



wwPDB EM Validation Summary Report ⓘ

Mar 25, 2026 – 03:53 PM UTC

PDB ID : 3JBT / pdb_00003jbt
EMDB ID : EMD-6480
Title : Atomic structure of the Apaf-1 apoptosome
Authors : Zhou, M.; Li, Y.; Hu, Q.; Bai, X.; Huang, W.; Yan, C.; Scheres, S.H.W.; Shi, Y.
Deposited on : 2015-10-15
Resolution : 3.80 Å (reported)
Based on initial models : 3J2T, 4RSZ

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:

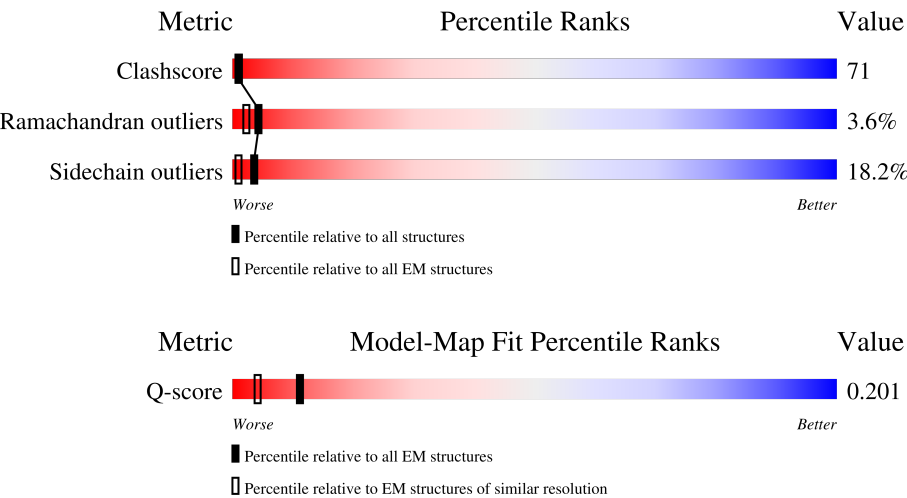
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.80 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	10198 (3.30 - 4.30)

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	1260	
1	C	1260	
1	E	1260	
1	G	1260	

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Mol	Chain	Length	Quality of chain
1	I	1260	50% 31%43%15%9%
1	K	1260	50% 31%43%15%9%
1	M	1260	50% 31%44%15%9%
2	B	105	94% 83%13%..
2	D	105	94% 83%13%..
2	F	105	94% 83%13%..
2	H	105	95% 83%13%..
2	J	105	94% 83%13%..
2	L	105	94% 83%13%..
2	N	105	94% 83%14%..

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 70252 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	1144	Total	C	N	O	S	0	0
			9139	5789	1569	1720	61		
1	C	1144	Total	C	N	O	S	0	0
			9139	5789	1569	1720	61		
1	E	1144	Total	C	N	O	S	0	0
			9139	5789	1569	1720	61		
1	G	1144	Total	C	N	O	S	0	0
			9139	5789	1569	1720	61		
1	I	1144	Total	C	N	O	S	0	0
			9139	5789	1569	1720	61		
1	K	1144	Total	C	N	O	S	0	0
			9139	5789	1569	1720	61		
1	M	1144	Total	C	N	O	S	0	0
			9139	5789	1569	1720	61		

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1249	LEU	-	expression tag	UNP O14727
A	1250	GLU	-	expression tag	UNP O14727
A	1251	HIS	-	expression tag	UNP O14727
A	1252	HIS	-	expression tag	UNP O14727
A	1253	HIS	-	expression tag	UNP O14727
A	1254	HIS	-	expression tag	UNP O14727
A	1255	HIS	-	expression tag	UNP O14727
A	1256	HIS	-	expression tag	UNP O14727
A	1257	HIS	-	expression tag	UNP O14727
A	1258	HIS	-	expression tag	UNP O14727
A	1259	HIS	-	expression tag	UNP O14727
A	1260	HIS	-	expression tag	UNP O14727
C	1249	LEU	-	expression tag	UNP O14727
C	1250	GLU	-	expression tag	UNP O14727
C	1251	HIS	-	expression tag	UNP O14727
C	1252	HIS	-	expression tag	UNP O14727

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1253	HIS	-	expression tag	UNP O14727
C	1254	HIS	-	expression tag	UNP O14727
C	1255	HIS	-	expression tag	UNP O14727
C	1256	HIS	-	expression tag	UNP O14727
C	1257	HIS	-	expression tag	UNP O14727
C	1258	HIS	-	expression tag	UNP O14727
C	1259	HIS	-	expression tag	UNP O14727
C	1260	HIS	-	expression tag	UNP O14727
E	1249	LEU	-	expression tag	UNP O14727
E	1250	GLU	-	expression tag	UNP O14727
E	1251	HIS	-	expression tag	UNP O14727
E	1252	HIS	-	expression tag	UNP O14727
E	1253	HIS	-	expression tag	UNP O14727
E	1254	HIS	-	expression tag	UNP O14727
E	1255	HIS	-	expression tag	UNP O14727
E	1256	HIS	-	expression tag	UNP O14727
E	1257	HIS	-	expression tag	UNP O14727
E	1258	HIS	-	expression tag	UNP O14727
E	1259	HIS	-	expression tag	UNP O14727
E	1260	HIS	-	expression tag	UNP O14727
G	1249	LEU	-	expression tag	UNP O14727
G	1250	GLU	-	expression tag	UNP O14727
G	1251	HIS	-	expression tag	UNP O14727
G	1252	HIS	-	expression tag	UNP O14727
G	1253	HIS	-	expression tag	UNP O14727
G	1254	HIS	-	expression tag	UNP O14727
G	1255	HIS	-	expression tag	UNP O14727
G	1256	HIS	-	expression tag	UNP O14727
G	1257	HIS	-	expression tag	UNP O14727
G	1258	HIS	-	expression tag	UNP O14727
G	1259	HIS	-	expression tag	UNP O14727
G	1260	HIS	-	expression tag	UNP O14727
I	1249	LEU	-	expression tag	UNP O14727
I	1250	GLU	-	expression tag	UNP O14727
I	1251	HIS	-	expression tag	UNP O14727
I	1252	HIS	-	expression tag	UNP O14727
I	1253	HIS	-	expression tag	UNP O14727
I	1254	HIS	-	expression tag	UNP O14727
I	1255	HIS	-	expression tag	UNP O14727
I	1256	HIS	-	expression tag	UNP O14727
I	1257	HIS	-	expression tag	UNP O14727
I	1258	HIS	-	expression tag	UNP O14727

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Chain	Residue	Modelled	Actual	Comment	Reference
I	1259	HIS	-	expression tag	UNP O14727
I	1260	HIS	-	expression tag	UNP O14727
K	1249	LEU	-	expression tag	UNP O14727
K	1250	GLU	-	expression tag	UNP O14727
K	1251	HIS	-	expression tag	UNP O14727
K	1252	HIS	-	expression tag	UNP O14727
K	1253	HIS	-	expression tag	UNP O14727
K	1254	HIS	-	expression tag	UNP O14727
K	1255	HIS	-	expression tag	UNP O14727
K	1256	HIS	-	expression tag	UNP O14727
K	1257	HIS	-	expression tag	UNP O14727
K	1258	HIS	-	expression tag	UNP O14727
K	1259	HIS	-	expression tag	UNP O14727
K	1260	HIS	-	expression tag	UNP O14727
M	1249	LEU	-	expression tag	UNP O14727
M	1250	GLU	-	expression tag	UNP O14727
M	1251	HIS	-	expression tag	UNP O14727
M	1252	HIS	-	expression tag	UNP O14727
M	1253	HIS	-	expression tag	UNP O14727
M	1254	HIS	-	expression tag	UNP O14727
M	1255	HIS	-	expression tag	UNP O14727
M	1256	HIS	-	expression tag	UNP O14727
M	1257	HIS	-	expression tag	UNP O14727
M	1258	HIS	-	expression tag	UNP O14727
M	1259	HIS	-	expression tag	UNP O14727
M	1260	HIS	-	expression tag	UNP O14727

- Molecule 2 is a protein called Cytochrome c.

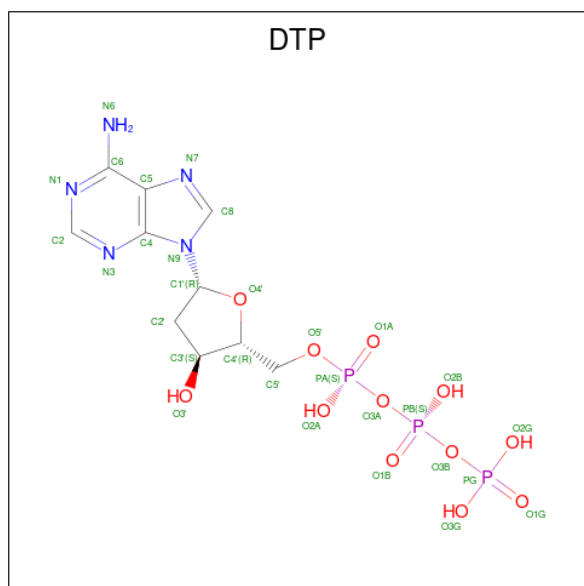
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	104	Total 823	C 524	N 144	O 151	S 4	0	0
2	D	104	Total 823	C 524	N 144	O 151	S 4	0	0
2	F	104	Total 823	C 524	N 144	O 151	S 4	0	0
2	H	104	Total 823	C 524	N 144	O 151	S 4	0	0
2	J	104	Total 823	C 524	N 144	O 151	S 4	0	0
2	L	104	Total 823	C 524	N 144	O 151	S 4	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	N	104	Total	C	N	O	S	0	0
			823	524	144	151	4		

- Molecule 3 is 2'-DEOXYADENOSINE 5'-TRIPHOSPHATE (CCD ID: DTP) (formula: $C_{10}H_{16}N_5O_{12}P_3$)



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			30	10	5	12	3	
3	C	1	Total	C	N	O	P	0
			30	10	5	12	3	
3	E	1	Total	C	N	O	P	0
			30	10	5	12	3	
3	G	1	Total	C	N	O	P	0
			30	10	5	12	3	
3	I	1	Total	C	N	O	P	0
			30	10	5	12	3	
3	K	1	Total	C	N	O	P	0
			30	10	5	12	3	
3	M	1	Total	C	N	O	P	0
			30	10	5	12	3	

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms	AltConf
4	C	1	Total 1 Mg 1	0
4	E	1	Total 1 Mg 1	0
4	G	1	Total 1 Mg 1	0
4	I	1	Total 1 Mg 1	0
4	K	1	Total 1 Mg 1	0
4	M	1	Total 1 Mg 1	0

- # HEM

Mol	Chain	Residues	Atoms					AltConf
5	B	1	Total 43	C 34	Fe 1	N 4	O 4	0
5	D	1	Total 43	C 34	Fe 1	N 4	O 4	0
5	F	1	Total 43	C 34	Fe 1	N 4	O 4	0
5	H	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



