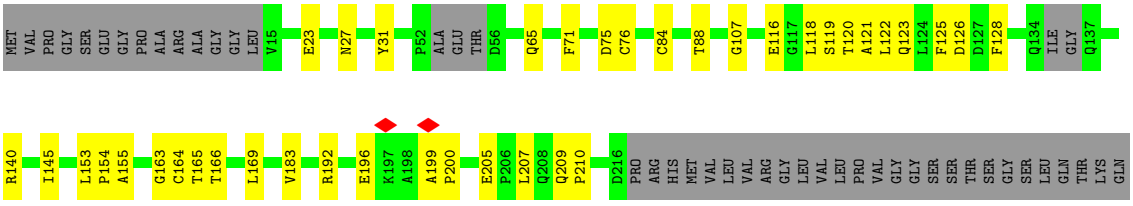
• Molecule 18: Mediator of RNA polymerase II transcription subunit 24

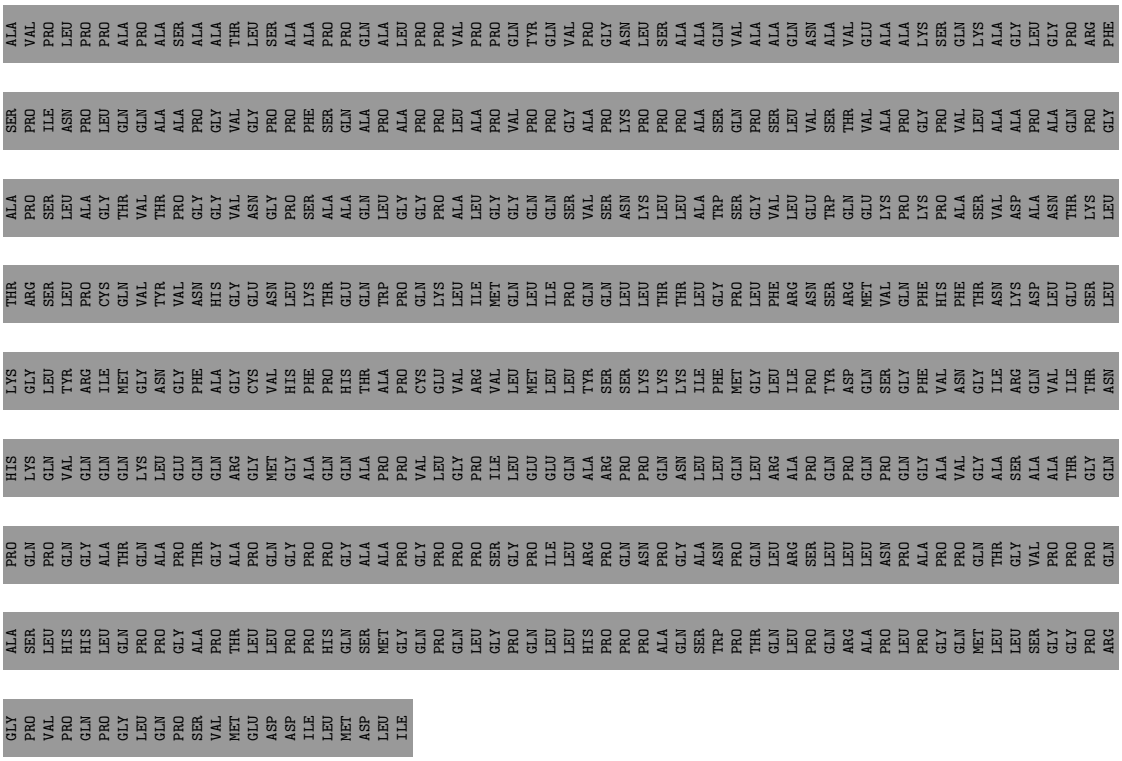
Chain S:



• Molecule 19: Mediator of RNA polymerase II transcription subunit 25

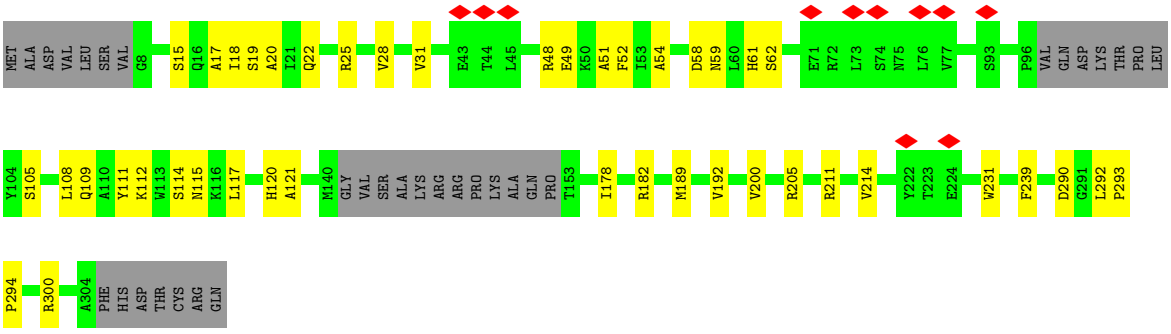
Chain T:





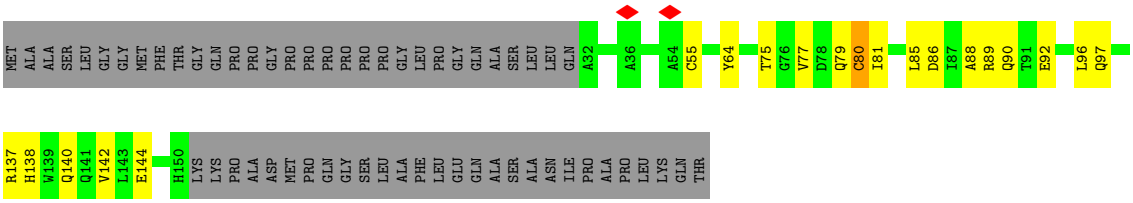
• Molecule 20: Mediator of RNA polymerase II transcription subunit 27

Chain V:



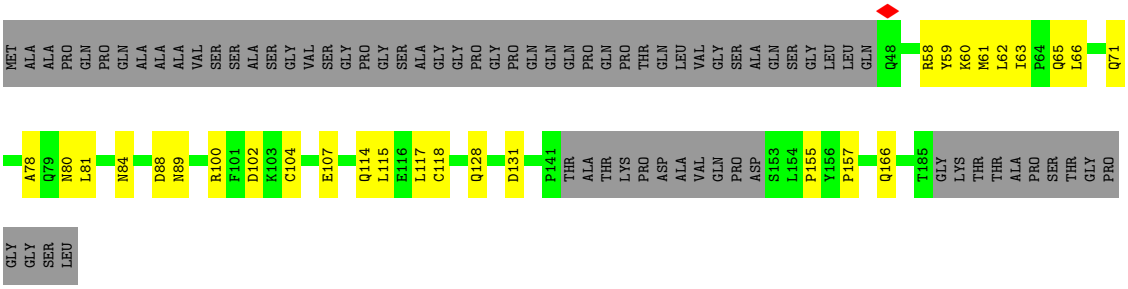
• Molecule 21: Mediator of RNA polymerase II transcription subunit 28

Chain W:

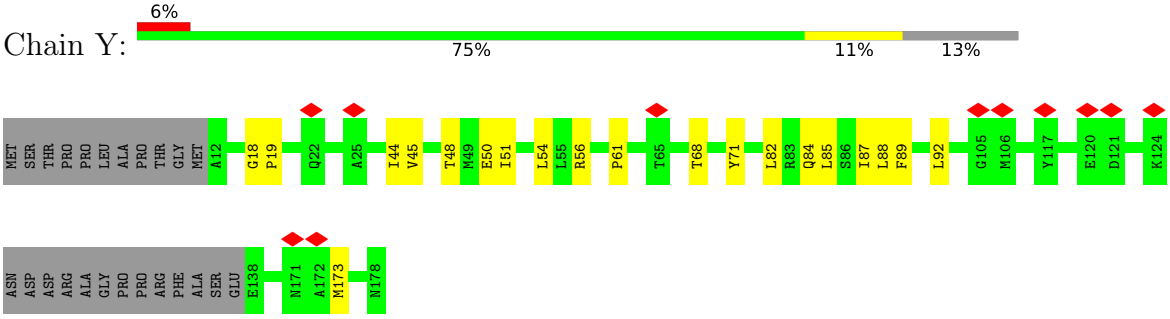


• Molecule 22: Mediator of RNA polymerase II transcription subunit 29

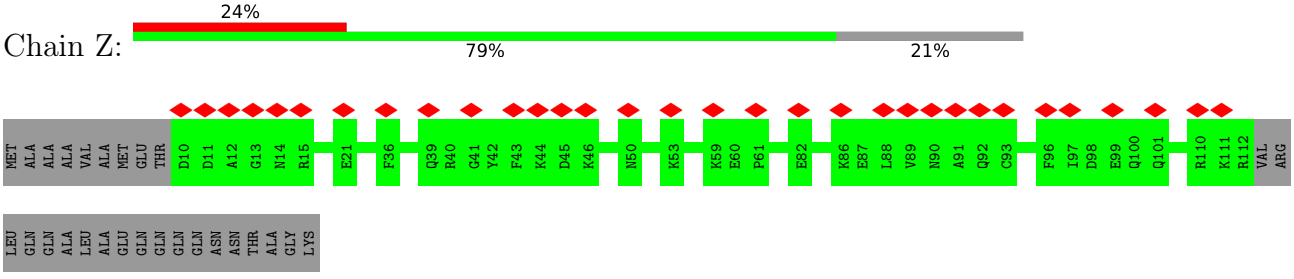
Chain X:



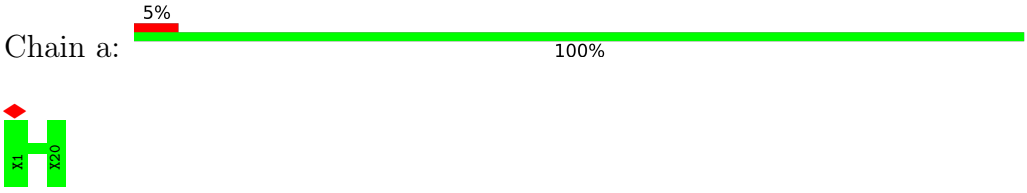
• Molecule 23: Mediator of RNA polymerase II transcription subunit 30



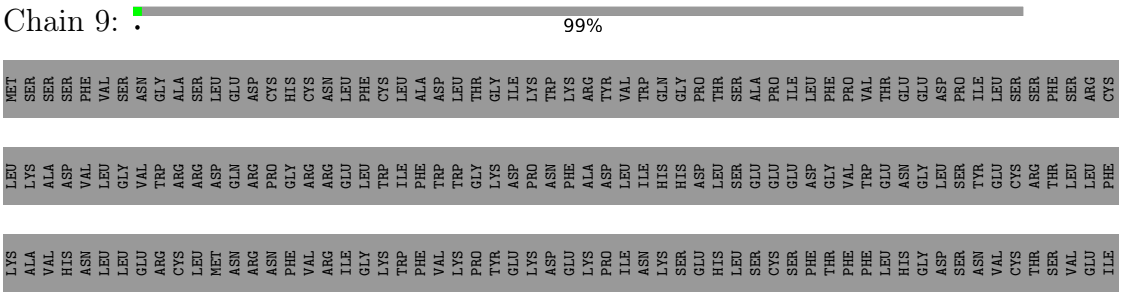
• Molecule 24: Mediator of RNA polymerase II transcription subunit 31

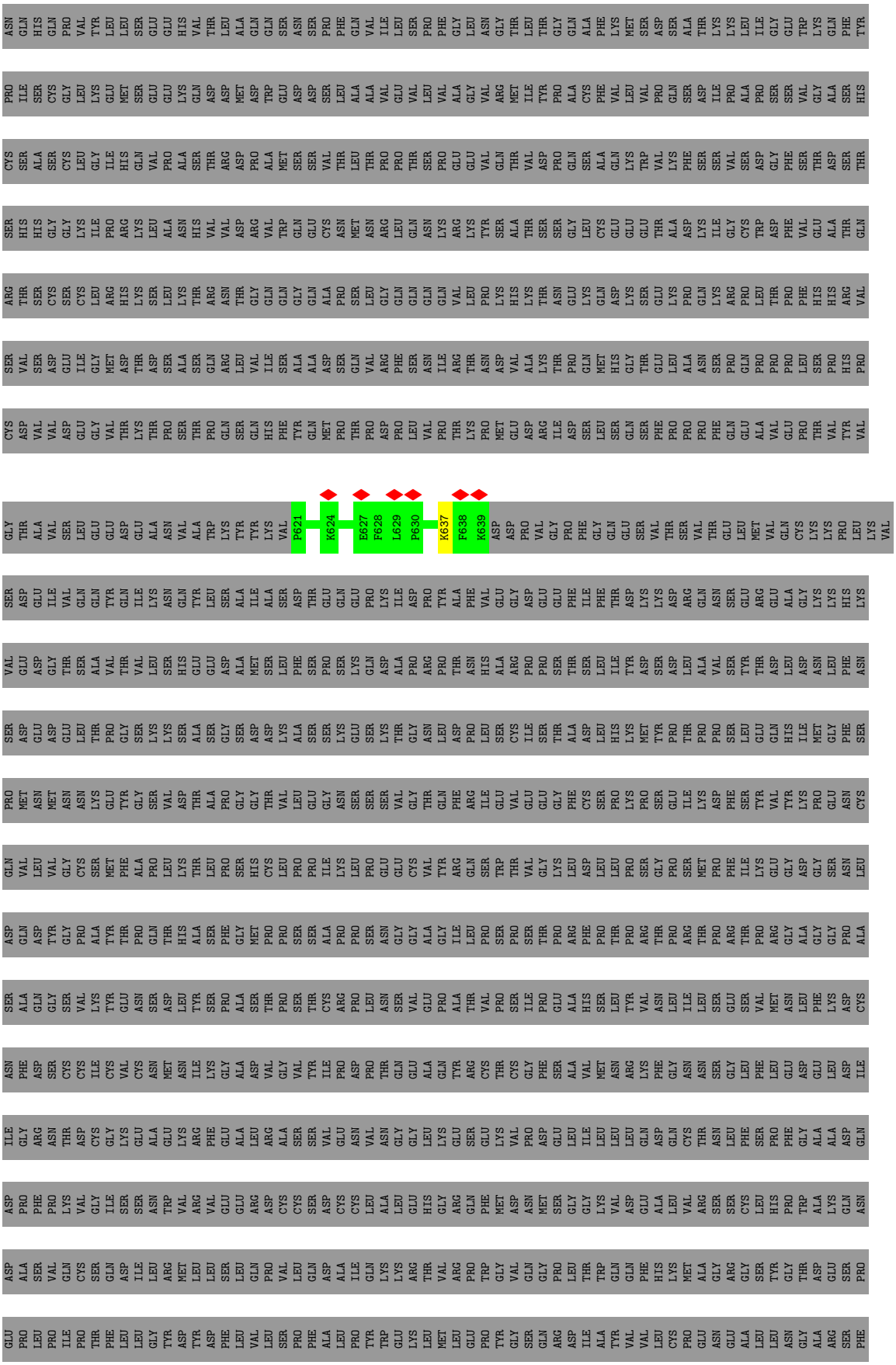


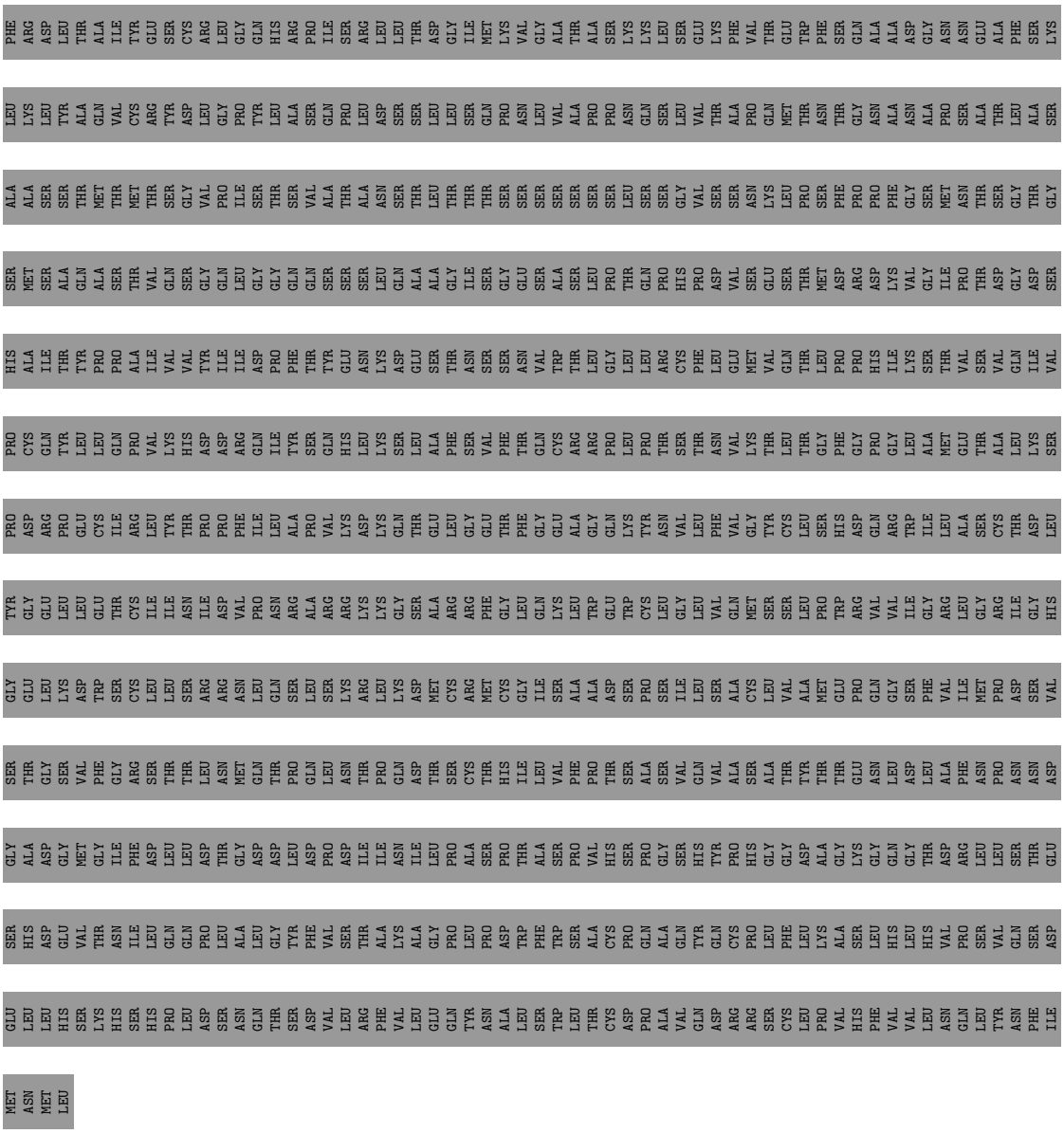
• Molecule 25: Unknown



• Molecule 26: Mediator of RNA polymerase II transcription subunit 13




F621
K624
E627
F628
L629
P630
K637
F638
K639


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

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	111331	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	22.5	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	36000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.621	Depositor
Minimum map value	-0.346	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	621.60004, 621.60004, 621.60004	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.11, 1.11, 1.11	Depositor

