



## wwPDB EM Validation Summary Report ⓘ

Oct 26, 2024 – 08:31 AM EDT

PDB ID : 5JUY  
EMDB ID : EMD-8178  
Title : Active human apoptosome with procaspase-9  
Authors : Cheng, T.C.; Hong, C.; Akey, I.V.; Yuan, S.; Akey, C.W.  
Deposited on : 2016-05-10  
Resolution : 4.10 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev113  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

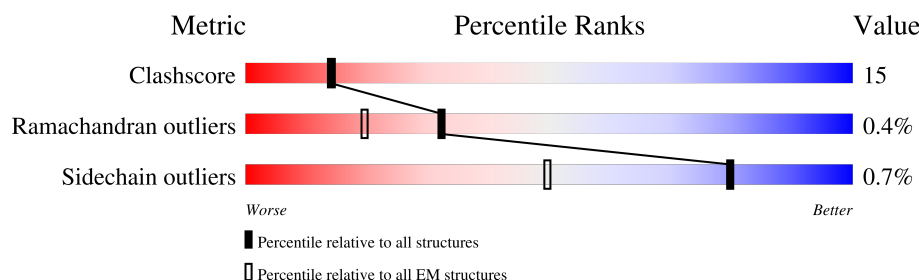
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	1248	
1	B	1248	
1	C	1248	
1	D	1248	
1	E	1248	
1	F	1248	
1	G	1248	
2	H	104	

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Mol	Chain	Length	Quality of chain
2	I	104	<div>81%</div> <div>56%44%</div>
2	J	104	<div>82%</div> <div>58%42%</div>
2	K	104	<div>81%</div> <div>58%42%</div>
2	L	104	<div>81%</div> <div>58%42%</div>
2	M	104	<div>80%</div> <div>59%41%</div>
2	N	104	<div>81%</div> <div>60%40%</div>
3	O	95	<div>95%</div> <div>76%20%•</div>
3	P	95	<div>99%</div> <div>76%19%5%</div>
3	Q	95	<div>100%</div> <div>77%19%•</div>
3	R	95	<div>100%</div> <div>77%19%•</div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 76058 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 Apoptotic protease-activating factor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1139	Total	C	N	O	S	0	0
			9099	5764	1563	1711	61		
1	B	1234	Total	C	N	O	S	0	0
			9861	6243	1694	1857	67		
1	C	1139	Total	C	N	O	S	0	0
			9099	5764	1563	1711	61		
1	D	1234	Total	C	N	O	S	0	0
			9861	6243	1694	1857	67		
1	E	1234	Total	C	N	O	S	0	0
			9861	6243	1694	1857	67		
1	F	1139	Total	C	N	O	S	0	0
			9099	5764	1563	1711	61		
1	G	1234	Total	C	N	O	S	0	0
			9861	6243	1694	1857	67		

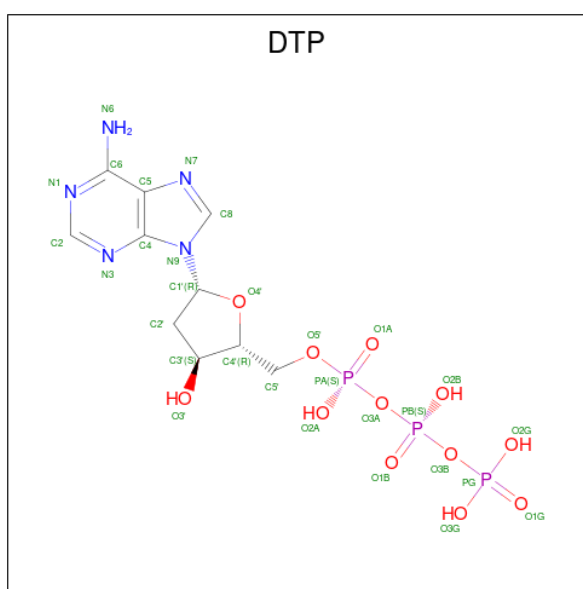
- Molecule 2 is a protein called Cytochrome c.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	104	Total	C	N	O	S	0	0
			814	517	143	150	4		
2	I	104	Total	C	N	O	S	0	0
			814	517	143	150	4		
2	J	104	Total	C	N	O	S	0	0
			814	517	143	150	4		
2	K	104	Total	C	N	O	S	0	0
			814	517	143	150	4		
2	L	104	Total	C	N	O	S	0	0
			814	517	143	150	4		
2	M	104	Total	C	N	O	S	0	0
			814	517	143	150	4		
2	N	104	Total	C	N	O	S	0	0
			814	517	143	150	4		

- Molecule 3 is a protein called Caspase-9.

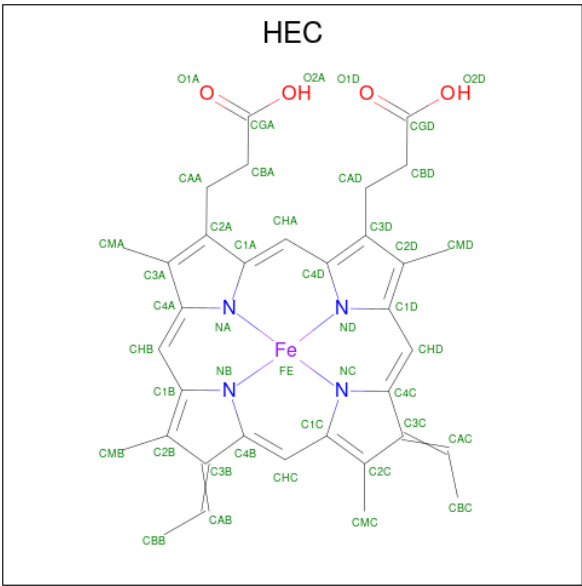
Mol	Chain	Residues	Atoms					AltConf	Trace
3	O	95	Total	C	N	O	S	0	0
			777	475	152	145	5		
3	P	95	Total	C	N	O	S	0	0
			777	475	152	145	5		
3	Q	95	Total	C	N	O	S	0	0
			777	475	152	145	5		
3	R	95	Total	C	N	O	S	0	0
			777	475	152	145	5		

- Molecule 4 is 2'-DEOXYADENOSINE 5'-TRIPHOSPHATE (three-letter code: DTP) (formula:  $C_{10}H_{16}N_5O_{12}P_3$ ).



Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			30	10	5	12	3	
4	B	1	Total	C	N	O	P	0
			30	10	5	12	3	
4	C	1	Total	C	N	O	P	0
			30	10	5	12	3	
4	D	1	Total	C	N	O	P	0
			30	10	5	12	3	
4	E	1	Total	C	N	O	P	0
			30	10	5	12	3	
4	F	1	Total	C	N	O	P	0
			30	10	5	12	3	
4	G	1	Total	C	N	O	P	0
			30	10	5	12	3	

- Molecule 5 is HEME C (three-letter code: HEC) (formula: C<sub>34</sub>H<sub>34</sub>FeN<sub>4</sub>O<sub>4</sub>).

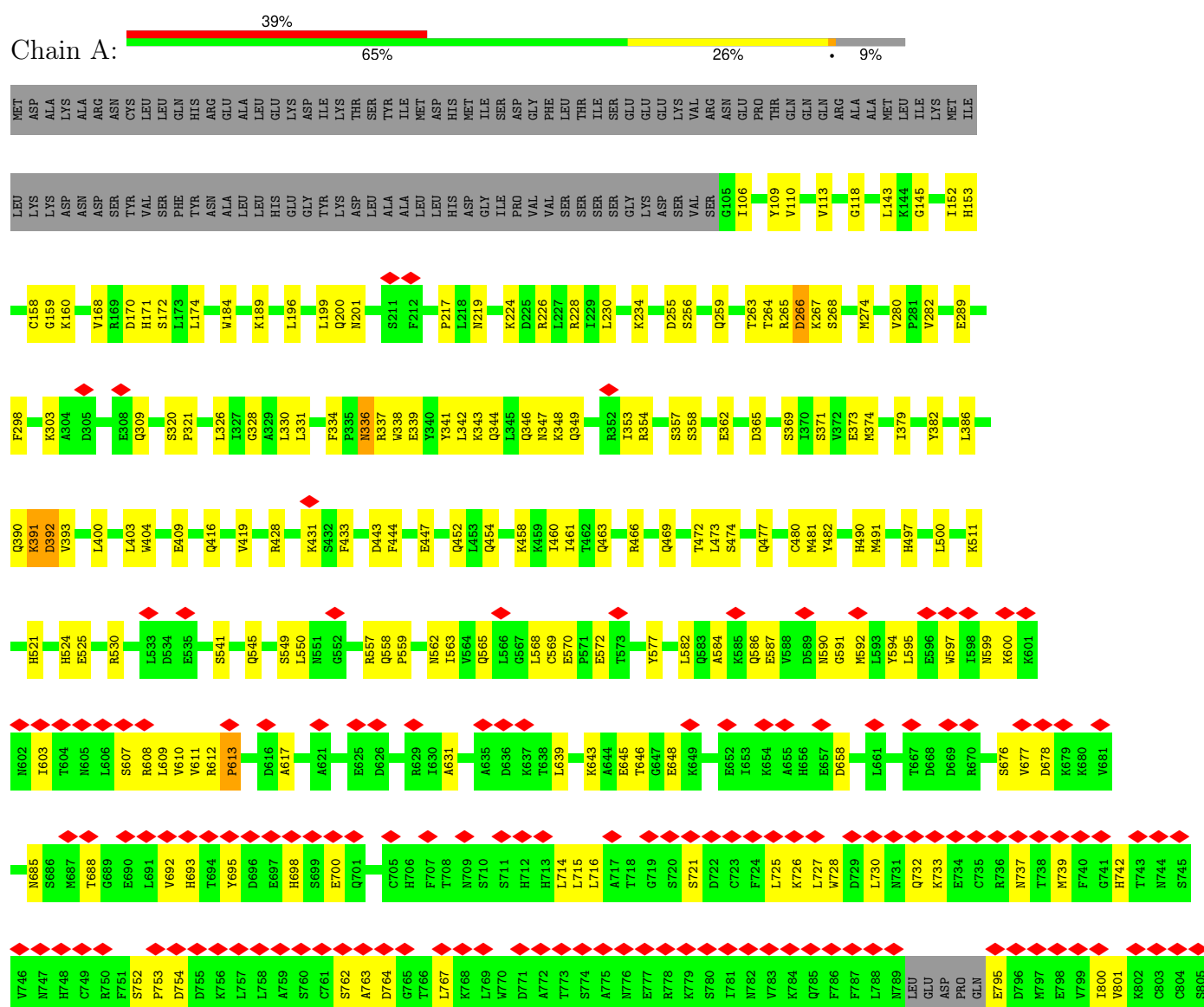


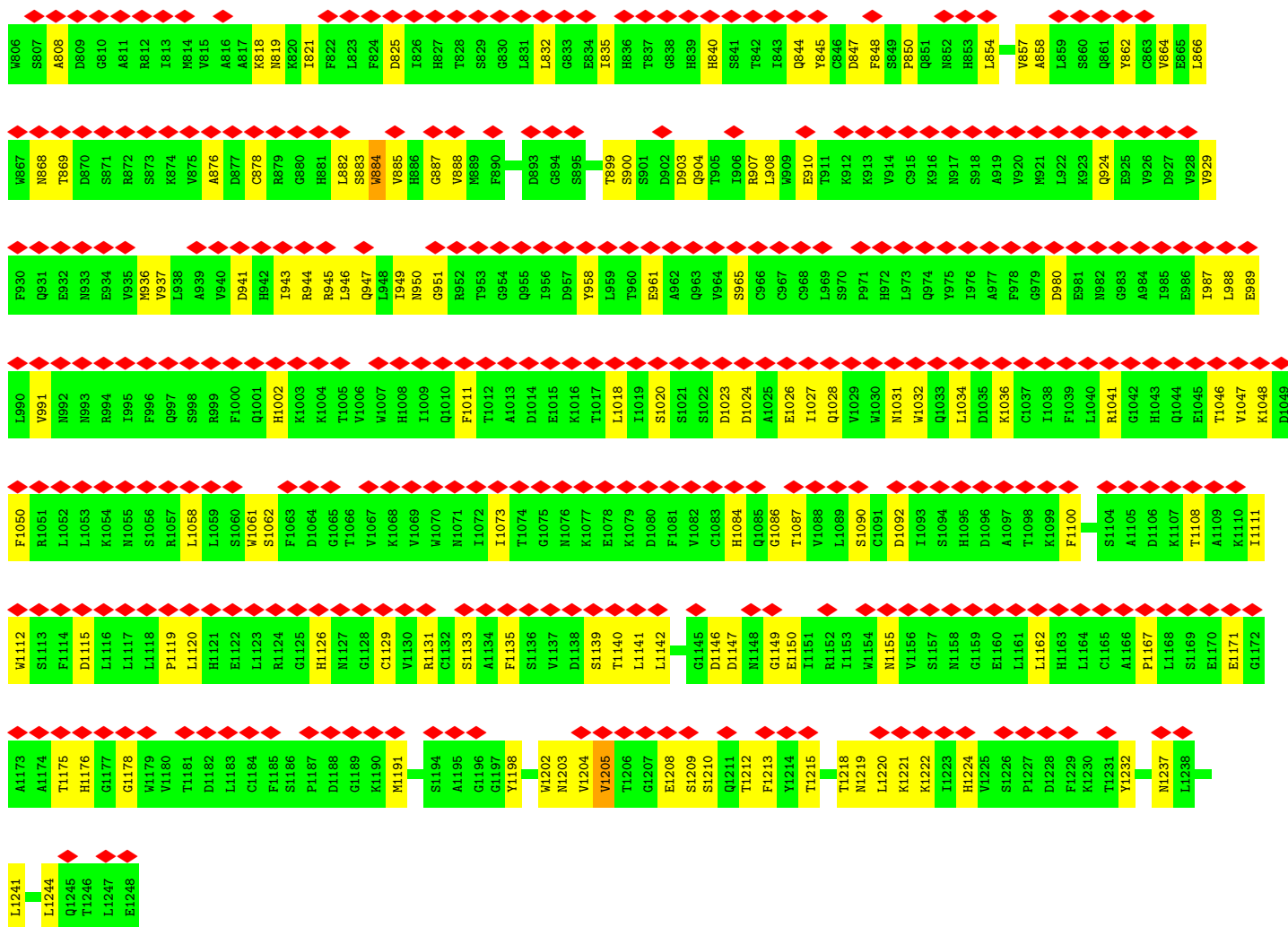
Mol	Chain	Residues	Atoms					AltConf
5	H	1	Total 43	C 34	Fe 1	N 4	O 4	0
5	I	1	Total 43	C 34	Fe 1	N 4	O 4	0
5	J	1	Total 43	C 34	Fe 1	N 4	O 4	0
5	K	1	Total 43	C 34	Fe 1	N 4	O 4	0
5	L	1	Total 43	C 34	Fe 1	N 4	O 4	0
5	M	1	Total 43	C 34	Fe 1	N 4	O 4	0
5	N	1	Total 43	C 34	Fe 1	N 4	O 4	0

### 3 Residue-property plots

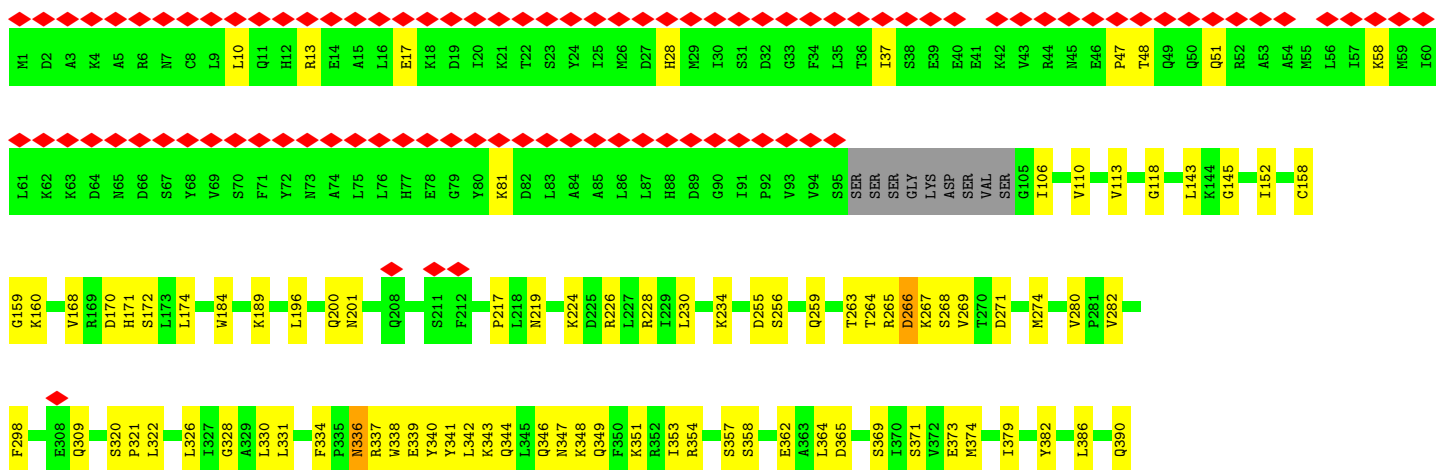
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Apoptotic protease-activating factor 1