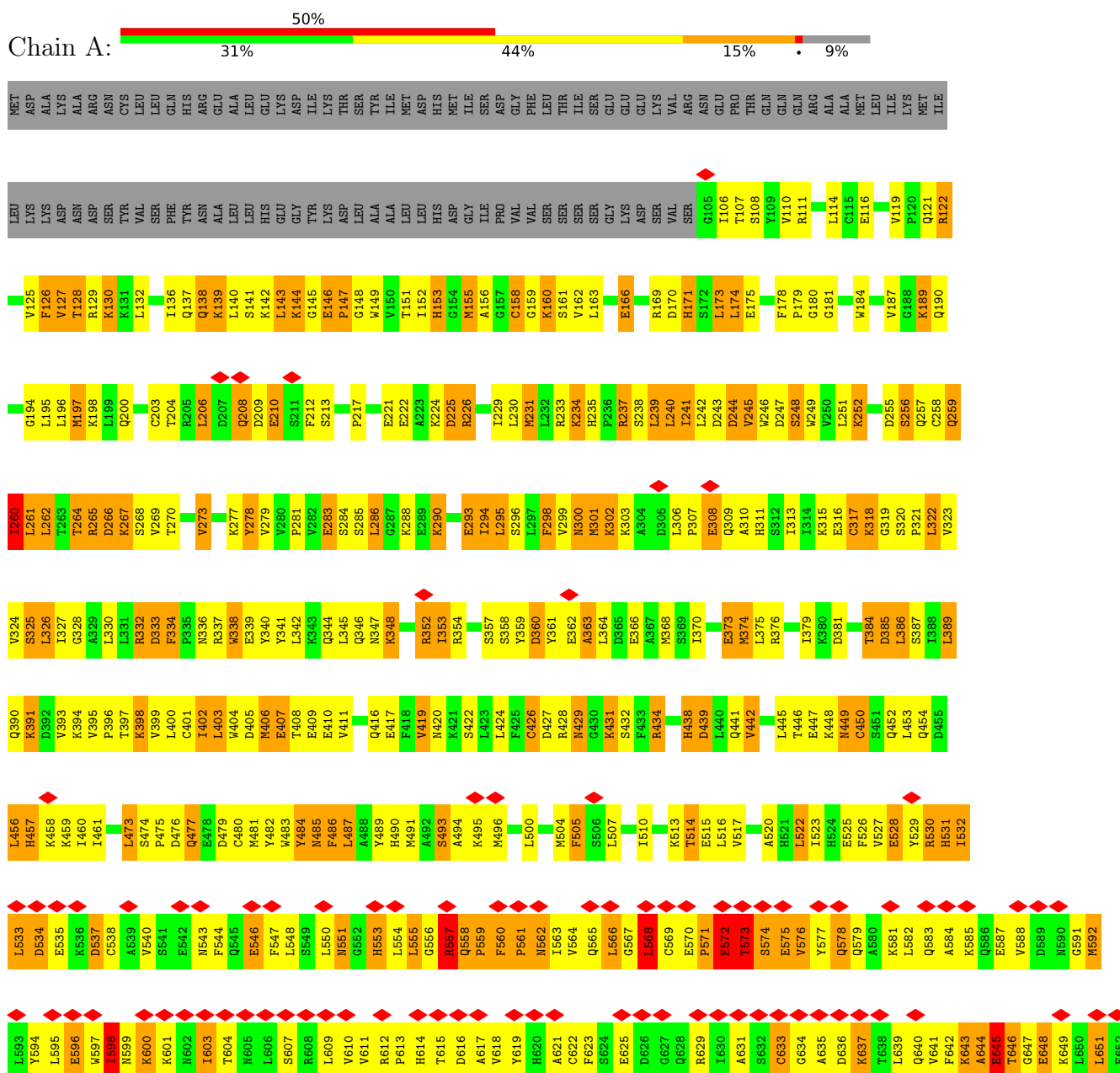
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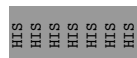
Mol	Chain	Residues	Atoms					AltConf
5	L	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
5	N	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

3 Residue-property plots

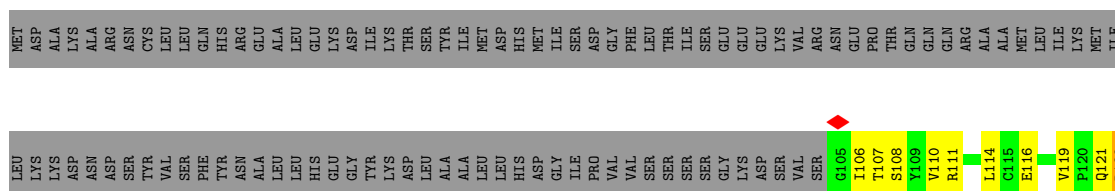
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

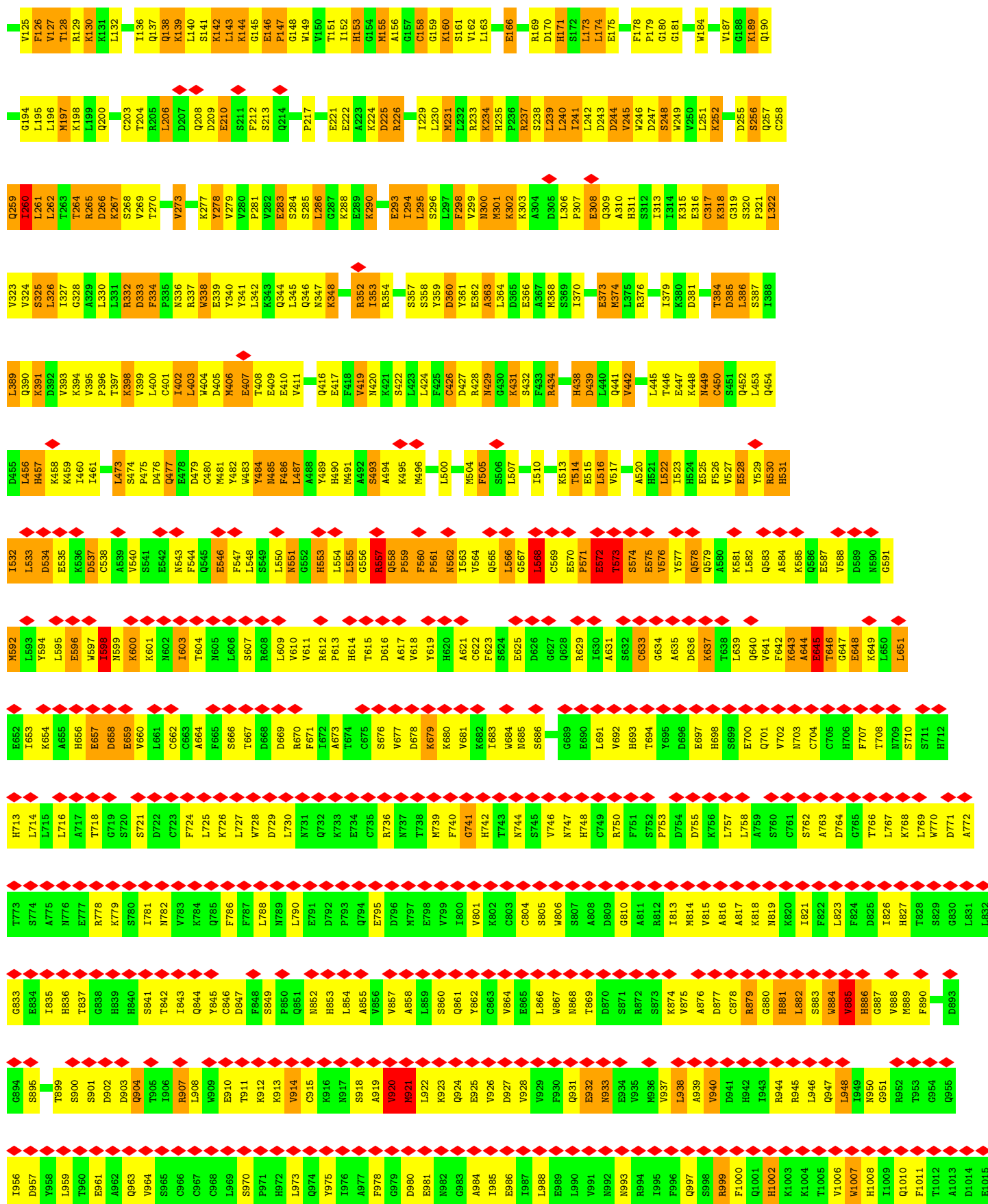
- Molecule 1: Apoptotic protease-activating factor 1



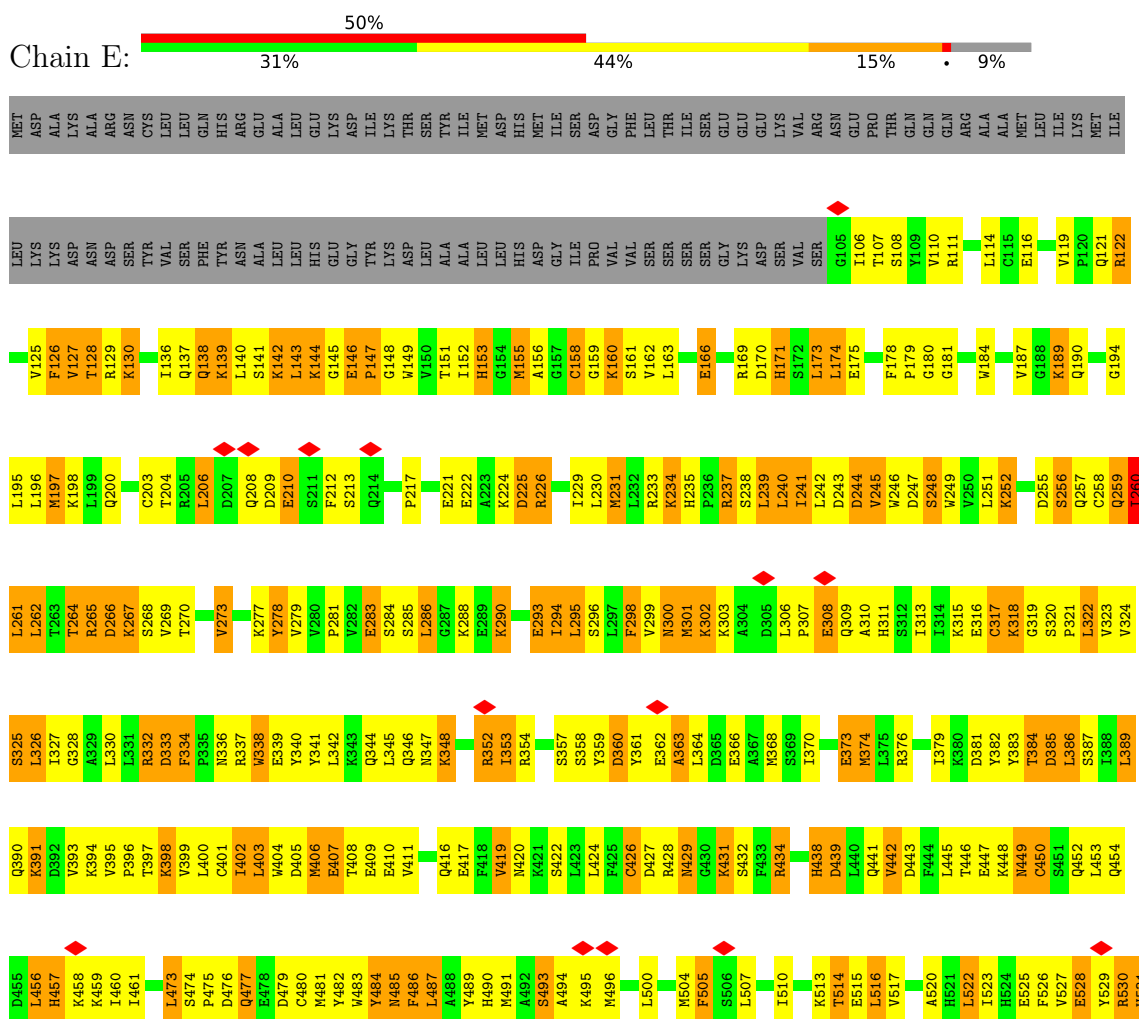


Chain C:





- Molecule 1: Apoptotic protease-activating factor 1



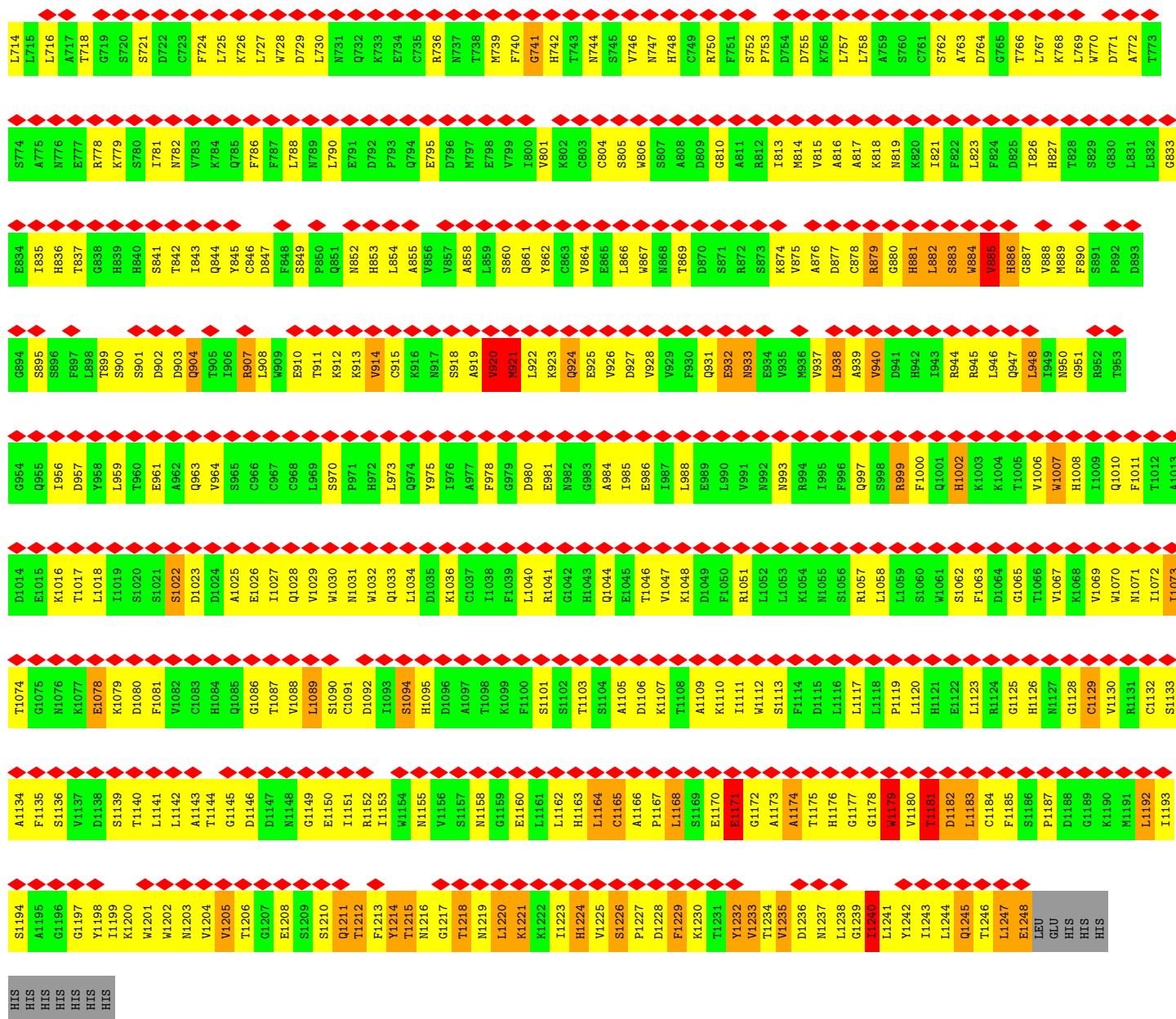


MET	ASP	ALA	LYS	ALA	LYS	ARG	ASN	CYS	LEU	LEU	GLN	HIS	ARG	GLU	ALA	LEU	LEU	GLY	ASP	ASP	GLY	ASP	GLY	VAL	ARG	ASN	GLU	PRO	THR	GLN	GLN	ARG	ALA	ALA	LEU	ILE	LYS	MET	ILE																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																						
LEU	LYS	LYS	ASP	ASN	ASP	ASP	TYR	VAL	SER	PHE	TYR	ASN	ALA	ALA	LEU	HIS	GLY	ASP	ILE	TYR	LYS	ASP	ALA	VAL	SER	ASN	G105	I106	T107	S108	Y109	R110	R111	C114	C115	E116	V119	G188	P120	Q121	R122																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																				

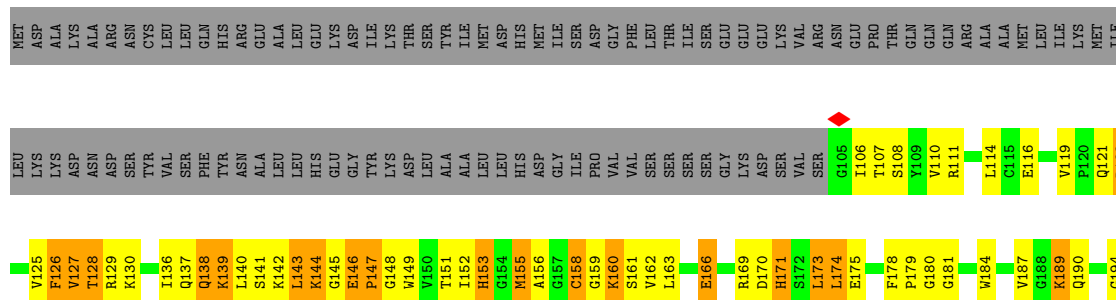


K391	D392	V393	K394	V395	P396	T397	K398	V399	L400	C401	I402	L403	W404	D405	M406	E407	T408	E409	E410	V411		Q416	E417	E418	V419	N420	K421	S422	L423	L424	F425	C426	D427	R428	S429	G430	K431		R434		H438	D439	L440	Q441	V442		L445	T446	E447	K448	N449	C450	S451	Q452	L453	Q454	D455	L456	H457																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																					
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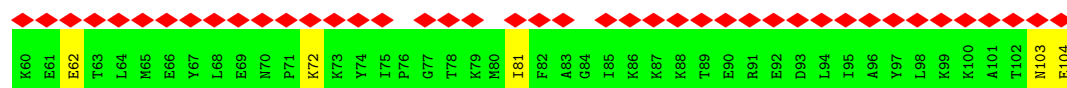
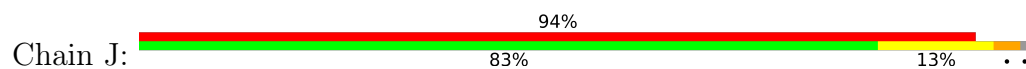
• Molecule 1: Apoptotic protease-activating factor 1



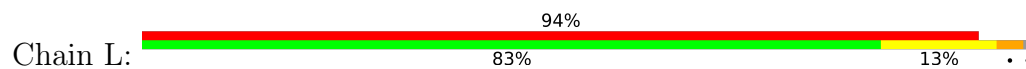
L1018	Y958	T899	I835	A775	L715	K654	Y594	D634	H457	K391	L326	L282	L195
I1019	L959	S900	H836	W776	L716	A655	L595	E535	K458	D392	I327	T263	L196
S1020	T960	S901	T837	E777	A717	H656	E596	K536	K459	V393	G328	T264	M197
S1021	E961	D902	G838	R778	T718	E657	E597	D837	I460	K394	A329	R265	K198
S1022	A962	D903	H839	K779	G719	S720	I598	C538	I461	V395	L330	D266	L199
D1023	Q963	D904	H840	S780	S721	C723	N599	A539	L473	T397	R332	S268	Q200
D1024	V964	T905	S841	L781	D722	F724	K601	E540	S474	K398	D333	V269	C203
A1025	S965	I906	T842	W782	C723	L725	N602	S541	D476	V334	F334	T270	T204
E1026	C966	R907	T843	K783	F724	K726	I603	E542	P475	L400	P335		R205
I1027	C967	L908	Q844	L784	C662	W728	L603	N543	Q477	C401	N336	V273	L206
C968	C968	F909	Y845	Q785	F665	L727	N605	Q545	E478	L402	R337	D207	
V1029	L969	E910	C846	F786	S666	D729	L606	E546	C480	W404	E339	Y278	Q208
W1030	S970	T911	D847	F787	T667	W728	S607	F547	Y482	M406	Y340	V279	D209
N1031	P971	K912	F848	L788	D668	R608	R608	L548	Y483	T408	K343	V280	E210
W1032	H972	F913	S849	W789	D669	D729	R609	S549	Y484	T408	Q344	V282	F212
Q1033	L973	Y914	P850	E791	E734	L730	L609	N550	F486	E409	Q344	E283	S213
L1034	C974	C915	Q851	D792	C735	N731	V610	G552	L487	V411	Q346	S285	
D1035	Y975	K916	H853	D793	R736	E671	V611	H553	A488	Q416	N347	L286	P217
K1036	I976	H917	L854	F793	K733	A673	R612	L554	Y489	E417	K288	E221	
C1037	A977	S918	A855	Q794	E734	T674	H614	G556	H490	F418	E289	E222	
I1038	F978	A919	W856	E795	C735	C675	T615	R557	A492	V419	I353	K224	
F1039	G979	Y920	H857	D796	R736	S676	D616	Q558	A494	K421	E293	R226	
L1040	D980	R921	A858	W797	N737	D677	A617	P559	K495	S422	S357	L229	
R1041	E981	L922	L859	E798	T738	D678	V618	F560	M496	L424	S296	L230	
G1042	N982	K923	S860	W799	W739	D678	Y619	P561		F425	D360	W231	
H1043	G983	Q924	Q861	I800	F740	K680	H620	N562	L500	C426	F298	L232	
Q1044	A984	E925	Y862	V801	H742	V681	A621	I563		D427	V299	R233	
E1045	I985	V926	C863	K802	T743	K682	C622	V564	M504	R428	E362	K234	
T1046	E986	D927	V864	C803	T743	L683	F623	Q565	F505	N429	N301	H235	
V1047	I987	Y928	C804	C804	N744	W684	S624	L566	S506	G430	K302	P236	
K1048	L988	Y929	L866	S805	S745	N685	E625	G567	L507	K431	K303	R237	
D1049	E989	F930	W867	W806	V746	S805	D626	L568		F433	A304	S238	
F1050	L990	Q931	H688	S807	N747	N747	G627	C569	I510	D305	L239	L238	
R1051	V991	E932	T869	A808	H748	E690	Q628	P571	K513	L306	L240	L241	
L1052	N992	N933	D870	D809	C749	E690	R629	E570	T514	P307	L242	L242	
L1053	N993	E934	S871	D810	R750	L691	I630	E572	E515	Q309	D243	D243	
K1054	R994	V935	R872	G810	F751	V692	A631	T573	L516	A310	D244	D244	
N1055	I995	H936	K872	A811	S752	H693	S632	S574	V517	H311	V245	V245	
S1056	F996	V937	S873	R812	F753	T694	C633	E575	A520	S312	D247	D247	
R1057	Q997	L938	K874	L813	D754	Y695	G634	V576		I313	S248	S248	
L1058	Q997	A939	W875	M814	D755	D696	A635	Y577	H521	I314	W249	W249	
I1059	R999	V940	A876	V815	K756	E697	D636	Q578	L522	K380	V250	V250	
S1060	D941	H942	C878	A816	L757	H698	K637	A580	E525	D381	L251	L251	
W1061	F1000	H942	R879	A817	L758	S699	T638	K581	F526	C318	C317	C317	
F1062	Q1001	L1943	G880	K818	A759	E700	L639	L582	S451	G319	G319	G319	
D1064	K1003	R944	H881	N819	S760	Q701	Q640	Q583	Q452	S320	S320	S320	
G1065	T1005	L946	L882	K820	C761	V702	V641	A584	Q453	L386	P321	Q257	
T1066	V1006	Q947	S883	L821	S762	W703	F642	K584	R530	L322	V323	Q258	
V1067	W1007	L948	W884	F822	A763	K643	K644	K585	H531	D455	V324	Q259	
K1068	H886	I949	Y885	L823	D764	C704	A644	E587	I532	L389	S325	L261	
V1069	G951	N950	T866	F824	T766	H706	E645	V588	L533	Q390			
W1070	I1009	G951	T766	D825	L767	F707	G647	D889					
N1071	Q1010	R952	L826	T826	K767	W708	E648	N590					
I1072	F1011	T953	W888	H827	L767	T708	K649	G591					
T1073	T1012	G954	N828	H827	L769	W709	L850	M592					
K1075	A1013	Q955	S829	T828	L769	S710	L651	L593					
T1074	D1014	E955	D771	H712	W770	S711	E652						
G1075	E1015	L956	Q830	H713	A772	H713	I653						
N1076	K1016	D957	L832	L831	T773	L714							
I1077	T1017		G833	E834	S774								