5 Model quality

5.1 Standard geometry

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	E	0.23	0/885	0.37	0/1230
2	A	0.23	0/2334	0.41	0/3247
3	B	0.23	0/782	0.34	0/1088
4	C	0.26	0/967	0.49	1/1333 (0.1%)
5	D	0.23	0/800	0.34	0/1116
6	F	0.22	0/361	0.33	0/501
7	G	0.23	0/604	0.33	0/841
8	H	0.22	0/584	0.43	0/802
9	I	0.24	0/7018	0.42	1/9683 (0.0%)
10	J	0.24	0/1207	0.42	0/1668
11	K	0.23	0/5165	0.47	1/7090 (0.0%)
12	L	0.24	0/3482	0.42	1/4795 (0.0%)
13	M	0.23	0/1163	0.42	0/1593
14	O	0.24	0/1027	0.39	0/1412
15	P	0.22	0/566	0.30	0/788
16	Q	0.24	0/758	0.38	0/1046
17	R	0.24	0/10024	0.41	0/13697
18	S	0.24	0/6059	0.40	0/8332
19	T	0.25	0/1320	0.43	0/1813
20	V	0.24	0/1765	0.41	0/2441
21	W	0.24	0/790	0.40	0/1083
22	X	0.24	0/872	0.41	0/1197
23	Y	0.25	0/1007	0.36	0/1375
24	Z	0.22	0/512	0.40	0/714
26	9	0.28	0/165	0.45	0/220
All	All	0.24	0/50217	0.41	4/69105 (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.

