



wwPDB EM Validation Summary Report ⓘ

Aug 6, 2026 – 10:27 AM EDT

PDB ID : 5JUY / pdb_00005juy
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

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:

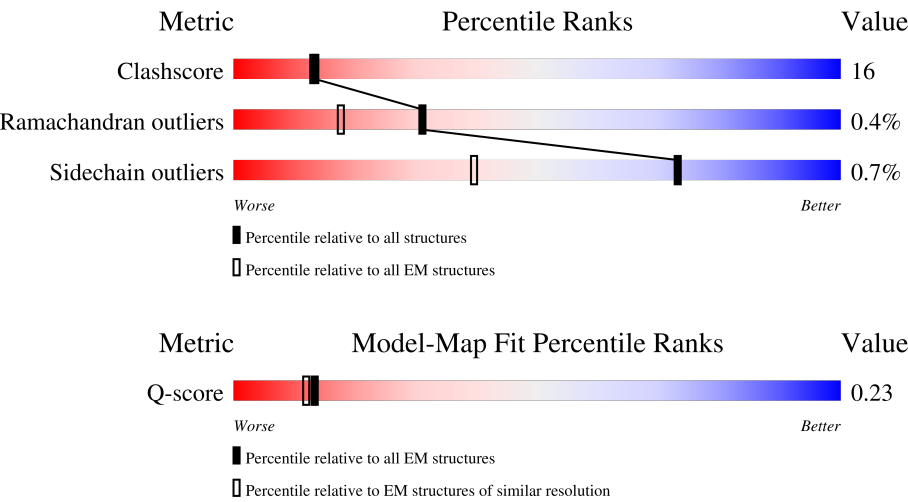
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance i

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

The reported resolution of this entry is 4.10 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	6458 (3.60 - 4.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	39% 63% 27% 9%
1	B	1248	46% 70% 28% ..
1	C	1248	39% 63% 27% 9%
1	D	1248	46% 70% 28% ..

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Mol	Chain	Length	Quality of chain
1	E	1248	
1	F	1248	
1	G	1248	
2	H	104	
2	I	104	
2	J	104	
2	K	104	
2	L	104	
2	M	104	
2	N	104	
3	O	95	
3	P	95	
3	Q	95	
3	R	95	

2 Entry composition [i](#)

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		

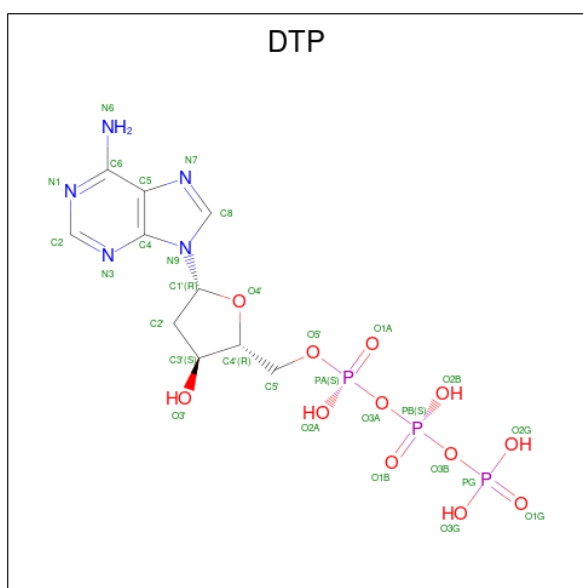
- Molecule 2 is a protein called Cytochrome c.

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.

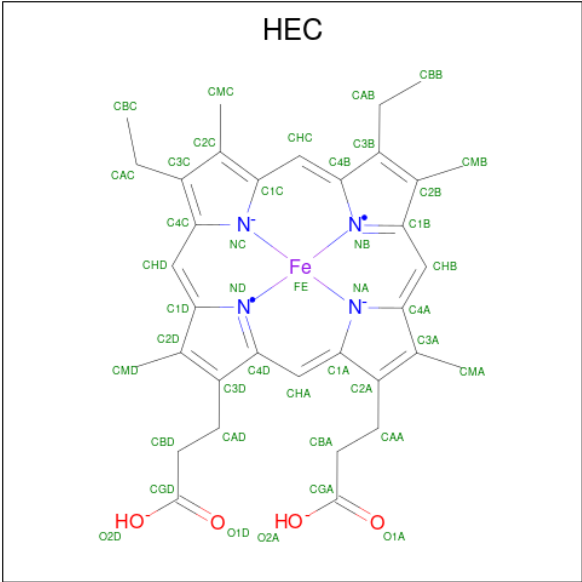
Mol	Chain	Residues	Atoms					AltConf	Trace
3	O	95	Total	C	N	O	S	0	0
			777	475	152	145	5		
3	P	95	Total	C	N	O	S	0	0
			777	475	152	145	5		
3	Q	95	Total	C	N	O	S	0	0
			777	475	152	145	5		
3	R	95	Total	C	N	O	S	0	0
			777	475	152	145	5		

- Molecule 4 is 2'-DEOXYADENOSINE 5'-TRIPHOSPHATE (CCD ID: 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 (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).

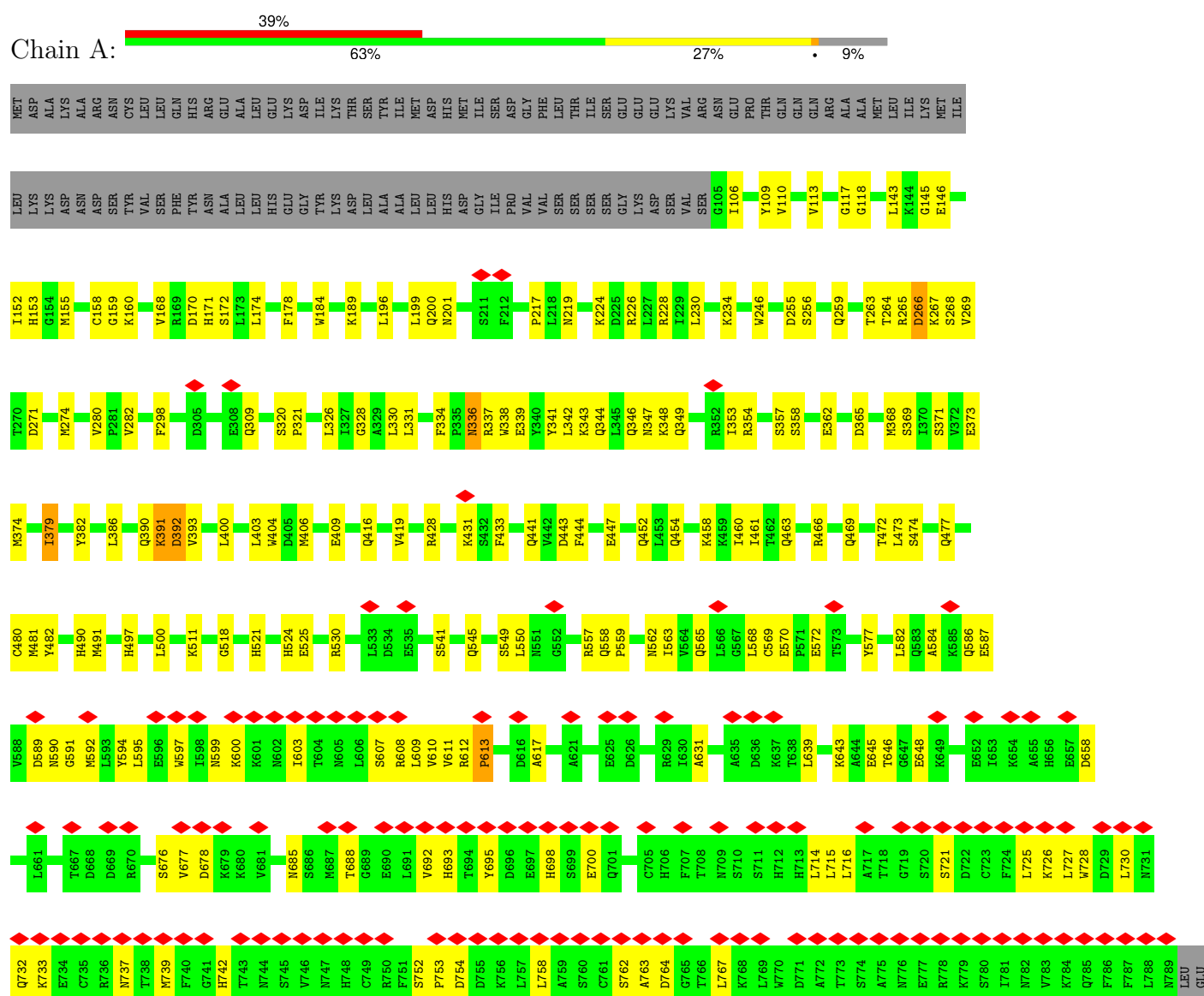


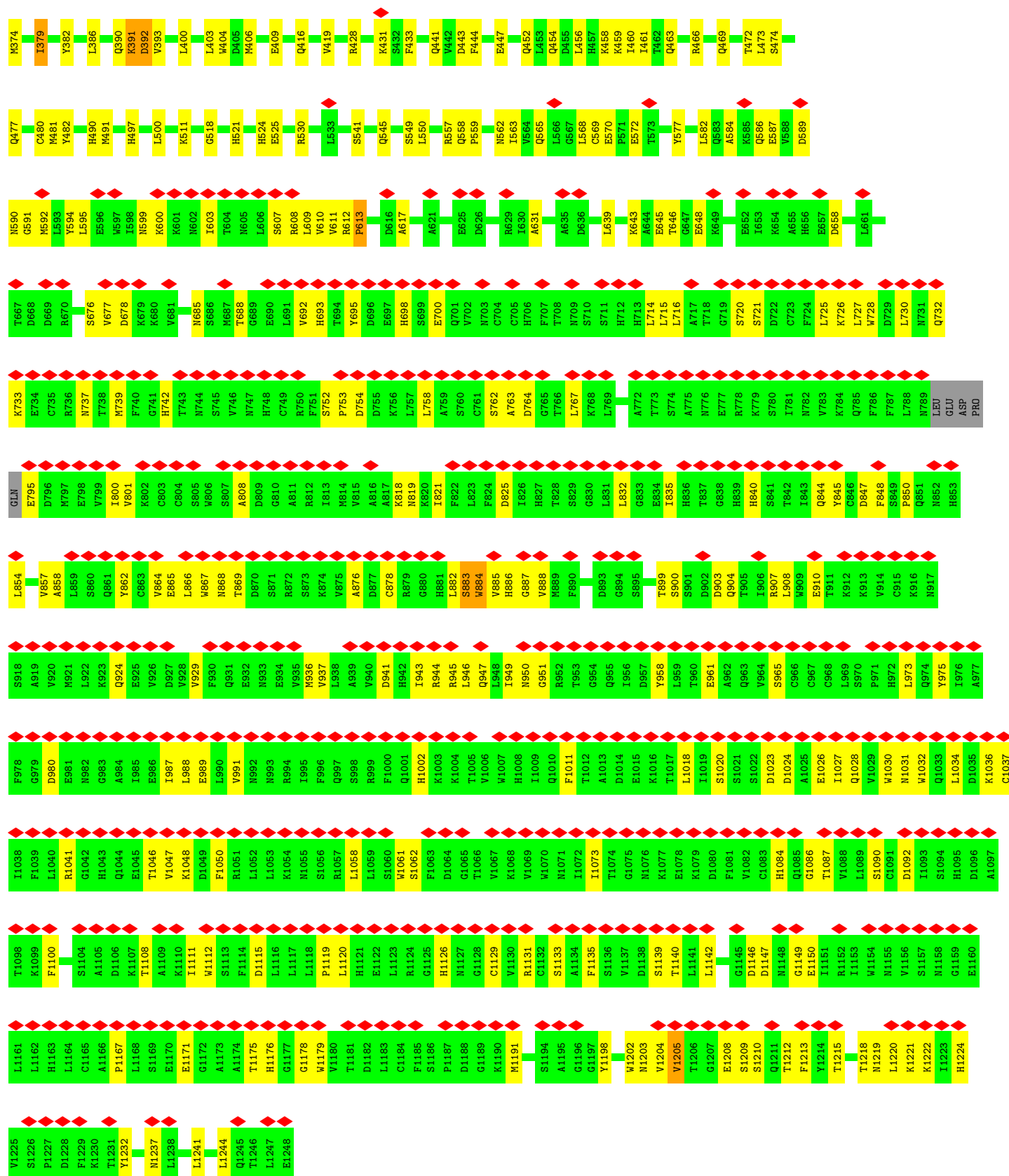
Mol	Chain	Residues	Atoms					AltConf
5	H	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
5	I	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
5	J	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
5	K	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
5	L	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
5	M	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
5	N	1	Total	C	Fe	N	O	0
			43	34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

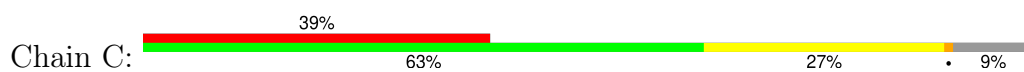
3 Residue-property plots

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.

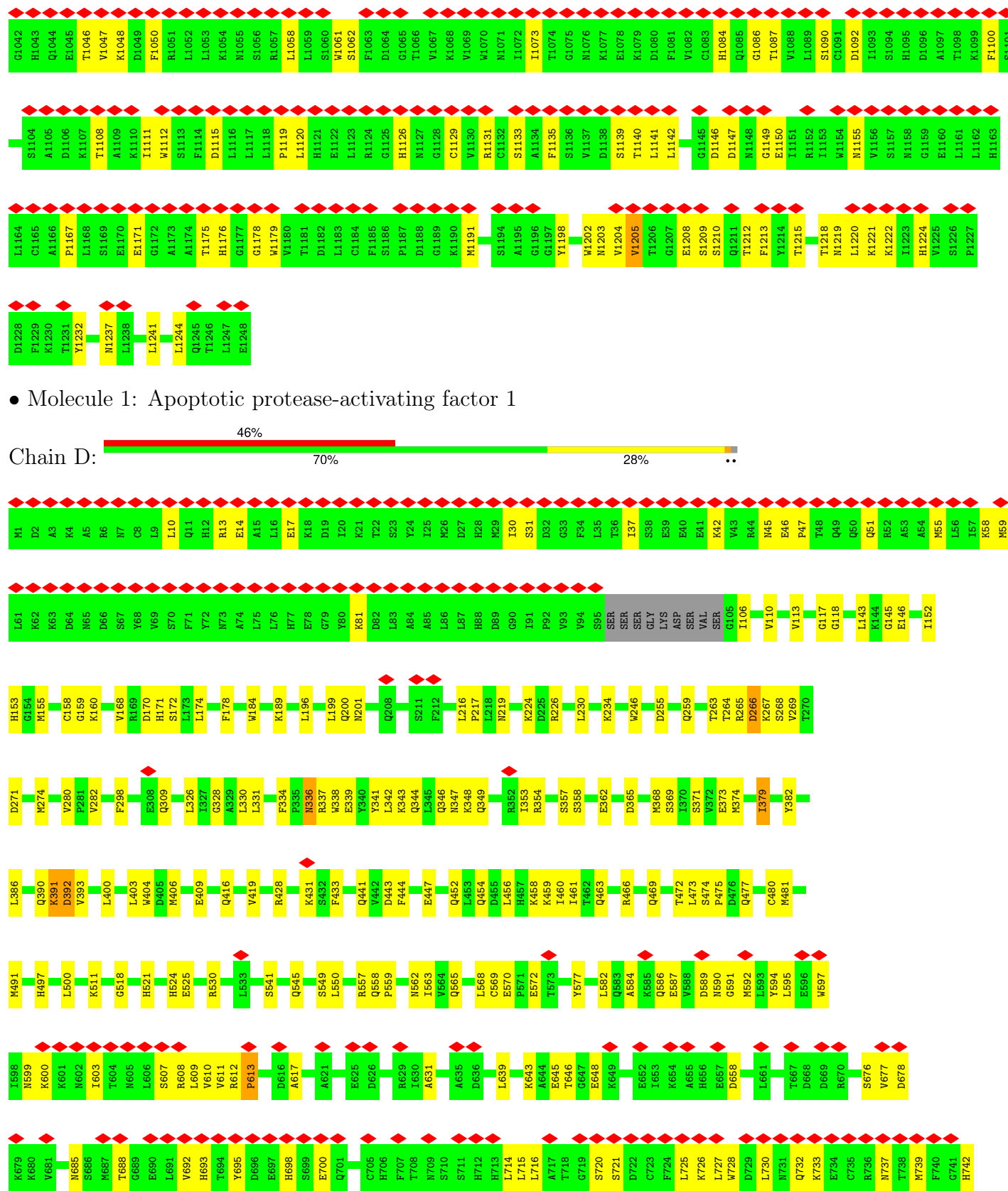
- Molecule 1: Apoptotic protease-activating factor 1