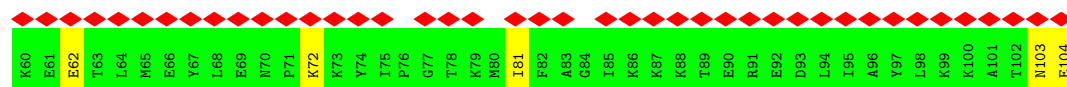
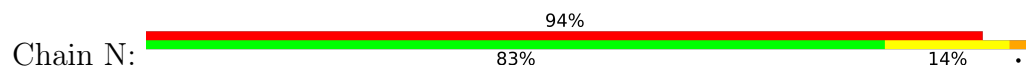
• Molecule 2: Cytochrome c



• Molecule 2: Cytochrome c



• Molecule 2: Cytochrome c



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C7	Depositor
Number of particles used	134919	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 (4k x 4k)	Depositor
Maximum map value	0.351	Depositor
Minimum map value	-0.239	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.04	Depositor
Map size ($\text{\AA}$)	422.40002, 422.40002, 422.40002	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.32, 1.32, 1.32	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.43	0/9337	0.88	30/12636 (0.2%)
1	C	0.43	0/9337	0.88	29/12636 (0.2%)
1	E	0.43	0/9337	0.88	31/12636 (0.2%)
1	G	0.43	0/9337	0.88	29/12636 (0.2%)
1	I	0.43	0/9337	0.88	30/12636 (0.2%)
1	K	0.43	0/9337	0.88	30/12636 (0.2%)
1	M	0.43	0/9337	0.88	30/12636 (0.2%)
2	B	0.84	0/839	0.94	1/1118 (0.1%)
2	D	0.84	0/839	0.94	1/1118 (0.1%)
2	F	0.84	0/839	0.94	1/1118 (0.1%)
2	H	0.84	0/839	0.94	1/1118 (0.1%)
2	J	0.84	0/839	0.94	1/1118 (0.1%)
2	L	0.84	0/839	0.94	1/1118 (0.1%)
2	N	0.84	0/839	0.94	1/1118 (0.1%)
All	All	0.48	0/71232	0.88	216/96278 (0.2%)

There are no bond length outliers.

The worst 5 of 216 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	264	THR	N-CA-C	9.10	120.78	108.23
1	C	264	THR	N-CA-C	9.09	120.78	108.23
1	A	264	THR	N-CA-C	9.09	120.77	108.23
1	M	264	THR	N-CA-C	9.08	120.75	108.23
1	G	264	THR	N-CA-C	9.07	120.75	108.23

There are no chirality outliers.

There are no planarity outliers.

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	9139	0	9005	1408	0
1	C	9139	0	9005	1409	0
1	E	9139	0	9005	1406	0
1	G	9139	0	9005	1417	0
1	I	9139	0	9005	1388	0
1	K	9139	0	9005	1393	0
1	M	9139	0	9005	1403	0
2	B	823	0	849	32	0
2	D	823	0	849	30	0
2	F	823	0	849	31	0
2	H	823	0	849	34	0
2	J	823	0	849	32	0
2	L	823	0	849	32	0
2	N	823	0	849	32	0
3	A	30	0	12	6	0
3	C	30	0	12	6	0
3	E	30	0	12	6	0
3	G	30	0	12	6	0
3	I	30	0	12	7	0
3	K	30	0	12	6	0
3	M	30	0	12	6	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
4	I	1	0	0	0	0
4	K	1	0	0	0	0
4	M	1	0	0	0	0
5	B	43	0	30	15	0
5	D	43	0	30	14	0
5	F	43	0	30	15	0
5	H	43	0	30	16	0
5	J	43	0	30	15	0
5	L	43	0	30	14	0
5	N	43	0	30	14	0
All	All	70252	0	69272	9859	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 71.

The worst 5 of 9859 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)
1:E:544:PHE:CE1	1:E:576:VAL:HG13	1.28	1.68
1:G:544:PHE:CE1	1:G:576:VAL:HG13	1.28	1.67
1:C:544:PHE:CE1	1:C:576:VAL:HG13	1.28	1.65
1:C:862:TYR:CD1	1:C:885:VAL:HG12	1.26	1.64
1:A:544:PHE:CE1	1:A:576:VAL:HG13	1.28	1.64

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	1142/1260 (91%)	999 (88%)	98 (9%)	45 (4%)	2	20
1	C	1142/1260 (91%)	999 (88%)	98 (9%)	45 (4%)	2	20
1	E	1142/1260 (91%)	999 (88%)	98 (9%)	45 (4%)	2	20
1	G	1142/1260 (91%)	999 (88%)	98 (9%)	45 (4%)	2	20
1	I	1142/1260 (91%)	999 (88%)	98 (9%)	45 (4%)	2	20
1	K	1142/1260 (91%)	999 (88%)	97 (8%)	46 (4%)	2	20
1	M	1142/1260 (91%)	999 (88%)	97 (8%)	46 (4%)	2	20
2	B	102/105 (97%)	100 (98%)	2 (2%)	0	100	100
2	D	102/105 (97%)	100 (98%)	2 (2%)	0	100	100
2	F	102/105 (97%)	100 (98%)	2 (2%)	0	100	100
2	H	102/105 (97%)	100 (98%)	2 (2%)	0	100	100
2	J	102/105 (97%)	100 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	L	102/105 (97%)	100 (98%)	2 (2%)	0	100	100
2	N	102/105 (97%)	100 (98%)	2 (2%)	0	100	100
All	All	8708/9555 (91%)	7693 (88%)	698 (8%)	317 (4%)	4	22

5 of 317 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	147	PRO
1	A	557	ARG
1	A	560	PHE
1	A	562	ASN
1	A	645	GLU

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	1027/1131 (91%)	829 (81%)	198 (19%)	1	9
1	C	1027/1131 (91%)	829 (81%)	198 (19%)	1	9
1	E	1027/1131 (91%)	829 (81%)	198 (19%)	1	9
1	G	1027/1131 (91%)	829 (81%)	198 (19%)	1	9
1	I	1027/1131 (91%)	829 (81%)	198 (19%)	1	9
1	K	1027/1131 (91%)	829 (81%)	198 (19%)	1	9
1	M	1027/1131 (91%)	829 (81%)	198 (19%)	1	9
2	B	86/87 (99%)	81 (94%)	5 (6%)	18	44
2	D	86/87 (99%)	81 (94%)	5 (6%)	18	44
2	F	86/87 (99%)	81 (94%)	5 (6%)	18	44
2	H	86/87 (99%)	81 (94%)	5 (6%)	18	44
2	J	86/87 (99%)	81 (94%)	5 (6%)	18	44
2	L	86/87 (99%)	81 (94%)	5 (6%)	18	44
2	N	86/87 (99%)	81 (94%)	5 (6%)	18	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	7791/8526 (91%)	6370 (82%)	1421 (18%)	3 12

5 of 1421 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	516	LEU
1	K	568	LEU
1	I	598	ILE
1	I	515	GLU
1	K	210	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 226 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	583	GLN
1	M	1219	ASN
1	I	521	HIS
1	M	1008	HIS
1	M	235	HIS

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](#)

Of 21 ligands modelled in this entry, 7 are monoatomic - leaving 14 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	HEM	L	201	2	50,50,50	1.55	7 (14%)	67,82,82	1.61	11 (16%)
5	HEM	F	201	2	50,50,50	1.55	7 (14%)	67,82,82	1.60	11 (16%)
3	DTP	K	1301	4	31,32,32	1.42	4 (12%)	46,50,50	1.78	9 (19%)
3	DTP	C	1301	4	31,32,32	1.43	4 (12%)	46,50,50	1.79	9 (19%)
3	DTP	A	1301	4	31,32,32	1.43	4 (12%)	46,50,50	1.79	9 (19%)
3	DTP	I	1301	4	31,32,32	1.43	4 (12%)	46,50,50	1.79	9 (19%)
5	HEM	D	201	2	50,50,50	1.55	8 (16%)	67,82,82	1.60	11 (16%)
3	DTP	M	1301	4	31,32,32	1.42	4 (12%)	46,50,50	1.79	9 (19%)
5	HEM	J	201	2	50,50,50	1.55	7 (14%)	67,82,82	1.61	11 (16%)
5	HEM	N	201	2	50,50,50	1.55	7 (14%)	67,82,82	1.61	11 (16%)
3	DTP	G	1301	4	31,32,32	1.43	4 (12%)	46,50,50	1.79	9 (19%)
5	HEM	H	201	2	50,50,50	1.55	7 (14%)	67,82,82	1.60	11 (16%)
5	HEM	B	201	2	50,50,50	1.55	8 (16%)	67,82,82	1.59	11 (16%)
3	DTP	E	1301	4	31,32,32	1.43	4 (12%)	46,50,50	1.79	9 (19%)

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	HEM	L	201	2	-	5/14/54/54	-
5	HEM	F	201	2	-	5/14/54/54	-
3	DTP	K	1301	4	-	7/22/34/34	0/3/3/3
3	DTP	C	1301	4	-	7/22/34/34	0/3/3/3
3	DTP	A	1301	4	-	7/22/34/34	0/3/3/3
3	DTP	I	1301	4	-	7/22/34/34	0/3/3/3
5	HEM	D	201	2	-	5/14/54/54	-
3	DTP	M	1301	4	-	7/22/34/34	0/3/3/3
5	HEM	J	201	2	-	5/14/54/54	-
5	HEM	N	201	2	-	5/14/54/54	-
3	DTP	G	1301	4	-	7/22/34/34	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	HEM	H	201	2	-	5/14/54/54	-
5	HEM	B	201	2	-	5/14/54/54	-
3	DTP	E	1301	4	-	7/22/34/34	0/3/3/3

The worst 5 of 79 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	201	HEM	FE-NB	5.11	2.10	1.94
5	J	201	HEM	FE-NB	5.11	2.10	1.94
5	H	201	HEM	FE-NB	5.10	2.10	1.94
5	D	201	HEM	FE-NB	5.10	2.10	1.94
5	L	201	HEM	FE-NB	5.10	2.10	1.94

The worst 5 of 140 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	1301	DTP	C5-C4-N3	-5.86	118.65	126.72
3	C	1301	DTP	C5-C4-N3	-5.86	118.65	126.72
3	G	1301	DTP	C5-C4-N3	-5.84	118.67	126.72
3	I	1301	DTP	C5-C4-N3	-5.84	118.67	126.72
3	A	1301	DTP	C5-C4-N3	-5.84	118.67	126.72

There are no chirality outliers.