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers

Mol	Chain	#Chirality outliers	#Planarity outliers
8	H	0	2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	168	PRO	CA-N-CD	-8.23	99.97	111.50
9	I	385	PRO	N-CA-CB	6.10	110.62	103.30
12	L	92	PRO	N-CA-CB	6.04	110.55	103.30
11	K	286	ALA	C-N-CA	6.02	136.75	121.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	H	82	SER	Peptide
8	H	85	SER	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	E	888	0	392	2	0
2	A	2339	0	1005	10	0
3	B	784	0	357	0	0
4	C	963	0	554	8	0
5	D	801	0	327	0	0
6	F	363	0	146	0	0
7	G	605	0	256	0	0
8	H	582	0	352	10	0
9	I	6892	0	5009	92	0
10	J	1171	0	1010	27	0
11	K	5051	0	4492	128	0
12	L	3424	0	2463	55	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	M	1140	0	832	17	0
14	O	1013	0	663	9	0
15	P	568	0	286	1	0
16	Q	754	0	448	13	0
17	R	9771	0	9126	269	0
18	S	5934	0	4713	105	0
19	T	1287	0	992	23	0
20	V	1726	0	1220	26	0
21	W	778	0	609	17	0
22	X	859	0	708	18	0
23	Y	994	0	777	16	0
24	Z	513	0	225	0	0
25	a	100	0	23	0	0
26	9	160	0	170	1	0
All	All	49460	0	37155	810	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 (810) 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)
17:R:620:ARG:HH21	17:R:656:LEU:HD22	1.45	0.81
18:S:117:CYS:O	18:S:120:LEU:HB3	1.82	0.80
11:K:203:LEU:HA	11:K:218:ALA:HB3	1.64	0.79
12:L:494:ASN:HA	12:L:500:VAL:HG12	1.66	0.78
12:L:393:PRO:HG2	12:L:397:PRO:HD2	1.65	0.77
17:R:1168:ILE:HA	17:R:1172:ILE:HD12	1.67	0.77
11:K:601:LEU:HA	11:K:605:LEU:HB2	1.68	0.76
13:M:53:ASP:HA	13:M:75:SER:HA	1.66	0.76
11:K:92:GLN:HB2	11:K:110:VAL:HA	1.67	0.75
12:L:549:PHE:HE2	12:L:570:ALA:HB3	1.51	0.75
13:M:135:LEU:HB2	13:M:142:LYS:HZ1	1.52	0.74
17:R:308:VAL:O	17:R:311:ALA:HB3	1.86	0.74
17:R:482:SER:HA	17:R:487:CYS:HB2	1.69	0.74
17:R:1198:GLN:HG3	17:R:1200:TYR:H	1.53	0.73
11:K:636:GLY:H	11:K:639:LEU:HD13	1.54	0.73
17:R:487:CYS:HB3	17:R:491:PRO:HG2	1.71	0.72
11:K:7:CYS:SG	11:K:8:GLU:N	2.63	0.71
10:J:631:ARG:HH21	10:J:637:HIS:H	1.37	0.71
9:I:399:ASP:O	9:I:400:HIS:ND1	2.24	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:446:PRO:HB2	11:K:480:LEU:HD13	1.73	0.71
17:R:651:ARG:HB2	17:R:961:LEU:HD13	1.70	0.70
17:R:714:ASP:O	17:R:717:GLN:HB2	1.91	0.70
11:K:92:GLN:HG3	11:K:111:GLY:H	1.56	0.69
20:V:48:ARG:O	20:V:51:ALA:HB3	1.93	0.68
11:K:181:LEU:HG	11:K:183:PRO:HD3	1.74	0.68
9:I:461:PHE:HD2	12:L:321:PRO:HG2	1.59	0.68
11:K:120:VAL:HB	11:K:169:ALA:HB1	1.76	0.68
17:R:1208:THR:O	17:R:1211:LEU:HB3	1.94	0.67
17:R:790:LEU:HD22	17:R:822:HIS:HB3	1.77	0.67
17:R:1023:LYS:HD3	17:R:1026:LEU:HB2	1.76	0.67
11:K:206:ILE:HG23	11:K:215:VAL:HB	1.75	0.67
11:K:587:LYS:NZ	11:K:590:GLU:O	2.25	0.67
17:R:571:LEU:HD13	17:R:1093:ARG:HD3	1.76	0.67
8:H:101:ARG:HH12	21:W:144:GLU:HA	1.59	0.67
18:S:174:ASN:HA	18:S:177:LEU:HD13	1.75	0.67
2:A:364:TYR:HA	2:A:373:CYS:HA	1.75	0.67
16:Q:103:GLN:O	16:Q:106:ARG:HB2	1.95	0.67
20:V:51:ALA:O	20:V:54:ALA:HB3	1.95	0.66
18:S:724:SER:O	18:S:727:ILE:HB	1.95	0.66
20:V:182:ARG:HG2	20:V:189:MET:H	1.59	0.66
12:L:324:VAL:HG23	12:L:329:ILE:HG22	1.75	0.66
17:R:1016:LEU:O	17:R:1020:ASP:N	2.28	0.66
19:T:164:CYS:SG	19:T:165:THR:N	2.67	0.66
17:R:377:LEU:HD13	17:R:428:ILE:HG22	1.77	0.66
20:V:114:SER:O	20:V:117:LEU:HB2	1.96	0.65
17:R:99:GLU:O	17:R:103:ASN:ND2	2.29	0.65
13:M:142:LYS:NZ	13:M:143:VAL:O	2.29	0.65
9:I:1348:PRO:HG2	9:I:1351:ALA:HB2	1.77	0.65
17:R:311:ALA:HA	17:R:331:TRP:HE1	1.62	0.65
17:R:1017:ARG:O	17:R:1020:ASP:HB2	1.96	0.65
9:I:837:PHE:O	9:I:862:GLN:NE2	2.31	0.64
9:I:664:ARG:HG3	9:I:675:GLN:HG2	1.78	0.64
11:K:236:VAL:HG11	11:K:242:ARG:HB2	1.79	0.64
11:K:491:VAL:HB	11:K:520:LEU:HD13	1.79	0.64
11:K:428:LEU:HB3	11:K:446:PRO:HA	1.78	0.64
17:R:777:ILE:HA	17:R:780:PHE:HB3	1.77	0.64
20:V:49:GLU:O	20:V:52:PHE:HB3	1.97	0.64
17:R:458:LEU:HG	17:R:459:GLN:HG2	1.79	0.64
13:M:131:ALA:HB2	13:M:148:ILE:HD13	1.80	0.64
11:K:25:CYS:HB2	11:K:34:ALA:HB3	1.80	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:S:412:GLU:HG2	18:S:413:PRO:HD3	1.80	0.63
17:R:1276:ASP:O	17:R:1280:ASN:ND2	2.31	0.63
18:S:243:THR:OG1	18:S:764:GLN:OE1	2.16	0.63
17:R:636:THR:O	17:R:817:ARG:NH2	2.24	0.63
11:K:217:ALA:HB1	11:K:227:VAL:HB	1.80	0.63
9:I:646:VAL:O	9:I:649:HIS:HB2	1.99	0.63
12:L:464:ASN:OD1	20:V:205:ARG:NE	2.31	0.63
17:R:1211:LEU:O	17:R:1214:ALA:HB3	1.99	0.63
11:K:168:ILE:HD11	11:K:181:LEU:HB2	1.79	0.63
13:M:24:GLN:HA	13:M:170:GLU:HA	1.81	0.63
17:R:1103:HIS:O	17:R:1106:HIS:ND1	2.31	0.63
9:I:896:MET:HA	9:I:908:GLN:HA	1.81	0.62
17:R:1275:TYR:HA	17:R:1278:LEU:HD12	1.81	0.62
17:R:173:ARG:O	17:R:177:LEU:N	2.32	0.62
17:R:283:VAL:HA	17:R:286:MET:HG2	1.80	0.62
22:X:80:ASN:O	22:X:84:ASN:ND2	2.33	0.62
17:R:654:THR:HA	17:R:690:THR:HG21	1.82	0.62
17:R:1067:TYR:HA	17:R:1070:LYS:HD2	1.81	0.62
18:S:348:LEU:HD13	18:S:385:ARG:HH21	1.64	0.62
2:A:460:ASP:O	18:S:7:LYS:NZ	2.32	0.62
19:T:125:PHE:HE2	19:T:140:ARG:HB3	1.65	0.62
9:I:448:ILE:HG21	9:I:506:LEU:HD12	1.81	0.61
8:H:96:ARG:O	12:L:367:TYR:OH	2.18	0.61
11:K:47:THR:HG23	11:K:70:GLU:H	1.65	0.61
11:K:198:ARG:HE	11:K:199:GLY:H	1.48	0.61
11:K:272:LYS:HE2	11:K:274:LEU:HB2	1.81	0.61
18:S:902:LEU:O	18:S:906:ILE:HG13	2.01	0.61
2:A:304:PHE:HA	2:A:397:THR:HA	1.82	0.61
17:R:452:LYS:O	17:R:455:HIS:HB3	2.00	0.61
9:I:705:LYS:NZ	10:J:669:GLU:OE1	2.31	0.60
11:K:676:LEU:O	11:K:680:LEU:HG	2.01	0.60
17:R:123:ARG:O	17:R:123:ARG:NH2	2.34	0.60
14:O:10:PRO:HG3	14:O:136:ARG:H	1.66	0.60
17:R:856:LYS:HG2	17:R:857:TYR:HB2	1.83	0.60
18:S:603:ILE:O	18:S:642:ARG:NH2	2.34	0.60
17:R:549:LYS:HA	17:R:552:HIS:HD2	1.66	0.60
18:S:316:VAL:HA	18:S:319:LYS:HD2	1.82	0.60
17:R:808:TYR:OH	17:R:933:TYR:O	2.19	0.60
9:I:968:PHE:HA	9:I:971:MET:HG2	1.84	0.60
12:L:594:PHE:HE2	12:L:617:ARG:HB2	1.67	0.60
17:R:785:PHE:HB3	17:R:788:LEU:HB2	1.84	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:R:1302:LYS:HA	17:R:1306:THR:HG22	1.82	0.60
20:V:108:LEU:O	20:V:111:TYR:HB2	2.02	0.60
11:K:368:LEU:O	11:K:384:ARG:NH2	2.35	0.59
11:K:47:THR:OG1	11:K:48:HIS:N	2.36	0.59
9:I:872:VAL:HA	9:I:875:LEU:HD12	1.85	0.59
17:R:281:ASP:O	17:R:285:ASN:ND2	2.36	0.59
4:C:171:ILE:HG13	4:C:172:PHE:H	1.66	0.59
11:K:675:LEU:HA	11:K:678:ARG:HG2	1.85	0.59
12:L:287:PRO:HB2	12:L:290:GLN:HB2	1.84	0.59
17:R:1065:ASP:OD1	17:R:1066:SER:N	2.34	0.59
11:K:599:GLN:HG3	11:K:803:VAL:HG22	1.85	0.59
11:K:484:PRO:O	11:K:488:GLN:N	2.34	0.59
17:R:340:PHE:HE1	17:R:576:ILE:HB	1.68	0.59
12:L:434:LYS:HD3	12:L:496:GLY:HA2	1.85	0.58
17:R:528:LEU:HD21	17:R:569:ARG:HB3	1.84	0.58
17:R:1151:LEU:O	17:R:1154:THR:OG1	2.21	0.58
17:R:1164:LEU:HD11	17:R:1211:LEU:HD21	1.84	0.58
17:R:1156:LEU:HD12	17:R:1160:TYR:HD2	1.67	0.58
17:R:149:PRO:HG2	17:R:152:VAL:HB	1.85	0.58
18:S:121:CYS:O	18:S:124:LEU:HB2	2.04	0.58
10:J:726:VAL:HG22	10:J:732:ALA:HB2	1.84	0.58
17:R:866:ILE:HG13	17:R:867:LEU:N	2.19	0.58
13:M:55:GLU:H	13:M:130:VAL:HG22	1.68	0.57
18:S:41:ASN:ND2	18:S:44:GLU:OE1	2.36	0.57
17:R:719:ILE:HG23	17:R:724:PRO:HD2	1.86	0.57
9:I:724:ARG:NH1	9:I:758:LEU:O	2.36	0.57
17:R:866:ILE:HD11	17:R:962:ARG:HE	1.69	0.57
18:S:124:LEU:O	18:S:127:ALA:HB3	2.03	0.57
17:R:66:PHE:O	17:R:70:GLN:NE2	2.34	0.57
2:A:455:GLN:HA	2:A:462:LEU:HA	1.86	0.57
11:K:642:LEU:O	11:K:646:MET:HG3	2.04	0.57
12:L:253:ALA:HB2	12:L:299:VAL:HG23	1.87	0.57
15:P:71:VAL:O	15:P:76:LEU:N	2.32	0.57
10:J:674:SER:OG	10:J:675:ILE:N	2.37	0.57
17:R:600:ILE:O	17:R:603:THR:HB	2.05	0.57
9:I:915:GLN:HE22	9:I:919:HIS:HB3	1.70	0.56
8:H:92:MET:O	8:H:96:ARG:HG3	2.05	0.56
9:I:241:THR:HA	9:I:252:ARG:H	1.69	0.56
10:J:640:TYR:O	10:J:644:VAL:HG22	2.05	0.56
11:K:78:ASP:OD1	11:K:124:TRP:NE1	2.32	0.56
16:Q:114:ARG:HA	16:Q:117:ILE:HD12	1.86	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:S:338:PHE:HD1	18:S:341:LEU:HD21	1.69	0.56
21:W:137:ARG:HD3	21:W:140:GLN:HE21	1.70	0.56
19:T:71:PHE:HZ	19:T:84:CYS:HB2	1.71	0.56
10:J:631:ARG:NH2	10:J:638:SER:H	2.04	0.56
11:K:206:ILE:HD12	11:K:271:LEU:HB3	1.87	0.56
17:R:56:HIS:O	17:R:56:HIS:ND1	2.39	0.56
17:R:190:LEU:HD21	17:R:198:HIS:H	1.71	0.56
17:R:847:ILE:HA	17:R:851:ASN:HD21	1.70	0.56
17:R:960:CYS:HB3	17:R:994:LEU:HD11	1.87	0.56
17:R:1088:PRO:HB2	17:R:1092:TRP:NE1	2.21	0.56
17:R:978:LEU:HD23	17:R:979:PRO:HD3	1.87	0.56
9:I:854:HIS:HD2	9:I:885:LEU:HD21	1.71	0.56
11:K:572:ALA:HA	11:K:643:ARG:HH12	1.70	0.56
16:Q:127:LEU:O	16:Q:131:GLU:HG2	2.06	0.56
17:R:179:PRO:HD3	17:R:1331:PHE:HD2	1.70	0.56
17:R:905:LYS:O	17:R:920:LYS:NZ	2.33	0.56
17:R:500:TYR:OH	17:R:546:ARG:NH2	2.39	0.55
9:I:913:LEU:HD23	9:I:921:ARG:HB3	1.87	0.55
17:R:83:LEU:O	17:R:87:VAL:HG23	2.06	0.55
17:R:717:GLN:O	17:R:720:MET:HG3	2.07	0.55
17:R:602:HIS:HE1	17:R:639:ASN:HD21	1.53	0.55
4:C:178:ASP:OD1	4:C:179:ALA:N	2.40	0.55
9:I:598:LYS:O	9:I:601:ILE:N	2.39	0.55
11:K:219:ALA:HB3	11:K:226:PRO:HG2	1.88	0.55
17:R:1165:HIS:HB3	17:R:1230:PHE:CZ	2.41	0.55
17:R:270:LEU:HA	17:R:273:VAL:HG22	1.88	0.55
17:R:712:CYS:HA	17:R:715:ILE:HD12	1.87	0.55
11:K:608:VAL:O	11:K:611:PHE:HB3	2.06	0.55
17:R:1224:LEU:O	17:R:1227:ILE:HG12	2.07	0.55
18:S:119:GLY:O	18:S:122:ARG:HB3	2.07	0.55
17:R:988:LEU:O	17:R:992:GLY:N	2.40	0.55
4:C:174:ARG:NH1	9:I:262:ASP:O	2.40	0.55
11:K:227:VAL:HG21	11:K:251:LEU:H	1.72	0.55
12:L:528:SER:O	12:L:532:VAL:HG23	2.07	0.55
17:R:1181:THR:HG23	17:R:1182:GLU:H	1.71	0.55
23:Y:45:VAL:O	23:Y:48:THR:OG1	2.22	0.55
11:K:516:MET:O	11:K:519:SER:OG	2.20	0.54
11:K:675:LEU:O	11:K:679:LEU:HG	2.07	0.54
14:O:40:CYS:HA	14:O:113:ARG:HA	1.90	0.54
17:R:561:PRO:O	17:R:951:TYR:OH	2.26	0.54
20:V:290:ASP:OD1	20:V:290:ASP:N	2.38	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:77:TRP:O	11:K:124:TRP:NE1	2.40	0.54
11:K:638:SER:O	11:K:642:LEU:HG	2.07	0.54
17:R:1145:TRP:O	17:R:1149:ILE:HG12	2.06	0.54
17:R:864:ARG:HE	17:R:962:ARG:NH2	2.06	0.54
12:L:329:ILE:HG13	12:L:340:SER:HA	1.89	0.54
22:X:60:LYS:HA	22:X:63:ILE:HD12	1.89	0.54
11:K:282:VAL:HG23	11:K:294:VAL:HA	1.90	0.54
14:O:114:GLY:O	14:O:125:LYS:NZ	2.37	0.54
20:V:109:GLN:NE2	21:W:64:TYR:OH	2.40	0.54
11:K:444:ILE:HG13	11:K:445:SER:H	1.73	0.54
17:R:1076:VAL:HG11	17:R:1145:TRP:CD1	2.42	0.54
19:T:118:LEU:O	19:T:121:ALA:HB3	2.07	0.54
9:I:314:LEU:O	9:I:318:THR:HG23	2.08	0.54
2:A:288:PHE:HA	2:A:295:ASN:HA	1.90	0.54
10:J:733:GLN:H	17:R:73:PRO:HG2	1.73	0.54
17:R:899:ARG:HE	17:R:928:TYR:HB2	1.72	0.54
17:R:1182:GLU:HB3	17:R:1184:VAL:HG12	1.90	0.54
17:R:1203:MET:O	17:R:1206:SER:OG	2.23	0.54
19:T:116:GLU:O	19:T:119:SER:OG	2.26	0.54
20:V:28:VAL:O	20:V:31:VAL:HB	2.08	0.54
9:I:674:HIS:HD1	9:I:674:HIS:H	1.56	0.54
11:K:53:LEU:HD13	11:K:61:VAL:HA	1.89	0.54
17:R:301:GLU:O	17:R:304:LEU:HG	2.08	0.54
17:R:864:ARG:HE	17:R:962:ARG:HH22	1.55	0.54
17:R:1130:VAL:HG21	17:R:1211:LEU:HD12	1.88	0.54
8:H:82:SER:O	8:H:84:TYR:N	2.41	0.53
11:K:170:VAL:HG21	11:K:216:VAL:HG11	1.90	0.53
11:K:514:LEU:O	11:K:517:LYS:HB2	2.08	0.53
17:R:175:ALA:O	17:R:1328:ARG:NH1	2.42	0.53
17:R:1069:CYS:O	17:R:1073:GLY:N	2.40	0.53
9:I:903:THR:HG23	9:I:905:THR:H	1.72	0.53
10:J:631:ARG:HH21	10:J:637:HIS:N	2.03	0.53
10:J:749:PHE:O	10:J:753:VAL:HG23	2.07	0.53
17:R:118:THR:O	17:R:122:VAL:HG23	2.08	0.53
16:Q:62:HIS:HA	16:Q:66:ALA:HB3	1.89	0.53
18:S:623:VAL:HA	18:S:676:LEU:HD11	1.89	0.53
9:I:1209:CYS:SG	9:I:1214:ARG:HB3	2.49	0.53
10:J:683:VAL:HA	10:J:686:LEU:HD23	1.91	0.53
11:K:605:LEU:O	11:K:608:VAL:HG22	2.09	0.53
9:I:965:LEU:HD13	9:I:968:PHE:HB2	1.90	0.53
11:K:143:PHE:HE1	11:K:466:GLU:HB3	1.73	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:R:967:PHE:HA	17:R:970:VAL:HG12	1.91	0.53
18:S:938:ARG:HH11	18:S:939:GLY:H	1.57	0.53
17:R:615:ILE:O	17:R:620:ARG:NH1	2.20	0.53
17:R:1069:CYS:HA	17:R:1072:ILE:HG12	1.91	0.53
18:S:175:ARG:HH22	18:S:221:LEU:HD13	1.74	0.53
22:X:81:LEU:HA	22:X:84:ASN:HD21	1.74	0.53
17:R:553:THR:HG23	17:R:554:LYS:H	1.74	0.53
21:W:75:THR:OG1	21:W:79:GLN:NE2	2.42	0.53
23:Y:82:LEU:O	23:Y:85:LEU:HG	2.09	0.53
14:O:64:TYR:N	14:O:75:CYS:O	2.42	0.52
9:I:1370:PHE:O	9:I:1392:ILE:N	2.42	0.52
11:K:236:VAL:HG23	11:K:237:VAL:H	1.74	0.52
9:I:649:HIS:HE2	12:L:559:GLU:C	2.13	0.52
17:R:240:SER:HA	17:R:1261:GLN:HG2	1.91	0.52
17:R:625:SER:O	17:R:629:THR:HG23	2.08	0.52
20:V:17:ALA:O	20:V:20:ALA:HB3	2.10	0.52
11:K:556:LEU:HD11	19:T:31:TYR:HE2	1.75	0.52
12:L:520:GLN:O	12:L:524:LEU:HG	2.09	0.52
17:R:1158:GLU:O	17:R:1162:ILE:HG12	2.08	0.52
18:S:133:ARG:O	18:S:136:ALA:HB3	2.10	0.52
22:X:104:CYS:O	22:X:107:GLU:HG3	2.10	0.52
11:K:200:ARG:HE	18:S:736:MET:HA	1.74	0.52
11:K:672:SER:O	11:K:676:LEU:HG	2.10	0.52
11:K:679:LEU:HD22	11:K:726:VAL:HG12	1.91	0.52
9:I:476:LEU:H	9:I:505:TRP:HZ2	1.58	0.52
18:S:217:ARG:O	18:S:221:LEU:HG	2.10	0.52
23:Y:82:LEU:HD13	23:Y:85:LEU:HD21	1.91	0.52
12:L:594:PHE:CE2	12:L:617:ARG:HB2	2.44	0.52
14:O:164:PHE:HD2	14:O:165:LEU:HD22	1.74	0.52
14:O:190:MET:O	14:O:193:TYR:HB2	2.10	0.52
18:S:841:TYR:O	18:S:897:ARG:NH2	2.40	0.52
17:R:755:ASN:O	17:R:759:ASN:ND2	2.42	0.52
18:S:110:CYS:SG	18:S:111:HIS:N	2.83	0.52
17:R:244:ASP:OD1	17:R:244:ASP:N	2.42	0.52
20:V:200:VAL:HG22	20:V:214:VAL:HG23	1.92	0.52
12:L:325:VAL:HG22	12:L:328:GLN:HB2	1.93	0.51
17:R:984:LEU:HD11	17:R:1026:LEU:HD22	1.91	0.51
22:X:166:GLN:HE21	23:Y:61:PRO:HD2	1.75	0.51
11:K:744:THR:OG1	11:K:745:LEU:N	2.43	0.51
9:I:311:LEU:HD21	9:I:376:LEU:HD11	1.90	0.51
9:I:915:GLN:NE2	9:I:919:HIS:O	2.43	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:365:HIS:O	12:L:368:VAL:HG22	2.09	0.51
17:R:767:TRP:HE3	17:R:792:LEU:HD22	1.75	0.51
17:R:866:ILE:HD13	17:R:966:VAL:HG22	1.93	0.51
17:R:999:ASP:N	17:R:999:ASP:OD1	2.44	0.51
8:H:88:LYS:O	8:H:92:MET:HG3	2.11	0.51
17:R:795:LYS:O	17:R:798:LEU:HB3	2.10	0.51
17:R:142:LEU:HA	17:R:145:ILE:HD12	1.92	0.51
22:X:128:GLN:HA	22:X:131:ASP:OD1	2.11	0.51
11:K:510:SER:O	11:K:513:ILE:HG12	2.10	0.51
17:R:770:MET:HA	17:R:773:GLU:HG2	1.93	0.51
16:Q:124:SER:O	16:Q:127:LEU:HB3	2.11	0.51
17:R:162:ALA:O	17:R:166:VAL:HG23	2.09	0.51
17:R:793:LEU:HA	17:R:796:MET:HG3	1.93	0.51
17:R:1064:GLU:O	17:R:1068:TYR:N	2.33	0.51
18:S:10:ILE:HD11	18:S:47:LEU:HD11	1.92	0.51
18:S:245:HIS:O	18:S:249:LEU:HG	2.10	0.51
18:S:298:GLU:HA	18:S:354:ARG:HH22	1.75	0.51
13:M:187:ARG:O	13:M:190:ALA:HB3	2.11	0.51
17:R:827:ALA:O	17:R:831:VAL:HG23	2.11	0.51
17:R:1220:SER:OG	17:R:1258:ARG:NE	2.43	0.51
20:V:59:ASN:O	20:V:62:SER:OG	2.19	0.51
22:X:66:LEU:HD11	22:X:115:LEU:HD13	1.92	0.51
11:K:125:LEU:HD11	11:K:163:PRO:HB2	1.93	0.51
11:K:272:LYS:HG3	11:K:274:LEU:H	1.76	0.51
17:R:601:LEU:O	17:R:605:LEU:HG	2.11	0.51
18:S:282:VAL:HA	18:S:285:ILE:HG22	1.91	0.51
19:T:123:GLN:O	19:T:126:ASP:HB2	2.11	0.51
10:J:680:GLN:HA	10:J:683:VAL:HG12	1.92	0.50
11:K:610:ASP:HA	11:K:613:LEU:HD12	1.92	0.50
10:J:723:GLU:H	10:J:735:PRO:HA	1.76	0.50
11:K:598:LEU:H	11:K:598:LEU:HD23	1.76	0.50
16:Q:61:MET:O	16:Q:66:ALA:N	2.35	0.50
8:H:99:TYR:OH	8:H:103:LYS:NZ	2.37	0.50
17:R:310:TYR:O	17:R:313:GLU:HB3	2.12	0.50
17:R:591:THR:HG23	17:R:597:ALA:HA	1.93	0.50
18:S:124:LEU:O	18:S:128:LEU:HD12	2.11	0.50
11:K:197:LEU:HD13	18:S:678:GLN:HE22	1.75	0.50
11:K:672:SER:O	11:K:675:LEU:HG	2.11	0.50
19:T:155:ALA:HB1	19:T:163:GLY:H	1.76	0.50
12:L:341:ILE:HD12	12:L:341:ILE:H	1.75	0.50
12:L:503:VAL:HG12	12:L:507:GLY:HA2	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:T:75:ASP:OD2	19:T:107:GLY:N	2.44	0.50
21:W:81:ILE:O	21:W:85:LEU:HG	2.11	0.50
17:R:688:ILE:HG21	17:R:719:ILE:HD11	1.94	0.50
17:R:866:ILE:HG13	17:R:867:LEU:H	1.76	0.50
10:J:718:SER:OG	10:J:719:VAL:N	2.44	0.50
17:R:374:TRP:O	17:R:378:GLN:HG2	2.12	0.50
17:R:890:LEU:HD13	17:R:987:LEU:HD21	1.94	0.50
17:R:999:ASP:O	17:R:1000:ARG:NE	2.43	0.50
9:I:484:MET:O	9:I:488:LEU:HG	2.11	0.50
17:R:617:PRO:HA	17:R:620:ARG:HG2	1.93	0.50
17:R:682:GLU:HB2	17:R:867:LEU:HD23	1.94	0.50
18:S:74:SER:HB3	18:S:120:LEU:HD12	1.93	0.50
18:S:168:THR:O	18:S:174:ASN:ND2	2.44	0.50
20:V:178:ILE:HG13	20:V:192:VAL:HG23	1.93	0.50
21:W:77:VAL:O	21:W:81:ILE:HG12	2.11	0.50
9:I:408:ILE:HG21	12:L:325:VAL:HG12	1.93	0.50
9:I:750:HIS:NE2	12:L:574:GLY:O	2.39	0.50
12:L:434:LYS:HE3	12:L:494:ASN:HB2	1.93	0.50
17:R:803:ILE:HG12	17:R:805:GLN:H	1.77	0.50
17:R:1227:ILE:HA	17:R:1230:PHE:HB3	1.94	0.50
20:V:15:SER:O	20:V:18:ILE:HB	2.12	0.50
11:K:492:GLU:O	11:K:495:HIS:ND1	2.44	0.49
17:R:187:ILE:O	17:R:191:TYR:N	2.41	0.49
17:R:601:LEU:HB3	17:R:605:LEU:HD11	1.94	0.49
11:K:536:THR:O	11:K:540:LEU:HG	2.12	0.49
17:R:10:GLU:O	17:R:14:LYS:N	2.41	0.49
17:R:1087:PHE:HB2	17:R:1088:PRO:HD3	1.93	0.49
17:R:1147:ASN:O	17:R:1151:LEU:HG	2.12	0.49
20:V:19:SER:O	20:V:22:GLN:HB2	2.12	0.49
11:K:93:ILE:HD13	11:K:167:TRP:HB3	1.92	0.49
17:R:1204:SER:O	17:R:1207:TYR:HB2	2.12	0.49
22:X:88:ASP:OD1	22:X:89:ASN:N	2.46	0.49
10:J:631:ARG:NH2	10:J:635:PHE:O	2.45	0.49
18:S:623:VAL:O	18:S:626:VAL:HG12	2.12	0.49
18:S:755:ARG:HG3	18:S:758:HIS:HB2	1.93	0.49
17:R:1072:ILE:HA	17:R:1075:LEU:HD23	1.95	0.49
18:S:94:VAL:O	18:S:98:LEU:HG	2.13	0.49
18:S:172:THR:H	18:S:175:ARG:HG3	1.78	0.49
20:V:120:HIS:CD2	21:W:77:VAL:HG11	2.47	0.49
11:K:373:ALA:HA	11:K:379:VAL:HG13	1.94	0.49
12:L:331:SER:HB2	12:L:339:LEU:HD12	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:117:ILE:HG23	16:Q:120:ARG:HH21	1.78	0.49
17:R:1213:HIS:O	17:R:1217:HIS:N	2.46	0.49
18:S:266:GLN:O	18:S:269:MET:HG2	2.13	0.49
11:K:748:SER:OG	11:K:749:THR:N	2.46	0.49
12:L:257:VAL:HB	12:L:341:ILE:HG13	1.95	0.49
17:R:1009:LEU:HD12	17:R:1012:TYR:HB2	1.95	0.49
2:A:375:PHE:N	2:A:440:PHE:O	2.34	0.48
9:I:885:LEU:HA	9:I:888:ILE:HG22	1.95	0.48
9:I:1372:LEU:N	9:I:1390:VAL:O	2.46	0.48
10:J:699:CYS:O	10:J:704:THR:N	2.40	0.48
17:R:647:SER:O	17:R:650:LEU:HB3	2.12	0.48
11:K:68:HIS:HE1	11:K:85:LEU:HD23	1.78	0.48
11:K:102:LEU:HD13	11:K:821:ARG:HA	1.94	0.48
11:K:737:LEU:HB3	11:K:739:PHE:CE2	2.47	0.48
12:L:537:GLN:O	21:W:89:ARG:NH2	2.45	0.48
12:L:642:SER:HA	21:W:97:GLN:HE21	1.78	0.48
17:R:639:ASN:O	17:R:817:ARG:NH2	2.39	0.48
20:V:290:ASP:HB2	20:V:300:ARG:HA	1.93	0.48
9:I:714:CYS:HB2	9:I:730:LEU:HD23	1.95	0.48
13:M:50:THR:OG1	13:M:133:GLY:O	2.30	0.48
17:R:1164:LEU:O	17:R:1168:ILE:HG12	2.13	0.48
17:R:1175:SER:OG	17:R:1176:SER:N	2.45	0.48
12:L:204:ASP:HA	12:L:220:PHE:HE2	1.77	0.48
2:A:468:ASP:O	2:A:476:SER:N	2.42	0.48
17:R:570:LEU:O	17:R:574:MET:HG2	2.13	0.48
17:R:767:TRP:O	17:R:771:THR:HG23	2.13	0.48
12:L:549:PHE:CE2	12:L:570:ALA:HB3	2.40	0.48
14:O:67:HIS:HA	14:O:71:TYR:HA	1.94	0.48
17:R:777:ILE:HG13	17:R:780:PHE:HD2	1.77	0.48
17:R:1051:HIS:HB3	17:R:1059:ASN:ND2	2.28	0.48
18:S:130:TRP:HA	18:S:133:ARG:HH11	1.78	0.48
9:I:690:LEU:HB3	9:I:714:CYS:SG	2.54	0.48
13:M:35:LEU:O	13:M:39:LEU:HG	2.13	0.48
14:O:38:THR:HA	14:O:115:THR:HA	1.95	0.48
17:R:564:VAL:O	17:R:567:TYR:HB3	2.14	0.48
18:S:539:ASN:HA	18:S:543:PRO:HD2	1.96	0.48
10:J:749:PHE:HB3	18:S:66:TYR:HE1	1.79	0.48
11:K:608:VAL:HG21	11:K:645:LEU:HD21	1.96	0.48
17:R:225:CYS:SG	17:R:226:SER:N	2.86	0.48
17:R:883:TYR:HE1	17:R:980:VAL:HB	1.79	0.48
9:I:928:TYR:HB3	9:I:963:PRO:HG3	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:R:685:ARG:HH21	17:R:724:PRO:HB3	1.79	0.47
17:R:1021:HIS:O	17:R:1024:ARG:HB3	2.13	0.47
17:R:1142:ILE:O	17:R:1146:MET:HG3	2.14	0.47
17:R:1310:VAL:HG22	17:R:1314:VAL:HG13	1.96	0.47
11:K:194:LEU:HD12	11:K:197:LEU:HD11	1.95	0.47
17:R:145:ILE:HD13	17:R:167:ILE:HD11	1.95	0.47
18:S:41:ASN:HD22	18:S:44:GLU:HB3	1.79	0.47
9:I:648:ALA:O	9:I:652:ALA:N	2.45	0.47
11:K:122:LEU:HA	11:K:122:LEU:HD23	1.73	0.47
11:K:286:ALA:HB3	11:K:290:THR:CB	2.44	0.47
12:L:306:PHE:HZ	12:L:327:ASN:H	1.62	0.47
11:K:661:PRO:HD2	11:K:663:TYR:CE1	2.49	0.47
11:K:754:LEU:HD11	11:K:760:ALA:H	1.78	0.47
17:R:180:ALA:O	17:R:184:VAL:HG23	2.13	0.47
17:R:1297:PHE:O	17:R:1301:MET:HG2	2.14	0.47
18:S:362:PHE:O	18:S:365:GLN:HG3	2.15	0.47
9:I:718:LEU:HD12	12:L:549:PHE:HA	1.96	0.47
11:K:515:ALA:O	11:K:518:ALA:HB3	2.14	0.47
17:R:179:PRO:HD3	17:R:1331:PHE:CD2	2.49	0.47