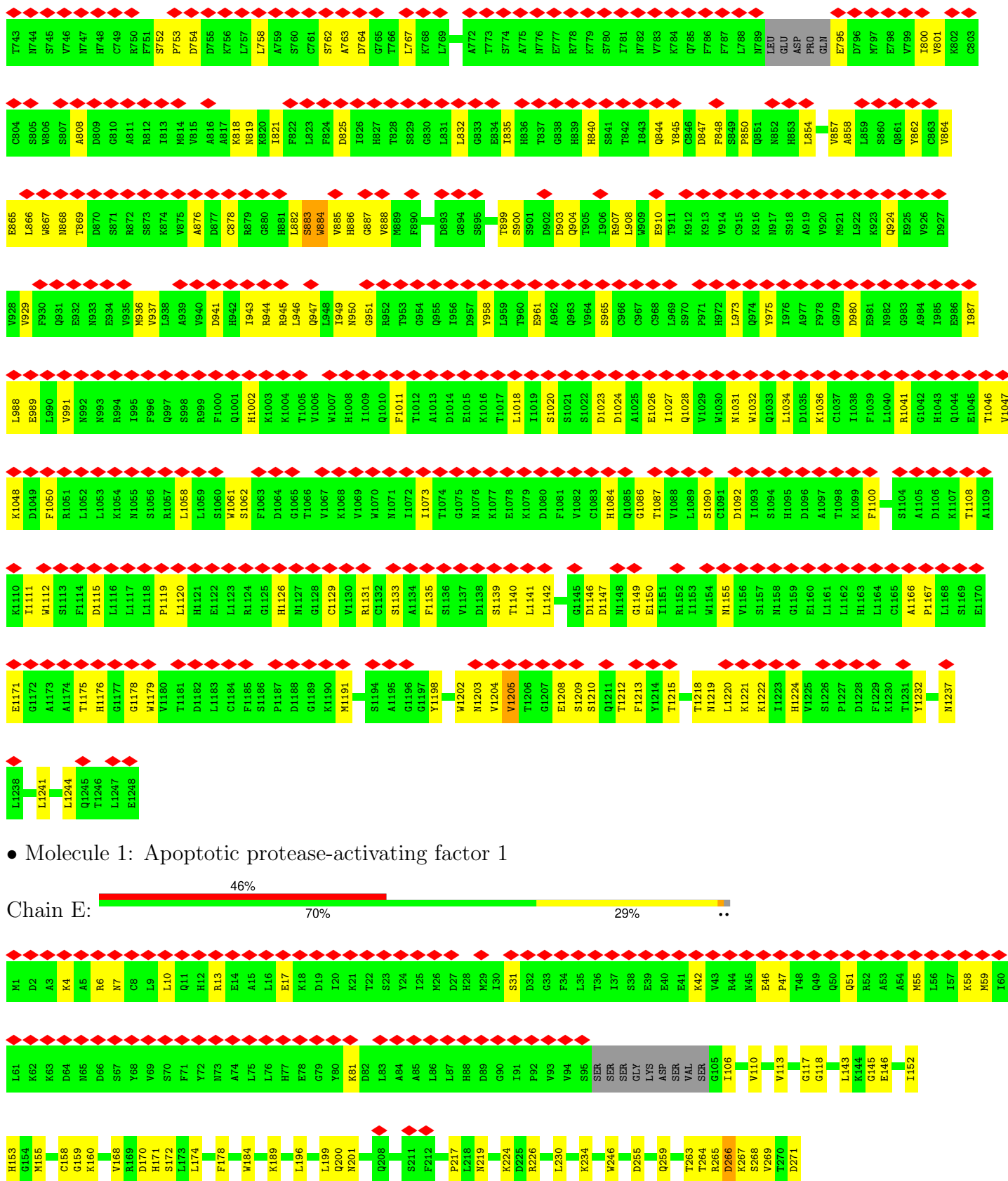


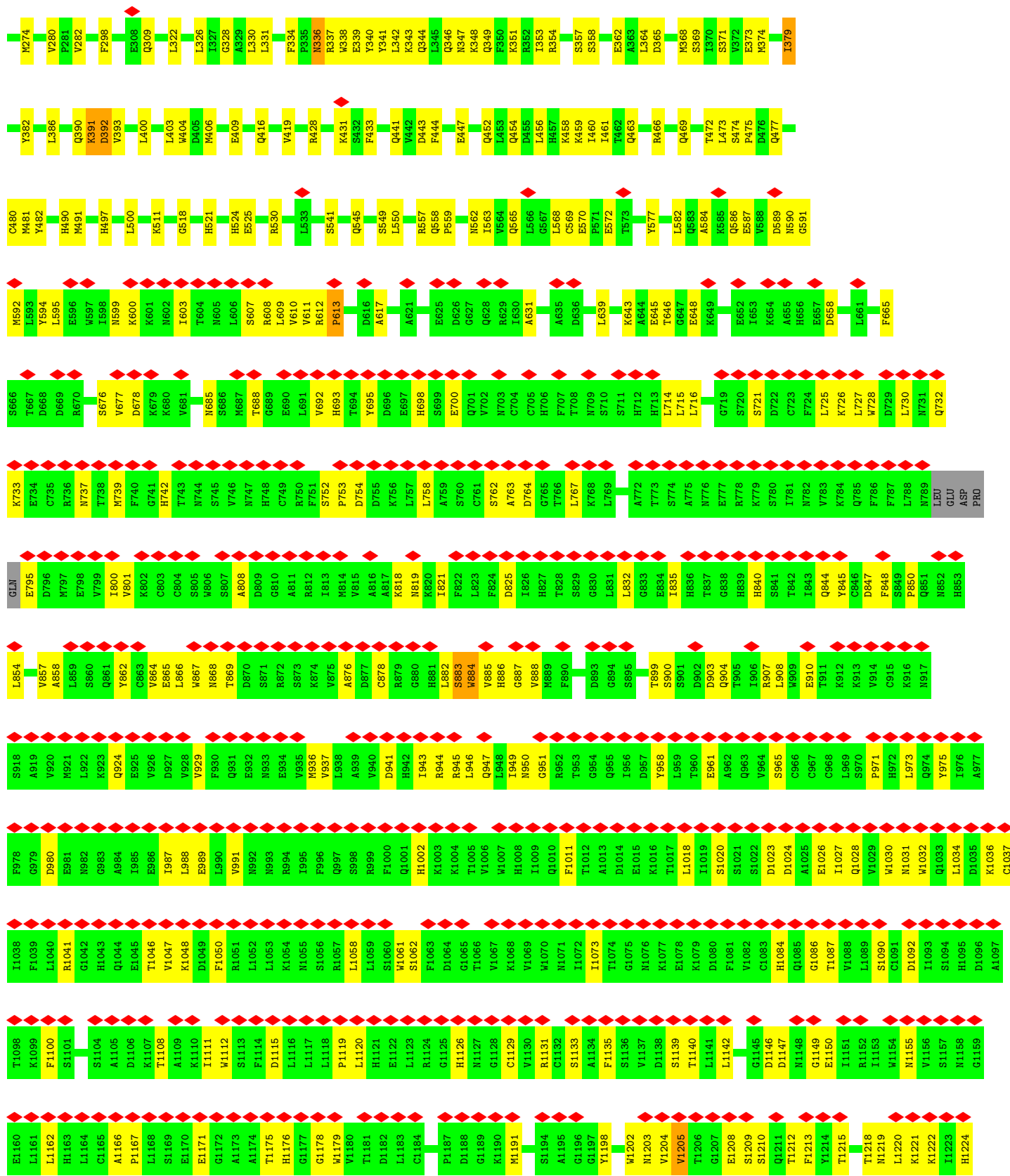




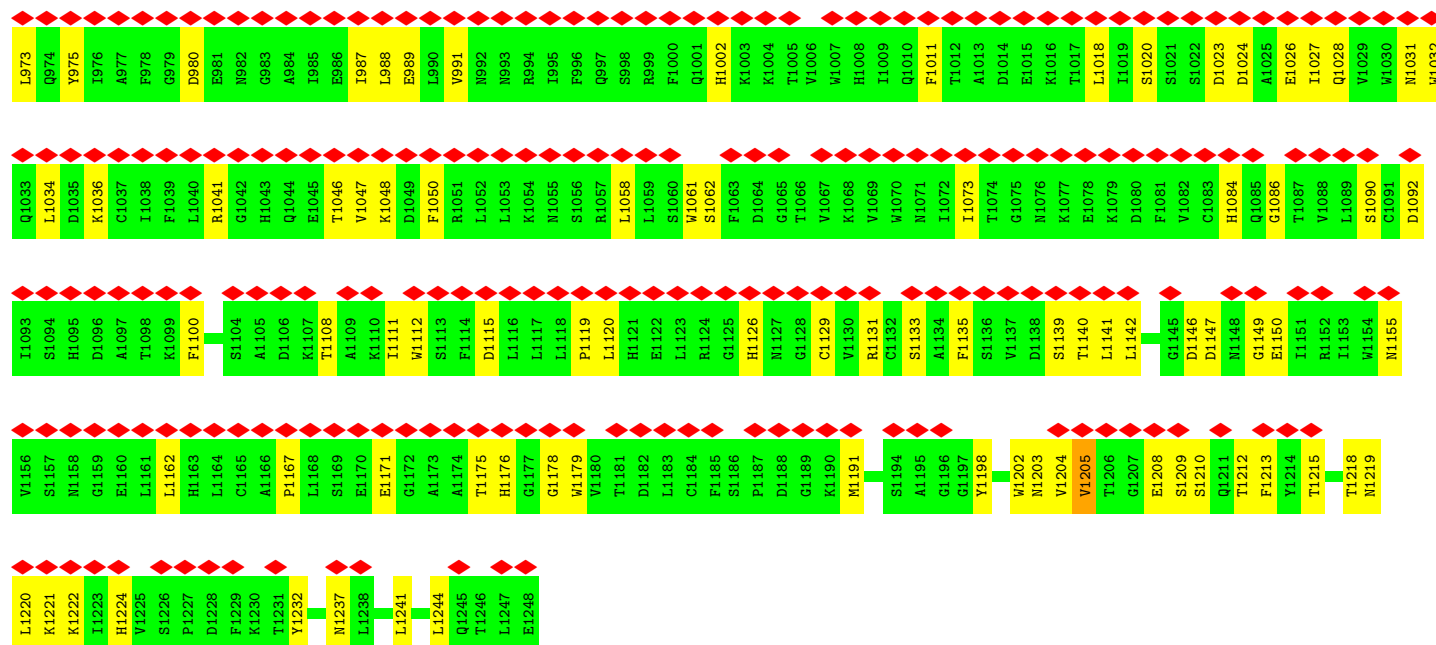
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ASP	LYS	G154	M274	L386	Y482	L594	V677	T738	E798	L859	L922	G983
ALA	ASP	M155	V280	Q390	H490	E596	D678	M739	V799	S860	K923	A984
LYS	ASN	C158	V282	K391	M491	M597	K679	F740	T800	Q861	Q924	L985
ARG	ASP	G159	F298	K392	H497	N599	K680	G741	V801	Y862	E925	E986
ASN	SER	K160	V308	V393	L500	K600	V681	H742	R802	C863	E926	L987
CYS	VAL	V168	F308	L400	L501	K601	N685	T743	C803	V864	V927	L988
LEU	SER	R169	Q309	L403	K511	M602	S686	M744	C804	E865	V928	E989
GLN	PHE	D170	Q309	M406	G518	L603	M687	S745	S805	L866	V929	L990
HIS	TYR	H171	L322	M404	H521	T604	T688	T746	M806	W867	F930	N992
ARG	ASN	S172	L326	E409	E525	M605	G689	M747	S807	N868	Q931	N993
GLU	ALA	L173	L327	E409	H521	L606	T688	H748	A808	T869	E932	N994
ALA	LEU	L174	L327	E409	H521	L606	T688	C749	D809	D870	N933	R994
LEU	LEU	F178	L327	E409	H521	L606	T688	H750	C810	S871	N934	R995
GLY	GLY	W184	L327	E409	H521	L606	T688	F751	A811	R872	N935	F996
LYS	TYR	K189	L327	E409	H521	L606	T688	S752	R812	S873	N936	Q997
ILE	ILE	L196	L327	E409	H521	L606	T688	P753	R813	K874	V937	S998
THR	ASP	L199	L327	E409	H521	L606	T688	D754	M814	V875	V940	S999
SER	LEU	Q200	L327	E409	H521	L606	T688	K755	M815	A876	D941	F1000
GLY	LEU	N201	L327	E409	H521	L606	T688	L757	A817	C878	H942	Q1001
ASP	ALA	Q208	L327	E409	H521	L606	T688	L758	K818	R879	I943	H1002
ILE	ALA	S211	L327	E409	H521	L606	T688	S759	M819	G880	R944	K1003
ASP	LEU	F212	L327	E409	H521	L606	T688	A760	R820	R881	R945	K1004
VAL	LEU	L216	L327	E409	H521	L606	T688	C761	R821	L882	L946	V1005
THR	SER	P217	L327	E409	H521	L606	T688	S762	F822	S883	Q947	V1006
ILE	GLY	N219	L327	E409	H521	L606	T688	A763	L823	W884	I948	V1007
GLY	ASP	K224	L327	E409	H521	L606	T688	D764	F824	V885	I949	H1008
LYS	SER	D225	L327	E409	H521	L606	T688	A765	D825	R886	N950	H1009
VAL	VAL	R226	L327	E409	H521	L606	T688	G766	T826	C887	G951	Q1010
ARG	SER	L230	L327	E409	H521	L606	T688	L767	T828	V888	A952	F1011
ASN	GLU	K234	L327	E409	H521	L606	T688	K768	S829	M889	T953	T1012
GLU	LYS	W246	L327	E409	H521	L606	T688	L769	C830	G890	G954	A1013
PRO	VAL	D255	L327	E409	H521	L606	T688	A770	L831	D893	Q955	I0104
GLN	GLN	Q259	L327	E409	H521	L606	T688	S771	L832	E894	D957	E1015
ALA	ALA	T263	L327	E409	H521	L606	T688	H713	E834	S895	Y958	K1016
ALA	ALA	T264	L327	E409	H521	L606	T688	L714	R835	T899	L960	T1017
MET	LEU	R265	L327	E409	H521	L606	T688	L715	R836	S901	E961	L1018
ILE	ILE	D266	L327	E409	H521	L606	T688	L716	T837	D902	A962	I1019
MET	LYS	E146	L327	E409	H521	L606	T688	L717	C838	Q903	Q963	S1020
LYS	VAL	S268	L327	E409	H521	L606	T688	A776	H839	Q904	V964	S1022
V269		T270	L327	E409	H521	L606	T688	S777	S840	T905	S965	D1023
ILE			L327	E409	H521	L606	T688	A778	R841	I906	C966	D1024
			L327	E409	H521	L606	T688	S779	T842	R907	C967	A1025
			L327	E409	H521	L606	T688	A779	R843	L908	C968	I0206
			L327	E409	H521	L606	T688	S780	T844	W909	C969	I1027
			L327	E409	H521	L606	T688	T781	L725	E910	S970	Q1028
			L327	E409	H521	L606	T688	T782	K726	T911	P971	V1029
			L327	E409	H521	L606	T688	V783	K727	K912	H972	W1030
			L327	E409	H521	L606	T688	A784	L727	R913	L973	N1031
			L327	E409	H521	L606	T688	S785	T728	C915	Q974	W1032
			L327	E409	H521	L606	T688	S786	T729	P850	Y975	L1034
			L327	E409	H521	L606	T688	L787	T730	Q851	I976	D1035
			L327	E409	H521	L606	T688	L788	D668	M852	A977	I0306
			L327	E409	H521	L606	T688	L789	D669	L854	F978	K1036
			L327	E409	H521	L606	T688	Q732	R670	V857	G979	C1037
			L327	E409	H521	L606	T688	K733			D980	I1038
			L327	E409	H521	L606	T688	E734			E981	F1039
			L327	E409	H521	L606	T688	C735				L1040
			L327	E409	H521	L606	T688	R736				R1041



