



wwPDB EM Validation Summary Report ⓘ

Mar 10, 2026 – 12:37 AM UTC

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:

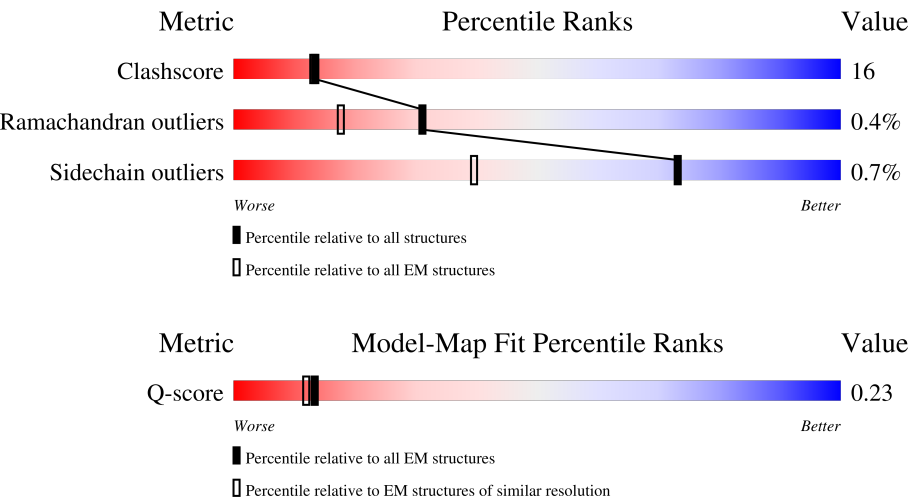
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.49

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

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		

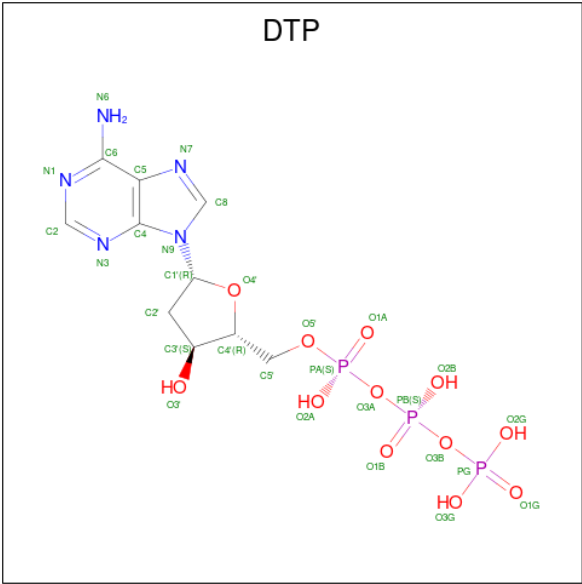
- Molecule 2 is a protein called Cytochrome c.

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.

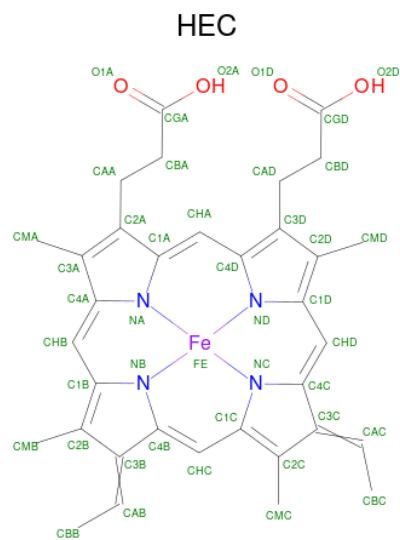
Mol	Chain	Residues	Atoms					AltConf	Trace
3	O	95	Total	C	N	O	S	0	0
			777	475	152	145	5		
3	P	95	Total	C	N	O	S	0	0
			777	475	152	145	5		
3	Q	95	Total	C	N	O	S	0	0
			777	475	152	145	5		
3	R	95	Total	C	N	O	S	0	0
			777	475	152	145	5		

- Molecule 4 is 2'-DEOXYADENOSINE 5'-TRIPHOSPHATE (CCD ID: DTP) (formula: C₁₀H₁₆N₅O₁₂P₃)



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: C₃₄H₃₄FeN₄O₄).

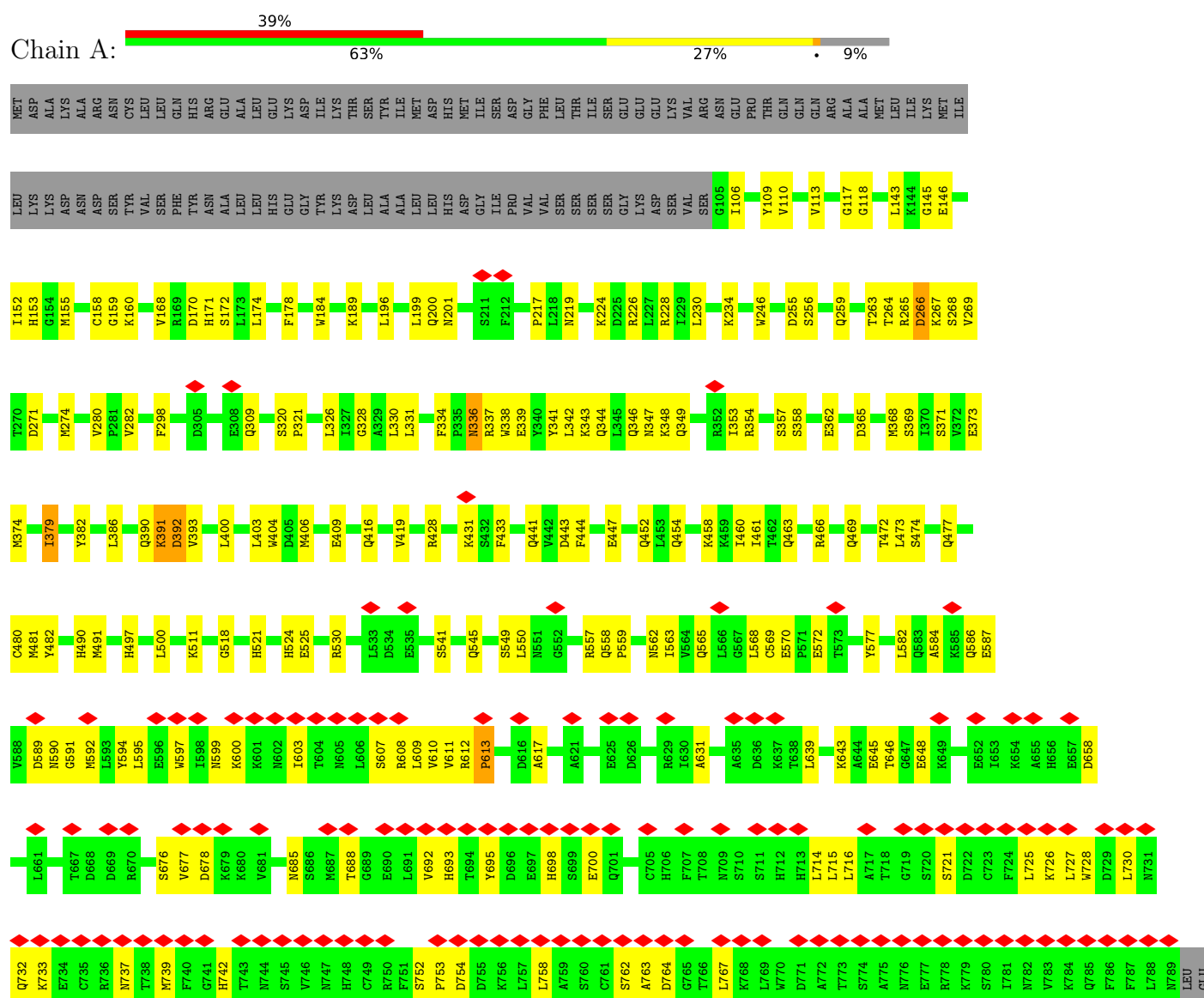


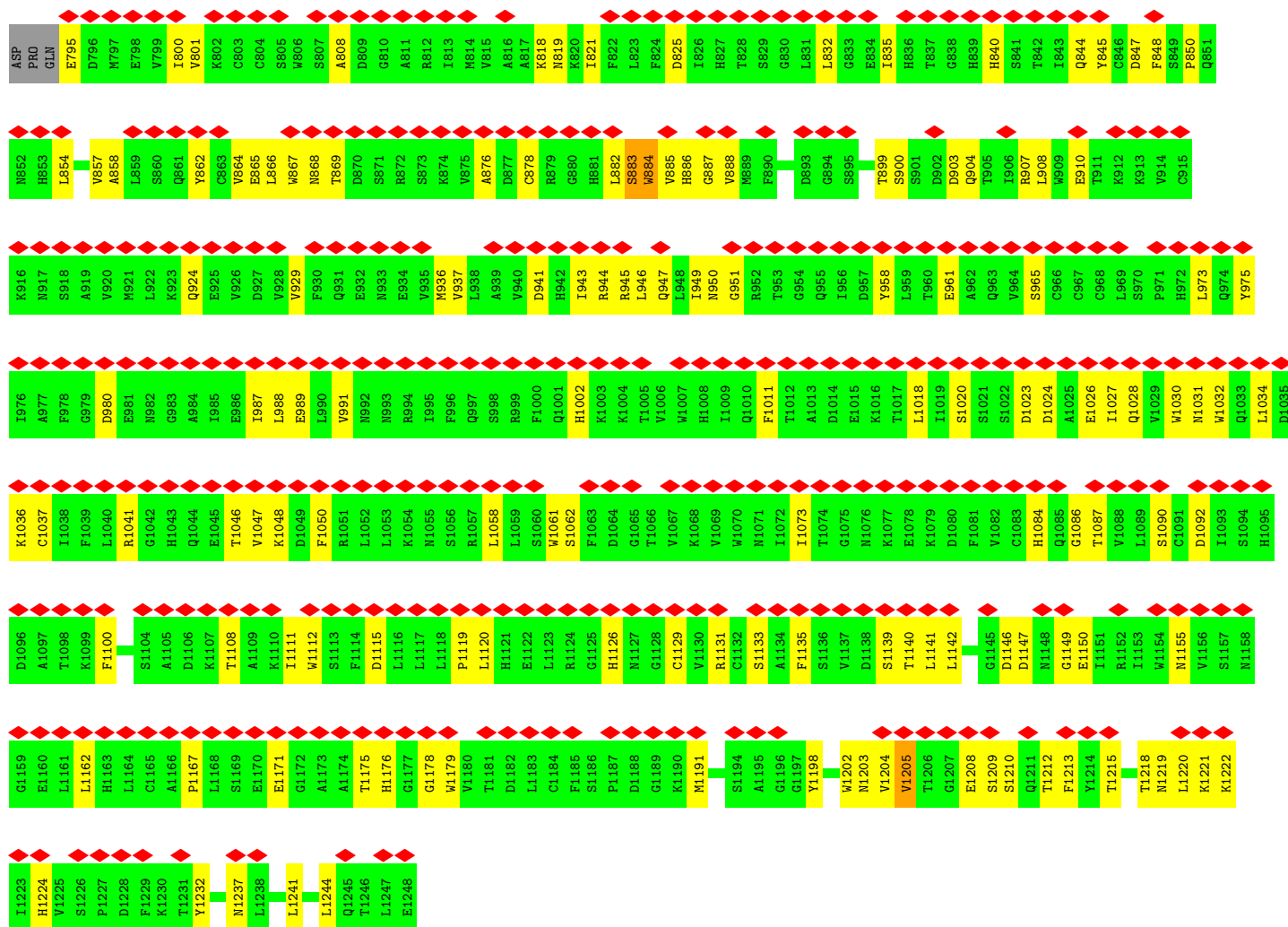
Mol	Chain	Residues	Atoms					AltConf
5	H	1	Total 43	C 34	Fe 1	N 4	O 4	0
5	I	1	Total 43	C 34	Fe 1	N 4	O 4	0
5	J	1	Total 43	C 34	Fe 1	N 4	O 4	0
5	K	1	Total 43	C 34	Fe 1	N 4	O 4	0
5	L	1	Total 43	C 34	Fe 1	N 4	O 4	0
5	M	1	Total 43	C 34	Fe 1	N 4	O 4	0
5	N	1	Total 43	C 34	Fe 1	N 4	O 4	0

3 Residue-property plots

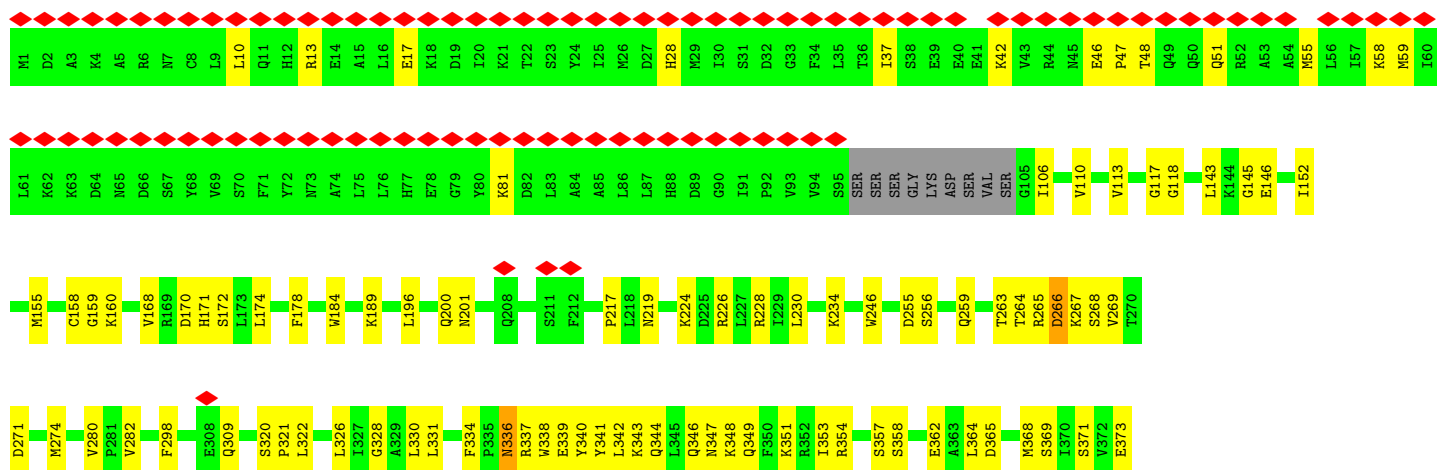
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

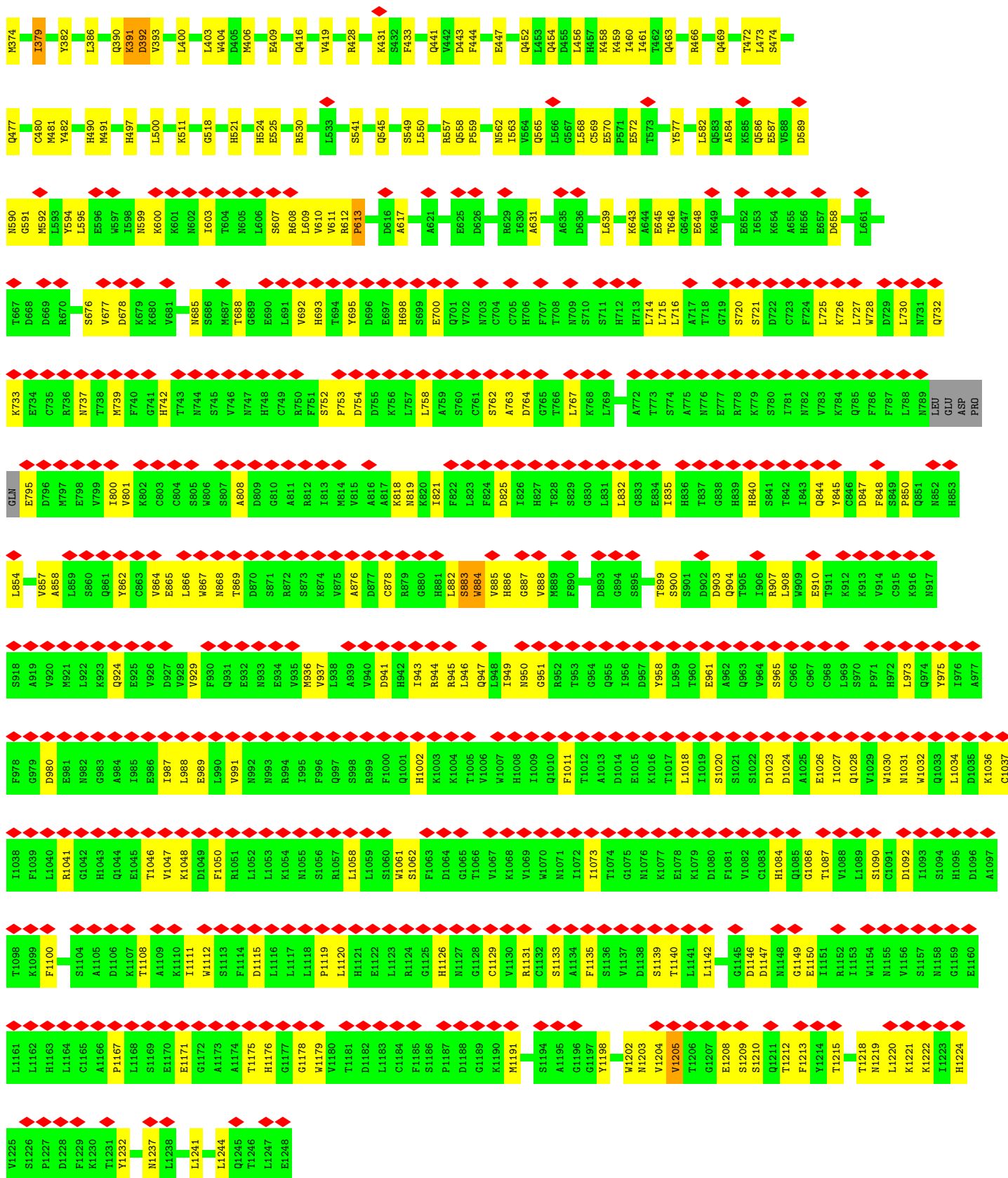
- Molecule 1: Apoptotic protease-activating factor 1



