



## Full wwPDB EM Validation Report ⓘ

May 12, 2024 – 05:07 pm BST

PDB ID : 6RDR  
EMDB ID : EMD-4828  
Title : Cryo-EM structure of Polytomella F-ATP synthase, Rotary substate 1D, monomer-masked refinement  
Authors : Murphy, B.J.; Klusch, N.; Yildiz, O.; Kuhlbrandt, W.  
Deposited on : 2019-04-12  
Resolution : 4.10 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

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

EMDB validation analysis : 0.0.1.dev92  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
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) : 2.36.2

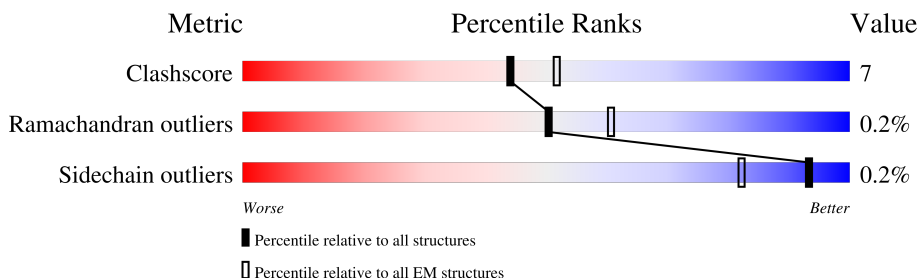
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.10 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	82	<div> <div>68%</div> <div>88%</div> <div>11%</div> <div>.</div> </div>
2	1	618	<div> <div>50%</div> <div>82%</div> <div>14%</div> <div>.</div> </div>
3	2	441	<div> <div>74%</div> <div>85%</div> <div>15%</div> </div>
4	3	325	<div> <div>51%</div> <div>65%</div> <div>11%</div> <div>25%</div> </div>
5	4	294	<div> <div>57%</div> <div>87%</div> <div>11%</div> <div>.</div> </div>
6	5	123	<div> <div>24%</div> <div>81%</div> <div>19%</div> </div>
7	6	151	<div> <div>48%</div> <div>73%</div> <div>9%</div> <div>18%</div> </div>
8	7	190	<div> <div>43%</div> <div>77%</div> <div>16%</div> <div>7%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	8	89	
10	9	97	
11	A	127	
11	B	127	
11	C	127	
11	D	127	
11	E	127	
11	F	127	
11	G	127	
11	H	127	
11	I	127	
11	J	127	
12	M	327	
13	P	229	
14	Q	74	
15	R	199	
16	S	317	
17	T	562	
17	U	562	
17	V	562	
18	X	574	
18	Y	574	
18	Z	574	

## 2 Entry composition

There are 22 unique types of molecules in this entry. The entry contains 53748 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 ASA-10: Polytomella F-ATP synthase associated subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	81	Total	C	N	O	S	0	0
			607	388	107	110	2		

- Molecule 2 is a protein called ATP synthase associated protein ASA1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	595	Total	C	N	O	S	0	0
			4661	2958	798	900	5		

- Molecule 3 is a protein called ASA-2: Polytomella F-ATP synthase associated subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	2	441	Total	C	N	O	0	0
			3163	2020	532	611		

- Molecule 4 is a protein called Mitochondrial F1F0 ATP synthase associated 32 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	245	Total	C	N	O	S	0	0
			1874	1204	299	370	1		

- Molecule 5 is a protein called Mitochondrial ATP synthase associated protein ASA4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	290	Total	C	N	O	S	0	0
			2177	1385	356	434	2		

- Molecule 6 is a protein called Mitochondrial F1F0 ATP synthase associated 14 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	5	123	Total	C	N	O	S	0	0
			986	640	172	170	4		

- Molecule 7 is a protein called Mitochondrial ATP synthase subunit ASA6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	124	Total	C	N	O	S	0	0
			926	599	154	172	1		

- Molecule 8 is a protein called Mitochondrial ATP synthase associated protein ASA7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	7	176	Total	C	N	O	S	0	0
			1347	860	227	259	1		

- Molecule 9 is a protein called Mitochondrial ATP synthase subunit ASA8.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	8	88	Total	C	N	O	0	0
			692	456	115	121		

- Molecule 10 is a protein called ASA-9: Polytomella F-ATP synthase associated subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	9	97	Total	C	N	O	S	0	0
			776	514	124	132	6		

- Molecule 11 is a protein called Mitochondrial ATP synthase subunit c.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	A	74	Total	C	N	O	S	0	0
			514	340	83	88	3		
11	B	74	Total	C	N	O	S	0	0
			514	340	83	88	3		
11	C	74	Total	C	N	O	S	0	0
			514	340	83	88	3		
11	D	74	Total	C	N	O	S	0	0
			514	340	83	88	3		
11	E	74	Total	C	N	O	S	0	0
			514	340	83	88	3		
11	F	74	Total	C	N	O	S	0	0
			514	340	83	88	3		
11	G	74	Total	C	N	O	S	0	0
			514	340	83	88	3		
11	H	74	Total	C	N	O	S	0	0
			514	340	83	88	3		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf	Trace
11	I	74	Total	C	N	O	S	0	0
			514	340	83	88	3		
11	J	74	Total	C	N	O	S	0	0
			514	340	83	88	3		

- Molecule 12 is a protein called Mitochondrial ATP synthase subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	217	Total	C	N	O	S	0	0
			1640	1077	267	288	8		

- Molecule 13 is a protein called Mitochondrial ATP synthase subunit OSCP.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	P	193	Total	C	N	O	S	0	0
			1532	988	250	290	4		

- Molecule 14 is a protein called epsilon: Polytomella F-ATP synthase epsilon subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Q	72	Total	C	N	O	S	0	0
			561	358	102	99	2		

- Molecule 15 is a protein called Mitochondrial ATP synthase subunit delta.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	R	177	Total	C	N	O	S	0	0
			1303	833	213	256	1		

- Molecule 16 is a protein called ATP synthase gamma chain, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	S	277	Total	C	N	O	S	0	0
			2130	1327	377	416	10		

- Molecule 17 is a protein called ATP synthase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	T	523	Total	C	N	O	S	0	0
			3979	2537	703	728	11		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf	Trace
17	U	523	Total	C	N	O	S	0	0
			3980	2537	703	729	11		
17	V	520	Total	C	N	O	S	0	0
			3962	2527	700	724	11		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	266	ARG	LYS	conflict	UNP A0ZW40
U	266	ARG	LYS	conflict	UNP A0ZW40
V	266	ARG	LYS	conflict	UNP A0ZW40

- Molecule 18 is a protein called ATP synthase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	X	542	Total	C	N	O	S	0	0
			4115	2586	696	820	13		
18	Y	521	Total	C	N	O	S	0	0
			3957	2485	670	789	13		
18	Z	538	Total	C	N	O	S	0	0
			4087	2568	692	814	13		

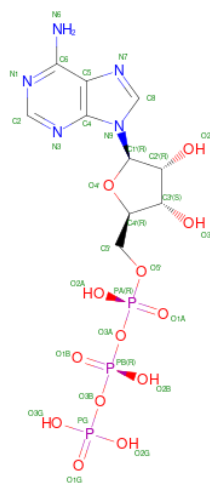
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	350	ALA	GLY	conflict	UNP A0ZW41
X	387	LEU	ARG	conflict	UNP A0ZW41
Y	350	ALA	GLY	conflict	UNP A0ZW41
Y	387	LEU	ARG	conflict	UNP A0ZW41
Z	350	ALA	GLY	conflict	UNP A0ZW41
Z	387	LEU	ARG	conflict	UNP A0ZW41

- Molecule 19 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
19	M	1	Total	Zn	0
			1	1	

- Molecule 20 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).



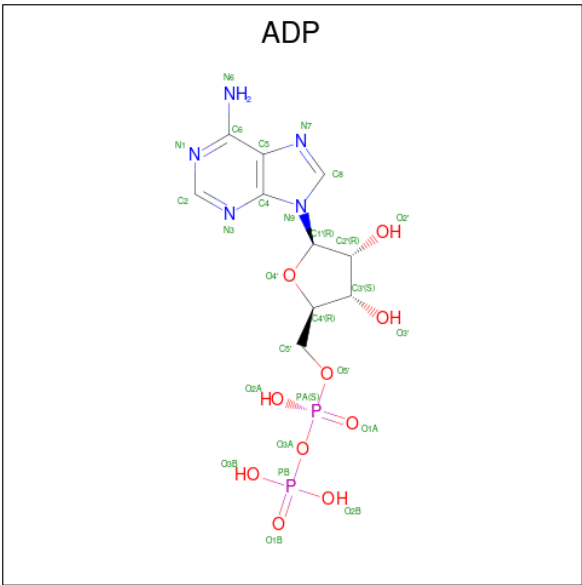
Mol	Chain	Residues	Atoms					AltConf
20	T	1	Total 31	C 10	N 5	O 13	P 3	0
20	U	1	Total 31	C 10	N 5	O 13	P 3	0
20	V	1	Total 31	C 10	N 5	O 13	P 3	0

- Molecule 21 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
21	T	1	Total Mg 1 1	0
21	U	1	Total Mg 1 1	0
21	V	1	Total Mg 1 1	0
21	X	1	Total Mg 1 1	0
21	Y	1	Total Mg 1 1	0

- Molecule 22 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$ ).



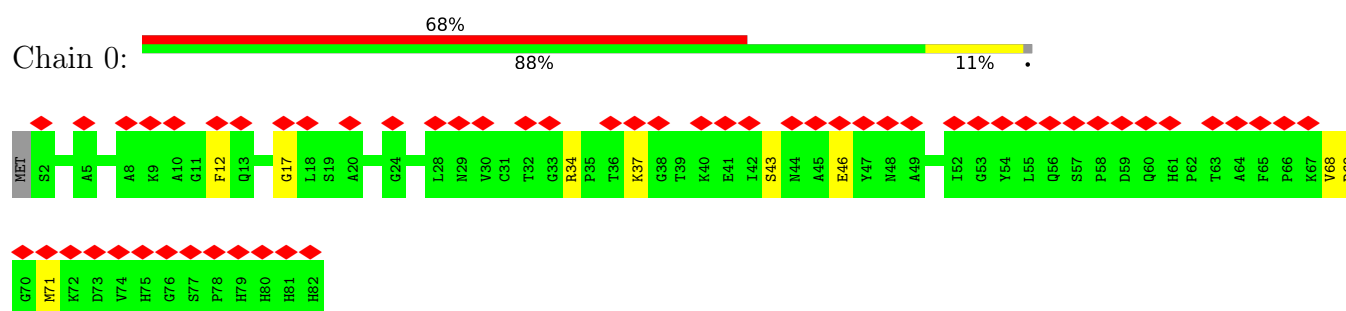


Mol	Chain	Residues	Atoms					AltConf
22	X	1	Total	C	N	O	P	0
			27	10	5	10	2	
22	Y	1	Total	C	N	O	P	0
			27	10	5	10	2	

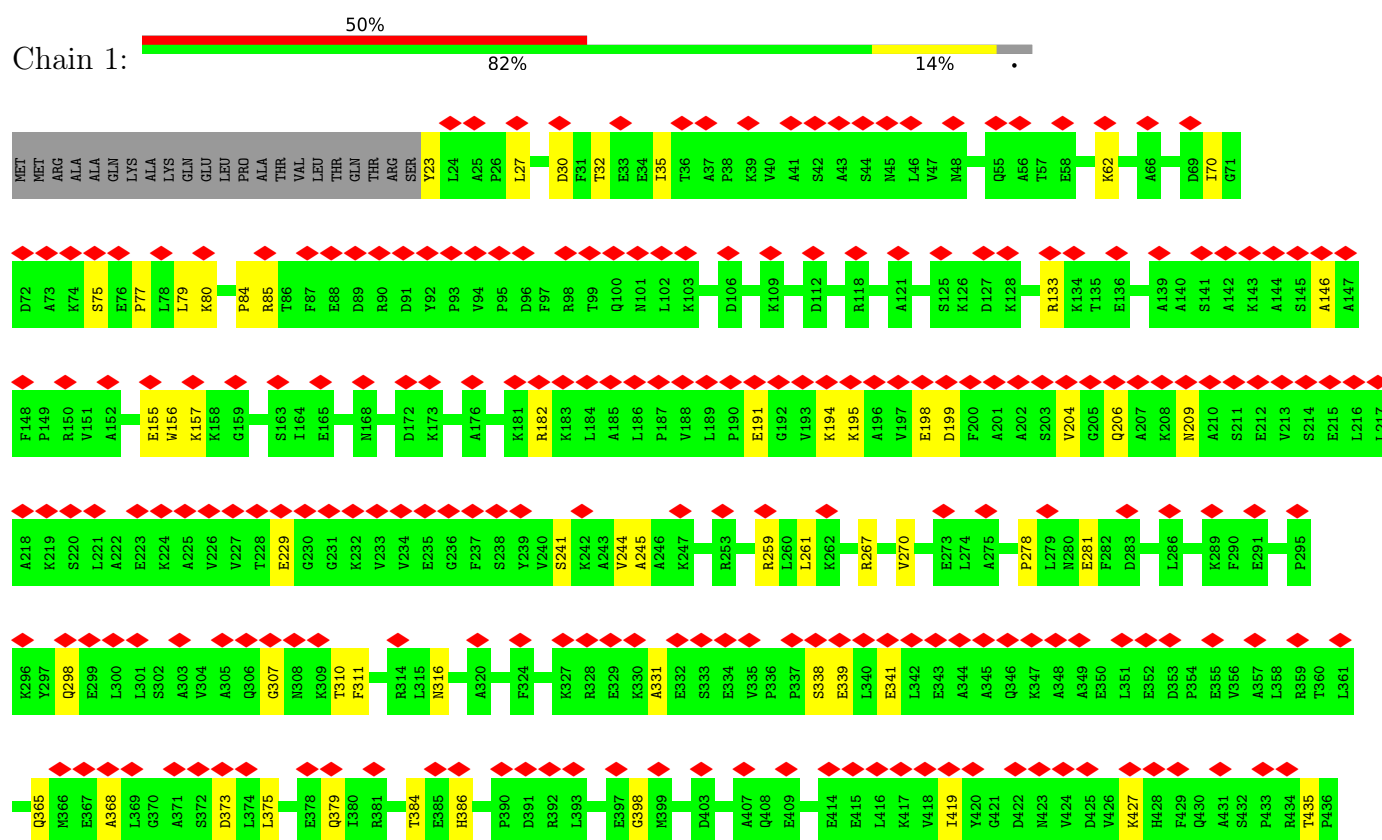
### 3 Residue-property plots

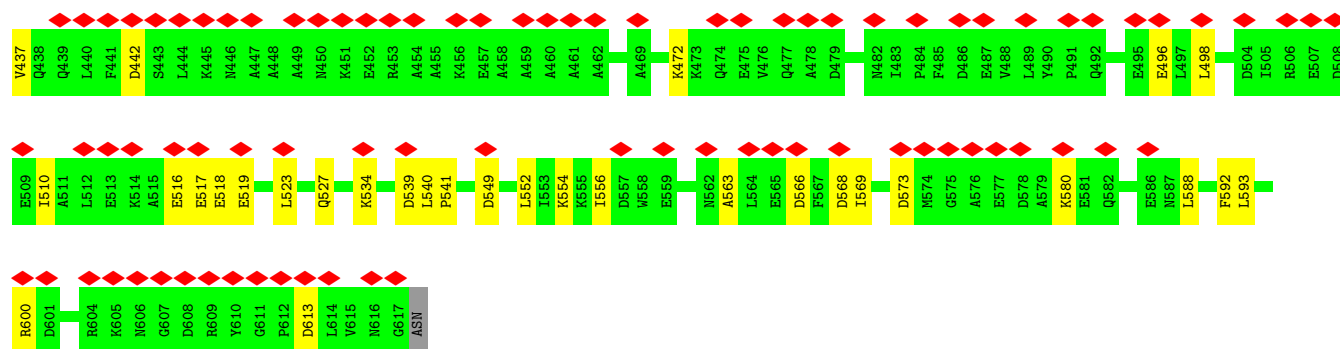
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: ASA-10: *Polytomella* F-ATP synthase associated subunit 10

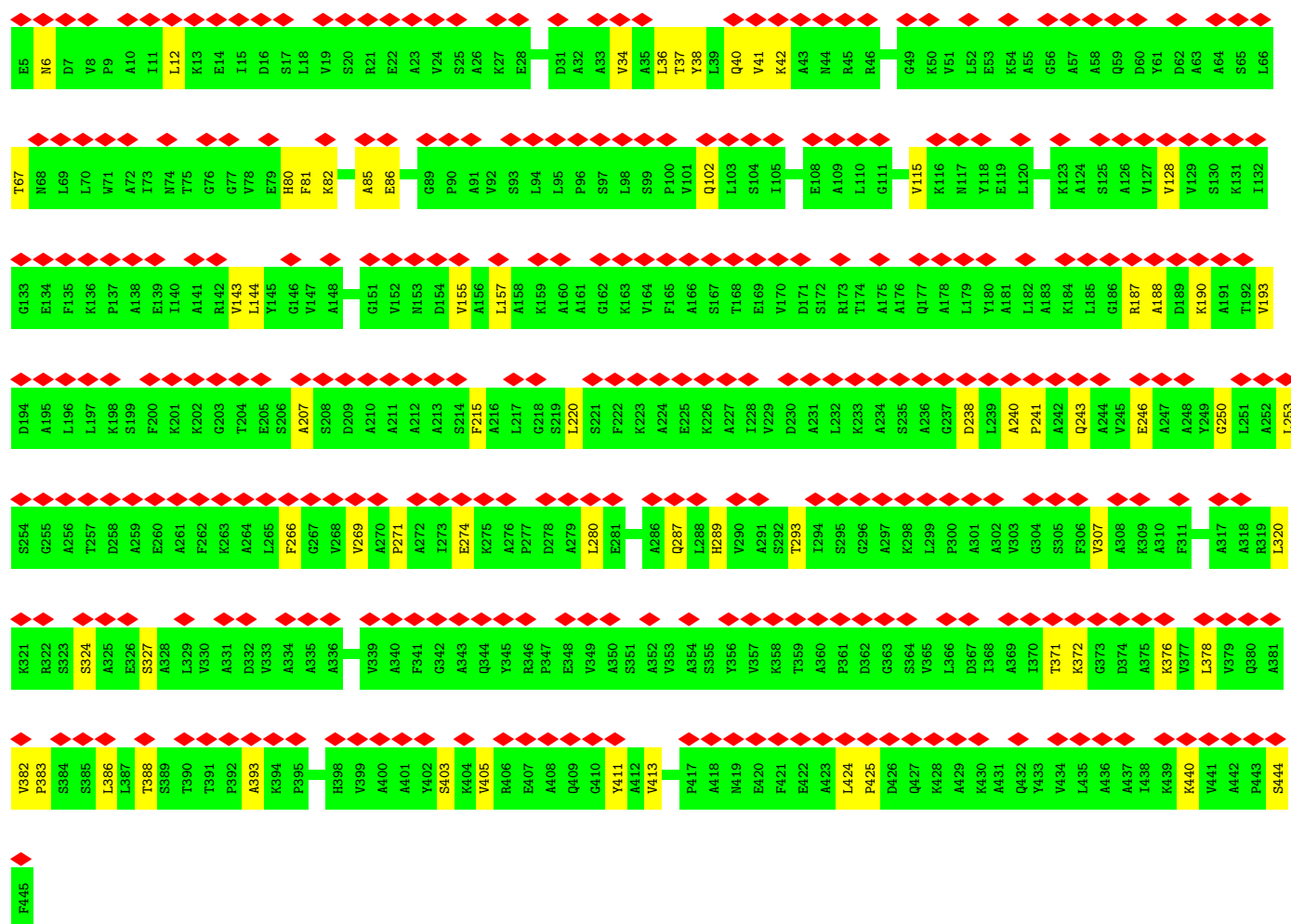
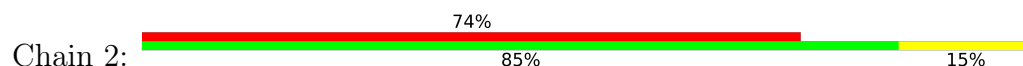


- Molecule 2: ATP synthase associated protein ASA1



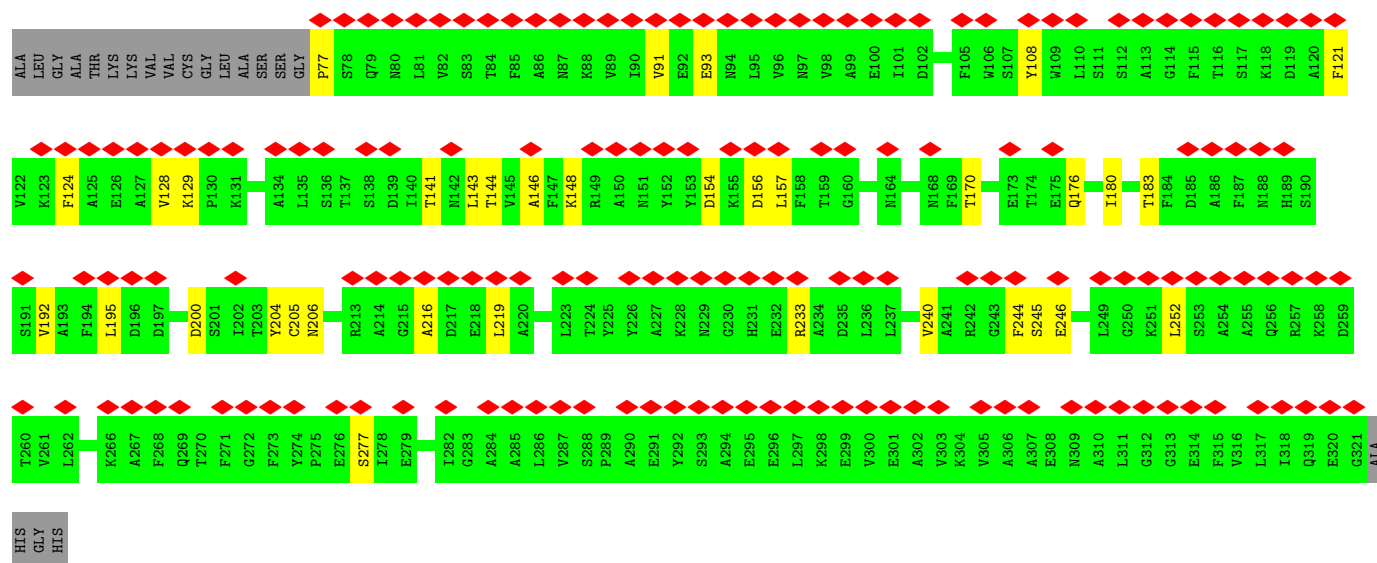


• Molecule 3: *Asa-2*: Polytomella F-ATP synthase associated subunit 2



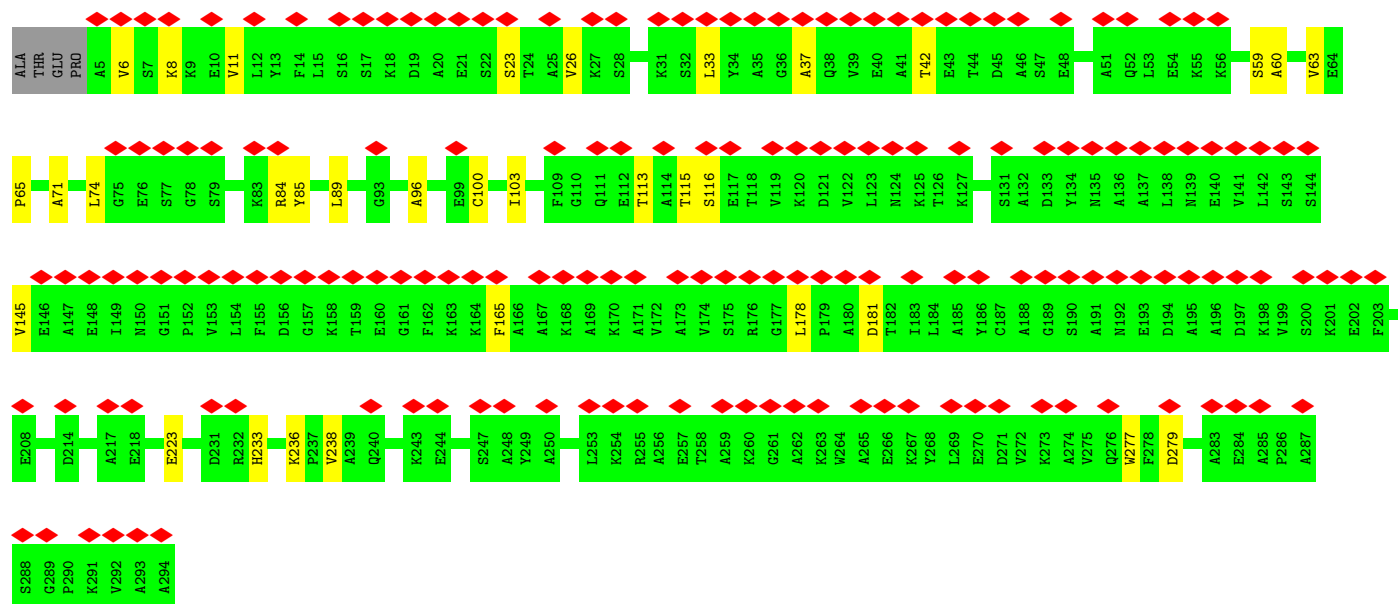
• Molecule 4: Mitochondrial F1F0 ATP synthase associated 32 kDa protein





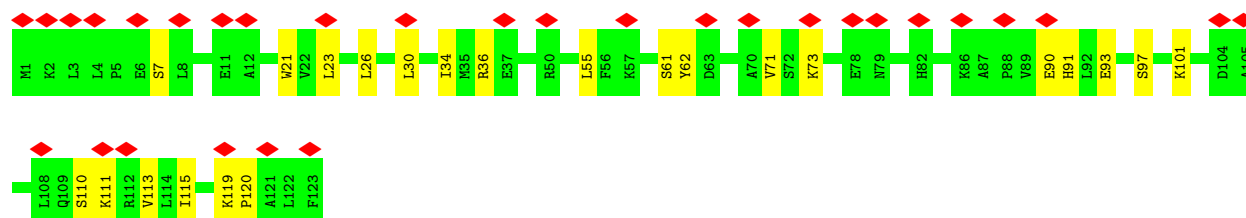
• Molecule 5: Mitochondrial ATP synthase associated protein ASA4