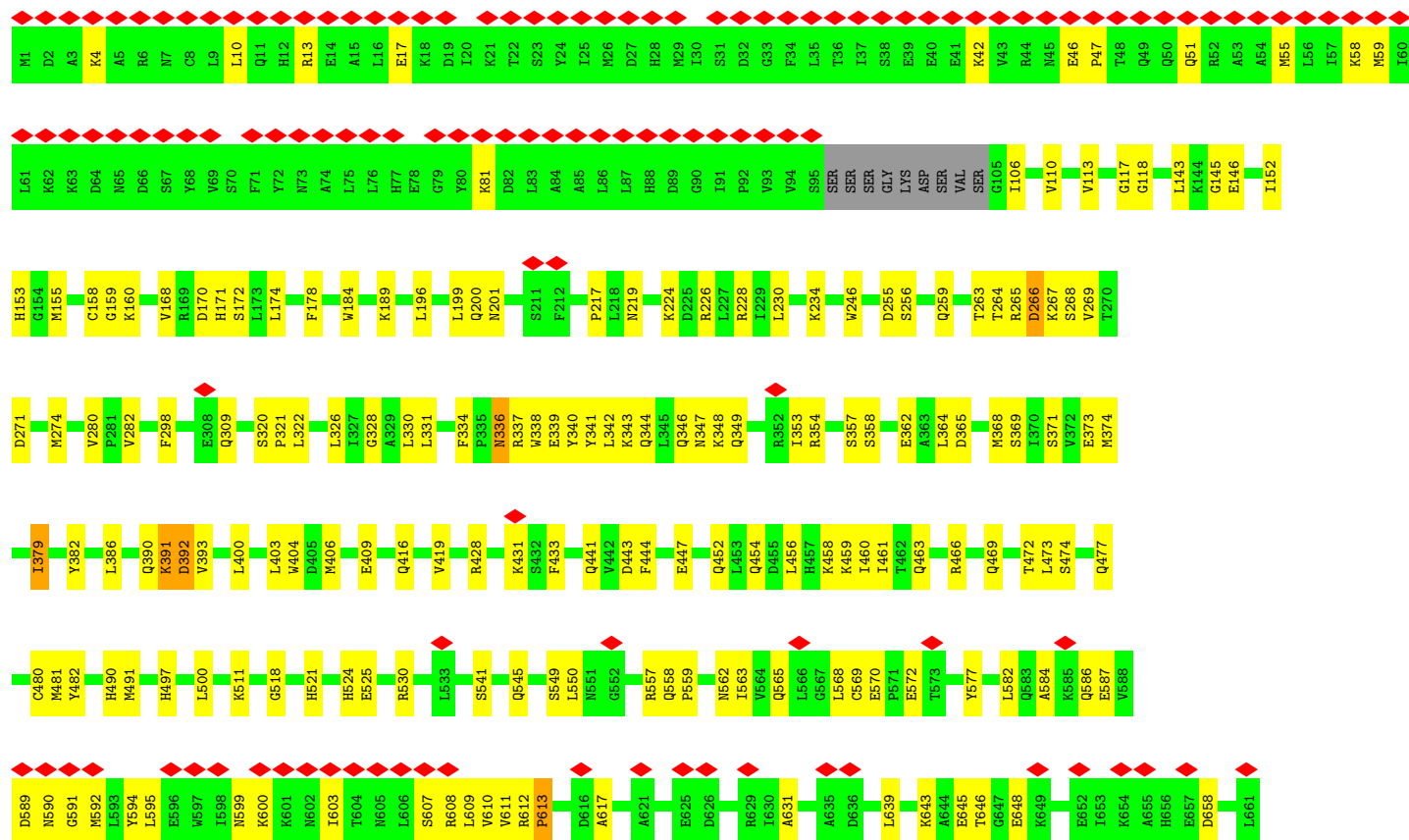


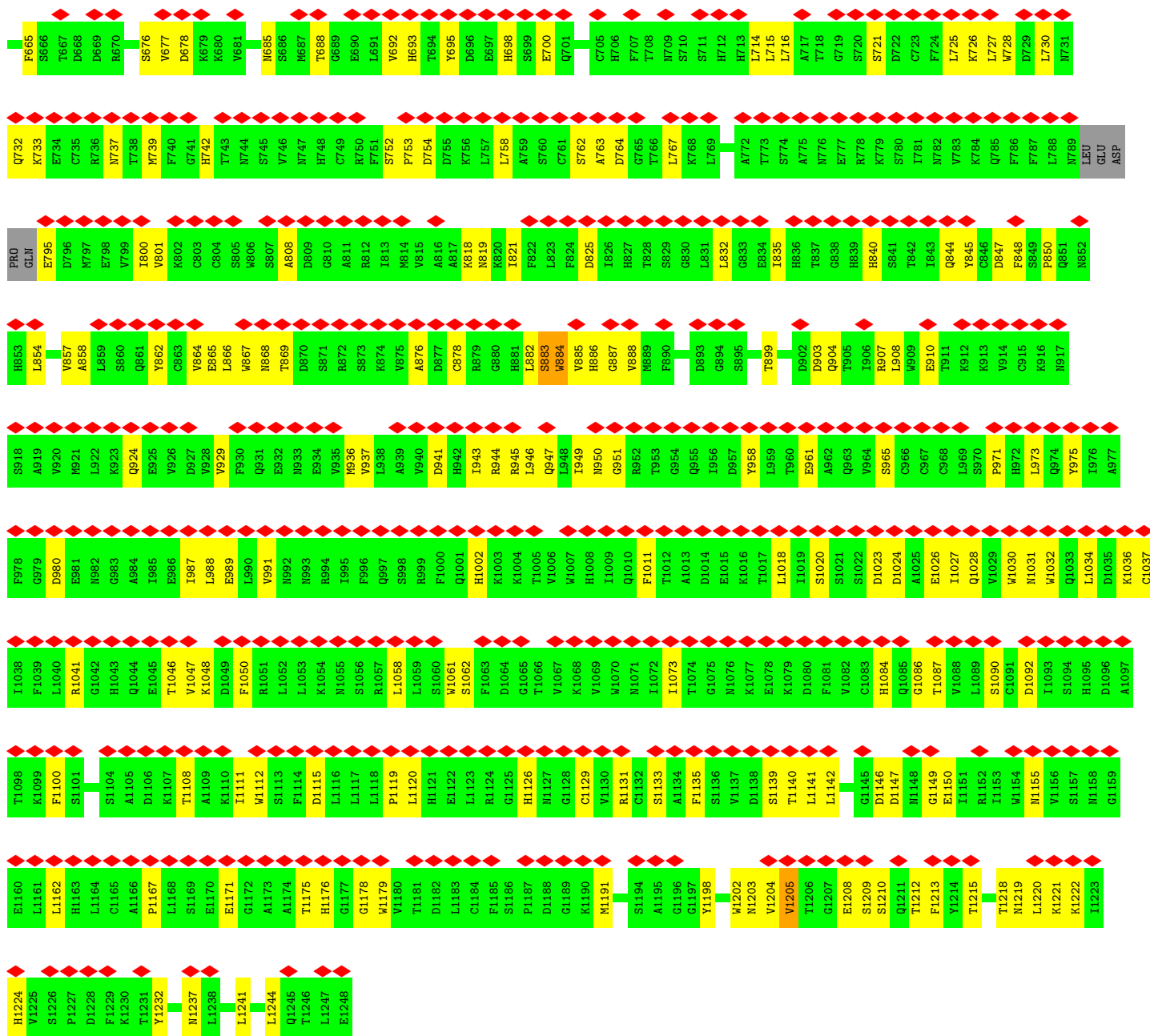




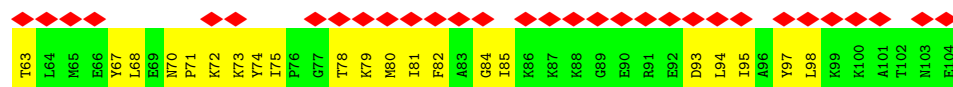
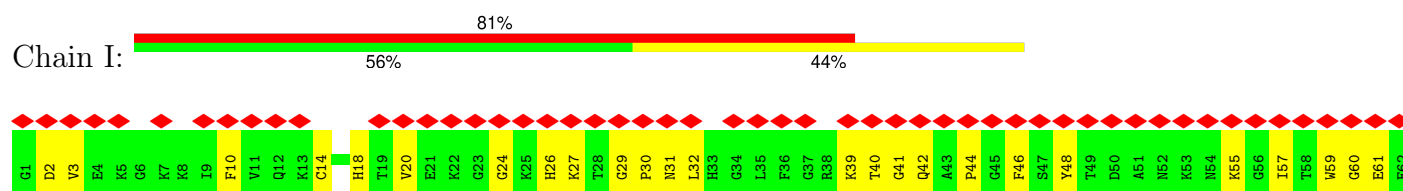


• Molecule 1: Apoptotic protease-activating factor 1

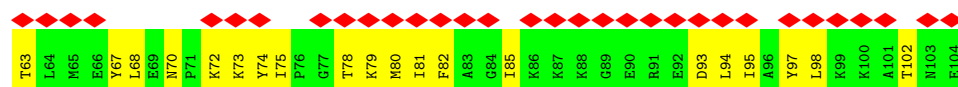
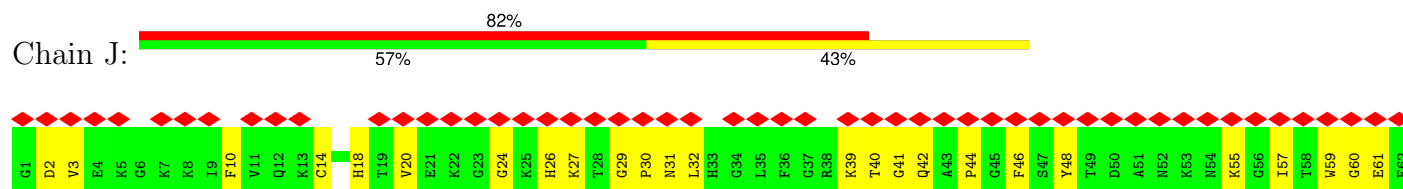




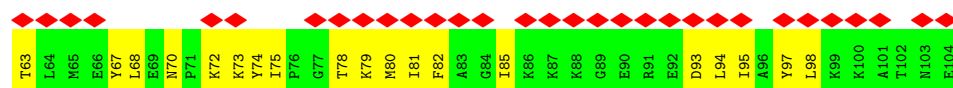
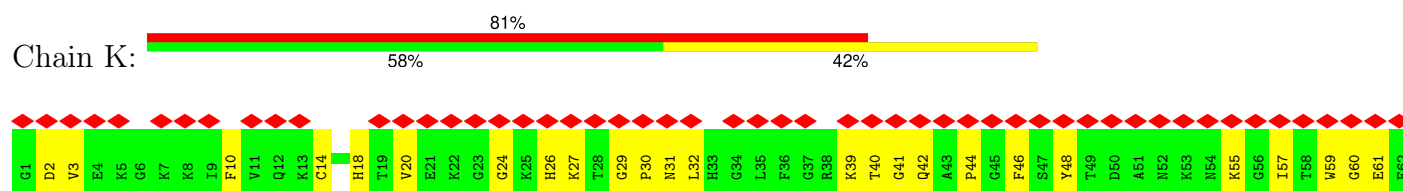
• Molecule 2: Cytochrome c



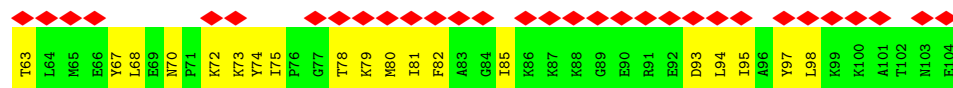
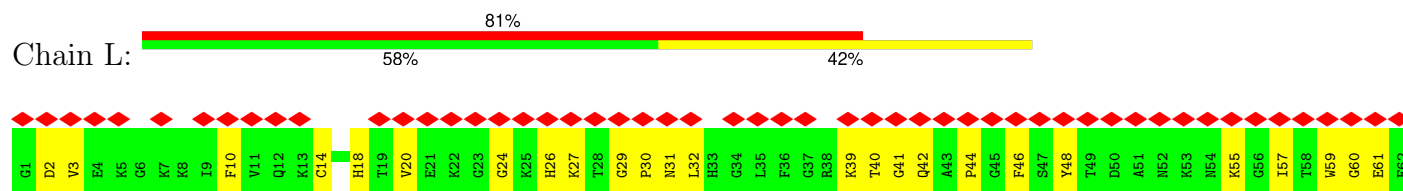
• Molecule 2: Cytochrome c



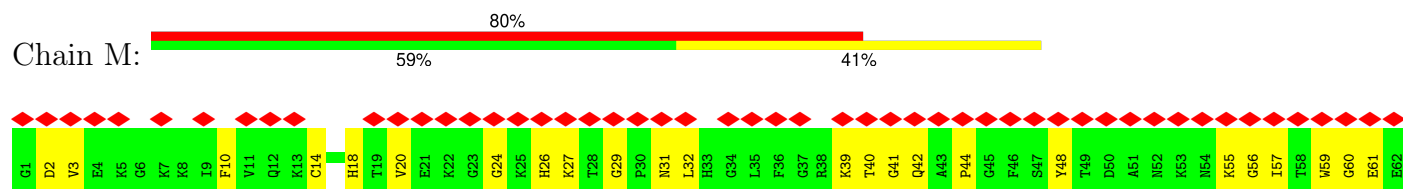
• Molecule 2: Cytochrome c

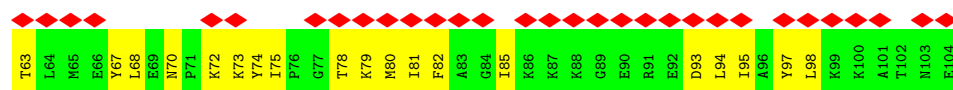


• Molecule 2: Cytochrome c

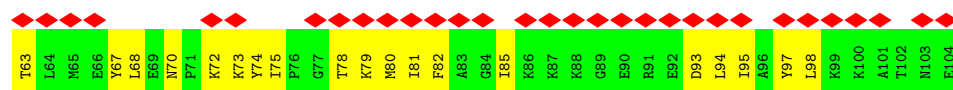
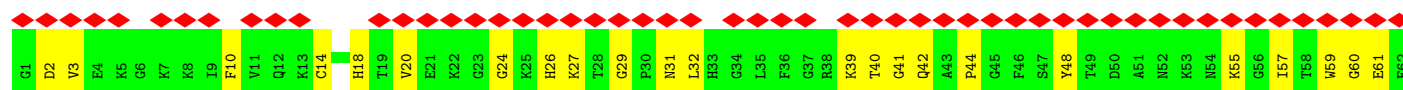
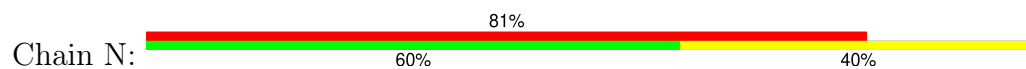


• Molecule 2: Cytochrome c

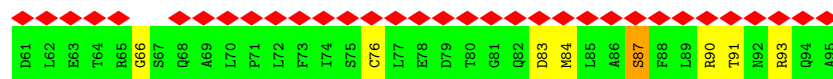
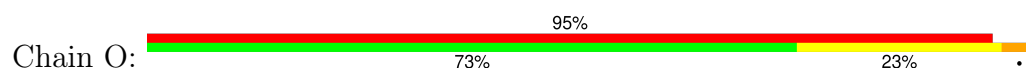




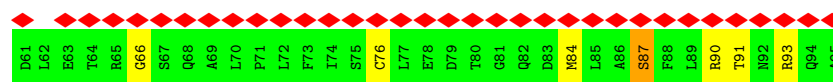
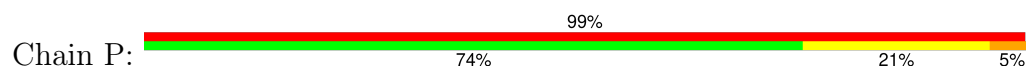
• Molecule 2: Cytochrome c



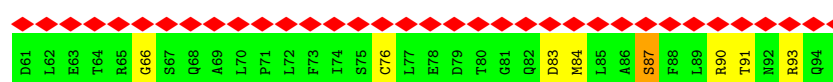
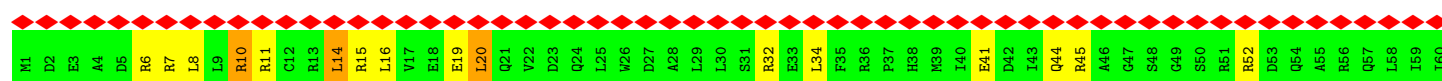
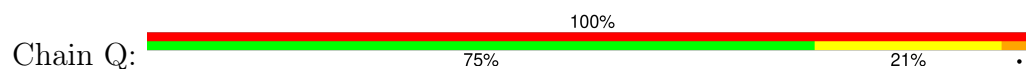
• Molecule 3: Caspase-9



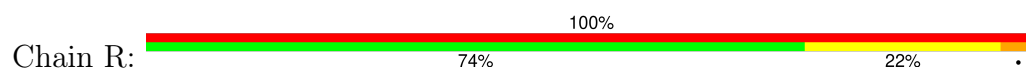
• Molecule 3: Caspase-9



• Molecule 3: Caspase-9



• Molecule 3: Caspase-9





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 (Å)	437.76, 437.76, 437.76	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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	0.42	1/9295 (0.0%)	0.80	14/12575 (0.1%)
1	B	0.49	1/10068 (0.0%)	0.80	14/13613 (0.1%)
1	C	0.42	1/9295 (0.0%)	0.80	14/12575 (0.1%)
1	D	0.48	1/10068 (0.0%)	0.80	14/13613 (0.1%)
1	E	0.49	1/10068 (0.0%)	0.80	14/13613 (0.1%)
1	F	0.42	1/9295 (0.0%)	0.80	14/12575 (0.1%)
1	G	0.49	1/10068 (0.0%)	0.80	14/13613 (0.1%)
2	H	0.31	0/830	0.73	0/1105
2	I	0.31	0/830	0.73	0/1105
2	J	0.31	0/830	0.73	0/1105
2	K	0.31	0/830	0.73	0/1105
2	L	0.31	0/830	0.73	0/1105
2	M	0.31	0/830	0.73	0/1105
2	N	0.31	0/830	0.73	0/1105
3	O	0.87	0/784	0.88	2/1051 (0.2%)
3	P	0.87	0/784	0.88	2/1051 (0.2%)
3	Q	0.87	0/784	0.88	1/1051 (0.1%)
3	R	0.87	0/784	0.88	2/1051 (0.2%)
All	All	0.47	7/77103 (0.0%)	0.80	105/104116 (0.1%)

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	11.07	1.50	1.33
1	B	168	VAL	C-N	11.04	1.50	1.33
1	A	168	VAL	C-N	11.04	1.50	1.33
1	E	168	VAL	C-N	11.04	1.50	1.33
1	D	168	VAL	C-N	11.02	1.50	1.33

The worst 5 of 105 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	178	PHE	CA-C-N	-8.62	112.95	121.65
1	G	178	PHE	C-N-CA	-8.62	112.95	121.65
1	E	178	PHE	CA-C-N	-8.60	112.97	121.65
1	E	178	PHE	C-N-CA	-8.60	112.97	121.65
1	B	178	PHE	CA-C-N	-8.58	112.98	121.65

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

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	309	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	9861	0	9736	317	0
1	C	9099	0	8968	306	0
1	D	9861	0	9736	324	0
1	E	9861	0	9736	329	0
1	F	9099	0	8968	317	0
1	G	9861	0	9736	319	0
2	H	814	0	833	58	0
2	I	814	0	833	58	0
2	J	814	0	833	59	0
2	K	814	0	833	56	0
2	L	814	0	833	57	0
2	M	814	0	833	58	0
2	N	814	0	833	55	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	2	0
5	I	43	0	32	2	0
5	J	43	0	32	2	0
5	K	43	0	32	2	0
5	L	43	0	32	2	0
5	M	43	0	32	2	0
5	N	43	0	32	2	0
All	All	76058	0	75112	2427	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 16.