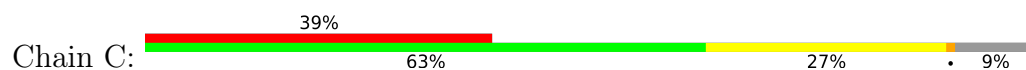


• Molecule 1: Apoptotic protease-activating factor 1

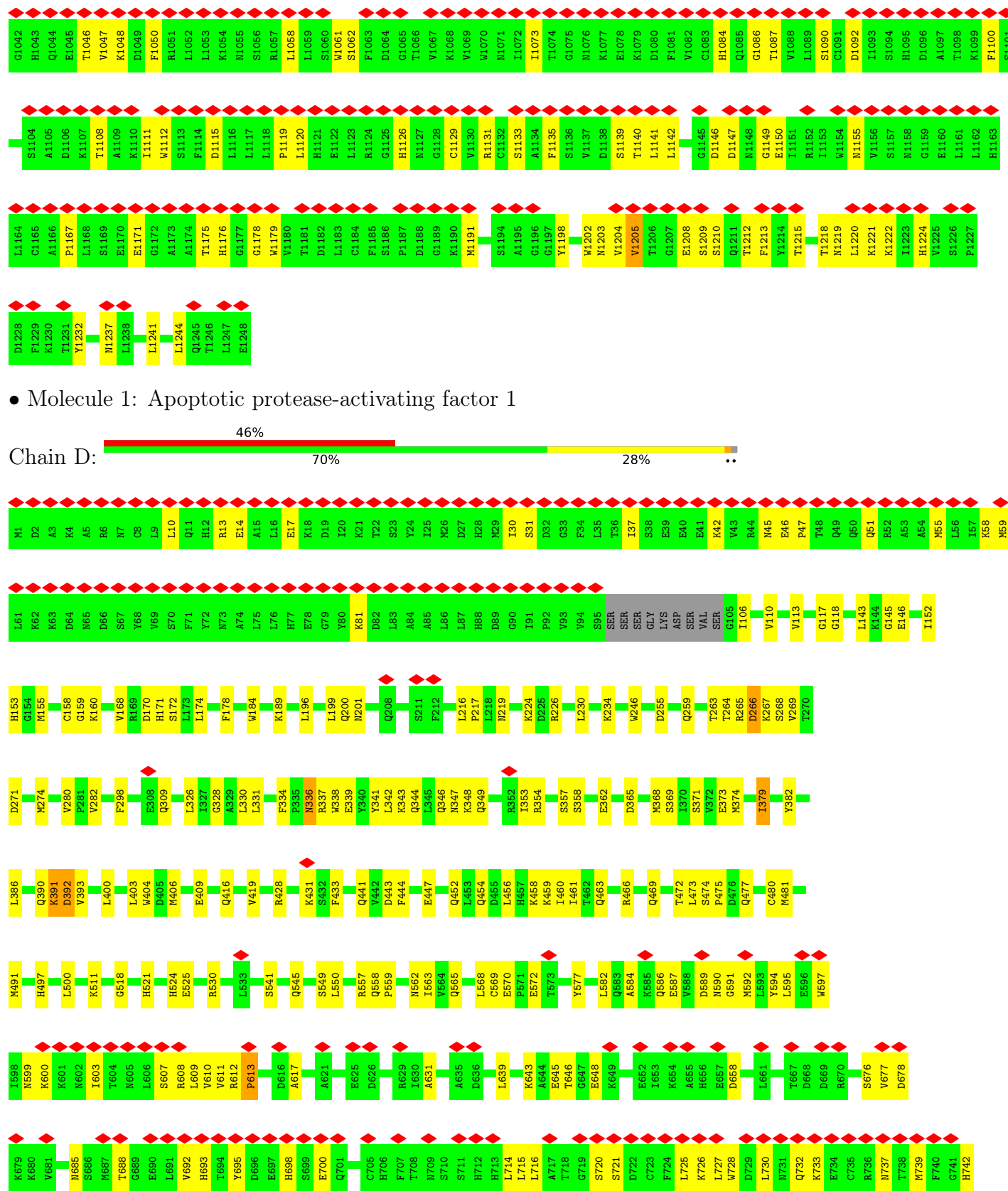




- Molecule 1: Apoptotic protease-activating factor 1

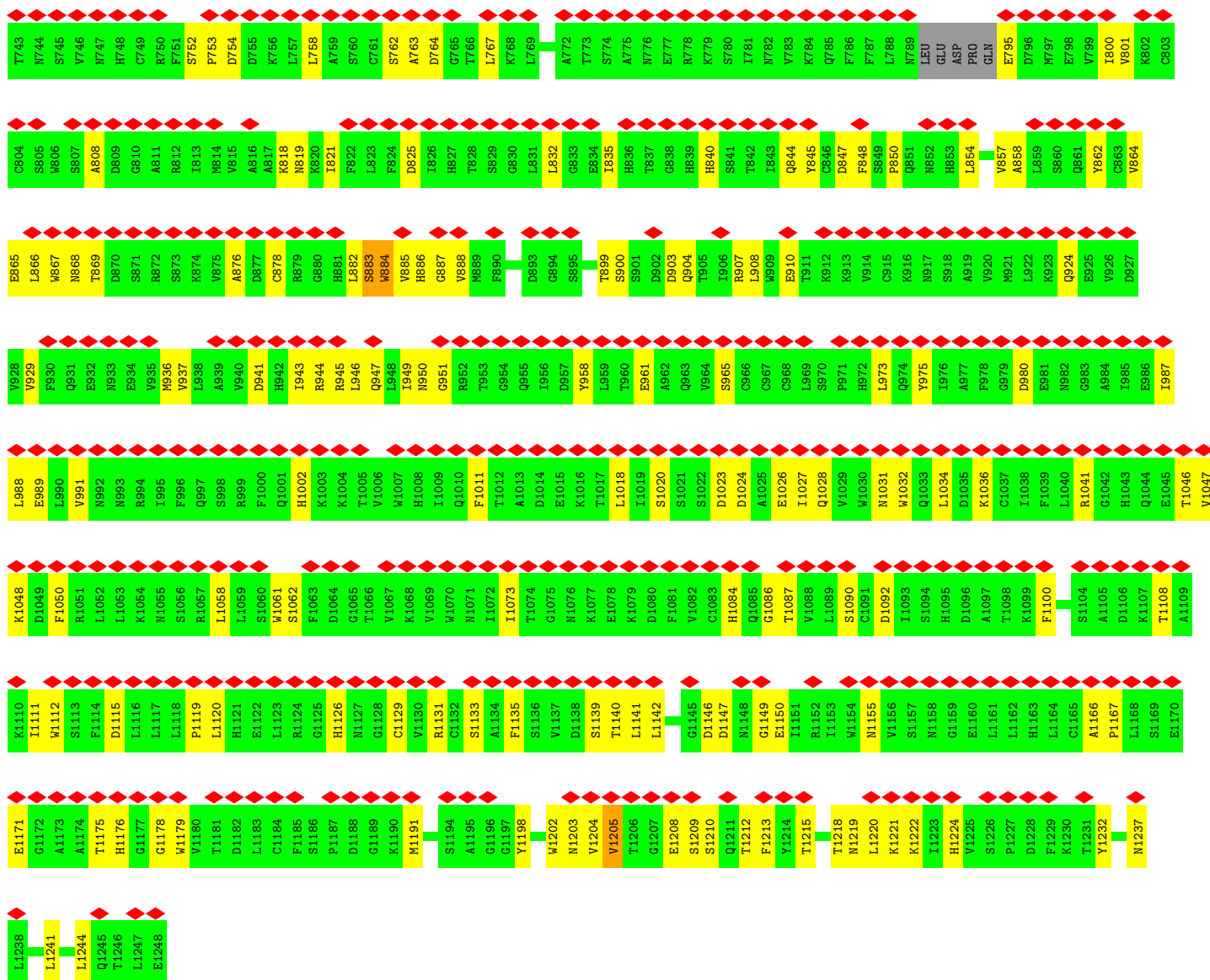


MET	LEU	H153	D271	M481	L593	S676	N737	N797	A858	N921	N982
ASP	LYS	G154	M274	Y482	L594	V677	T738	E798	L859	L922	G983
ALA	ASP	M155	L386	L595	E596	D678	M739	V799	S860	E923	A984
LYS	ASN	C158	V280	M491	M597	K679	F740	T800	Q861	Q924	L985
ARG	ASP	G159	K391	H497	L598	K680	G741	V801	Y862	E925	E986
ASN	SER	K160	V282	H497	N599	V681	H742	R802	C863	V926	L987
CYS	TYR	V168	F298	L500	K600	V681	T743	R803	E864	V927	L988
LEU	SER	R169	F308	K601	H602	V682	M744	C804	E865	V928	E989
GLN	PHE	D170	Q309	K611	L603	V683	S745	S805	L866	V929	L990
HIS	TYR	H171	Q309	G518	L604	V684	T746	M806	W867	F930	N992
ARG	ASN	S172	L322	H521	T604	V685	M747	S807	N868	Q931	N993
GLU	ALA	L173	L326	G518	H605	V686	H748	A808	T869	E932	R994
ALA	LEU	L174	L326	H521	L606	V687	C749	D809	D870	N933	R995
LEU	LEU	F178	L327	H521	L607	V688	H750	C810	S871	E934	F996
GLY	GLY	W184	L328	H522	L608	V689	F751	A811	R872	V935	F997
LYS	TYR	K189	L330	E409	L609	V690	S752	R812	S873	M936	Q997
ILE	ILE	L196	L331	Q416	V610	V691	F753	R813	K874	V937	S998
THR	ASP	L199	L331	V419	V611	V692	D754	R814	V875	V940	F1000
SER	LEU	L199	L331	L533	V612	V693	K755	R815	D876	D941	Q1001
GLY	ALA	Q200	L334	S541	P613	V694	L757	A816	A877	H942	H1002
ASP	ALA	N201	F334	Q545	D615	V695	L758	A817	C878	I943	K1003
ILE	LEU	Q208	P335	Q549	A617	V696	S759	K818	R879	R944	K1004
GLY	LEU	S211	N336	E700	A617	V697	A760	R819	G880	R945	L1005
ASP	ASP	F212	W338	L550	A621	V698	S761	R820	H881	L946	V1006
PRO	ASP	L216	Y340	R557	E625	V699	G762	F822	L882	Q947	W1007
VAL	VAL	L217	L341	P559	D626	V700	A763	L823	S883	I948	H1008
THR	VAL	P217	L342	N562	D627	V701	D764	F824	W884	I949	N1009
ILE	SER	N219	L343	L563	D628	V702	G765	D825	H885	G951	Q1010
GLY	SER	K224	L344	L564	D629	V703	L766	R826	R886	A952	T1012
LYS	GLY	R226	L345	Q452	D630	V704	T767	H827	H887	T953	A1013
VAL	VAL	L230	L346	L453	D631	V705	L768	T828	V888	G954	D1014
ASN	GLU	K234	L347	Q454	D632	V706	K769	C830	M889	G955	E1015
PRO	ASP	W246	L348	D455	D633	V707	L770	L831	R890	L956	D1016
GLN	SER	D255	L349	L456	D634	V708	D771	L832	D891	D957	L1017
ARG	VAL	Q259	L350	L457	D635	V709	S774	L833	T899	N958	L1018
ALA	SER	T263	L351	K458	D636	V710	A775	L834	S901	E961	I1019
ALA	GLU	T264	L352	K459	D637	V711	M776	L835	D902	A962	S1020
MET	PRO	R265	L353	I460	D638	V712	E777	L836	D903	Q963	S1021
LEU	THR	D266	L354	I461	D639	V713	R778	E837	Q904	V964	S1022
ILE	GLN	E146	L355	Q463	D640	V714	S779	E838	T905	S965	D1023
MET	GLN	S268	L356	Q464	D641	V715	A780	E839	I906	C966	D1024
LYS	GLN	V269	L357	R466	D642	V716	M781	H840	R907	C967	A1025
ILE	ARG	T270	L358	Q469	D643	V717	T782	S841	S908	C968	E1026
	ALA		L359	T472	D644	V718	L783	T842	R909	C969	I1027
	ALA		L360	L473	D645	V719	V784	R843	E910	S970	Q1028
	ALA		L361	S474	D646	V720	K785	Q844	T911	P971	V1029
	ALA		L362	Q477	D647	V721	Q786	Y845	K912	H972	W1030
	ALA		L363	C480	D648	V722	L787	Y846	L913	L973	N1031
	ALA		L364		D649	V723	D788	D847	C915	Q974	W1032
	ALA		L365		D650	V724	L789	F848	S849	Y975	L1034
	ALA		L366		D651	V725	L790	R849	P851	I976	D1035
	ALA		L367		D652	V726	L791	T850	N852	A977	K1036
	ALA		L368		D653	V727	L792	Q732	L854	C1037	I1038
	ALA		L369		D654	V728	L793	K733	V857	F1039	L1040
	ALA		L370		D655	V729	L794	E734			
	ALA		L371		D656	V730	L795	C735			
	ALA		L372		D657	V731	L796	R736			
	ALA		L373		D658	V732	L797				
	ALA		L374		D659	V733	L798				
	ALA		L375		D660	V734	L799				
	ALA		L376		D661	V735	L800				
	ALA		L377		D662	V736	L801				
	ALA		L378		D663	V737	L802				
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	ALA		L381		D666	V740	L805				
	ALA		L382		D667	V741	L806				
	ALA		L383		D668	V742	L807				
	ALA		L384		D669	V743	L808				
	ALA		L385		D670	V744	L809				
	ALA		L386		D671	V745	L810				
	ALA		L387		D672	V746	L811				
	ALA		L388		D673	V747	L812				
	ALA		L389		D674	V748	L813				
	ALA		L390		D675	V749	L814				
	ALA		L391		D676	V750	L815				
	ALA		L392		D677	V751	L816				
	ALA		L393		D678	V752	L817				
	ALA		L394		D679	V753	L818				
	ALA		L395		D680	V754	L819				
	ALA		L396		D681	V755	L820				
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	ALA		L401		D686	V760	L825				
	ALA		L402		D687	V761	L826				
	ALA		L403		D688	V762	L827				
	ALA		L404		D689	V763	L828				
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	ALA		L406		D691	V765	L830				
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	ALA		L408		D693	V767	L832				
	ALA		L409		D694	V768	L833				
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	ALA		L411		D696	V770	L835				
	ALA		L412		D697	V771	L836				
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	ALA		L414		D699	V773	L838				
	ALA		L415		D700	V774	L839				
	ALA		L416		D701	V775	L840				
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	ALA		L433		D718	V792	L857				
	ALA		L434		D719	V793	L858				
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	ALA		L436		D721	V795	L860				
	ALA		L437		D722	V796	L861				
	ALA		L438		D723	V797	L862				
	ALA		L439		D724	V798	L863				
	ALA		L440		D725	V799	L864				
	ALA		L441		D726	V800	L865				
	ALA		L442		D727	V801	L866				
	ALA		L443		D728	V802	L867				
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	ALA		L445		D730	V804	L869				
	ALA		L446		D731	V805	L870				
	ALA		L447		D732	V806	L871				
	ALA		L448		D733	V807	L872				
	ALA		L449		D734	V808	L873				
	ALA		L450		D735	V809	L874				
	ALA		L451		D736	V810	L875				
	ALA		L452		D737	V811	L876				
	ALA		L453		D738	V812	L877				
	ALA		L454		D739	V813	L878				
	ALA		L455		D740	V814	L879				
	ALA		L456		D741	V815	L880				
	ALA		L457		D742	V816	L881				
	ALA		L458		D743	V817	L882				
	ALA		L459		D744	V818	L883				
	ALA		L460		D745	V819	L884				
	ALA		L461		D746	V820	L885				
	ALA		L462		D747	V821	L886				
	ALA		L463		D748	V822	L887				
	ALA		L464		D749	V823	L888				
	ALA		L465		D750	V824	L889				
	ALA		L466		D751	V825	L890				
	ALA		L467		D752	V826	L891				
	ALA		L468		D753	V827	L892				