Chain 4: 57% 87% 11%

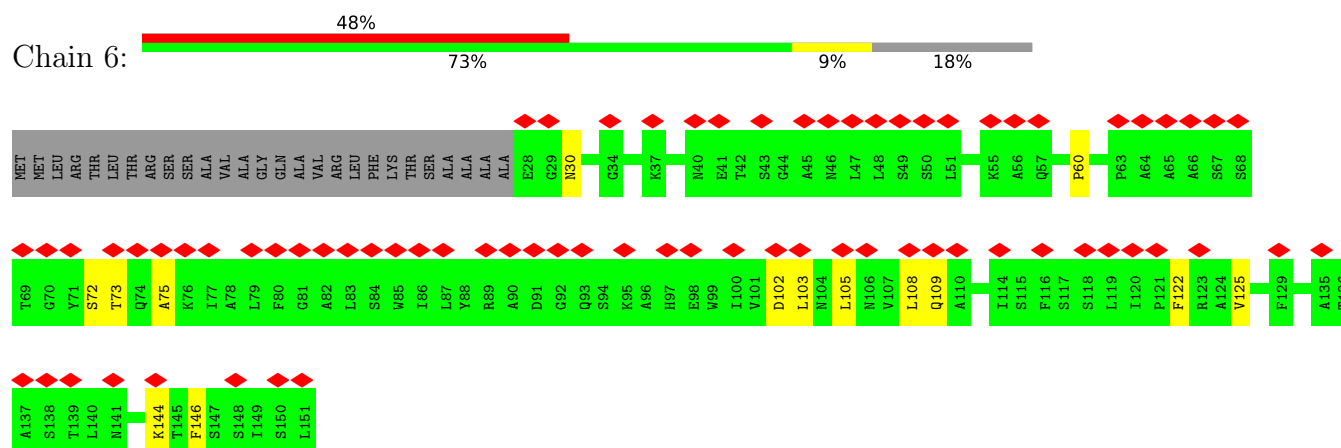


• Molecule 6: Mitochondrial F1F0 ATP synthase associated 14 kDa protein

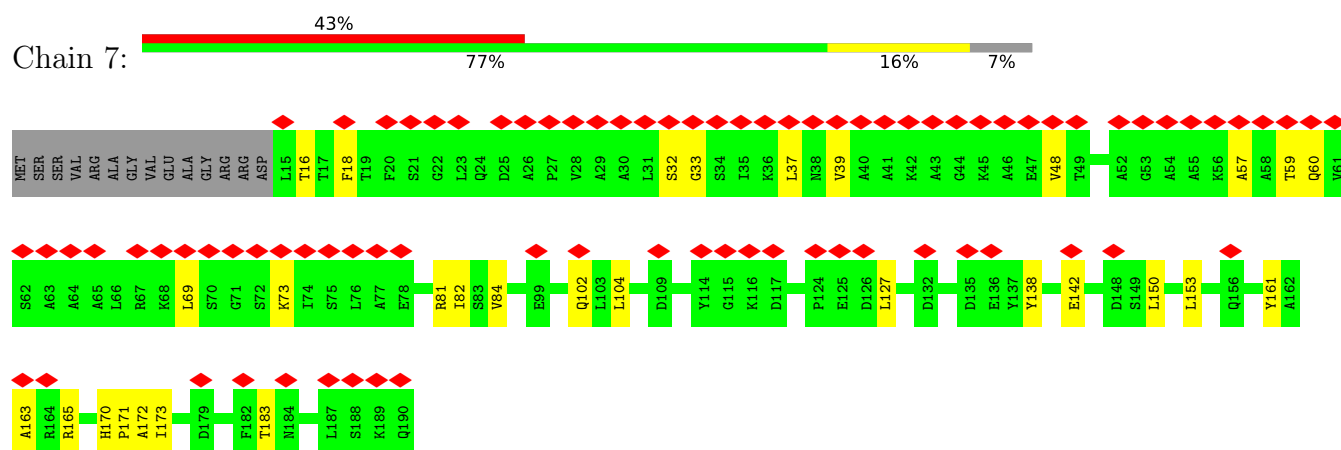
Chain 5: 24% 81% 19%



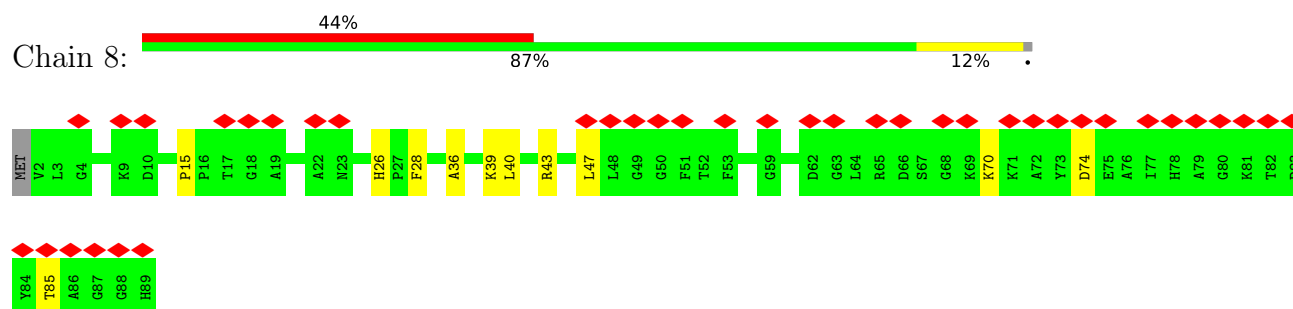
- Molecule 7: Mitochondrial ATP synthase subunit ASA6



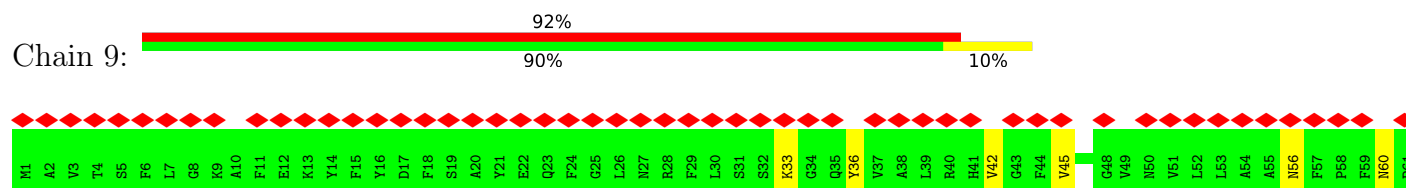
- Molecule 8: Mitochondrial ATP synthase associated protein ASA7

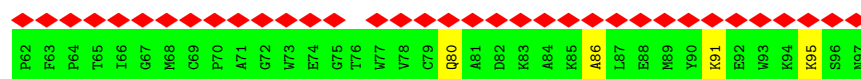


- Molecule 9: Mitochondrial ATP synthase subunit ASA8

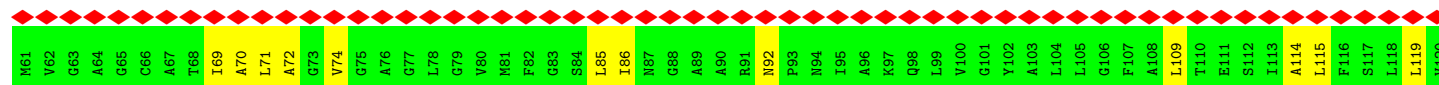
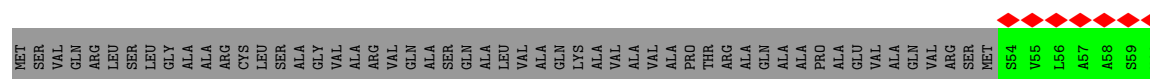


- Molecule 10: ASA-9: Polytomella F-ATP synthase associated subunit 9

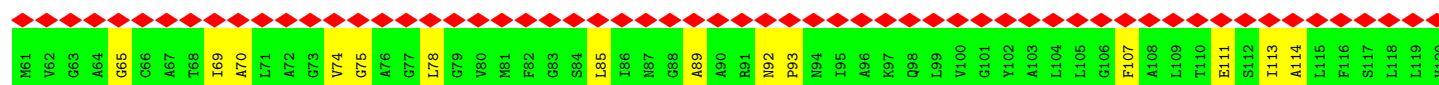
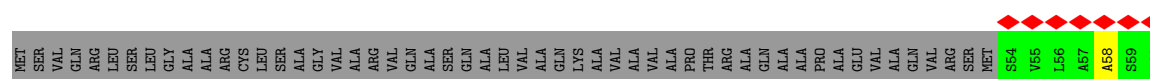




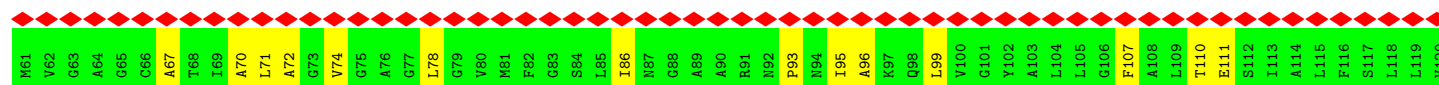
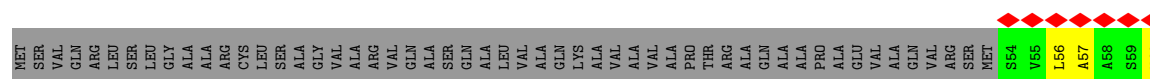
- Molecule 11: Mitochondrial ATP synthase subunit c



- Molecule 11: Mitochondrial ATP synthase subunit c

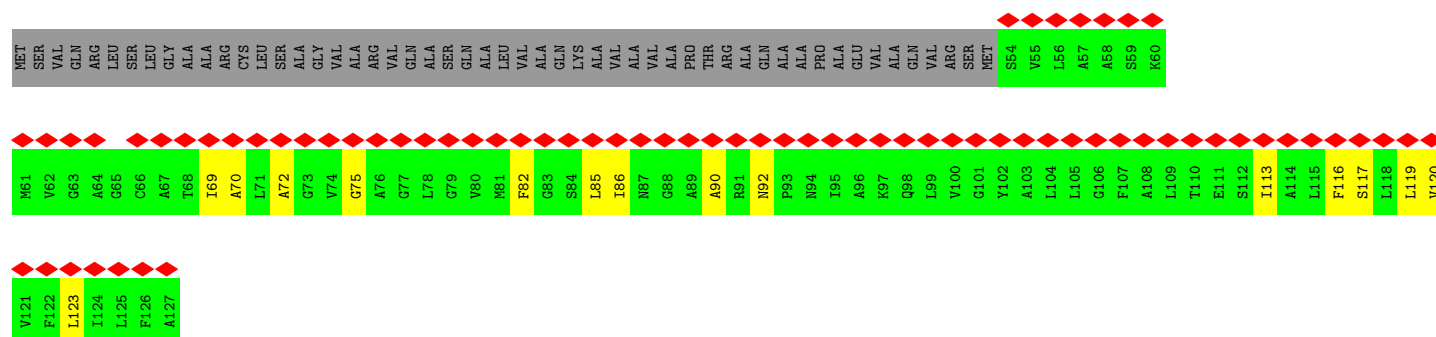


- Molecule 11: Mitochondrial ATP synthase subunit c

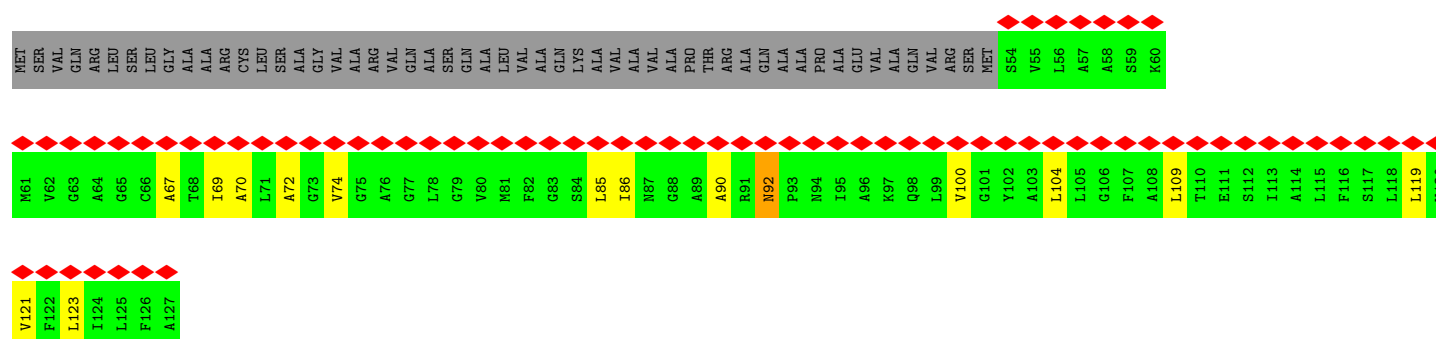


- Molecule 11: Mitochondrial ATP synthase subunit c

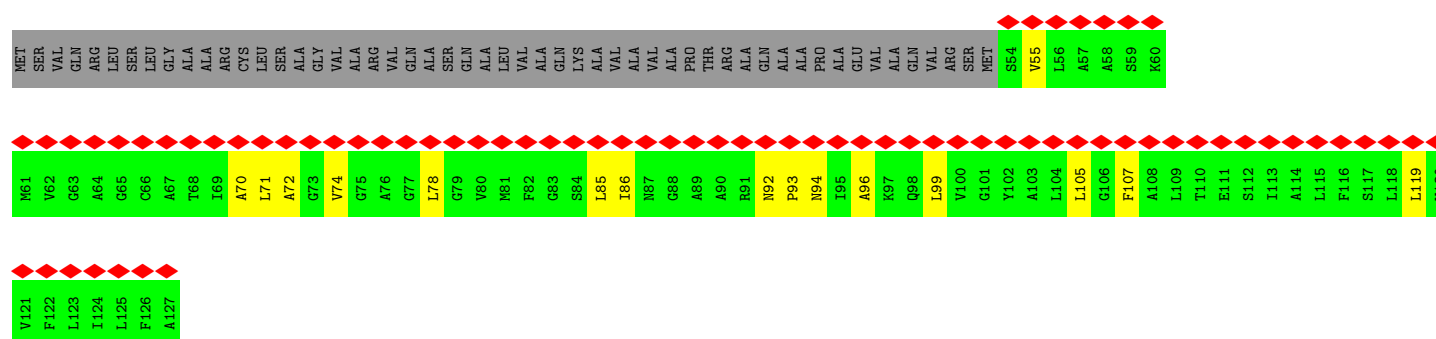




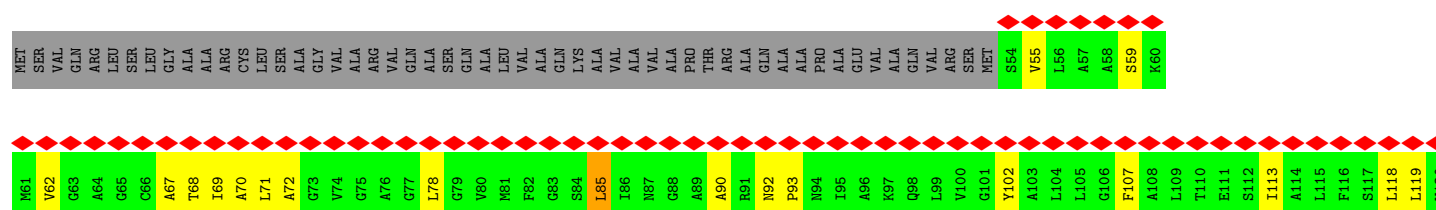
• Molecule 11: Mitochondrial ATP synthase subunit c



• Molecule 11: Mitochondrial ATP synthase subunit c

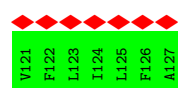
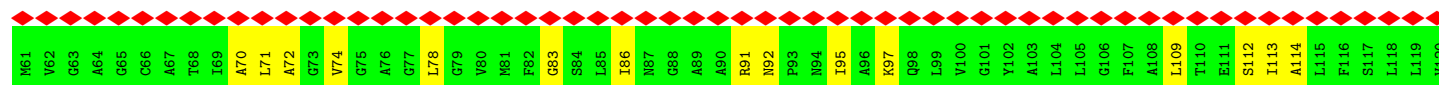
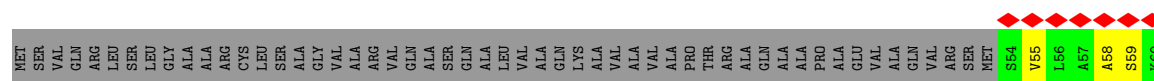


• Molecule 11: Mitochondrial ATP synthase subunit c

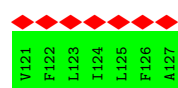
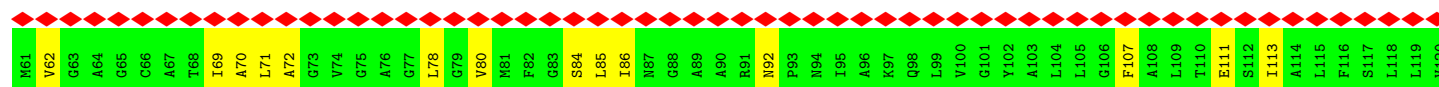
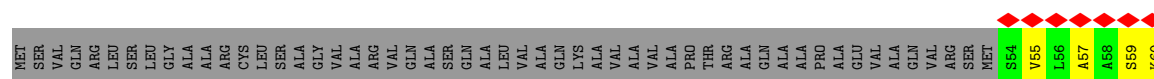




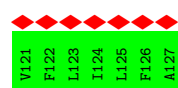
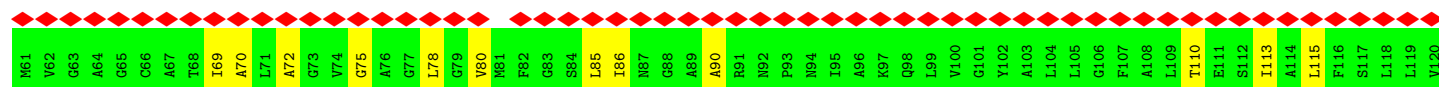
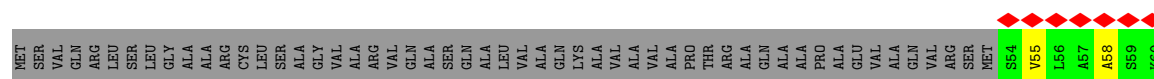
• Molecule 11: Mitochondrial ATP synthase subunit c



• Molecule 11: Mitochondrial ATP synthase subunit c



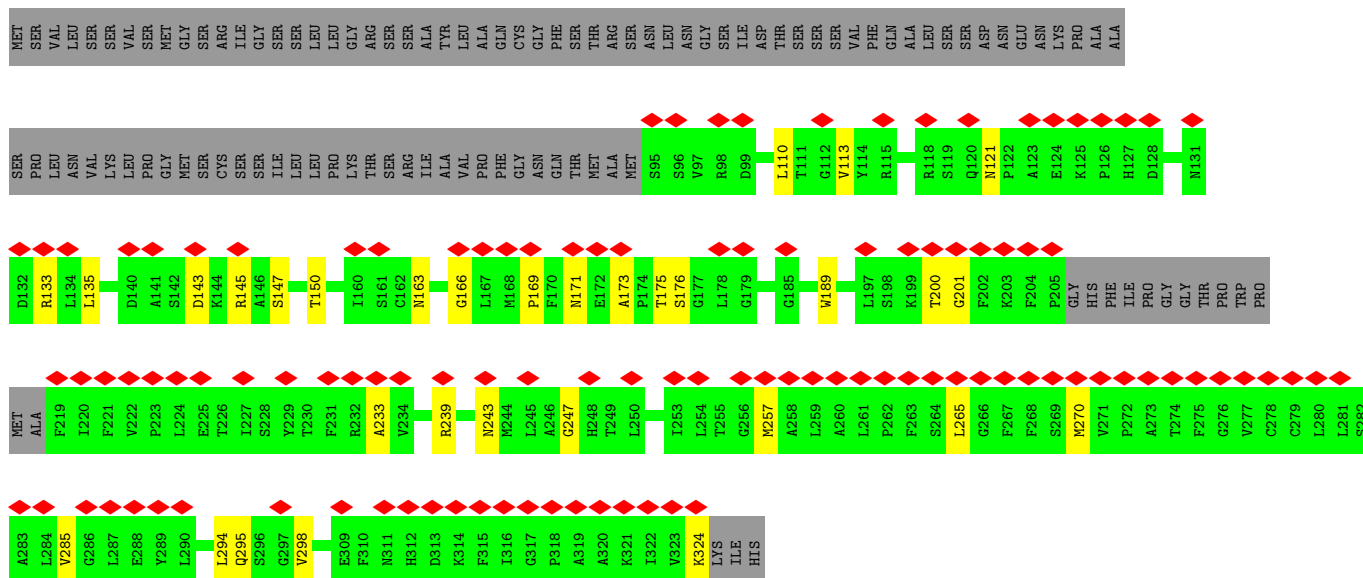
• Molecule 11: Mitochondrial ATP synthase subunit c



• Molecule 12: Mitochondrial ATP synthase subunit 6



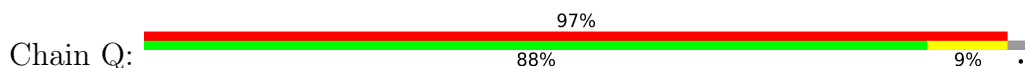




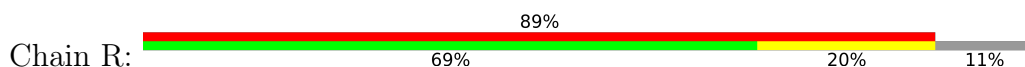
• Molecule 13: Mitochondrial ATP synthase subunit OSCP



• Molecule 14: epsilon: Polytomella F-ATP synthase epsilon subunit

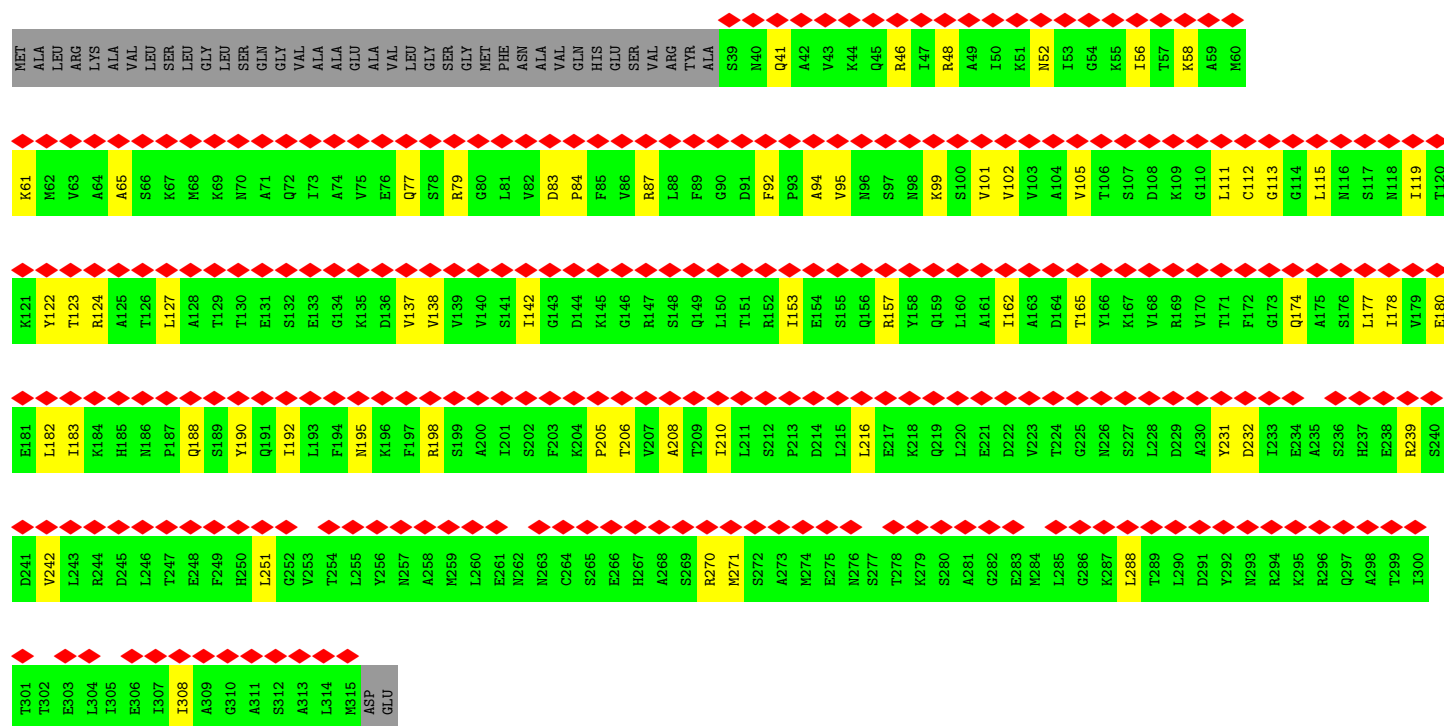
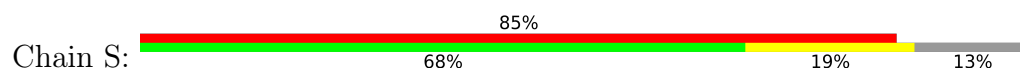


• Molecule 15: Mitochondrial ATP synthase subunit delta

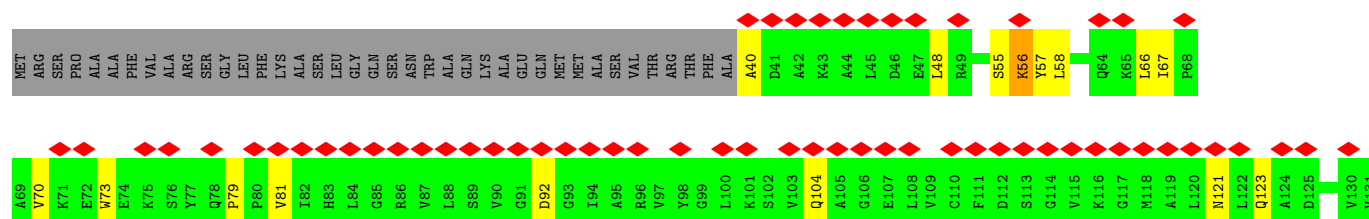
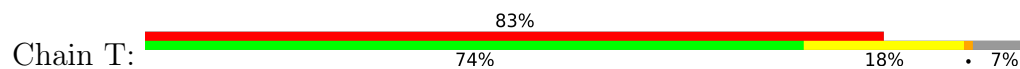