17:R:602:HIS:CE1	17:R:639:ASN:HD21	2.31	0.47
18:S:755:ARG:O	18:S:759:THR:HG23	2.14	0.47
23:Y:44:ILE:O	23:Y:48:THR:HG23	2.14	0.47
9:I:718:LEU:O	12:L:549:PHE:HB3	2.14	0.47
17:R:907:ASN:ND2	17:R:996:LYS:HB3	2.29	0.47
17:R:1077:ASP:OD1	17:R:1081:GLY:HA3	2.15	0.47
9:I:854:HIS:CE1	9:I:878:LEU:HD11	2.50	0.47
9:I:1371:PHE:HA	9:I:1391:PRO:HA	1.97	0.47
11:K:774:LEU:H	11:K:774:LEU:HD23	1.80	0.47
17:R:175:ALA:HB1	17:R:1328:ARG:HH12	1.78	0.47
17:R:282:MET:HA	17:R:285:ASN:HD21	1.79	0.47
17:R:378:GLN:NE2	17:R:536:LYS:HE3	2.30	0.47
17:R:808:TYR:O	17:R:811:LEU:HG	2.15	0.47
18:S:68:ILE:HG21	18:S:100:ILE:HD11	1.97	0.47
18:S:227:SER:OG	18:S:228:MET:N	2.48	0.47
22:X:114:GLN:O	22:X:117:LEU:HG	2.15	0.47
2:A:374:TYR:HA	2:A:440:PHE:H	1.80	0.47
11:K:434:ASP:OD1	11:K:434:ASP:N	2.48	0.47
11:K:582:VAL:HA	11:K:585:ASN:HB2	1.96	0.47
17:R:423:PHE:HE1	17:R:454:HIS:HD2	1.63	0.47
17:R:637:ASN:HA	17:R:817:ARG:HE	1.78	0.47
17:R:697:VAL:HA	17:R:698:THR:HA	1.51	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:R:821:ALA:O	17:R:825:THR:HG23	2.14	0.47
17:R:980:VAL:O	17:R:983:SER:OG	2.25	0.47
17:R:1156:LEU:HD12	17:R:1160:TYR:CD2	2.48	0.47
18:S:218:CYS:O	18:S:222:ILE:HG12	2.15	0.47
11:K:57:HIS:HA	11:K:759:ARG:HH22	1.80	0.47
18:S:833:ARG:O	18:S:833:ARG:HD3	2.15	0.47
20:V:58:ASP:O	20:V:61:HIS:HB2	2.14	0.47
16:Q:101:ARG:O	16:Q:104:GLN:HB3	2.14	0.47
17:R:1065:ASP:O	17:R:1068:TYR:HB2	2.15	0.47
17:R:1149:ILE:HA	17:R:1152:ILE:HD12	1.96	0.47
17:R:1266:CYS:O	17:R:1270:ILE:HG12	2.15	0.47
17:R:1275:TYR:CZ	17:R:1298:LEU:HD11	2.50	0.47
20:V:214:VAL:HG13	20:V:239:PHE:HB3	1.97	0.47
11:K:47:THR:N	11:K:68:HIS:O	2.49	0.46
17:R:1273:ALA:O	17:R:1277:MET:HG2	2.15	0.46
17:R:1315:GLU:HA	17:R:1318:ILE:HG22	1.97	0.46
19:T:205:GLU:O	19:T:207:LEU:N	2.43	0.46
9:I:643:PHE:O	9:I:646:VAL:HG12	2.15	0.46
12:L:195:ARG:NE	16:Q:88:LEU:O	2.48	0.46
17:R:1016:LEU:HD11	17:R:1019:ARG:HE	1.79	0.46
9:I:690:LEU:HD23	9:I:691:LEU:N	2.31	0.46
9:I:1190:LEU:HD12	9:I:1211:PRO:HB2	1.98	0.46
11:K:74:CYS:SG	11:K:84:LEU:N	2.79	0.46
11:K:198:ARG:NE	11:K:199:GLY:H	2.13	0.46
17:R:1269:GLU:HA	17:R:1272:VAL:HG12	1.97	0.46
17:R:1276:ASP:O	17:R:1279:LEU:HG	2.15	0.46
18:S:834:HIS:H	18:S:835:ARG:NH1	2.12	0.46
20:V:292:LEU:O	20:V:294:PRO:HD2	2.15	0.46
17:R:451:LEU:HD22	17:R:454:HIS:CE1	2.50	0.46
11:K:176:VAL:HG23	11:K:177:THR:H	1.80	0.46
11:K:236:VAL:HG23	11:K:237:VAL:N	2.31	0.46
17:R:616:GLN:HE22	17:R:618:HIS:HB3	1.80	0.46
17:R:641:LEU:HD23	17:R:641:LEU:H	1.80	0.46
17:R:1044:LEU:O	17:R:1067:TYR:OH	2.23	0.46
17:R:1078:THR:HG23	17:R:1100:PRO:HG2	1.98	0.46
18:S:44:GLU:HA	18:S:47:LEU:HG	1.97	0.46
18:S:298:GLU:HA	18:S:354:ARG:NH2	2.31	0.46
9:I:542:ASN:HB3	9:I:556:ILE:HG12	1.98	0.46
17:R:329:LEU:O	17:R:333:HIS:ND1	2.35	0.46
17:R:774:ASN:HA	17:R:777:ILE:HG22	1.97	0.46
18:S:781:LEU:O	18:S:785:ILE:HG12	2.14	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:V:121:ALA:HB1	23:Y:56:ARG:HG3	1.97	0.46
9:I:343:LEU:HD13	9:I:345:VAL:HG23	1.97	0.46
9:I:599:ASP:HA	9:I:600:ASN:HA	1.50	0.46
17:R:768:LYS:O	17:R:771:THR:OG1	2.28	0.46
19:T:75:ASP:OD1	19:T:76:CYS:N	2.45	0.46
4:C:171:ILE:HD13	9:I:273:HIS:HA	1.97	0.46
9:I:699:ILE:O	9:I:703:THR:OG1	2.31	0.46
18:S:700:PRO:HB2	18:S:703:ARG:HB2	1.97	0.46
9:I:496:ILE:HG13	9:I:497:PRO:HD3	1.98	0.46
11:K:176:VAL:HG23	11:K:177:THR:N	2.31	0.46
11:K:549:SER:O	11:K:553:PRO:HD3	2.15	0.46
11:K:609:GLY:O	11:K:612:VAL:HG22	2.15	0.46
12:L:220:PHE:HA	12:L:235:PRO:HD2	1.97	0.46
17:R:109:TRP:NE1	17:R:149:PRO:HD3	2.31	0.46
20:V:25:ARG:O	20:V:28:VAL:HG22	2.16	0.46
23:Y:51:ILE:HA	23:Y:54:LEU:HD12	1.97	0.46
8:H:101:ARG:NH1	21:W:144:GLU:HA	2.30	0.46
9:I:1215:PHE:O	9:I:1219:VAL:HG13	2.16	0.46
17:R:1158:GLU:HB3	17:R:1159:PRO:HD3	1.98	0.46
18:S:141:ARG:HA	18:S:141:ARG:HD3	1.70	0.46
12:L:432:GLN:O	12:L:435:HIS:HB3	2.17	0.45
17:R:882:CYS:O	17:R:886:ILE:HG13	2.17	0.45
9:I:520:THR:OG1	9:I:521:ILE:N	2.49	0.45
10:J:627:LEU:HD12	22:X:78:ALA:HB1	1.99	0.45
11:K:198:ARG:HE	11:K:199:GLY:N	2.13	0.45
17:R:452:LYS:HG3	17:R:453:LEU:HD12	1.98	0.45
9:I:724:ARG:O	9:I:725:THR:OG1	2.32	0.45
10:J:740:ARG:HG2	10:J:744:TYR:HD2	1.81	0.45
17:R:1075:LEU:O	17:R:1078:THR:OG1	2.31	0.45
18:S:915:ALA:HA	18:S:918:HIS:CE1	2.51	0.45
11:K:586:LEU:HD12	11:K:587:LYS:N	2.31	0.45
12:L:441:ARG:O	12:L:444:ALA:HB3	2.16	0.45
12:L:492:GLN:HB3	12:L:502:VAL:HG23	1.98	0.45
16:Q:105:LEU:O	16:Q:108:LEU:HB3	2.16	0.45
17:R:177:LEU:HD22	17:R:178:LEU:HD23	1.97	0.45
18:S:915:ALA:HB1	18:S:919:THR:HB	1.99	0.45
12:L:287:PRO:HB3	12:L:289:TRP:CZ2	2.52	0.45
18:S:218:CYS:HA	18:S:221:LEU:HD12	1.99	0.45
18:S:360:THR:O	18:S:364:LEU:HG	2.16	0.45
21:W:137:ARG:O	21:W:140:GLN:HG3	2.16	0.45
11:K:482:VAL:HG22	11:K:483:GLN:H	1.82	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:R:790:LEU:HD23	17:R:826:PHE:HB2	1.99	0.45
19:T:192:ARG:O	19:T:196:GLU:HG2	2.17	0.45
8:H:86:SER:O	8:H:90:CYS:N	2.45	0.45
17:R:72:SER:O	17:R:76:ILE:HG12	2.17	0.45
17:R:674:THR:HG23	17:R:675:VAL:H	1.82	0.45
17:R:731:THR:O	17:R:973:ARG:NH2	2.42	0.45
17:R:786:PRO:HB2	17:R:787:PRO:HD3	1.99	0.45
18:S:169:LEU:HD12	18:S:218:CYS:HB2	1.99	0.45
18:S:263:LEU:O	18:S:267:LEU:HG	2.17	0.45
12:L:287:PRO:HB3	12:L:289:TRP:CE2	2.51	0.45
18:S:245:HIS:CE1	18:S:249:LEU:HD11	2.52	0.45
18:S:716:VAL:HG22	18:S:765:LEU:HD13	1.97	0.45
11:K:85:LEU:HD11	11:K:106:TRP:CZ2	2.52	0.45
12:L:339:LEU:HD23	12:L:339:LEU:HA	1.84	0.45
12:L:592:VAL:HG13	12:L:622:GLU:HA	1.98	0.45
17:R:1005:LEU:O	17:R:1008:THR:OG1	2.27	0.45
18:S:182:LYS:HD3	18:S:183:LEU:HD23	1.99	0.45
19:T:23:GLU:N	19:T:145:ILE:O	2.50	0.45
4:C:178:ASP:O	4:C:181:LEU:HB3	2.17	0.45
11:K:431:VAL:HA	11:K:441:MET:HG3	1.99	0.45
17:R:967:PHE:O	17:R:971:ILE:N	2.49	0.45
19:T:119:SER:O	19:T:122:LEU:HB3	2.17	0.45
9:I:496:ILE:N	9:I:497:PRO:HD2	2.31	0.44
11:K:443:ARG:HH12	11:K:476:TRP:HE1	1.65	0.44
13:M:55:GLU:HA	13:M:73:ARG:HG2	2.00	0.44
17:R:598:TRP:O	17:R:600:ILE:N	2.49	0.44
17:R:1061:TRP:HE1	17:R:1115:LEU:HD12	1.82	0.44
18:S:766:LEU:HA	18:S:769:ILE:HG22	1.99	0.44
18:S:766:LEU:O	18:S:769:ILE:HG22	2.17	0.44
18:S:915:ALA:HA	18:S:918:HIS:NE2	2.32	0.44
19:T:65:GLN:HB2	19:T:88:THR:HA	1.98	0.44
23:Y:68:THR:HA	23:Y:71:TYR:CE1	2.52	0.44
23:Y:84:GLN:O	23:Y:87:ILE:HG22	2.17	0.44
9:I:903:THR:OG1	9:I:904:ASN:N	2.50	0.44
17:R:804:SER:O	17:R:805:GLN:HG3	2.17	0.44
17:R:1072:ILE:O	17:R:1075:LEU:HB2	2.18	0.44
17:R:1248:VAL:O	17:R:1252:VAL:HG12	2.17	0.44
18:S:574:GLU:O	18:S:578:SER:OG	2.31	0.44
21:W:138:HIS:O	21:W:142:VAL:HG13	2.17	0.44
9:I:902:ARG:HD3	9:I:903:THR:HB	1.99	0.44
11:K:117:ASP:N	11:K:173:SER:OG	2.46	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:R:67:ILE:HD12	17:R:79:LEU:HG	2.00	0.44
17:R:1158:GLU:HA	17:R:1161:TRP:NE1	2.32	0.44
11:K:225:SER:N	11:K:226:PRO:HD3	2.32	0.44
12:L:471:SER:OG	12:L:494:ASN:ND2	2.45	0.44
17:R:549:LYS:HA	17:R:552:HIS:CD2	2.51	0.44
21:W:92:GLU:O	21:W:96:LEU:HG	2.17	0.44
9:I:727:VAL:HG22	9:I:754:THR:HG22	1.98	0.44
11:K:72:ILE:HG22	11:K:87:ALA:HB2	2.00	0.44
17:R:144:LYS:HD2	17:R:144:LYS:HA	1.87	0.44
17:R:591:THR:HG21	17:R:600:ILE:HD11	1.99	0.44
17:R:963:PHE:CZ	17:R:991:LEU:HD22	2.53	0.44
18:S:732:THR:HA	18:S:735:HIS:CE1	2.52	0.44
18:S:743:CYS:O	18:S:747:ILE:HG12	2.18	0.44
9:I:380:HIS:NE2	9:I:383:PRO:HB3	2.31	0.44
9:I:495:ILE:HG13	9:I:496:ILE:N	2.32	0.44
11:K:733:GLN:NE2	11:K:734:PRO:O	2.51	0.44
17:R:331:TRP:CZ3	17:R:371:HIS:HB3	2.53	0.44
18:S:659:GLU:O	18:S:663:ILE:HG12	2.18	0.44
18:S:742:PHE:CZ	18:S:746:LEU:HD11	2.53	0.44
12:L:196:LYS:HB3	12:L:202:LEU:HA	2.00	0.44
13:M:57:VAL:HA	13:M:71:ARG:HA	2.00	0.44
4:C:172:PHE:HA	4:C:175:GLN:HB3	1.99	0.44
9:I:1356:PRO:HA	9:I:1357:PRO:HD3	1.87	0.44
10:J:688:PRO:HG3	12:L:619:PRO:HA	2.00	0.44
12:L:535:VAL:HG21	12:L:637:MET:HB3	1.98	0.44
17:R:63:ILE:O	17:R:67:ILE:HG12	2.17	0.44
17:R:767:TRP:HA	17:R:770:MET:HG2	2.00	0.44
18:S:903:PHE:CE2	18:S:946:PRO:HG3	2.53	0.44
19:T:153:LEU:N	19:T:154:PRO:HD2	2.33	0.44
19:T:209:GLN:N	19:T:210:PRO:HD2	2.33	0.44
9:I:648:ALA:HA	9:I:651:VAL:HG22	2.00	0.44
9:I:679:VAL:O	9:I:680:GLU:HG2	2.18	0.44
11:K:644:GLU:O	11:K:648:VAL:HG13	2.18	0.44
11:K:667:SER:O	11:K:671:ASP:N	2.51	0.44
17:R:537:MET:SD	17:R:537:MET:N	2.88	0.44
18:S:726:SER:O	18:S:729:ILE:HB	2.18	0.44
22:X:58:ARG:NH1	22:X:118:CYS:SG	2.87	0.44
1:E:183:ALA:O	1:E:187:PHE:N	2.49	0.43
17:R:738:PRO:HB2	17:R:741:ALA:HB2	2.00	0.43
17:R:1020:ASP:O	17:R:1023:LYS:HB3	2.18	0.43
17:R:1024:ARG:NH2	17:R:1057:GLU:OE1	2.50	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:R:1088:PRO:HB2	17:R:1092:TRP:HE1	1.80	0.43
17:R:1302:LYS:NZ	17:R:1332:ILE:O	2.51	0.43
18:S:250:LEU:HD13	18:S:727:ILE:HG21	1.99	0.43
11:K:122:LEU:HB3	11:K:123:SER:H	1.69	0.43
17:R:685:ARG:NH2	17:R:871:MET:HG2	2.33	0.43
9:I:947:TYR:HE2	9:I:1175:ALA:H	1.66	0.43
13:M:146:TYR:O	13:M:167:TYR:HA	2.19	0.43
17:R:424:ALA:O	17:R:428:ILE:HG23	2.18	0.43
8:H:101:ARG:HH22	21:W:144:GLU:HA	1.83	0.43
11:K:120:VAL:HG21	11:K:170:VAL:HB	2.00	0.43
17:R:591:THR:HA	17:R:594:LYS:HB3	2.00	0.43
17:R:1109:CYS:SG	17:R:1110:VAL:N	2.91	0.43
9:I:1226:GLN:HA	9:I:1229:ILE:HG22	1.99	0.43
11:K:143:PHE:CE1	11:K:466:GLU:HB3	2.54	0.43
11:K:207:ALA:HA	11:K:214:ILE:HG23	1.99	0.43
11:K:636:GLY:O	11:K:640:GLY:N	2.47	0.43
12:L:474:LYS:HE2	12:L:474:LYS:HB3	1.81	0.43
17:R:845:LYS:O	17:R:849:ILE:HG22	2.18	0.43
17:R:856:LYS:HA	17:R:857:TYR:HA	1.60	0.43
18:S:668:LEU:O	18:S:671:MET:HG3	2.18	0.43
18:S:673:ALA:HA	18:S:676:LEU:HD13	2.00	0.43
9:I:464:LEU:HG	12:L:323:ILE:HG22	2.00	0.43
11:K:809:ARG:NH2	19:T:27:ASN:O	2.51	0.43
13:M:132:LYS:HG2	13:M:149:PHE:CE2	2.54	0.43
16:Q:102:ASN:O	16:Q:105:LEU:HG	2.18	0.43
17:R:560:ALA:N	17:R:561:PRO:HD2	2.33	0.43
17:R:842:GLN:HG2	17:R:846:CYS:SG	2.58	0.43
1:E:185:VAL:O	13:M:71:ARG:NH2	2.51	0.43
17:R:340:PHE:HZ	17:R:572:VAL:HB	1.84	0.43
11:K:567:LEU:O	11:K:570:ILE:HG12	2.18	0.43
17:R:866:ILE:HD11	17:R:962:ARG:HG2	2.01	0.43
17:R:1300:HIS:CE1	17:R:1304:MET:HG3	2.54	0.43
23:Y:89:PHE:HD1	23:Y:92:LEU:HD12	1.83	0.43
18:S:333:ASP:OD1	18:S:334:VAL:N	2.50	0.43
20:V:112:LYS:O	20:V:115:ASN:HB2	2.19	0.43
21:W:88:ALA:O	21:W:92:GLU:HG2	2.18	0.43
17:R:600:ILE:HG13	17:R:601:LEU:N	2.33	0.43
17:R:976:GLU:HG2	17:R:977:LEU:H	1.84	0.43
18:S:817:SER:O	18:S:820:SER:OG	2.33	0.43
26:9:637:LYS:HD3	26:9:637:LYS:HA	1.91	0.43
11:K:680:LEU:O	11:K:683:LEU:HG	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:192:TRP:CE2	12:L:293:LEU:HD21	2.54	0.42
18:S:314:PRO:O	18:S:318:VAL:HG23	2.19	0.42
22:X:65:GLN:N	22:X:65:GLN:OE1	2.51	0.42
9:I:685:ASN:OD1	9:I:685:ASN:N	2.52	0.42
10:J:740:ARG:O	10:J:744:TYR:HB2	2.19	0.42
10:J:749:PHE:HB3	18:S:66:TYR:CE1	2.54	0.42
17:R:80:TYR:CG	17:R:121:LEU:HD12	2.53	0.42
17:R:964:LEU:HB3	17:R:965:PRO:HD3	2.00	0.42
4:C:37:SER:HA	4:C:38:ASN:HA	1.71	0.42
9:I:1259:SER:N	9:I:1260:PRO:HD2	2.34	0.42
11:K:478:ILE:HA	11:K:481:HIS:CD2	2.54	0.42
12:L:302:CYS:HA	12:L:305:ILE:HG22	2.01	0.42
17:R:122:VAL:HA	17:R:125:ILE:HG22	2.01	0.42
17:R:570:LEU:HB3	17:R:573:TYR:HB2	2.00	0.42
17:R:888:LEU:O	17:R:892:LYS:HG2	2.18	0.42
18:S:664:MET:HA	18:S:667:ILE:HG22	2.00	0.42
18:S:719:LYS:O	18:S:761:ARG:NH2	2.52	0.42
18:S:796:TRP:HB3	18:S:917:PRO:HG3	2.01	0.42
23:Y:89:PHE:O	23:Y:92:LEU:HB2	2.20	0.42
9:I:415:ALA:HB1	9:I:462:VAL:HG21	2.01	0.42
9:I:1347:ILE:H	9:I:1360:PRO:HG2	1.84	0.42
11:K:471:THR:HG23	11:K:473:TYR:H	1.85	0.42
17:R:476:LEU:HA	17:R:531:LEU:HD21	2.01	0.42
17:R:704:SER:HB3	17:R:707:ILE:HD13	2.01	0.42
17:R:901:SER:O	17:R:904:VAL:HG13	2.19	0.42
23:Y:50:GLU:O	23:Y:54:LEU:HG	2.19	0.42
9:I:293:LYS:HA	9:I:293:LYS:HD2	1.71	0.42
9:I:830:TRP:CE3	9:I:837:PHE:HE1	2.37	0.42
11:K:381:MET:O	11:K:390:MET:HG3	2.20	0.42
11:K:390:MET:SD	11:K:450:HIS:NE2	2.92	0.42
16:Q:105:LEU:HA	16:Q:108:LEU:HB3	2.00	0.42
17:R:587:GLN:O	17:R:590:PRO:HD2	2.19	0.42
17:R:727:TRP:NE1	17:R:874:HIS:HB2	2.34	0.42
17:R:1017:ARG:HD2	17:R:1018:ASN:N	2.33	0.42
17:R:1246:LEU:HD11	17:R:1294:ILE:HD11	2.02	0.42
18:S:161:CYS:SG	18:S:162:LEU:N	2.92	0.42
18:S:805:THR:HG22	18:S:924:TRP:CD1	2.55	0.42
19:T:199:ALA:HB3	19:T:200:PRO:HD3	2.01	0.42
23:Y:51:ILE:HD12	23:Y:54:LEU:HD12	2.02	0.42
10:J:621:PRO:HB3	22:X:71:GLN:NE2	2.34	0.42
11:K:194:LEU:H	11:K:194:LEU:HD23	1.83	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:430:LEU:HD12	11:K:430:LEU:HA	1.90	0.42
11:K:612:VAL:HA	11:K:615:LEU:HG	2.02	0.42
9:I:332:VAL:N	9:I:344:SER:O	2.52	0.42
9:I:915:GLN:NE2	9:I:919:HIS:HB3	2.35	0.42
9:I:1218:SER:O	9:I:1222:ARG:HG2	2.19	0.42
17:R:764:TYR:O	17:R:768:LYS:HG2	2.19	0.42
17:R:840:GLY:HA2	17:R:843:LEU:HD13	2.00	0.42
17:R:1112:LEU:HD13	17:R:1117:VAL:HG21	2.02	0.42
18:S:502:ALA:HA	18:S:506:GLY:HA2	2.02	0.42
4:C:168:PRO:HD2	4:C:168:PRO:O	2.19	0.42
9:I:928:TYR:OH	9:I:1223:ARG:NH1	2.41	0.42
11:K:506:GLN:O	11:K:510:SER:OG	2.37	0.42
13:M:57:VAL:O	13:M:126:ASP:N	2.50	0.42
17:R:540:ILE:HG13	17:R:541:HIS:N	2.35	0.42
18:S:41:ASN:ND2	18:S:44:GLU:HB3	2.34	0.42
13:M:38:ARG:HE	13:M:38:ARG:HB2	1.70	0.42
18:S:786:LEU:HB2	18:S:787:PRO:HD3	2.01	0.42
11:K:440:SER:OG	11:K:441:MET:N	2.51	0.42
11:K:459:GLN:O	11:K:462:LEU:HG	2.19	0.42
17:R:214:PRO:HB2	17:R:1188:PHE:CE1	2.54	0.42
17:R:650:LEU:O	17:R:654:THR:HG23	2.19	0.42
17:R:672:PRO:HB3	17:R:676:LEU:HD12	2.01	0.42
17:R:895:ASP:OD1	17:R:895:ASP:N	2.52	0.42
2:A:265:MET:HA	2:A:300:PRO:HA	2.01	0.41
9:I:278:ASP:O	9:I:281:HIS:HB3	2.20	0.41
9:I:646:VAL:HG13	9:I:647:LEU:N	2.35	0.41
9:I:689:ARG:HA	9:I:715:THR:HA	2.02	0.41
11:K:722:SER:O	11:K:725:LEU:HG	2.20	0.41
17:R:743:PHE:HB3	17:R:746:ASN:HD21	1.85	0.41
18:S:277:PRO:HG2	18:S:280:LEU:HB2	2.01	0.41
19:T:145:ILE:HD12	19:T:183:VAL:O	2.20	0.41
9:I:307:LEU:O	9:I:311:LEU:HD23	2.19	0.41
9:I:561:LEU:HA	9:I:570:LEU:HD22	2.01	0.41
17:R:972:HIS:HB2	17:R:1008:THR:HG22	2.02	0.41
18:S:978:GLN:O	18:S:982:LYS:HG2	2.21	0.41
9:I:481:LEU:O	9:I:485:GLU:HG2	2.21	0.41
9:I:877:VAL:O	9:I:881:THR:HG22	2.19	0.41
9:I:1223:ARG:O	9:I:1226:GLN:HG3	2.20	0.41
11:K:127:ASN:HD21	11:K:149:ARG:HB2	1.85	0.41
11:K:593:LEU:HD22	11:K:652:TRP:HH2	1.85	0.41
12:L:287:PRO:O	12:L:291:THR:HG23	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:R:680:SER:O	17:R:680:SER:OG	2.30	0.41
17:R:1249:TYR:O	17:R:1253:GLY:N	2.42	0.41
18:S:267:LEU:HA	18:S:270:VAL:HG22	2.03	0.41
2:A:454:PHE:O	2:A:463:VAL:N	2.49	0.41
9:I:561:LEU:HA	9:I:570:LEU:HD13	2.03	0.41
10:J:691:LEU:O	10:J:709:CYS:HA	2.19	0.41
11:K:579:ILE:HA	11:K:582:VAL:HG22	2.02	0.41
12:L:332:GLN:HE21	12:L:335:PRO:HA	1.85	0.41
14:O:154:TRP:CD1	14:O:157:LEU:HD11	2.55	0.41
17:R:536:LYS:HA	17:R:573:TYR:HE1	1.85	0.41
18:S:297:PRO:HG3	18:S:305:TRP:CD1	2.56	0.41
22:X:155:PRO:HB2	22:X:157:PRO:HD2	2.02	0.41
9:I:691:LEU:HD13	10:J:682:GLU:HG3	2.02	0.41
17:R:94:PRO:HG2	17:R:128:GLY:HA2	2.02	0.41
17:R:1176:SER:O	17:R:1178:THR:N	2.53	0.41
9:I:443:ALA:HB3	9:I:461:PHE:HD1	1.86	0.41
11:K:73:THR:H	11:K:86:SER:HG	1.68	0.41
11:K:129:VAL:HG21	11:K:467:TYR:HE1	1.85	0.41
12:L:329:ILE:CG1	12:L:340:SER:HA	2.49	0.41
16:Q:106:ARG:HA	16:Q:109:GLN:HE21	1.85	0.41
17:R:680:SER:HB2	17:R:683:LEU:HB2	2.03	0.41
18:S:42:LEU:O	18:S:79:LEU:HD23	2.20	0.41
19:T:120:THR:O	19:T:123:GLN:HB3	2.21	0.41
22:X:59:TYR:CE2	22:X:63:ILE:HD11	2.56	0.41
11:K:734:PRO:C	11:K:735:LEU:HD12	2.41	0.41
17:R:91:LEU:HB3	17:R:92:LEU:HD12	2.03	0.41
17:R:125:ILE:HD12	17:R:125:ILE:HA	1.89	0.41
17:R:782:VAL:HG23	17:R:783:GLN:HG3	2.02	0.41
17:R:993:GLY:HA2	17:R:1036:ASP:OD1	2.21	0.41
18:S:221:LEU:O	18:S:225:ILE:HG12	2.20	0.41
22:X:58:ARG:O	22:X:61:MET:HG2	2.21	0.41
23:Y:88:LEU:O	23:Y:92:LEU:HG	2.21	0.41
9:I:664:ARG:O	9:I:668:SER:N	2.53	0.41
17:R:490:LEU:HB3	17:R:491:PRO:HD3	2.03	0.41
17:R:540:ILE:HG13	17:R:541:HIS:H	1.86	0.41
17:R:843:LEU:O	17:R:847:ILE:HG12	2.21	0.41
18:S:174:ASN:O	18:S:178:LEU:HG	2.20	0.41
18:S:709:LEU:HG	18:S:710:THR:N	2.36	0.41
9:I:284:VAL:O	9:I:288:LEU:N	2.53	0.41
9:I:775:ASP:O	9:I:779:ILE:HG12	2.21	0.41
10:J:637:HIS:CE1	11:K:777:TYR:H	2.37	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:156:LEU:O	11:K:156:LEU:HD23	2.21	0.41
11:K:209:THR:OG1	11:K:210:GLY:N	2.54	0.41
11:K:455:LYS:O	11:K:458:LEU:HG	2.21	0.41
17:R:144:LYS:O	17:R:147:THR:HG22	2.21	0.41
17:R:617:PRO:O	17:R:620:ARG:HG2	2.20	0.41
17:R:1154:THR:HG22	17:R:1219:SER:HB3	2.02	0.41
18:S:305:TRP:O	18:S:309:THR:HG23	2.21	0.41
18:S:412:GLU:HG2	18:S:413:PRO:CD	2.50	0.41
19:T:166:THR:O	19:T:169:LEU:HG	2.20	0.41
20:V:105:SER:HA	20:V:108:LEU:HD13	2.03	0.41
21:W:55:CYS:HB3	21:W:80:CYS:HB2	1.88	0.41
21:W:86:ASP:O	21:W:90:GLN:HG2	2.20	0.41
22:X:62:LEU:O	22:X:66:LEU:HD12	2.21	0.41
8:H:96:ARG:HD3	23:Y:173:MET:SD	2.61	0.41
11:K:593:LEU:HD23	11:K:594:ASP:H	1.86	0.41
12:L:391:PRO:HG3	12:L:398:PHE:HD1	1.86	0.41
17:R:592:VAL:HA	17:R:597:ALA:HB2	2.03	0.41
17:R:820:VAL:HG23	17:R:821:ALA:H	1.86	0.41
17:R:892:LYS:HA	17:R:892:LYS:HD2	1.86	0.41
17:R:918:HIS:HD2	17:R:921:HIS:NE2	2.19	0.41
17:R:1221:ILE:HG23	17:R:1222:GLY:H	1.86	0.41
18:S:5:ASN:O	18:S:8:GLN:HG2	2.21	0.41
18:S:675:VAL:HG13	18:S:676:LEU:HD12	2.03	0.41
18:S:769:ILE:HD12	18:S:769:ILE:HA	1.85	0.41
20:V:211:ARG:HG3	20:V:231:TRP:HH2	1.86	0.41
9:I:408:ILE:HA	9:I:411:VAL:HG12	2.03	0.40
10:J:740:ARG:HG2	10:J:744:TYR:CD2	2.56	0.40
11:K:675:LEU:O	11:K:678:ARG:HG2	2.21	0.40
12:L:474:LYS:HG2	12:L:491:LEU:HD12	2.03	0.40
17:R:540:ILE:HG13	17:R:541:HIS:ND1	2.36	0.40
17:R:681:GLU:HB2	17:R:824:ARG:HH22	1.85	0.40
18:S:48:GLU:CD	18:S:60:ILE:HG21	2.42	0.40
19:T:125:PHE:HA	19:T:128:PHE:CD2	2.56	0.40
9:I:446:VAL:HG13	9:I:458:LEU:HD23	2.03	0.40
10:J:646:ALA:O	10:J:649:ALA:HB3	2.20	0.40
17:R:684:ASN:O	17:R:688:ILE:HG23	2.21	0.40
17:R:713:LYS:HB2	17:R:713:LYS:HE2	1.90	0.40
18:S:262:PRO:O	18:S:265:GLU:HG2	2.22	0.40
22:X:100:ARG:HG3	22:X:102:ASP:HB3	2.03	0.40
17:R:685:ARG:O	17:R:688:ILE:HG12	2.21	0.40
17:R:727:TRP:HB2	17:R:732:LEU:HD21	2.02	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:R:927:LYS:HE2	17:R:927:LYS:HB3	1.86	0.40
18:S:267:LEU:HD12	18:S:319:LYS:HE2	2.03	0.40
18:S:495:PHE:HE2	18:S:616:VAL:HG21	1.86	0.40
9:I:927:MET:HA	9:I:959:PHE:HB2	2.03	0.40
11:K:644:GLU:HA	11:K:647:VAL:HG12	2.04	0.40
12:L:288:HIS:O	12:L:291:THR:OG1	2.25	0.40
13:M:194:LYS:N	13:M:195:PRO:HD2	2.37	0.40
17:R:972:HIS:HD2	17:R:1008:THR:HA	1.86	0.40
17:R:1107:VAL:O	17:R:1111:GLU:HG3	2.20	0.40
23:Y:18:GLY:HA2	23:Y:19:PRO:HD3	1.92	0.40
18:S:696:TRP:CG	18:S:697:ASN:N	2.89	0.40
18:S:760:LEU:O	18:S:764:GLN:HG2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	E	173/268 (65%)	160 (92%)	13 (8%)	0	100 100
2	A	462/1575 (29%)	420 (91%)	42 (9%)	0	100 100
3	B	154/270 (57%)	152 (99%)	2 (1%)	0	100 100
4	C	172/246 (70%)	152 (88%)	18 (10%)	2 (1%)	13 50
5	D	159/233 (68%)	156 (98%)	3 (2%)	0	100 100
6	F	69/142 (49%)	66 (96%)	3 (4%)	0	100 100
7	G	120/135 (89%)	119 (99%)	1 (1%)	0	100 100
8	H	101/117 (86%)	89 (88%)	9 (9%)	3 (3%)	4 31
9	I	1075/1459 (74%)	943 (88%)	132 (12%)	0	100 100
10	J	165/789 (21%)	136 (82%)	29 (18%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
11	K	710/828 (86%)	578 (81%)	132 (19%)	0	100 100
12	L	545/649 (84%)	463 (85%)	81 (15%)	1 (0%)	47 81
13	M	176/208 (85%)	160 (91%)	16 (9%)	0	100 100
14	O	164/212 (77%)	153 (93%)	11 (7%)	0	100 100
15	P	110/144 (76%)	106 (96%)	4 (4%)	0	100 100
16	Q	129/200 (64%)	117 (91%)	12 (9%)	0	100 100
17	R	1291/1367 (94%)	1116 (86%)	175 (14%)	0	100 100
18	S	901/987 (91%)	811 (90%)	90 (10%)	0	100 100
19	T	191/745 (26%)	166 (87%)	25 (13%)	0	100 100
20	V	272/311 (88%)	231 (85%)	40 (15%)	1 (0%)	34 72
21	W	117/178 (66%)	110 (94%)	7 (6%)	0	100 100
22	X	123/199 (62%)	117 (95%)	6 (5%)	0	100 100
23	Y	150/178 (84%)	133 (89%)	17 (11%)	0	100 100
24	Z	101/131 (77%)	99 (98%)	2 (2%)	0	100 100
26	9	17/2171 (1%)	13 (76%)	4 (24%)	0	100 100
All	All	7647/13742 (56%)	6766 (88%)	874 (11%)	7 (0%)	54 85