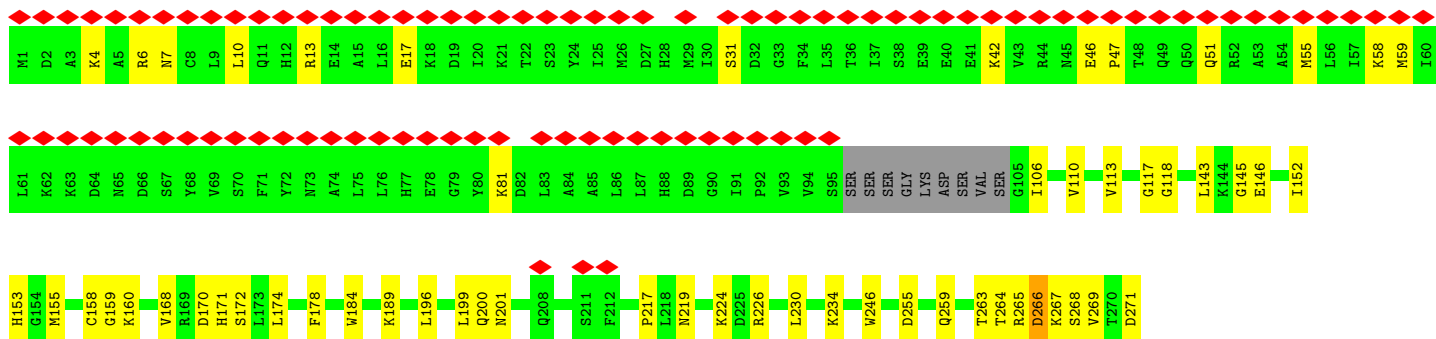


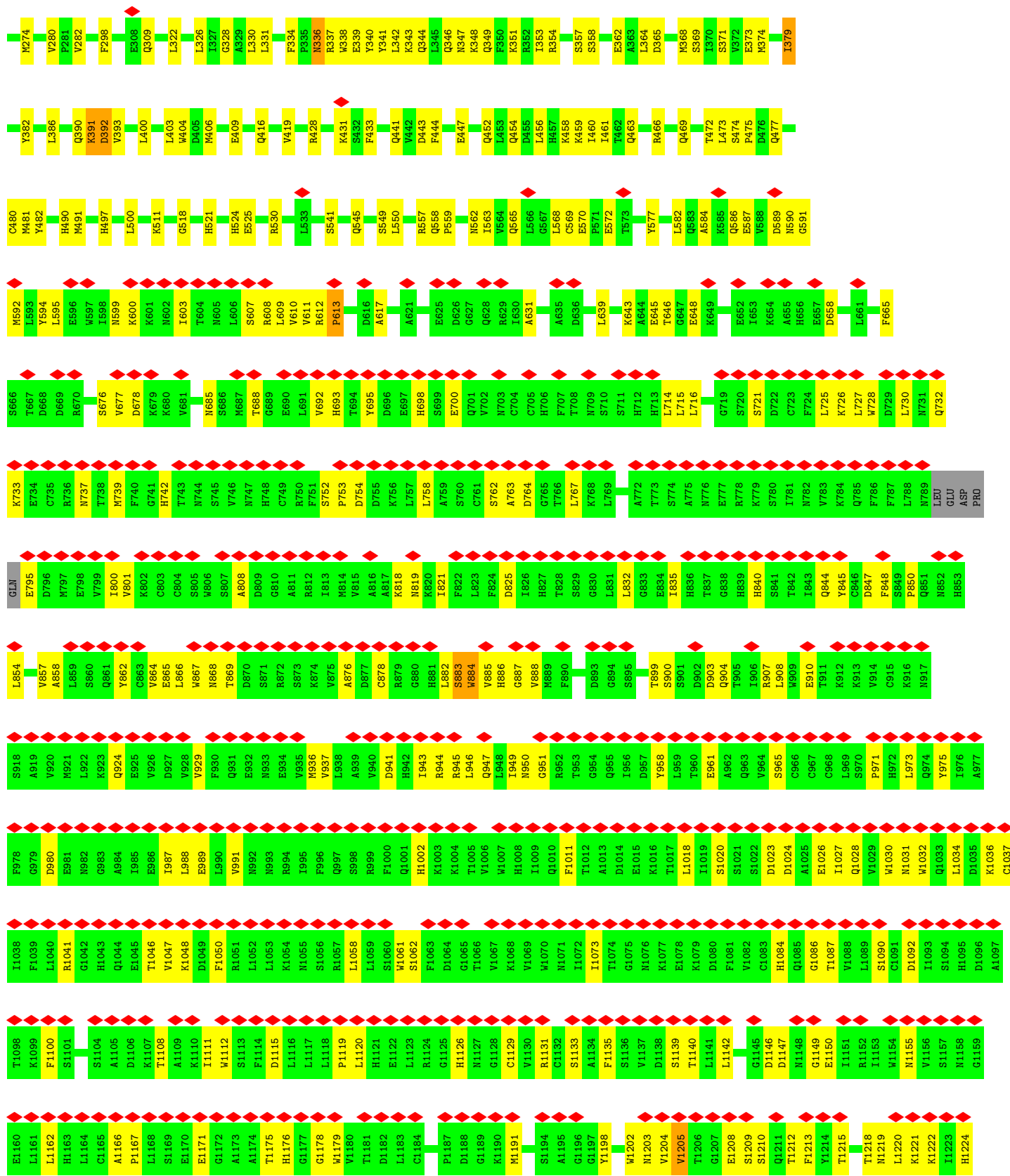
• Molecule 1: Apoptotic protease-activating factor 1

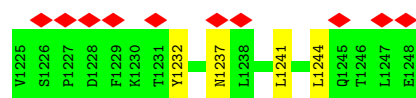




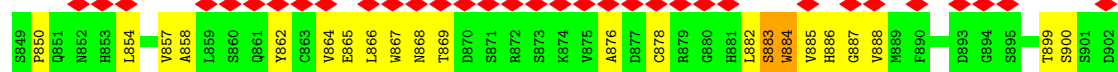
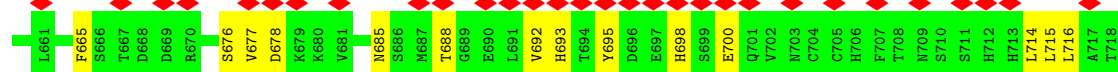
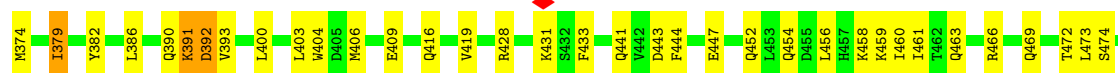
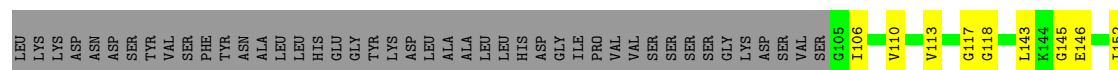
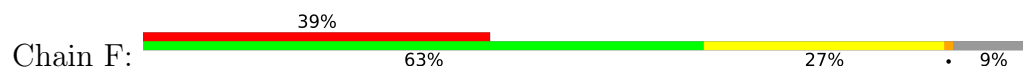
• Molecule 1: Apoptotic protease-activating factor 1

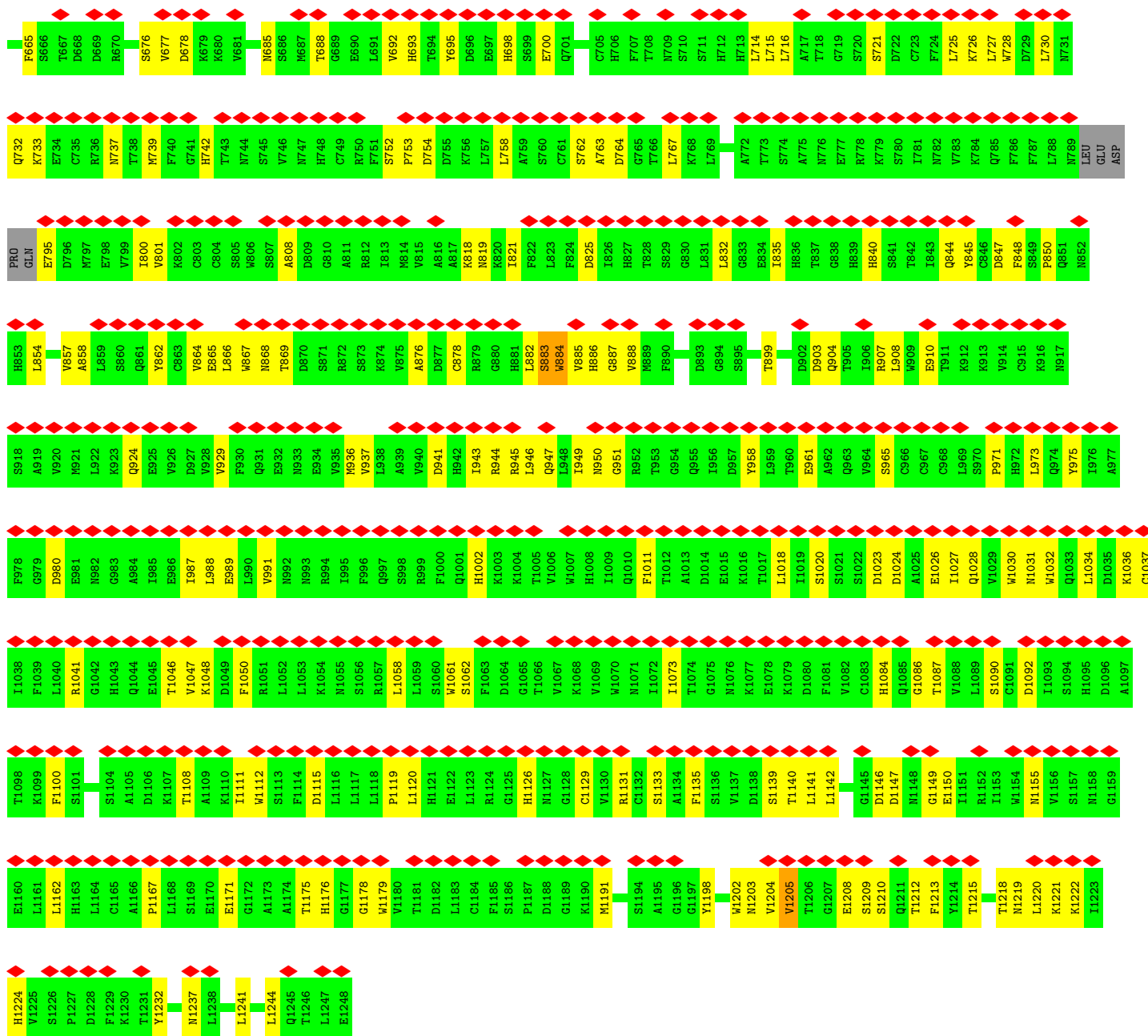




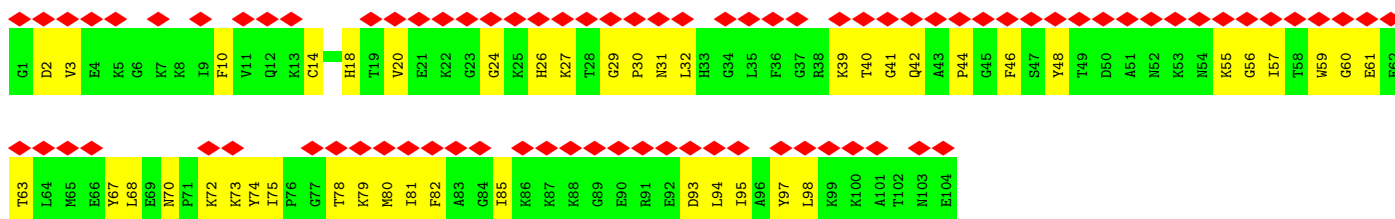
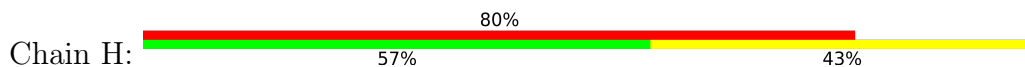


● Molecule 1: Apoptotic protease-activating factor 1

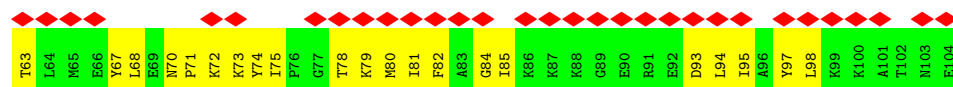
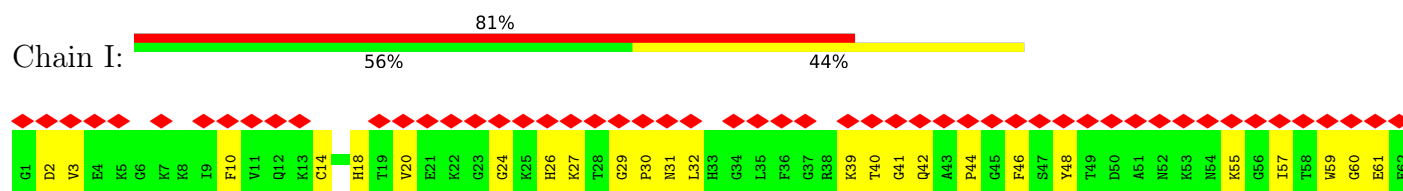




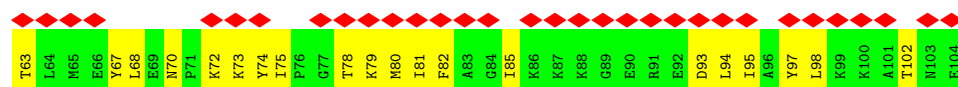
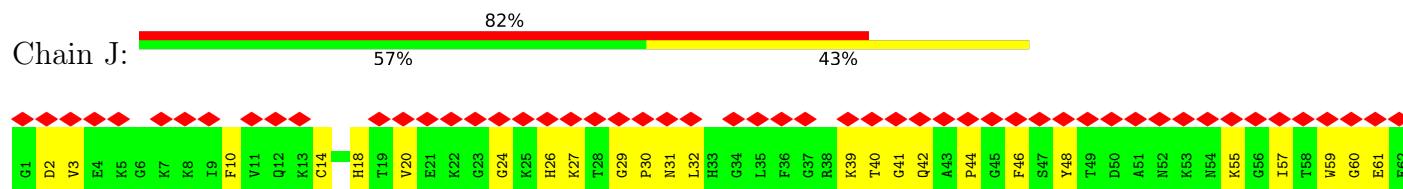
- Molecule 2: Cytochrome c



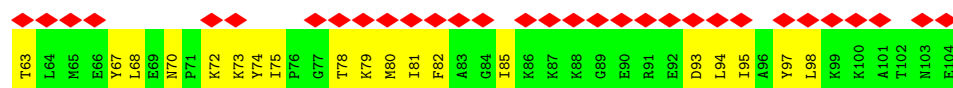
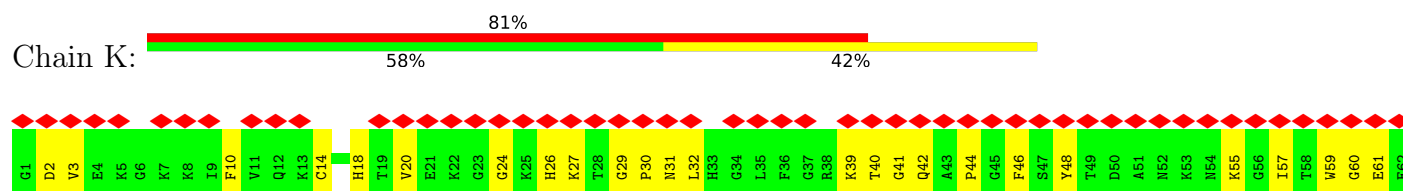
- Molecule 2: Cytochrome c



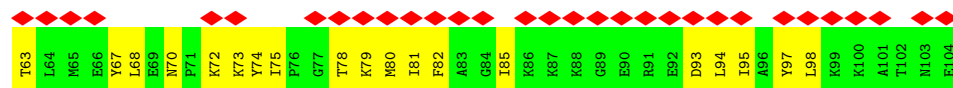
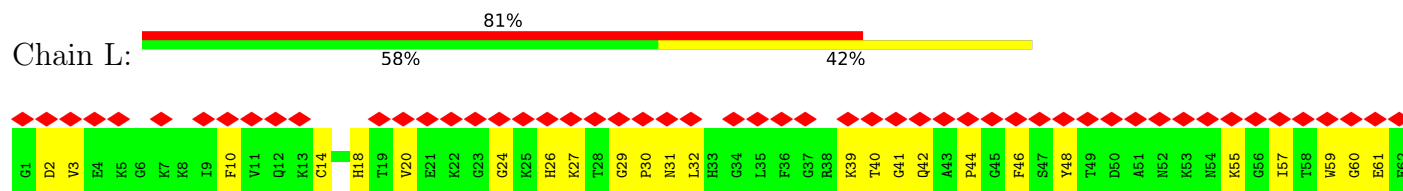
• Molecule 2: Cytochrome c