5 of 84 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1301	DTP	C5'-O5'-PA-O2A
3	A	1301	DTP	C5'-O5'-PA-O3A
3	A	1301	DTP	O4'-C1'-N9-C8
3	A	1301	DTP	O4'-C1'-N9-C4
3	C	1301	DTP	C5'-O5'-PA-O2A

There are no ring outliers.

14 monomers are involved in 146 short contacts:

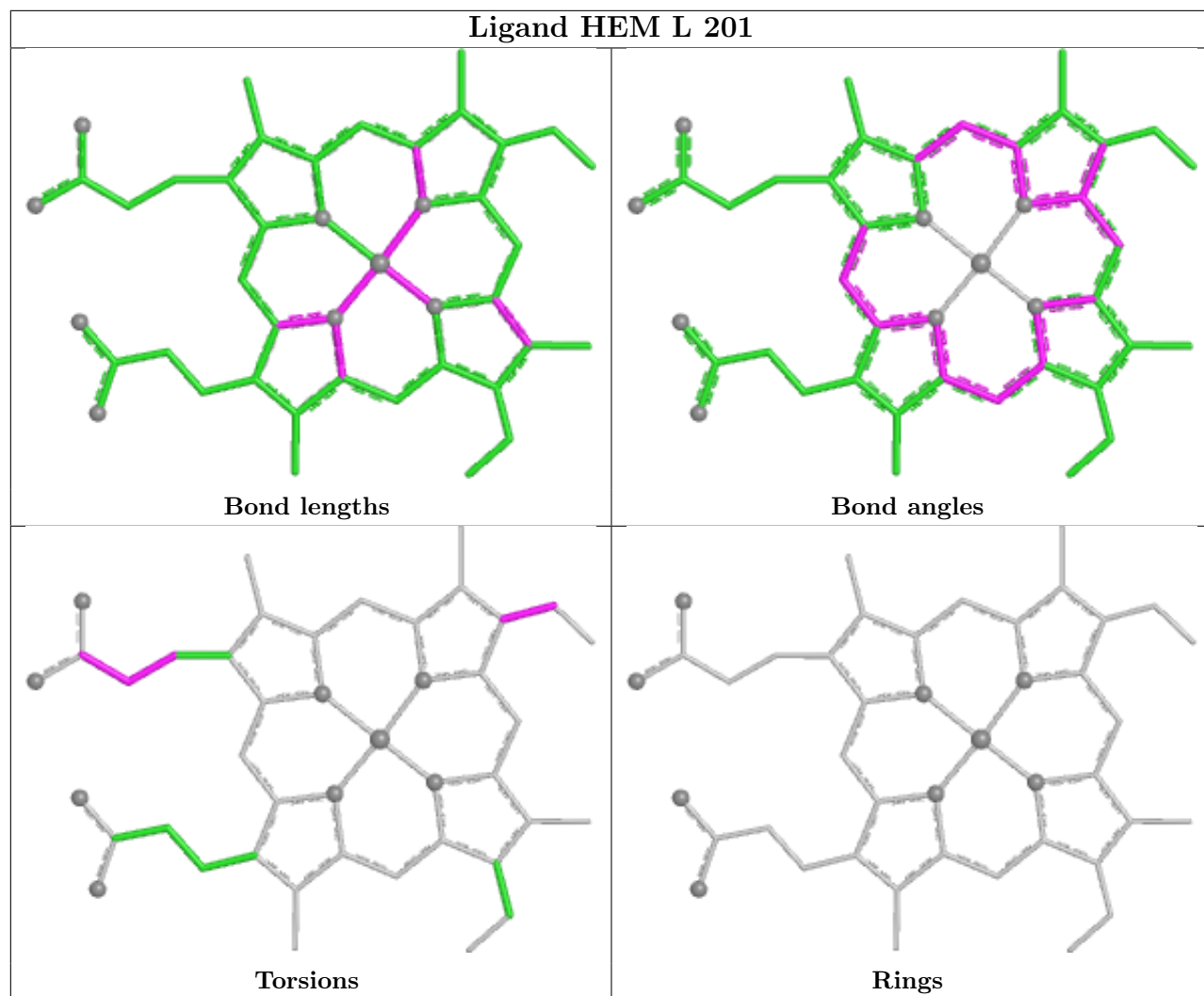
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	L	201	HEM	14	0
5	F	201	HEM	15	0
3	K	1301	DTP	6	0
3	C	1301	DTP	6	0

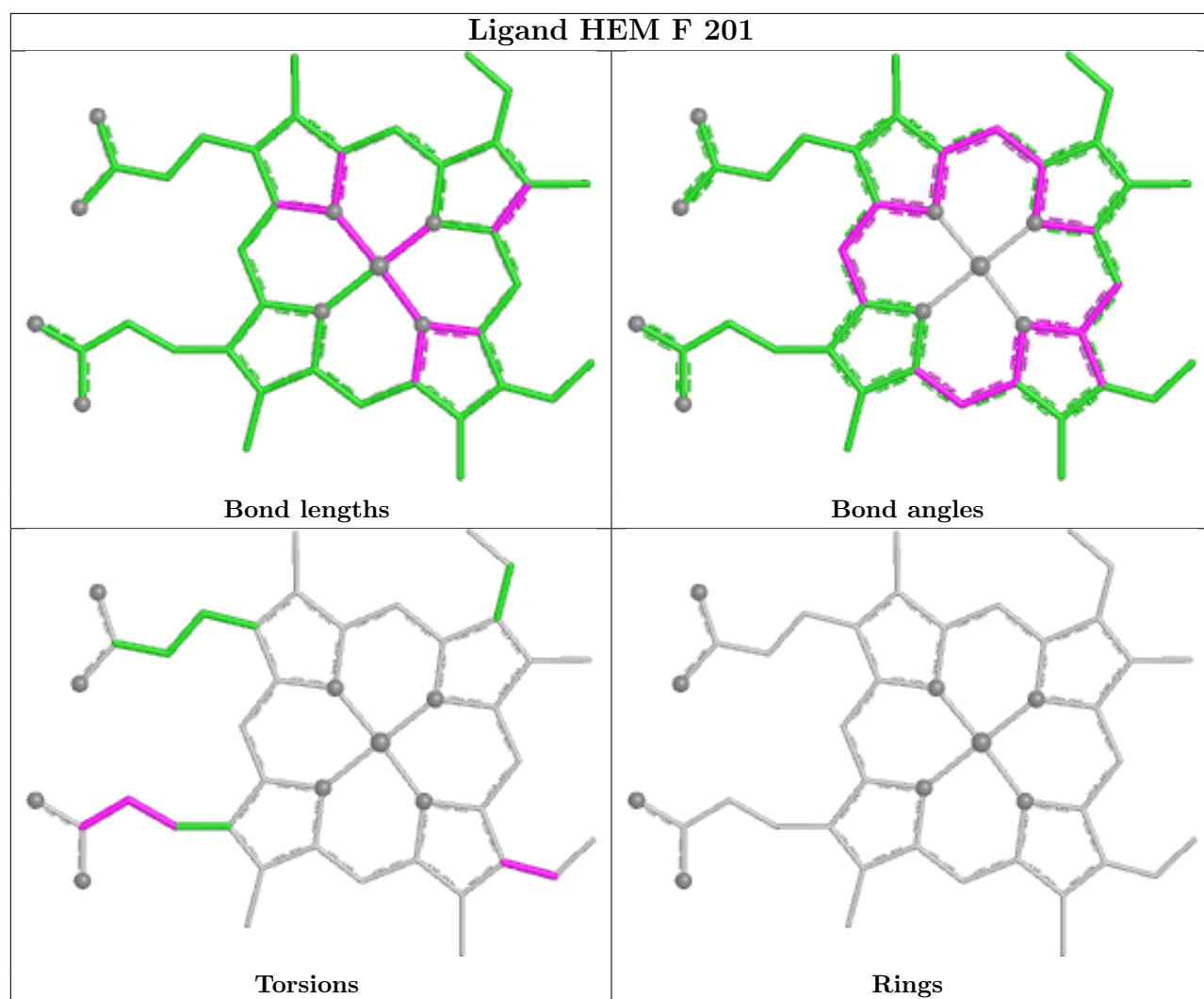
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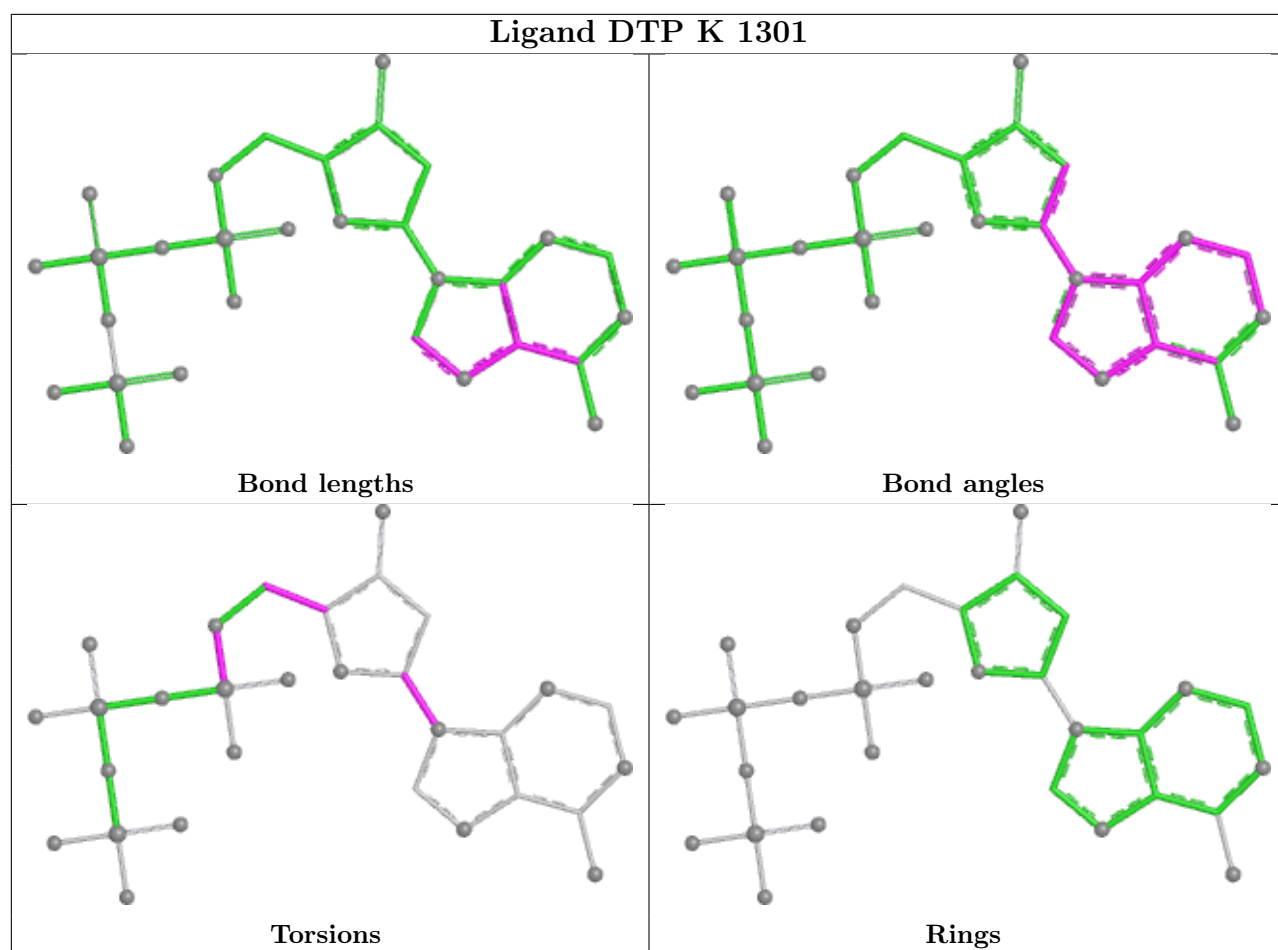
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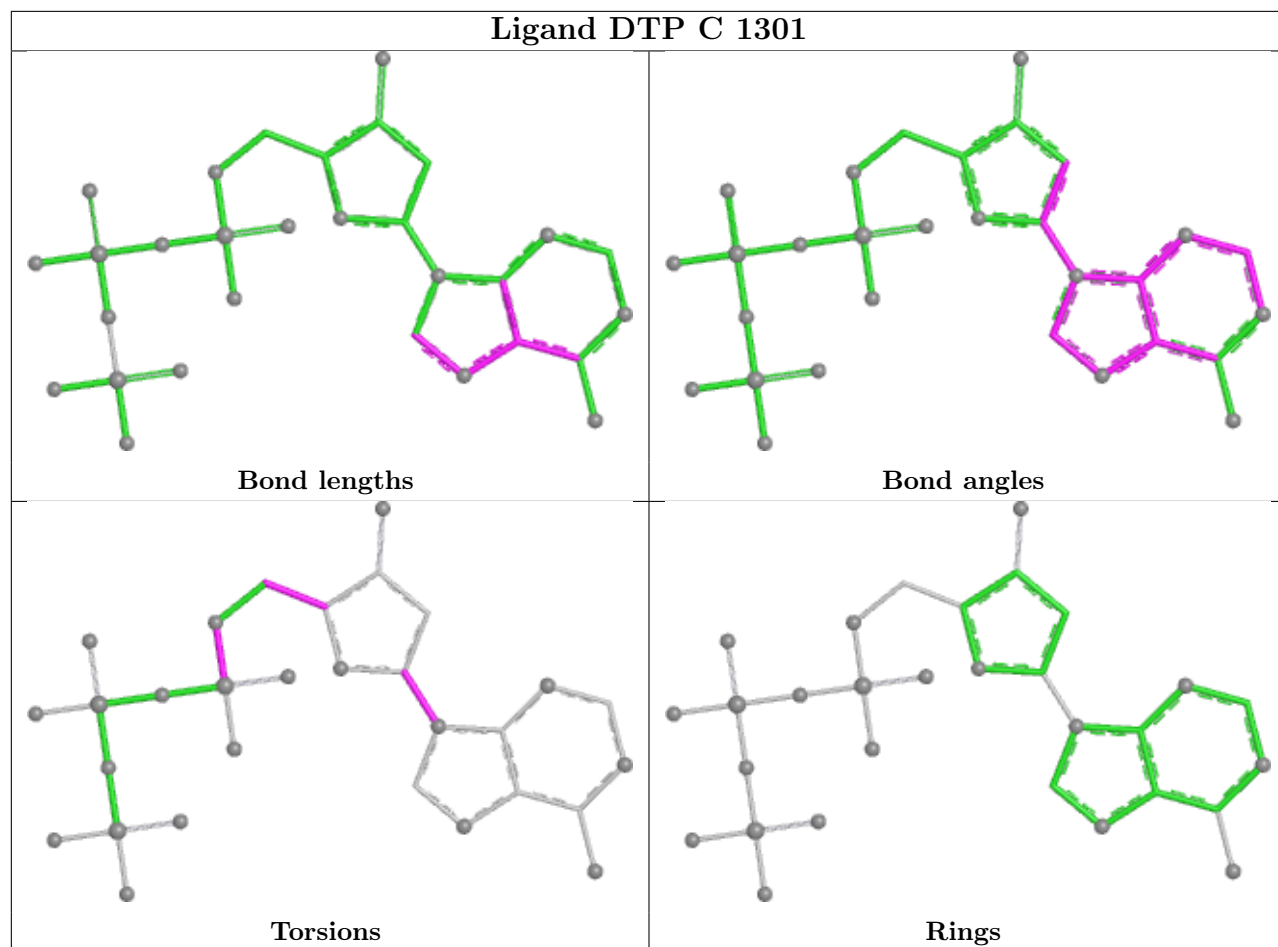
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1301	DTP	6	0
3	I	1301	DTP	7	0
5	D	201	HEM	14	0
3	M	1301	DTP	6	0
5	J	201	HEM	15	0
5	N	201	HEM	14	0
3	G	1301	DTP	6	0
5	H	201	HEM	16	0
5	B	201	HEM	15	0
3	E	1301	DTP	6	0