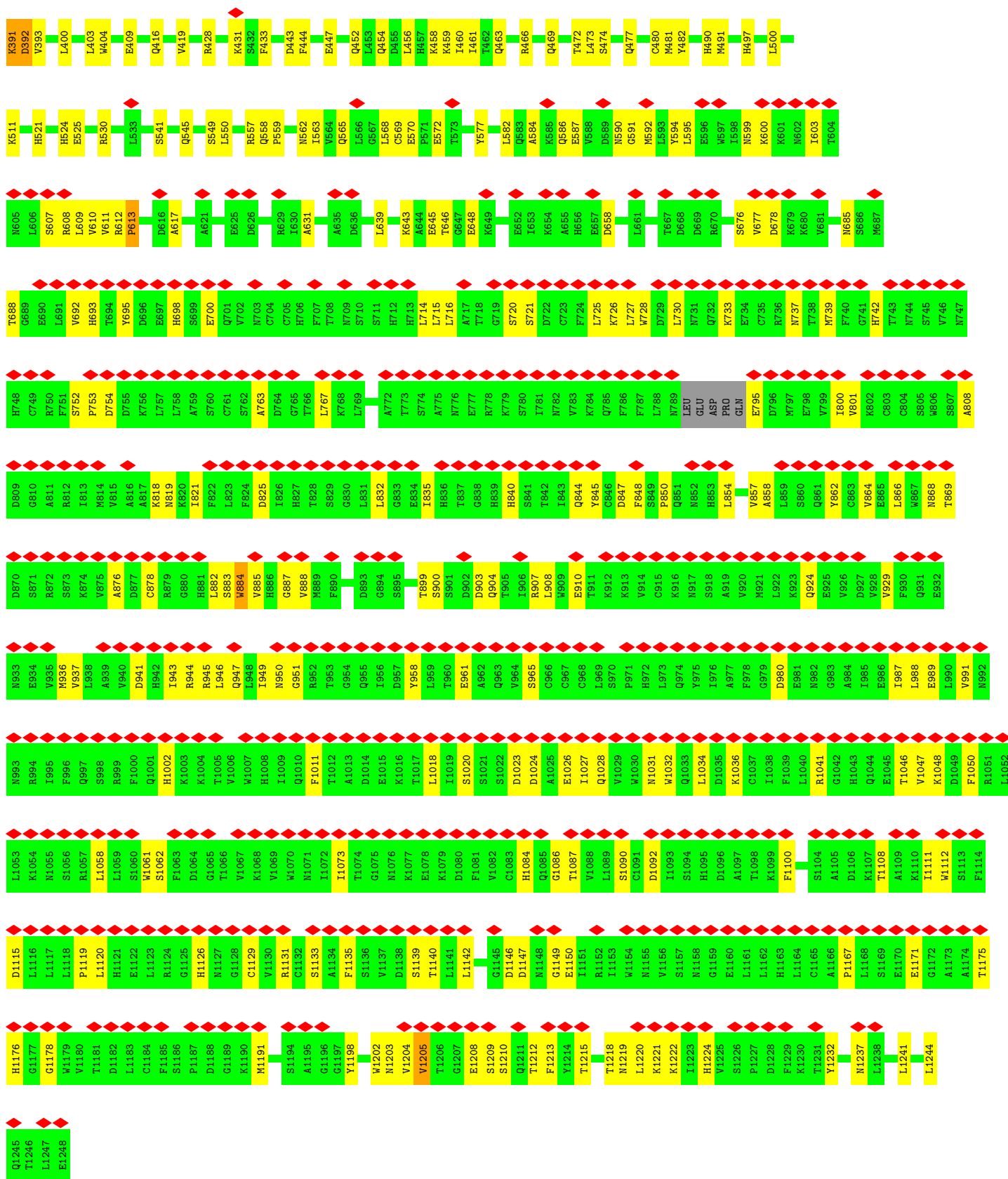




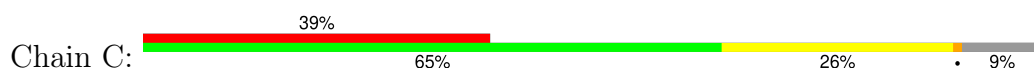
• Molecule 1: Apoptotic protease-activating factor 1



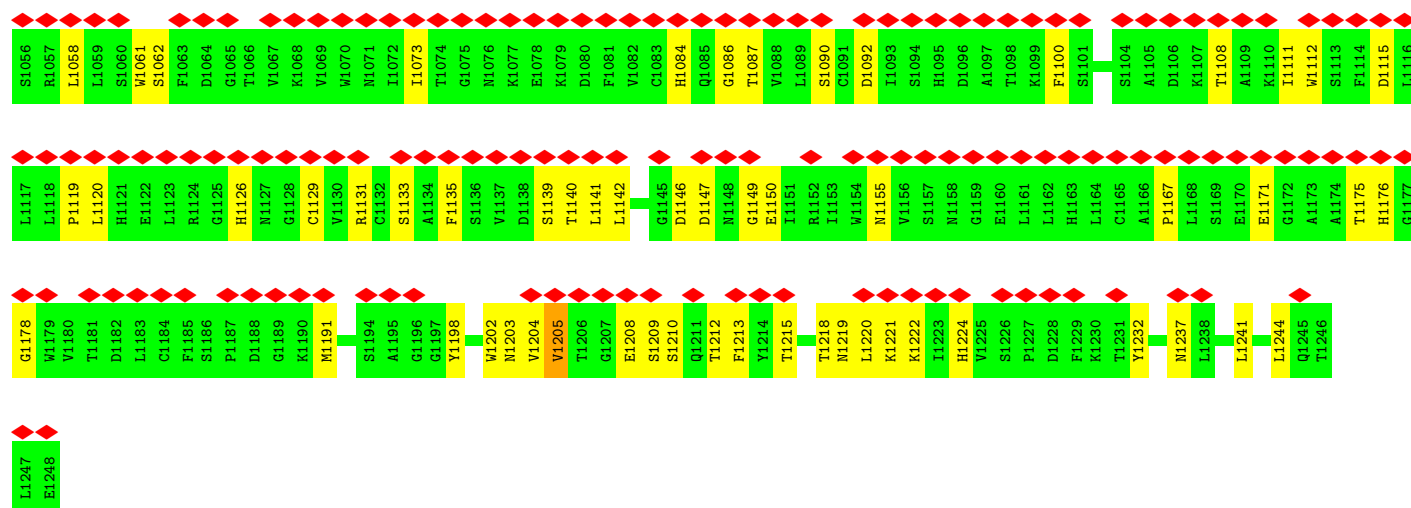




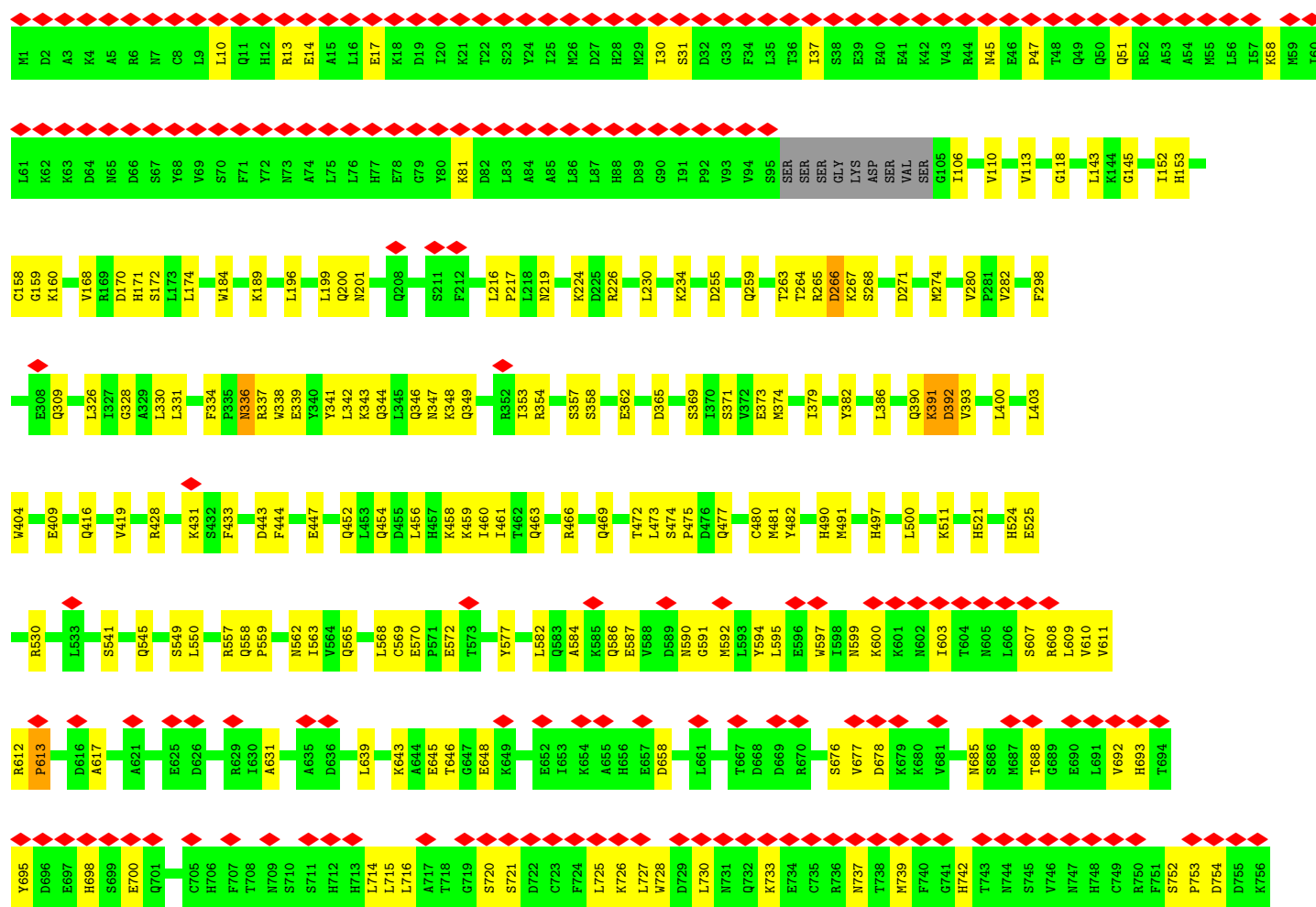
• Molecule 1: Apoptotic protease-activating factor 1

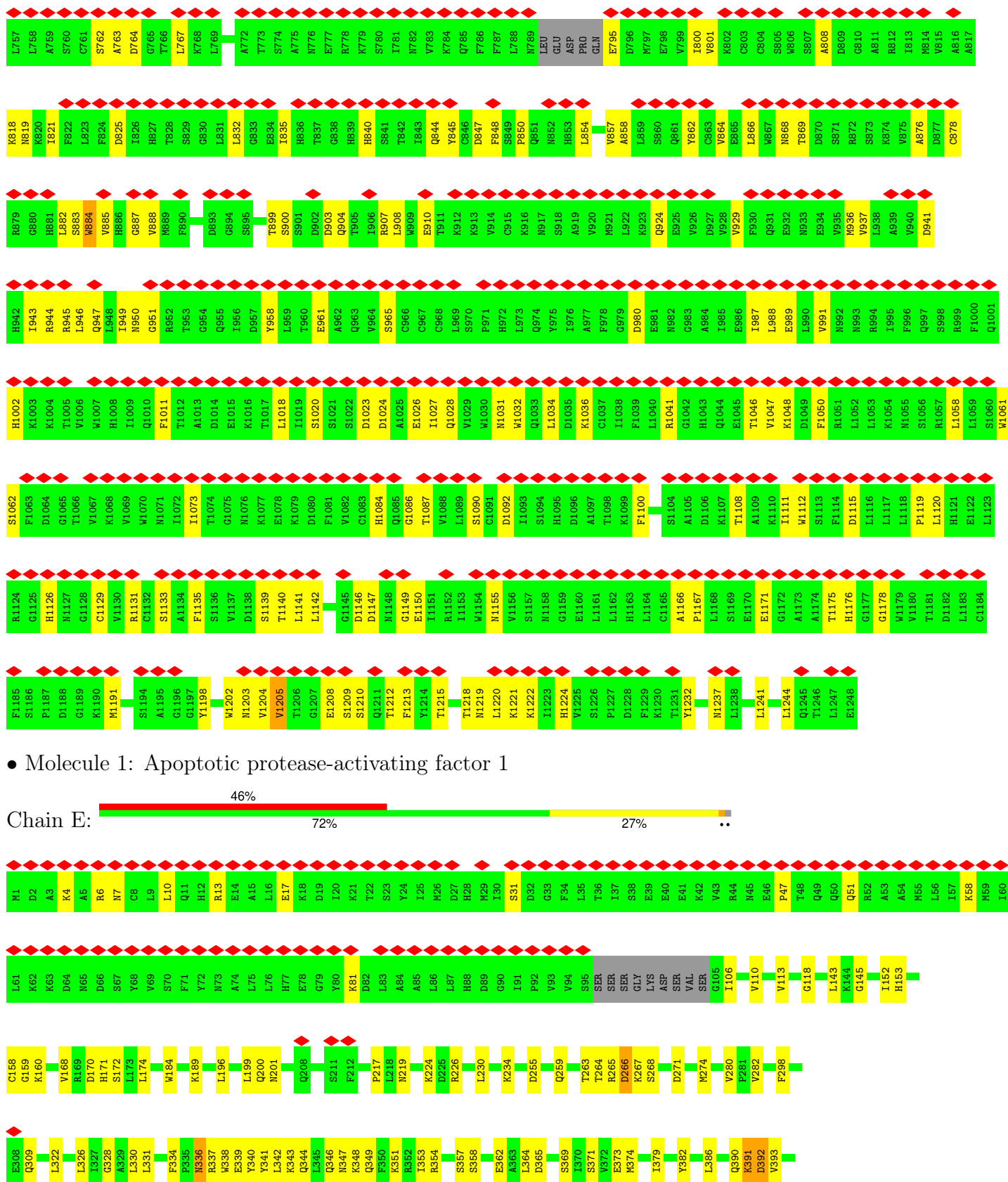


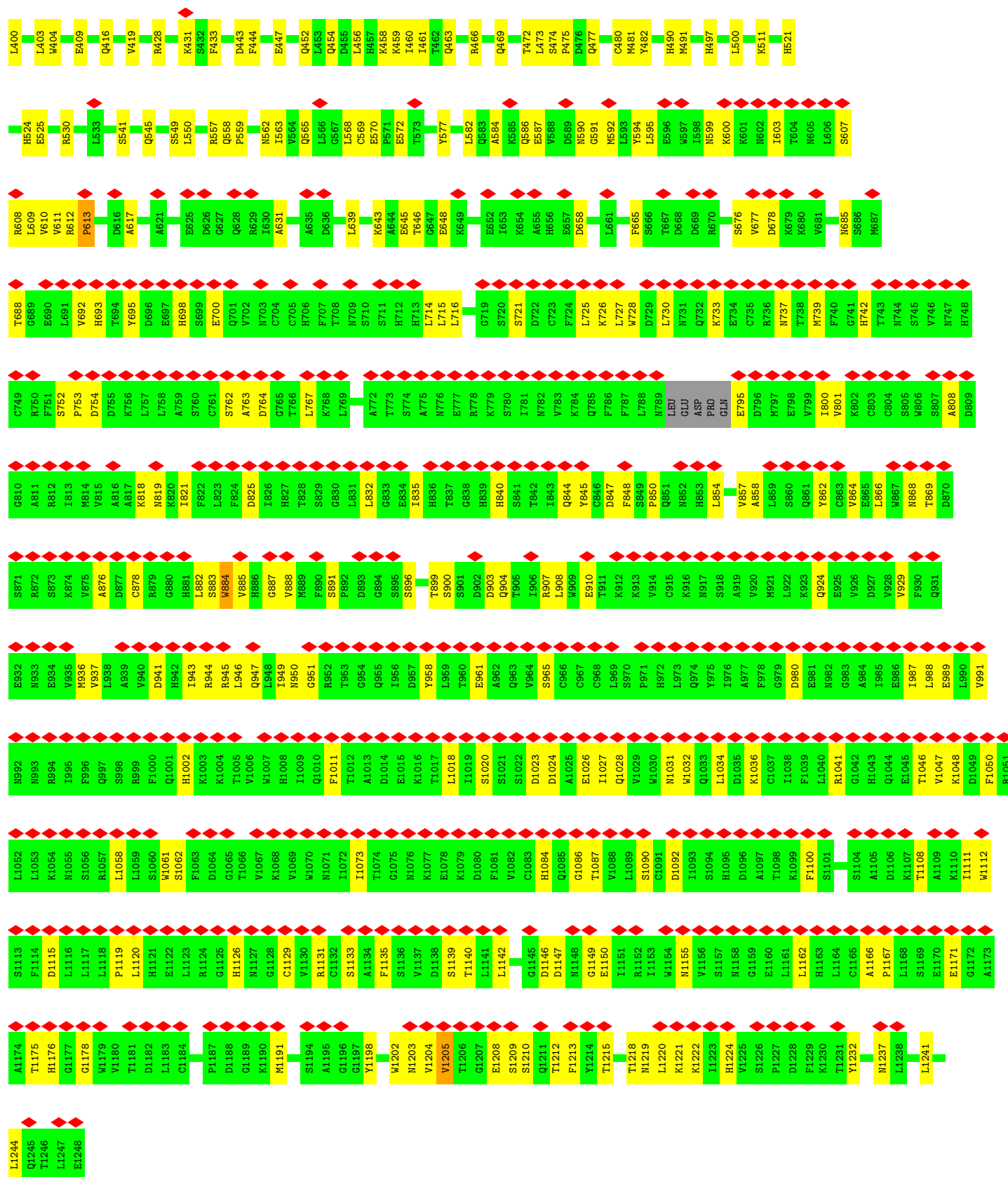
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ASP	LYS	G159	Q308	L400	H524	R608	V692	S752	R812	S873	M936	Q997
ALA	ASP	K160	Q309	L403	E525	L609	H693	P753	I813	R874	V937	S998
LYS	ASN	V168	L322	M403	R530	V610	T694	D754	M814	V875	V940	R999
ASN	ASP	D170	L326	E409	L533	P613	D696	K756	V815	A876	D941	F1000
ASN	SER	H171	L327	Q416	S541	D616	E697	L757	A816	C878	I942	H1002
CYS	TYR	S172	A328	Q419	Q545	A617	H698	L758	R819	R879	I943	K1003
LEU	VAL	L174	L330	V419	Q549	A621	S699	A759	R820	G880	R944	K1004
GLN	PHE	L174	L331	R428	L550	E625	E700	S760	I821	H881	R945	K1005
HIS	TYR	W184	L331	K431	S549	D626	Q701	C761	F822	L882	Q947	V1006
ARG	ALA	W184	L331	K431	L550	D626	W702	A763	L823	S883	I948	W1007
GLU	LEU	K189	F334	K431	L550	D626	W703	A763	R824	W884	I949	H1008
ALA	LEU	L196	N336	S432	R557	D626	C704	D764	D825	V885	N950	I1009
GLY	GLU	L199	R337	F433	Q558	R629	C705	D764	I826	H886	G951	Q1010
ASP	TYR	Q200	W338	D443	P559	L630	H706	T766	H827	C887	R952	T1012
ILE	LYS	N201	E339	F444	Q558	A631	W707	L767	S829	V888	T953	A1013
THR	ASP	Q208	Y341	E447	N562	D636	S710	L767	G830	F889	Q954	D1014
THR	LEU	S211	L342	E447	V564	D636	S711	K768	L832	D893	D957	E1015
ALA	ALA	F212	K343	Q452	Q565	L639	S712	L769	G833	C894	Y958	K1016
MET	LEU	L216	Q344	L453	L566	L639	H712	W770	E834	S895	T959	T1017
HIS	LEU	L216	Q344	L453	L566	L639	H712	A772	R835	T899	T960	L1018
MET	ASP	L218	Q344	L453	L566	L639	H712	T773	H836	S901	E961	I1019
ILE	ASP	L218	Q344	L453	L566	L639	H712	S774	H836	D902	A962	S1021
ASP	PRO	N219	F350	L453	L566	L639	H712	A775	H836	Q903	Q963	S1022
VAL	VAL	K224	R352	I460	L566	L639	H712	E777	T837	Q904	V964	D1023
PHE	SER	R226	L353	I461	L566	L639	H712	K778	G838	T905	S965	D1024
LEU	THR	R226	R354	T462	L566	L639	H712	K779	H839	R906	C966	A1025
THR	SER	L230	R354	Q463	L566	L639	H712	S780	H840	R907	C967	E1026
SER	SER	K234	S357	R466	L566	L639	H712	T781	S841	L908	C968	I1027
GLY	LYS	D255	S358	Q469	L566	L639	H712	T782	T842	W909	C969	Q1028
LYS	ASP	D255	E362	Q469	L566	L639	H712	W783	I843	E910	L969	V1029
VAL	SER	Q259	A363	Q469	L566	L639	H712	W784	Q844	T911	S970	W1030
ARG	SER	T263	L364	T472	L566	L639	H712	K785	Y845	K912	P971	I1031
GLU	GLU	T264	R365	L473	L566	L639	H712	F786	D847	K913	L973	W1032
PRO	THR	D266	D365	S474	L566	L639	H712	F787	F848	V914	L973	Q1033
GLN	GLN	K267	D365	S474	L566	L639	H712	L788	S849	C915	Q974	L1034
GLN	GLN	S268	M374	Y482	L566	L639	H712	W789	Q851	K916	Y975	L1035
ARG	ARG	V269	M374	Y482	L566	L639	H712	LEU	N852	N917	Y976	K1036
ALA	ALA	D271	L379	H490	L566	L639	H712	ASP	H853	S918	A977	I1037
MET	ALA	M274	L386	M491	L566	L639	H712	PRO	L854	A919	F978	C1037
LEU	LEU	V280	L386	M491	L566	L639	H712	GLN	V857	V920	Q979	I1038
ILE	LYS	P281	L386	M491	L566	L639	H712	E795	W857	N921	D980	F1039
MET	LYS	V282	L386	M491	L566	L639	H712	D796	A858	L922	E981	L1040
ILE	LYS	V282	L386	M491	L566	L639	H712	W797	L859	Q923	E981	R1041
								E798	S860	Q924	G983	G1042
								W799	Q861	Y925	A984	H1043
								T800	Y862	Y926	L985	Q1044
								V801	C863	D927	E986	E1045
								K802	W864	V928	I987	T1046
								C803	L866	V929	L988	V1047
								C804	W867	F930	L988	K1048
								S805	N868	Q931	E989	D1049
								W806	T869	E932	L990	L1052
								S807	D870	N933	W991	L1053
								A808	S871	N992	I992	K1054
								D809	C749	R993	I993	N1055
								G810		I995		