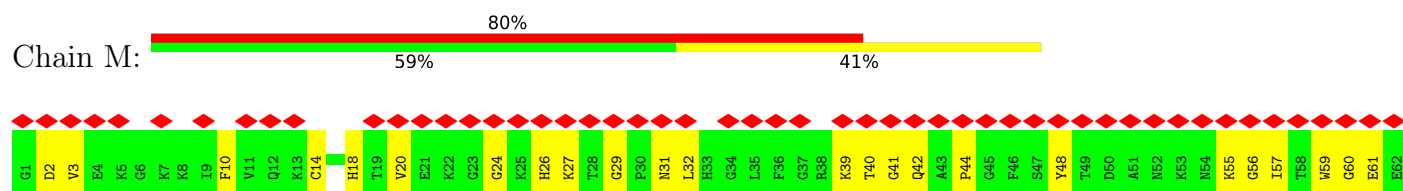
• Molecule 2: Cytochrome c

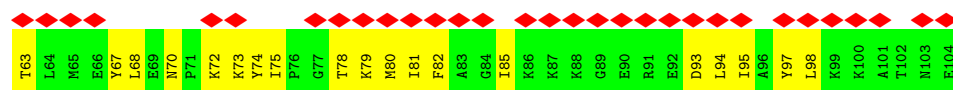


• Molecule 2: Cytochrome c

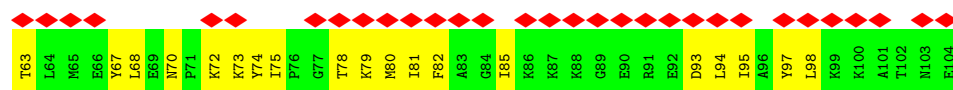
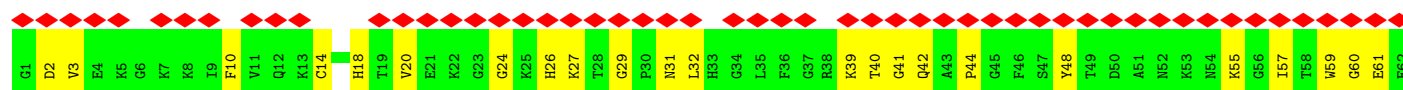
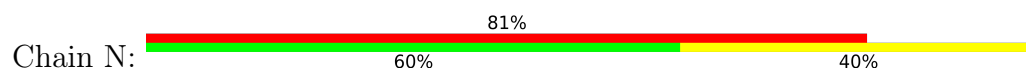


• Molecule 2: Cytochrome c

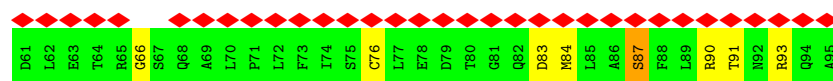
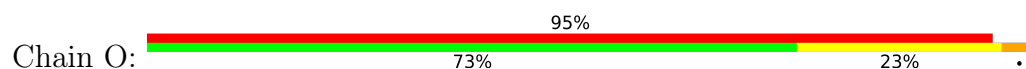




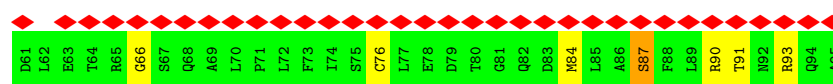
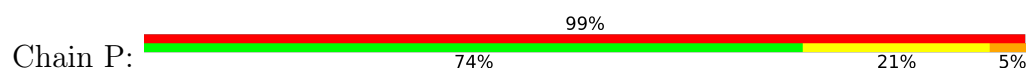
• Molecule 2: Cytochrome c



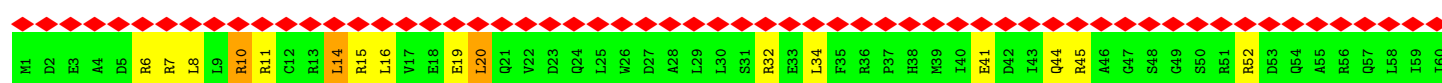
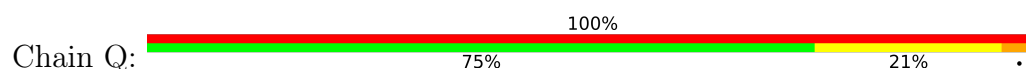
• Molecule 3: Caspase-9



• Molecule 3: Caspase-9



• Molecule 3: Caspase-9



• Molecule 3: Caspase-9



M1	D2	E3	A4	D5	R6	R7	L8	L9	R10	R11	G12	R13	L14	R15	L16	V17	F18	E19	L20	G21	V22	D23	G24	L25	V26	D27	A28	L29	L30	S31	R32	E33	L34	F35	R36	F37	H38	R39	T40	E41	D42	T43	D44	R45	A46	G47	S48	G49	S50	R51	R52	D53	O54	A55	R56	G57	L58	I59	T60
D61	L62	E63	T64	R65	G66	S67	G68	A69	L70	P71	L72	F73	I74	S75	C76	L77	E78	D79	T80	G81	R82	D83	M84	L85	A86	S87	F88	L89	R90	T91	N92	R93	Q94	A95																									

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
4	DTP	A	1301	-	31,32,32	3.51	12 (38%)	46,50,50	2.02	11 (23%)
5	HEC	M	500	-	46,50,50	2.02	7 (15%)	58,82,82	1.13	2 (3%)
4	DTP	C	1301	-	31,32,32	3.51	12 (38%)	46,50,50	2.02	11 (23%)
5	HEC	K	500	-	46,50,50	2.02	7 (15%)	58,82,82	1.14	2 (3%)
5	HEC	J	500	-	46,50,50	2.01	7 (15%)	58,82,82	1.13	2 (3%)
4	DTP	F	1301	-	31,32,32	3.51	12 (38%)	46,50,50	2.02	11 (23%)
5	HEC	N	500	-	46,50,50	2.01	7 (15%)	58,82,82	1.14	2 (3%)
4	DTP	B	1301	-	31,32,32	3.50	12 (38%)	46,50,50	2.02	11 (23%)
5	HEC	L	500	-	46,50,50	2.01	7 (15%)	58,82,82	1.13	2 (3%)
5	HEC	I	500	-	46,50,50	2.01	7 (15%)	58,82,82	1.13	2 (3%)
5	HEC	H	500	-	46,50,50	2.02	7 (15%)	58,82,82	1.12	2 (3%)
4	DTP	G	1301	-	31,32,32	3.51	12 (38%)	46,50,50	2.02	11 (23%)
4	DTP	D	1301	-	31,32,32	3.52	12 (38%)	46,50,50	2.02	11 (23%)
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
4	DTP	A	1301	-	-	8/22/34/34	0/3/3/3
5	HEC	M	500	-	-	1/14/54/54	-
4	DTP	C	1301	-	-	8/22/34/34	0/3/3/3
5	HEC	K	500	-	-	1/14/54/54	-
5	HEC	J	500	-	-	1/14/54/54	-
4	DTP	F	1301	-	-	8/22/34/34	0/3/3/3
5	HEC	N	500	-	-	1/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	DTP	B	1301	-	-	8/22/34/34	0/3/3/3
5	HEC	L	500	-	-	1/14/54/54	-
5	HEC	I	500	-	-	1/14/54/54	-
5	HEC	H	500	-	-	1/14/54/54	-
4	DTP	G	1301	-	-	8/22/34/34	0/3/3/3
4	DTP	D	1301	-	-	8/22/34/34	0/3/3/3
4	DTP	E	1301	-	-	8/22/34/34	0/3/3/3

The worst 5 of 133 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 91 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 63 torsion outliers are listed below:

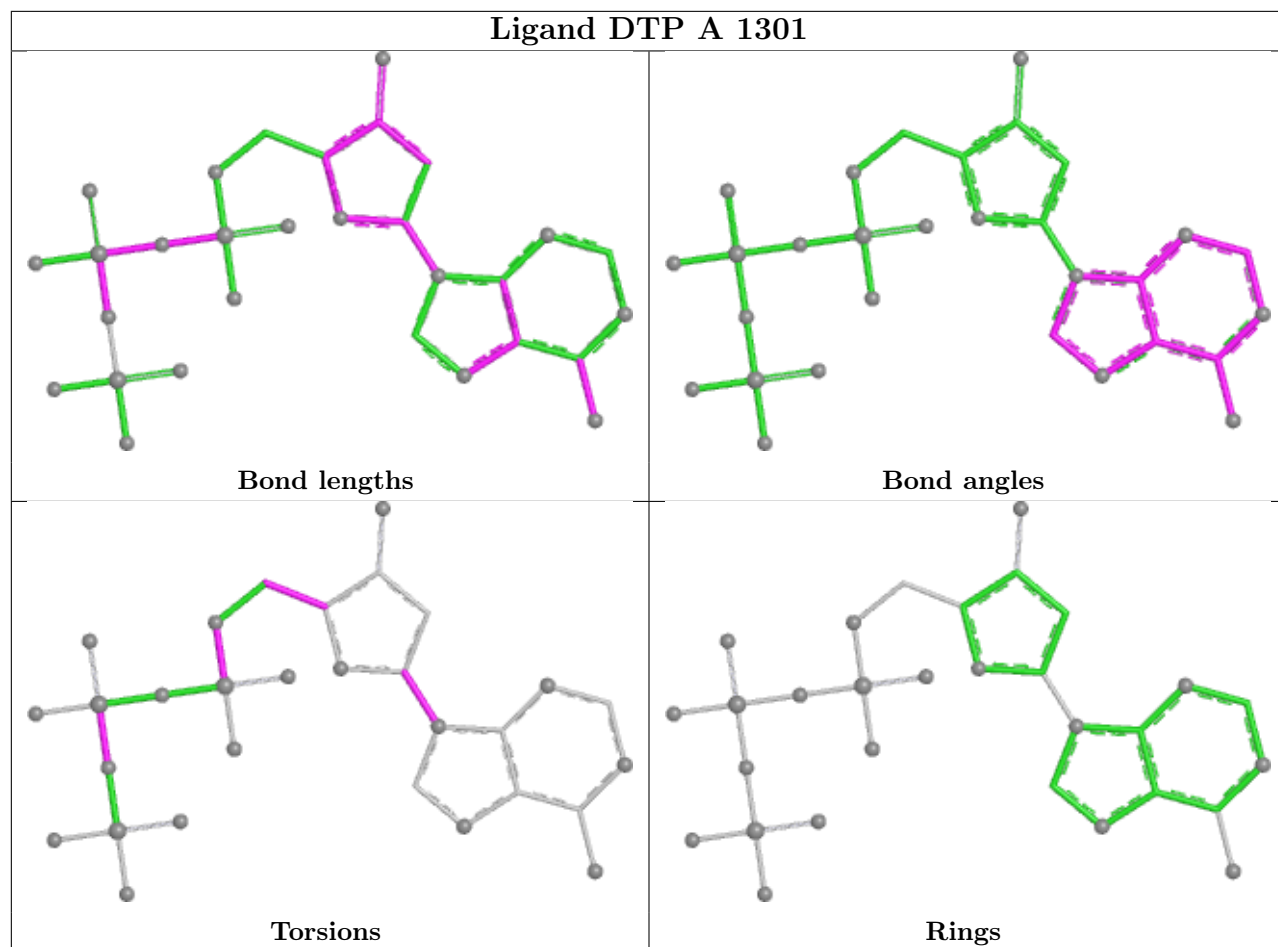
Mol	Chain	Res	Type	Atoms
4	A	1301	DTP	C5'-O5'-PA-O1A
4	A	1301	DTP	C5'-O5'-PA-O2A
4	A	1301	DTP	C5'-O5'-PA-O3A
4	A	1301	DTP	O4'-C4'-C5'-O5'
4	B	1301	DTP	C5'-O5'-PA-O1A

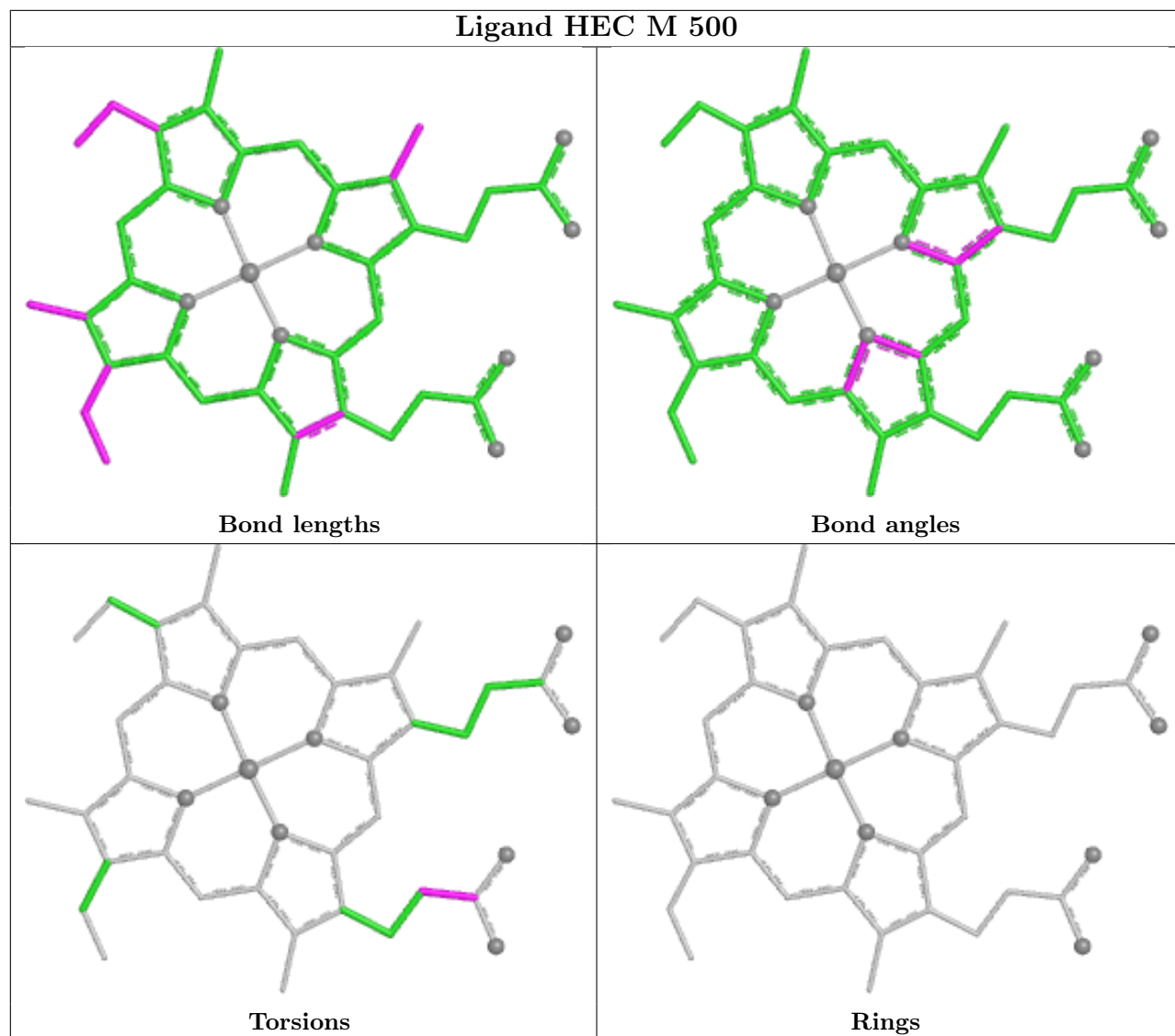
There are no ring outliers.

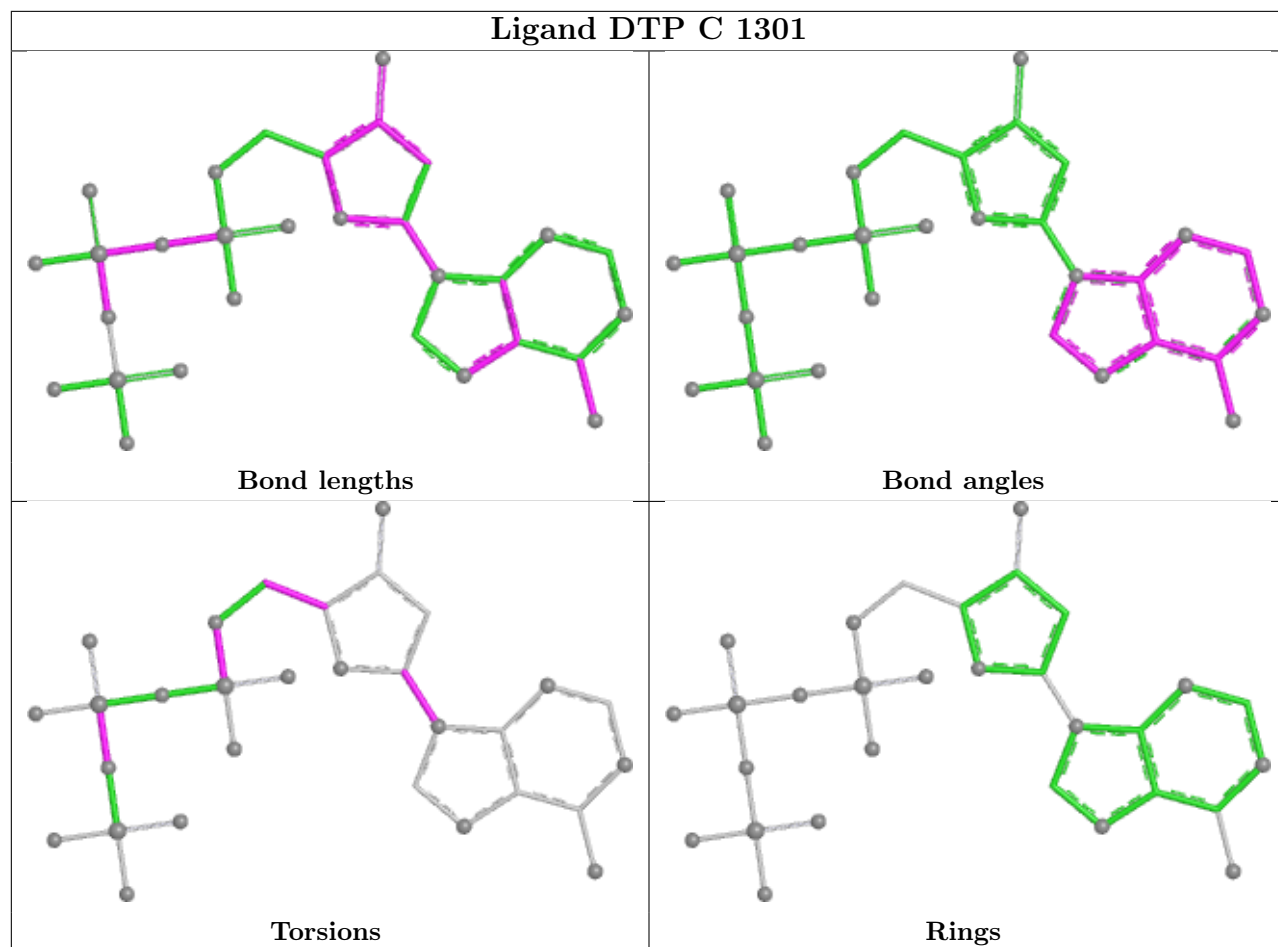
14 monomers are involved in 35 short contacts:

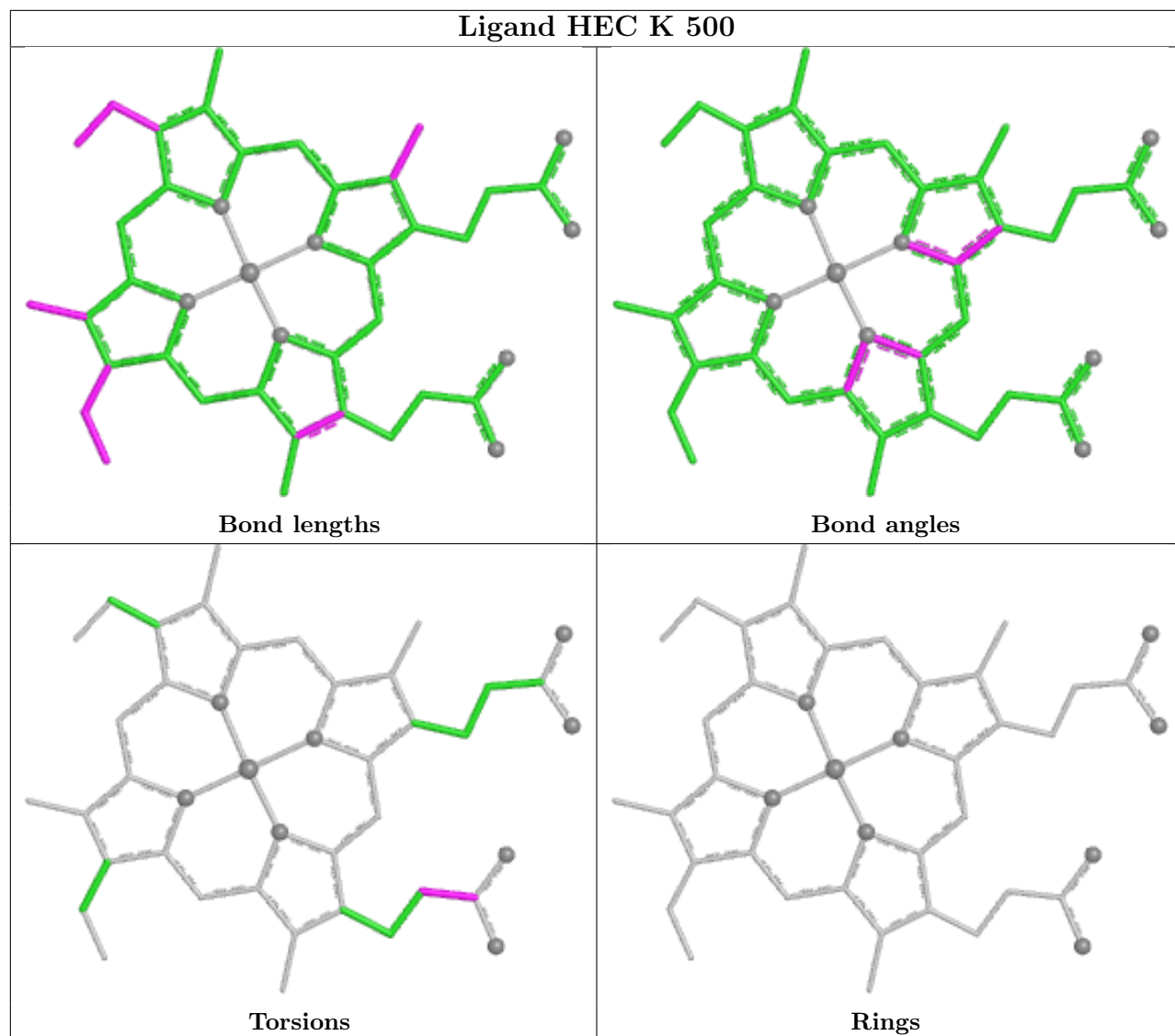
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1301	DTP	3	0
5	M	500	HEC	2	0
4	C	1301	DTP	3	0
5	K	500	HEC	2	0
5	J	500	HEC	2	0
4	F	1301	DTP	3	0
5	N	500	HEC	2	0
4	B	1301	DTP	3	0
5	L	500	HEC	2	0
5	I	500	HEC	2	0
5	H	500	HEC	2	0
4	G	1301	DTP	3	0
4	D	1301	DTP	3	0
4	E	1301	DTP	3	0

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.