The worst 5 of 2427 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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 [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1135/1248 (91%)	1045 (92%)	84 (7%)	6 (0%)	24	61
1	B	1228/1248 (98%)	1138 (93%)	84 (7%)	6 (0%)	24	61
1	C	1135/1248 (91%)	1045 (92%)	84 (7%)	6 (0%)	24	61
1	D	1228/1248 (98%)	1138 (93%)	84 (7%)	6 (0%)	24	61
1	E	1228/1248 (98%)	1138 (93%)	84 (7%)	6 (0%)	24	61
1	F	1135/1248 (91%)	1045 (92%)	84 (7%)	6 (0%)	24	61
1	G	1228/1248 (98%)	1138 (93%)	84 (7%)	6 (0%)	24	61
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	R	93/95 (98%)	92 (99%)	1 (1%)	0	100	100
All	All	9403/9844 (96%)	8741 (93%)	620 (7%)	42 (0%)	31	65

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
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%)	86	85
1	B	1106/1119 (99%)	1101 (100%)	5 (0%)	81	82
1	C	1022/1119 (91%)	1019 (100%)	3 (0%)	86	85
1	D	1106/1119 (99%)	1101 (100%)	5 (0%)	81	82
1	E	1106/1119 (99%)	1101 (100%)	5 (0%)	81	82
1	F	1022/1119 (91%)	1019 (100%)	3 (0%)	86	85
1	G	1106/1119 (99%)	1101 (100%)	5 (0%)	81	82
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%)	76 (90%)	8 (10%)	8	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	P	84/84 (100%)	77 (92%)	7 (8%)	10	32
3	Q	84/84 (100%)	76 (90%)	8 (10%)	8	27
3	R	84/84 (100%)	76 (90%)	8 (10%)	8	27
All	All	8414/8757 (96%)	8354 (99%)	60 (1%)	73	79

5 of 60 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	884	TRP
3	R	34	LEU
3	O	87	SER
3	R	20	LEU
3	R	93	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 196 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	785	GLN
1	F	827	HIS
1	E	844	GLN
1	F	469	GLN
1	F	1076	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	L	500	2	50,50,50	1.91	9 (18%)	68,82,82	1.54	5 (7%)
4	DTP	A	1301	-	31,32,32	3.51	12 (38%)	46,50,50	2.02	11 (23%)
4	DTP	F	1301	-	31,32,32	3.51	12 (38%)	46,50,50	2.02	11 (23%)
5	HEC	M	500	2	50,50,50	1.91	9 (18%)	68,82,82	1.54	5 (7%)
4	DTP	B	1301	-	31,32,32	3.50	12 (38%)	46,50,50	2.02	11 (23%)
5	HEC	I	500	2	50,50,50	1.91	9 (18%)	68,82,82	1.55	5 (7%)
4	DTP	G	1301	-	31,32,32	3.51	12 (38%)	46,50,50	2.02	11 (23%)
5	HEC	J	500	2	50,50,50	1.91	9 (18%)	68,82,82	1.54	5 (7%)
5	HEC	K	500	2	50,50,50	1.91	9 (18%)	68,82,82	1.55	5 (7%)
4	DTP	D	1301	-	31,32,32	3.52	12 (38%)	46,50,50	2.02	11 (23%)
4	DTP	C	1301	-	31,32,32	3.51	12 (38%)	46,50,50	2.02	11 (23%)
5	HEC	N	500	2	50,50,50	1.91	9 (18%)	68,82,82	1.54	5 (7%)
5	HEC	H	500	2	50,50,50	1.91	9 (18%)	68,82,82	1.53	5 (7%)
4	DTP	E	1301	-	31,32,32	3.51	12 (38%)	46,50,50	2.03	11 (23%)

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	L	500	2	-	5/14/54/54	-
4	DTP	A	1301	-	-	8/22/34/34	0/3/3/3
4	DTP	F	1301	-	-	8/22/34/34	0/3/3/3
5	HEC	M	500	2	-	5/14/54/54	-
4	DTP	B	1301	-	-	8/22/34/34	0/3/3/3
5	HEC	I	500	2	-	5/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	DTP	G	1301	-	-	8/22/34/34	0/3/3/3
5	HEC	J	500	2	-	5/14/54/54	-
5	HEC	K	500	2	-	5/14/54/54	-
4	DTP	D	1301	-	-	8/22/34/34	0/3/3/3
4	DTP	C	1301	-	-	8/22/34/34	0/3/3/3
5	HEC	N	500	2	-	5/14/54/54	-
5	HEC	H	500	2	-	5/14/54/54	-
4	DTP	E	1301	-	-	8/22/34/34	0/3/3/3

The worst 5 of 147 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 112 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1301	DTP	N3-C2-N1	-5.67	120.00	128.58
4	G	1301	DTP	N3-C2-N1	-5.67	120.01	128.58
4	E	1301	DTP	N3-C2-N1	-5.66	120.01	128.58
4	C	1301	DTP	N3-C2-N1	-5.64	120.04	128.58
4	A	1301	DTP	N3-C2-N1	-5.64	120.04	128.58

There are no chirality outliers.

5 of 91 torsion outliers are listed below:

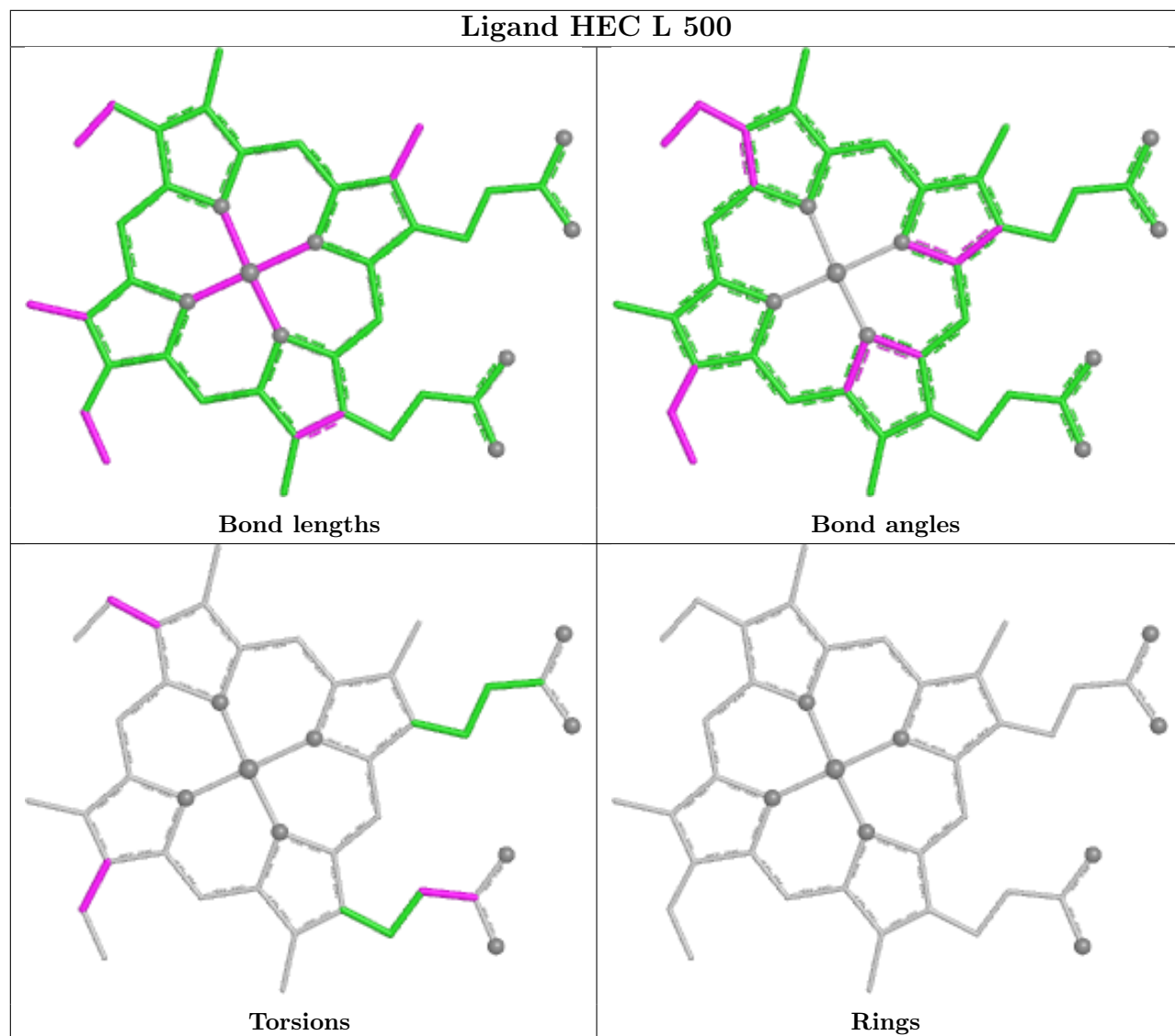
Mol	Chain	Res	Type	Atoms
4	A	1301	DTP	C5'-O5'-PA-O1A
4	A	1301	DTP	C5'-O5'-PA-O2A
4	A	1301	DTP	C5'-O5'-PA-O3A
4	A	1301	DTP	O4'-C4'-C5'-O5'
4	B	1301	DTP	C5'-O5'-PA-O1A

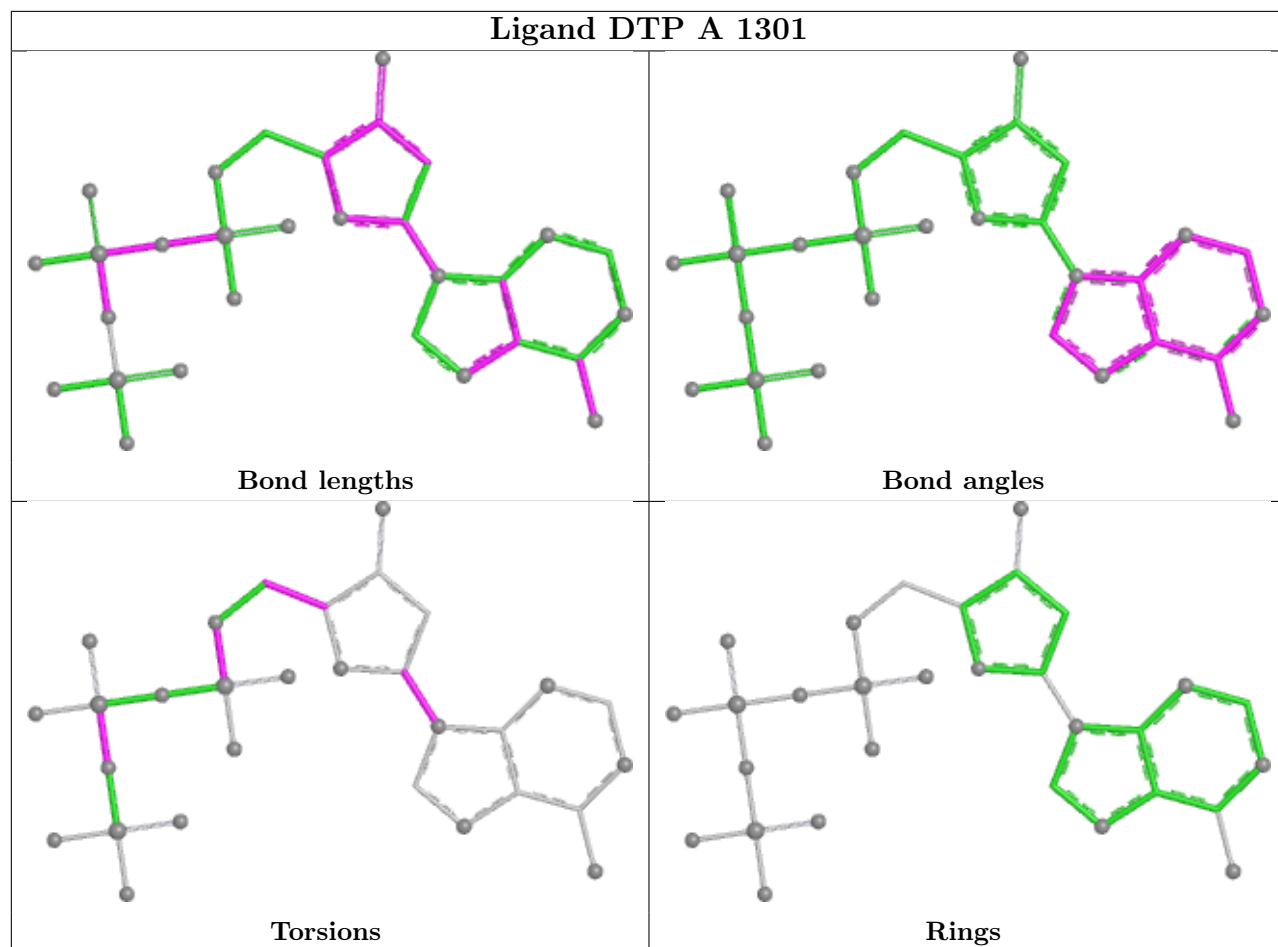
There are no ring outliers.

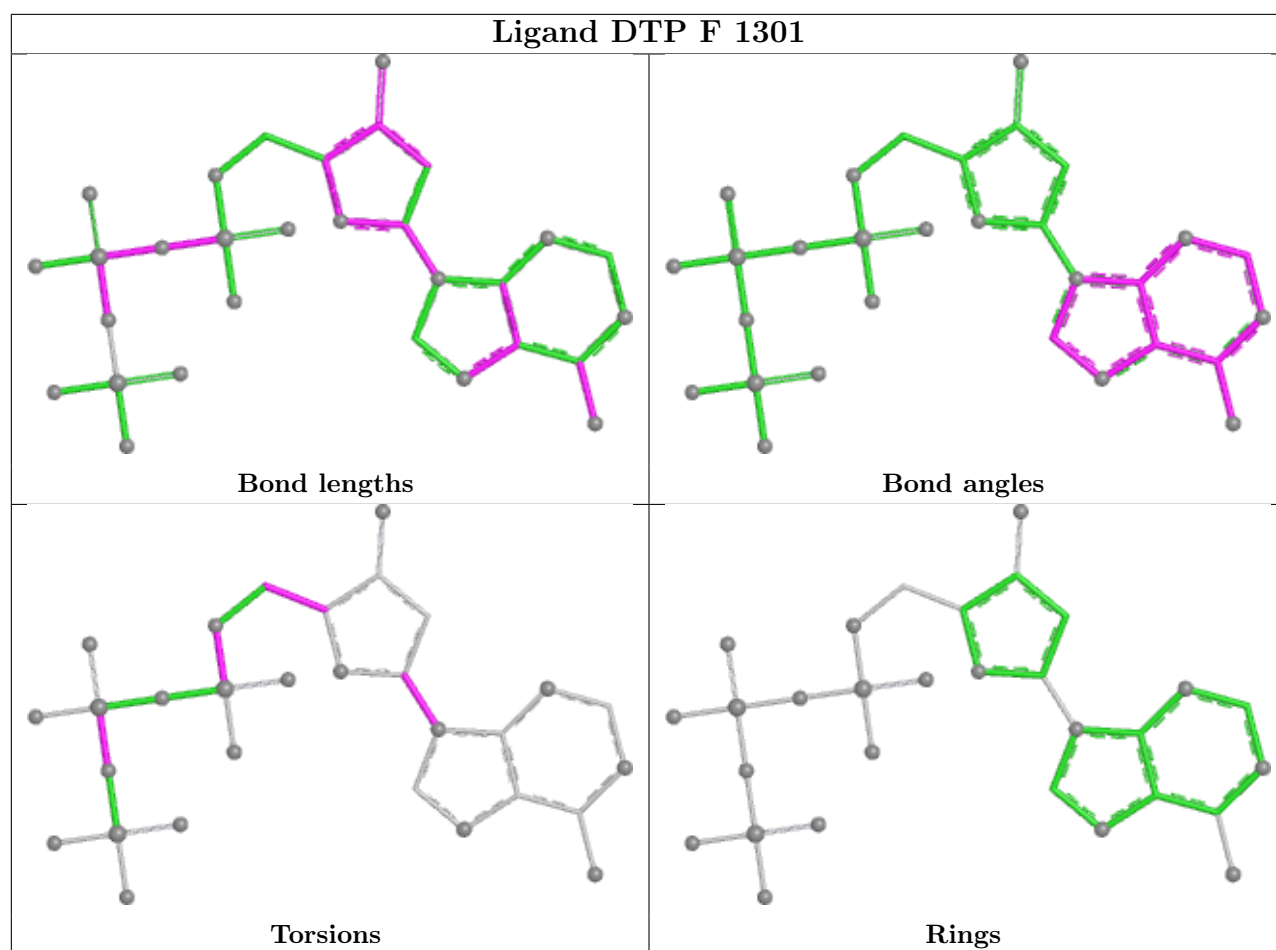
14 monomers are involved in 35 short contacts:

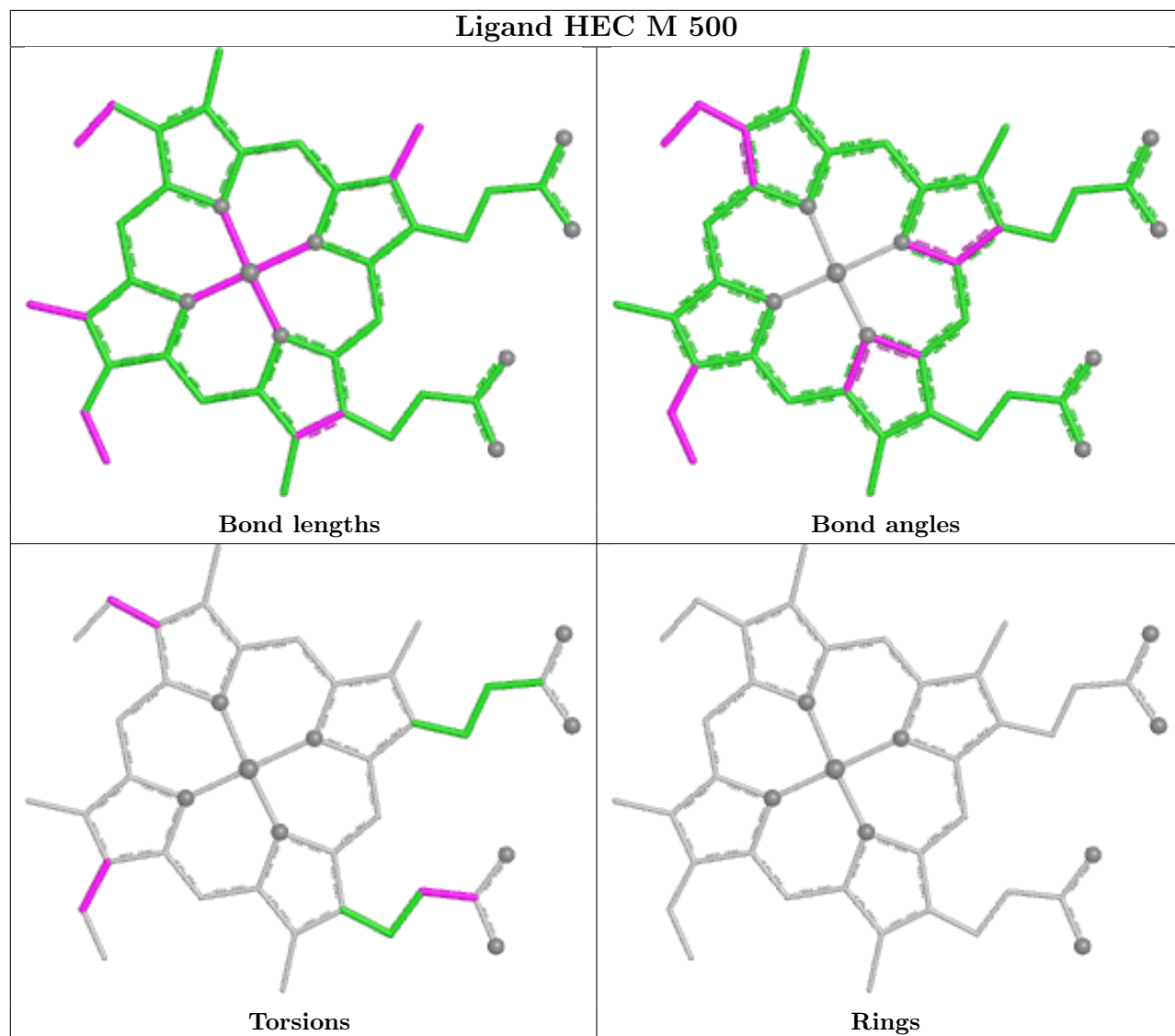
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	L	500	HEC	2	0
4	A	1301	DTP	3	0
4	F	1301	DTP	3	0
5	M	500	HEC	2	0
4	B	1301	DTP	3	0
5	I	500	HEC	2	0
4	G	1301	DTP	3	0
5	J	500	HEC	2	0
5	K	500	HEC	2	0
4	D	1301	DTP	3	0
4	C	1301	DTP	3	0
5	N	500	HEC	2	0
5	H	500	HEC	2	0
4	E	1301	DTP	3	0

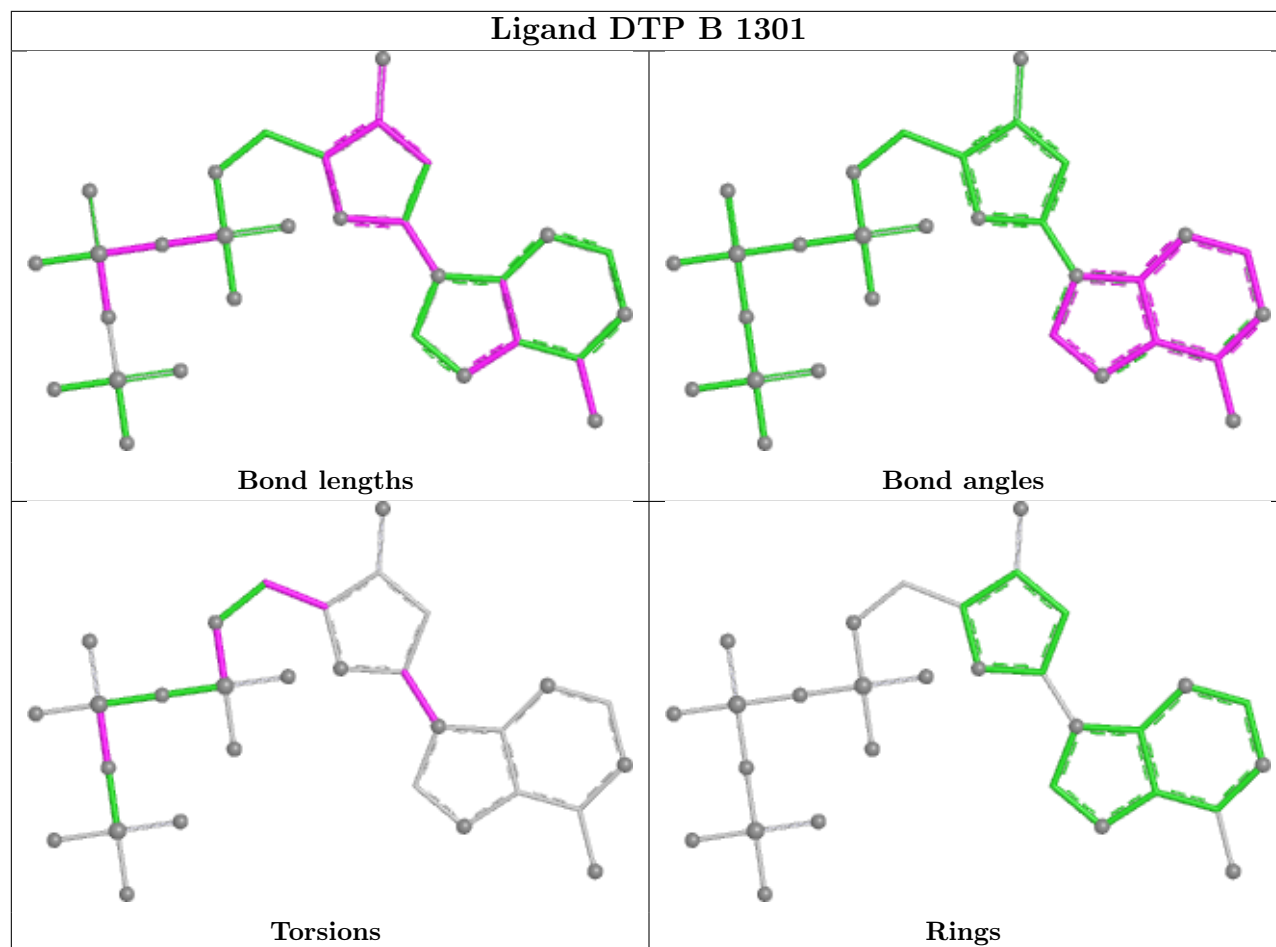
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