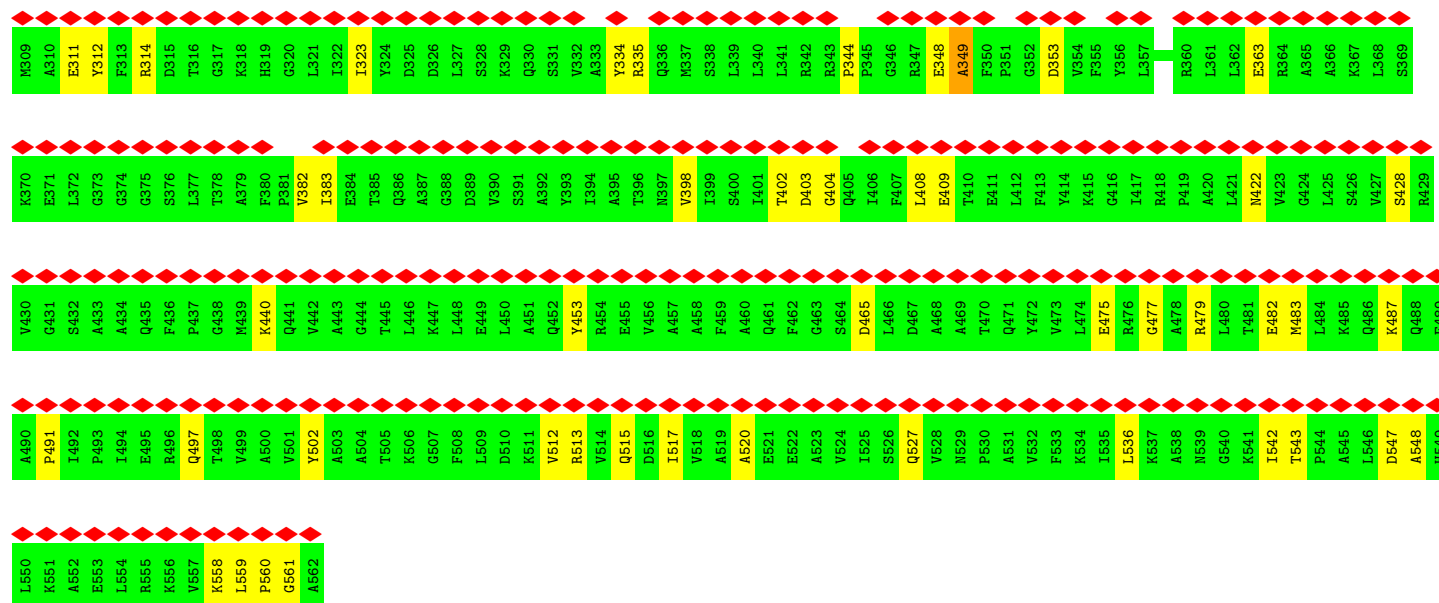
• Molecule 16: ATP synthase gamma chain, mitochondrial



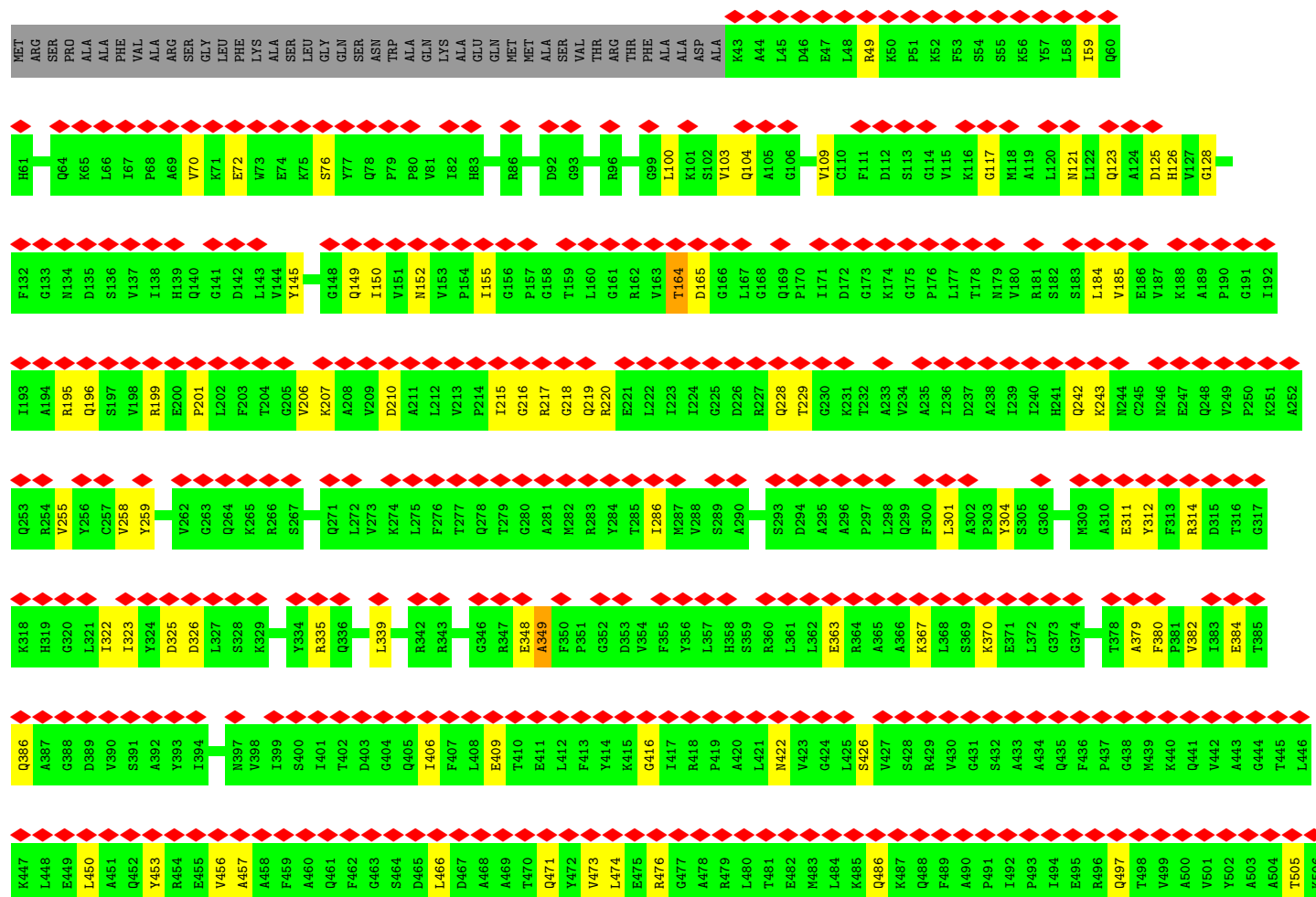
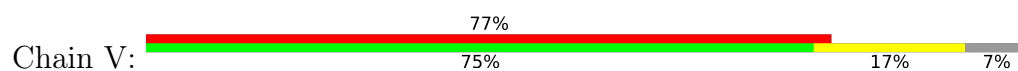
• Molecule 17: ATP synthase subunit alpha

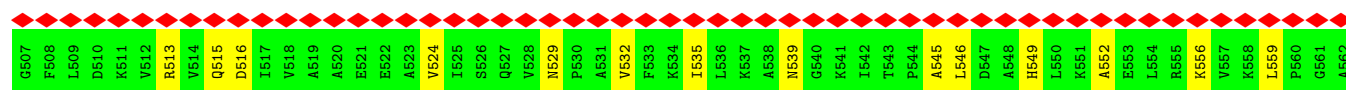




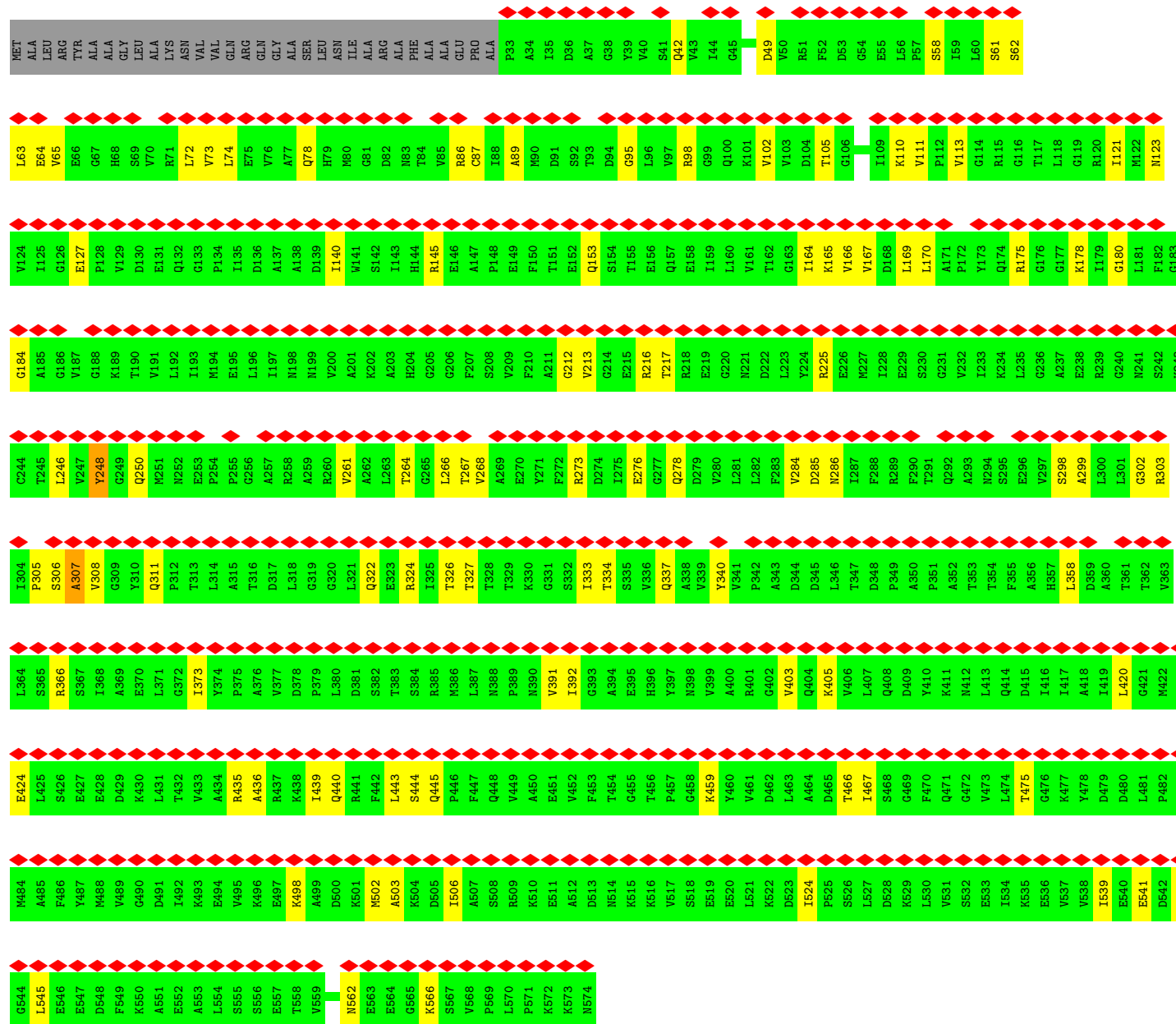
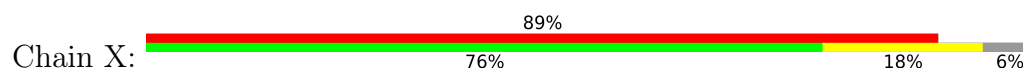


• Molecule 17: ATP synthase subunit alpha

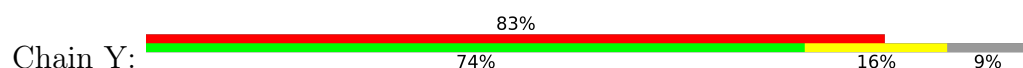


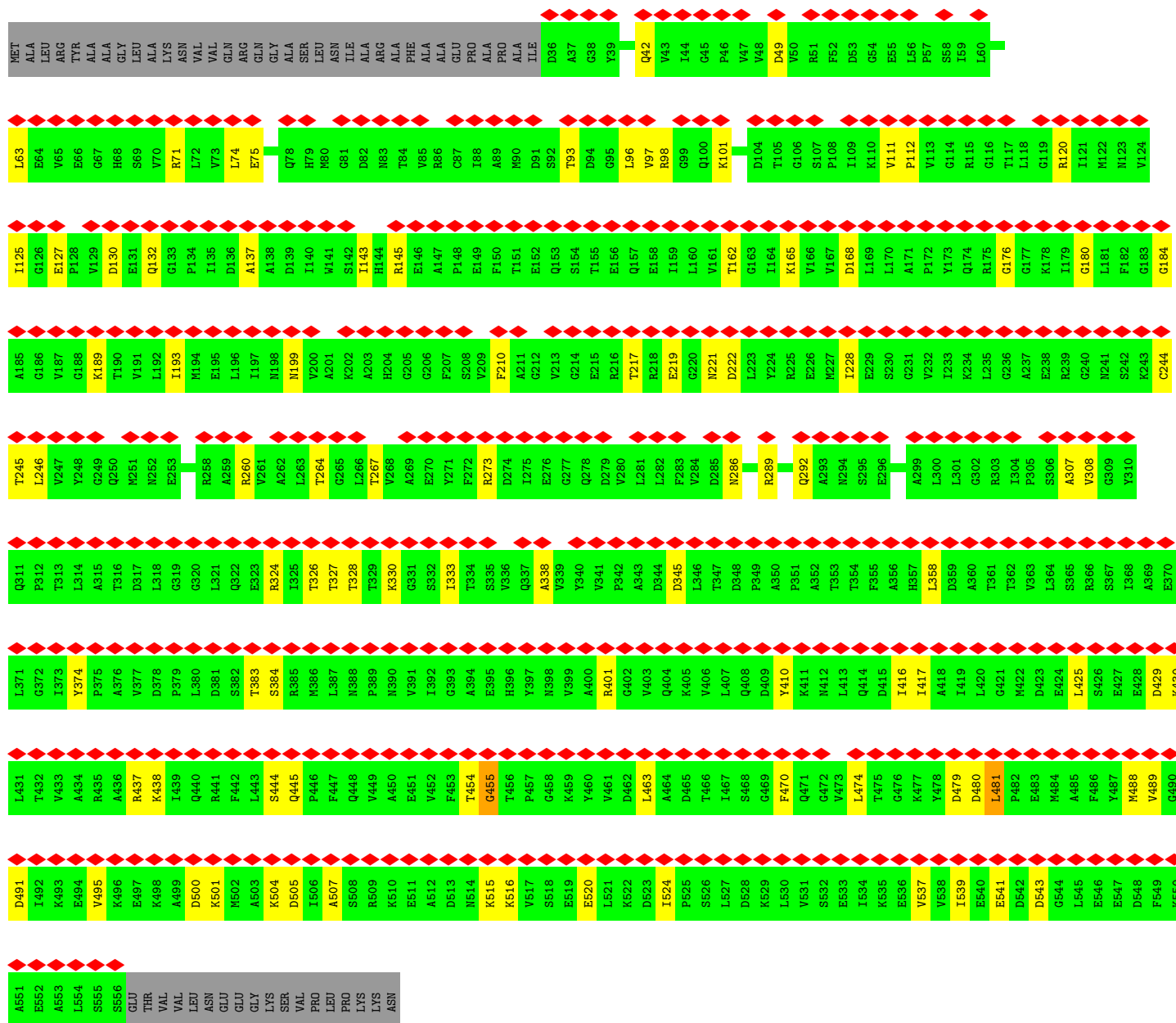


• Molecule 18: ATP synthase subunit beta

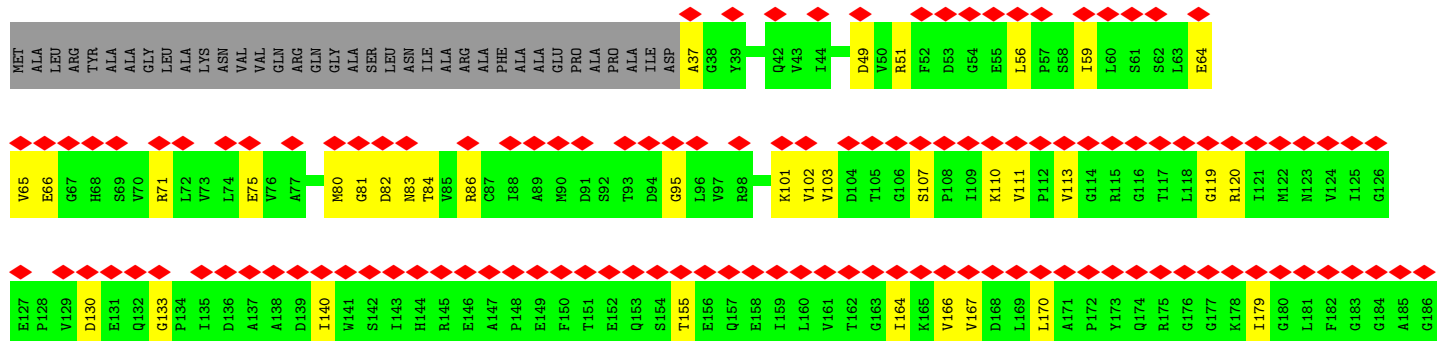
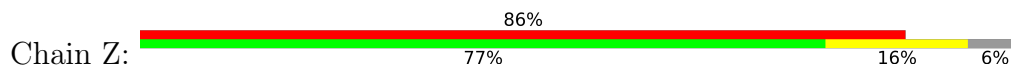


• Molecule 18: ATP synthase subunit beta





● Molecule 18: ATP synthase subunit beta



D548	M488	E428	I368	A307	V247	V187
F549	V489	D429	A369	V308	Y248	G188
K550	G490	K430	E370	G309	G249	G189
A551	D491	L431	L371	Y310	Q250	T190
E552	I492	T432	G372	Q311	M251	V191
A553	K493	V433	L373		N252	L192
L554	E494	A434	Y374	L314	L253	I193
S555	V495	R435	F375	A315	P254	M194
S556	K496	A436	A376	T316	P255	E195
E557	E497	R437	V377	D317	G256	L196
T558	K498	K438	D378	L318	A257	I197
V559	A499	I439	F379	G319	R258	N198
V560	D500	Q440	L380	G320	A259	N199
L561	K501	R441	D381	L321	R260	V200
N562	M502	F442	S382	Q322	V261	A201
E563	A503	L443	T383	E323	A262	K202
E564	K504	S444	S384	R324	L263	A203
G565	D505	Q445	A385	T325	T264	H204
K566	I506	P446	K386	T326	G265	G205
S567	A507	F447	L387	T327	L266	G206
V568	S508	Q448	K388	T328	V268	F207
P569	R509	V449	P389	T329	A269	S208
L570	K510	A450	N390	K330	E270	V209
P571	E511	E451	V391	G331	Y271	F210
K572	A512	V452	L392	S332	F272	A211
K573	D513	F453	G393	I333	R273	G212
N574	N514	T454	A394	T334	D274	V213
	K515	G455	E395	S335	I275	G214
	K516	T456	H396	V336	E276	E215
	V517	P457	Y397	Q337	G277	R216
	S518	G458	N398	A338	Q278	T217
	E519	K459	V399	V339	D279	R218
	E520	Y460	A400	Y340	V280	E219
L521	V461	V461	R401	V341	G220	G220
K522	D462	D462	G402	P342	L281	N221
D523	Y403	L463	V403	A343	D282	D222
I524	A464	A464	Q404	D344	F283	L223
P525	D465	D465	K405	D345	V284	L223
S526	T466	T466	V406	L346	D285	Y224
L527	I467	T467	V407	T347	N286	R225
D528	S468	S468	L407	D348	E226	E226
K529	G469	G469	D409	P349	M227	M227
L530	F470	F470	Y410	A350	I228	I228
V531	Q471	Q471	K411	P351	F290	E229
S532	G472	G472	M412	A352	T291	S230
E533	V473	V473	L413	Q292	G292	G231
I534	L474	L474	Q414	A293	A293	V232
K535	T475	T475	D415	T354	N294	I233
E536	G476	G476	I416	F355	M295	K234
V537	K477	K477	I417	A356	S295	L235
V538	Y478	Y478	L358	H357	E296	G236
I539	D479	D479	A418	V297	S298	A237
E540	D480	D480	P359	A299	A299	E238
E541	L481	L481	A360	L300	L300	R239
D542	P482	P482	L420	T361	L301	G240
D543	E483	E483	G421	T362	G302	N241
G544	M484	M484	M422	V363	R303	G241
L545	A485	A485	D423	L364	I304	N241
E546	F486	F486	E424	S365	P305	S242
			L425	R366	S306	K243
			S426	S367		T244
			E427			L246

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	27039	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	35	Depositor
Minimum defocus (nm)	-400	Depositor
Maximum defocus (nm)	-5000	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.106	Depositor
Minimum map value	-0.062	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	505.44, 505.44, 505.44	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.053, 1.053, 1.053	Depositor



## 5 Model quality

### 5.1 Standard geometry

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

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	0	0.33	0/628	0.50	0/856
2	1	0.33	0/4750	0.49	0/6434
3	2	0.32	0/3212	0.51	0/4371
4	3	0.33	0/1911	0.52	1/2601 (0.0%)
5	4	0.33	0/2216	0.48	0/3000
6	5	0.37	0/1011	0.57	0/1376
7	6	0.35	0/946	0.55	0/1287
8	7	0.38	0/1374	0.51	0/1865
9	8	0.36	0/715	0.54	0/974
10	9	0.31	0/802	0.49	0/1084
11	A	0.32	0/520	0.54	0/704
11	B	0.32	0/520	0.53	0/704
11	C	0.30	0/519	0.51	0/701
11	D	0.28	0/520	0.55	1/704 (0.1%)
11	E	0.29	0/520	0.53	0/704
11	F	0.30	0/520	0.60	0/704
11	G	0.29	0/520	0.57	0/704
11	H	0.28	0/520	0.56	0/704
11	I	0.30	0/520	0.60	0/704
11	J	0.30	0/520	0.59	0/704
12	M	0.37	0/1683	0.57	0/2295
13	P	0.34	0/1553	0.54	0/2093
14	Q	0.29	0/574	0.49	0/774
15	R	0.31	0/1336	0.52	0/1827
16	S	0.29	0/2153	0.53	0/2901
17	T	0.38	0/4048	0.56	1/5481 (0.0%)
17	U	0.40	0/4049	0.56	0/5481
17	V	0.39	0/4031	0.55	0/5456
18	X	0.38	0/4176	0.55	0/5659
18	Y	0.38	0/4015	0.55	1/5440 (0.0%)
18	Z	0.36	0/4147	0.54	0/5619
All	All	0.35	0/54529	0.54	4/73911 (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
6	5	0	1
17	T	0	2
17	U	0	1
17	V	0	1
18	X	0	1
18	Y	0	1
18	Z	0	2
All	All	0	9

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	T	167	LEU	CA-CB-CG	7.06	131.54	115.30
4	3	77	PRO	N-CA-CB	5.98	110.48	103.30
11	D	119	LEU	CA-CB-CG	5.31	127.52	115.30
18	Y	481	LEU	CA-CB-CG	5.18	127.21	115.30

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	5	119	LYS	Peptide
17	T	348	GLU	Peptide
17	T	492	ILE	Peptide
17	U	348	GLU	Peptide
17	V	348	GLU	Peptide
18	X	307	ALA	Peptide
18	Y	307	ALA	Peptide
18	Z	307	ALA	Peptide
18	Z	503	ALA	Mainchain

## 5.2 Too-close contacts

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

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	607	0	584	7	0
2	1	4661	0	4695	61	0
3	2	3163	0	3262	38	0
4	3	1874	0	1826	22	0
5	4	2177	0	2169	28	0
6	5	986	0	1021	19	0
7	6	926	0	941	11	0
8	7	1347	0	1345	28	0
9	8	692	0	694	9	0
10	9	776	0	757	7	0
11	A	514	0	554	15	0
11	B	514	0	554	16	0
11	C	514	0	553	20	0
11	D	514	0	554	14	0
11	E	514	0	554	14	0
11	F	514	0	554	15	0
11	G	514	0	554	18	0
11	H	514	0	554	16	0
11	I	514	0	554	18	0
11	J	514	0	554	15	0
12	M	1640	0	1665	23	0
13	P	1532	0	1603	28	0
14	Q	561	0	565	5	0
15	R	1303	0	1266	30	0
16	S	2130	0	2180	44	0
17	T	3979	0	4119	72	0
17	U	3980	0	4119	68	0
17	V	3962	0	4105	61	0
18	X	4115	0	4137	64	0
18	Y	3957	0	3966	64	0
18	Z	4087	0	4110	59	0
19	M	1	0	0	0	0
20	T	31	0	12	0	0
20	U	31	0	12	0	0
20	V	31	0	12	0	0
21	T	1	0	0	0	0
21	U	1	0	0	0	0
21	V	1	0	0	0	0
21	X	1	0	0	0	0
21	Y	1	0	0	0	0
22	X	27	0	12	0	0
22	Y	27	0	12	1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	53748	0	54728	751	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 7.