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	H	86	SER
4	C	168	PRO
8	H	83	SER
8	H	85	SER
20	V	293	PRO
4	C	182	ILE
12	L	393	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	
4	C	25/223 (11%)	25 (100%)	0	100	100
8	H	13/98 (13%)	13 (100%)	0	100	100
9	I	387/1276 (30%)	386 (100%)	1 (0%)	92	95
10	J	100/693 (14%)	99 (99%)	1 (1%)	76	86
11	K	419/729 (58%)	418 (100%)	1 (0%)	93	96
12	L	182/572 (32%)	182 (100%)	0	100	100
13	M	61/183 (33%)	61 (100%)	0	100	100
14	O	44/177 (25%)	44 (100%)	0	100	100
16	Q	23/173 (13%)	23 (100%)	0	100	100
17	R	952/1231 (77%)	952 (100%)	0	100	100
18	S	395/867 (46%)	390 (99%)	5 (1%)	69	82
19	T	90/598 (15%)	90 (100%)	0	100	100
20	V	96/279 (34%)	96 (100%)	0	100	100
21	W	52/153 (34%)	51 (98%)	1 (2%)	57	75
22	X	65/164 (40%)	65 (100%)	0	100	100
23	Y	61/157 (39%)	61 (100%)	0	100	100
26	9	19/1912 (1%)	19 (100%)	0	100	100
All	All	2984/9485 (32%)	2975 (100%)	9 (0%)	92	95