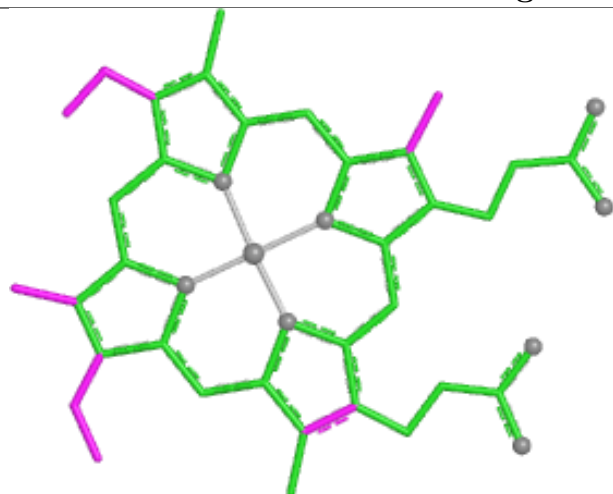




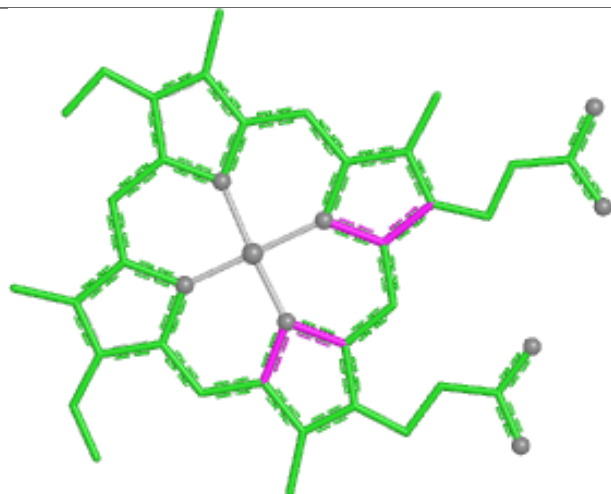




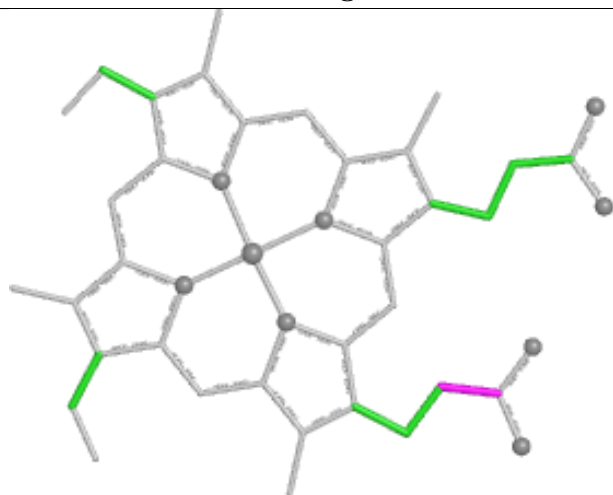
Ligand HEC J 500



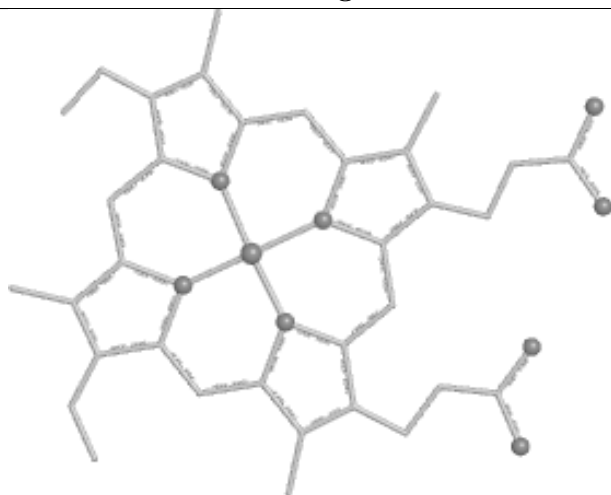
Bond lengths



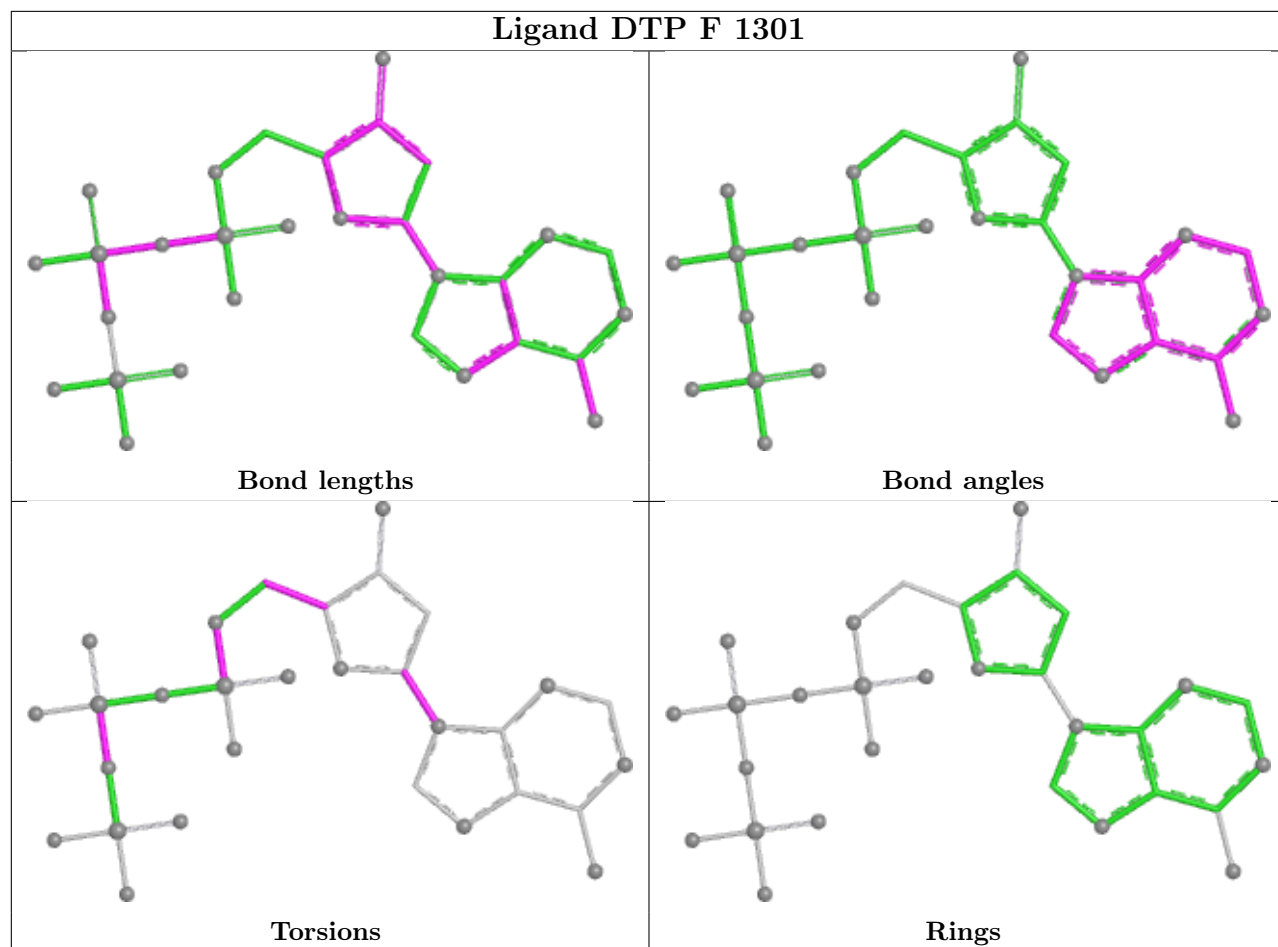
Bond angles

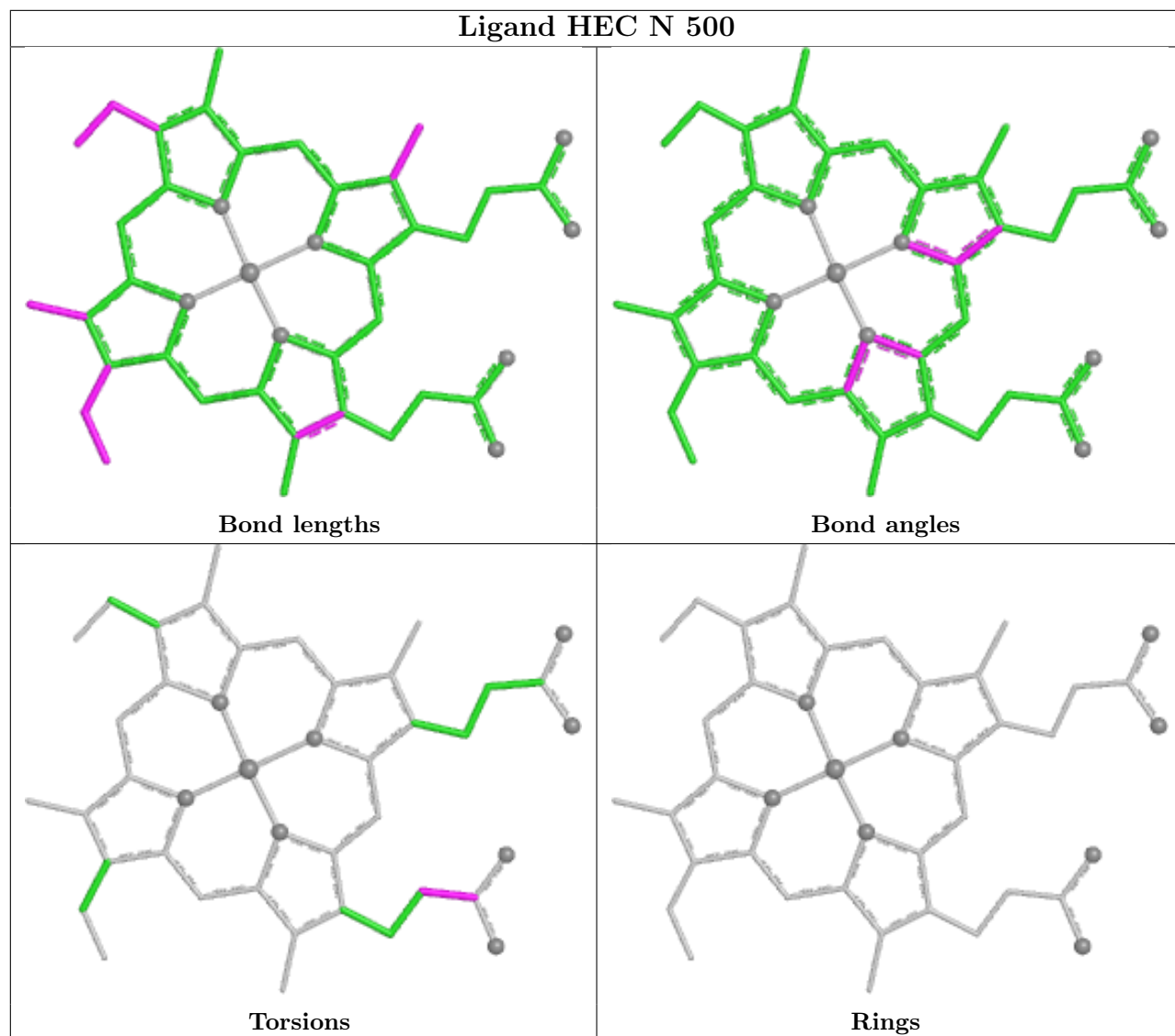


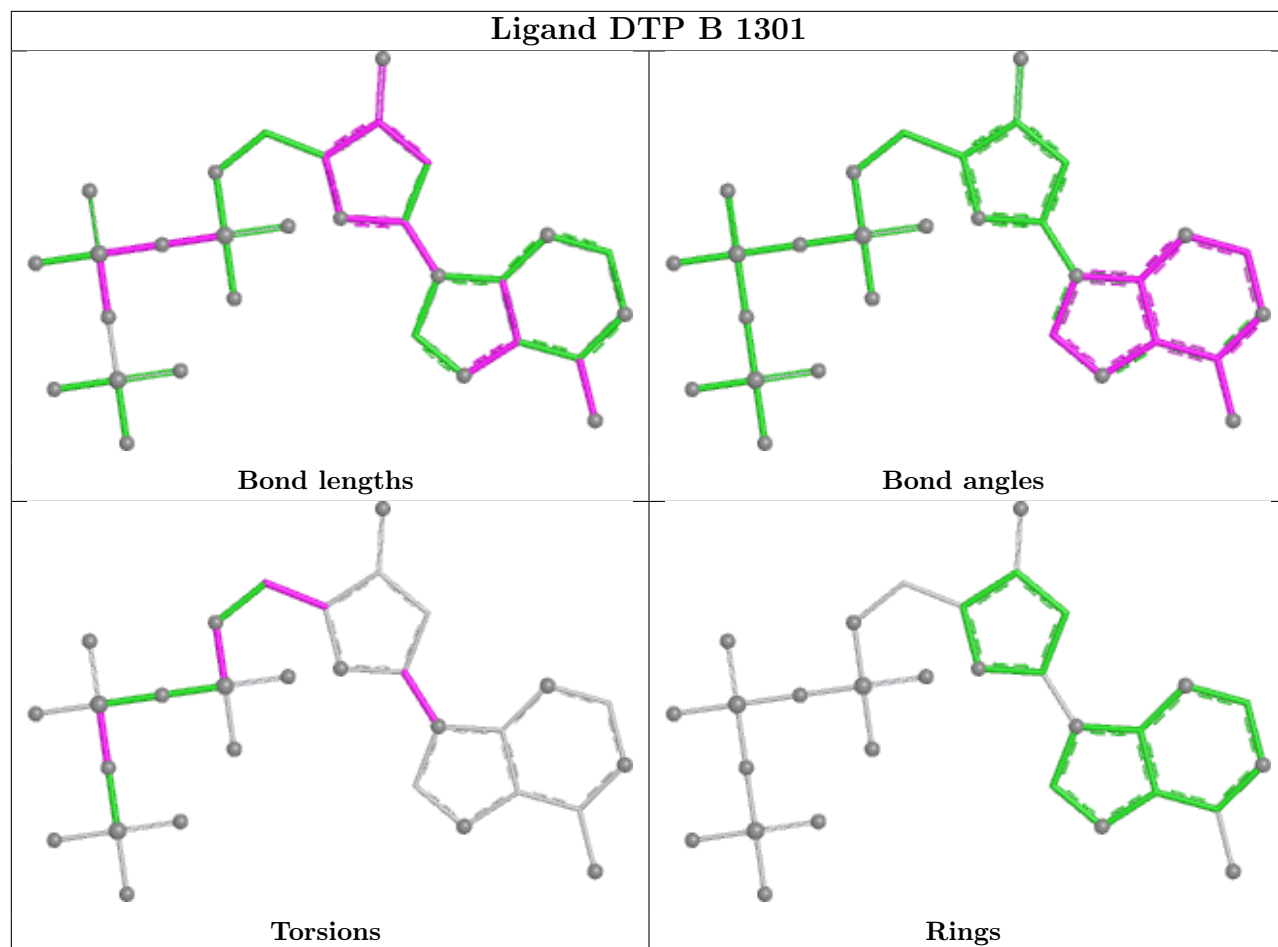
Torsions

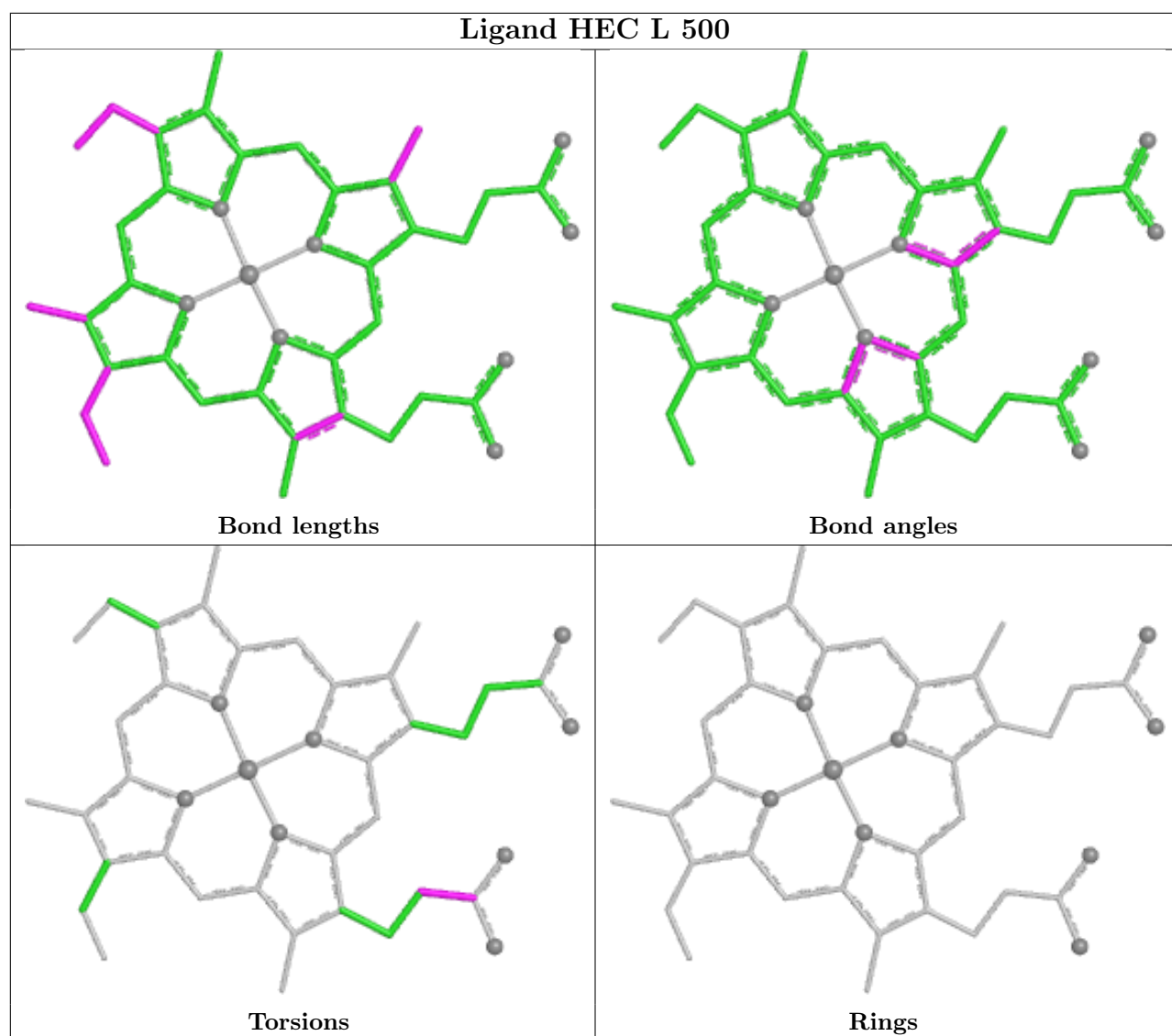


Rings

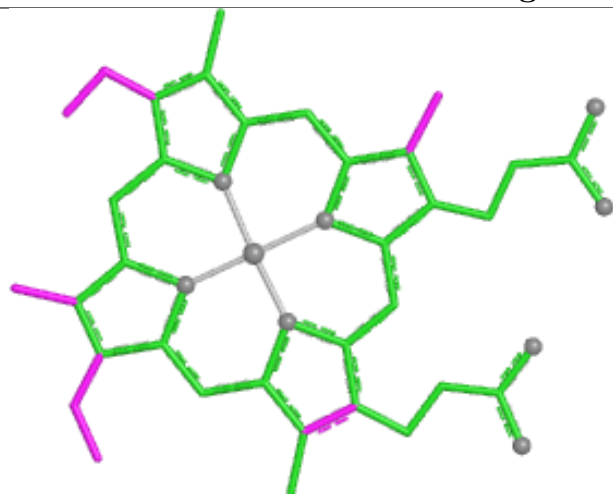




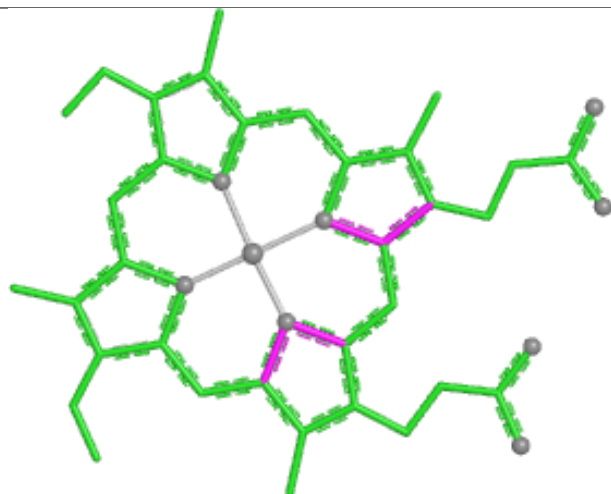




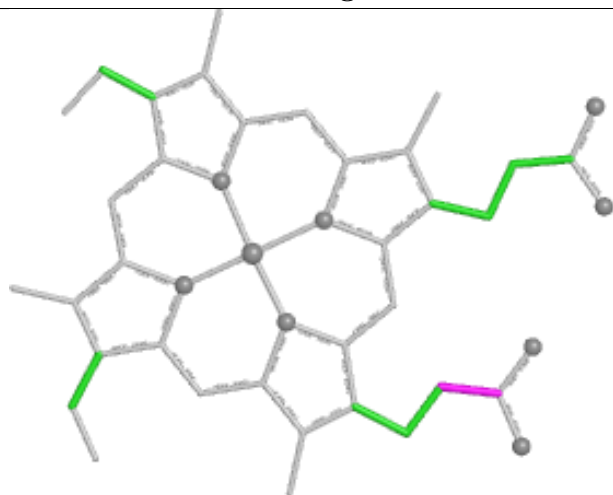
Ligand HEC I 500



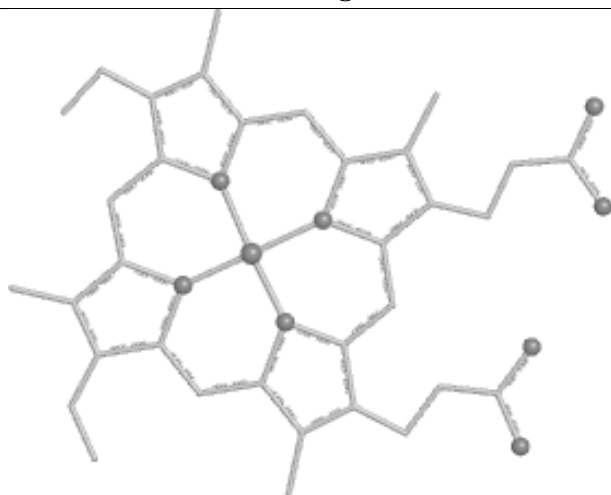
Bond lengths



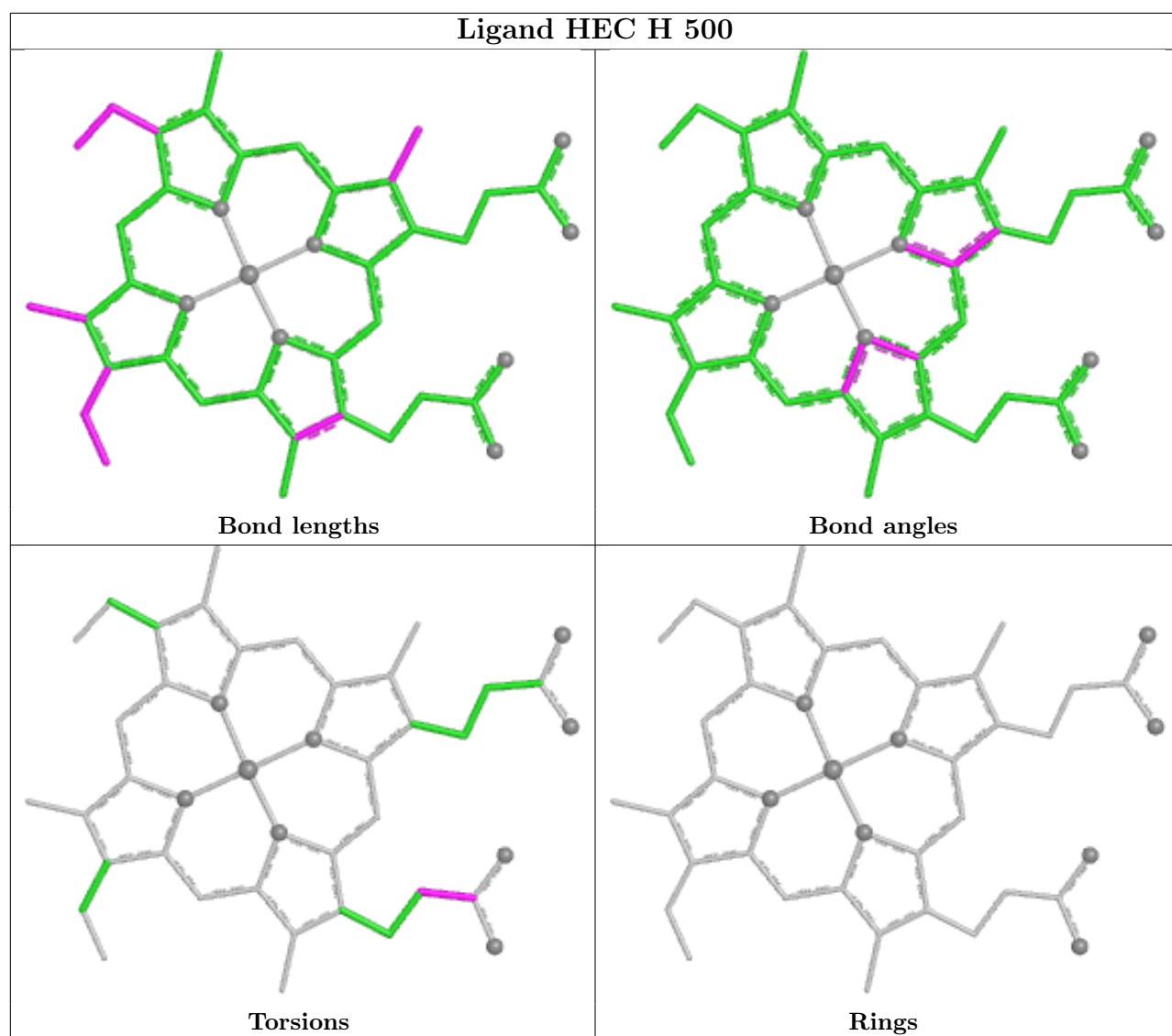
Bond angles

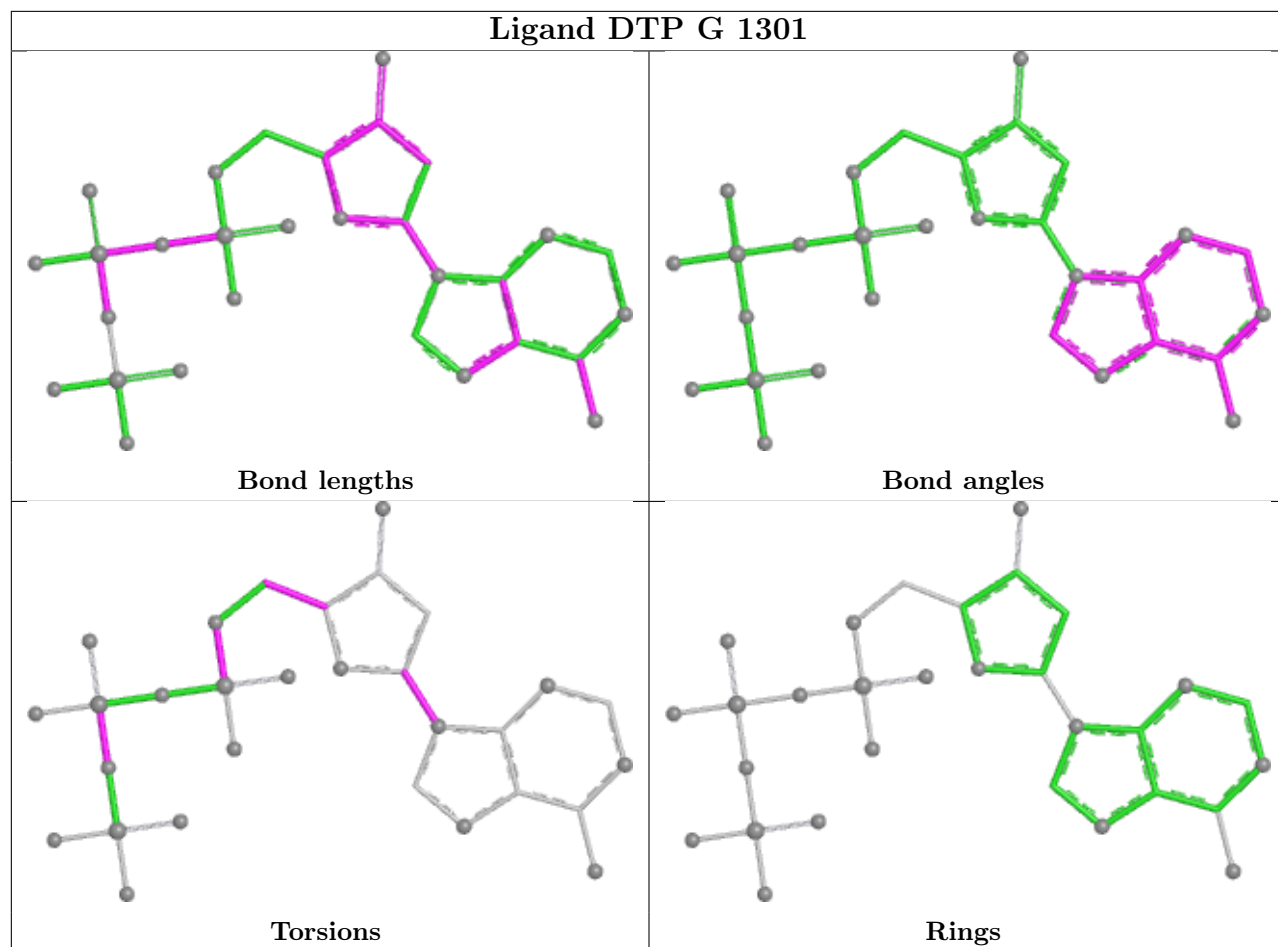


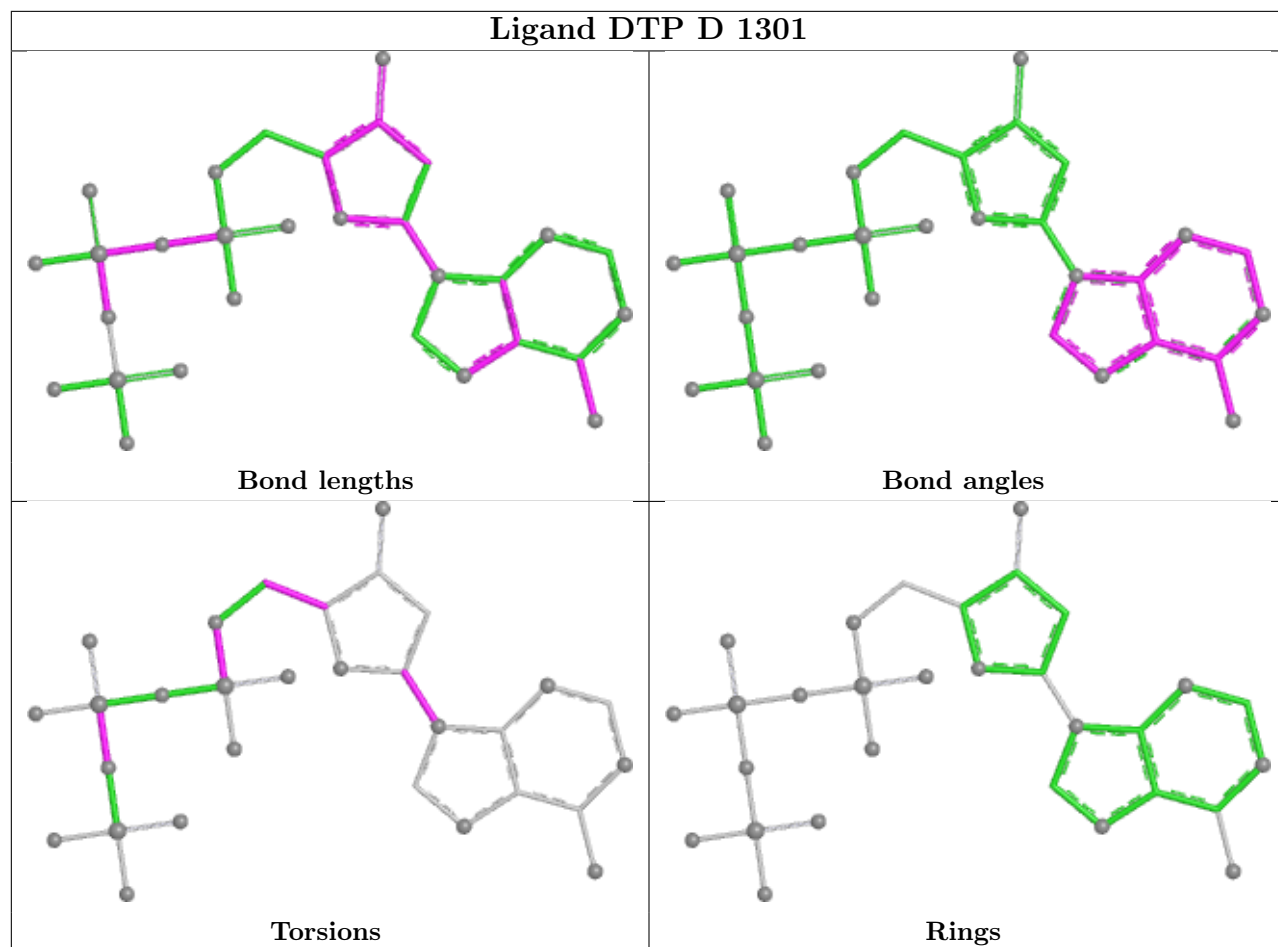
Torsions

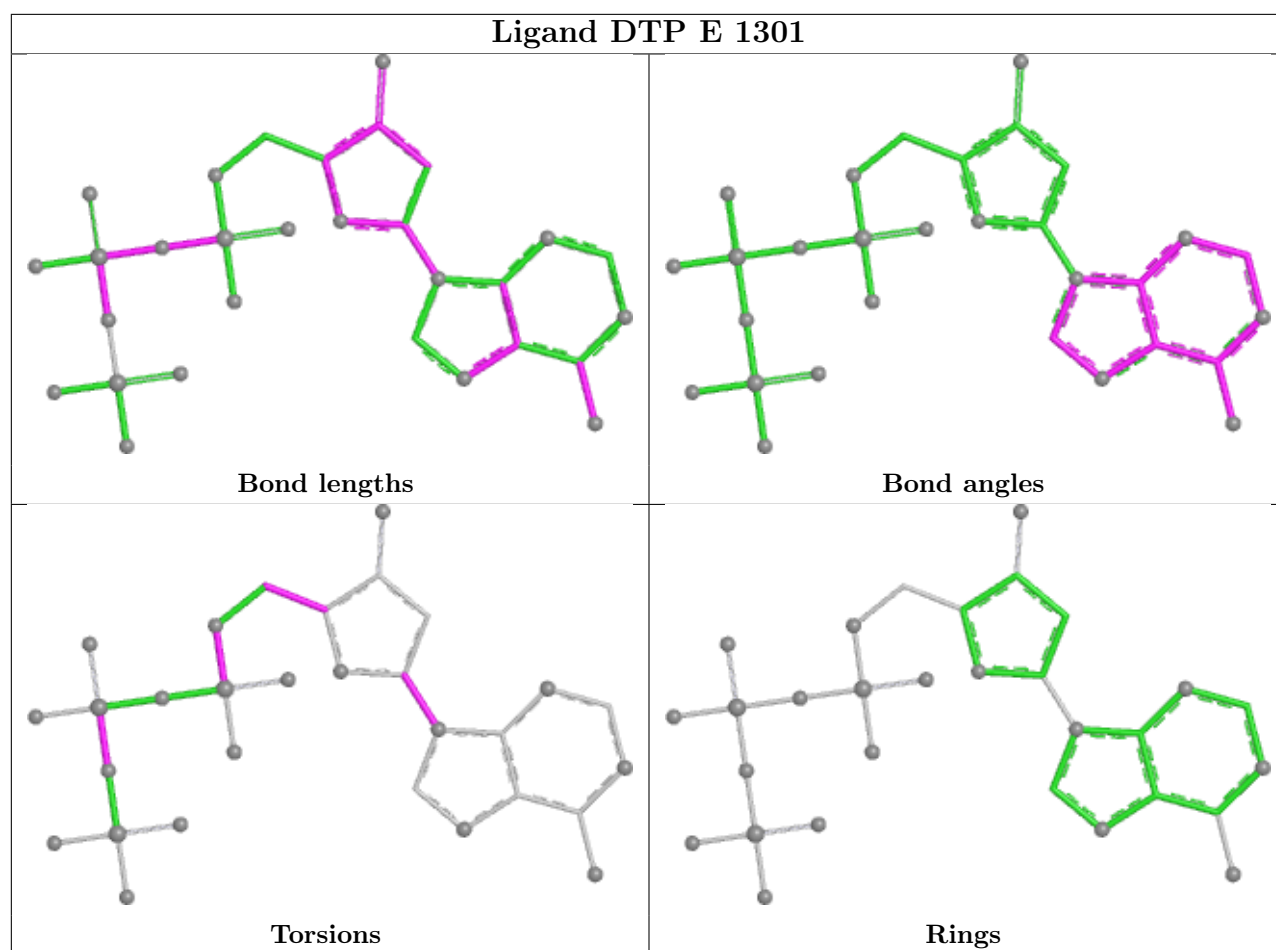


Rings









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.

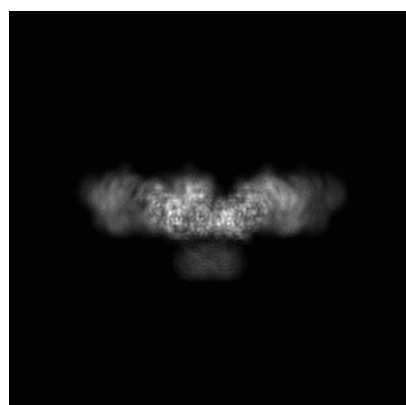
6 Map visualisation [i](#)

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.