All (751) 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)
11:I:107:PHE:CZ	11:I:111:GLU:OE2	1.91	1.24
18:X:503:ALA:O	18:X:506:ILE:HG12	1.38	1.23
13:P:184:LEU:HD23	13:P:184:LEU:H	1.26	0.98
11:C:111:GLU:OE1	11:D:113:ILE:HD11	1.67	0.94
18:X:503:ALA:O	18:X:506:ILE:CG1	2.23	0.86
11:I:107:PHE:CE1	11:I:111:GLU:OE2	2.33	0.82
18:X:498:LYS:O	18:X:502:MET:HG2	1.79	0.82
11:C:78:LEU:HD21	11:C:111:GLU:OE2	1.82	0.78
17:V:535:ILE:O	17:V:539:ASN:HB2	1.85	0.76
11:I:107:PHE:HZ	11:I:111:GLU:OE2	1.68	0.75
13:P:184:LEU:HD23	13:P:184:LEU:N	2.02	0.75
11:B:123:LEU:HD12	12:M:257:MET:SD	2.27	0.74
11:B:107:PHE:O	11:B:111:GLU:HG2	1.88	0.73
11:G:119:LEU:O	11:G:123:LEU:HB2	1.90	0.72
17:U:383:ILE:HG13	17:U:398:VAL:HG11	1.73	0.71
15:R:129:VAL:HB	15:R:146:VAL:HG21	1.72	0.70
11:B:93:PRO:HG3	11:C:95:ILE:HD13	1.76	0.66
17:V:242:GLN:HE21	17:V:255:VAL:HG11	1.59	0.66
17:U:229:THR:HG22	17:U:229:THR:O	1.96	0.66
9:8:26:HIS:HD2	9:8:28:PHE:H	1.44	0.65
18:Y:501:LYS:O	18:Y:505:ASP:HB2	1.97	0.65
2:1:316:ASN:HD21	2:1:331:ALA:H	1.44	0.65
17:T:335:ARG:HD2	17:T:349:ALA:HB3	1.79	0.64
18:Y:286:ASN:H	18:Y:338:ALA:HB3	1.63	0.64
17:U:512:VAL:HG22	17:U:561:GLY:HA3	1.80	0.64
13:P:187:GLN:O	13:P:188:GLU:O	2.14	0.64
18:Z:273:ARG:HD3	18:Z:333:ILE:HG13	1.80	0.64
2:1:84:PRO:HG2	6:5:71:VAL:HG11	1.78	0.64
11:C:107:PHE:CE1	11:C:111:GLU:HG3	2.32	0.63
17:U:185:VAL:HG23	17:U:186:GLU:HG2	1.80	0.63
18:X:327:THR:HG22	18:X:333:ILE:H	1.64	0.62
18:X:403:VAL:HG23	18:X:439:ILE:HD12	1.80	0.62
15:R:55:THR:HB	16:S:83:ASP:OD1	1.99	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:H:86:ILE:HG21	11:I:85:LEU:HA	1.82	0.62
11:I:72:ALA:HB2	11:J:70:ALA:HA	1.81	0.62
13:P:155:THR:HB	13:P:201:GLU:HB2	1.82	0.62
17:T:153:VAL:HG11	17:T:305:SER:HB2	1.82	0.62
17:U:246:ASN:HD21	17:U:255:VAL:H	1.47	0.62
16:S:48:ARG:O	16:S:52:ASN:ND2	2.33	0.62
18:Z:179:ILE:HB	18:Z:336:VAL:HA	1.82	0.62
11:C:107:PHE:CE1	11:C:111:GLU:CG	2.83	0.61
13:P:153:TYR:HA	13:P:185:VAL:HG12	1.82	0.61
5:4:8:LYS:NZ	5:4:42:THR:OG1	2.34	0.61
11:F:72:ALA:HB2	11:G:70:ALA:HA	1.83	0.61
4:3:129:LYS:NZ	4:3:156:ASP:OD1	2.34	0.60
17:V:311:GLU:HG2	17:V:314:ARG:HE	1.65	0.60
11:I:71:LEU:HD12	11:J:113:ILE:HG23	1.83	0.60
11:C:86:ILE:HG21	11:D:85:LEU:HA	1.83	0.60
18:X:64:GLU:HG2	18:X:73:VAL:HG12	1.83	0.60
11:I:78:LEU:HB3	11:J:110:THR:HG22	1.84	0.60
11:I:80:VAL:HG12	11:J:80:VAL:HG11	1.82	0.60
17:T:326:ASP:H	17:T:382:VAL:HB	1.66	0.60
3:2:128:VAL:HG21	3:2:143:VAL:HG11	1.83	0.60
17:U:409:GLU:OE2	17:U:422:ASN:ND2	2.35	0.60
11:D:86:ILE:HG21	11:E:85:LEU:HA	1.84	0.59
11:H:71:LEU:HD12	11:I:113:ILE:HD12	1.84	0.59
18:Z:306:SER:OG	18:Z:307:ALA:N	2.33	0.59
18:X:373:ILE:HG23	18:X:444:SER:HB2	1.84	0.59
16:S:119:ILE:HA	16:S:122:TYR:HB2	1.84	0.59
17:V:155:ILE:HD12	17:V:312:TYR:HB2	1.83	0.59
15:R:58:LYS:O	15:R:139:ASN:ND2	2.36	0.59
17:V:100:LEU:HD13	17:V:103:VAL:HG21	1.85	0.59
17:V:215:ILE:HG23	17:V:219:GLN:HE21	1.67	0.59
17:T:314:ARG:NH1	17:T:364:ARG:O	2.36	0.59
3:2:403:SER:HB2	3:2:413:VAL:HG11	1.85	0.59
17:T:495:GLU:HG2	17:T:496:ARG:HG3	1.85	0.59
17:U:210:ASP:HB2	17:U:497:GLN:HE22	1.67	0.59
18:Z:209:VAL:HG22	18:Z:245:THR:HB	1.84	0.59
3:2:67:THR:HG21	3:2:102:GLN:HB3	1.85	0.58
18:Z:419:ILE:HG13	18:Z:420:LEU:HD12	1.84	0.58
11:C:107:PHE:O	11:C:111:GLU:HG2	2.02	0.58
17:T:543:THR:HG22	17:T:545:ALA:H	1.67	0.58
18:Y:425:LEU:HB3	18:Y:429:ASP:HB2	1.84	0.58
18:X:273:ARG:NH1	18:X:326:THR:O	2.37	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:U:479:ARG:NH1	17:U:513:ARG:O	2.37	0.58
18:Z:164:ILE:HB	18:Z:167:VAL:HG22	1.85	0.58
11:C:72:ALA:HB2	11:D:70:ALA:HA	1.85	0.58
11:I:86:ILE:HG21	11:J:85:LEU:HA	1.86	0.58
17:V:409:GLU:OE1	17:V:422:ASN:ND2	2.37	0.58
2:1:259:ARG:NH1	2:1:516:GLU:OE2	2.37	0.57
11:B:107:PHE:CE1	11:B:111:GLU:OE2	2.56	0.57
15:R:136:VAL:HG22	15:R:142:THR:HG22	1.85	0.57
17:V:228:GLN:HG2	18:Y:383:THR:HG21	1.85	0.57
18:Z:120:ARG:NH1	18:Z:133:GLY:O	2.37	0.57
3:2:86:GLU:HG3	5:4:84:ARG:HD3	1.87	0.57
2:1:554:LYS:NZ	4:3:170:THR:O	2.37	0.57
11:B:74:VAL:HG11	11:B:114:ALA:HB2	1.85	0.57
17:V:453:TYR:HA	17:V:456:VAL:HG12	1.86	0.57
4:3:219:LEU:HD22	4:3:240:VAL:HG13	1.85	0.57
9:8:36:ALA:HA	9:8:40:LEU:HB3	1.87	0.57
11:A:74:VAL:HG12	11:J:75:GLY:HA3	1.86	0.57
18:X:78:GLN:HB2	18:X:86:ARG:HB3	1.87	0.57
11:C:107:PHE:CZ	11:C:111:GLU:HG3	2.40	0.57
11:E:119:LEU:O	11:E:123:LEU:HB2	2.05	0.57
17:U:207:LYS:NZ	17:U:483:MET:SD	2.78	0.57
11:H:91:ARG:NH1	16:S:232:ASP:OD1	2.37	0.57
18:Y:273:ARG:NH1	18:Y:326:THR:O	2.38	0.57
17:U:270:ALA:HB1	18:Z:155:THR:HG22	1.87	0.56
18:X:65:VAL:HG12	18:X:102:VAL:HG22	1.87	0.56
3:2:207:ALA:HB3	3:2:238:ASP:HB2	1.87	0.56
11:A:92:ASN:ND2	11:J:90:ALA:O	2.38	0.56
13:P:205:ARG:HD2	17:T:81:VAL:CG1	2.35	0.56
17:V:384:GLU:OE2	17:V:386:GLN:NE2	2.39	0.56
17:V:335:ARG:HD2	17:V:349:ALA:HB3	1.86	0.56
18:Y:143:ILE:O	18:Y:324:ARG:NH2	2.39	0.56
15:R:90:VAL:HB	15:R:117:GLU:HB2	1.87	0.56
17:T:254:ARG:NH2	18:Y:541:GLU:OE1	2.39	0.56
11:A:74:VAL:HG21	11:A:114:ALA:HB2	1.87	0.56
2:1:206:GLN:O	2:1:209:ASN:ND2	2.39	0.56
11:E:86:ILE:HG21	11:F:85:LEU:HA	1.88	0.56
11:I:57:ALA:HA	11:I:60:LYS:HG2	1.88	0.56
13:P:209:MET:CE	17:T:79:PRO:HG2	2.35	0.56
3:2:36:LEU:HD22	3:2:41:VAL:HG11	1.88	0.56
11:D:120:VAL:HA	11:D:123:LEU:HB2	1.88	0.56
18:Y:120:ARG:NH1	18:Y:132:GLN:O	2.38	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:V:201:PRO:O	17:V:217:ARG:NH2	2.39	0.55
17:U:335:ARG:HD2	17:U:349:ALA:HB3	1.88	0.55
2:1:62:LYS:HD3	2:1:146:ALA:HB2	1.88	0.55
3:2:42:LYS:NZ	8:7:69:LEU:O	2.39	0.55
5:4:74:LEU:HD22	5:4:223:GLU:HG3	1.89	0.55
17:U:479:ARG:NH1	17:U:512:VAL:O	2.37	0.55
18:Y:145:ARG:HH22	18:Y:267:THR:HG23	1.72	0.55
18:Z:445:GLN:NE2	18:Z:459:LYS:O	2.40	0.55
11:G:72:ALA:HB2	11:H:70:ALA:HA	1.88	0.55
16:S:111:LEU:HB2	16:S:270:ARG:HE	1.72	0.55
9:8:70:LYS:NZ	9:8:74:ASP:OD2	2.39	0.55
4:3:91:VAL:HG23	4:3:93:GLU:H	1.72	0.55
4:3:144:THR:HG21	4:3:180:ILE:HG12	1.89	0.55
8:7:39:VAL:HA	8:7:48:VAL:HA	1.88	0.55
2:1:539:ASP:N	2:1:539:ASP:OD1	2.39	0.55
17:T:185:VAL:HG23	17:T:186:GLU:HG2	1.90	0.54
17:V:123:GLN:OE1	17:V:126:HIS:NE2	2.40	0.54
2:1:155:GLU:OE2	2:1:157:LYS:NZ	2.40	0.54
11:E:72:ALA:HB2	11:F:70:ALA:HA	1.88	0.54
16:S:41:GLN:NE2	18:Y:345:ASP:OD2	2.40	0.54
17:T:201:PRO:HA	17:T:216:GLY:HA2	1.89	0.54
17:U:140:GLN:HE22	18:Z:83:ASN:H	1.54	0.54
17:V:210:ASP:HB2	17:V:497:GLN:HE22	1.72	0.54
1:0:43:SER:OG	1:0:46:GLU:OE1	2.25	0.54
2:1:435:THR:HG22	2:1:437:VAL:H	1.71	0.54
13:P:109:LEU:HB3	13:P:119:LYS:HD2	1.88	0.54
16:S:165:THR:OG1	16:S:174:GLN:NE2	2.41	0.54
16:S:190:TYR:HB2	16:S:210:ILE:HB	1.90	0.54
5:4:71:ALA:HB2	8:7:84:VAL:HG12	1.90	0.54
17:T:283:ARG:NH2	17:T:284:TYR:OH	2.41	0.54
18:Z:113:VAL:HG12	18:Z:268:VAL:HG12	1.88	0.54
4:3:216:ALA:HB3	4:3:252:LEU:HD11	1.90	0.54
16:S:56:ILE:HD11	18:Y:416:ILE:HG12	1.90	0.54
17:T:202:LEU:HB2	17:T:217:ARG:HG2	1.90	0.54
17:U:155:ILE:HD12	17:U:312:TYR:HB2	1.89	0.54
17:V:529:ASN:HD21	18:Z:527:LEU:HD23	1.73	0.54
2:1:600:ARG:NH1	4:3:200:ASP:OD2	2.40	0.54
18:X:391:VAL:HG23	18:X:392:ILE:HG23	1.89	0.54
18:Y:42:GLN:HB3	18:Y:49:ASP:HB2	1.90	0.54
18:Y:444:SER:OG	18:Y:488:MET:SD	2.65	0.54
18:Y:454:THR:OG1	18:Y:455:GLY:N	2.41	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:V:406:ILE:HA	17:V:426:SER:HB2	1.91	0.53
18:Y:374:TYR:HB3	22:Y:601:ADP:C6	2.44	0.53
13:P:74:LEU:HD13	13:P:138:THR:HG22	1.89	0.53
16:S:65:ALA:HB2	16:S:271:MET:HG3	1.89	0.53
17:V:125:ASP:OD1	17:V:125:ASP:N	2.41	0.53
2:1:85:ARG:HG2	6:5:71:VAL:HB	1.89	0.53
2:1:267:ARG:NH1	2:1:519:GLU:OE1	2.33	0.53
17:V:258:VAL:HG22	17:V:286:ILE:HB	1.90	0.53
6:5:113:VAL:HG12	6:5:115:ILE:H	1.73	0.53
14:Q:49:GLN:NE2	14:Q:63:TYR:OH	2.42	0.53
17:T:486:GLN:NE2	17:T:490:ALA:O	2.42	0.53
2:1:30:ASP:N	2:1:30:ASP:OD1	2.41	0.53
2:1:566:ASP:N	2:1:566:ASP:OD1	2.41	0.53
17:U:543:THR:O	17:U:547:ASP:N	2.40	0.53
18:Y:210:PHE:HB3	18:Y:246:LEU:HD23	1.90	0.53
1:0:12:PHE:HB3	7:6:75:ALA:HB2	1.90	0.53
1:0:17:GLY:O	6:5:21:TRP:NE1	2.42	0.53
2:1:613:ASP:OD2	4:3:233:ARG:NH2	2.42	0.53
5:4:115:THR:HB	13:P:193:LYS:HA	1.91	0.53
5:4:181:ASP:OD1	5:4:181:ASP:N	2.41	0.53
15:R:55:THR:HB	16:S:83:ASP:CG	2.29	0.53
18:X:62:SER:HG	18:X:105:THR:HG1	1.53	0.53
3:2:188:ALA:HB2	3:2:220:LEU:HD22	1.90	0.53
11:A:85:LEU:HA	11:J:86:ILE:HG21	1.90	0.53
18:X:266:LEU:HD21	18:X:324:ARG:HB2	1.91	0.53
18:Y:180:GLY:HA3	18:Y:358:LEU:HD13	1.90	0.53
12:M:163:ASN:ND2	12:M:175:THR:OG1	2.42	0.53
5:4:89:LEU:HB3	8:7:172:ALA:HB2	1.90	0.53
11:I:55:VAL:O	11:I:59:SER:HB3	2.09	0.53
18:Z:119:GLY:N	18:Z:244:CYS:O	2.42	0.53
17:T:121:ASN:OD1	17:T:121:ASN:N	2.40	0.52
2:1:32:THR:OG1	8:7:163:ALA:O	2.28	0.52
18:Y:71:ARG:NH2	18:Y:127:GLU:OE2	2.42	0.52
17:U:261:ALA:HB1	17:U:264:GLN:HG3	1.90	0.52
17:V:164:THR:OG1	17:V:165:ASP:N	2.43	0.52
5:4:71:ALA:O	5:4:84:ARG:NH1	2.42	0.52
11:B:75:GLY:HA3	11:C:74:VAL:HG22	1.90	0.52
17:U:344:PRO:HD2	18:X:299:ALA:HB1	1.92	0.52
17:V:220:ARG:HH11	18:Z:216:ARG:HB3	1.73	0.52
11:G:69:ILE:HA	11:H:70:ALA:HB2	1.92	0.52
11:A:70:ALA:HB2	11:J:69:ILE:HA	1.91	0.52