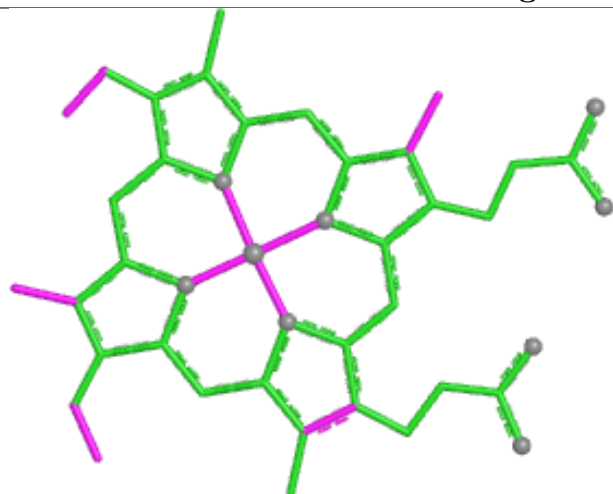




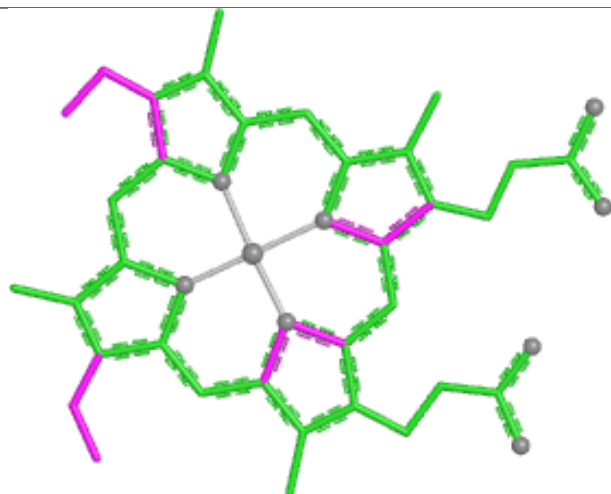




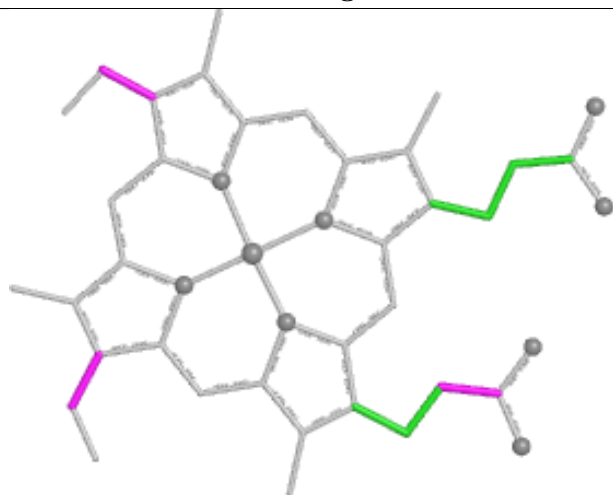
Ligand HEC I 500



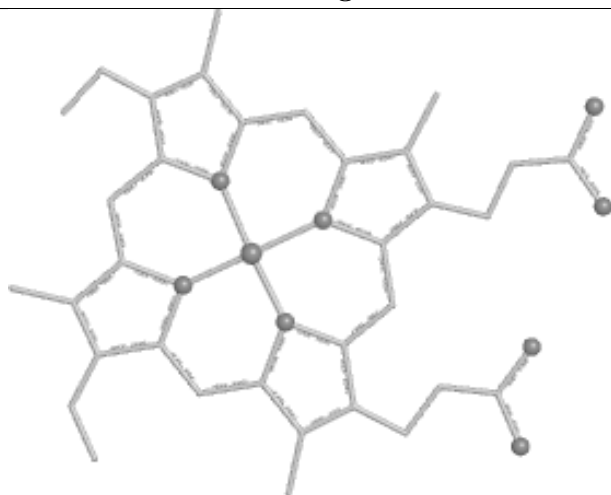
Bond lengths



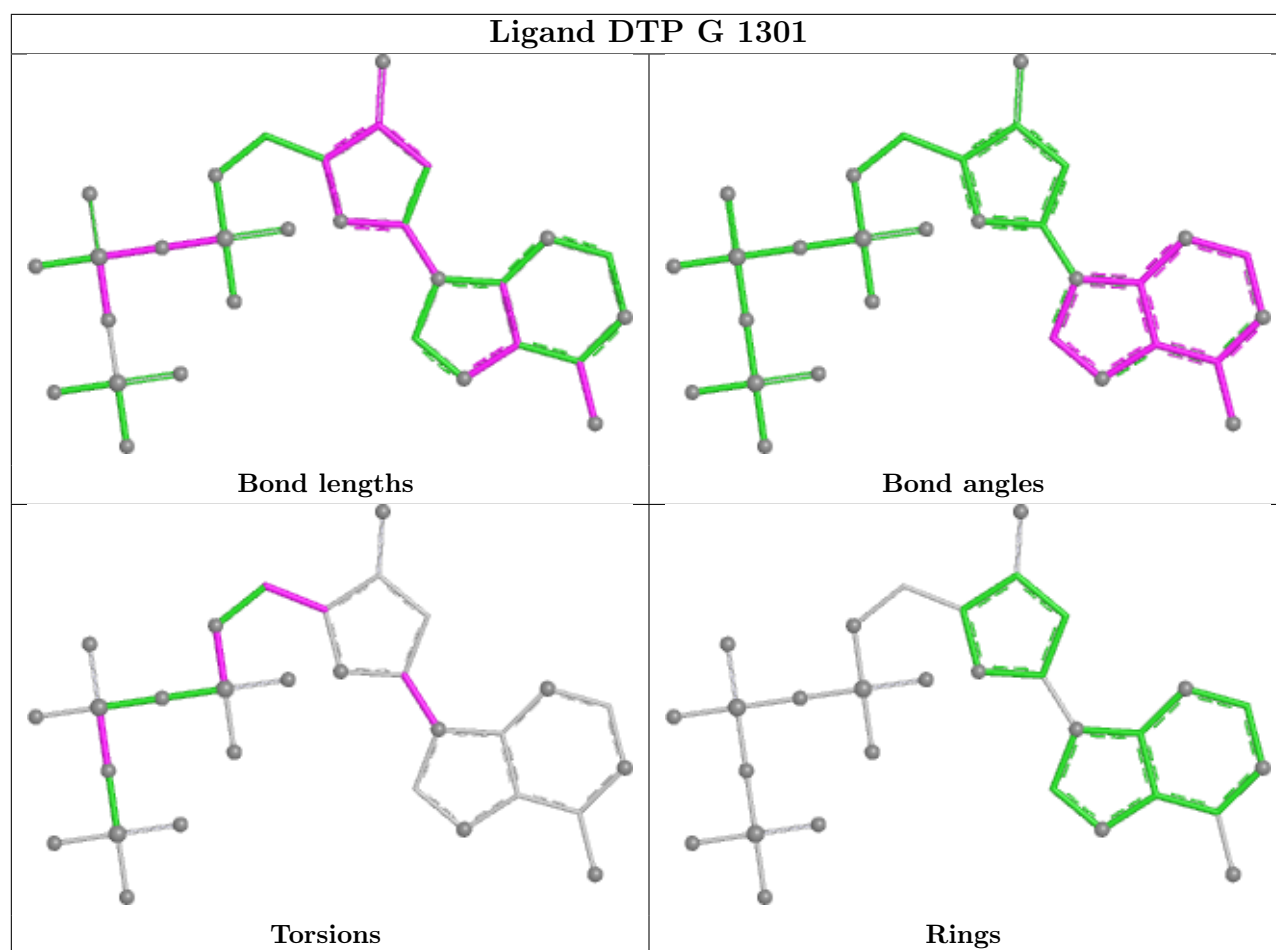
Bond angles



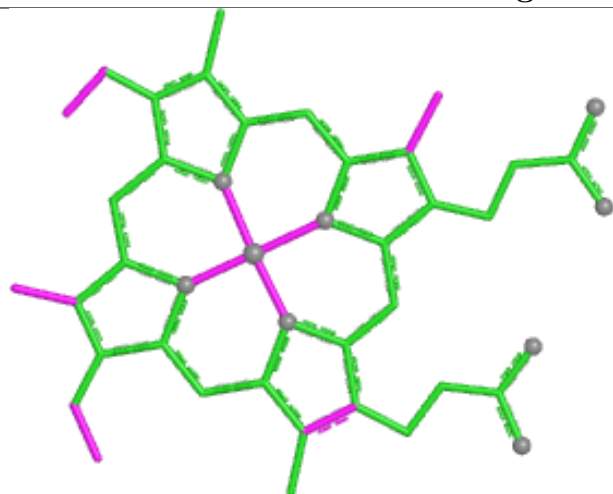
Torsions



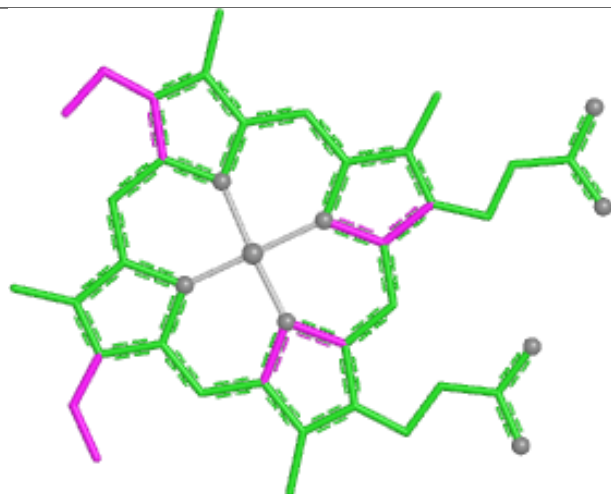
Rings



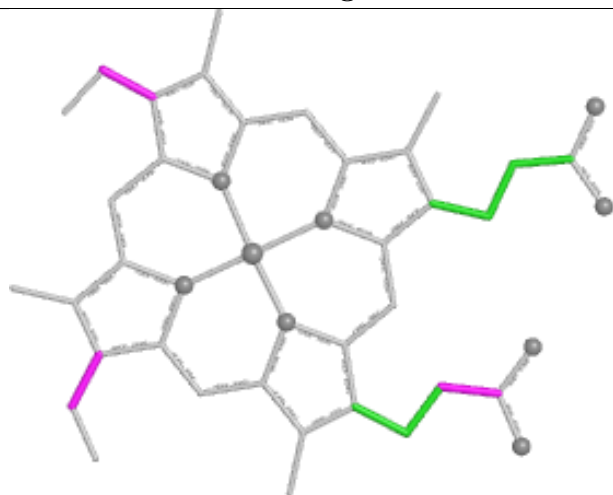
Ligand HEC J 500



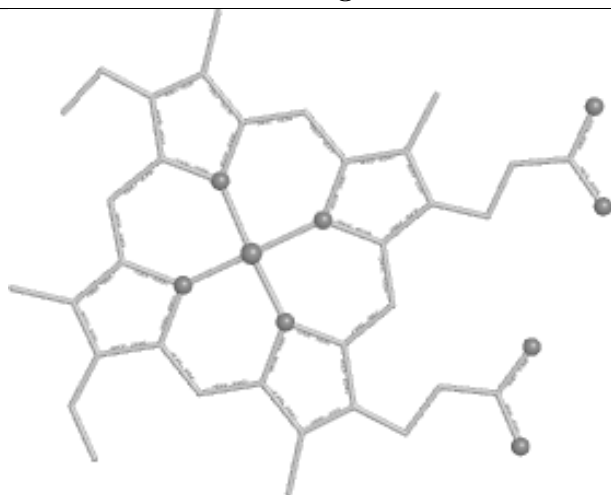
Bond lengths



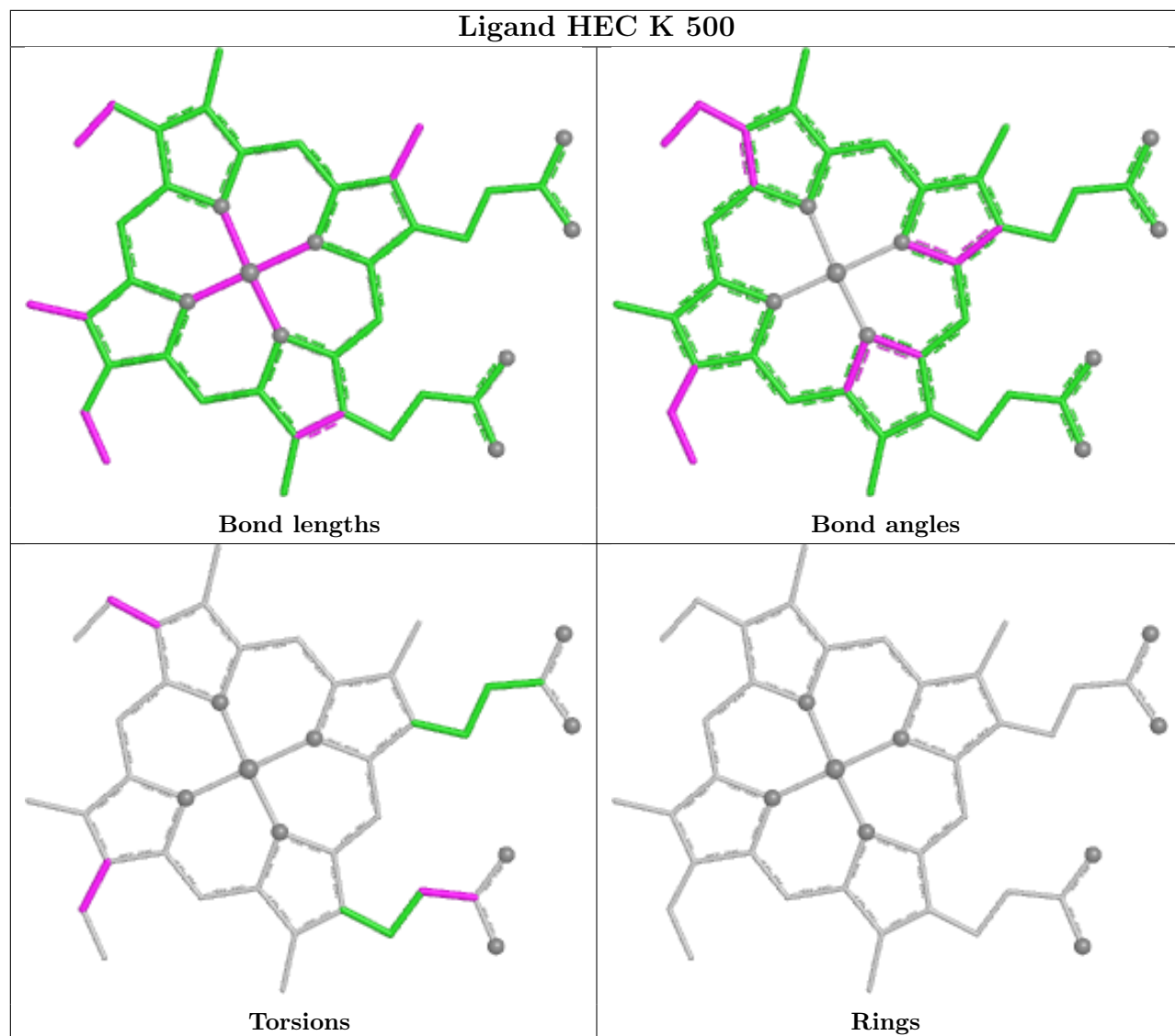
Bond angles

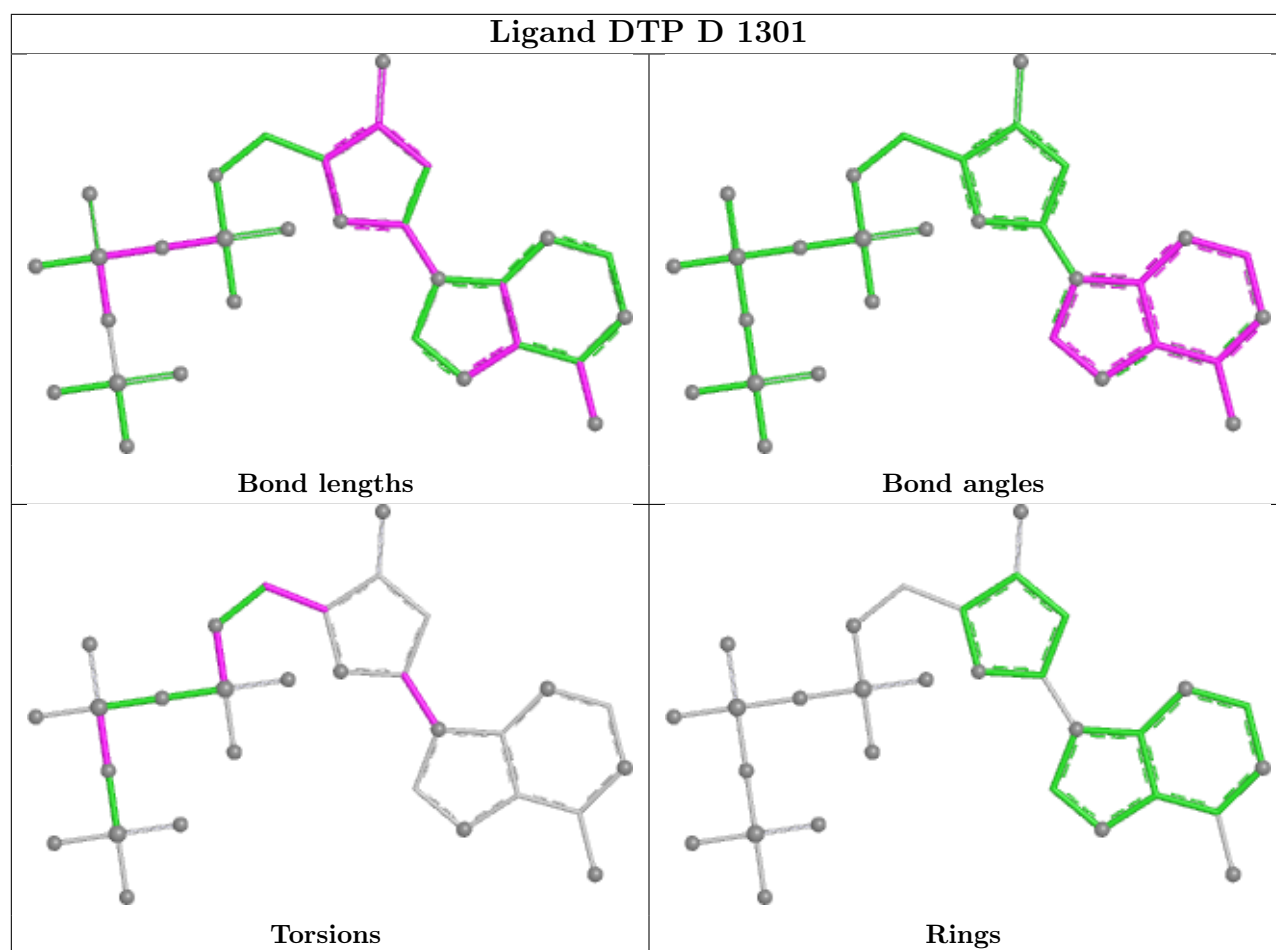


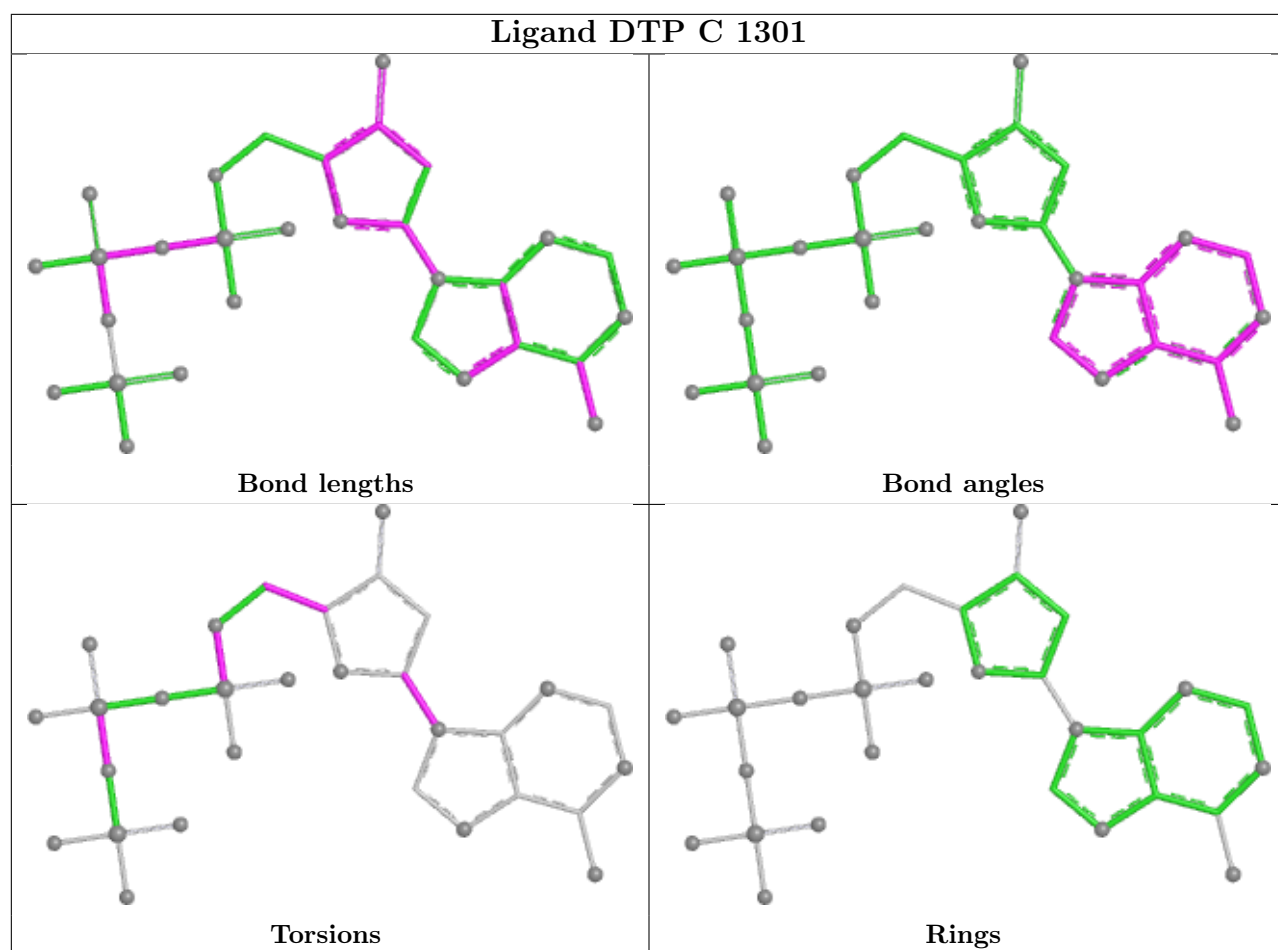
Torsions

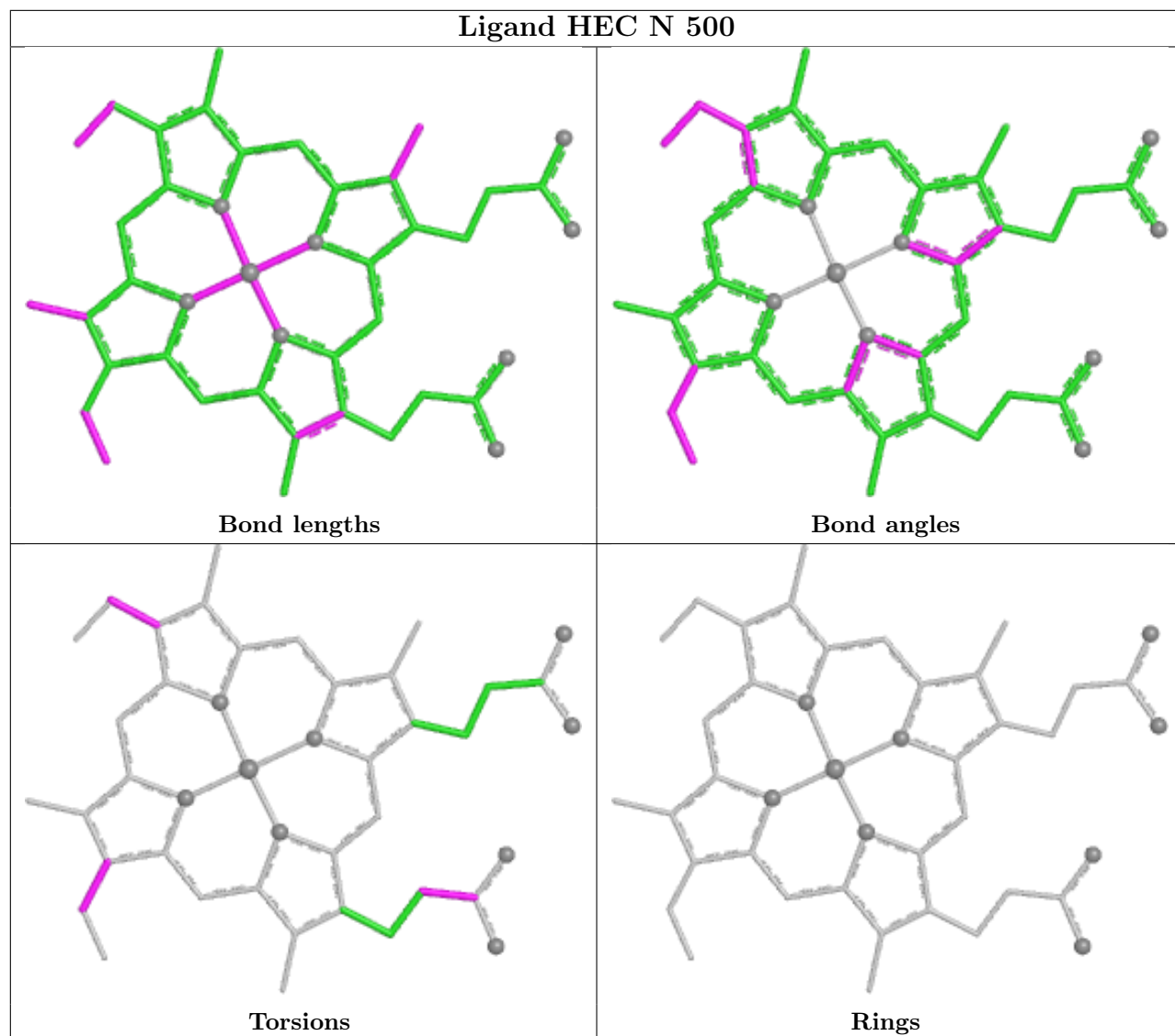


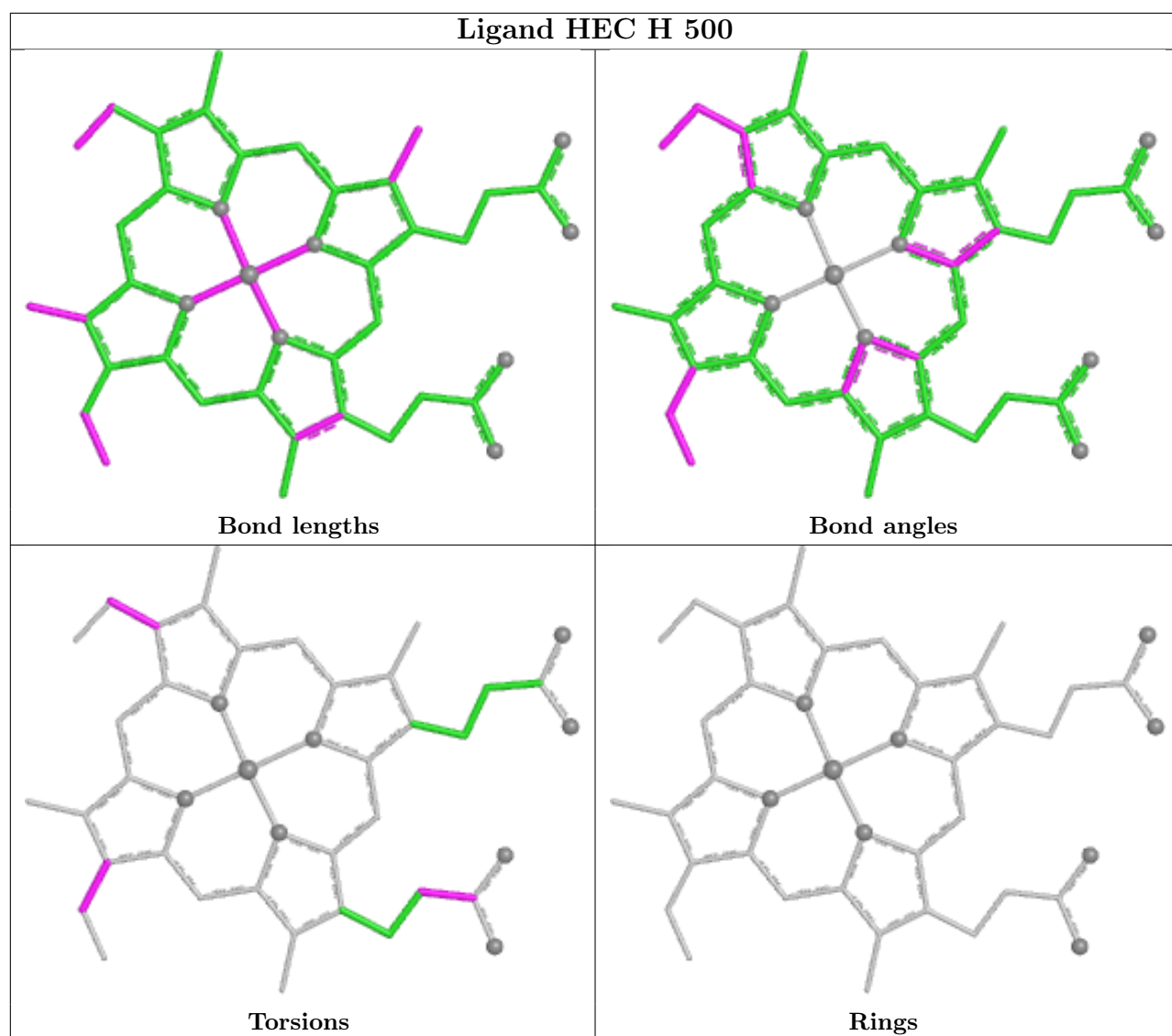
Rings

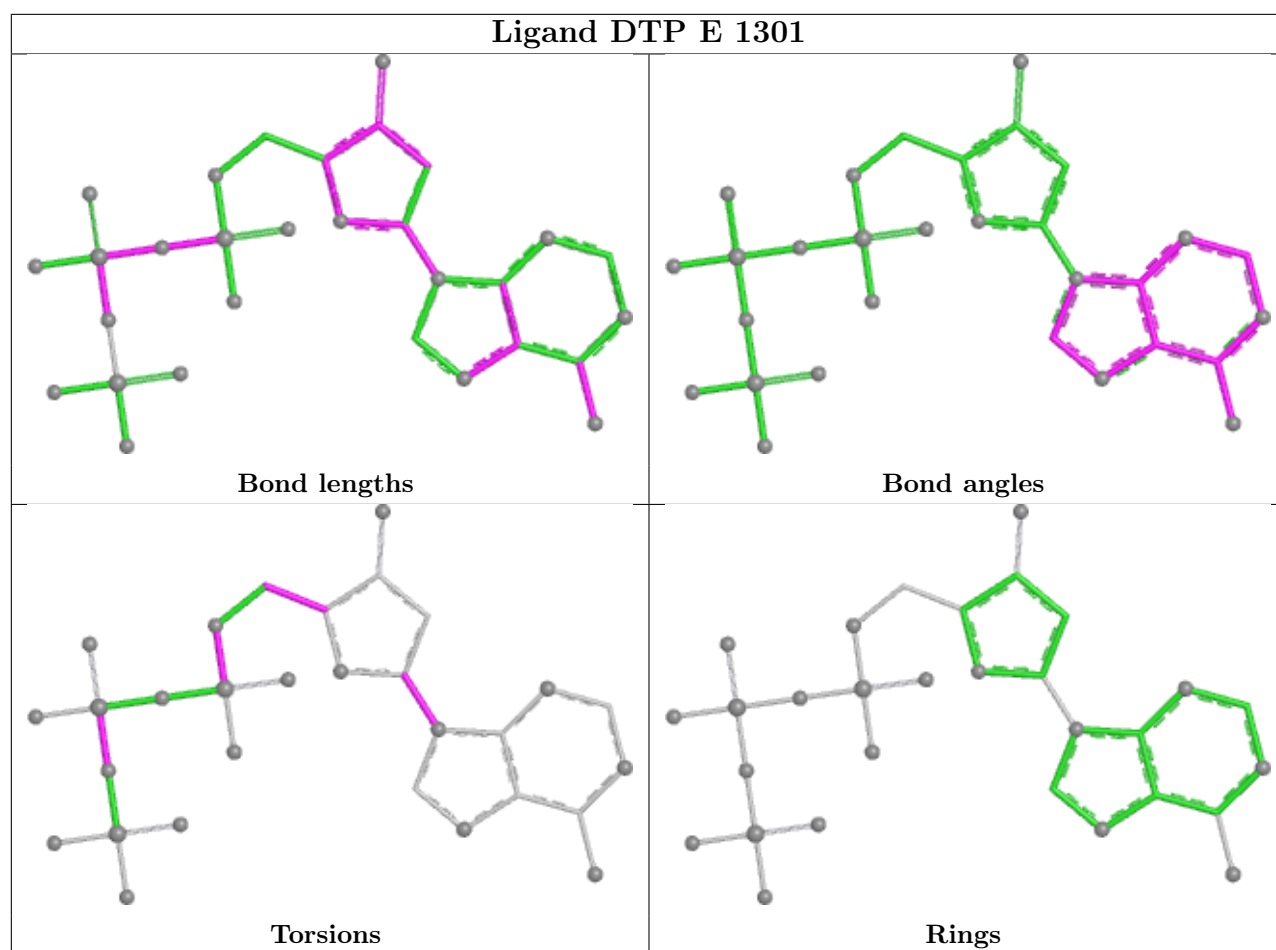












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

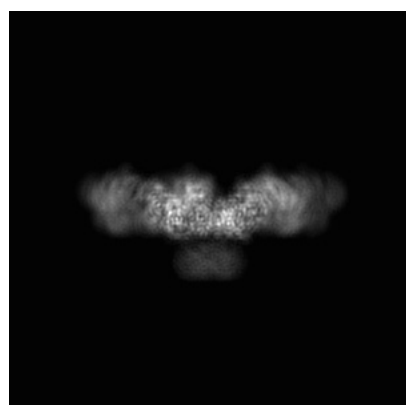
6 Map visualisation [i](#)

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.

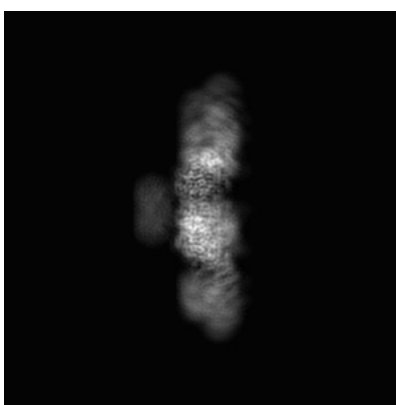
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