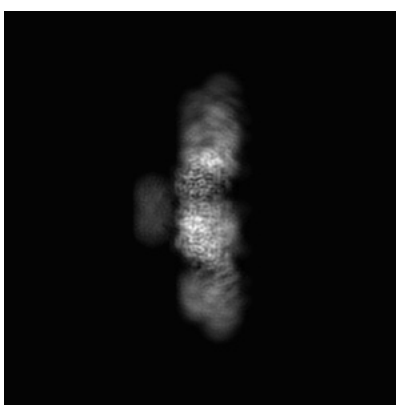
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

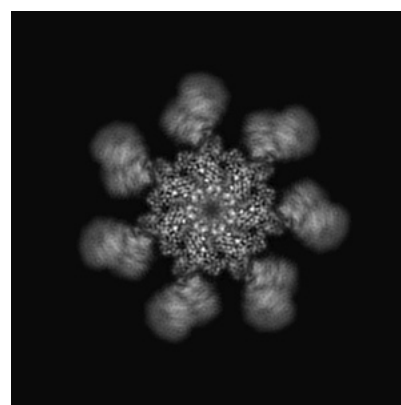
6.1.1 Primary map



X



Y

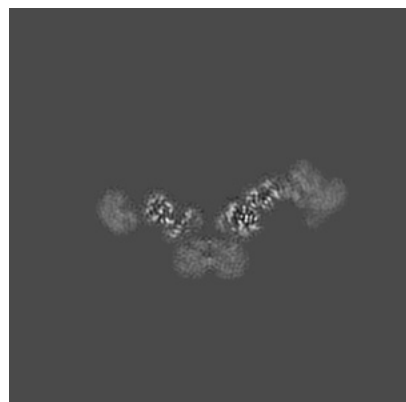


Z

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

6.2 Central slices [i](#)

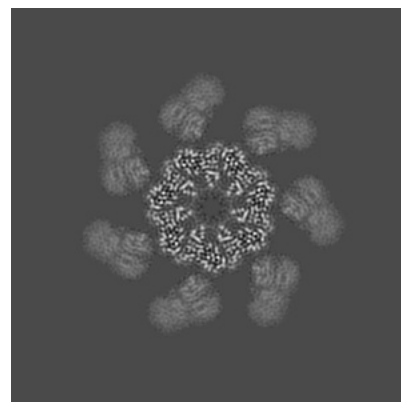
6.2.1 Primary map



X Index: 160



Y Index: 160



Z Index: 160

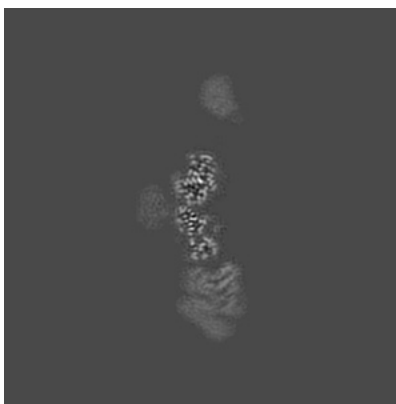
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

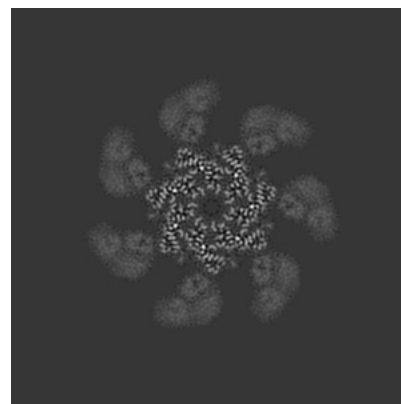
6.3.1 Primary map



X Index: 146



Y Index: 135

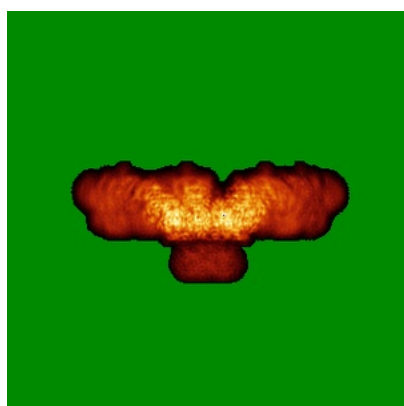


Z Index: 157

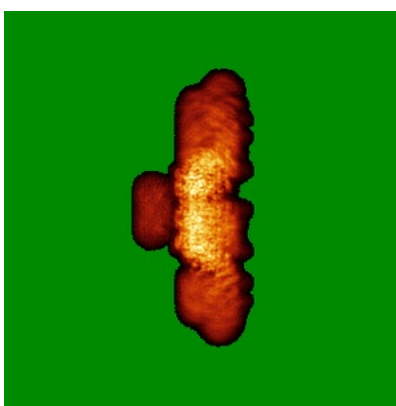
The images above show the largest variance slices of the map in three orthogonal directions.

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

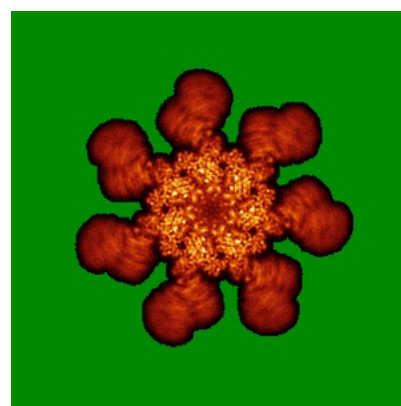
6.4.1 Primary map



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

This section was not generated.