• Molecule 1: Apoptotic protease-activating factor 1

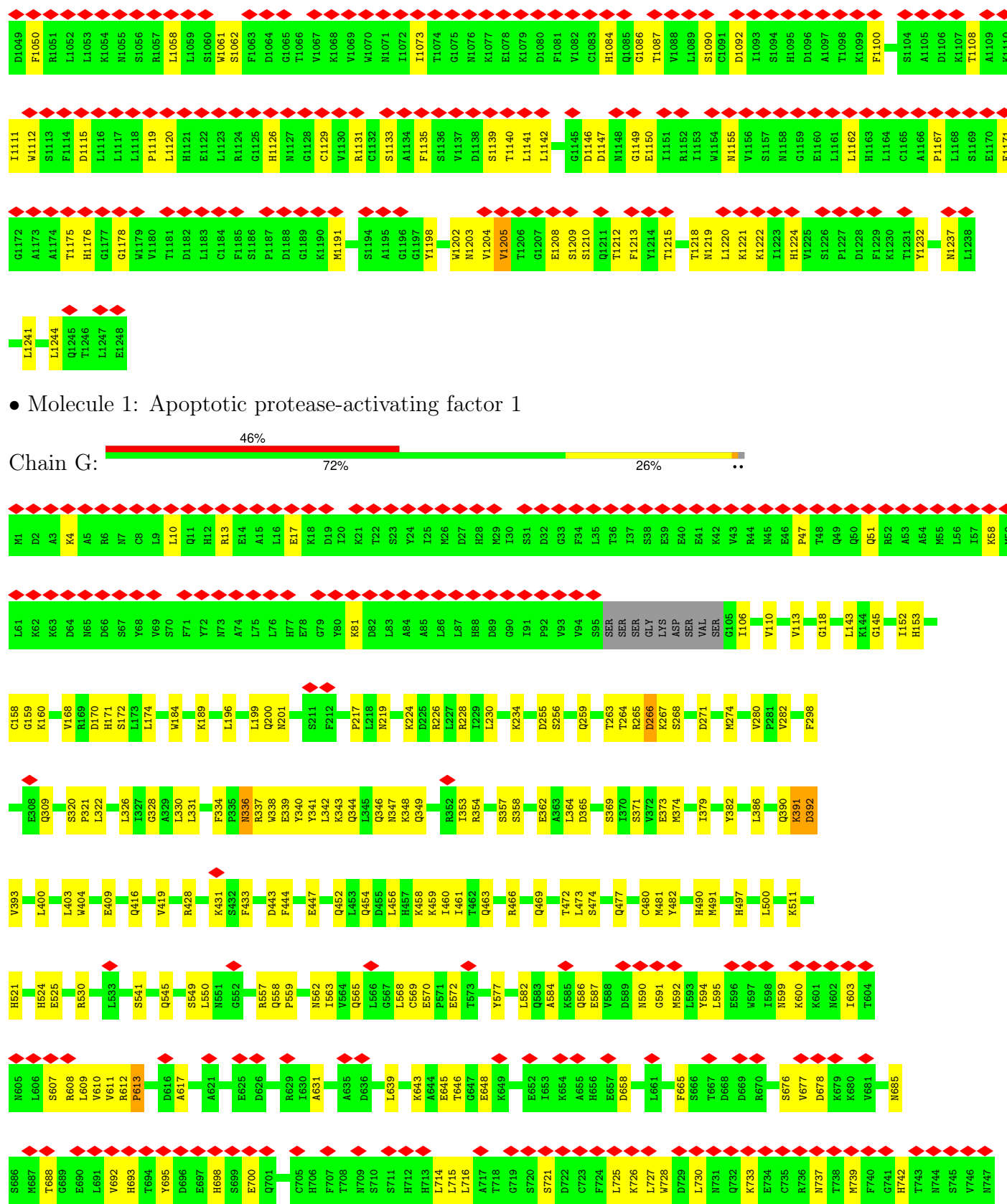


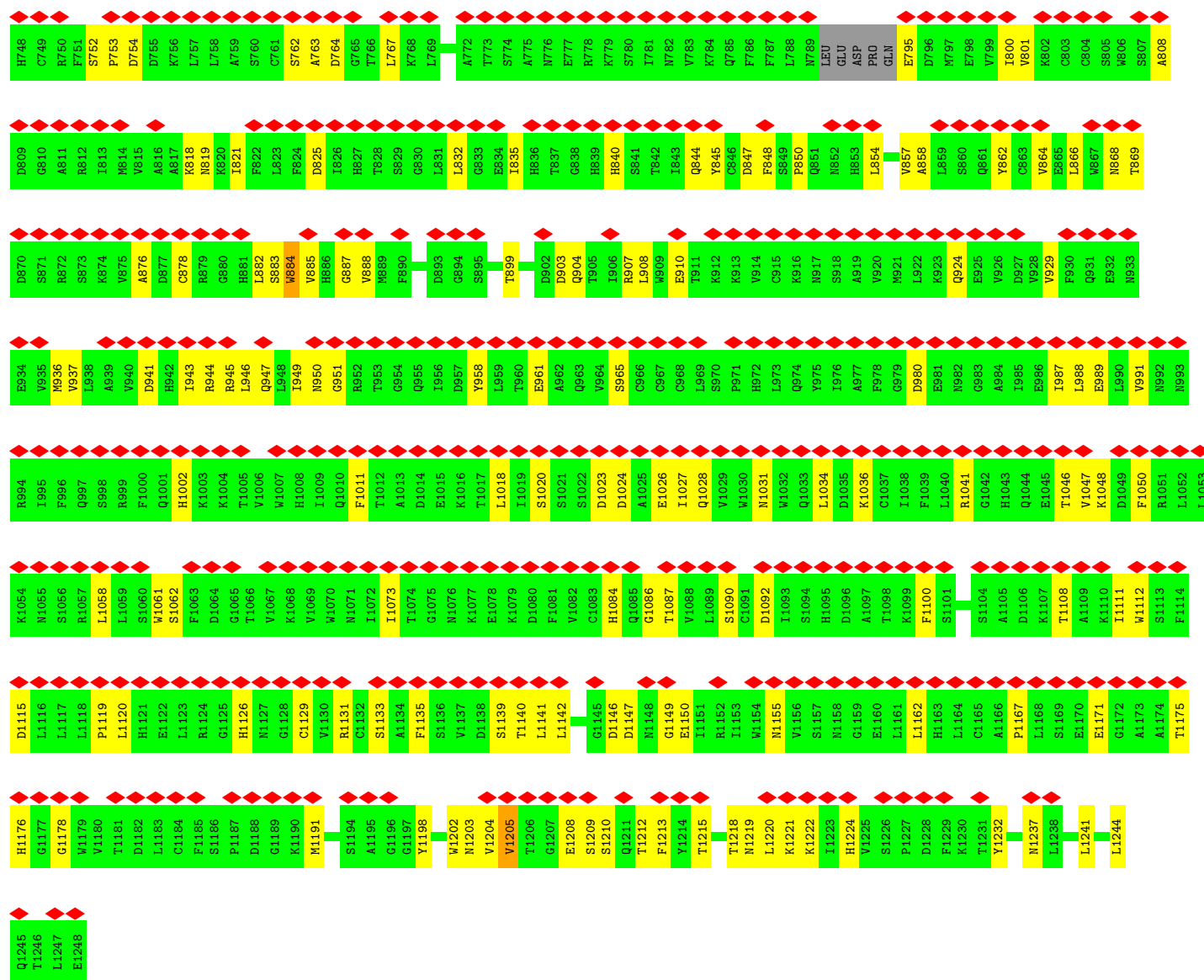




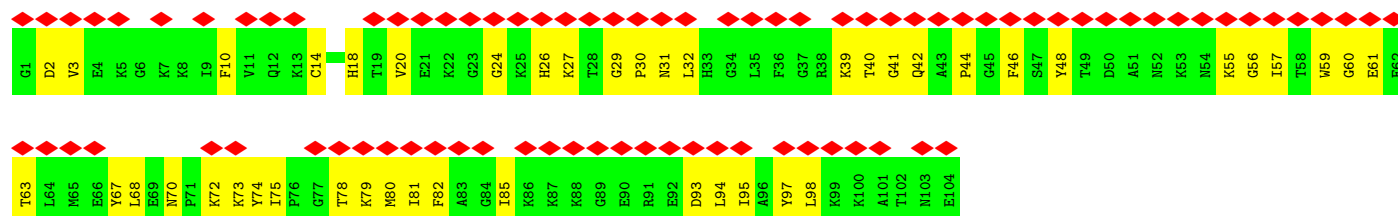
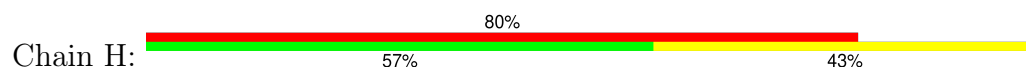
- Molecule 1: Apoptotic protease-activating factor 1



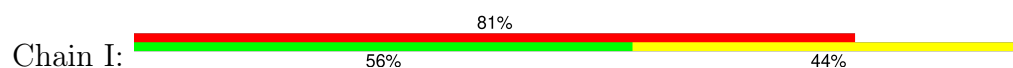




• Molecule 2: Cytochrome c



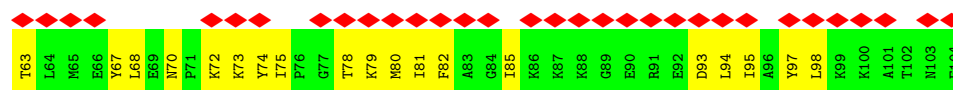
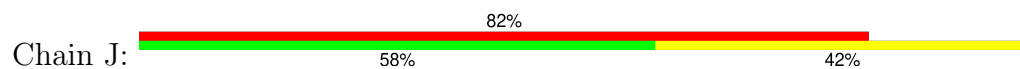
• Molecule 2: Cytochrome c



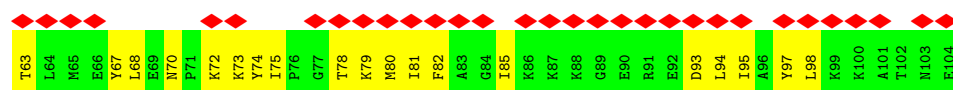
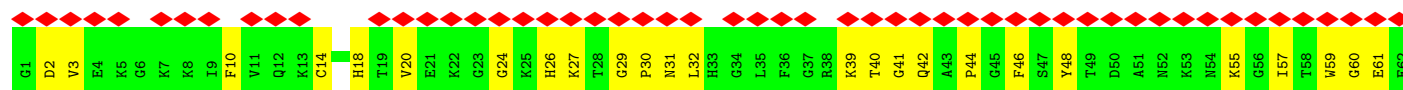
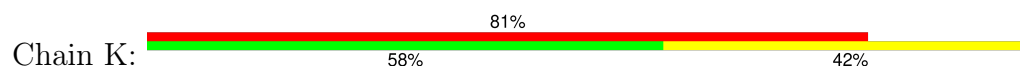




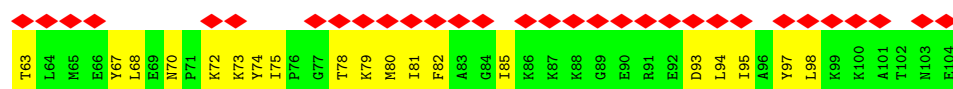
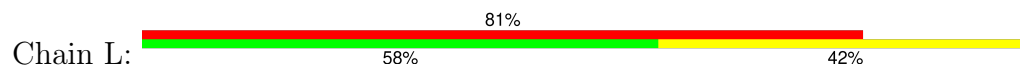
• Molecule 2: Cytochrome c



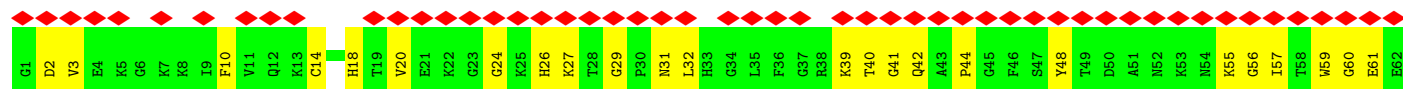
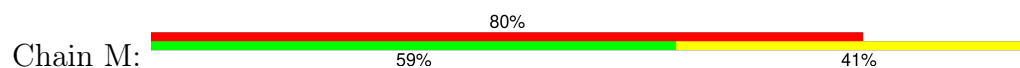
• Molecule 2: Cytochrome c

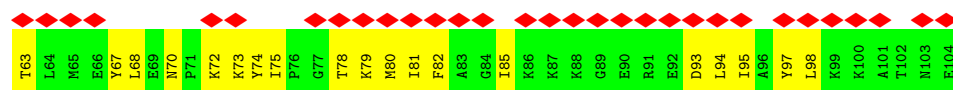


• Molecule 2: Cytochrome c

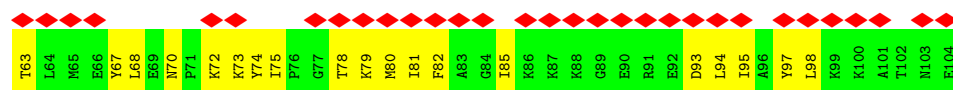
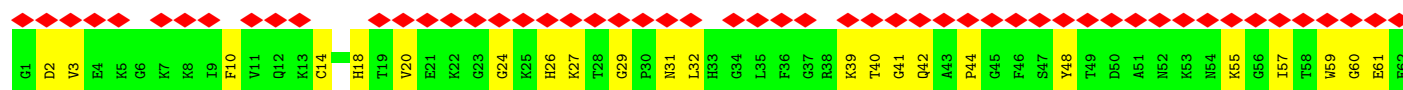
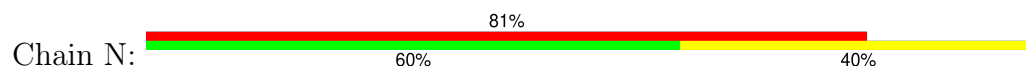


• Molecule 2: Cytochrome c

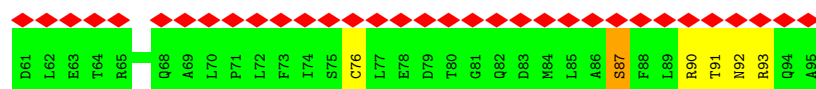
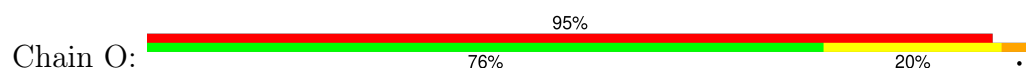




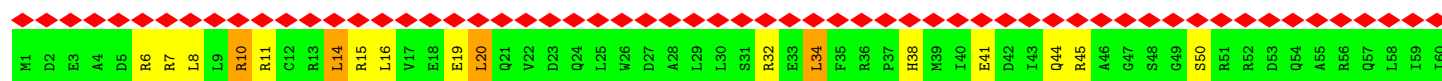
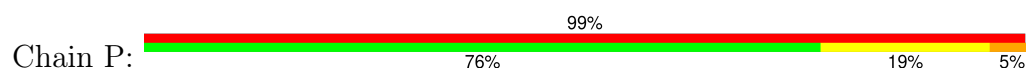
• Molecule 2: Cytochrome c



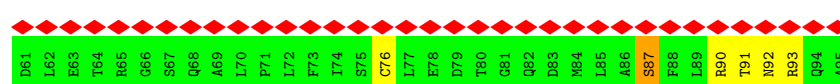
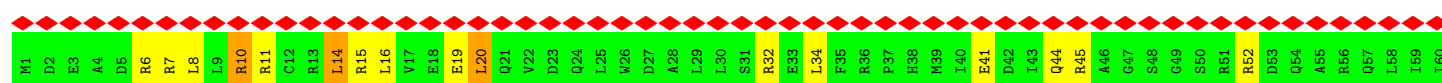
• Molecule 3: Caspase-9



• Molecule 3: Caspase-9



• Molecule 3: Caspase-9



• Molecule 3: Caspase-9



D61	L62	E63	T64	R65	G66	S67	Q68	A69	L70	P71	L72	F73	I74	S75	C76	L77	E78	D79	T80	G81	Q82	D83	M84	L85	A86	S87	F88	L89	R90	T91	N92	R93	Q94	A95
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## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C7	Depositor
Number of particles used	92867	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 ( $e^-/\text{\AA}^2$ )	1.8	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	81000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.198	Depositor
Minimum map value	-0.084	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.03	Depositor
Map size ( $\text{\AA}$ )	437.76, 437.76, 437.76	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.368, 1.368, 1.368	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: DTP, HEC

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.33	1/9295 (0.0%)	0.46	0/12575
1	B	0.37	1/10068 (0.0%)	0.47	0/13613
1	C	0.33	1/9295 (0.0%)	0.46	0/12575
1	D	0.36	1/10068 (0.0%)	0.47	0/13613
1	E	0.36	1/10068 (0.0%)	0.47	0/13613
1	F	0.33	1/9295 (0.0%)	0.47	0/12575
1	G	0.37	1/10068 (0.0%)	0.47	0/13613
2	H	0.25	0/830	0.42	0/1105
2	I	0.25	0/830	0.42	0/1105
2	J	0.25	0/830	0.42	0/1105
2	K	0.25	0/830	0.42	0/1105
2	L	0.25	0/830	0.42	0/1105
2	M	0.25	0/830	0.42	0/1105
2	N	0.25	0/830	0.42	0/1105
3	O	0.60	0/784	0.61	0/1051
3	P	0.60	0/784	0.61	0/1051
3	Q	0.60	0/784	0.61	0/1051
3	R	0.60	0/784	0.61	0/1051
All	All	0.36	7/77103 (0.0%)	0.47	0/104116

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	F	0	1
1	G	0	1
All	All	0	7

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	168	VAL	C-N	6.96	1.50	1.34
1	B	168	VAL	C-N	6.94	1.50	1.34
1	A	168	VAL	C-N	6.94	1.50	1.34
1	E	168	VAL	C-N	6.94	1.50	1.34
1	D	168	VAL	C-N	6.93	1.50	1.34

There are no bond angle outliers.