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	I	902	ARG
10	J	740	ARG
11	K	741	ARG
18	S	133	ARG
18	S	385	ARG
18	S	487	ARG
18	S	833	ARG
18	S	938	ARG
21	W	80	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
9	I	799	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	I	854	HIS
10	J	629	ASN
10	J	637	HIS
11	K	48	HIS
11	K	68	HIS
11	K	134	HIS
11	K	270	HIS
11	K	380	HIS
12	L	332	GLN
12	L	372	ASN
12	L	457	GLN
13	M	134	HIS
16	Q	109	GLN
17	R	103	ASN
17	R	285	ASN
17	R	378	GLN
17	R	534	HIS
17	R	552	HIS
17	R	602	HIS
17	R	664	GLN
17	R	684	ASN
17	R	726	ASN
17	R	730	HIS
17	R	907	ASN
17	R	918	HIS
17	R	1028	HIS
17	R	1059	ASN
17	R	1165	HIS
17	R	1320	ASN
18	S	41	ASN
18	S	71	GLN
18	S	370	GLN
18	S	678	GLN
18	S	758	HIS
20	V	109	GLN
20	V	120	HIS
20	V	252	HIS
21	W	79	GLN
21	W	97	GLN
22	X	83	GLN
22	X	84	ASN
22	X	166	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
23	Y	81	HIS

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

There are no chain breaks in this entry.

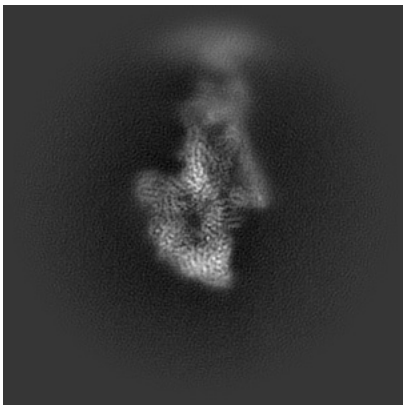
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-40971. These allow visual inspection of the internal detail of the map and identification of artifacts.

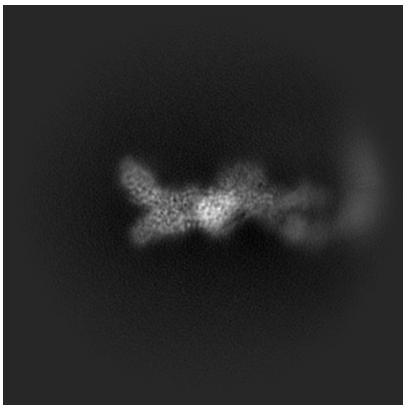
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

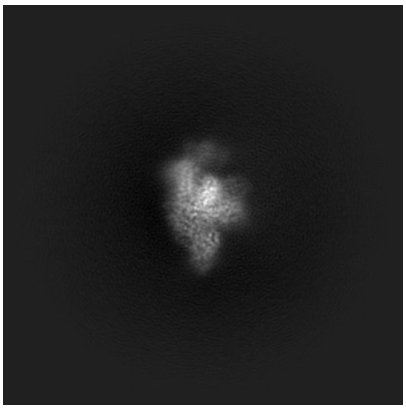
6.1.1 Primary map



X

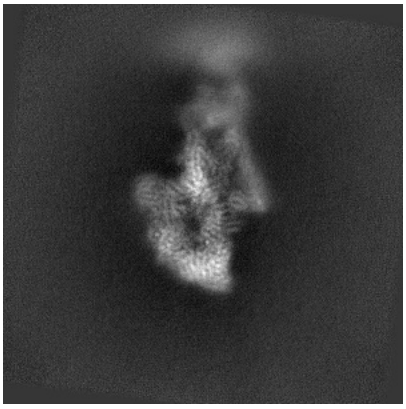


Y

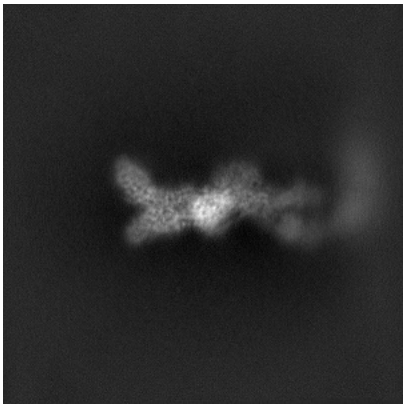


Z

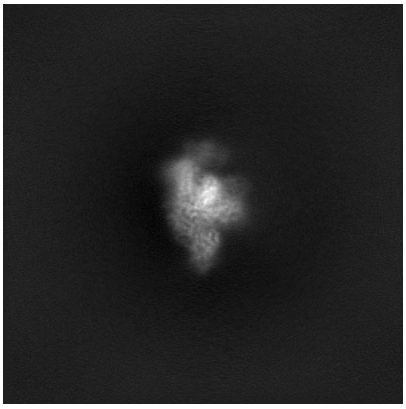
6.1.2 Raw map



X



Y

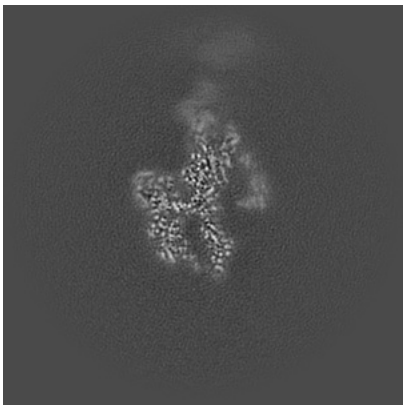


Z

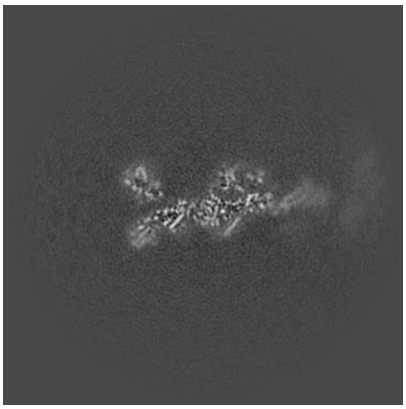
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

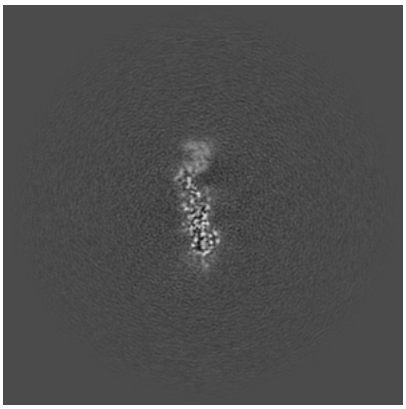
6.2.1 Primary map



X Index: 280

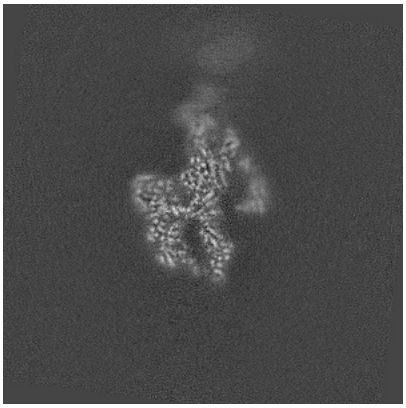


Y Index: 280

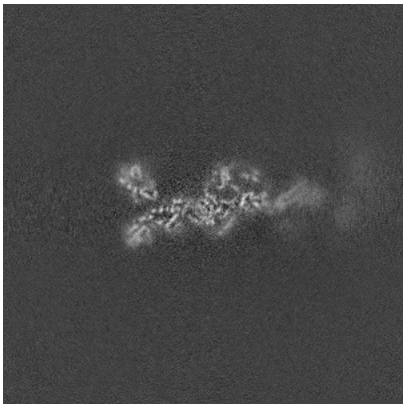


Z Index: 280

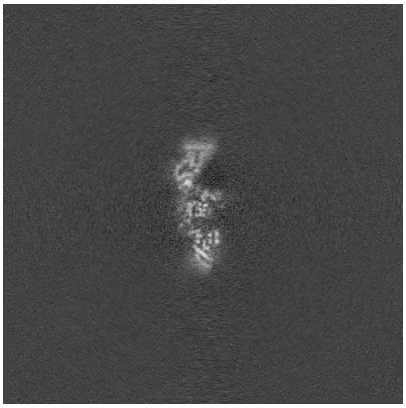
6.2.2 Raw map



X Index: 280



Y Index: 280

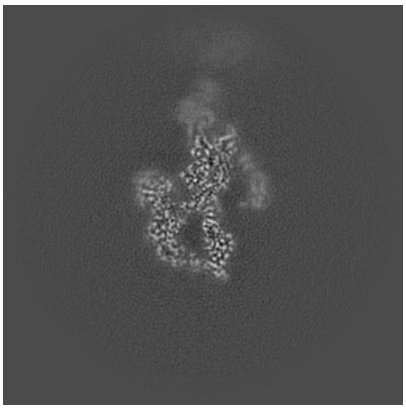


Z Index: 280

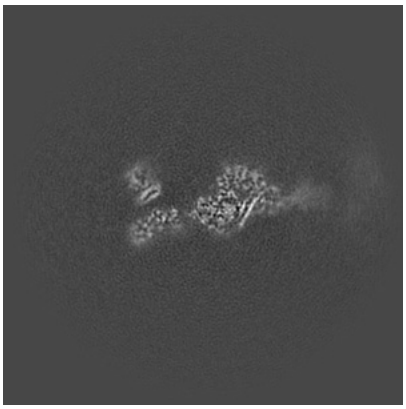
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