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:U:157:PRO:HB3	18:X:545:LEU:HB3	1.92	0.52
18:Z:244:CYS:SG	18:Z:245:THR:N	2.82	0.52
8:7:170:HIS:HD2	8:7:172:ALA:H	1.56	0.52
15:R:104:HIS:HB3	15:R:136:VAL:HG11	1.90	0.52
18:X:63:LEU:HB2	18:X:74:LEU:HB2	1.92	0.52
2:1:568:ASP:HB2	2:1:580:LYS:HE3	1.90	0.52
4:3:121:PHE:HA	4:3:124:PHE:HB2	1.91	0.52
17:T:543:THR:O	17:T:547:ASP:N	2.36	0.52
18:Z:49:ASP:OD2	18:Z:86:ARG:NH2	2.43	0.52
3:2:6:ASN:HA	8:7:57:ALA:HA	1.91	0.52
11:C:71:LEU:HD23	11:D:117:SER:HB2	1.91	0.52
18:X:213:VAL:HG22	18:X:261:VAL:HG13	1.91	0.52
17:U:254:ARG:NH2	18:X:543:ASP:OD1	2.43	0.51
17:V:150:ILE:O	17:V:152:ASN:ND2	2.43	0.51
10:9:80:GLN:HB3	10:9:86:ALA:HB2	1.91	0.51
11:B:65:GLY:HA2	11:C:67:ALA:HB2	1.92	0.51
11:B:69:ILE:HA	11:C:70:ALA:HB2	1.92	0.51
11:D:72:ALA:HB2	11:E:70:ALA:HA	1.91	0.51
17:T:415:LYS:O	18:X:405:LYS:NZ	2.42	0.51
17:T:479:ARG:NH1	17:T:512:VAL:O	2.42	0.51
17:U:311:GLU:OE1	17:U:314:ARG:NH1	2.43	0.51
17:U:475:GLU:OE1	17:U:479:ARG:NH1	2.44	0.51
8:7:170:HIS:HB3	8:7:173:ILE:HB	1.91	0.51
18:Z:439:ILE:HG23	18:Z:470:PHE:HE1	1.76	0.51
1:0:34:ARG:NH2	6:5:7:SER:OG	2.43	0.51
3:2:85:ALA:HB3	5:4:84:ARG:HG3	1.92	0.51
11:A:72:ALA:HB2	11:B:70:ALA:HA	1.93	0.51
16:S:210:ILE:HG21	16:S:251:LEU:HB2	1.92	0.51
17:T:196:GLN:OE1	17:T:367:LYS:NZ	2.42	0.51
11:A:69:ILE:HG23	11:B:69:ILE:HG13	1.92	0.51
14:Q:25:ASP:OD1	14:Q:28:ARG:NH1	2.44	0.51
18:X:166:VAL:HG23	18:X:170:LEU:HD12	1.92	0.51
15:R:49:GLU:HB2	16:S:206:THR:HG22	1.93	0.51
16:S:119:ILE:HD13	16:S:195:ASN:HD21	1.76	0.51
18:X:123:ASN:HD21	18:X:127:GLU:HB2	1.75	0.51
7:6:72:SER:OG	7:6:73:THR:N	2.43	0.51
15:R:74:PHE:HE2	15:R:81:LEU:HD12	1.74	0.51
2:1:365:GLN:HE21	2:1:386:HIS:HD2	1.58	0.51
3:2:215:PHE:HA	3:2:250:GLY:HA3	1.92	0.51
6:5:91:HIS:ND1	8:7:138:TYR:OH	2.33	0.51
16:S:192:ILE:HB	16:S:208:ALA:HB3	1.92	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:T:250:PRO:HD3	18:Y:537:VAL:HG11	1.93	0.51
2:1:182:ARG:HA	2:1:229:GLU:HA	1.92	0.51
2:1:310:THR:OG1	2:1:311:PHE:N	2.43	0.51
16:S:190:TYR:N	16:S:210:ILE:O	2.44	0.51
17:U:205:GLY:N	17:U:210:ASP:OD2	2.43	0.51
17:U:229:THR:HG22	17:U:408:LEU:HB3	1.94	0.50
2:1:191:GLU:HA	2:1:194:LYS:HG2	1.93	0.50
16:S:195:ASN:HA	16:S:205:PRO:HA	1.93	0.50
18:X:175:ARG:O	18:X:334:THR:OG1	2.29	0.50
11:E:85:LEU:HD11	11:E:100:VAL:HG22	1.93	0.50
16:S:101:VAL:HG11	16:S:182:LEU:HD22	1.93	0.50
11:C:78:LEU:HD11	11:D:113:ILE:HG13	1.92	0.50
12:M:169:PRO:O	12:M:171:ASN:ND2	2.44	0.50
17:T:135:ASP:OD1	17:T:135:ASP:N	2.44	0.50
18:X:145:ARG:HH12	18:X:267:THR:HG23	1.76	0.50
3:2:190:LYS:HA	3:2:193:VAL:HG12	1.94	0.50
9:8:26:HIS:CD2	9:8:28:PHE:H	2.25	0.50
17:T:195:ARG:NH2	18:Y:217:THR:OG1	2.44	0.50
17:V:195:ARG:NH2	17:V:363:GLU:O	2.44	0.50
18:Z:248:TYR:HB3	18:Z:250:GLN:HE21	1.76	0.50
5:4:60:ALA:HA	5:4:63:VAL:HG12	1.93	0.50
16:S:112:CYS:HB2	16:S:115:LEU:HB3	1.94	0.50
18:X:562:ASN:OD1	18:X:566:LYS:N	2.43	0.50
2:1:206:GLN:HB2	2:1:209:ASN:HD21	1.75	0.50
3:2:246:GLU:OE1	3:2:287:GLN:NE2	2.45	0.50
13:P:209:MET:HG2	17:T:79:PRO:HB3	1.94	0.50
17:U:112:ASP:OD1	17:U:143:LEU:N	2.42	0.50
17:V:416:GLY:O	18:Y:401:ARG:NH2	2.42	0.50
18:X:166:VAL:HB	18:X:443:LEU:HB3	1.93	0.50
17:T:311:GLU:OE1	17:T:314:ARG:NH2	2.45	0.49
6:5:110:SER:OG	6:5:111:LYS:N	2.45	0.49
18:Y:328:THR:HG23	18:Y:330:LYS:H	1.77	0.49
18:Z:110:LYS:HB3	18:Z:140:ILE:HG22	1.93	0.49
3:2:271:PRO:HA	3:2:274:GLU:HB2	1.94	0.49
7:6:102:ASP:HA	7:6:105:LEU:HB2	1.94	0.49
11:A:70:ALA:HA	11:J:72:ALA:HB2	1.93	0.49
11:A:92:ASN:N	11:A:92:ASN:OD1	2.44	0.49
11:J:115:LEU:HD11	12:M:239:ARG:HB2	1.94	0.49
16:S:137:VAL:HB	16:S:157:ARG:HD2	1.94	0.49
17:V:476:ARG:NH1	17:V:505:THR:O	2.34	0.49
18:Y:520:GLU:HG3	18:Y:524:ILE:HB	1.92	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:154:ASP:HB3	4:3:157:LEU:HB3	1.95	0.49
11:A:119:LEU:O	11:A:123:LEU:HB2	2.12	0.49
18:Y:125:ILE:HG13	18:Y:127:GLU:HG3	1.95	0.49
2:1:563:ALA:HA	9:8:39:LYS:HE2	1.94	0.49
11:A:86:ILE:HD13	11:B:85:LEU:HD13	1.95	0.49
17:T:403:ASP:O	17:T:429:ARG:NH2	2.40	0.49
17:U:517:ILE:HA	17:U:520:ALA:HB3	1.94	0.49
11:H:83:GLY:O	11:I:84:SER:OG	2.28	0.49
18:Y:491:ASP:OD1	18:Y:491:ASP:N	2.42	0.49
3:2:371:THR:HG22	3:2:376:LYS:HG2	1.93	0.49
11:I:107:PHE:CZ	11:I:111:GLU:CD	2.80	0.49
13:P:136:GLU:O	13:P:140:ASN:ND2	2.46	0.49
17:T:134:ASN:ND2	17:T:136:SER:OG	2.46	0.49
17:T:136:SER:O	18:X:58:SER:OG	2.31	0.49
17:U:100:LEU:O	18:X:98:ARG:NH2	2.46	0.49
17:U:402:THR:HG22	17:U:404:GLY:H	1.78	0.49
2:1:307:GLY:HA3	2:1:534:LYS:HE3	1.93	0.49
4:3:148:LYS:HB2	4:3:183:THR:HG22	1.93	0.49
13:P:78:ILE:HD11	13:P:138:THR:HG21	1.93	0.49
16:S:112:CYS:SG	16:S:113:GLY:N	2.85	0.49
18:Z:37:ALA:N	18:Z:102:VAL:O	2.46	0.49
3:2:34:VAL:HA	3:2:37:THR:HG22	1.94	0.49
15:R:143:ASP:OD1	16:S:87:ARG:NH2	2.40	0.49
17:T:235:ALA:HB1	17:T:323:ILE:HD13	1.95	0.49
17:U:136:SER:HA	18:Z:59:ILE:HB	1.95	0.49
18:X:180:GLY:HA3	18:X:358:LEU:HD13	1.95	0.49
17:T:323:ILE:HG12	17:T:380:PHE:HB2	1.93	0.49
2:1:368:ALA:O	2:1:379:GLN:NE2	2.46	0.48
11:A:71:LEU:HD22	11:B:113:ILE:HG23	1.94	0.48
17:U:536:LEU:HD11	17:U:542:ILE:HG12	1.95	0.48
2:1:593:LEU:HD22	4:3:204:TYR:HB2	1.95	0.48
11:G:67:ALA:HB3	11:G:121:VAL:HG23	1.94	0.48
18:X:111:VAL:HG11	18:X:264:THR:HG23	1.94	0.48
7:6:122:PHE:HA	7:6:125:VAL:HG12	1.96	0.48
12:M:200:THR:OG1	12:M:201:GLY:N	2.46	0.48
18:Y:504:LYS:O	18:Y:507:ALA:HB3	2.14	0.48
2:1:70:ILE:HG13	2:1:133:ARG:HH11	1.78	0.48
10:9:91:LYS:O	10:9:95:LYS:NZ	2.47	0.48
15:R:164:LEU:HD13	15:R:188:TYR:HB2	1.96	0.48
17:V:516:ASP:OD1	17:V:516:ASP:N	2.47	0.48
2:1:35:ILE:HD12	8:7:173:ILE:HG23	1.96	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:245:SER:OG	4:3:246:GLU:N	2.47	0.48
4:3:246:GLU:OE2	12:M:133:ARG:NH2	2.39	0.48
5:4:238:VAL:HG21	8:7:142:GLU:HG2	1.96	0.48
11:G:62:VAL:HB	11:H:59:SER:HB2	1.94	0.48
13:P:172:LYS:O	13:P:176:LYS:NZ	2.46	0.48
16:S:99:LYS:H	16:S:188:GLN:HG2	1.77	0.48
17:U:344:PRO:HB3	18:X:305:PRO:HG3	1.96	0.48
18:X:284:VAL:HB	18:X:337:GLN:HG2	1.95	0.48
5:4:277:TRP:NE1	17:T:40:ALA:O	2.44	0.48
17:U:222:LEU:N	17:U:402:THR:HG21	2.29	0.48
17:U:527:GLN:OE1	17:U:558:LYS:N	2.46	0.48
17:V:185:VAL:HG22	17:V:304:TYR:HB3	1.96	0.48
8:7:165:ARG:NH2	8:7:171:PRO:O	2.47	0.48
11:E:104:LEU:HD21	11:F:105:LEU:HD21	1.96	0.48
12:M:239:ARG:O	12:M:243:ASN:HB2	2.13	0.48
17:U:242:GLN:HE21	17:U:255:VAL:HB	1.78	0.48
17:V:259:TYR:OH	17:V:325:ASP:OD2	2.23	0.48
18:X:178:LYS:NZ	18:X:322:GLN:O	2.45	0.48
18:Y:500:ASP:OD1	18:Y:500:ASP:N	2.47	0.48
6:5:61:SER:O	6:5:61:SER:OG	2.31	0.48
11:D:113:ILE:HD13	11:D:116:PHE:HD2	1.78	0.48
17:V:218:GLY:HA3	17:V:367:LYS:HB2	1.96	0.48
18:Z:81:GLY:O	18:Z:84:THR:OG1	2.31	0.48
11:E:90:ALA:O	11:F:92:ASN:ND2	2.47	0.47
18:Y:75:GLU:OE1	18:Y:260:ARG:NE	2.47	0.47
18:Z:231:GLY:O	18:Z:234:LYS:NZ	2.46	0.47
4:3:141:THR:HG21	4:3:176:GLN:HG2	1.96	0.47
16:S:101:VAL:HG22	16:S:138:VAL:HB	1.95	0.47
17:T:190:PRO:O	17:T:195:ARG:NH1	2.46	0.47
17:T:220:ARG:NH2	17:T:363:GLU:OE2	2.47	0.47
17:T:376:SER:OG	17:T:377:LEU:N	2.47	0.47
7:6:60:PRO:HB3	9:8:15:PRO:HB2	1.96	0.47
11:H:72:ALA:HB2	11:I:70:ALA:HA	1.97	0.47
11:H:74:VAL:HG11	11:H:114:ALA:HB2	1.95	0.47
17:T:283:ARG:NH1	18:Y:543:ASP:OD1	2.46	0.47
17:U:78:GLN:OE1	17:U:86:ARG:NH1	2.47	0.47
2:1:27:LEU:HB3	17:T:58:LEU:HD22	1.97	0.47
11:G:78:LEU:HD11	11:G:107:PHE:HD1	1.80	0.47
16:S:46:ARG:HH21	16:S:288:LEU:HD11	1.80	0.47
17:V:466:LEU:HG	17:V:471:GLN:HG3	1.95	0.47
18:X:216:ARG:O	18:X:250:GLN:NE2	2.47	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:4:279:ASP:OD2	8:7:81:ARG:NH1	2.47	0.47
15:R:168:SER:O	15:R:168:SER:OG	2.31	0.47
16:S:79:ARG:HH22	16:S:198:ARG:HD2	1.80	0.47
2:1:384:THR:HG21	2:1:398:GLY:HA3	1.96	0.47
3:2:372:LYS:NZ	3:2:444:SER:O	2.44	0.47
6:5:97:SER:O	6:5:101:LYS:NZ	2.45	0.47
10:9:42:VAL:HA	10:9:45:VAL:HG12	1.97	0.47
11:F:71:LEU:HA	11:F:74:VAL:HG22	1.96	0.47
11:F:86:ILE:HG21	11:G:85:LEU:HA	1.97	0.47
11:G:90:ALA:O	11:H:92:ASN:ND2	2.39	0.47
16:S:105:VAL:HB	16:S:142:ILE:HD12	1.96	0.47
17:T:227:ARG:HG2	17:T:228:GLN:HG2	1.96	0.47
17:T:548:ALA:HB3	18:Y:524:ILE:HG12	1.96	0.47
17:V:524:VAL:HG23	17:V:559:LEU:HD21	1.96	0.47
18:Y:515:LYS:HG3	18:Y:516:LYS:H	1.80	0.47
3:2:38:TYR:HD1	8:7:37:LEU:HD11	1.80	0.47
5:4:145:VAL:HG21	5:4:165:PHE:HA	1.96	0.47
9:8:43:ARG:NH1	12:M:143:ASP:O	2.47	0.47
18:Y:500:ASP:O	18:Y:504:LYS:HB2	2.14	0.47
4:3:244:PHE:O	4:3:277:SER:OG	2.33	0.47
11:D:90:ALA:O	11:E:92:ASN:ND2	2.48	0.47
17:U:84:LEU:HD23	17:U:143:LEU:HD12	1.97	0.47
18:X:164:ILE:HB	18:X:167:VAL:HB	1.97	0.47
18:Z:266:LEU:HD21	18:Z:325:ILE:HG12	1.97	0.47
17:V:323:ILE:HG12	17:V:380:PHE:HB2	1.96	0.47
11:C:57:ALA:HA	11:C:60:LYS:HG2	1.96	0.46
12:M:121:ASN:O	12:M:145:ARG:NH1	2.48	0.46
15:R:161:LYS:HE3	15:R:192:GLU:HG2	1.96	0.46
17:U:453:TYR:CG	17:U:477:GLY:HA3	2.50	0.46
18:Z:51:ARG:NH1	18:Z:82:ASP:OD2	2.43	0.46
11:F:78:LEU:HD11	11:F:107:PHE:HA	1.96	0.46
12:M:110:LEU:HA	12:M:113:VAL:HG12	1.96	0.46
17:U:58:LEU:HA	17:U:61:HIS:HB3	1.96	0.46
2:1:194:LYS:NZ	2:1:198:GLU:OE2	2.44	0.46
11:E:92:ASN:OD1	11:E:92:ASN:N	2.47	0.46
17:T:367:LYS:HG3	17:T:376:SER:HB2	1.98	0.46
17:T:409:GLU:OE1	17:T:422:ASN:ND2	2.49	0.46
17:U:192:ILE:HG12	18:X:217:THR:HG23	1.97	0.46
17:V:76:SER:O	17:V:76:SER:OG	2.32	0.46
18:Y:184:GLY:O	18:Y:189:LYS:NZ	2.41	0.46
18:Y:244:CYS:SG	18:Y:245:THR:N	2.89	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:F:96:ALA:HA	11:F:99:LEU:HB3	1.96	0.46
11:J:78:LEU:HD23	11:J:78:LEU:HA	1.82	0.46
13:P:209:MET:HE2	17:T:79:PRO:HG2	1.96	0.46
2:1:245:ALA:HB1	2:1:498:LEU:HD13	1.97	0.46
3:2:155:VAL:HG12	3:2:187:ARG:HD2	1.98	0.46
18:Z:206:GLY:HA2	18:Z:278:GLN:HE21	1.79	0.46
5:4:6:VAL:HG11	5:4:11:VAL:HB	1.97	0.46
16:S:95:VAL:HG21	16:S:216:LEU:HD21	1.98	0.46
17:U:222:LEU:H	17:U:402:THR:HG21	1.80	0.46
17:U:502:TYR:OH	17:U:547:ASP:OD1	2.34	0.46
18:Y:63:LEU:HB2	18:Y:74:LEU:HB2	1.98	0.46
2:1:569:ILE:O	2:1:573:ASP:HB2	2.15	0.46
4:3:128:VAL:HG21	4:3:143:LEU:HD11	1.97	0.46
15:R:137:HIS:HA	16:S:231:TYR:HE1	1.79	0.46
18:X:435:ARG:NH2	18:X:475:THR:O	2.49	0.46
2:1:338:SER:OG	2:1:339:GLU:N	2.48	0.46
3:2:324:SER:HA	3:2:327:SER:HB3	1.98	0.46
12:M:295:GLN:HA	12:M:298:VAL:HG12	1.97	0.46
13:P:64:GLU:OE1	13:P:66:GLN:NE2	2.49	0.46
18:X:110:LYS:HB3	18:X:140:ILE:HG22	1.97	0.46
18:Z:170:LEU:HD22	18:Z:404:GLN:HG3	1.98	0.46
17:T:548:ALA:HA	17:T:551:LYS:HG2	1.96	0.46
18:X:165:LYS:HG2	18:X:466:THR:HG22	1.98	0.46
18:Y:438:LYS:NZ	18:Y:481:LEU:O	2.40	0.46
2:1:156:TRP:O	8:7:102:GLN:NE2	2.50	0.45
5:4:178:LEU:HD11	8:7:183:THR:HG21	1.98	0.45
17:T:225:GLY:O	17:T:385:THR:OG1	2.33	0.45
2:1:278:PRO:HG2	2:1:281:GLU:HB2	1.97	0.45
11:I:59:SER:HA	11:I:62:VAL:HG12	1.97	0.45
16:S:58:LYS:HA	16:S:61:LYS:HD3	1.98	0.45
17:T:456:VAL:HG23	17:T:474:LEU:HD12	1.96	0.45
17:U:119:ALA:HA	17:U:129:VAL:HG12	1.98	0.45
18:X:184:GLY:O	18:X:366:ARG:NH2	2.42	0.45
18:Y:383:THR:OG1	18:Y:384:SER:N	2.50	0.45
18:Y:425:LEU:HB2	18:Y:430:LYS:HG3	1.98	0.45
18:Z:64:GLU:OE1	18:Z:71:ARG:NE	2.48	0.45
8:7:59:THR:OG1	8:7:60:GLN:N	2.49	0.45
11:E:67:ALA:HB3	11:E:121:VAL:HG23	1.98	0.45
11:G:118:LEU:HA	11:G:121:VAL:HG12	1.98	0.45
17:U:428:SER:O	17:U:428:SER:OG	2.32	0.45
5:4:113:THR:O	5:4:116:SER:OG	2.31	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:G:59:SER:HA	11:G:62:VAL:HG12	1.97	0.45
17:V:326:ASP:H	17:V:382:VAL:HB	1.81	0.45
18:Z:101:LYS:HE2	18:Z:103:VAL:HG12	1.98	0.45
2:1:373:ASP:OD1	2:1:373:ASP:N	2.45	0.45
7:6:109:GLN:NE2	12:M:166:GLY:O	2.49	0.45
11:A:109:LEU:HD13	12:M:294:LEU:HD23	1.98	0.45
17:T:481:THR:O	17:T:485:LYS:NZ	2.50	0.45
17:V:70:VAL:HG12	17:V:72:GLU:H	1.82	0.45
18:Z:75:GLU:OE2	18:Z:260:ARG:NE	2.44	0.45
3:2:382:VAL:HG13	3:2:386:LEU:HB2	1.97	0.45
11:D:92:ASN:OD1	11:D:92:ASN:N	2.50	0.45
15:R:73:ASN:HB3	15:R:75:TYR:CZ	2.51	0.45
17:V:339:LEU:HD11	17:V:349:ALA:HB1	1.99	0.45
11:F:92:ASN:N	11:F:92:ASN:OD1	2.50	0.45
17:U:195:ARG:NH2	17:U:363:GLU:O	2.49	0.45
18:Y:193:ILE:HD11	18:Y:338:ALA:HB2	1.98	0.45
18:Y:480:ASP:OD1	18:Y:480:ASP:N	2.47	0.45
18:Z:417:ILE:HG23	18:Z:422:MET:HA	1.99	0.45
11:G:93:PRO:HG3	11:H:95:ILE:HD13	1.99	0.45
18:Z:166:VAL:HG23	18:Z:170:LEU:HD12	1.99	0.45
11:B:78:LEU:HD23	11:B:78:LEU:HA	1.86	0.45
11:F:71:LEU:HD22	11:G:113:ILE:HD12	1.99	0.45
18:Y:410:TYR:OH	18:Y:437:ARG:NE	2.50	0.45
2:1:23:TYR:HB2	8:7:82:ILE:HD11	1.97	0.44
2:1:298:GLN:HE22	7:6:144:LYS:HB3	1.82	0.44
15:R:33:PHE:HA	15:R:36:VAL:HG12	1.99	0.44
15:R:86:LYS:HE3	15:R:118:LEU:HD12	2.00	0.44
18:Z:66:GLU:HG2	18:Z:101:LYS:HD3	1.98	0.44
3:2:144:LEU:HD13	3:2:157:LEU:HD22	1.98	0.44
5:4:145:VAL:HG11	5:4:165:PHE:HB2	2.00	0.44
13:P:49:THR:HA	17:V:59:ILE:HD11	1.99	0.44
15:R:79:SER:HA	16:S:77:GLN:HB3	1.99	0.44
17:U:134:ASN:OD1	17:U:134:ASN:N	2.50	0.44
18:Y:165:LYS:HE3	18:Y:445:GLN:HB2	1.98	0.44
18:Y:168:ASP:HB3	18:Y:463:LEU:HD13	1.99	0.44
2:1:552:LEU:HD22	2:1:588:LEU:HD21	2.00	0.44
11:G:68:THR:HB	11:G:121:VAL:HG21	1.98	0.44
11:I:92:ASN:OD1	11:I:92:ASN:N	2.50	0.44
17:T:155:ILE:HD12	17:T:312:TYR:HB2	2.00	0.44
18:X:42:GLN:HG2	18:X:49:ASP:HB2	1.99	0.44
18:X:436:ALA:O	18:X:440:GLN:HB2	2.18	0.44

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:388:THR:HB	3:2:393:ALA:HA	1.99	0.44
13:P:184:LEU:N	13:P:184:LEU:CD2	2.73	0.44
17:T:151:VAL:HG11	17:T:301:LEU:HD21	1.99	0.44
17:U:513:ARG:HH11	17:U:515:GLN:HG3	1.82	0.44
2:1:195:LYS:O	2:1:199:ASP:HB2	2.17	0.44
6:5:26:LEU:HD23	12:M:150:THR:HG23	2.00	0.44
6:5:30:LEU:O	6:5:34:ILE:N	2.39	0.44
7:6:30:ASN:OD1	7:6:30:ASN:N	2.50	0.44
10:9:33:LYS:HA	10:9:36:TYR:HB3	1.99	0.44
13:P:222:VAL:HG23	17:T:66:LEU:HD11	1.99	0.44
17:V:456:VAL:HG13	17:V:474:LEU:HD13	2.00	0.44
18:Y:120:ARG:NE	18:Y:130:ASP:OD2	2.41	0.44
2:1:204:VAL:HG23	2:1:206:GLN:HG2	2.00	0.44
17:U:559:LEU:HD12	17:U:560:PRO:HD2	2.00	0.44
17:V:104:GLN:HB3	18:Z:95:GLY:HA2	2.00	0.44
5:4:65:PRO:HG3	17:T:56:LYS:HB2	2.00	0.44
16:S:84:PRO:HA	16:S:87:ARG:HG2	1.98	0.44
17:T:164:THR:HA	17:T:170:PRO:HA	1.99	0.44
3:2:80:HIS:CE1	3:2:82:LYS:HB3	2.52	0.44
8:7:73:LYS:HA	8:7:73:LYS:HD3	1.82	0.44
11:D:69:ILE:HD12	11:E:69:ILE:HB	2.00	0.44
15:R:106:PRO:HB2	16:S:231:TYR:HA	1.99	0.44
17:U:240:ILE:HG22	17:U:491:PRO:HG3	2.00	0.44
17:V:150:ILE:HB	17:V:184:LEU:HD22	2.00	0.44
18:Y:289:ARG:NH1	18:Y:292:GLN:OE1	2.46	0.44
18:Z:287:ILE:HD12	18:Z:290:PHE:HB3	2.00	0.44
2:1:270:VAL:HG13	2:1:527:GLN:HB2	2.00	0.44
5:4:33:LEU:HD23	5:4:37:ALA:HB3	1.99	0.44
5:4:85:TYR:HH	8:7:161:TYR:HH	1.59	0.44
9:8:43:ARG:NH2	12:M:147:SER:OG	2.45	0.44
11:D:82:PHE:HZ	11:E:109:LEU:HD23	1.83	0.44
13:P:101:ARG:HG2	13:P:126:ALA:HB1	2.00	0.44
16:S:180:GLU:HA	16:S:183:ILE:HB	2.00	0.44
16:S:308:ILE:HD11	18:Z:305:PRO:HG2	1.99	0.44
17:V:109:VAL:N	17:V:117:GLY:O	2.46	0.44
18:X:298:SER:HB2	18:X:311:GLN:HE21	1.82	0.44
18:Z:107:SER:HB2	18:Z:110:LYS:HE2	1.99	0.44
18:Z:573:LYS:HA	18:Z:573:LYS:HD3	1.84	0.44
6:5:30:LEU:HD13	12:M:110:LEU:HG	1.99	0.43
17:T:498:THR:HA	17:T:501:VAL:HG12	1.99	0.43
17:V:453:TYR:O	17:V:457:ALA:N	2.50	0.43