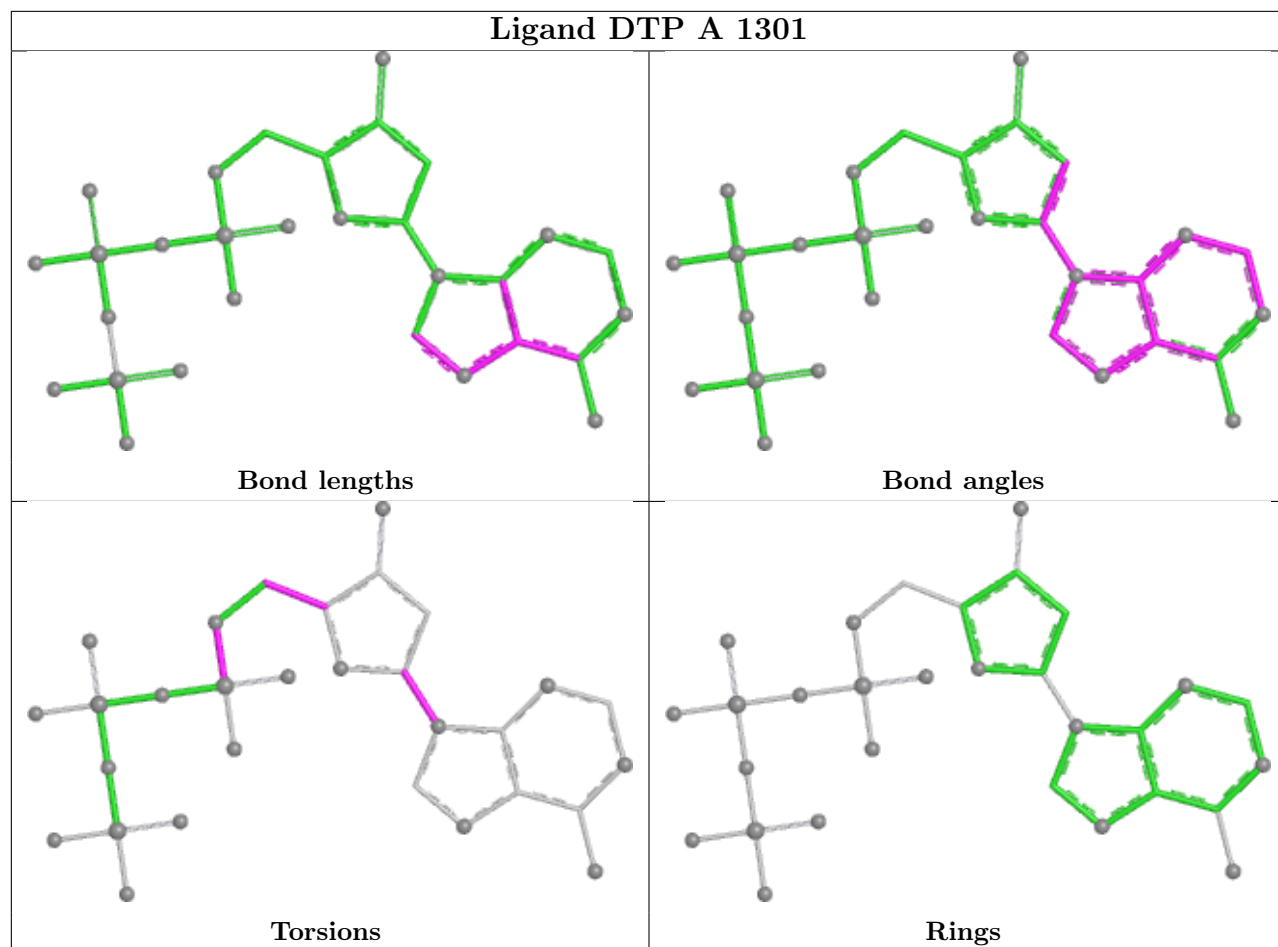
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