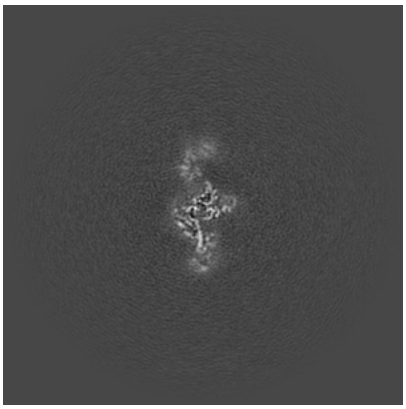
6.3.1 Primary map



X Index: 284

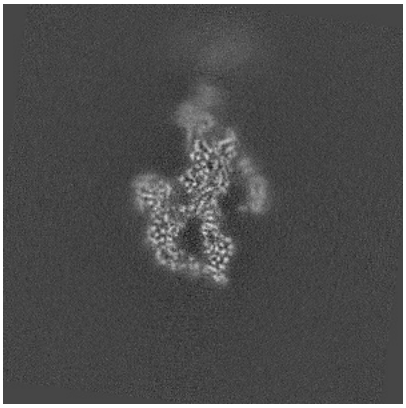


Y Index: 274

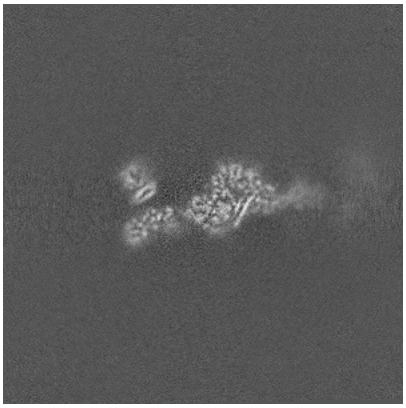


Z Index: 303

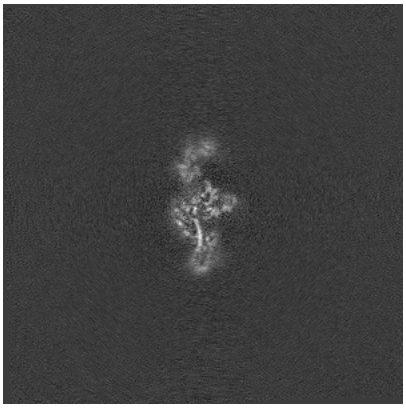
6.3.2 Raw map



X Index: 284



Y Index: 273

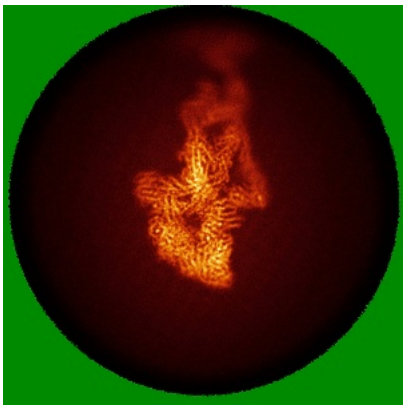


Z Index: 295

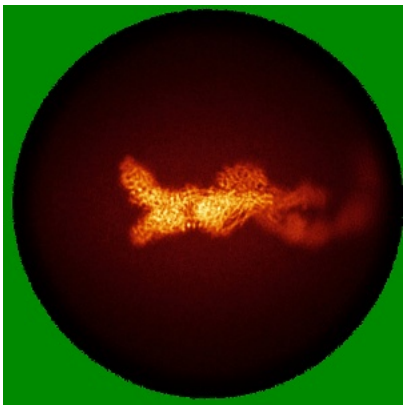
The images above show the largest variance slices of the map in three orthogonal directions.

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

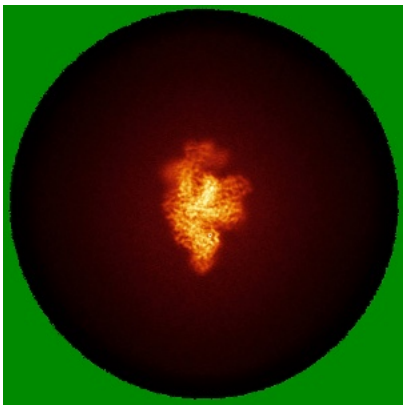
6.4.1 Primary map



X

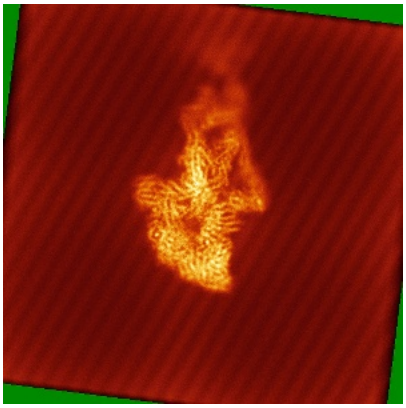


Y

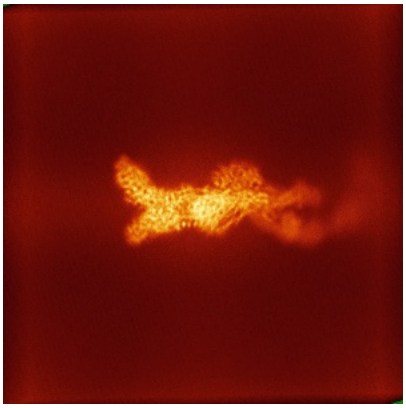


Z

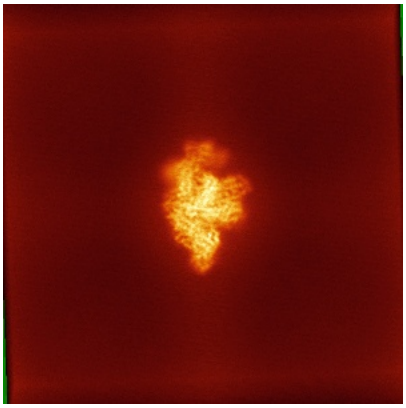
6.4.2 Raw map



X



Y

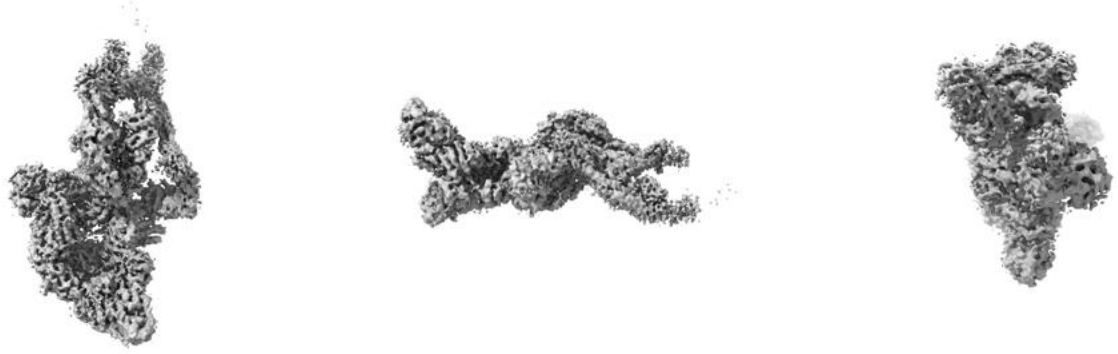


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

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

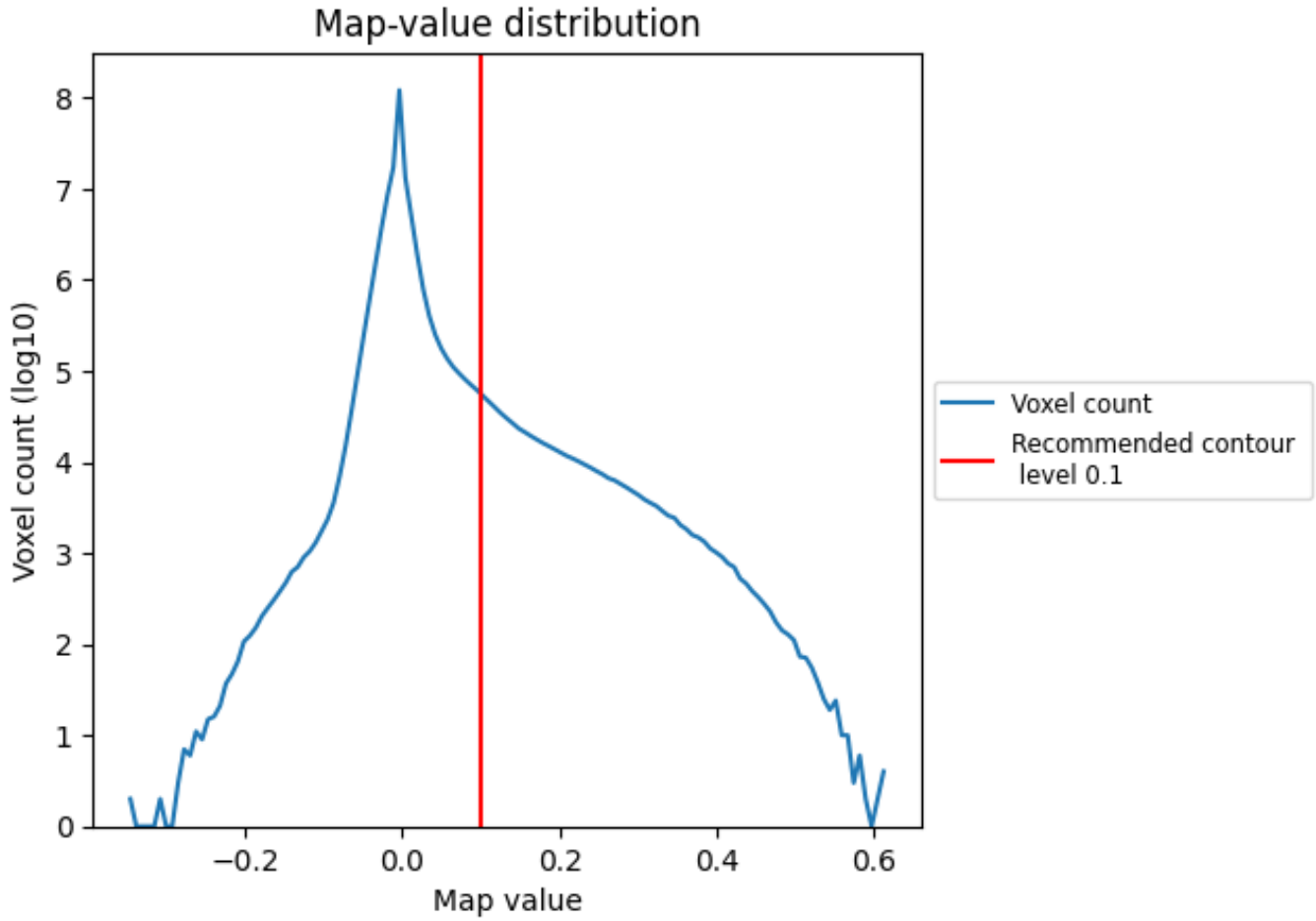
6.6 Mask visualisation (i)

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

7 Map analysis

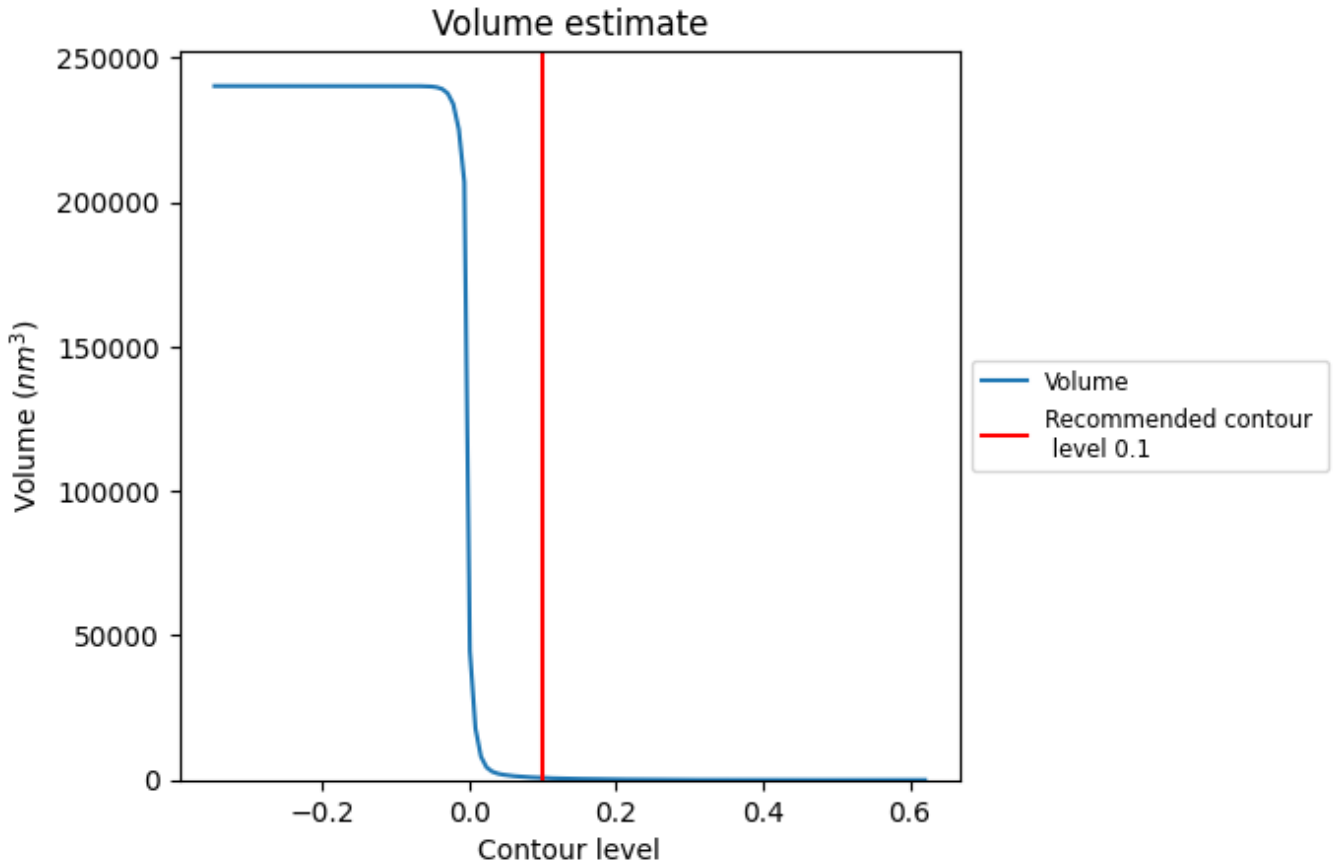
This section contains the results of statistical analysis of the map.

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.