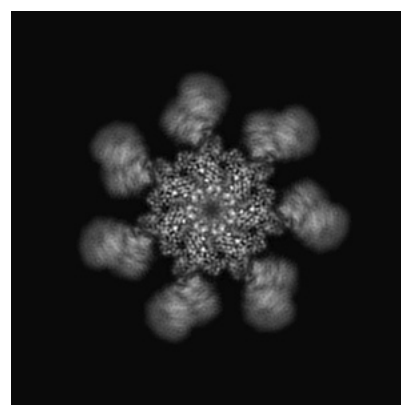
6.1.1 Primary map



X



Y

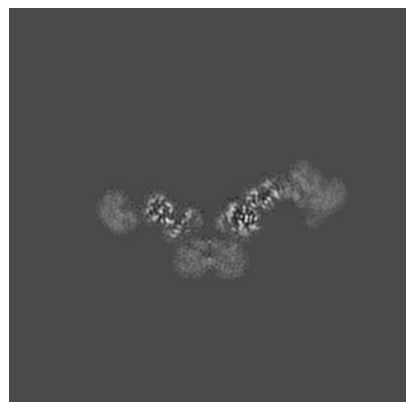


Z

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

6.2 Central slices [i](#)

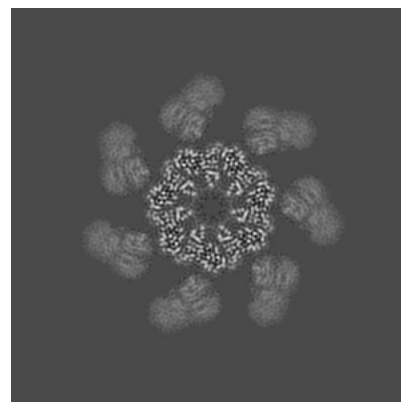
6.2.1 Primary map



X Index: 160



Y Index: 160



Z Index: 160

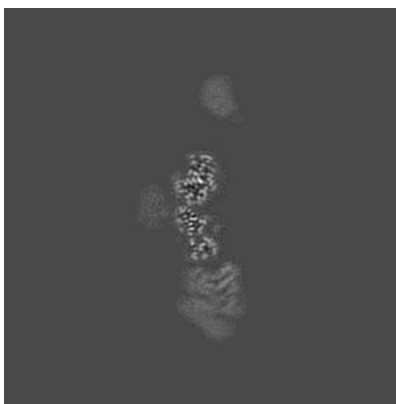
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

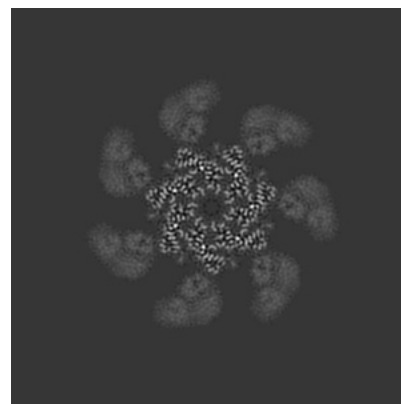
6.3.1 Primary map



X Index: 146



Y Index: 135

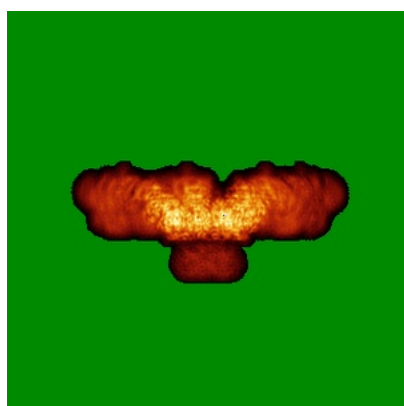


Z Index: 157

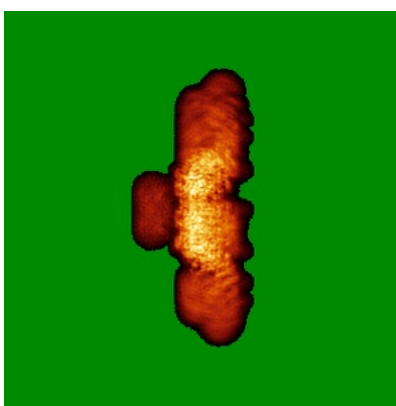
The images above show the largest variance slices of the map in three orthogonal directions.

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

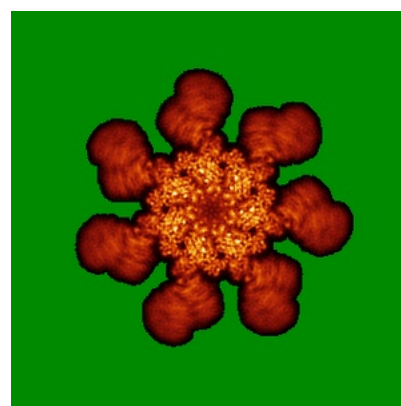
6.4.1 Primary map



X



Y

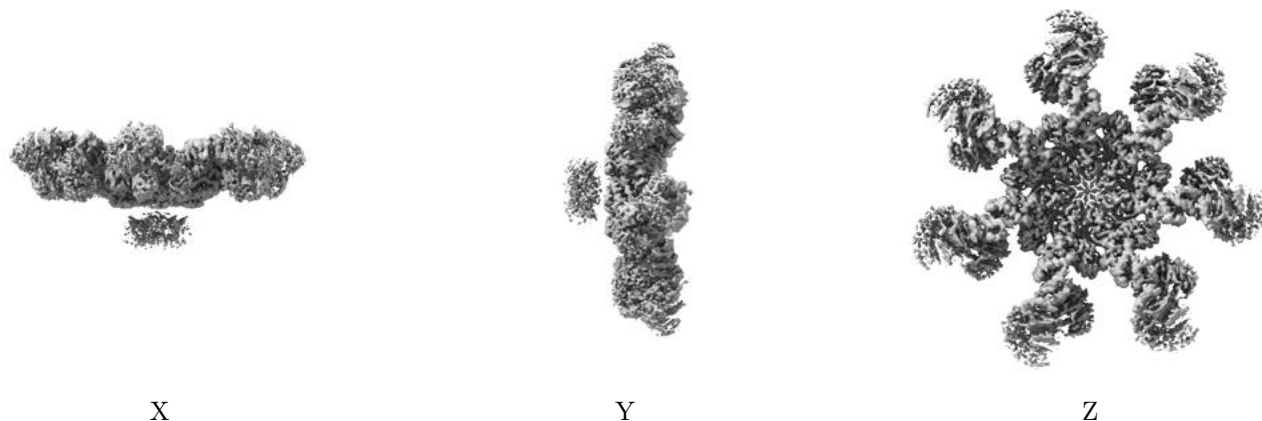


Z

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.

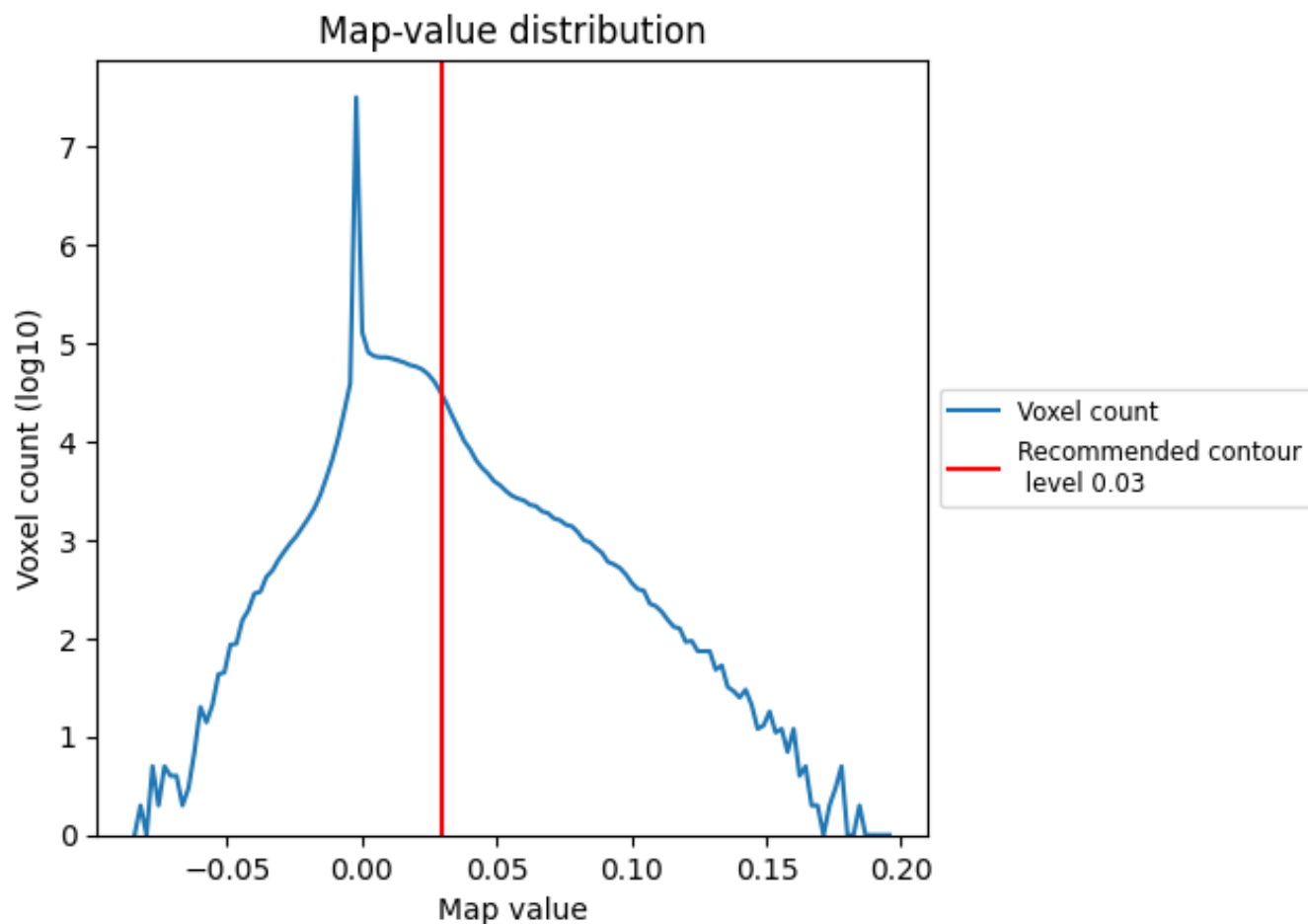
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