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:V:513:ARG:HH11	17:V:515:GLN:HE21	1.66	0.43
18:Z:130:ASP:OD1	18:Z:130:ASP:N	2.51	0.43
2:1:75:SER:O	2:1:75:SER:OG	2.36	0.43
8:7:32:SER:OG	8:7:33:GLY:N	2.51	0.43
12:M:265:LEU:HD13	12:M:270:MET:HG2	2.00	0.43
18:X:169:LEU:HD21	18:X:403:VAL:HG11	1.99	0.43
3:2:81:PHE:HE1	3:2:115:VAL:HA	1.82	0.43
4:3:277:SER:OG	4:3:277:SER:O	2.32	0.43
11:H:97:LYS:HA	11:H:97:LYS:HD3	1.79	0.43
16:S:239:ARG:HA	16:S:242:VAL:HG12	2.00	0.43
17:T:256:TYR:HE1	17:T:318:LYS:HD2	1.83	0.43
17:V:545:ALA:O	17:V:549:HIS:ND1	2.50	0.43
18:Z:255:PRO:HA	18:Z:258:ARG:HB2	2.01	0.43
18:Z:266:LEU:HD13	18:Z:324:ARG:HD3	2.00	0.43
3:2:241:PRO:HB2	3:2:280:LEU:HD11	2.00	0.43
3:2:440:LYS:HB2	3:2:440:LYS:HE3	1.75	0.43
4:3:205:CYS:O	4:3:206:ASN:ND2	2.51	0.43
11:A:115:LEU:HD11	12:M:247:GLY:HA2	2.01	0.43
15:R:55:THR:O	15:R:58:LYS:NZ	2.45	0.43
17:T:472:TYR:OH	17:T:476:ARG:NH1	2.51	0.43
17:U:108:LEU:HG	17:U:151:VAL:HG12	2.01	0.43
18:X:276:GLU:HB3	18:X:278:GLN:HE21	1.83	0.43
6:5:30:LEU:HA	6:5:30:LEU:HD23	1.84	0.43
17:T:291:THR:N	17:T:294:ASP:OD1	2.51	0.43
17:T:367:LYS:HA	17:T:376:SER:HA	2.01	0.43
17:U:207:LYS:HE2	17:U:207:LYS:HB3	1.77	0.43
10:9:56:ASN:OD1	10:9:56:ASN:N	2.51	0.43
17:U:482:GLU:HG3	17:U:517:ILE:HB	2.00	0.43
18:Z:80:MET:HG2	18:Z:86:ARG:HB2	2.00	0.43
6:5:23:LEU:HD22	9:8:47:LEU:HD23	2.00	0.43
17:T:92:ASP:OD2	18:X:303:ARG:NE	2.44	0.43
18:Y:176:GLY:O	18:Y:327:THR:OG1	2.26	0.43
18:Y:539:ILE:HG22	18:Y:541:GLU:HG2	2.01	0.43
1:0:69:PRO:HD2	10:9:60:ASN:HD22	1.83	0.43
5:4:233:HIS:CG	8:7:153:LEU:HD11	2.53	0.43
13:P:187:GLN:O	13:P:188:GLU:C	2.57	0.43
16:S:102:VAL:HG11	16:S:127:LEU:HD22	2.00	0.43
16:S:119:ILE:O	16:S:123:THR:OG1	2.35	0.43
17:T:67:ILE:HA	17:T:70:VAL:HG12	2.01	0.43
18:Y:165:LYS:NZ	18:Y:489:VAL:O	2.45	0.43
3:2:266:PHE:HA	3:2:269:VAL:HG22	2.01	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:B:58:ALA:HB2	11:C:56:LEU:HD12	2.00	0.43
11:H:55:VAL:HA	11:H:58:ALA:HB3	2.00	0.43
11:H:78:LEU:HD23	11:H:78:LEU:HA	1.85	0.43
17:T:516:ASP:O	17:T:520:ALA:N	2.50	0.43
17:U:236:ILE:HG23	17:U:276:PHE:HE2	1.84	0.43
18:X:61:SER:OG	18:X:62:SER:N	2.52	0.43
15:R:37:TRP:HH2	15:R:45:LEU:HB2	1.84	0.42
17:T:123:GLN:O	18:Y:98:ARG:NH1	2.44	0.42
17:U:559:LEU:HG	17:U:561:GLY:H	1.84	0.42
17:V:199:ARG:HA	17:V:199:ARG:HD3	1.89	0.42
18:Y:273:ARG:HD3	18:Y:333:ILE:HG13	2.01	0.42
18:Y:481:LEU:HD21	18:Y:495:VAL:HG12	2.00	0.42
18:Z:266:LEU:HA	18:Z:266:LEU:HD23	1.85	0.42
17:U:88:LEU:HG	17:U:98:TYR:HB2	2.01	0.42
18:X:445:GLN:NE2	18:X:459:LYS:O	2.52	0.42
2:1:593:LEU:HD13	4:3:204:TYR:HD2	1.84	0.42
8:7:104:LEU:HD23	8:7:104:LEU:HA	1.90	0.42
11:I:69:ILE:HD12	11:J:69:ILE:HB	2.01	0.42
17:T:326:ASP:OD1	17:T:329:LYS:NZ	2.51	0.42
18:Y:228:ILE:HD13	18:Y:228:ILE:HA	1.90	0.42
5:4:100:CYS:HB3	5:4:103:ILE:HD12	2.00	0.42
16:S:162:ILE:HG21	16:S:178:ILE:HD12	2.02	0.42
17:T:246:ASN:HA	17:T:249:VAL:HG22	2.01	0.42
18:Y:470:PHE:O	18:Y:474:LEU:HB2	2.20	0.42
18:Z:375:PRO:HD2	18:Z:444:SER:HA	2.01	0.42
5:4:233:HIS:HA	5:4:236:LYS:HE2	2.01	0.42
11:F:55:VAL:HG12	11:G:55:VAL:HG11	2.02	0.42
17:U:548:ALA:HB3	18:X:524:ILE:HG12	2.02	0.42
17:V:206:VAL:HG13	17:V:486:GLN:HG3	2.00	0.42
18:Y:101:LYS:HE2	18:Y:101:LYS:HB2	1.87	0.42
18:Z:522:LYS:HG3	18:Z:523:ASP:H	1.85	0.42
3:2:12:LEU:HD12	3:2:12:LEU:HA	1.89	0.42
4:3:192:VAL:HA	4:3:195:LEU:HD12	2.01	0.42
17:T:55:SER:O	17:T:57:TYR:N	2.52	0.42
18:Z:64:GLU:OE2	18:Z:71:ARG:NH1	2.52	0.42
2:1:510:ILE:HD12	2:1:510:ILE:HA	1.88	0.42
8:7:127:LEU:HD12	8:7:127:LEU:HA	1.85	0.42
11:G:71:LEU:HD23	11:G:71:LEU:HA	1.92	0.42
12:M:189:TRP:CD2	12:M:233:ALA:HB2	2.55	0.42
14:Q:10:ARG:HA	14:Q:10:ARG:HD3	1.86	0.42
17:U:154:PRO:HD2	17:U:168:GLY:HA3	2.01	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:U:487:LYS:HE2	17:U:487:LYS:HB3	1.91	0.42
18:X:113:VAL:HG12	18:X:268:VAL:HG22	2.01	0.42
3:2:378:LEU:HG	3:2:411:TYR:HB3	2.02	0.42
4:3:108:TYR:HA	4:3:146:ALA:HB2	2.02	0.42
13:P:52:GLN:HB3	17:V:59:ILE:HG12	2.02	0.42
17:T:104:GLN:HG2	18:Y:97:VAL:HG22	2.02	0.42
17:T:160:LEU:HD23	17:T:160:LEU:HA	1.89	0.42
17:T:260:VAL:HG11	17:T:306:GLY:HA3	2.02	0.42
18:Y:111:VAL:HG11	18:Y:264:THR:HG23	2.02	0.42
18:Y:438:LYS:HE3	18:Y:479:ASP:HA	2.01	0.42
18:Z:325:ILE:HG23	18:Z:333:ILE:HG22	2.01	0.42
18:Z:425:LEU:HD12	18:Z:429:ASP:HB3	2.01	0.42
2:1:77:PRO:HB2	2:1:80:LYS:HB2	2.01	0.42
2:1:592:PHE:HE1	6:5:55:LEU:HD13	1.84	0.42
7:6:108:LEU:HG	12:M:285:VAL:HG21	2.01	0.42
11:C:107:PHE:HA	11:C:110:THR:HG22	2.01	0.42
13:P:208:ASP:HB3	13:P:213:LYS:HG2	2.02	0.42
15:R:33:PHE:HD2	16:S:94:ALA:HB2	1.85	0.42
16:S:177:LEU:HD23	16:S:177:LEU:HA	1.94	0.42
17:V:301:LEU:HD23	17:V:301:LEU:HA	1.91	0.42
18:Z:213:VAL:HG22	18:Z:261:VAL:HG13	2.02	0.42
1:0:37:LYS:HD2	1:0:37:LYS:HA	1.81	0.42
17:T:195:ARG:HA	17:T:195:ARG:HD3	1.79	0.42
18:X:74:LEU:HB3	18:X:87:CYS:HB3	2.02	0.42
18:X:212:GLY:HA2	18:X:285:ASP:HB3	2.02	0.42
18:X:467:ILE:HD12	18:X:467:ILE:HA	1.82	0.42
2:1:517:GLU:HG2	2:1:518:GLU:HG3	2.02	0.41
10:9:95:LYS:HB3	10:9:95:LYS:HE3	1.88	0.41
15:R:198:LYS:HA	15:R:198:LYS:HD2	1.88	0.41
17:T:48:LEU:HD23	17:T:48:LEU:HA	1.92	0.41
18:X:248:TYR:HD1	18:X:248:TYR:HA	1.75	0.41
2:1:549:ASP:OD2	2:1:549:ASP:N	2.52	0.41
3:2:289:HIS:HD2	3:2:307:VAL:HG23	1.85	0.41
7:6:103:LEU:HD23	7:6:103:LEU:HA	1.88	0.41
8:7:16:THR:OG1	8:7:18:PHE:O	2.38	0.41
12:M:135:LEU:HD23	12:M:135:LEU:HA	1.94	0.41
12:M:173:ALA:HB3	12:M:176:SER:HB3	2.02	0.41
13:P:103:LYS:HA	13:P:103:LYS:HD2	1.75	0.41
17:V:322:ILE:HG23	17:V:379:ALA:HA	2.02	0.41
2:1:261:LEU:HD23	2:1:261:LEU:HA	1.91	0.41
14:Q:31:LEU:HD22	15:R:154:GLN:HG3	2.02	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:T:250:PRO:HD2	17:T:253:GLN:HE21	1.85	0.41
17:U:140:GLN:HB3	18:Z:56:LEU:HD12	2.02	0.41
17:U:229:THR:O	17:U:229:THR:CG2	2.66	0.41
17:U:334:TYR:OH	17:U:353:ASP:OD2	2.36	0.41
17:V:201:PRO:HA	17:V:216:GLY:HA2	2.01	0.41
18:X:121:ILE:HG12	18:X:246:LEU:HD12	2.02	0.41
18:X:566:LYS:HB3	18:X:566:LYS:HE3	1.88	0.41
2:1:338:SER:HB3	2:1:341:GLU:HG3	2.02	0.41
6:5:62:TYR:OH	7:6:146:PHE:O	2.32	0.41
11:H:109:LEU:O	11:H:112:SER:OG	2.35	0.41
13:P:217:GLU:HG3	17:T:73:TRP:HZ2	1.85	0.41
15:R:86:LYS:NZ	15:R:125:GLU:OE2	2.37	0.41
17:V:207:LYS:H	17:V:486:GLN:NE2	2.19	0.41
17:V:532:VAL:HG23	17:V:546:LEU:HD11	2.03	0.41
18:Z:346:LEU:HD22	18:Z:355:PHE:HE1	1.84	0.41
18:Z:363:VAL:HB	18:Z:378:ASP:HB3	2.01	0.41
2:1:241:SER:HB3	2:1:244:VAL:HG12	2.01	0.41
11:F:96:ALA:HB1	11:G:102:TYR:HE2	1.86	0.41
11:G:92:ASN:OD1	11:G:92:ASN:N	2.53	0.41
13:P:77:PHE:HA	13:P:80:LEU:HB2	2.02	0.41
13:P:120:LYS:HD3	13:P:120:LYS:HA	1.85	0.41
17:U:235:ALA:HB1	17:U:323:ILE:HG12	2.00	0.41
17:U:353:ASP:OD1	17:U:353:ASP:N	2.44	0.41
17:V:196:GLN:HE21	17:V:367:LYS:HE3	1.85	0.41
18:Y:162:THR:O	18:Y:199:ASN:ND2	2.40	0.41
18:Y:219:GLU:HA	18:Y:222:ASP:HB2	2.03	0.41
18:Y:500:ASP:O	18:Y:504:LYS:CG	2.68	0.41
18:Z:516:LYS:HZ3	18:Z:519:GLU:HA	1.86	0.41
2:1:419:ILE:HG21	2:1:442:ASP:HB2	2.02	0.41
5:4:59:SER:OG	5:4:96:ALA:O	2.30	0.41
11:B:92:ASN:OD1	11:B:92:ASN:N	2.53	0.41
1:0:68:VAL:N	1:0:71:MET:SD	2.87	0.41
3:2:253:LEU:HD23	3:2:253:LEU:HA	1.85	0.41
8:7:150:LEU:HD23	8:7:153:LEU:HD12	2.01	0.41
11:B:89:ALA:HB3	11:C:99:LEU:HD21	2.03	0.41
15:R:89:VAL:O	15:R:100:VAL:N	2.43	0.41
17:T:192:ILE:O	18:Y:221:ASN:ND2	2.52	0.41
17:T:342:ARG:NH1	18:X:302:GLY:O	2.53	0.41
17:V:149:GLN:HB3	17:V:152:ASN:HD21	1.86	0.41
18:Z:65:VAL:HG22	18:Z:102:VAL:HG22	2.02	0.41
3:2:240:ALA:H	3:2:243:GLN:HE21	1.68	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:5:90:GLU:HA	6:5:93:GLU:HG2	2.03	0.41
11:A:69:ILE:HB	11:J:69:ILE:HD12	2.02	0.41
11:C:60:LYS:HD2	11:C:125:LEU:HD23	2.03	0.41
17:T:199:ARG:HE	17:T:199:ARG:HB3	1.73	0.41
17:T:236:ILE:HD13	17:T:236:ILE:HA	1.93	0.41
17:U:223:ILE:HB	17:U:382:VAL:HG22	2.02	0.41
17:V:121:ASN:O	17:V:128:GLY:N	2.52	0.41
2:1:523:LEU:HD23	2:1:523:LEU:HA	1.89	0.41
2:1:540:LEU:HD12	2:1:541:PRO:HD2	2.03	0.41
3:2:40:GLN:HG2	8:7:69:LEU:HD13	2.02	0.41
3:2:293:THR:HG21	3:2:405:VAL:HG23	2.03	0.41
3:2:320:LEU:HD23	3:2:320:LEU:HA	1.91	0.41
5:4:23:SER:HA	5:4:26:VAL:HG12	2.03	0.41
6:5:73:LYS:HD2	6:5:73:LYS:HA	1.92	0.41
11:D:75:GLY:HA3	11:E:74:VAL:HG22	2.02	0.41
11:F:94:ASN:H	15:R:101:LYS:HG3	1.86	0.41
11:H:113:ILE:HD13	11:H:113:ILE:HA	1.90	0.41
12:M:324:LYS:HE2	12:M:324:LYS:HB3	1.94	0.41
13:P:38:LYS:HE2	13:P:38:LYS:HB2	1.97	0.41
14:Q:27:LEU:HD23	15:R:148:GLU:HB3	2.02	0.41
16:S:124:ARG:HD2	16:S:153:ILE:HG21	2.03	0.41
17:U:94:ILE:HG12	17:U:130:VAL:HG12	2.03	0.41
17:U:104:GLN:HB3	18:X:95:GLY:HA2	2.03	0.41
17:U:402:THR:HG22	17:U:403:ASP:N	2.35	0.41
17:U:465:ASP:OD1	17:U:465:ASP:N	2.47	0.41
17:V:49:ARG:HD3	17:V:49:ARG:HA	1.92	0.41
17:V:370:LYS:HD3	17:V:370:LYS:HA	1.88	0.41
18:X:420:LEU:HD13	18:X:424:GLU:HG2	2.03	0.41
18:Z:294:ASN:HA	18:Z:297:VAL:HG22	2.03	0.41
11:J:55:VAL:HA	11:J:58:ALA:HB3	2.03	0.41
18:X:72:LEU:HD11	18:X:89:ALA:HB1	2.02	0.41
18:Z:111:VAL:HG11	18:Z:264:THR:HG23	2.03	0.41
2:1:79:LEU:N	2:1:496:GLU:OE2	2.42	0.40
3:2:424:LEU:HA	3:2:425:PRO:HD3	1.87	0.40
11:F:93:PRO:HD2	15:R:101:LYS:HB2	2.03	0.40
17:U:135:ASP:N	17:U:135:ASP:OD1	2.54	0.40
17:U:440:LYS:HE2	17:U:440:LYS:HB3	1.87	0.40
17:V:145:TYR:HB3	18:Z:560:VAL:HB	2.03	0.40
18:X:306:SER:OG	18:X:307:ALA:N	2.54	0.40
2:1:316:ASN:HD22	2:1:316:ASN:HA	1.70	0.40
2:1:472:LYS:HD2	2:1:472:LYS:HA	1.82	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:C:93:PRO:HA	11:C:96:ALA:HB2	2.04	0.40
18:X:225:ARG:HA	18:X:225:ARG:HD3	1.87	0.40
18:X:539:ILE:HG22	18:X:541:GLU:HG2	2.03	0.40
18:Z:318:LEU:HD12	18:Z:318:LEU:HA	1.92	0.40
8:7:170:HIS:CD2	8:7:172:ALA:H	2.39	0.40
17:V:426:SER:O	17:V:426:SER:OG	2.39	0.40
17:V:552:ALA:O	17:V:556:LYS:NZ	2.53	0.40
18:X:286:ASN:HD21	18:X:340:TYR:HB2	1.85	0.40
2:1:556:ILE:HG21	6:5:36:ARG:HA	2.03	0.40
16:S:105:VAL:HG23	16:S:142:ILE:HB	2.03	0.40
17:V:450:LEU:HD23	17:V:450:LEU:HA	1.95	0.40
18:Y:93:THR:HB	18:Y:96:LEU:HD12	2.02	0.40
2:1:375:LEU:HA	2:1:427:LYS:HD3	2.02	0.40
3:2:82:LYS:HG3	5:4:84:ARG:HD2	2.03	0.40
5:4:89:LEU:HA	5:4:89:LEU:HD23	1.84	0.40
15:R:28:ALA:HB3	16:S:92:PHE:HD1	1.86	0.40
17:V:456:VAL:HG11	17:V:473:VAL:HG23	2.03	0.40
18:X:153:GLN:HE22	18:X:326:THR:HG21	1.87	0.40
18:Y:112:PRO:HB3	18:Y:137:ALA:HA	2.04	0.40
18:Y:417:ILE:HD11	18:Y:425:LEU:HD11	2.03	0.40
18:Z:210:PHE:HB3	18:Z:246:LEU:HD23	2.02	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	79/82 (96%)	72 (91%)	7 (9%)	0	100	100
2	1	593/618 (96%)	571 (96%)	22 (4%)	0	100	100
3	2	439/441 (100%)	419 (95%)	19 (4%)	1 (0%)	47	80
4	3	243/325 (75%)	233 (96%)	10 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	4	288/294 (98%)	277 (96%)	11 (4%)	0	100	100
6	5	121/123 (98%)	113 (93%)	7 (6%)	1 (1%)	19	58
7	6	122/151 (81%)	112 (92%)	10 (8%)	0	100	100
8	7	174/190 (92%)	169 (97%)	5 (3%)	0	100	100
9	8	86/89 (97%)	78 (91%)	8 (9%)	0	100	100
10	9	95/97 (98%)	84 (88%)	11 (12%)	0	100	100
11	A	72/127 (57%)	70 (97%)	2 (3%)	0	100	100
11	B	72/127 (57%)	70 (97%)	2 (3%)	0	100	100
11	C	71/127 (56%)	69 (97%)	2 (3%)	0	100	100
11	D	72/127 (57%)	72 (100%)	0	0	100	100
11	E	72/127 (57%)	69 (96%)	3 (4%)	0	100	100
11	F	72/127 (57%)	69 (96%)	3 (4%)	0	100	100
11	G	72/127 (57%)	72 (100%)	0	0	100	100
11	H	72/127 (57%)	71 (99%)	1 (1%)	0	100	100
11	I	72/127 (57%)	70 (97%)	2 (3%)	0	100	100
11	J	72/127 (57%)	71 (99%)	1 (1%)	0	100	100
12	M	213/327 (65%)	208 (98%)	5 (2%)	0	100	100
13	P	191/229 (83%)	177 (93%)	13 (7%)	1 (0%)	29	67
14	Q	70/74 (95%)	67 (96%)	3 (4%)	0	100	100
15	R	175/199 (88%)	165 (94%)	10 (6%)	0	100	100
16	S	275/317 (87%)	261 (95%)	14 (5%)	0	100	100
17	T	521/562 (93%)	484 (93%)	34 (6%)	3 (1%)	25	63
17	U	521/562 (93%)	494 (95%)	26 (5%)	1 (0%)	47	80
17	V	518/562 (92%)	492 (95%)	25 (5%)	1 (0%)	47	80
18	X	540/574 (94%)	502 (93%)	37 (7%)	1 (0%)	47	80
18	Y	519/574 (90%)	479 (92%)	38 (7%)	2 (0%)	34	71
18	Z	536/574 (93%)	500 (93%)	34 (6%)	2 (0%)	34	71
All	All	7038/8234 (86%)	6660 (95%)	365 (5%)	13 (0%)	50	80

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	P	188	GLU

Continued on next page...



*Continued from previous page...*

Mol	Chain	Res	Type
18	X	308	VAL
18	Z	308	VAL
3	2	383	PRO
17	T	56	LYS
17	T	493	PRO
17	V	349	ALA
17	T	349	ALA
17	U	349	ALA
18	Y	308	VAL
18	Z	307	ALA
6	5	120	PRO
18	Y	455	GLY

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	63/64 (98%)	63 (100%)	0	100	100
2	1	493/512 (96%)	493 (100%)	0	100	100
3	2	312/312 (100%)	312 (100%)	0	100	100
4	3	195/258 (76%)	195 (100%)	0	100	100
5	4	220/223 (99%)	220 (100%)	0	100	100
6	5	107/107 (100%)	107 (100%)	0	100	100
7	6	96/115 (84%)	96 (100%)	0	100	100
8	7	140/150 (93%)	140 (100%)	0	100	100
9	8	71/72 (99%)	70 (99%)	1 (1%)	67	80
10	9	79/79 (100%)	79 (100%)	0	100	100
11	A	50/86 (58%)	50 (100%)	0	100	100
11	B	50/86 (58%)	50 (100%)	0	100	100
11	C	50/86 (58%)	50 (100%)	0	100	100
11	D	50/86 (58%)	50 (100%)	0	100	100

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	E	50/86 (58%)	49 (98%)	1 (2%)	55	73
11	F	50/86 (58%)	49 (98%)	1 (2%)	55	73
11	G	50/86 (58%)	49 (98%)	1 (2%)	55	73
11	H	50/86 (58%)	50 (100%)	0	100	100
11	I	50/86 (58%)	50 (100%)	0	100	100
11	J	50/86 (58%)	50 (100%)	0	100	100
12	M	178/272 (65%)	178 (100%)	0	100	100
13	P	171/196 (87%)	170 (99%)	1 (1%)	86	92
14	Q	56/58 (97%)	56 (100%)	0	100	100
15	R	134/151 (89%)	133 (99%)	1 (1%)	84	90
16	S	235/265 (89%)	235 (100%)	0	100	100
17	T	419/448 (94%)	417 (100%)	2 (0%)	88	93
17	U	419/448 (94%)	419 (100%)	0	100	100
17	V	418/448 (93%)	415 (99%)	3 (1%)	84	90
18	X	449/469 (96%)	448 (100%)	1 (0%)	93	96
18	Y	430/469 (92%)	430 (100%)	0	100	100
18	Z	446/469 (95%)	446 (100%)	0	100	100
All	All	5631/6445 (87%)	5619 (100%)	12 (0%)	93	96

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	8	85	THR
11	E	92	ASN
11	F	119	LEU
11	G	85	LEU
13	P	184	LEU
15	R	115	VAL
17	T	180	VAL
17	T	220	ARG
17	V	164	THR
17	V	229	THR
17	V	243	LYS
18	X	248	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (95)

such sidechains are listed below:

Mol	Chain	Res	Type
1	0	48	ASN
2	1	65	GLN
2	1	100	GLN
2	1	209	ASN
2	1	285	GLN
2	1	298	GLN
2	1	316	ASN
2	1	365	GLN
2	1	587	ASN
2	1	606	ASN
3	2	122	ASN
3	2	243	GLN
3	2	289	HIS
3	2	380	GLN
4	3	164	ASN
4	3	179	GLN
4	3	188	ASN
4	3	206	ASN
5	4	38	GLN
5	4	240	GLN
6	5	29	GLN
6	5	117	GLN
7	6	106	ASN
8	7	90	GLN
8	7	102	GLN
8	7	123	HIS
8	7	170	HIS
9	8	26	HIS
10	9	60	ASN
11	A	94	ASN
11	B	94	ASN
11	F	87	ASN
11	F	98	GLN
11	G	87	ASN
11	H	87	ASN
11	I	94	ASN
11	I	98	GLN
11	J	98	GLN
12	M	108	ASN
12	M	163	ASN
13	P	65	ASN
13	P	140	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
13	P	220	ASN
13	P	223	ASN
14	Q	40	GLN
14	Q	46	HIS
14	Q	49	GLN
15	R	38	ASN
15	R	53	ASN
15	R	83	GLN
15	R	171	GLN
16	S	52	ASN
16	S	174	GLN
16	S	293	ASN
17	T	64	GLN
17	T	134	ASN
17	T	441	GLN
17	T	497	GLN
17	T	529	ASN
17	U	61	HIS
17	U	123	GLN
17	U	140	GLN
17	U	179	ASN
17	U	242	GLN
17	U	246	ASN
17	U	248	GLN
17	U	358	HIS
17	U	497	GLN
17	U	549	HIS
17	V	64	GLN
17	V	104	GLN
17	V	152	ASN
17	V	196	GLN
17	V	219	GLN
17	V	241	HIS
17	V	242	GLN
17	V	264	GLN
17	V	278	GLN
17	V	486	GLN
17	V	497	GLN
17	V	515	GLN
18	X	68	HIS
18	X	199	ASN
18	X	278	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
18	X	311	GLN
18	X	412	ASN
18	X	471	GLN
18	Y	83	ASN
18	Y	278	GLN
18	Z	199	ASN
18	Z	250	GLN
18	Z	278	GLN
18	Z	294	ASN
18	Z	404	GLN
18	Z	440	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 6 are monoatomic - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
20	ATP	T	1001	21	26,33,33	0.90	1 (3%)	31,52,52	1.69	6 (19%)
22	ADP	Y	601	21	24,29,29	0.65	0	29,45,45	0.70	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	ADP	X	601	21	24,29,29	0.95	1 (4%)	29,45,45	1.54	5 (17%)
20	ATP	U	1001	21	26,33,33	0.92	1 (3%)	31,52,52	1.72	5 (16%)
20	ATP	V	1001	21	26,33,33	0.93	1 (3%)	31,52,52	1.68	5 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	ATP	T	1001	21	-	3/18/38/38	0/3/3/3
22	ADP	Y	601	21	-	0/12/32/32	0/3/3/3
22	ADP	X	601	21	-	3/12/32/32	0/3/3/3
20	ATP	U	1001	21	-	2/18/38/38	0/3/3/3
20	ATP	V	1001	21	-	2/18/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	X	601	ADP	C5-C4	2.31	1.47	1.40
20	V	1001	ATP	C5-C4	2.24	1.46	1.40
20	T	1001	ATP	C5-C4	2.23	1.46	1.40
20	U	1001	ATP	C5-C4	2.20	1.46	1.40

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	T	1001	ATP	PB-O3B-PG	-4.70	116.69	132.83
20	U	1001	ATP	PB-O3B-PG	-4.53	117.28	132.83
20	V	1001	ATP	PA-O3A-PB	-4.35	117.89	132.83
20	V	1001	ATP	PB-O3B-PG	-4.03	119.00	132.83
22	X	601	ADP	PA-O3A-PB	-3.80	119.77	132.83
20	U	1001	ATP	C3'-C2'-C1'	3.80	106.70	100.98
20	T	1001	ATP	PA-O3A-PB	-3.80	119.79	132.83
22	X	601	ADP	N3-C2-N1	-3.46	123.27	128.68
20	U	1001	ATP	PA-O3A-PB	-3.40	121.16	132.83
20	V	1001	ATP	N3-C2-N1	-3.23	123.62	128.68
22	X	601	ADP	C3'-C2'-C1'	3.22	105.82	100.98
20	T	1001	ATP	N3-C2-N1	-3.10	123.83	128.68
20	U	1001	ATP	N3-C2-N1	-3.06	123.90	128.68

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	V	1001	ATP	C3'-C2'-C1'	2.96	105.44	100.98
20	U	1001	ATP	C4-C5-N7	-2.94	106.33	109.40
20	V	1001	ATP	C4-C5-N7	-2.52	106.78	109.40
22	X	601	ADP	C4-C5-N7	-2.38	106.92	109.40
20	T	1001	ATP	C3'-C2'-C1'	2.37	104.54	100.98
22	X	601	ADP	O3B-PB-O2B	2.31	116.47	107.64
22	Y	601	ADP	C5-C6-N6	2.27	123.81	120.35
20	T	1001	ATP	C4-C5-N7	-2.05	107.27	109.40
20	T	1001	ATP	O3G-PG-O2G	2.00	115.29	107.64

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	T	1001	ATP	C5'-O5'-PA-O1A
20	T	1001	ATP	C5'-O5'-PA-O3A
22	X	601	ADP	C5'-O5'-PA-O1A
22	X	601	ADP	C5'-O5'-PA-O3A
20	T	1001	ATP	C5'-O5'-PA-O2A
22	X	601	ADP	C5'-O5'-PA-O2A
20	U	1001	ATP	PA-O3A-PB-O2B
20	V	1001	ATP	PA-O3A-PB-O2B
20	U	1001	ATP	PA-O3A-PB-O1B
20	V	1001	ATP	PA-O3A-PB-O1B

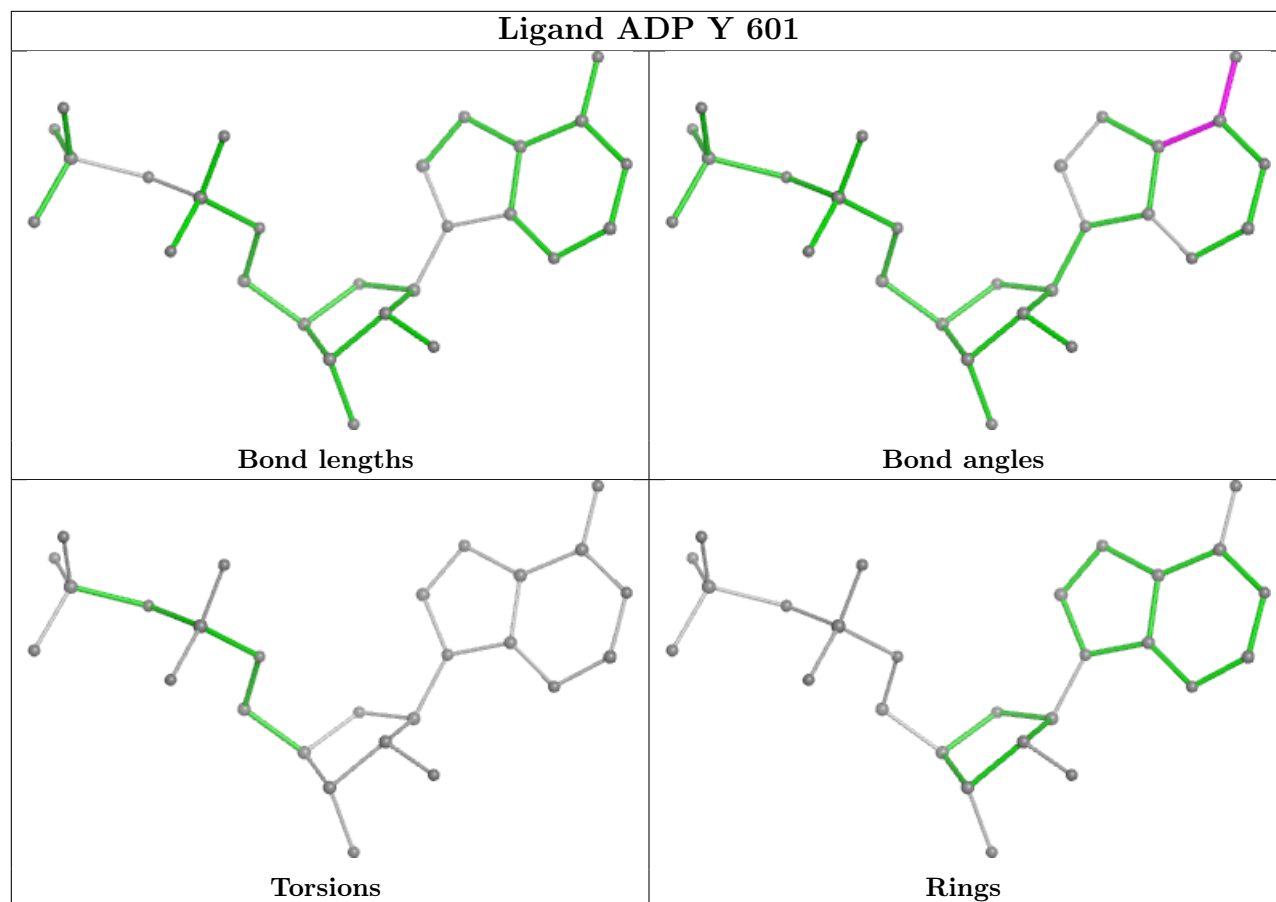
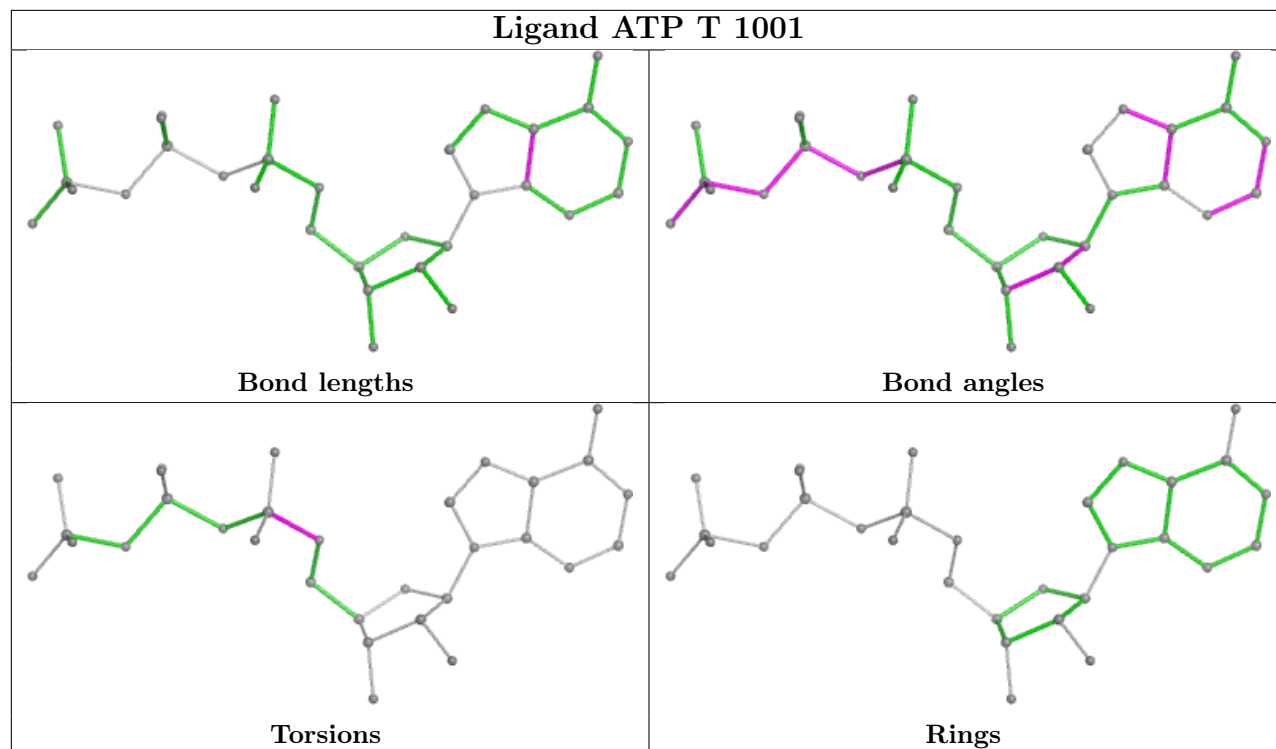
There are no ring outliers.