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	336	ASN	Peptide
1	B	336	ASN	Peptide
1	C	336	ASN	Peptide
1	D	336	ASN	Peptide
1	E	336	ASN	Peptide

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9099	0	8967	296	0
1	B	9861	0	9736	300	0
1	C	9099	0	8968	293	0
1	D	9861	0	9736	310	0
1	E	9861	0	9736	313	0
1	F	9099	0	8968	300	0
1	G	9861	0	9736	300	0
2	H	814	0	833	59	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	I	814	0	833	58	0
2	J	814	0	833	59	0
2	K	814	0	833	57	0
2	L	814	0	833	58	0
2	M	814	0	833	59	0
2	N	814	0	833	56	0
3	O	777	0	787	21	0
3	P	777	0	787	28	0
3	Q	777	0	786	39	0
3	R	777	0	787	29	0
4	A	30	0	9	3	0
4	B	30	0	9	3	0
4	C	30	0	9	3	0
4	D	30	0	9	3	0
4	E	30	0	9	3	0
4	F	30	0	9	3	0
4	G	30	0	9	3	0
5	H	43	0	32	4	0
5	I	43	0	32	4	0
5	J	43	0	32	4	0
5	K	43	0	32	4	0
5	L	43	0	32	4	0
5	M	43	0	32	4	0
5	N	43	0	32	4	0
All	All	76058	0	75112	2327	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 15.

The worst 5 of 2327 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)
3:Q:52:ARG:HD3	3:R:38:HIS:CE1	1.20	1.66
3:Q:52:ARG:CD	3:R:38:HIS:CE1	2.01	1.40
1:E:884:TRP:CH2	2:L:79:LYS:HA	1.68	1.28
1:D:884:TRP:CH2	2:K:79:LYS:HA	1.68	1.28
1:G:884:TRP:CH2	2:N:79:LYS:HA	1.68	1.28

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	A	1135/1248 (91%)	1045 (92%)	84 (7%)	6 (0%)	25	62
1	B	1228/1248 (98%)	1138 (93%)	84 (7%)	6 (0%)	25	62
1	C	1135/1248 (91%)	1045 (92%)	84 (7%)	6 (0%)	25	62
1	D	1228/1248 (98%)	1138 (93%)	84 (7%)	6 (0%)	25	62
1	E	1228/1248 (98%)	1138 (93%)	84 (7%)	6 (0%)	25	62
1	F	1135/1248 (91%)	1045 (92%)	84 (7%)	6 (0%)	25	62
1	G	1228/1248 (98%)	1138 (93%)	84 (7%)	6 (0%)	25	62
2	H	102/104 (98%)	98 (96%)	4 (4%)	0	100	100
2	I	102/104 (98%)	98 (96%)	4 (4%)	0	100	100
2	J	102/104 (98%)	98 (96%)	4 (4%)	0	100	100
2	K	102/104 (98%)	98 (96%)	4 (4%)	0	100	100
2	L	102/104 (98%)	98 (96%)	4 (4%)	0	100	100
2	M	102/104 (98%)	98 (96%)	4 (4%)	0	100	100
2	N	102/104 (98%)	98 (96%)	4 (4%)	0	100	100
3	O	93/95 (98%)	92 (99%)	1 (1%)	0	100	100
3	P	93/95 (98%)	92 (99%)	1 (1%)	0	100	100
3	Q	93/95 (98%)	92 (99%)	1 (1%)	0	100	100
3	R	93/95 (98%)	92 (99%)	1 (1%)	0	100	100
All	All	9403/9844 (96%)	8741 (93%)	620 (7%)	42 (0%)	32	67

5 of 42 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1073	ILE
1	B	1073	ILE
1	C	1073	ILE
1	D	1073	ILE

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Mol	Chain	Res	Type
1	E	1073	ILE

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1022/1119 (91%)	1019 (100%)	3 (0%)	91	92
1	B	1106/1119 (99%)	1101 (100%)	5 (0%)	86	90
1	C	1022/1119 (91%)	1019 (100%)	3 (0%)	91	92
1	D	1106/1119 (99%)	1101 (100%)	5 (0%)	86	90
1	E	1106/1119 (99%)	1101 (100%)	5 (0%)	86	90
1	F	1022/1119 (91%)	1019 (100%)	3 (0%)	91	92
1	G	1106/1119 (99%)	1101 (100%)	5 (0%)	86	90
2	H	84/84 (100%)	84 (100%)	0	100	100
2	I	84/84 (100%)	84 (100%)	0	100	100
2	J	84/84 (100%)	84 (100%)	0	100	100
2	K	84/84 (100%)	84 (100%)	0	100	100
2	L	84/84 (100%)	84 (100%)	0	100	100
2	M	84/84 (100%)	84 (100%)	0	100	100
2	N	84/84 (100%)	84 (100%)	0	100	100
3	O	84/84 (100%)	77 (92%)	7 (8%)	9	30
3	P	84/84 (100%)	77 (92%)	7 (8%)	9	30
3	Q	84/84 (100%)	77 (92%)	7 (8%)	9	30
3	R	84/84 (100%)	77 (92%)	7 (8%)	9	30
All	All	8414/8757 (96%)	8357 (99%)	57 (1%)	80	86

5 of 57 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	884	TRP

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Mol	Chain	Res	Type
3	R	92	ASN
3	O	93	ARG
3	R	87	SER
3	Q	93	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 123 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	924	GLN
2	I	70	ASN
1	E	819	ASN
2	H	70	ASN
3	Q	44	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

14 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	HEC	I	500	-	32,50,50	2.16	5 (15%)	30,82,82	1.66	4 (13%)
5	HEC	N	500	-	32,50,50	2.16	5 (15%)	30,82,82	1.68	5 (16%)
4	DTP	F	1301	-	28,32,32	3.51	11 (39%)	35,50,50	2.24	3 (8%)
4	DTP	A	1301	-	28,32,32	3.51	11 (39%)	35,50,50	2.24	3 (8%)
5	HEC	K	500	-	32,50,50	2.17	5 (15%)	30,82,82	1.67	4 (13%)
5	HEC	J	500	-	32,50,50	2.17	5 (15%)	30,82,82	1.66	4 (13%)
5	HEC	M	500	-	32,50,50	2.16	5 (15%)	30,82,82	1.67	4 (13%)
4	DTP	E	1301	-	28,32,32	3.51	11 (39%)	35,50,50	2.25	3 (8%)
5	HEC	H	500	-	32,50,50	2.17	5 (15%)	30,82,82	1.67	5 (16%)
4	DTP	G	1301	-	28,32,32	3.52	11 (39%)	35,50,50	2.24	3 (8%)
4	DTP	C	1301	-	28,32,32	3.51	11 (39%)	35,50,50	2.24	3 (8%)
4	DTP	B	1301	-	28,32,32	3.51	11 (39%)	35,50,50	2.24	3 (8%)
4	DTP	D	1301	-	28,32,32	3.52	11 (39%)	35,50,50	2.24	3 (8%)
5	HEC	L	500	-	32,50,50	2.16	5 (15%)	30,82,82	1.67	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
5	HEC	I	500	-	-	1/10/54/54	-
5	HEC	N	500	-	-	1/10/54/54	-
4	DTP	F	1301	-	-	6/18/34/34	0/3/3/3
4	DTP	A	1301	-	-	6/18/34/34	0/3/3/3
5	HEC	K	500	-	-	1/10/54/54	-
5	HEC	J	500	-	-	1/10/54/54	-
5	HEC	M	500	-	-	1/10/54/54	-
4	DTP	E	1301	-	-	6/18/34/34	0/3/3/3
5	HEC	H	500	-	-	1/10/54/54	-
4	DTP	G	1301	-	-	6/18/34/34	0/3/3/3
4	DTP	C	1301	-	-	6/18/34/34	0/3/3/3
4	DTP	B	1301	-	-	6/18/34/34	0/3/3/3
4	DTP	D	1301	-	-	6/18/34/34	0/3/3/3
5	HEC	L	500	-	-	1/10/54/54	-

The worst 5 of 112 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1301	DTP	C2'-C3'	-12.34	1.21	1.52
4	G	1301	DTP	C2'-C3'	-12.33	1.21	1.52
4	F	1301	DTP	C2'-C3'	-12.33	1.21	1.52
4	A	1301	DTP	C2'-C3'	-12.31	1.21	1.52
4	E	1301	DTP	C2'-C3'	-12.31	1.21	1.52

The worst 5 of 52 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	1301	DTP	C5-C6-N6	9.00	134.02	120.31
4	F	1301	DTP	C5-C6-N6	8.98	133.98	120.31
4	B	1301	DTP	C5-C6-N6	8.97	133.98	120.31
4	A	1301	DTP	C5-C6-N6	8.96	133.97	120.31
4	C	1301	DTP	C5-C6-N6	8.95	133.94	120.31

There are no chirality outliers.

5 of 49 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1301	DTP	C5'-O5'-PA-O1A
4	A	1301	DTP	C5'-O5'-PA-O2A
4	A	1301	DTP	C5'-O5'-PA-O3A
4	A	1301	DTP	O4'-C4'-C5'-O5'
4	B	1301	DTP	C5'-O5'-PA-O1A

There are no ring outliers.

14 monomers are involved in 49 short contacts:

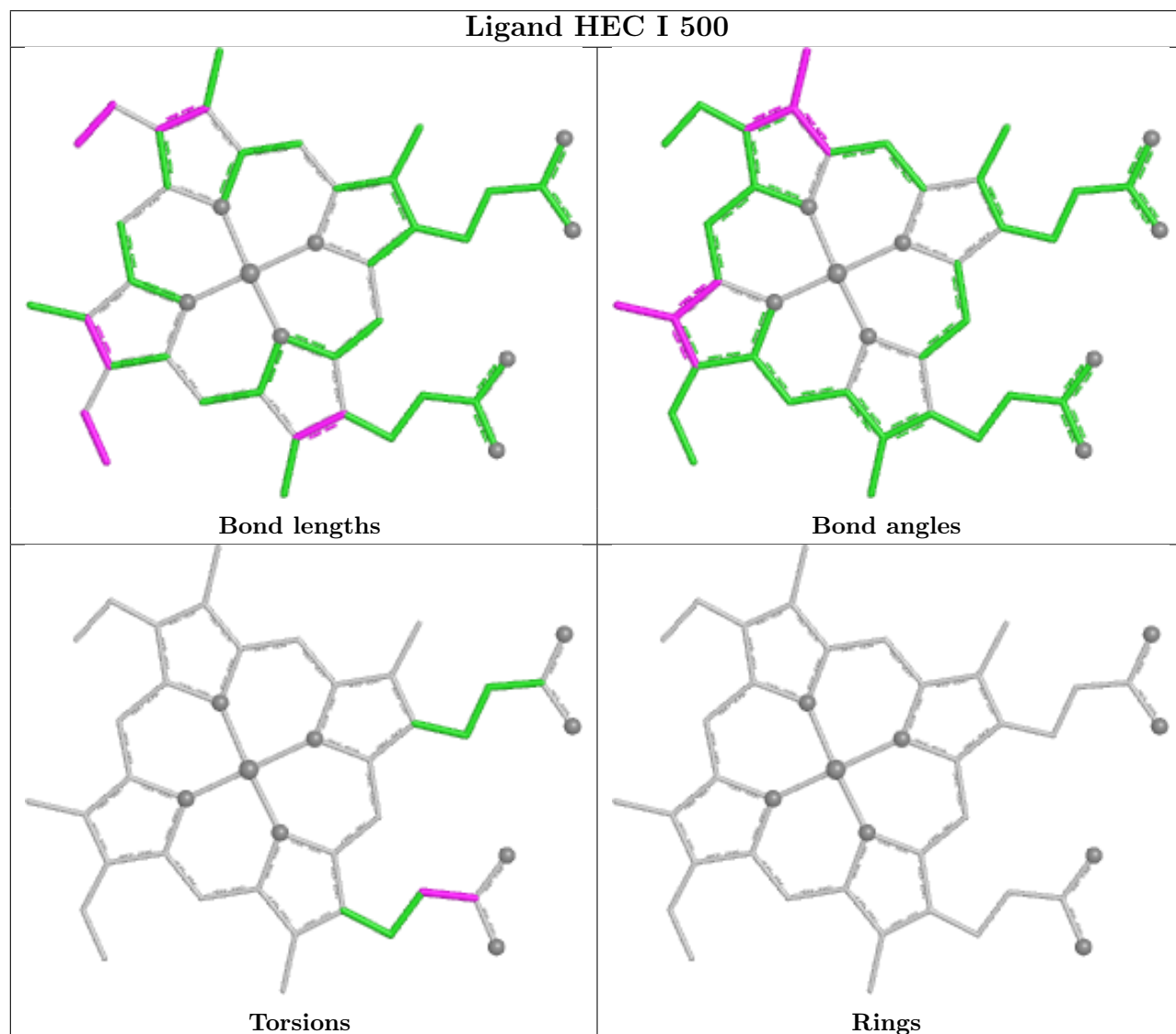
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	I	500	HEC	4	0
5	N	500	HEC	4	0
4	F	1301	DTP	3	0
4	A	1301	DTP	3	0
5	K	500	HEC	4	0
5	J	500	HEC	4	0
5	M	500	HEC	4	0
4	E	1301	DTP	3	0
5	H	500	HEC	4	0
4	G	1301	DTP	3	0
4	C	1301	DTP	3	0
4	B	1301	DTP	3	0
4	D	1301	DTP	3	0