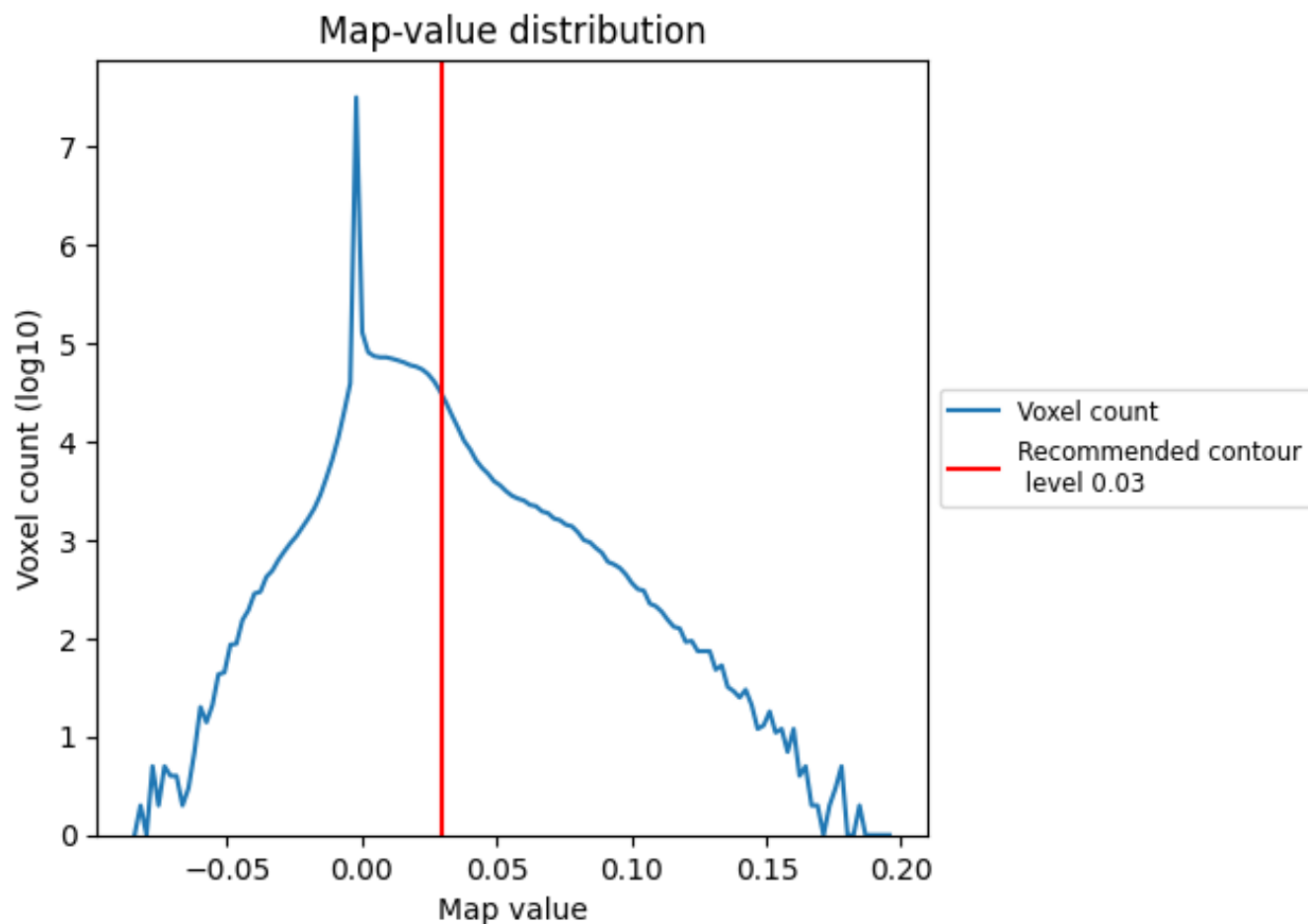
6.6 Mask visualisation

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

7 Map analysis [i](#)

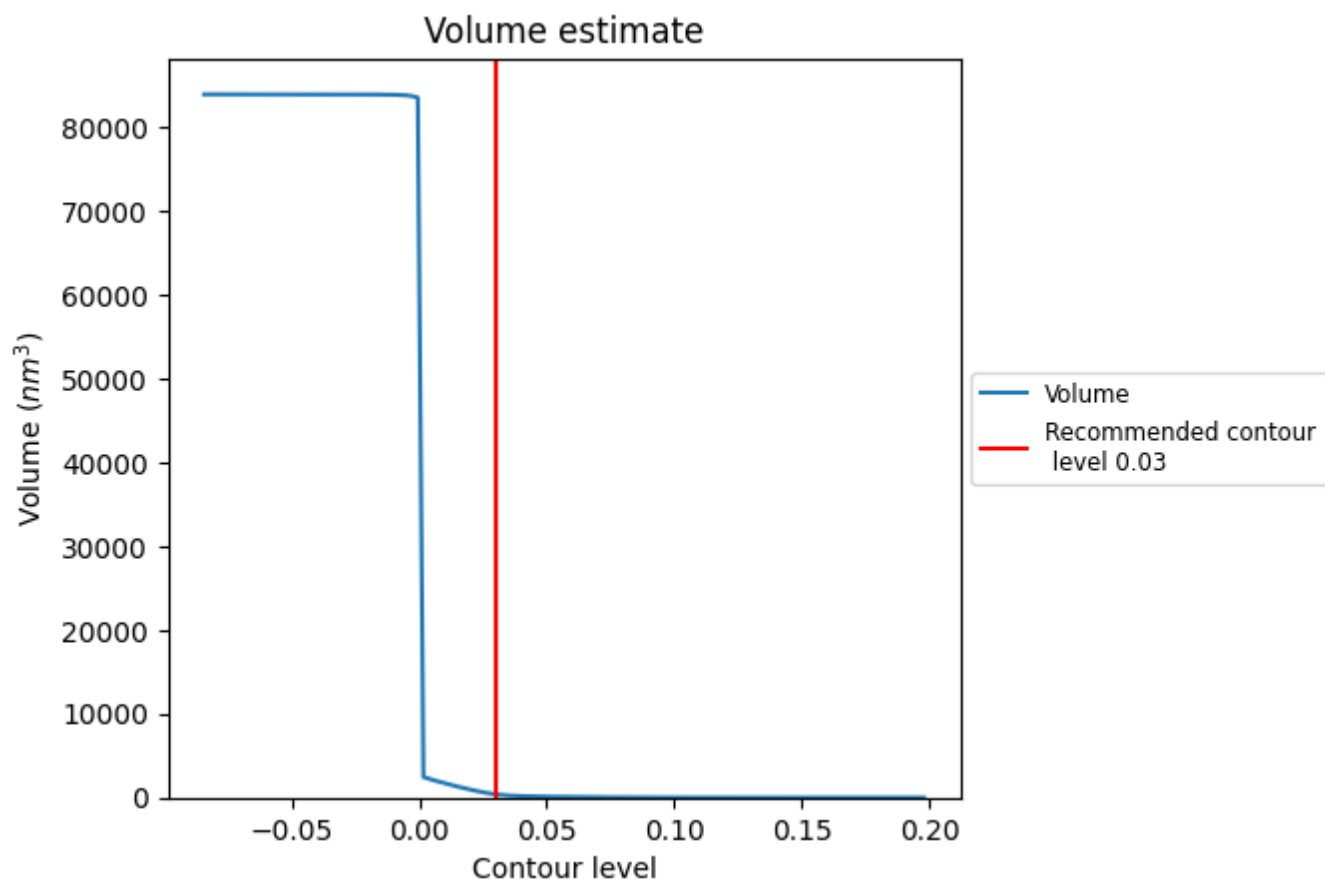
This section contains the results of statistical analysis of the map.

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.

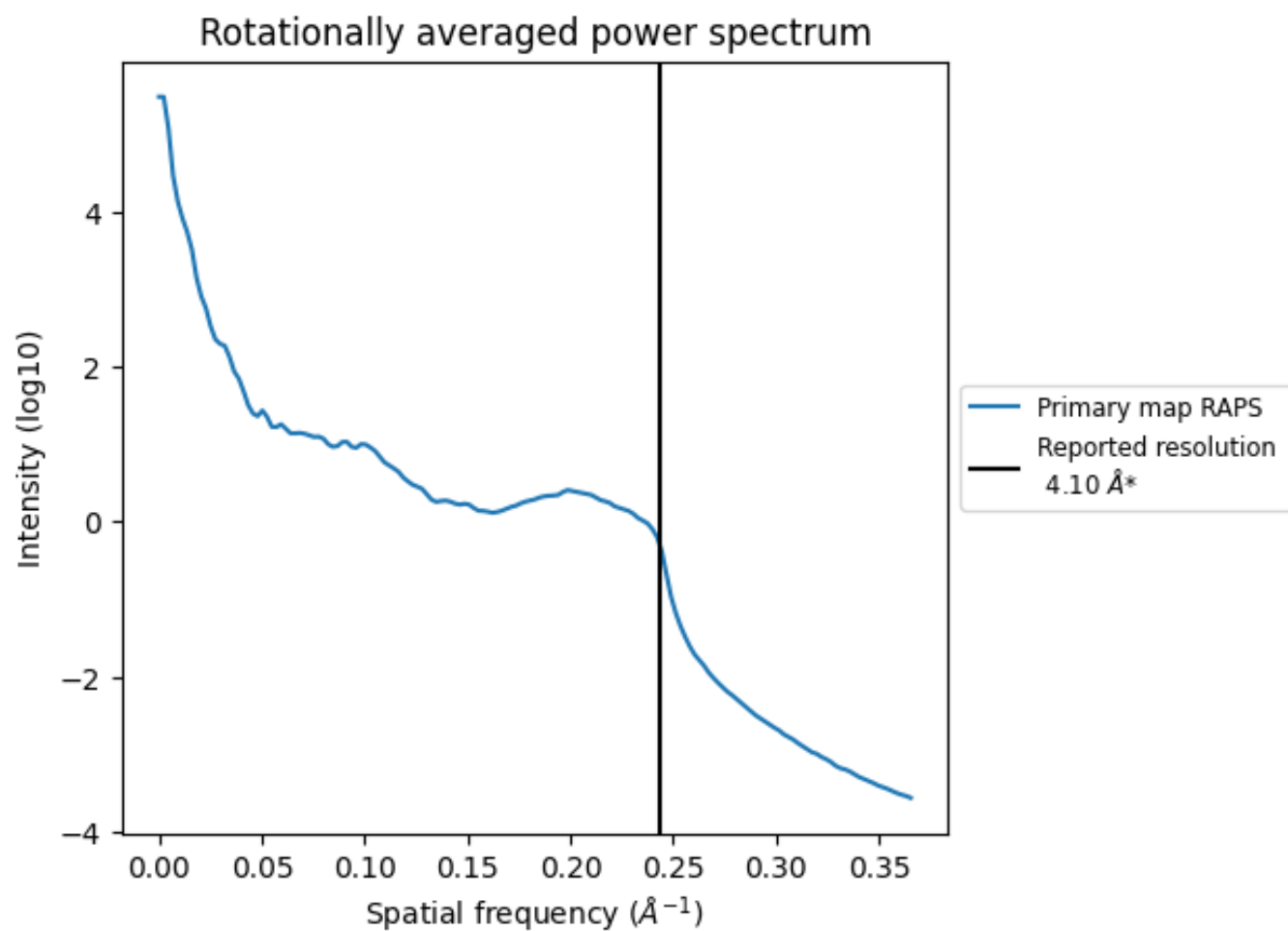
7.2 Volume estimate [i](#)



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

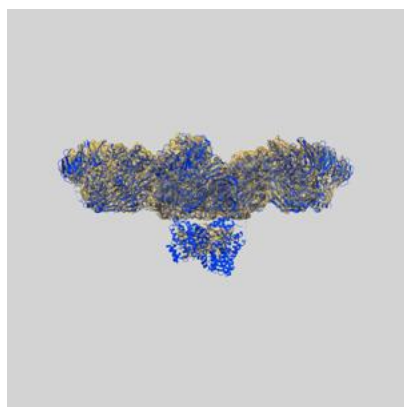
8 Fourier-Shell correlation

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

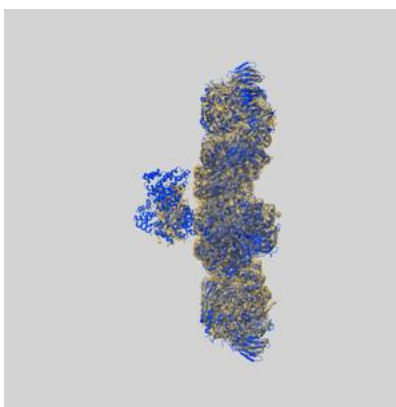
9 Map-model fit [i](#)

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](#).

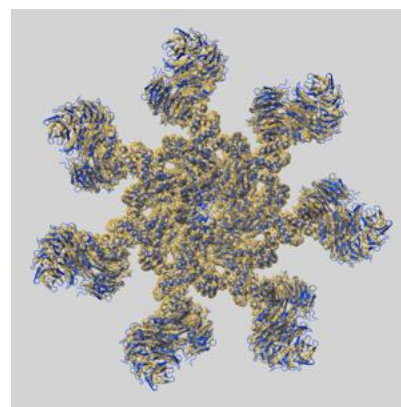
9.1 Map-model overlay [i](#)



X



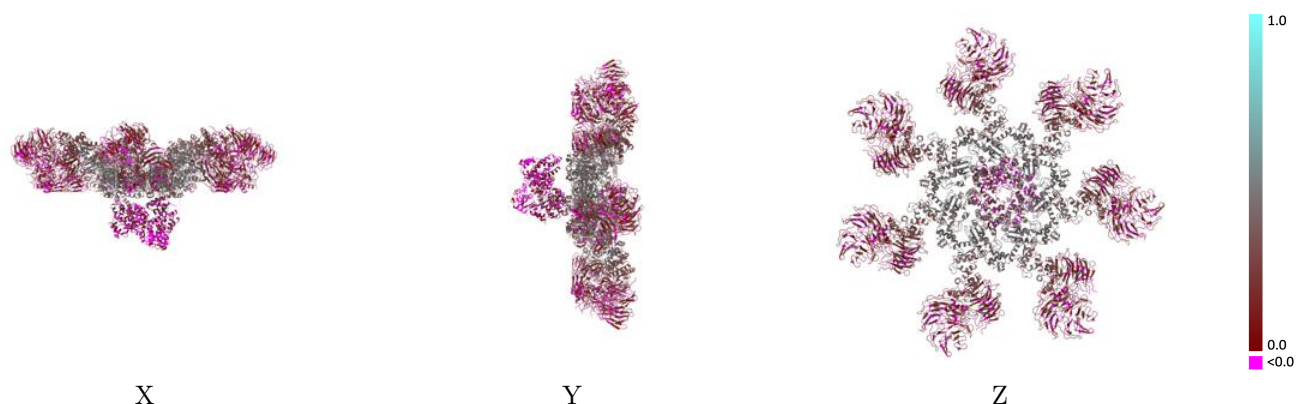
Y



Z

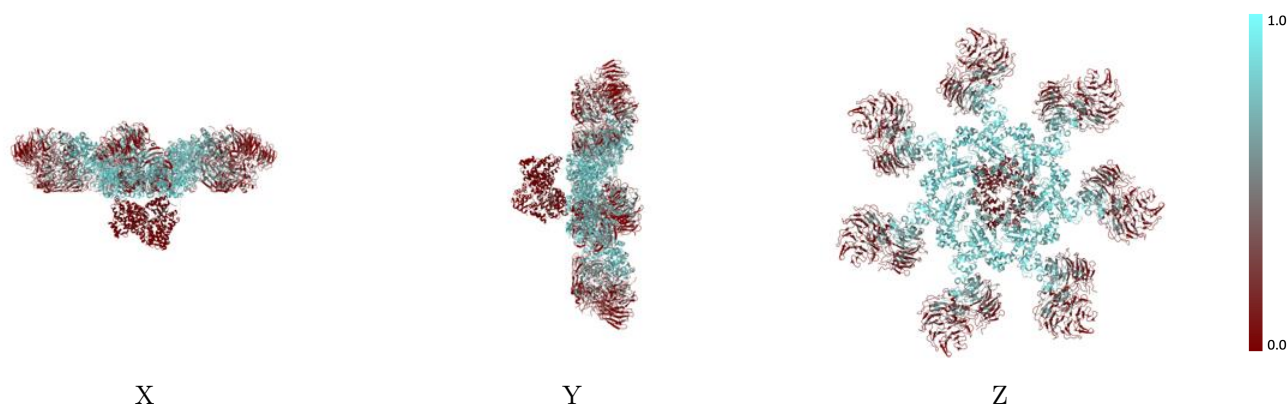
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



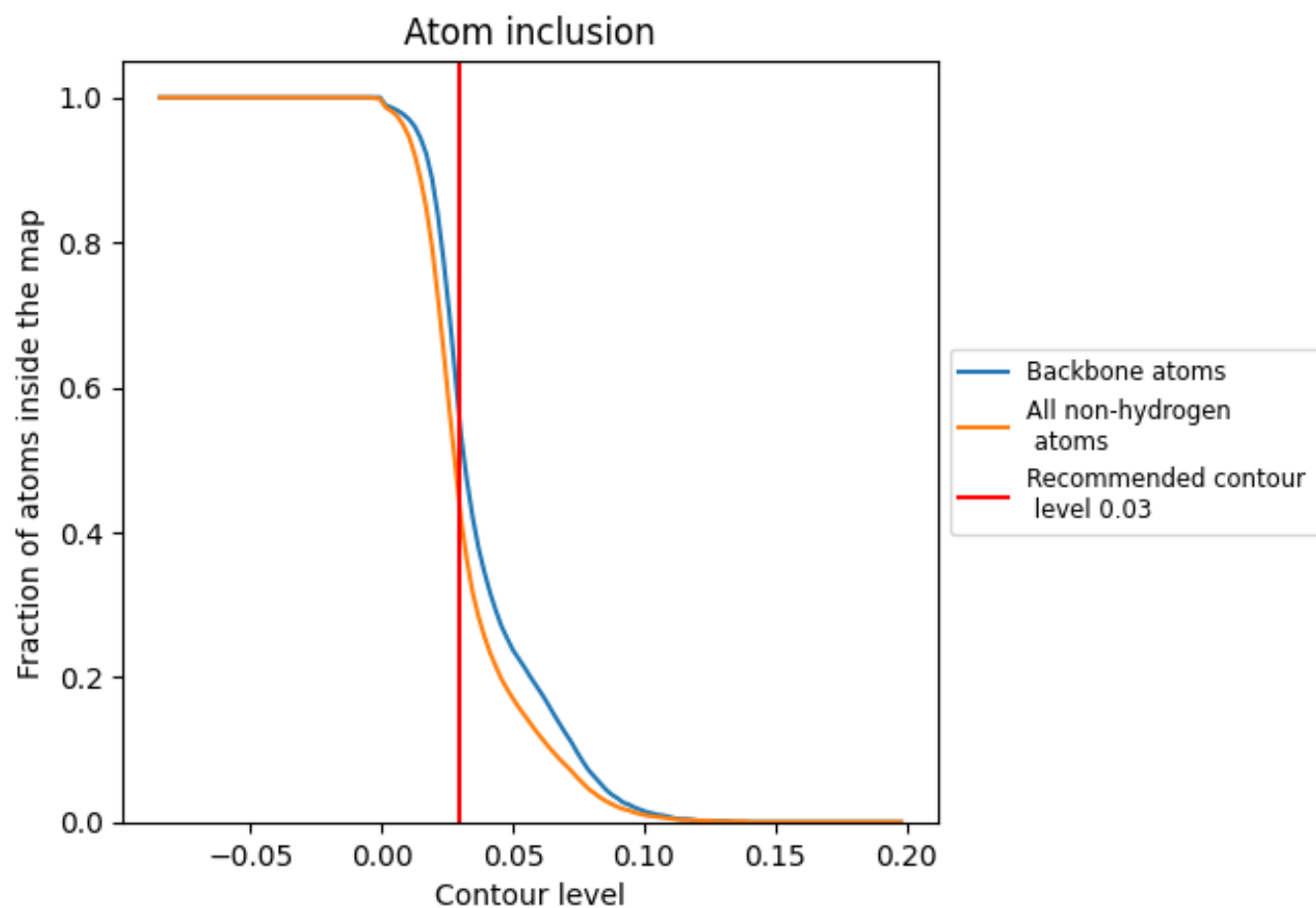
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	 -0.0120
R	 0.0040	 -0.0460