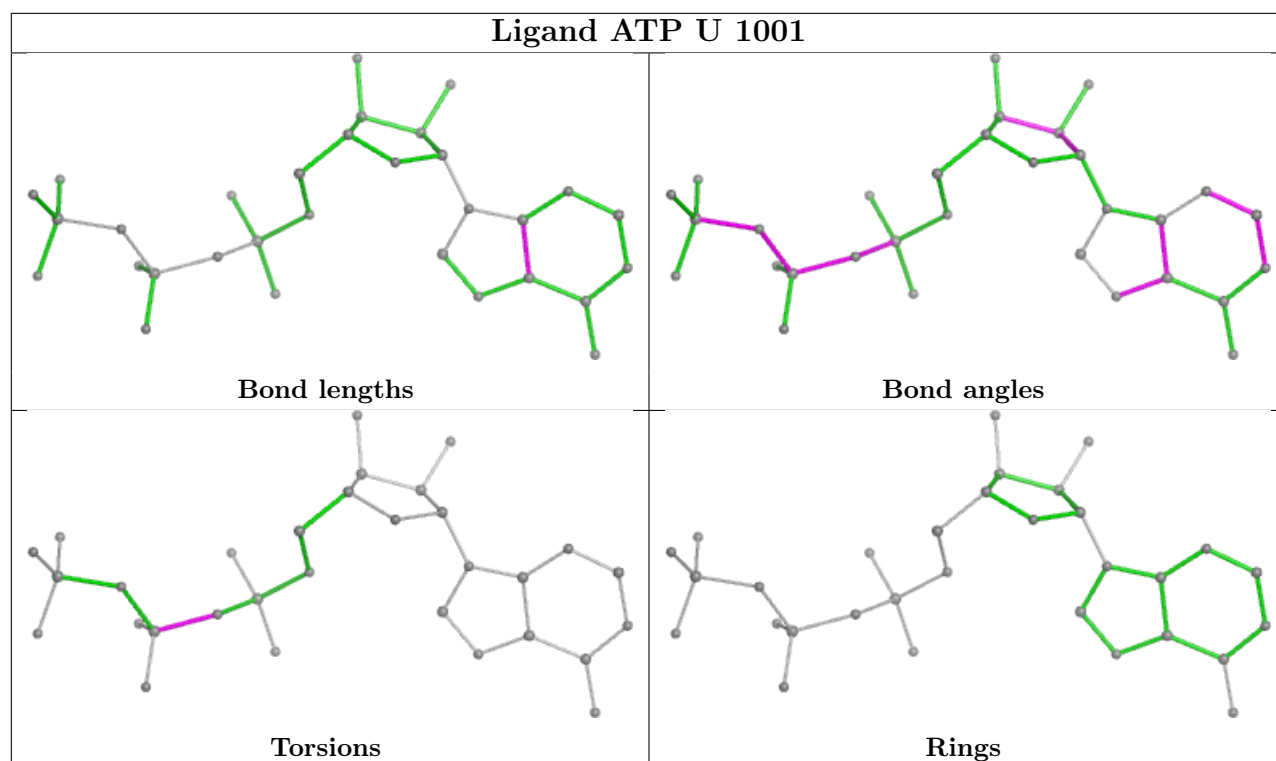
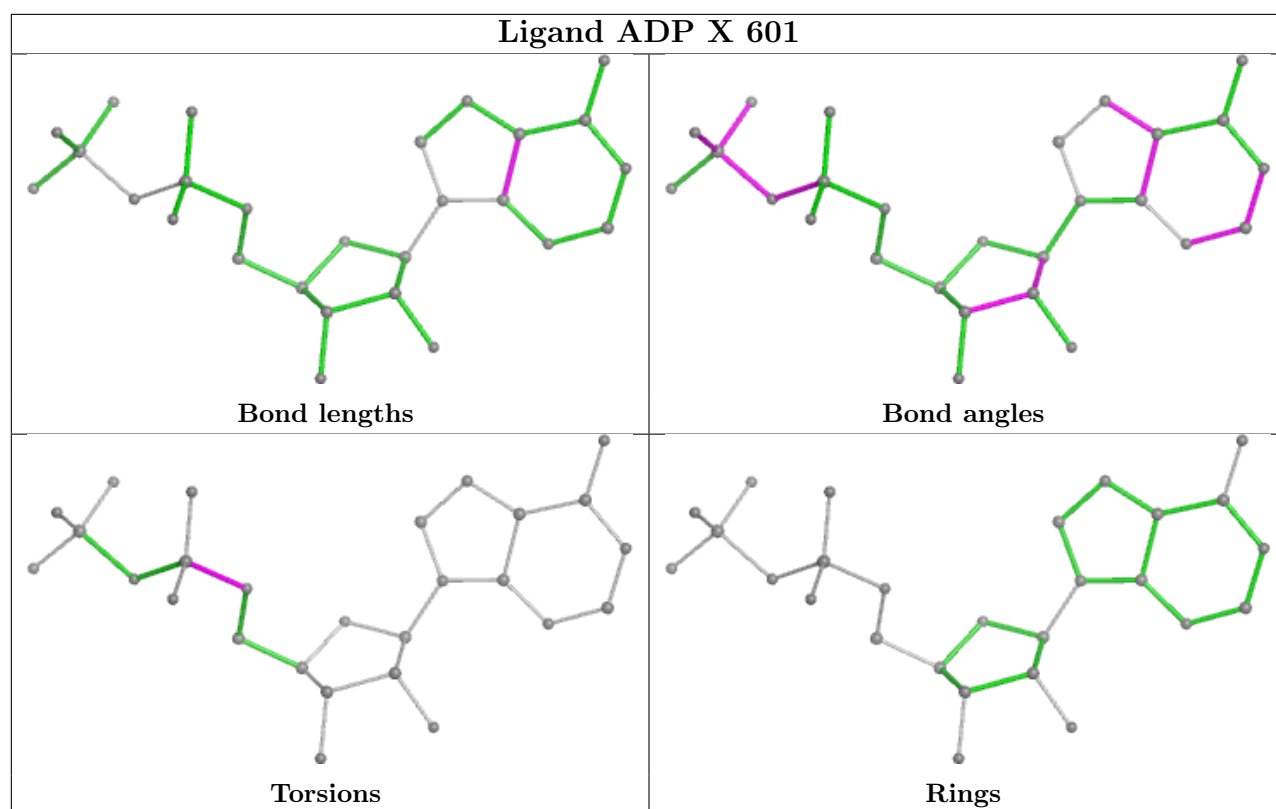
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	Y	601	ADP	1	0

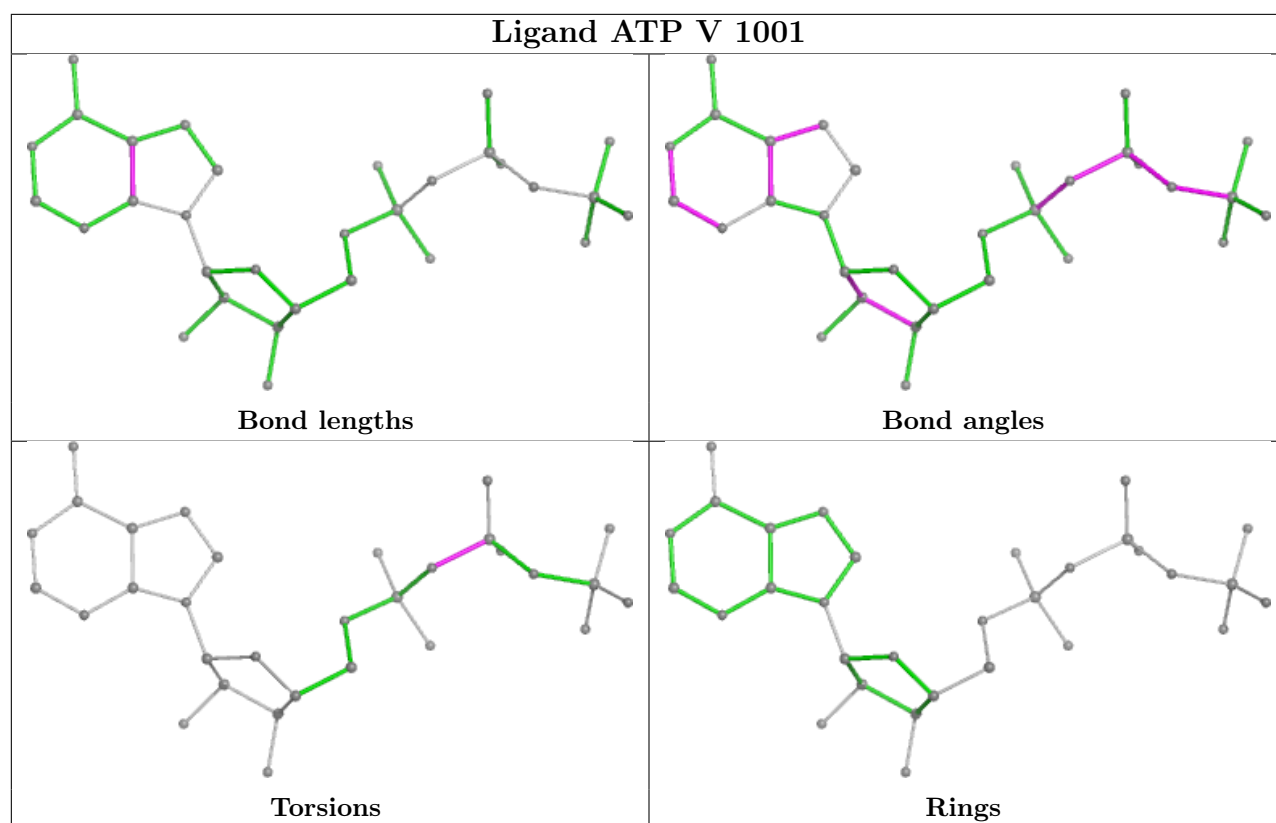
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient

equivalents in the CSD to analyse the geometry.









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
11	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	126:PHE	C	127:ALA	N	3.25

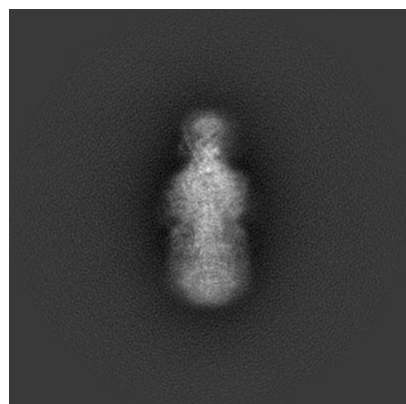
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4828. These allow visual inspection of the internal detail of the map and identification of artifacts.

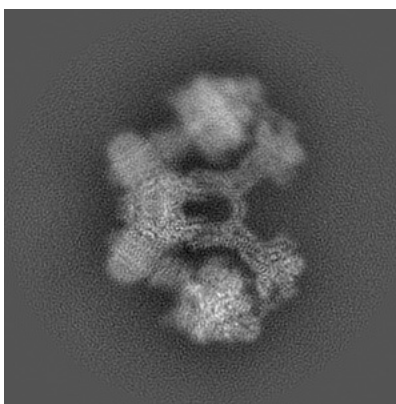
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

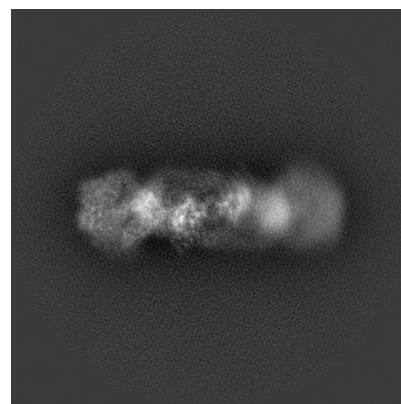
#### 6.1.1 Primary map



X

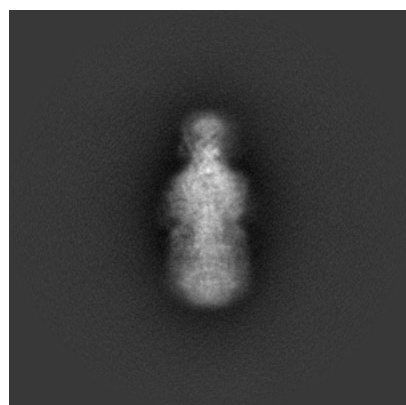


Y

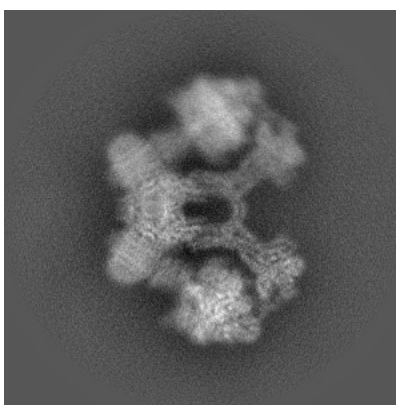


Z

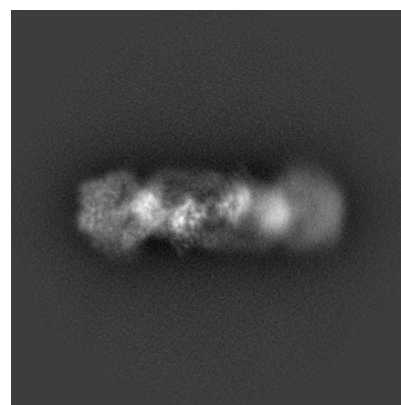
#### 6.1.2 Raw map



X



Y

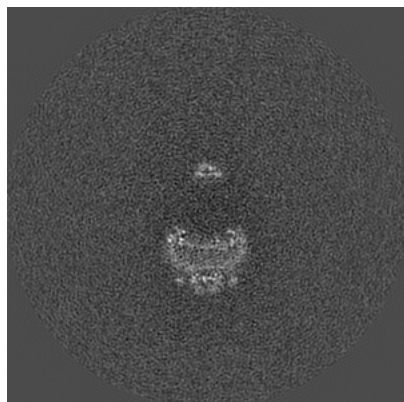


Z

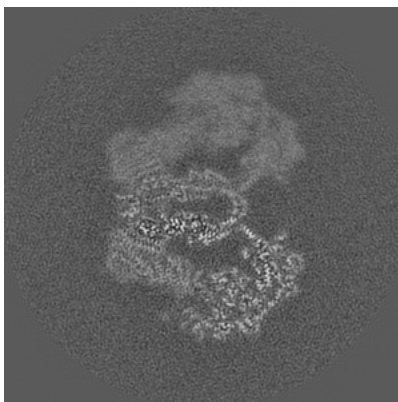
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

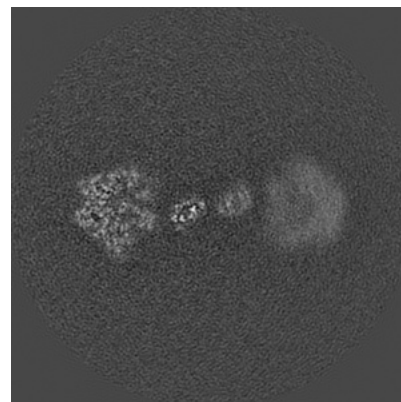
### 6.2.1 Primary map



X Index: 240

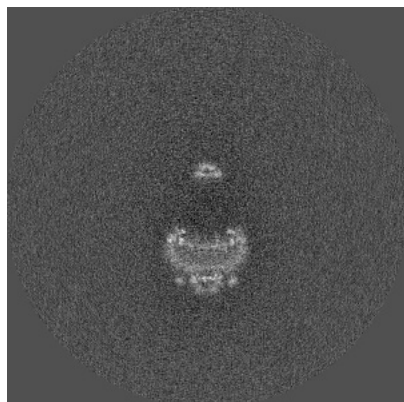


Y Index: 240

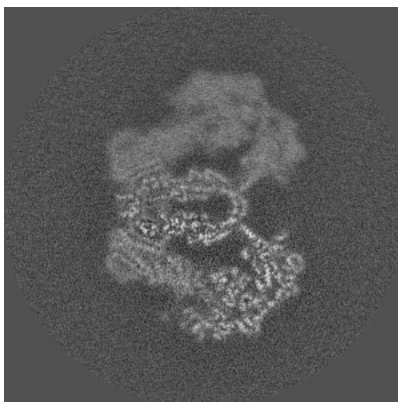


Z Index: 240

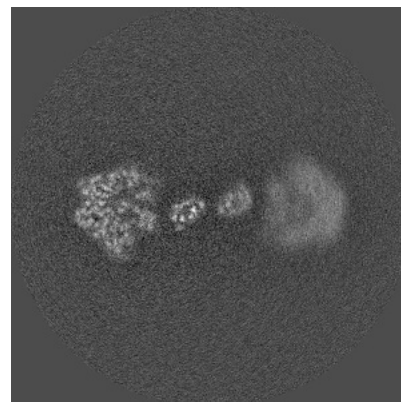
### 6.2.2 Raw map



X Index: 240



Y Index: 240

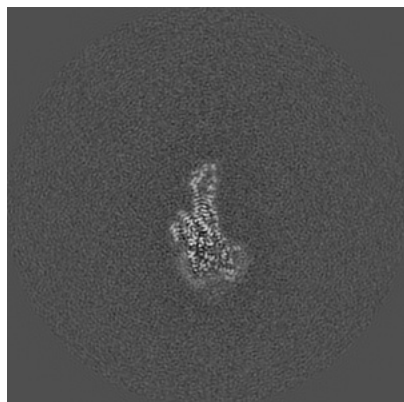


Z Index: 240

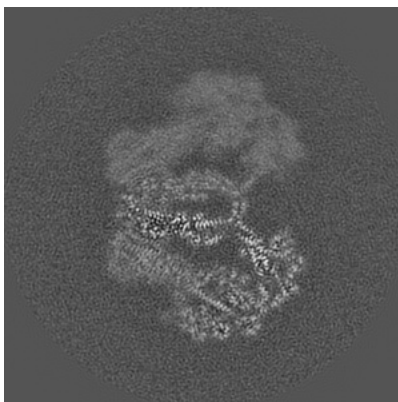
The images above show central slices of the map in three orthogonal directions.

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

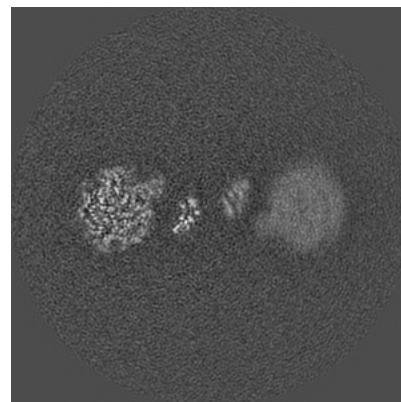
### 6.3.1 Primary map



X Index: 217

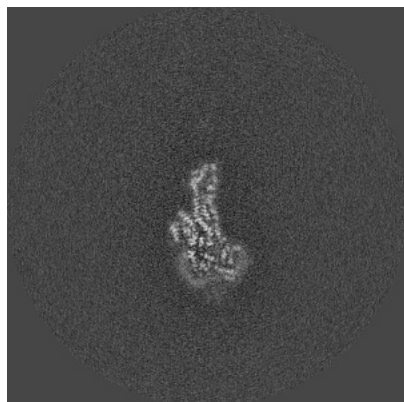


Y Index: 236

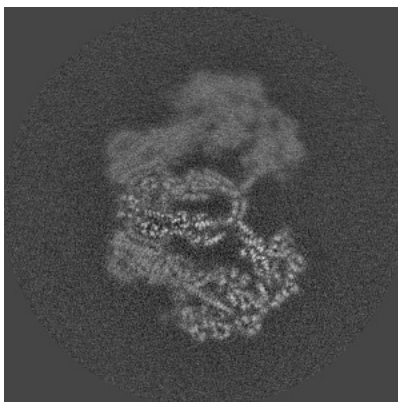


Z Index: 262

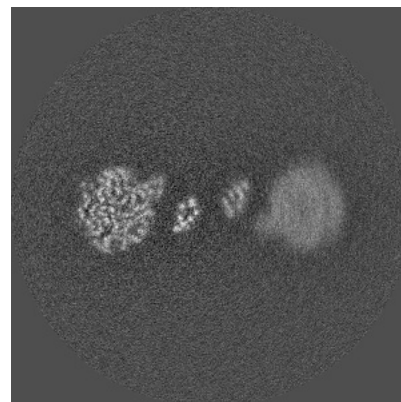
### 6.3.2 Raw map



X Index: 217



Y Index: 237



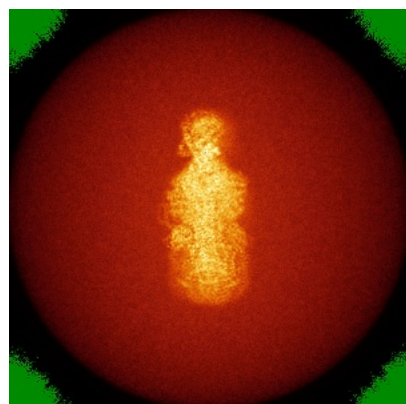
Z Index: 261

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

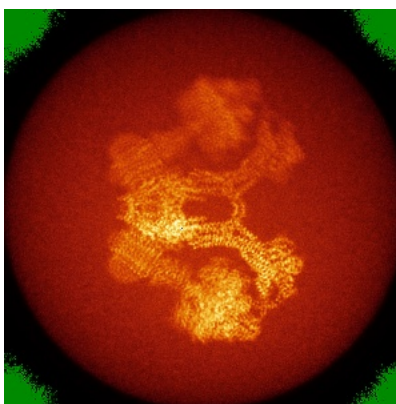


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

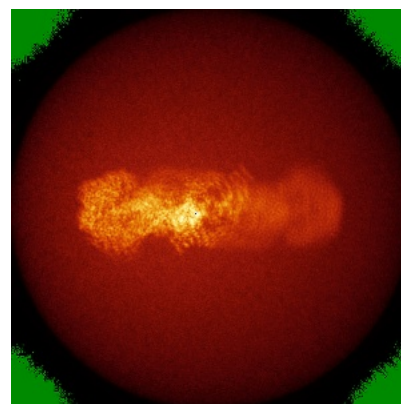
### 6.4.1 Primary map



X

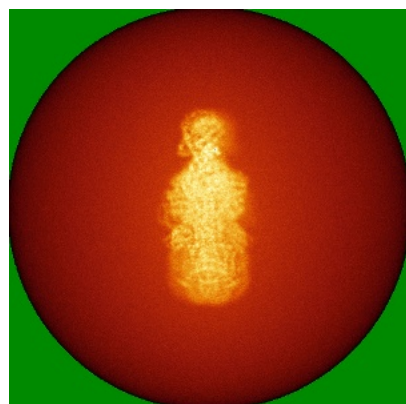


Y

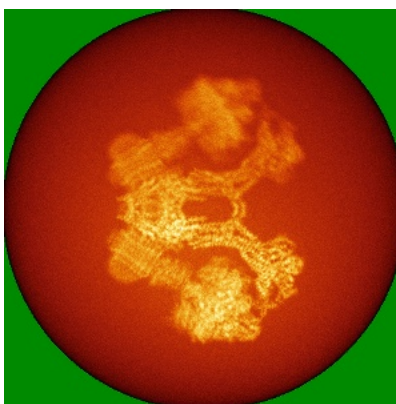


Z

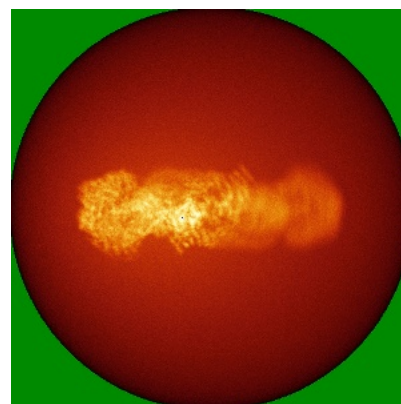
### 6.4.2 Raw map



X



Y

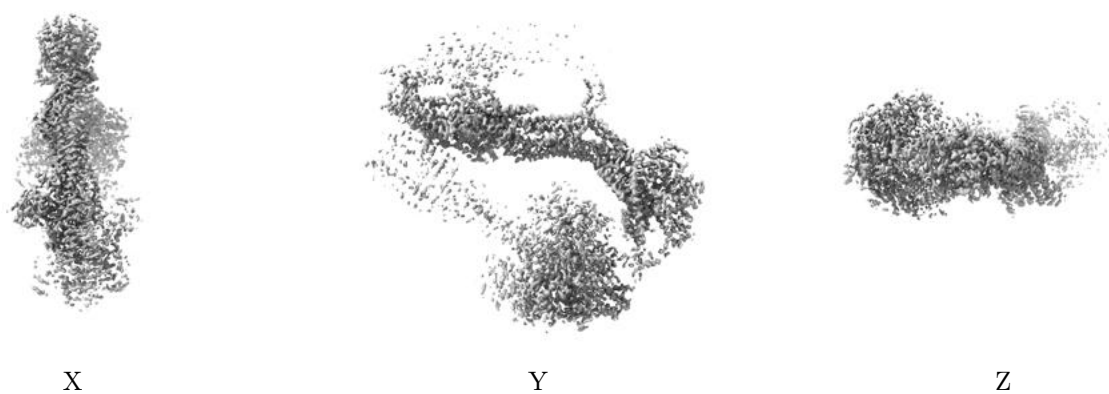


Z

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

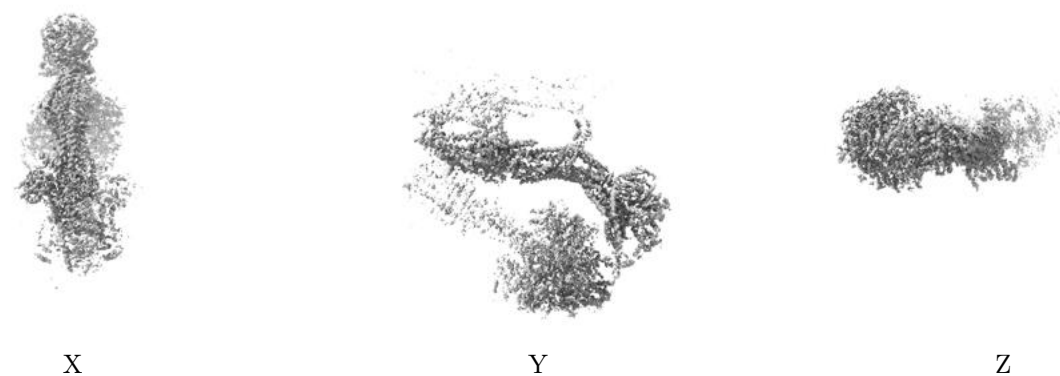
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