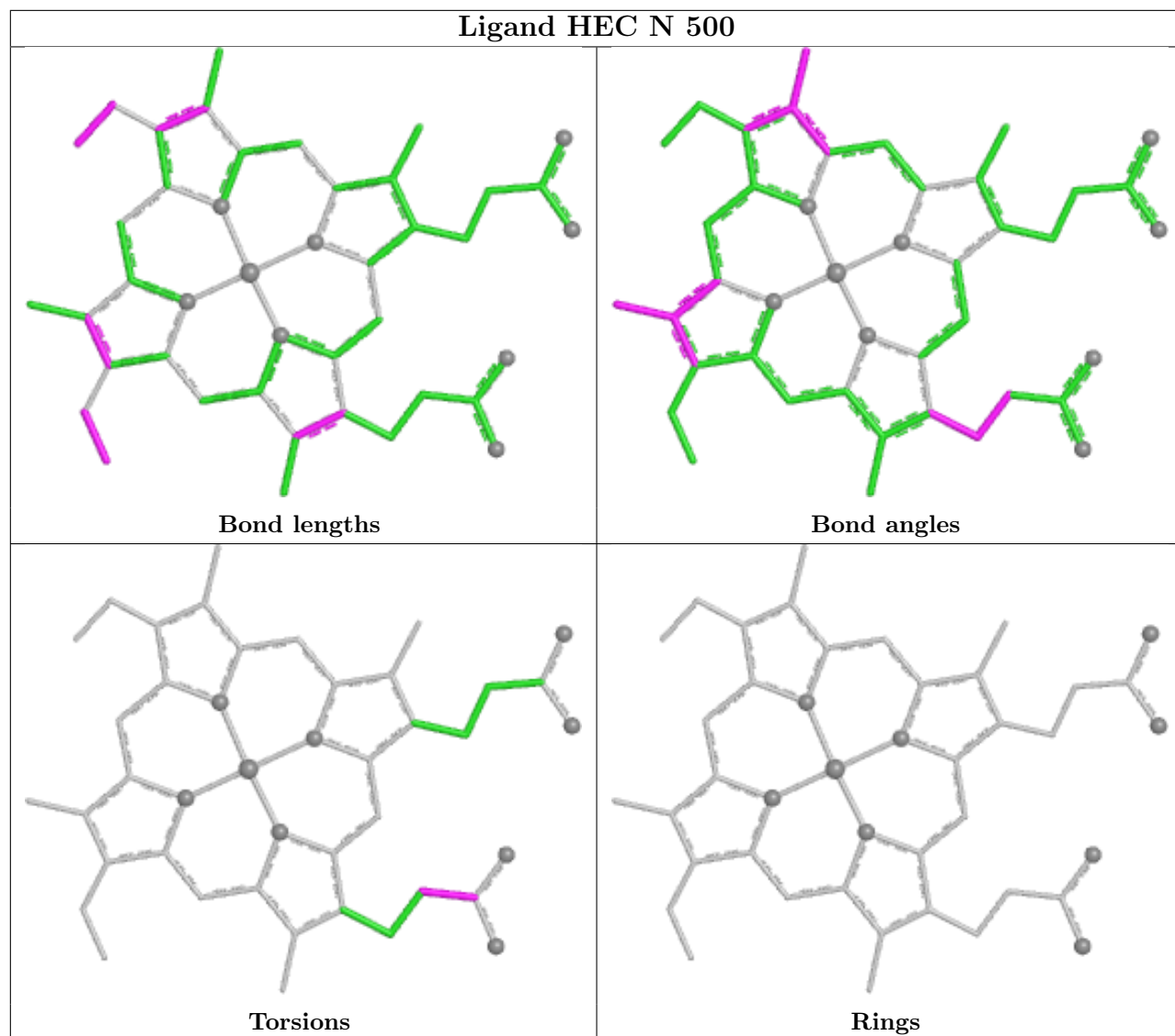
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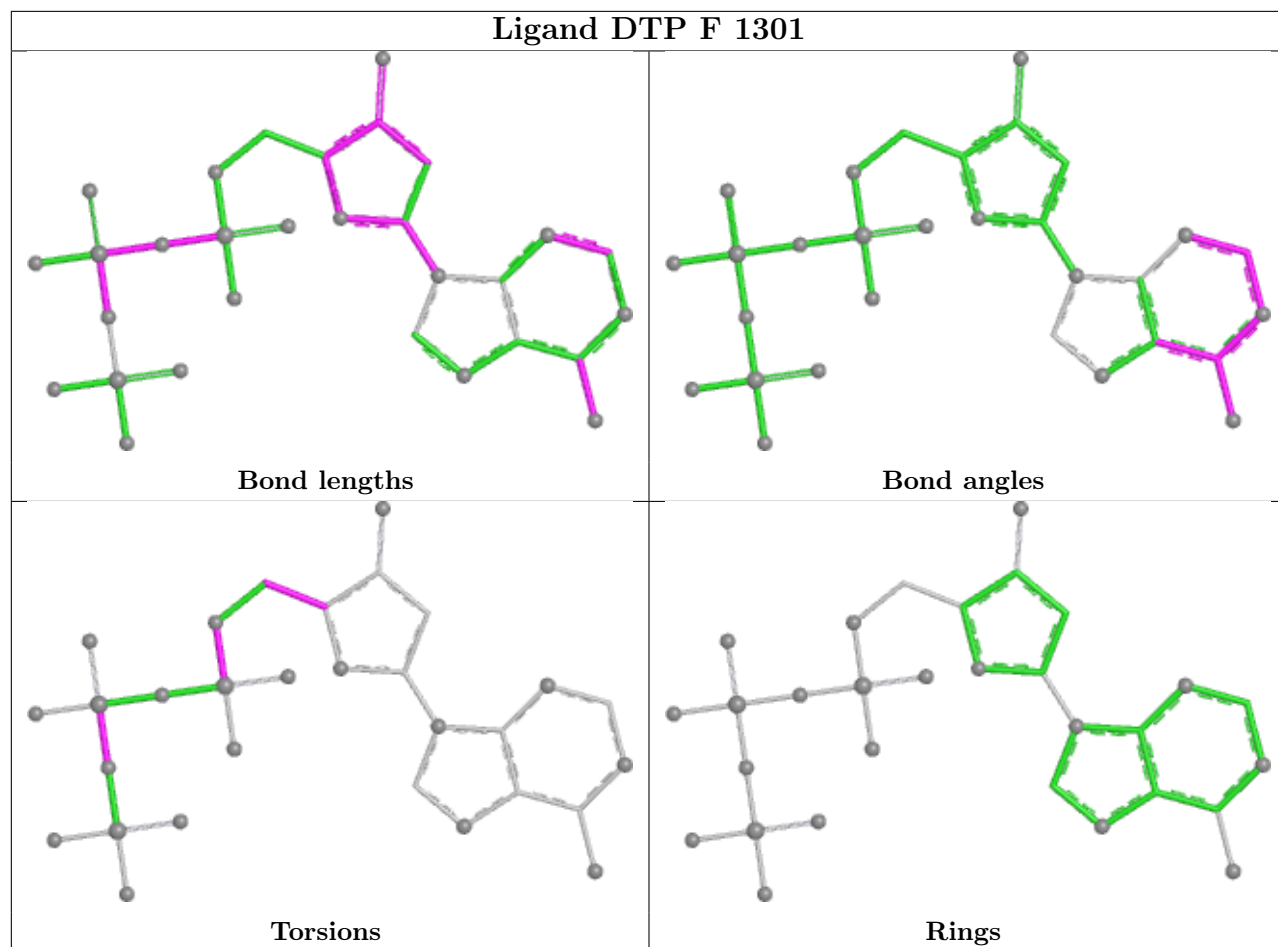
*Continued from previous page...*

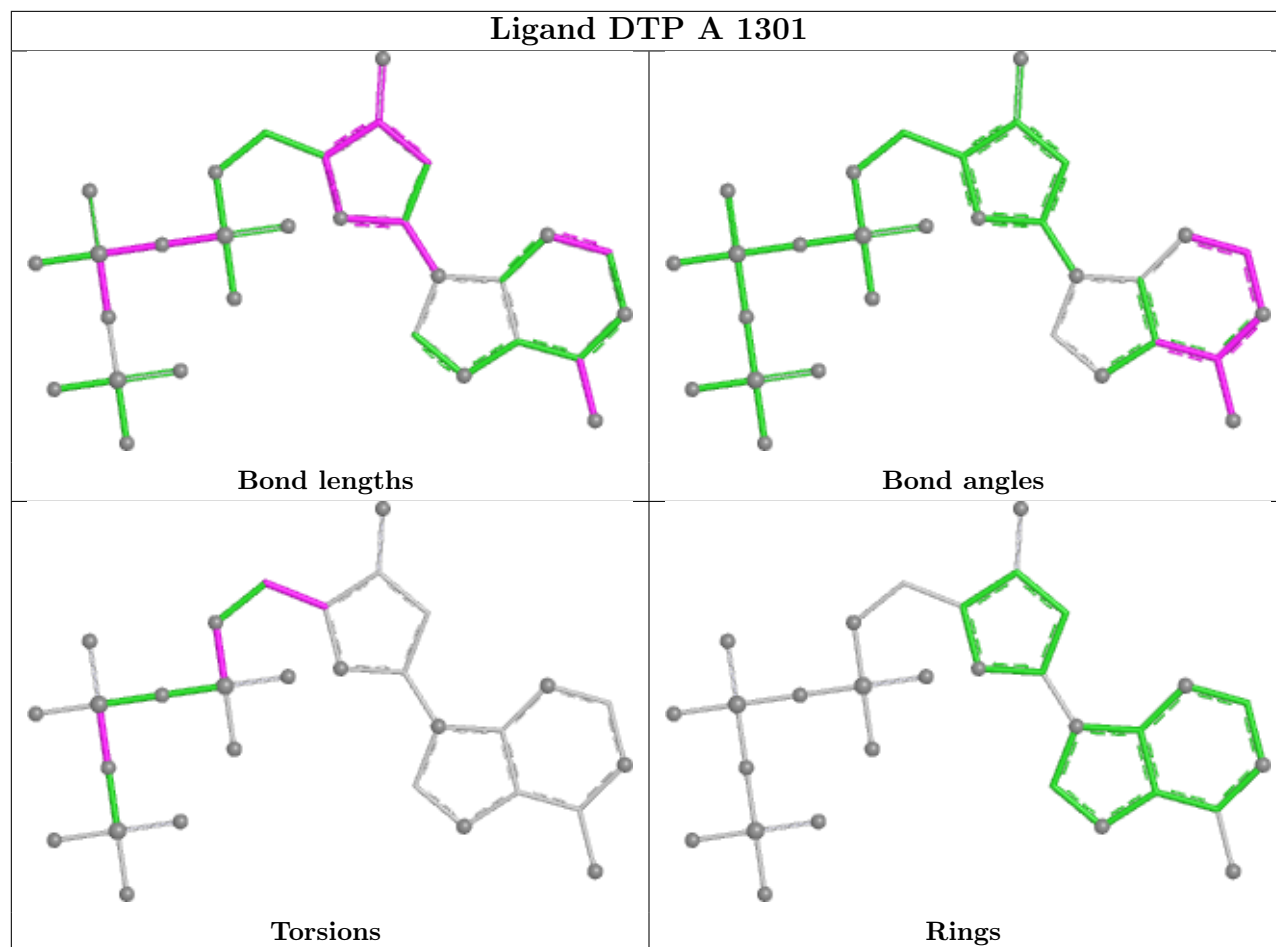
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	L	500	HEC	4	0

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.