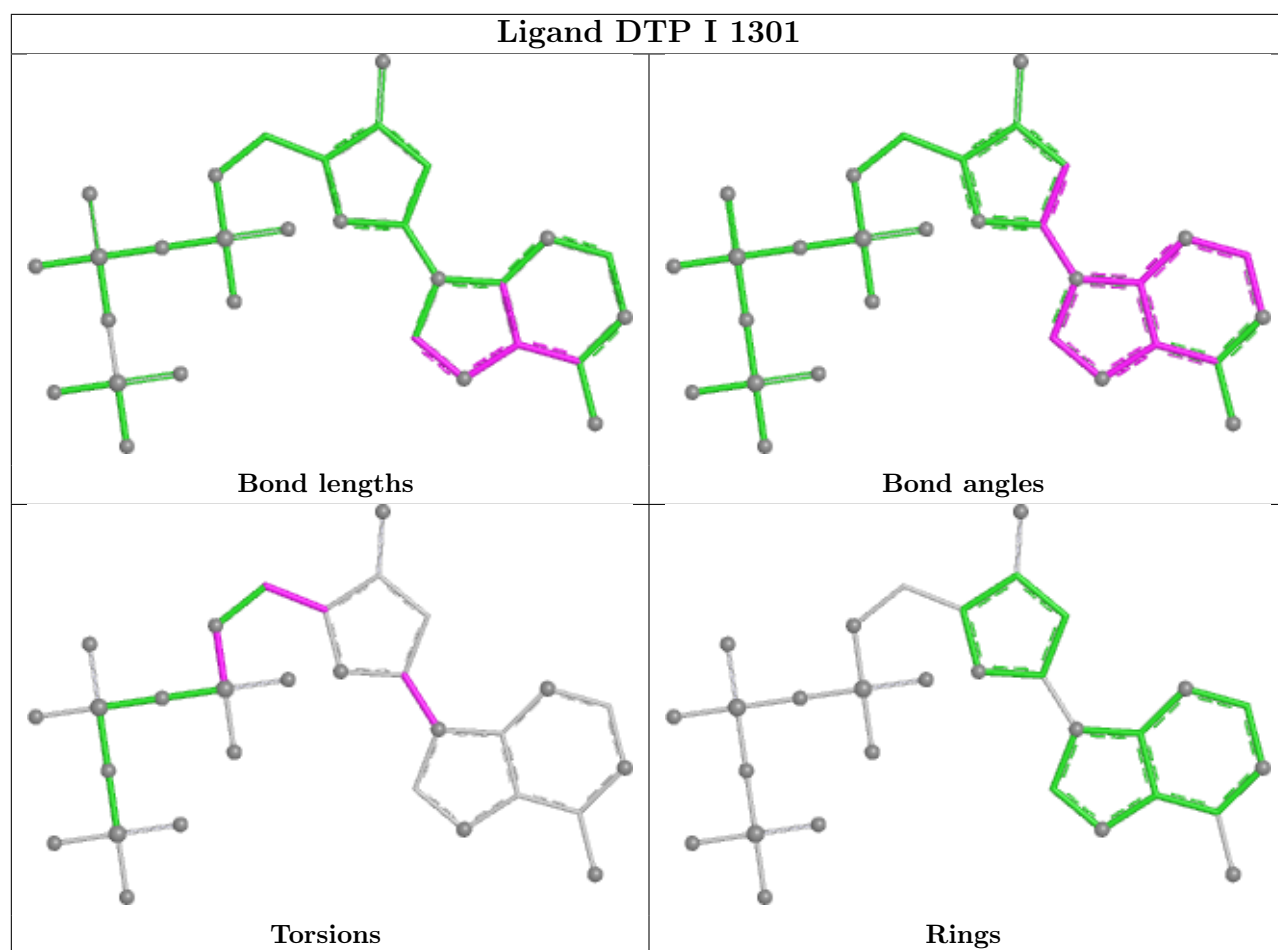


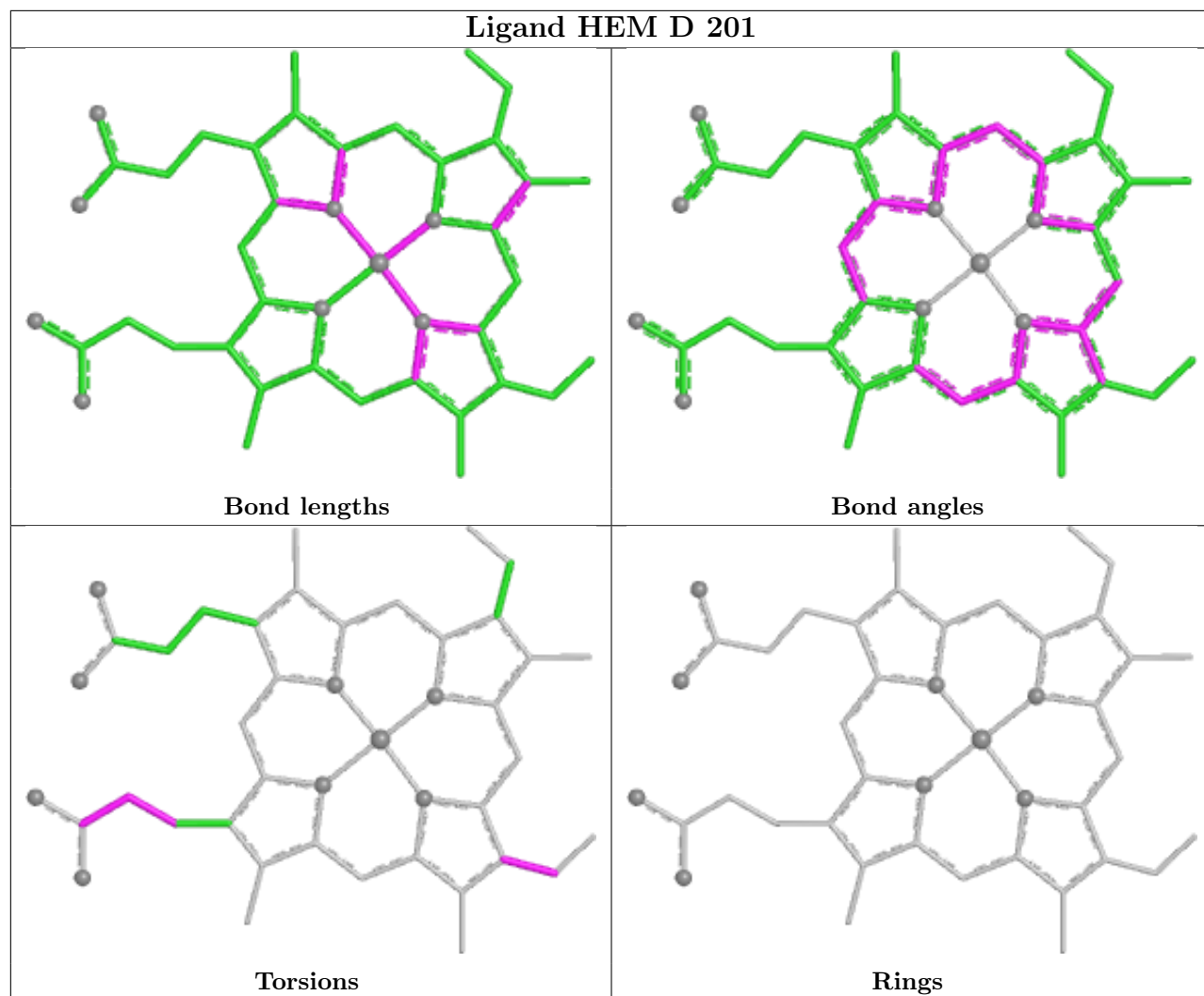


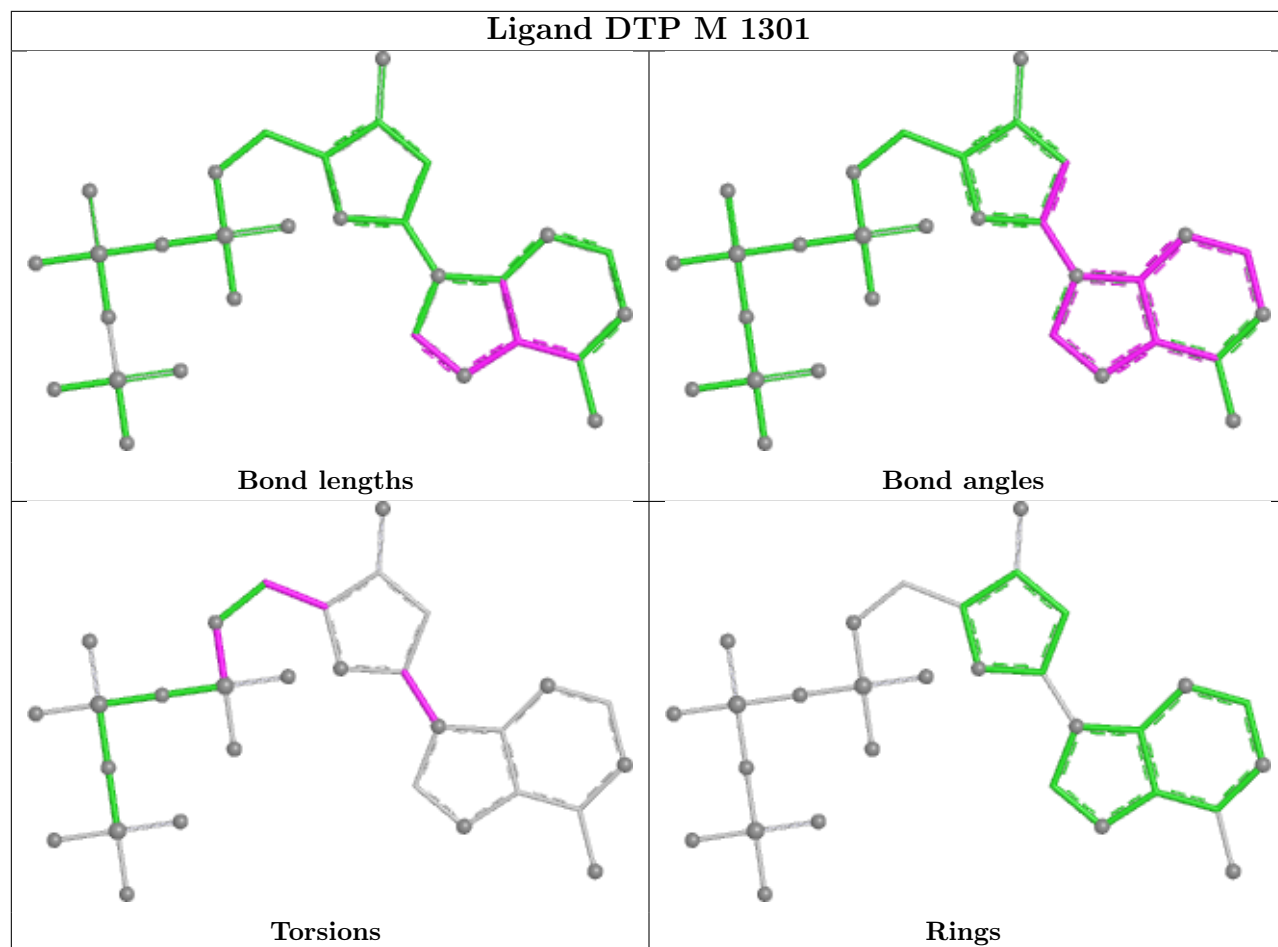