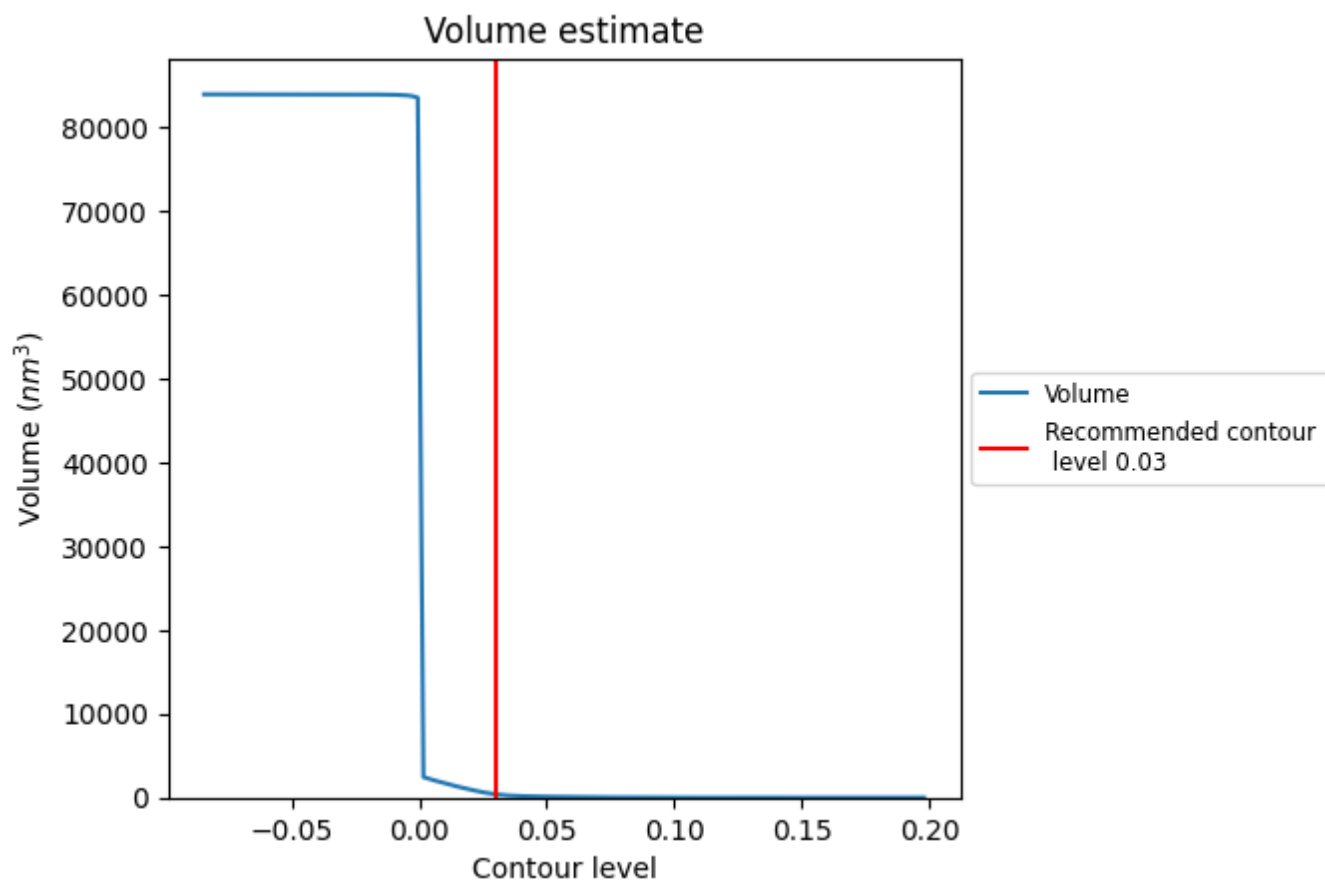
This section contains the results of statistical analysis of the map.

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.

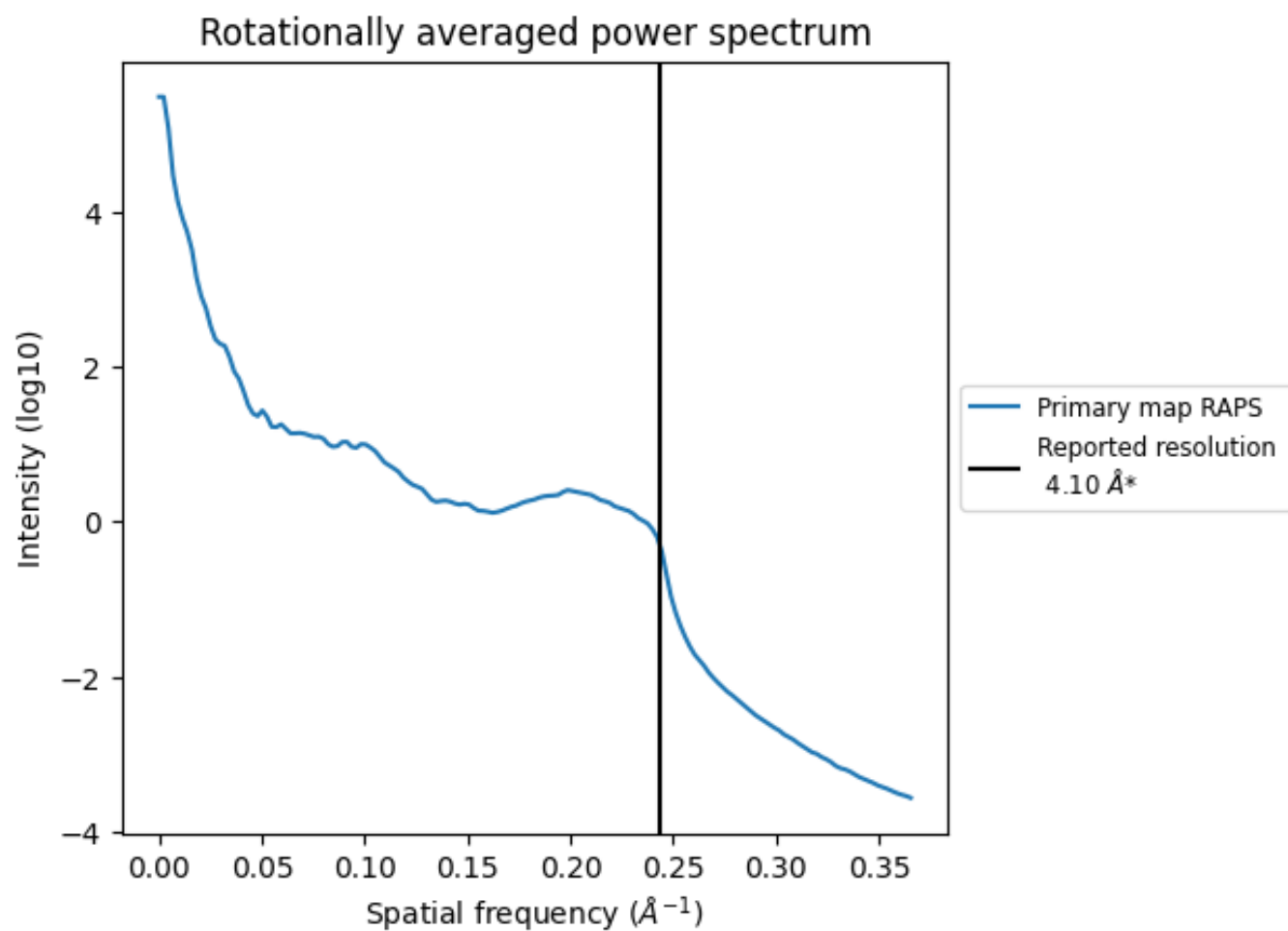
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 389 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⁻¹

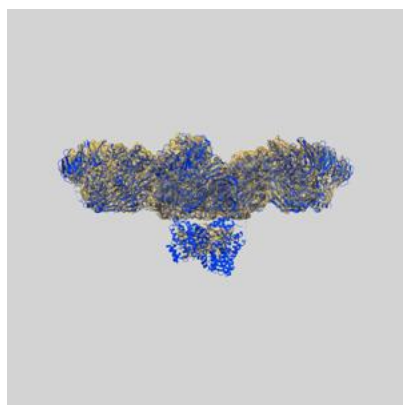
8 Fourier-Shell correlation

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

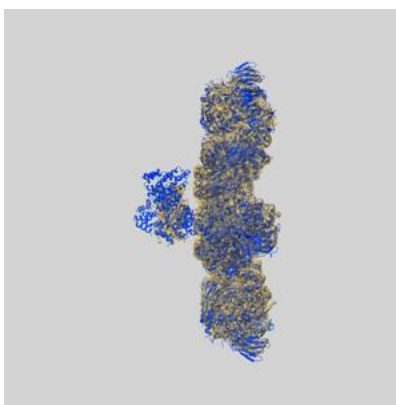
9 Map-model fit [i](#)

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](#).

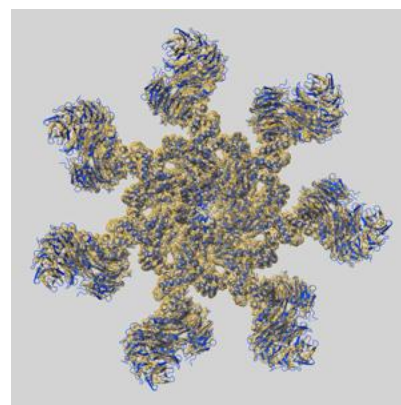
9.1 Map-model overlay [i](#)



X



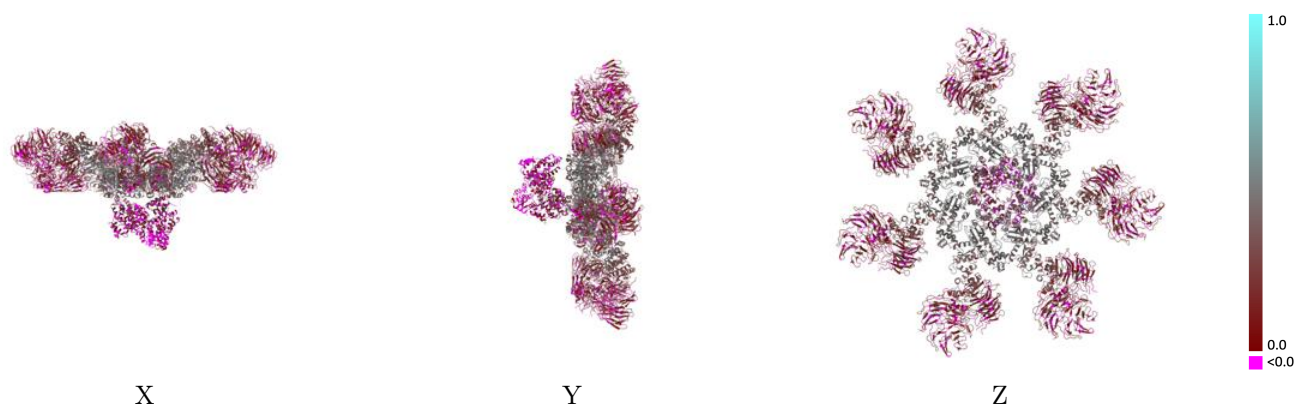
Y



Z

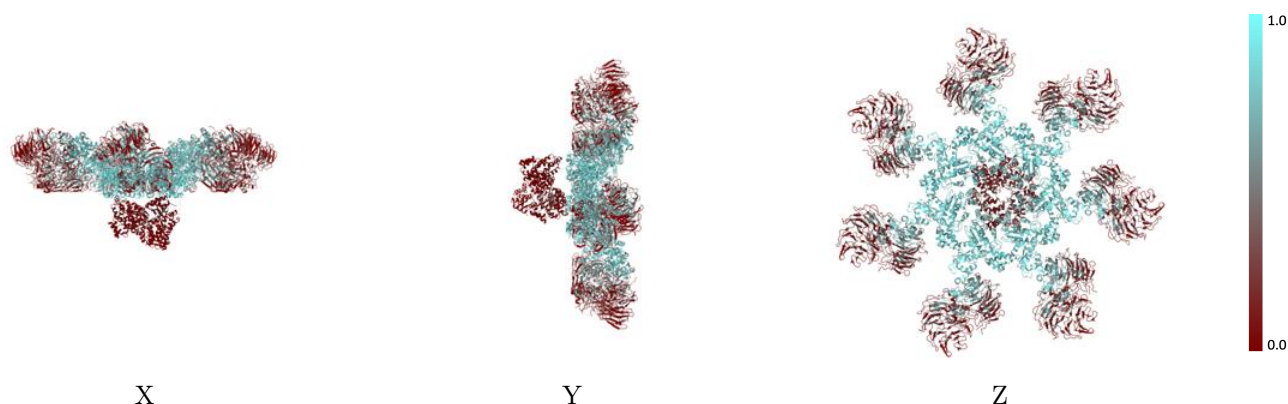
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



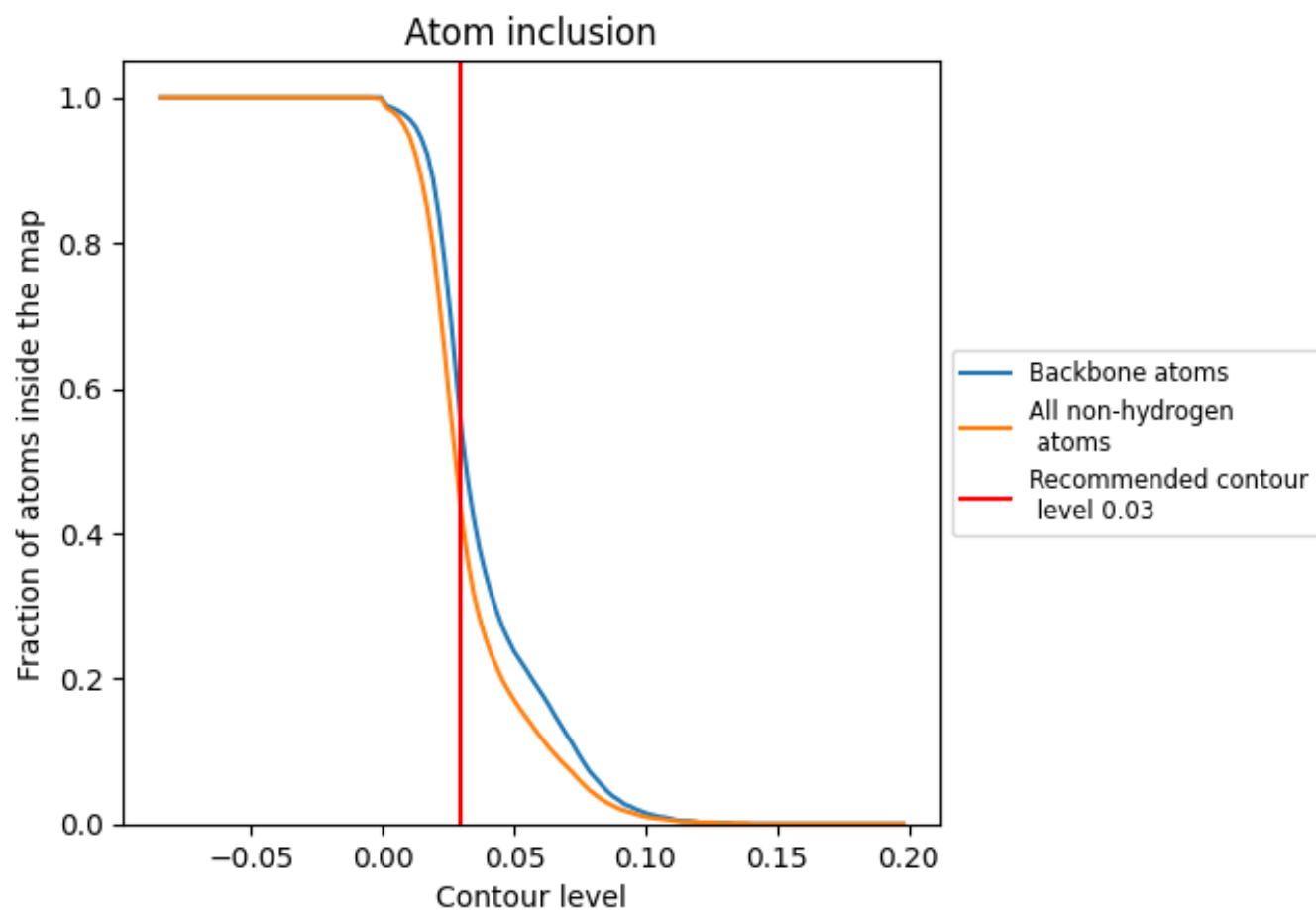
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

1.0
0.0
<0.0