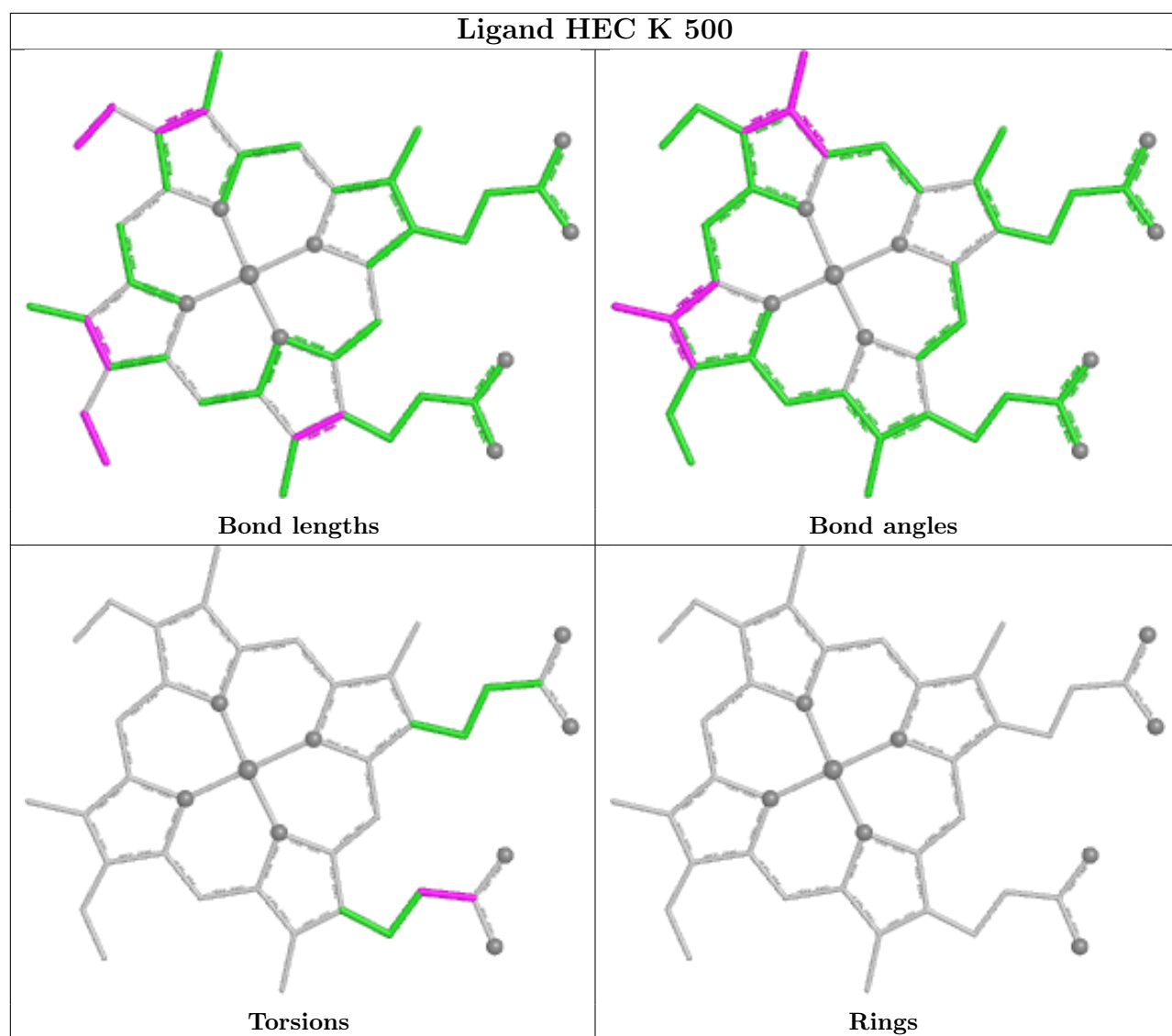




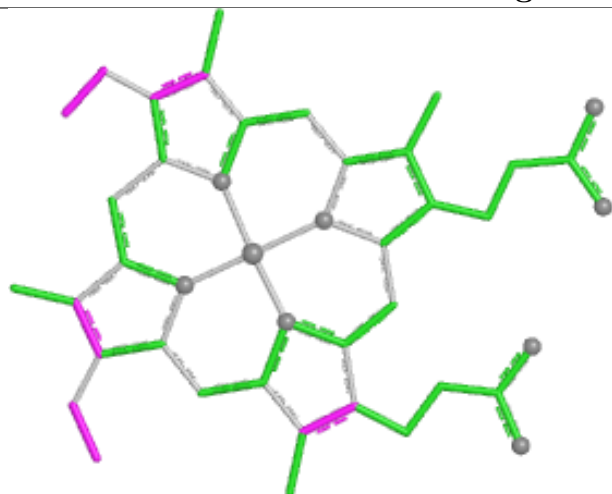




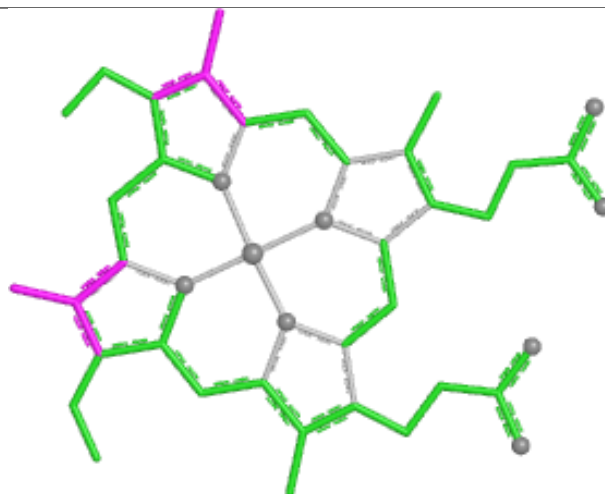




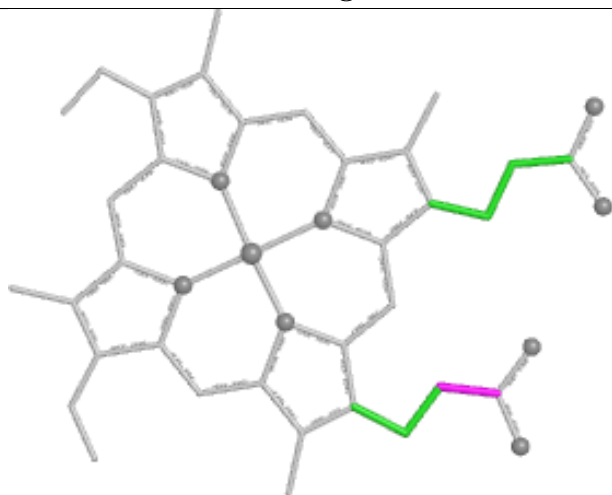
## Ligand HEC J 500



Bond lengths



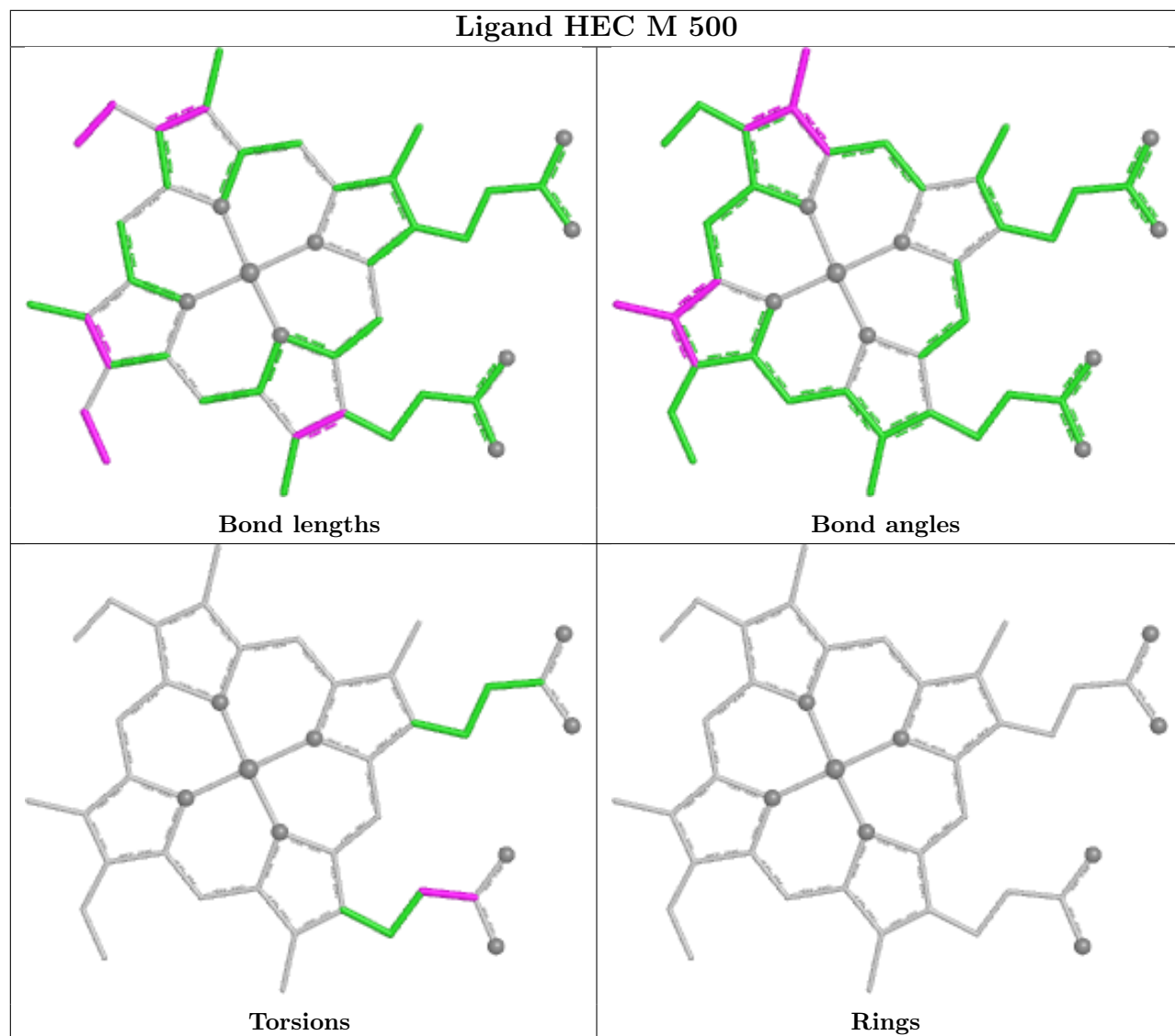
Bond angles

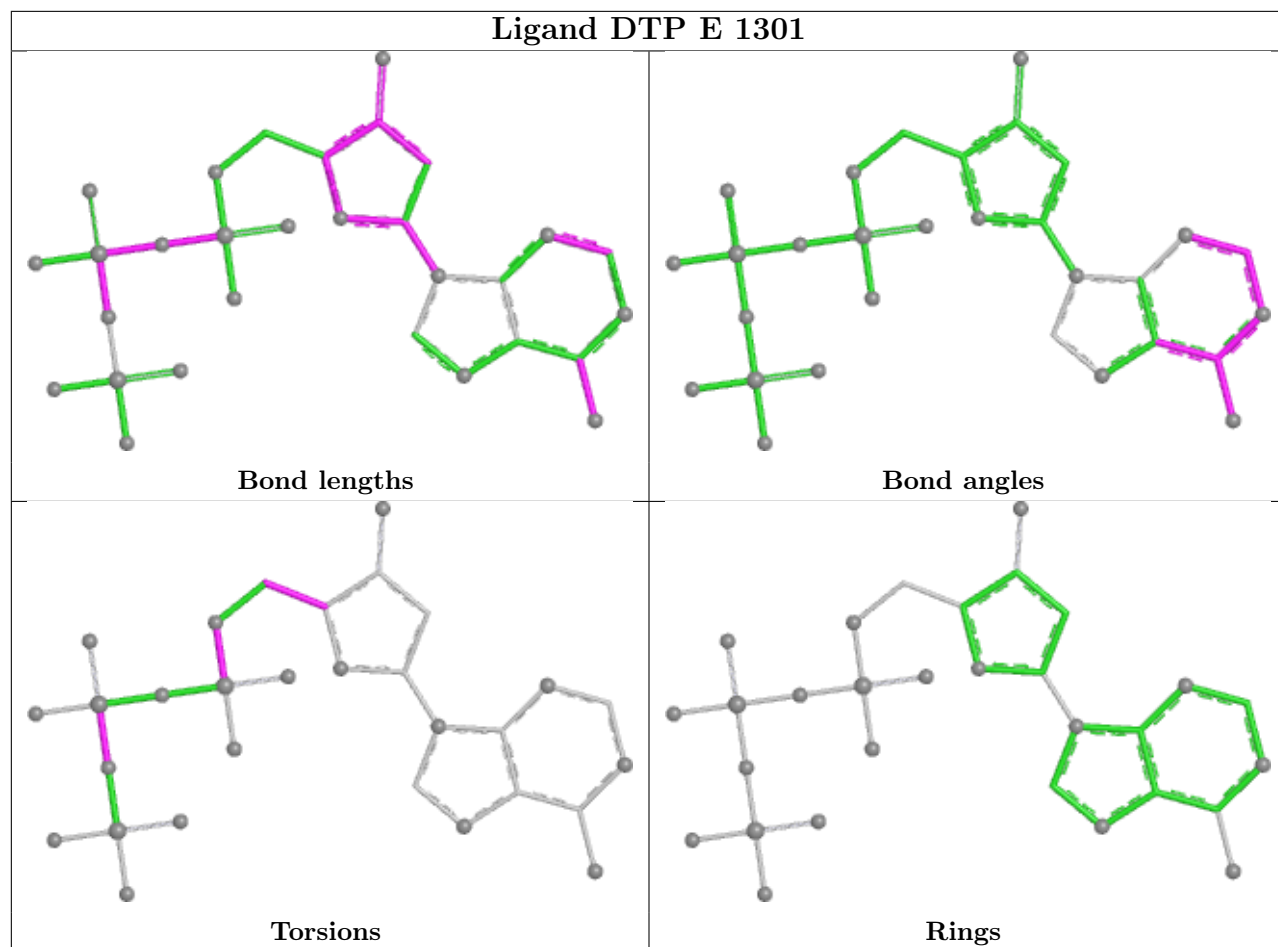


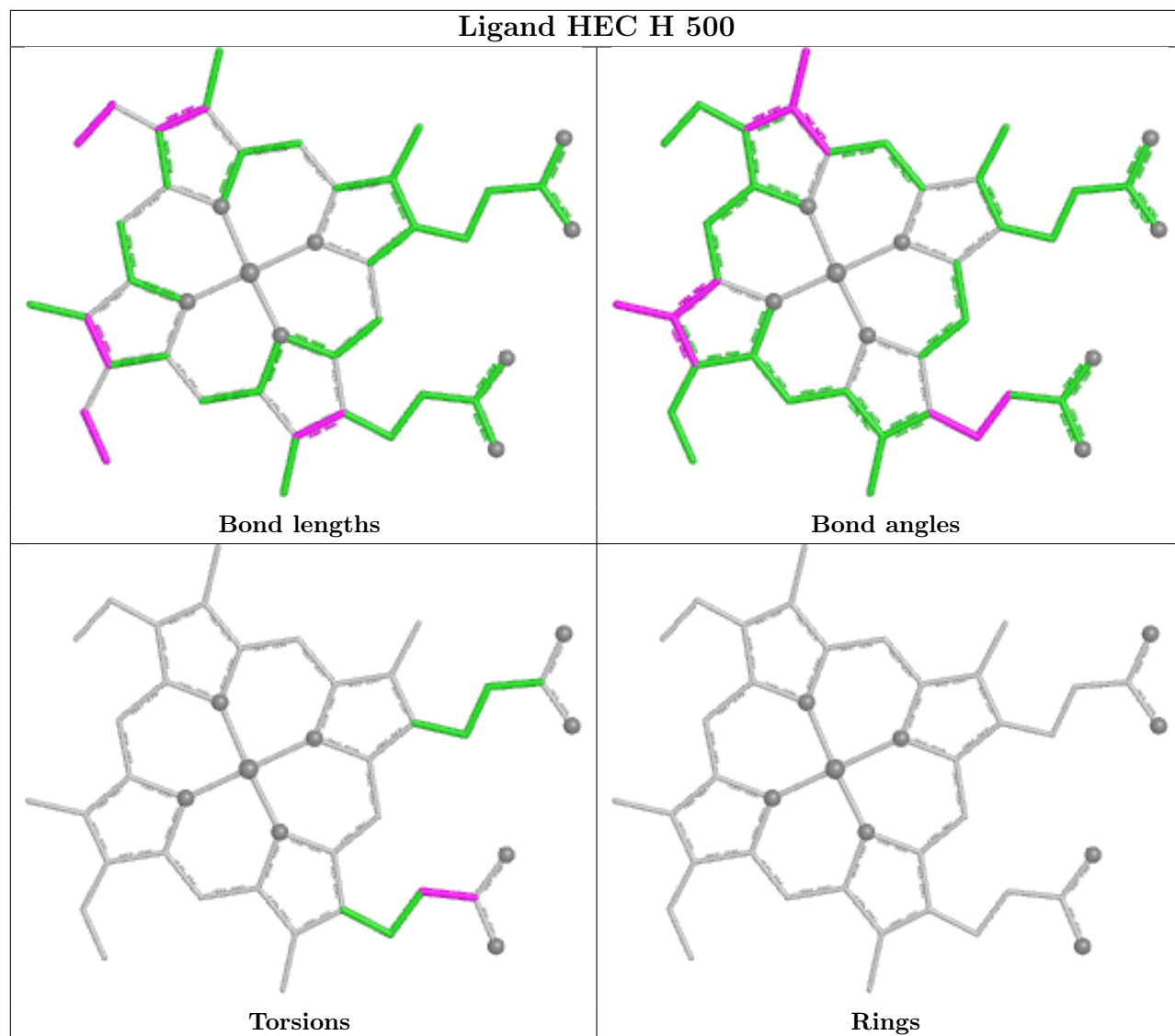
Torsions

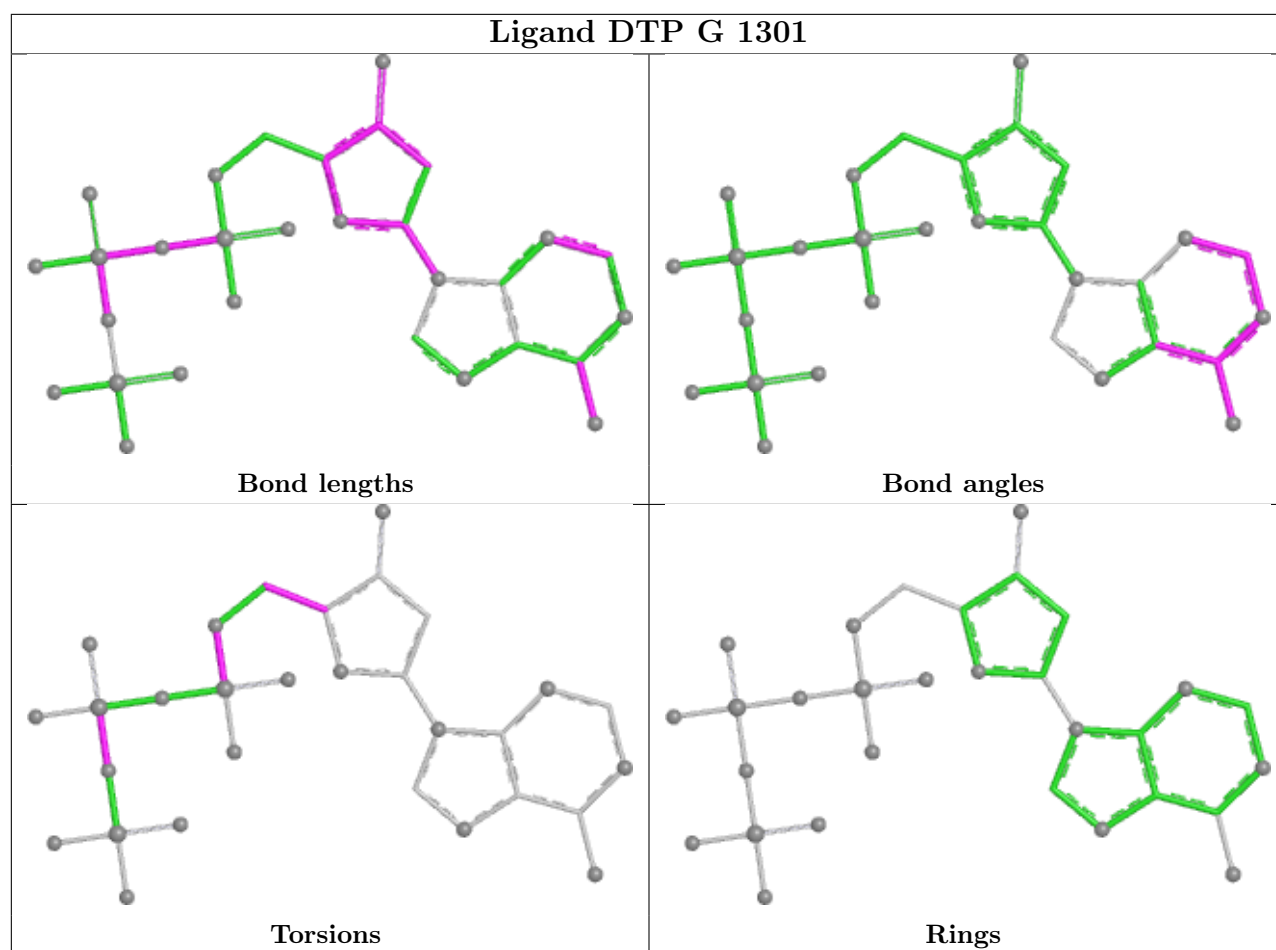


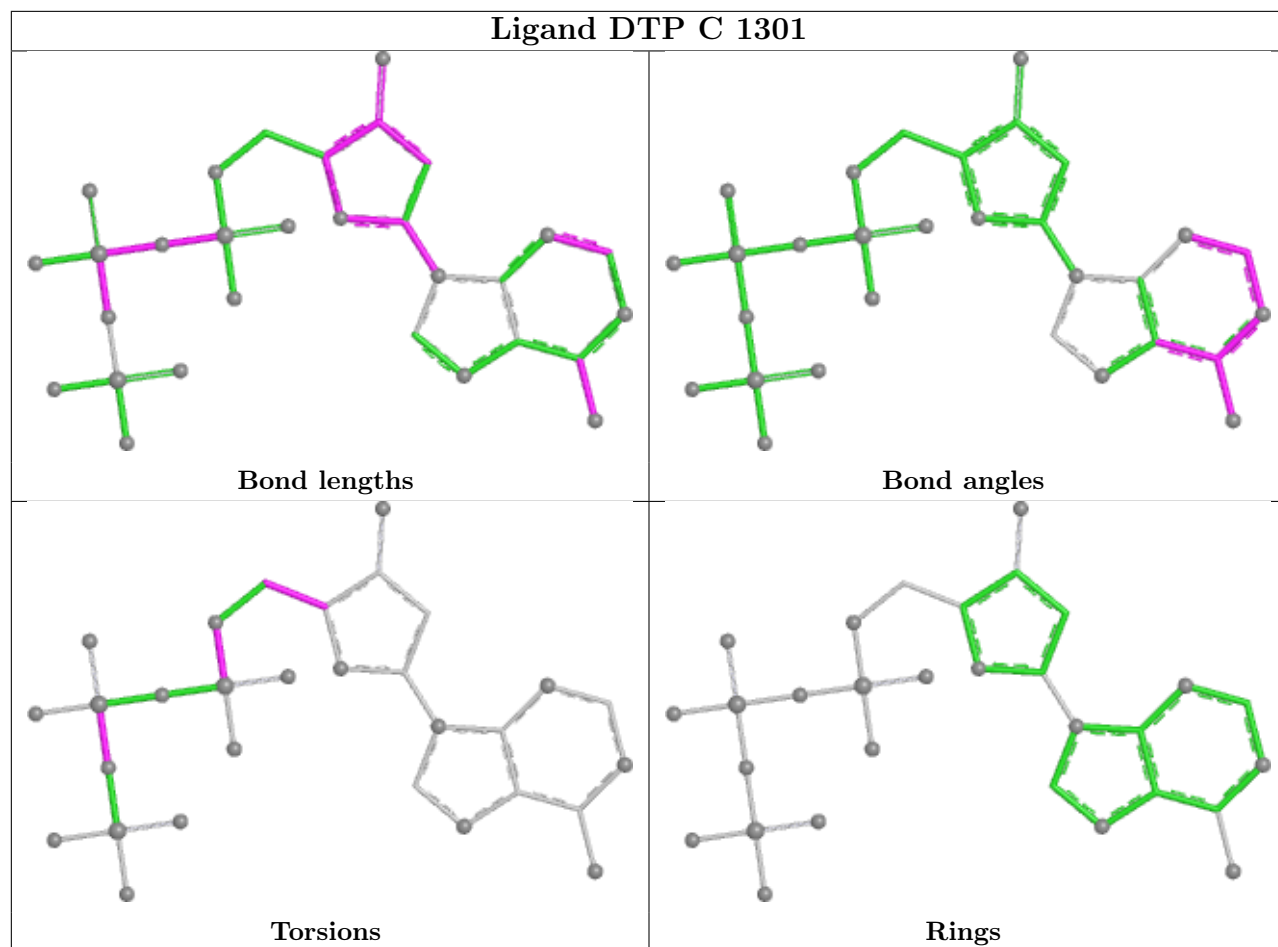
Rings

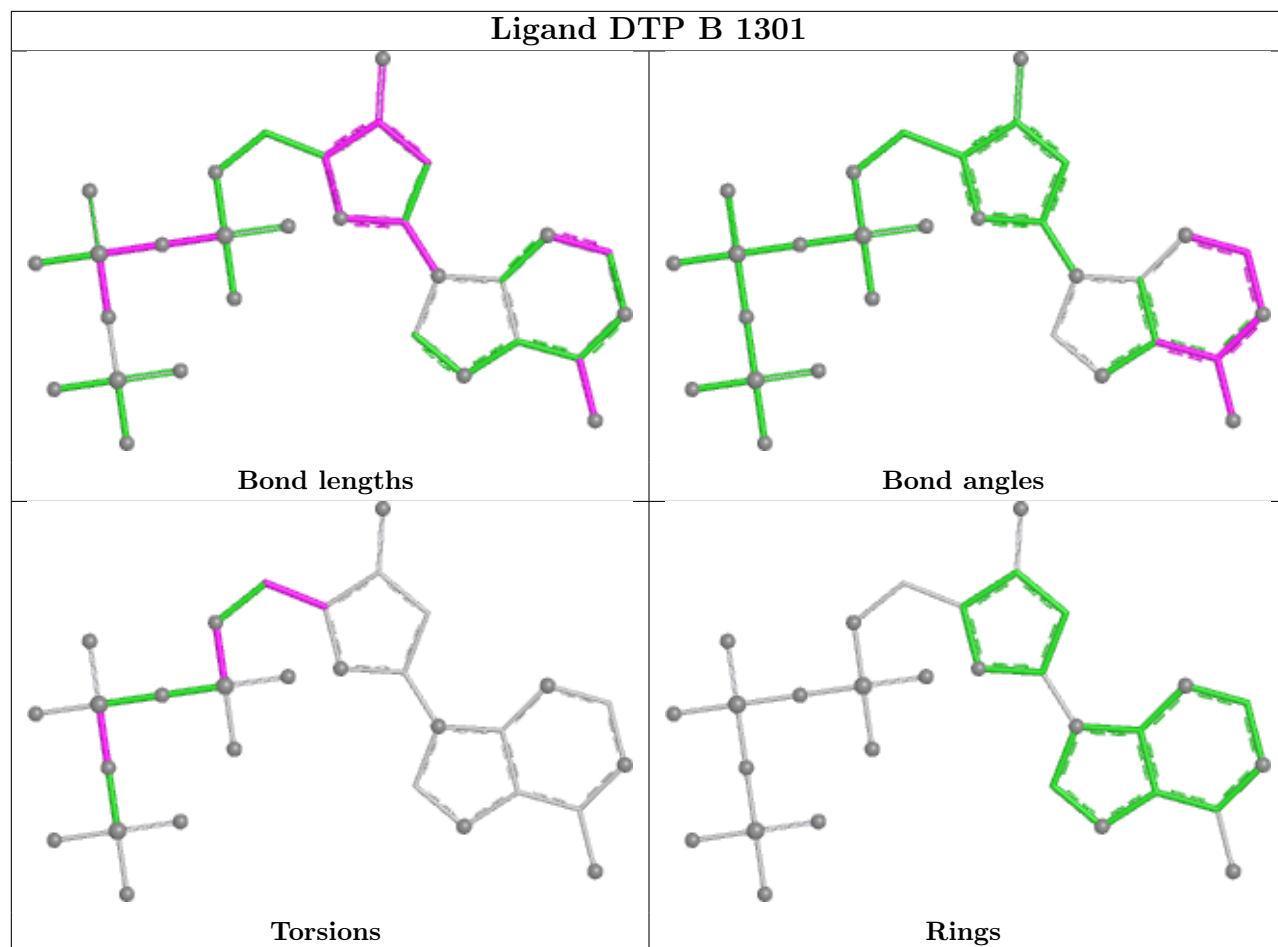




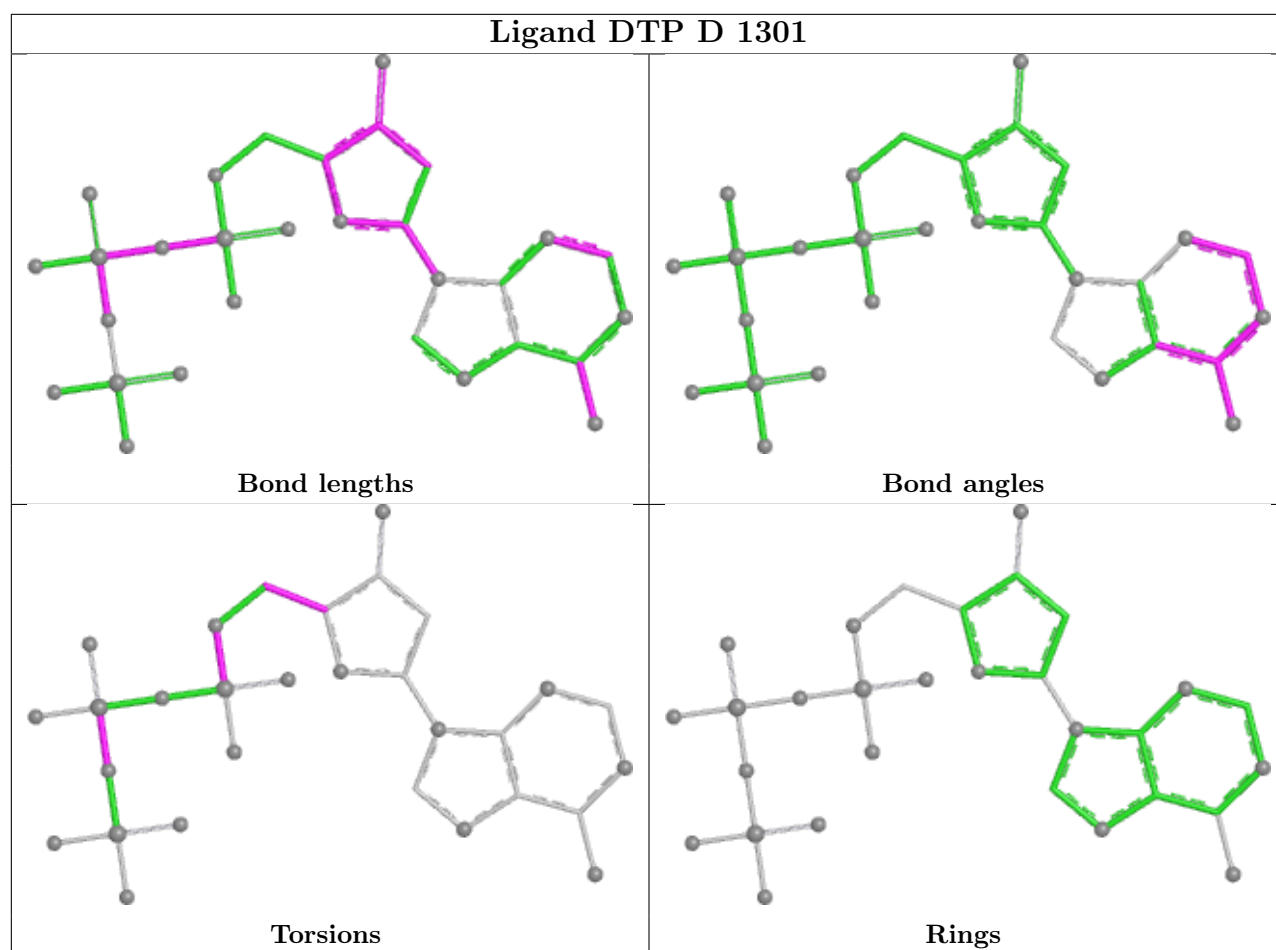


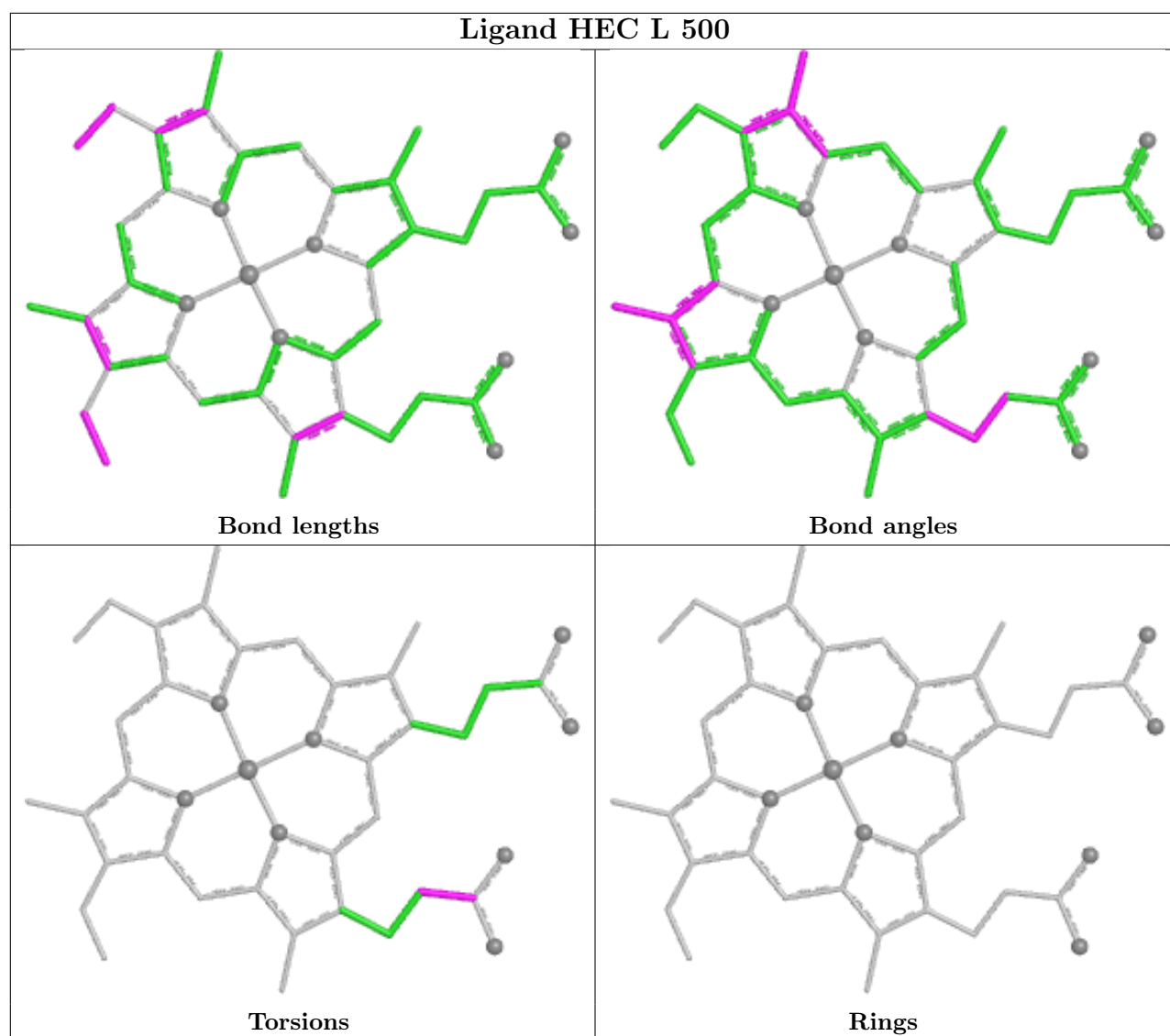












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

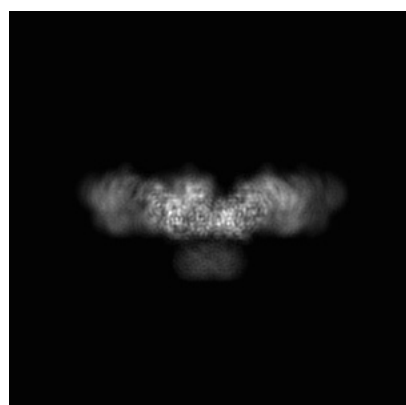
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8178. These allow visual inspection of the internal detail of the map and identification of artifacts.

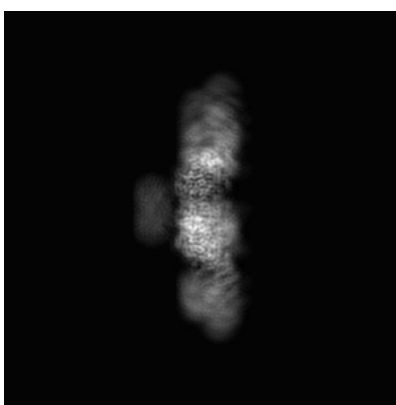
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

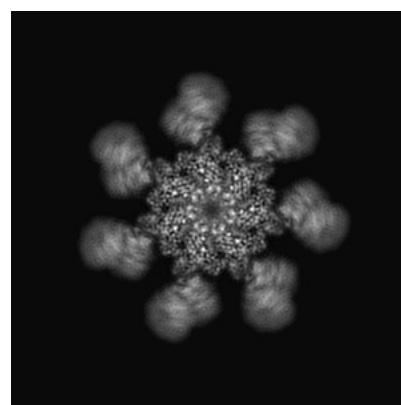
#### 6.1.1 Primary map



X



Y

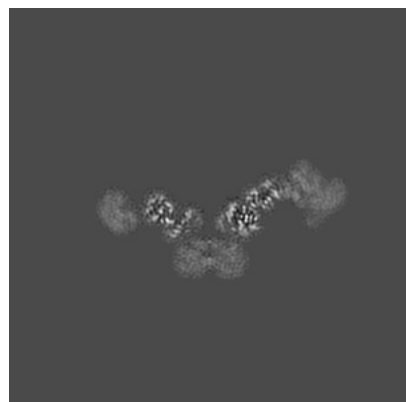