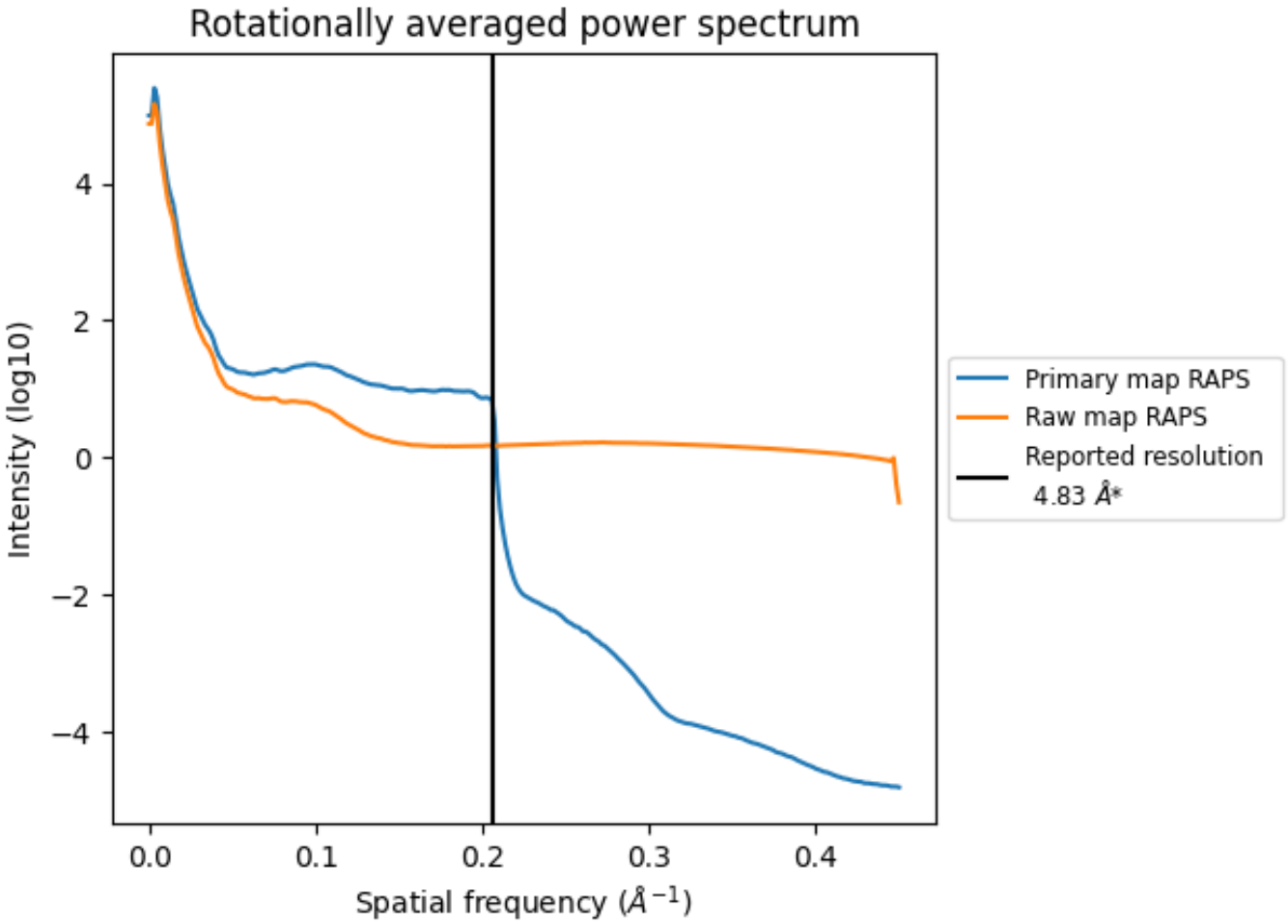
7.2 Volume estimate



The volume at the recommended contour level is 718 nm^3; this corresponds to an approximate mass of 648 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)

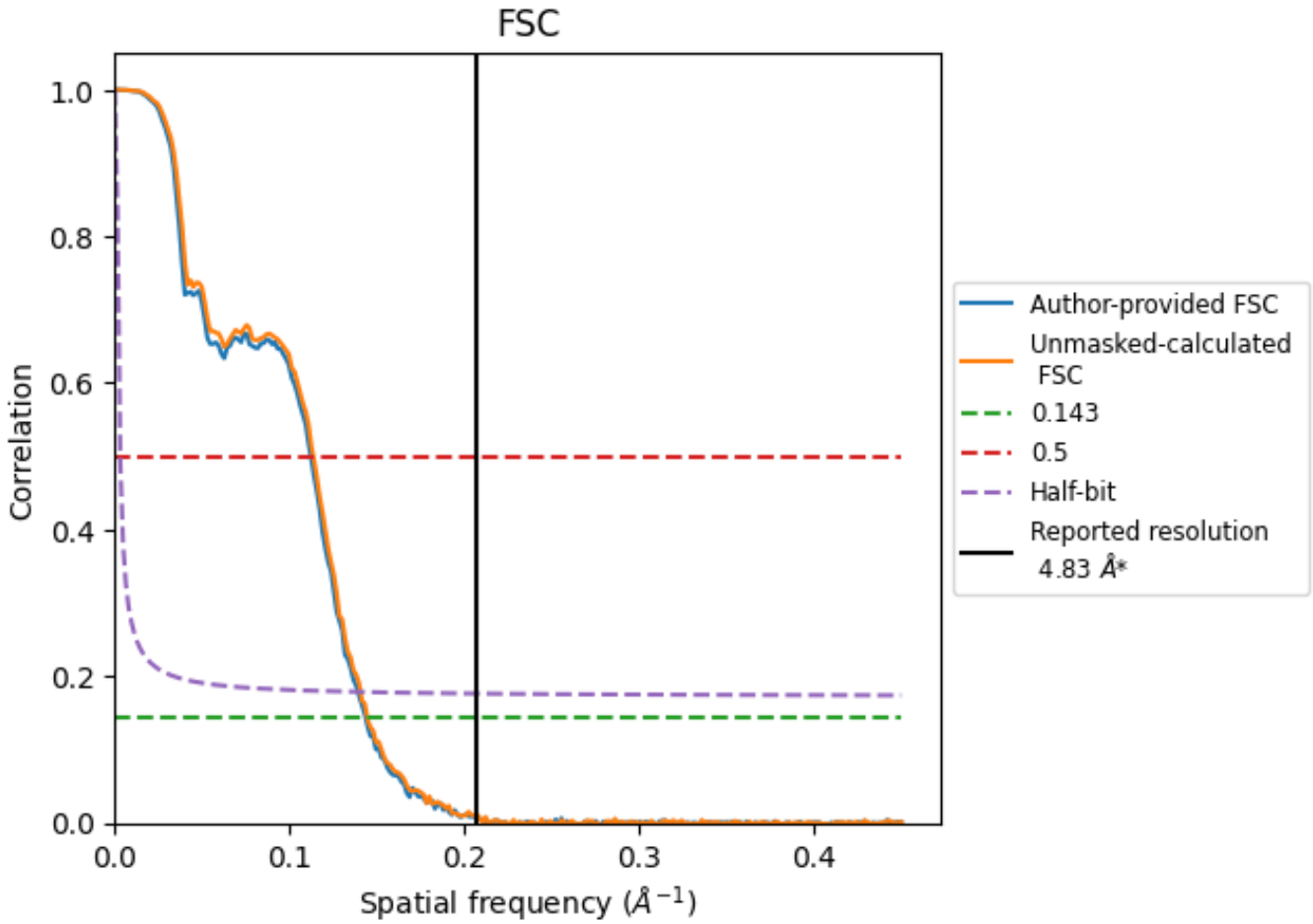


*Reported resolution corresponds to spatial frequency of 0.207 $Å^{-1}$

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.207 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.83	-	-
Author-provided FSC curve	6.96	8.90	7.18
Unmasked-calculated*	6.92	8.80	7.11

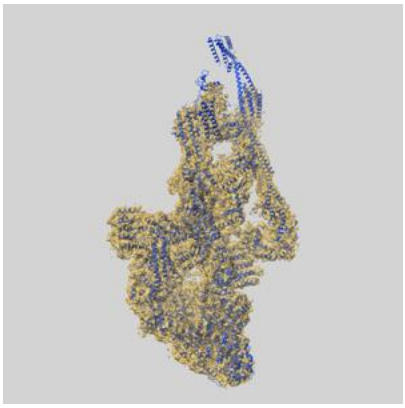
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 6.96 differs from the reported value 4.83 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.92 differs from the reported value 4.83 by more than 10 %

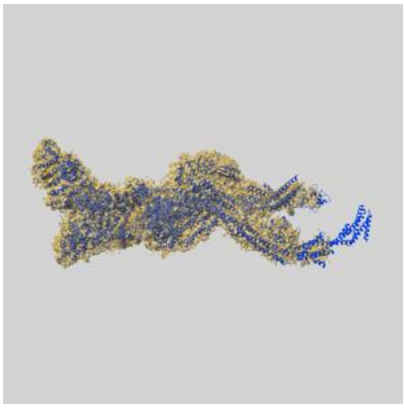
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-40971 and PDB model 8T1L. Per-residue inclusion information can be found in section 3 on page 8.

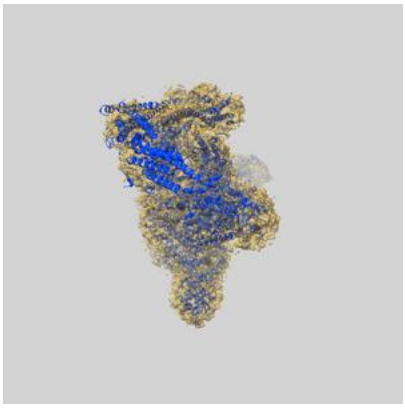
9.1 Map-model overlay



X



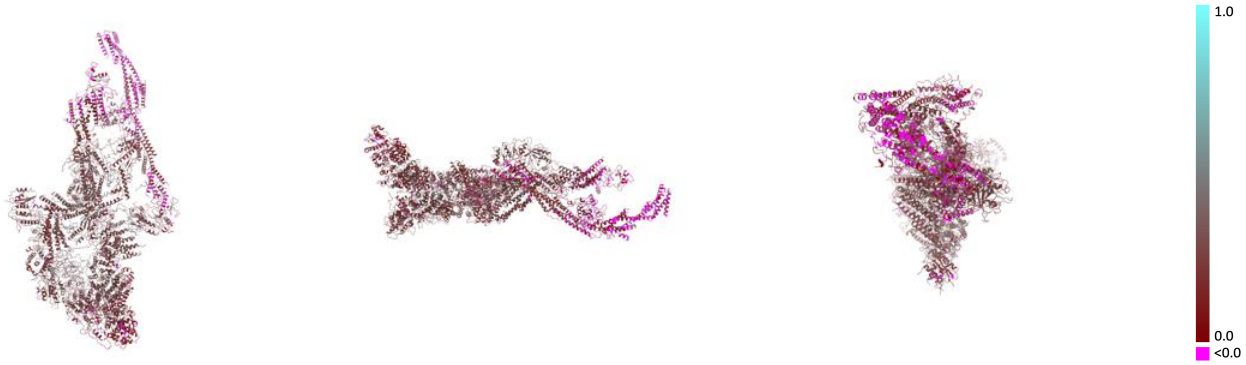
Y



Z

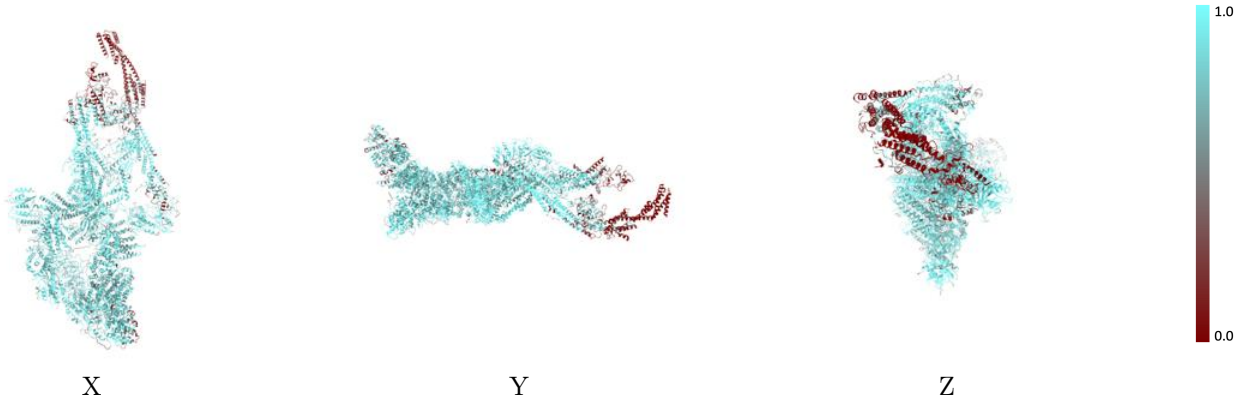
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



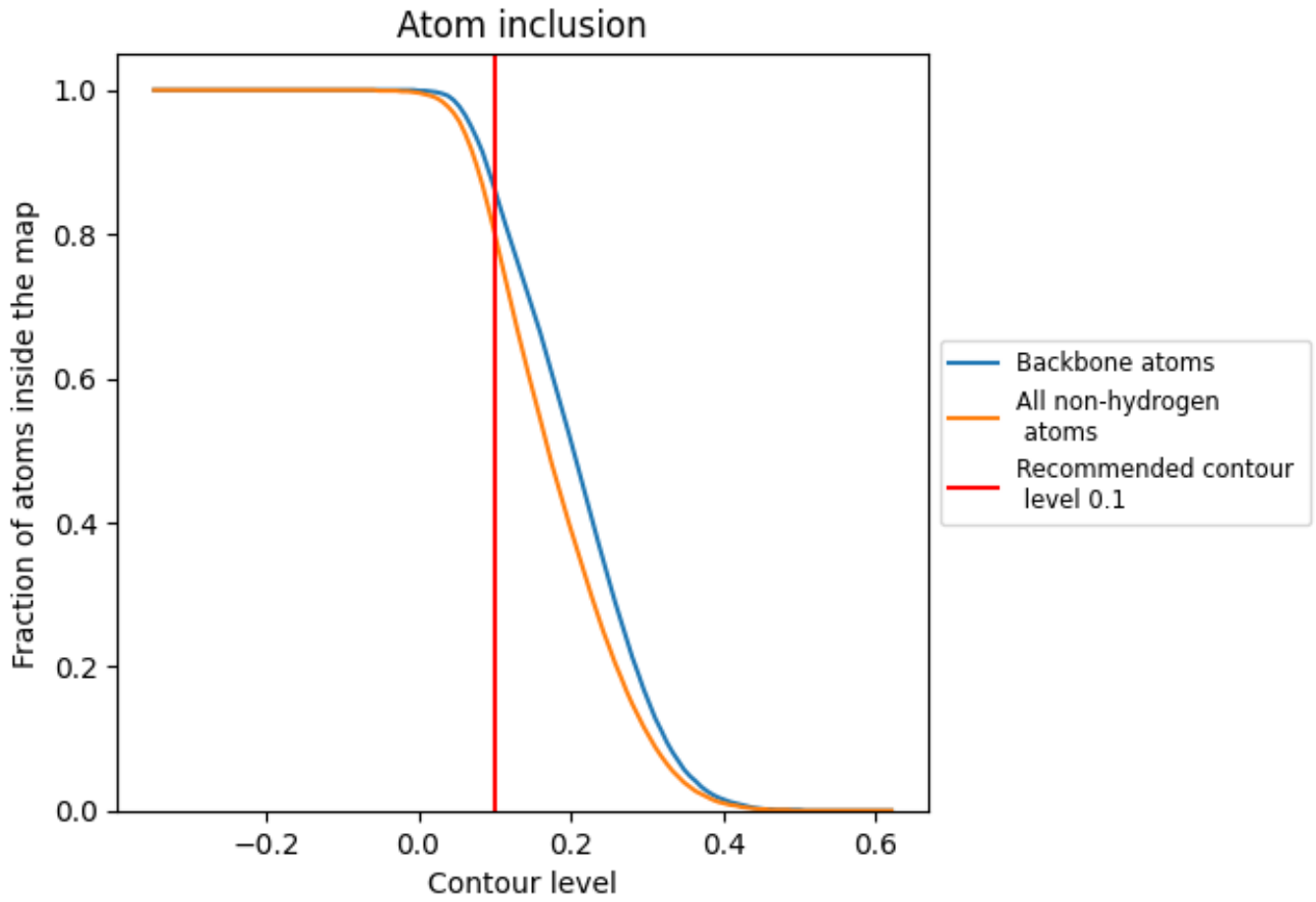
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).

9.4 Atom inclusion (i)



At the recommended contour level, 86% of all backbone atoms, 80% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8020	0.2470
9	0.4750	0.1650
A	0.8390	0.2250
B	0.6940	0.1400
C	0.4310	0.1550
D	0.4160	0.0960
E	0.4980	0.1370
F	0.7490	0.1570
G	0.0430	0.0540
H	0.7920	0.2050
I	0.8130	0.2680
J	0.8700	0.2860
K	0.8660	0.2830
L	0.8260	0.2780
M	0.9250	0.2940
O	0.9420	0.3050
P	0.4470	0.1080
Q	0.8040	0.2150
R	0.8090	0.2300
S	0.8670	0.2700
T	0.8990	0.2750
V	0.9020	0.3150
W	0.8860	0.2840
X	0.8740	0.2650
Y	0.8510	0.2470
Z	0.6300	0.1590
a	0.8900	0.2320