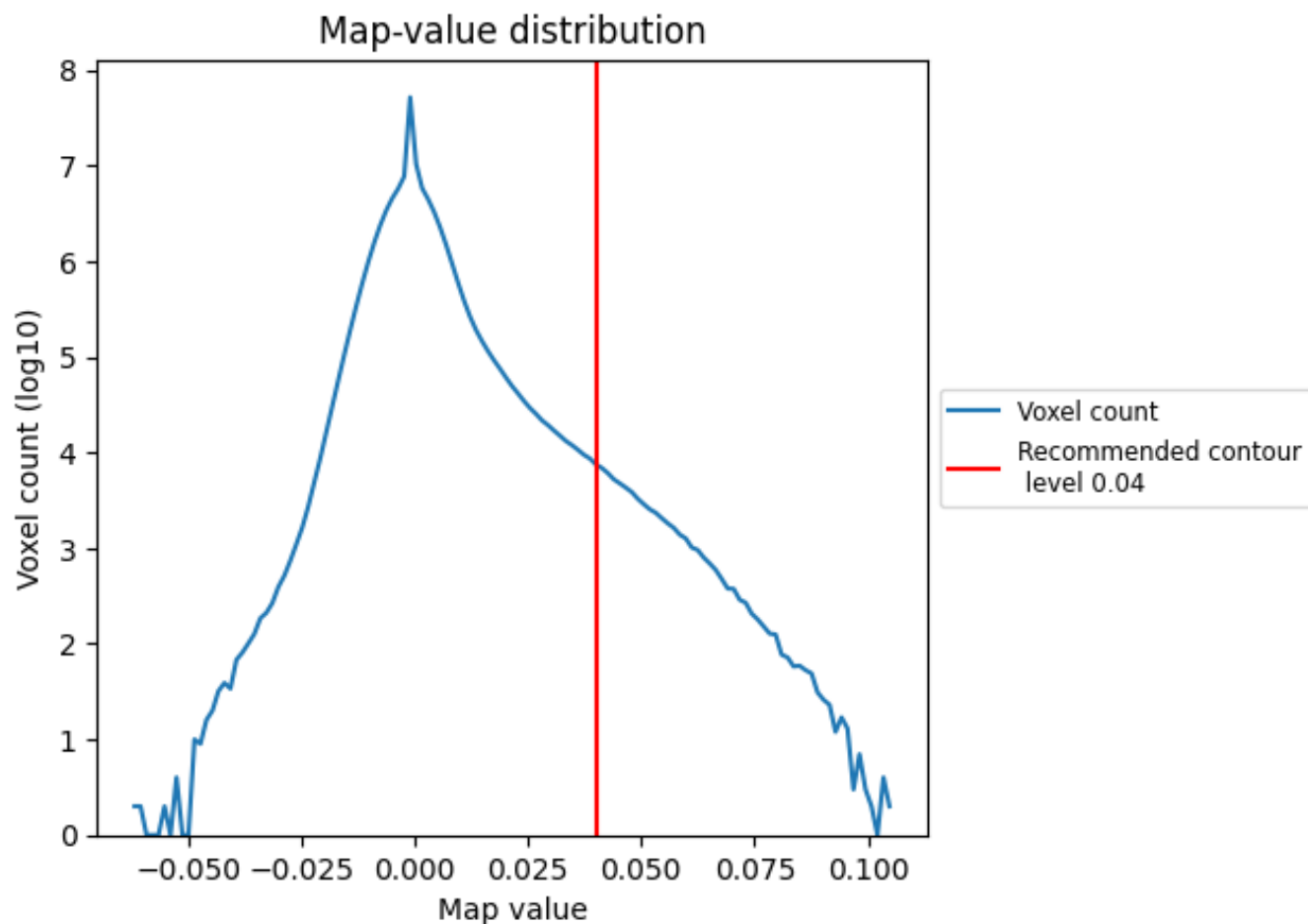
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

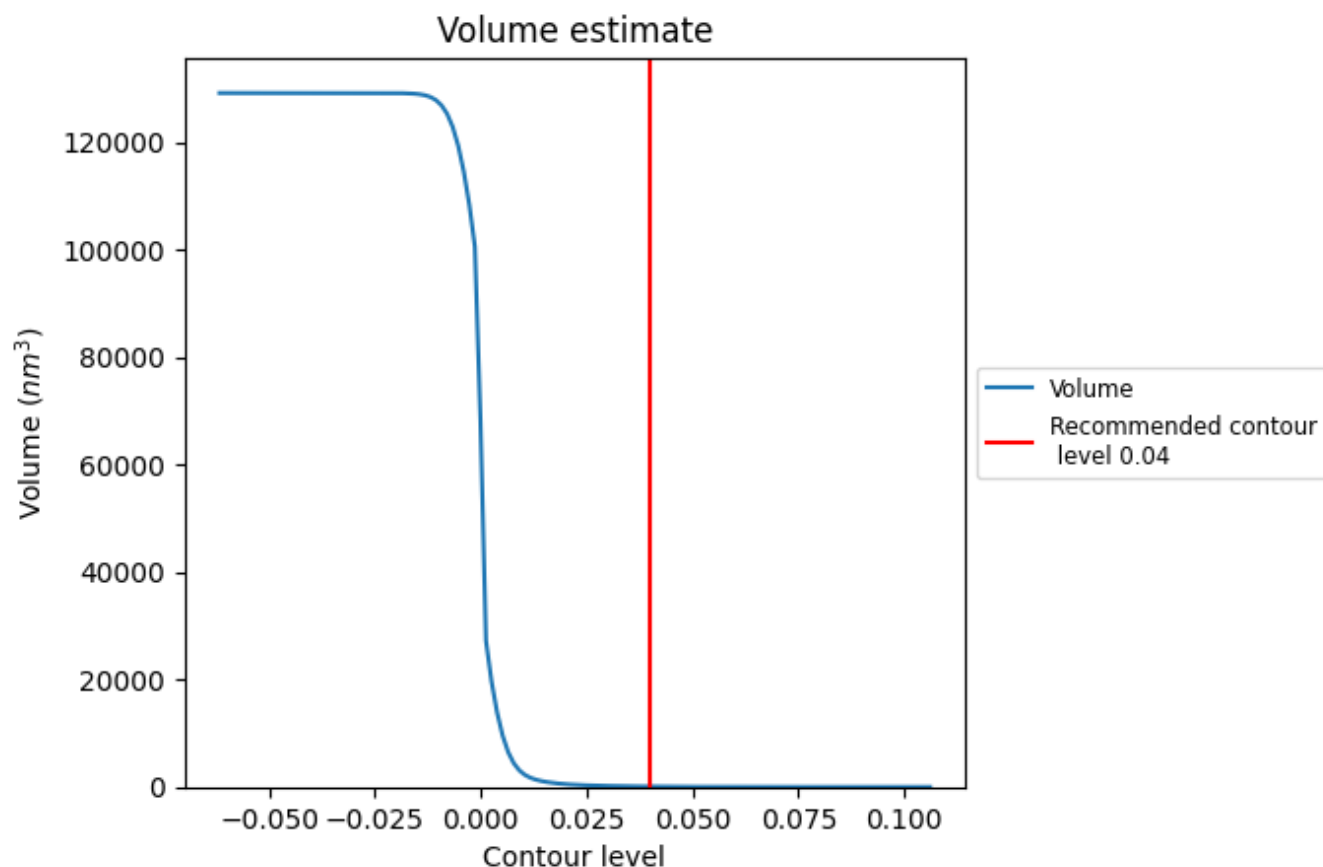
This section contains the results of statistical analysis of the map.

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



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

## 7.2 Volume estimate [i](#)

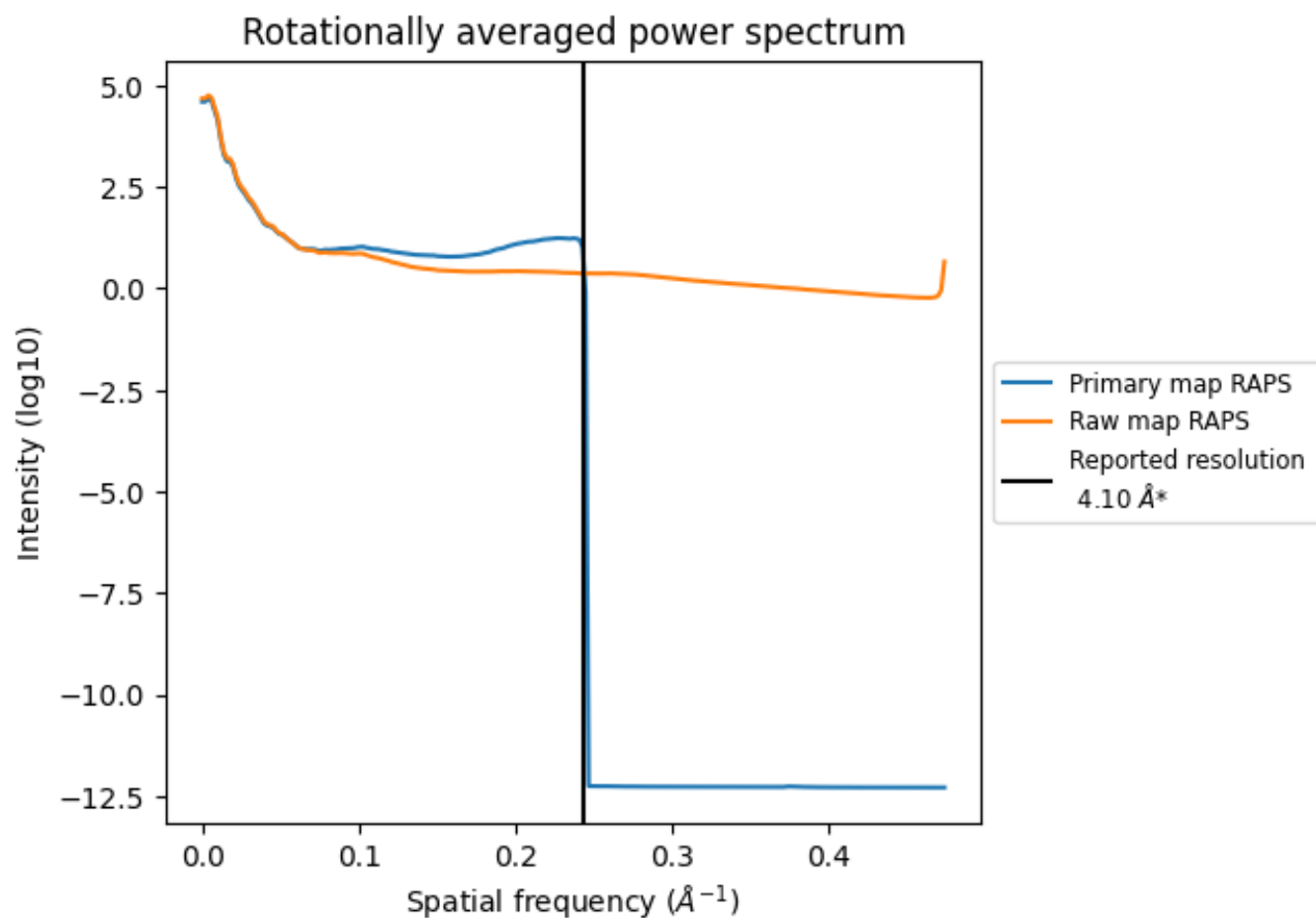


The volume at the recommended contour level is 76  $\text{nm}^3$ ; this corresponds to an approximate mass of 69 kDa.

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



### 7.3 Rotationally averaged power spectrum ⓘ

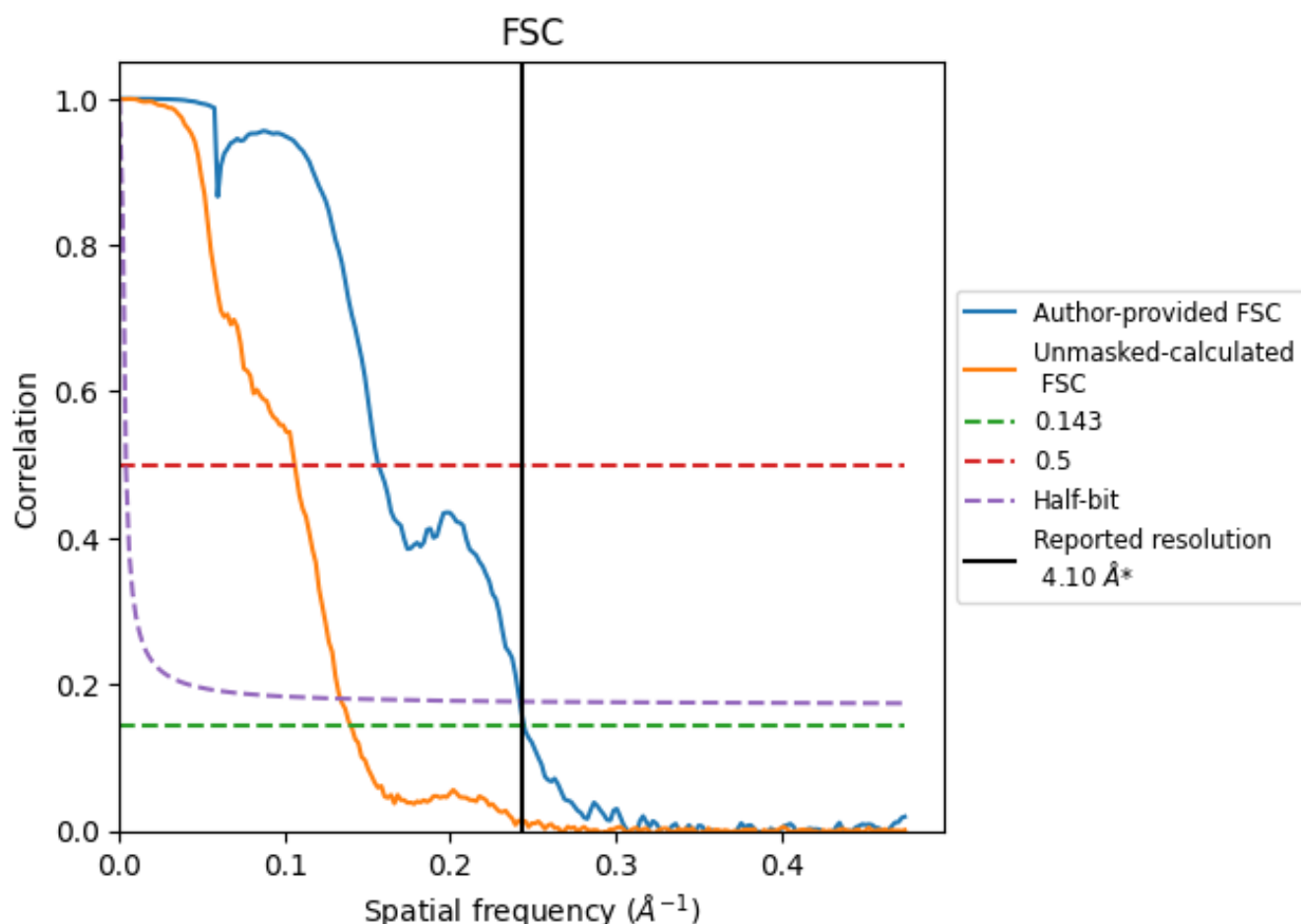


\*Reported resolution corresponds to spatial frequency of  $0.244 \text{ \AA}^{-1}$

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.244 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

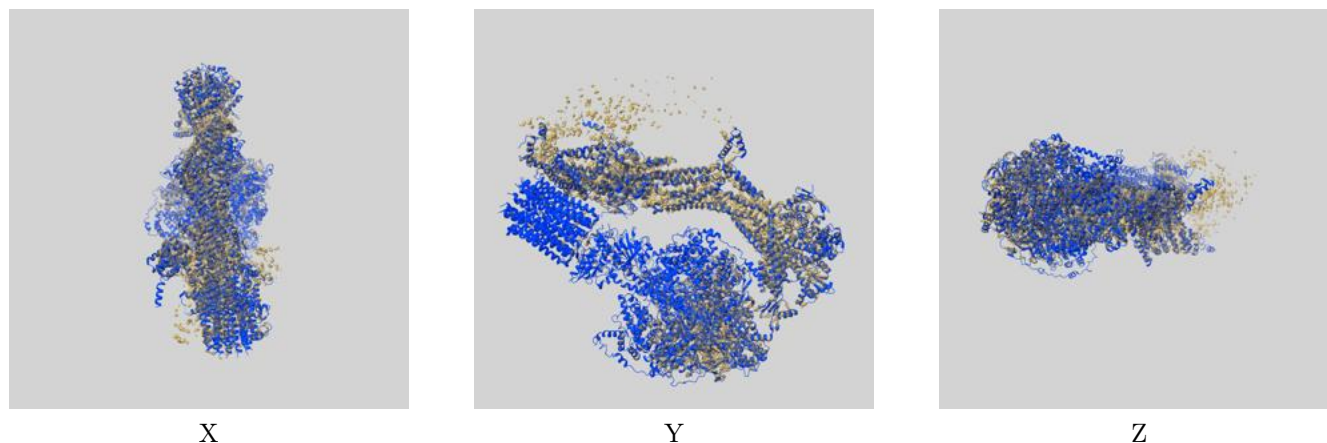
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.10	-	-
Author-provided FSC curve	4.09	6.39	4.13
Unmasked-calculated*	7.15	9.44	7.48

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.15 differs from the reported value 4.1 by more than 10 %

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

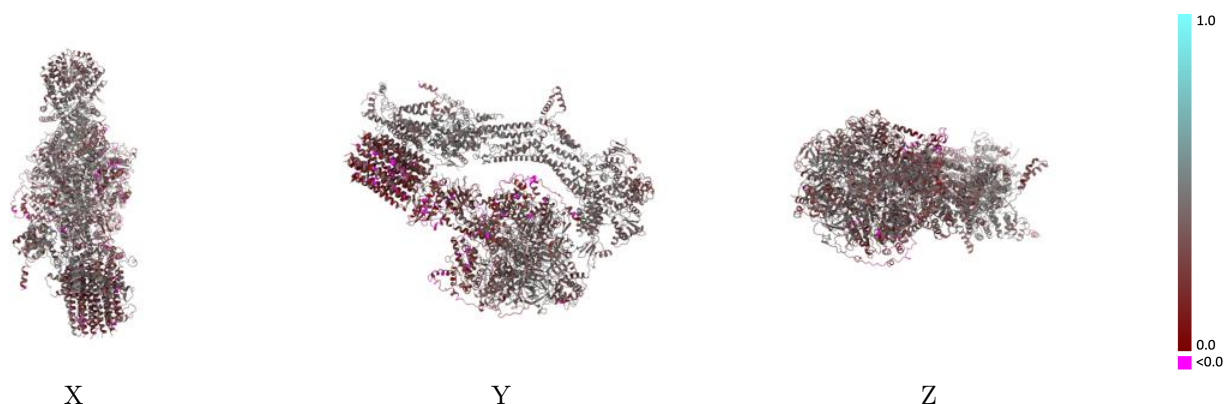
This section contains information regarding the fit between EMDB map EMD-4828 and PDB model 6RDR. Per-residue inclusion information can be found in section [3](#) on page [10](#).

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



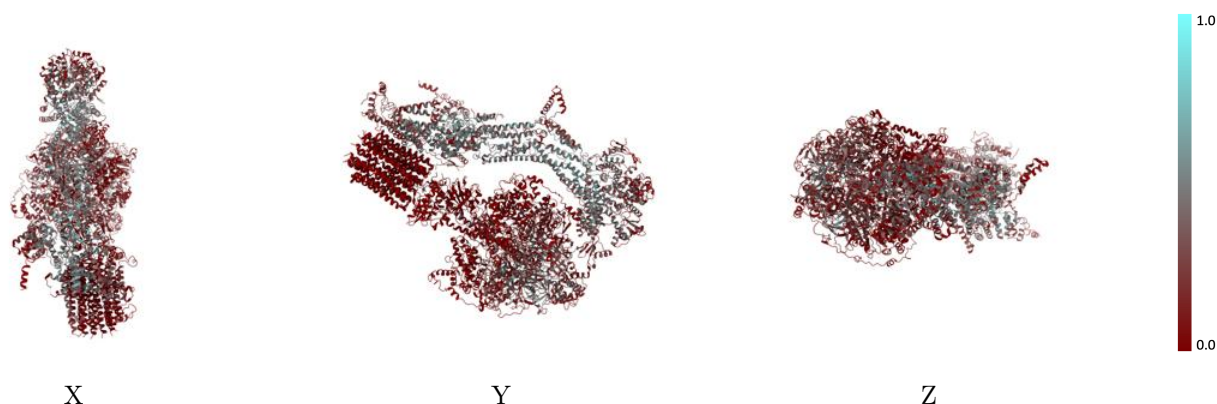
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



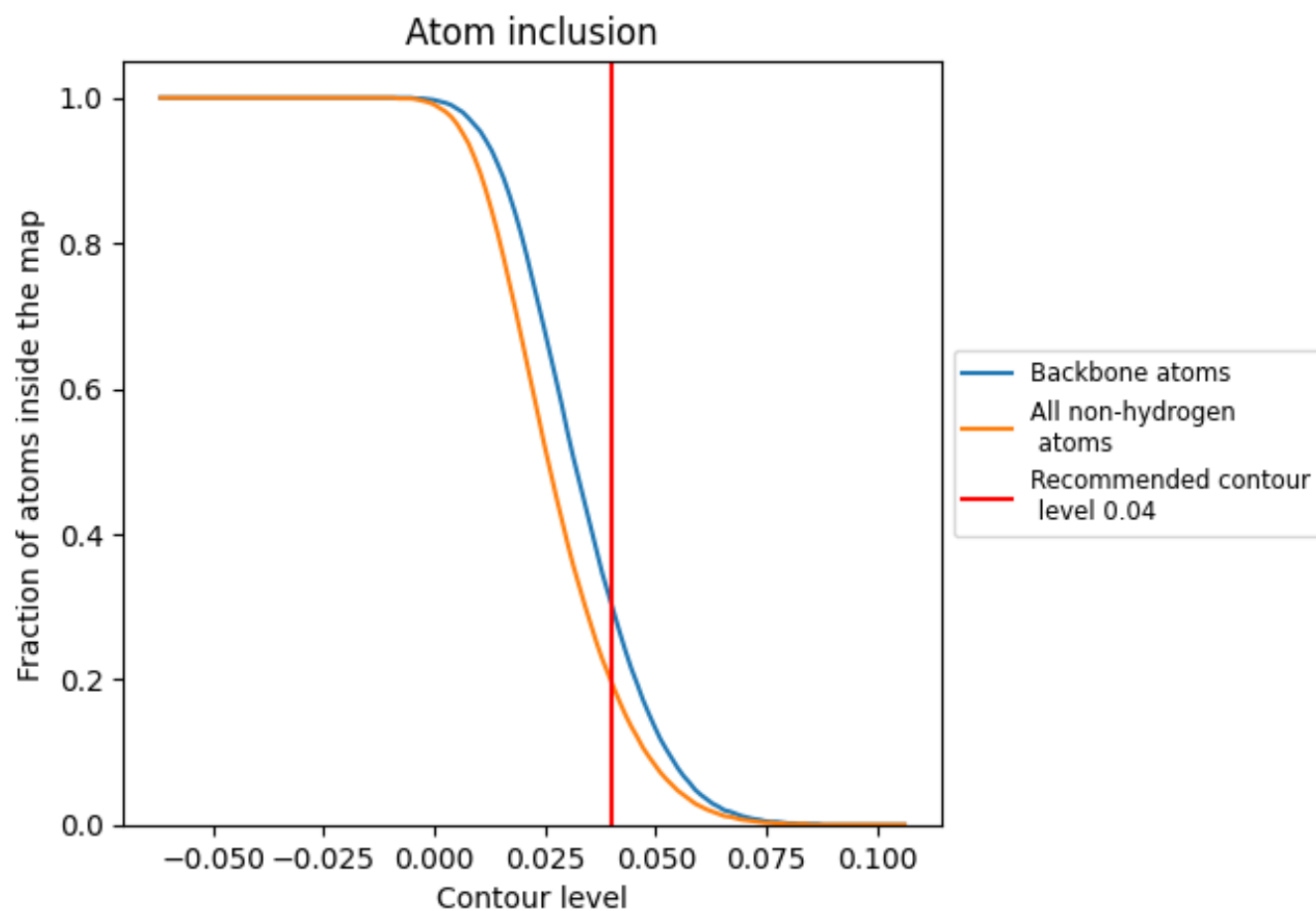
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.04).

































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 30% of all backbone atoms, 20% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.1960	 0.3500
0	 0.3060	 0.4240
1	 0.3910	 0.4360
2	 0.2690	 0.3890
3	 0.2870	 0.3920
4	 0.3480	 0.4080
5	 0.4900	 0.4570
6	 0.3690	 0.4390
7	 0.4280	 0.4280
8	 0.4130	 0.4480
9	 0.1570	 0.3750
A	 0.0330	 0.3270
B	 0.0120	 0.2720
C	 0.0160	 0.2270
D	 0.0200	 0.2380
E	 0.0290	 0.2040
F	 0.0160	 0.2290
G	 0.0060	 0.1810
H	 0.0100	 0.1990
I	 0.0160	 0.2510
J	 0.0610	 0.2970
M	 0.3590	 0.4290
P	 0.2240	 0.3740
Q	 0.0040	 0.2090
R	 0.0140	 0.2230
S	 0.0620	 0.2970
T	 0.1510	 0.3430
U	 0.1570	 0.3270
V	 0.1910	 0.3600
X	 0.0940	 0.3270
Y	 0.1230	 0.3300
Z	 0.1230	 0.3160