Z

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

### 6.2 Central slices [i](#)

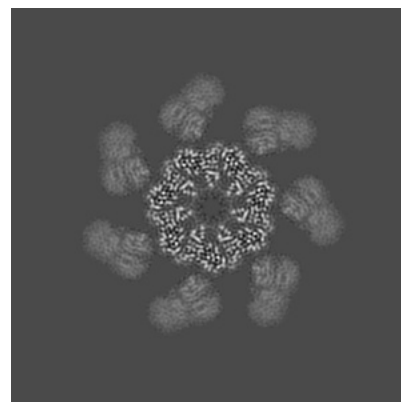
#### 6.2.1 Primary map



X Index: 160



Y Index: 160



Z Index: 160

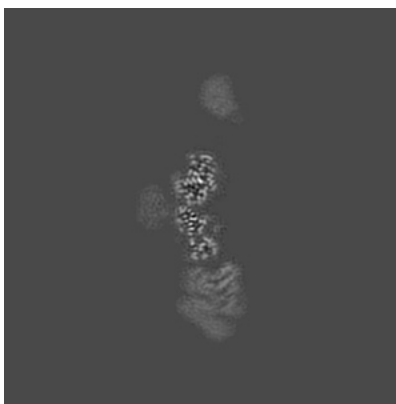
The images above show central slices of the map in three orthogonal directions.

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

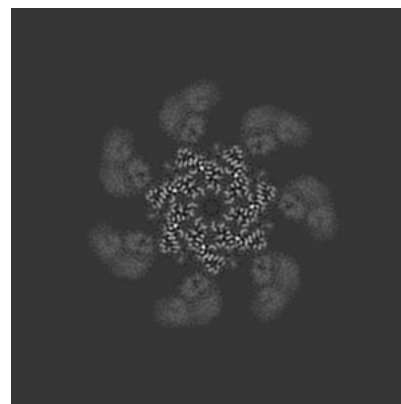
### 6.3.1 Primary map



X Index: 146



Y Index: 135

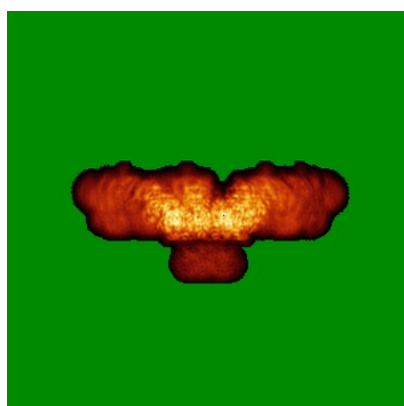


Z Index: 157

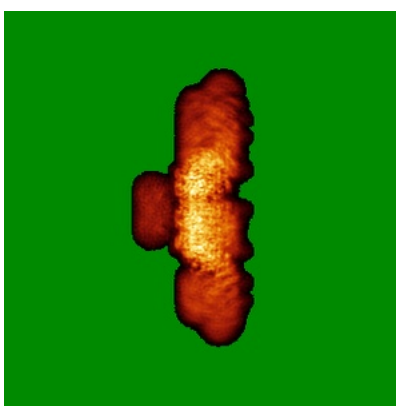
The images above show the largest variance slices of the map in three orthogonal directions.

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

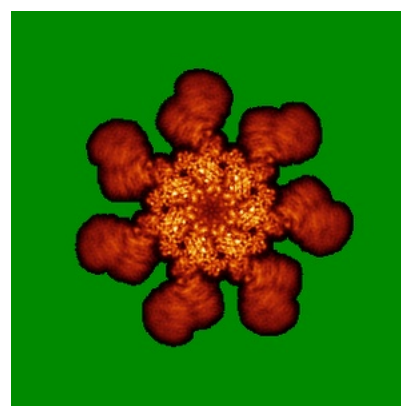
### 6.4.1 Primary map



X



Y

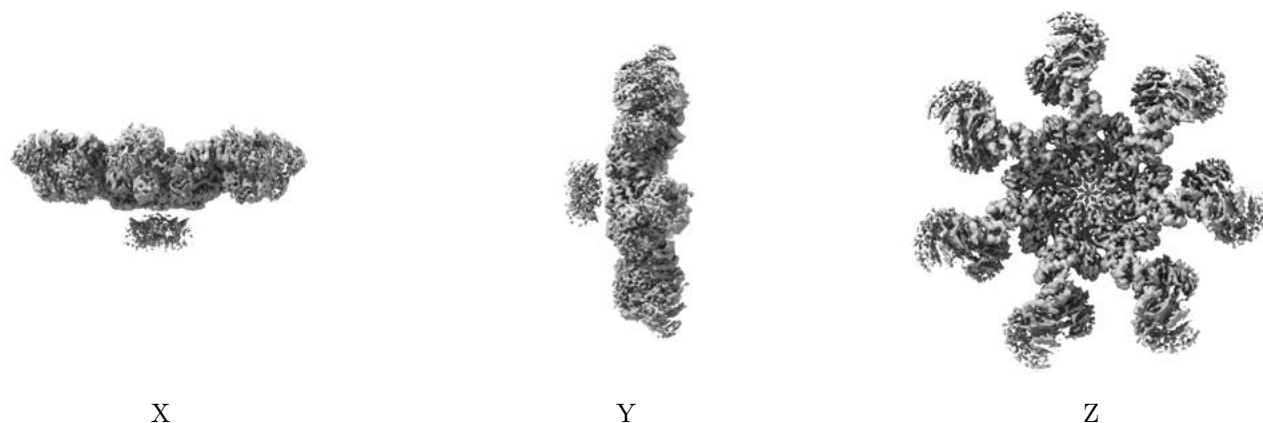


Z

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 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

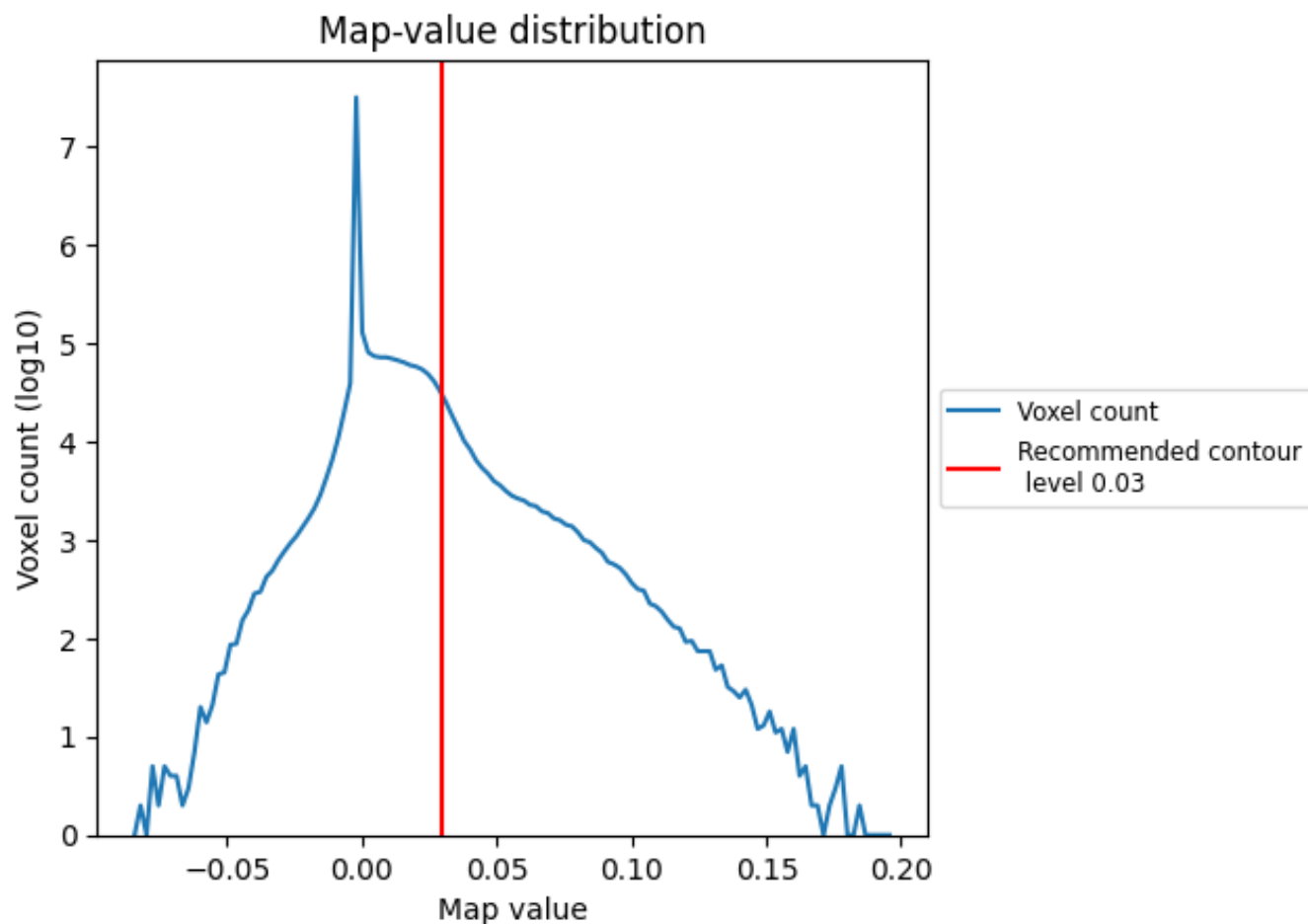
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

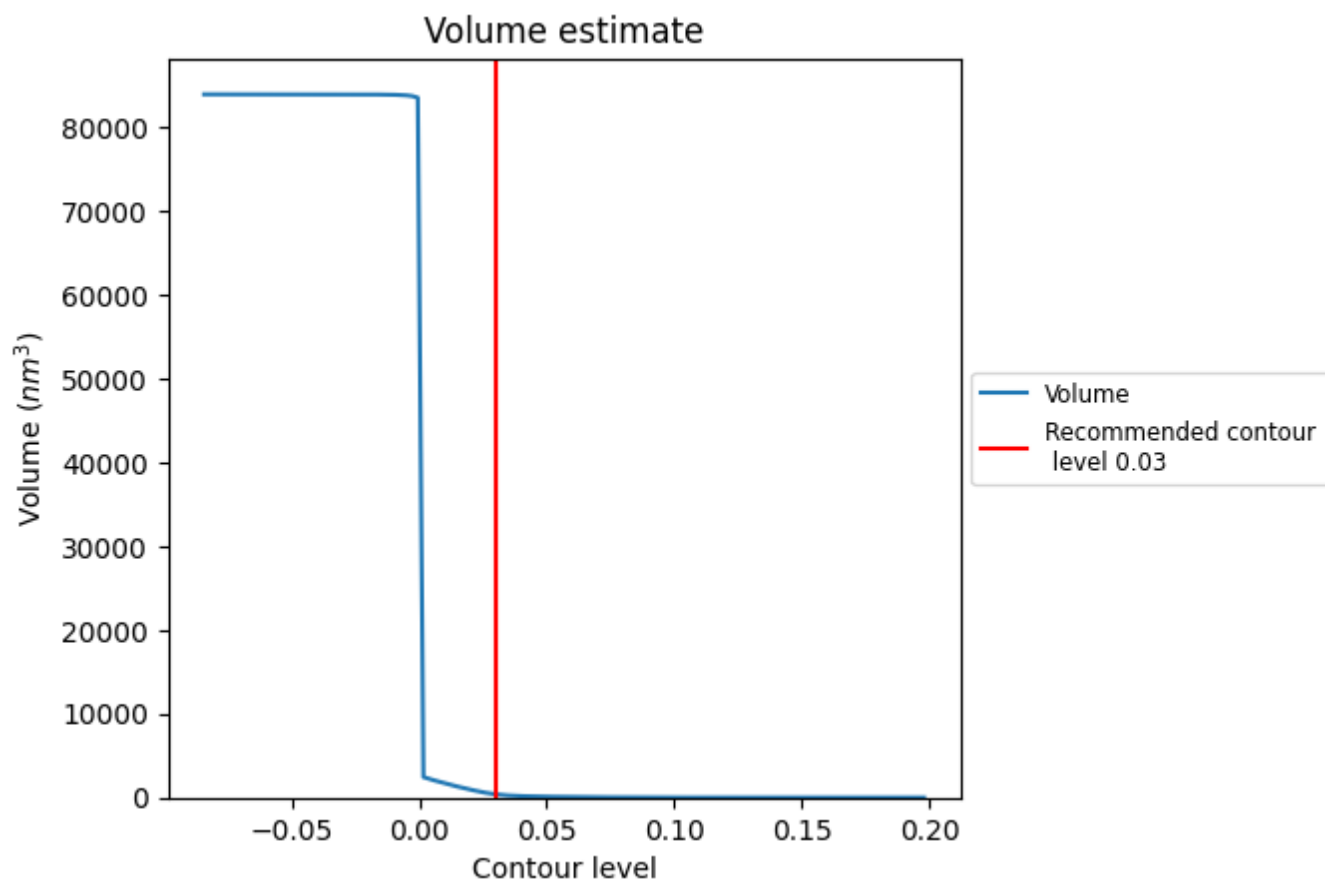
This section contains the results of statistical analysis of the map.

### 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.

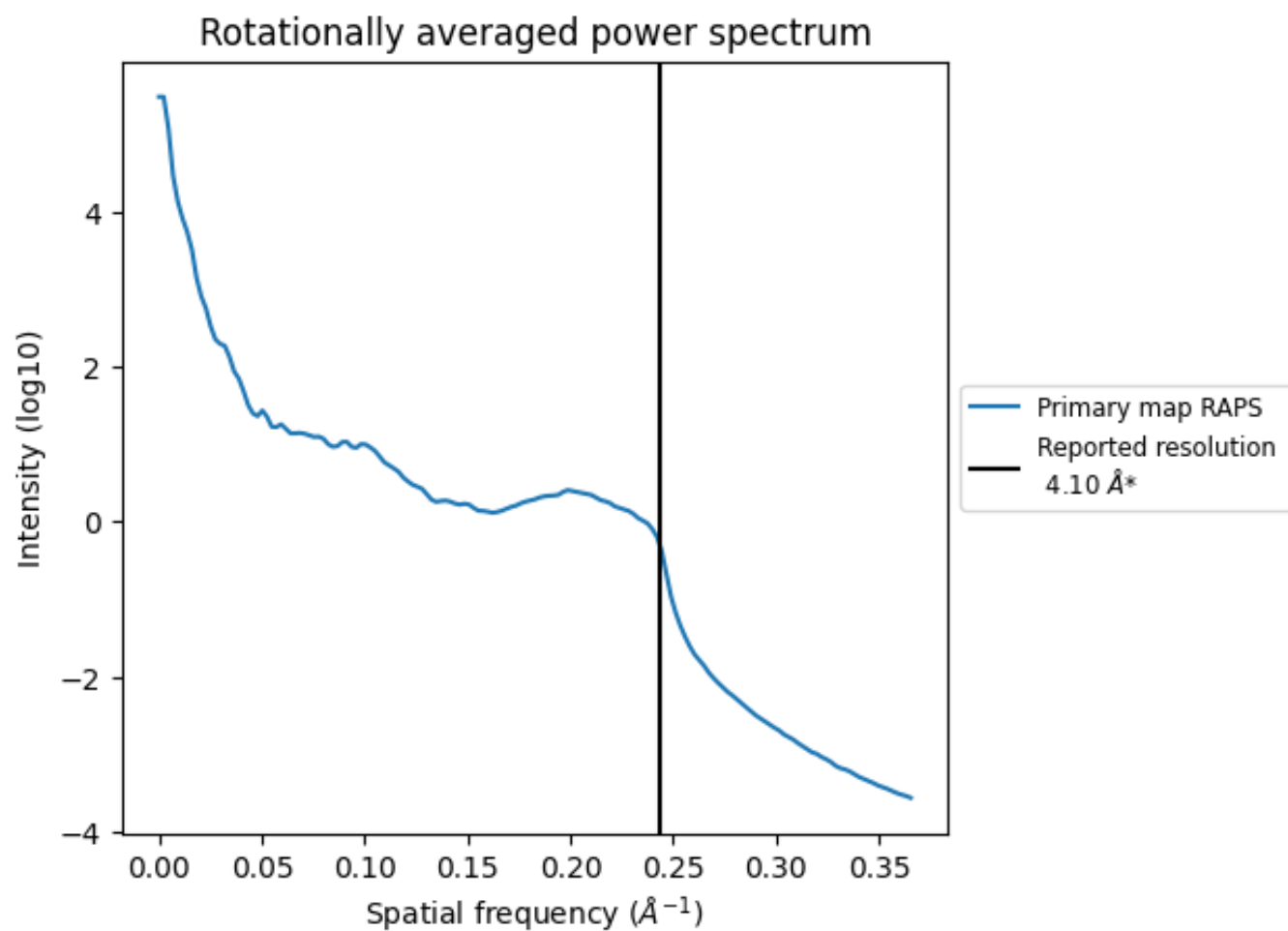
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 389  $\text{nm}^3$ ; this corresponds to an approximate mass of 352 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 Å<sup>-1</sup>



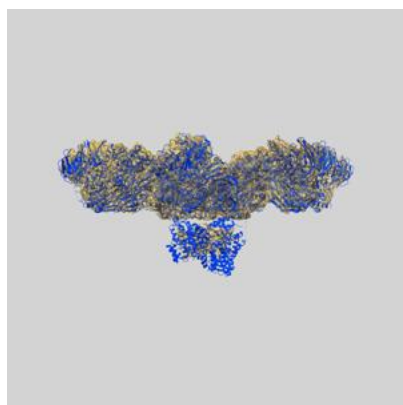
## 8 Fourier-Shell correlation

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

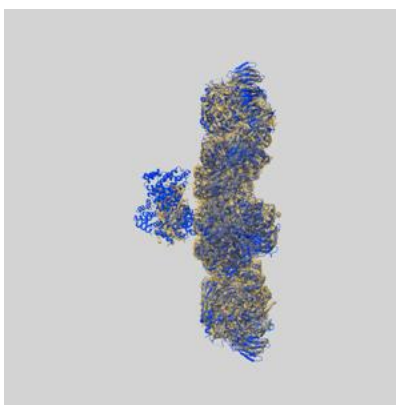
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-8178 and PDB model 5JUY. Per-residue inclusion information can be found in section [3](#) on page [7](#).

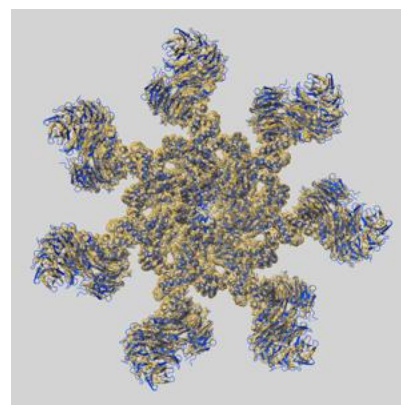
### 9.1 Map-model overlay [i](#)



X



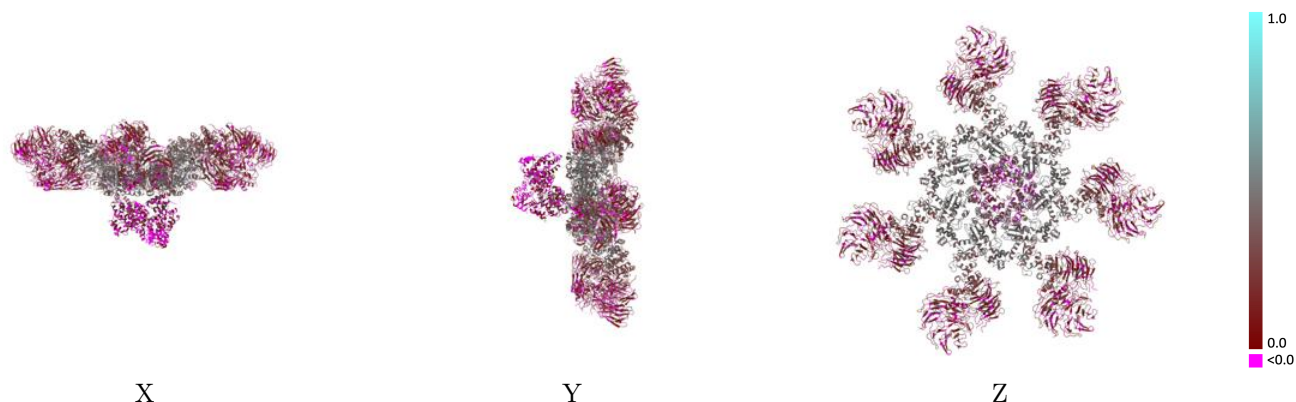
Y



Z

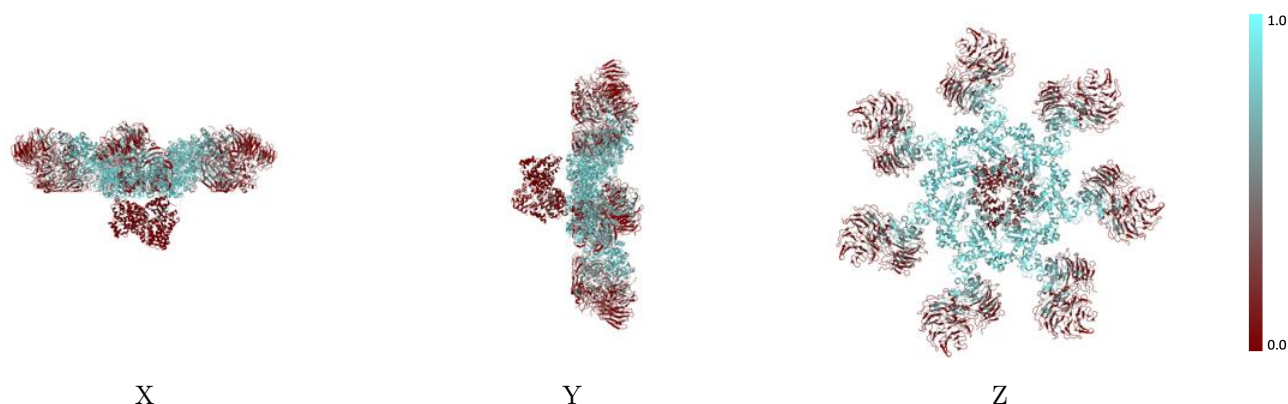
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



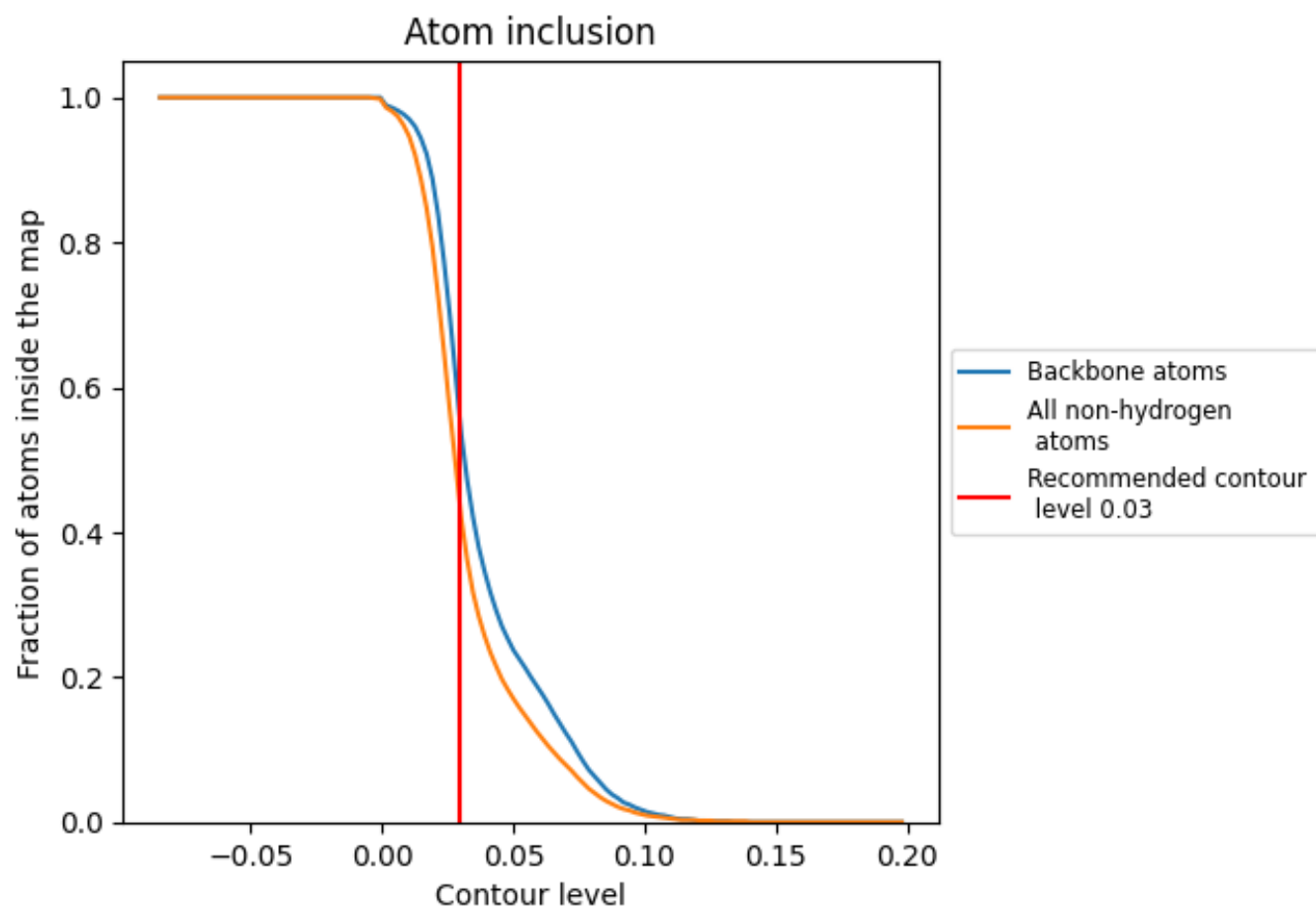
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.03).







































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 55% of all backbone atoms, 43% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4290	 0.2300
A	 0.4830	 0.2610
B	 0.4490	 0.2420
C	 0.4820	 0.2620
D	 0.4510	 0.2410
E	 0.4490	 0.2460
F	 0.4810	 0.2590
G	 0.4510	 0.2500
H	 0.2400	 0.1010
I	 0.2420	 0.1010
J	 0.2360	 0.1010
K	 0.2460	 0.1060
L	 0.2400	 0.1040
M	 0.2380	 0.1050
N	 0.2360	 0.1030
O	 0.1050	 0.0880
P	 0.0350	 0.0600
Q	 0.0040	 -0.0130
R	 0.0040	 -0.0470