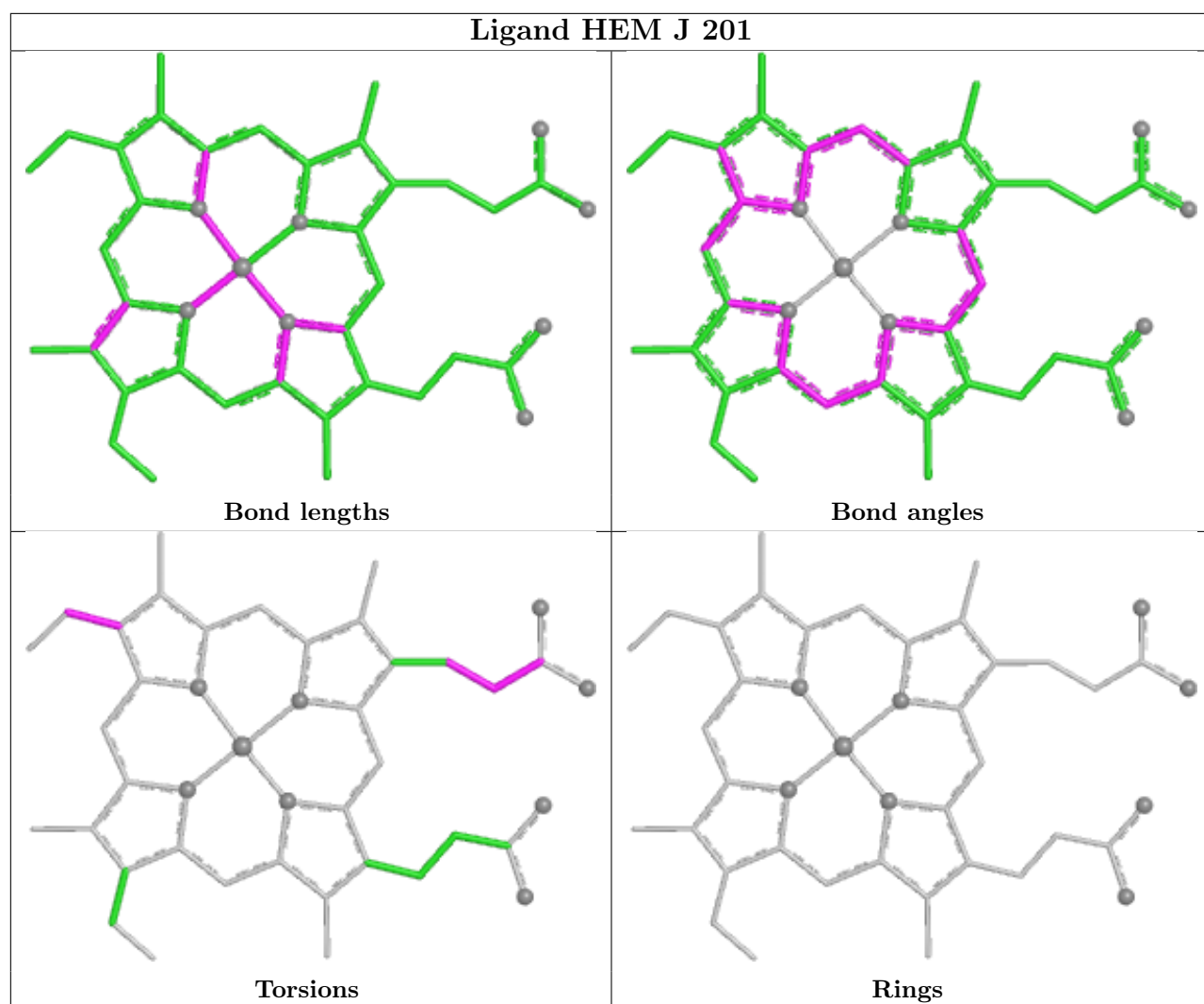


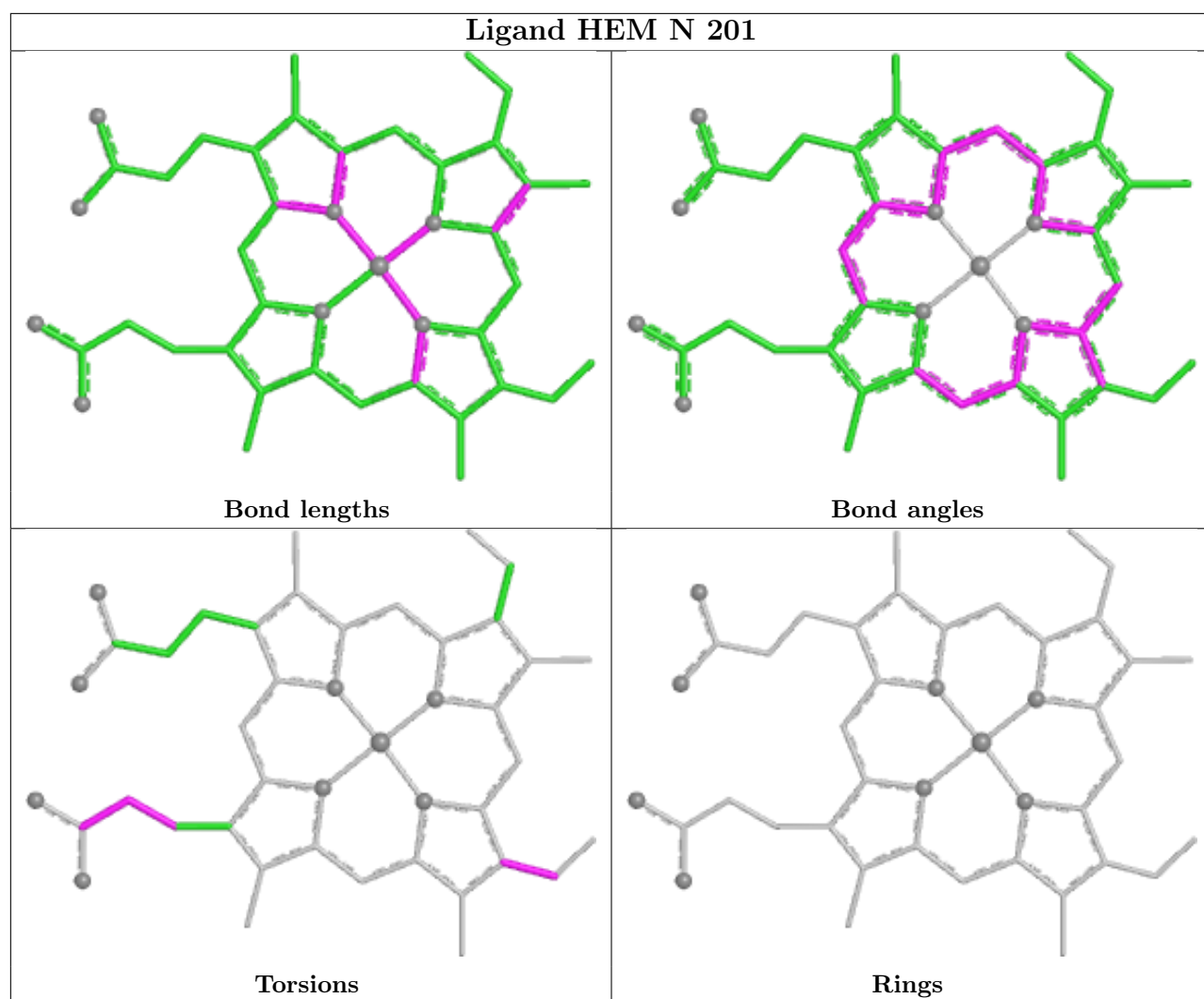


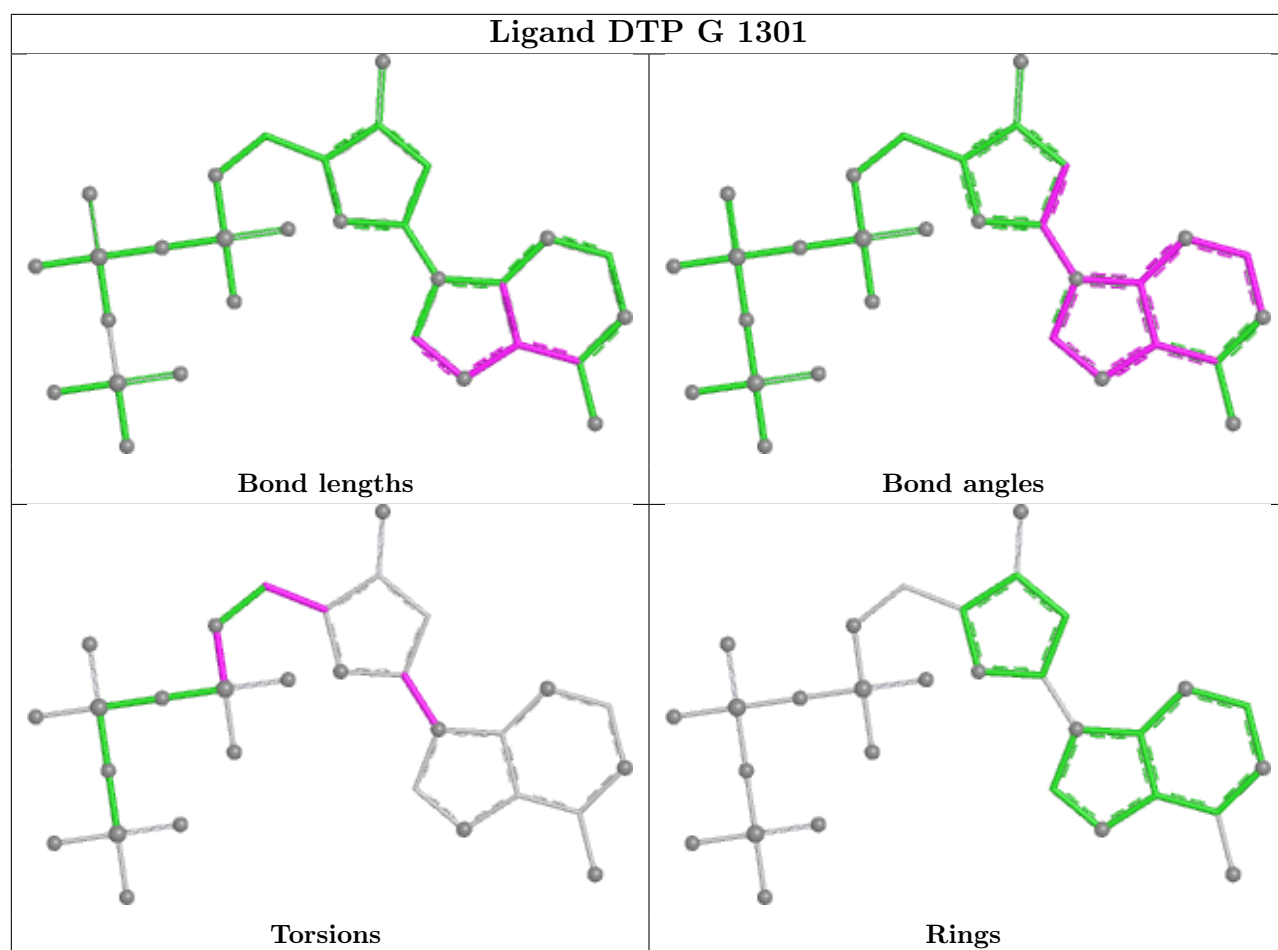


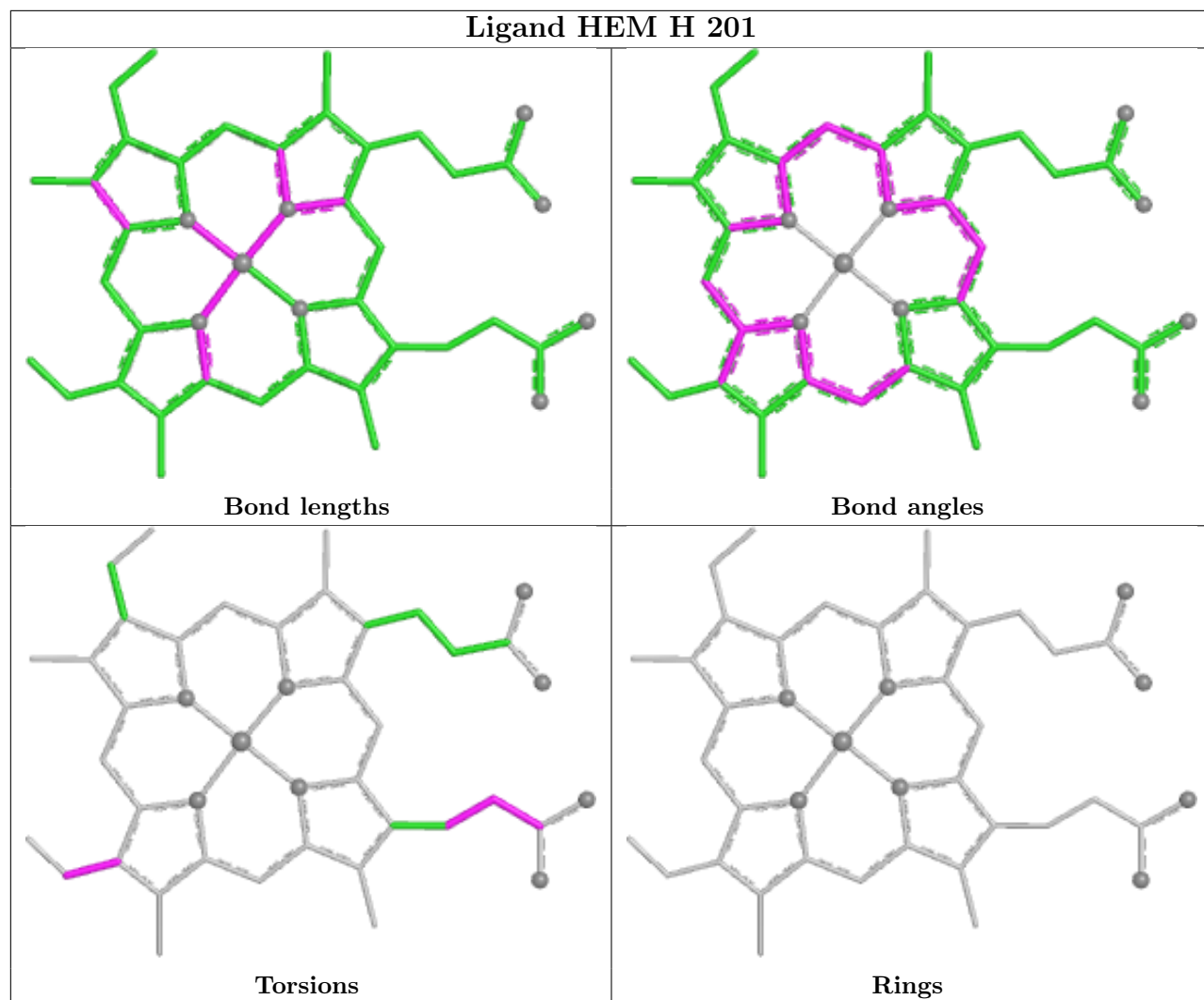


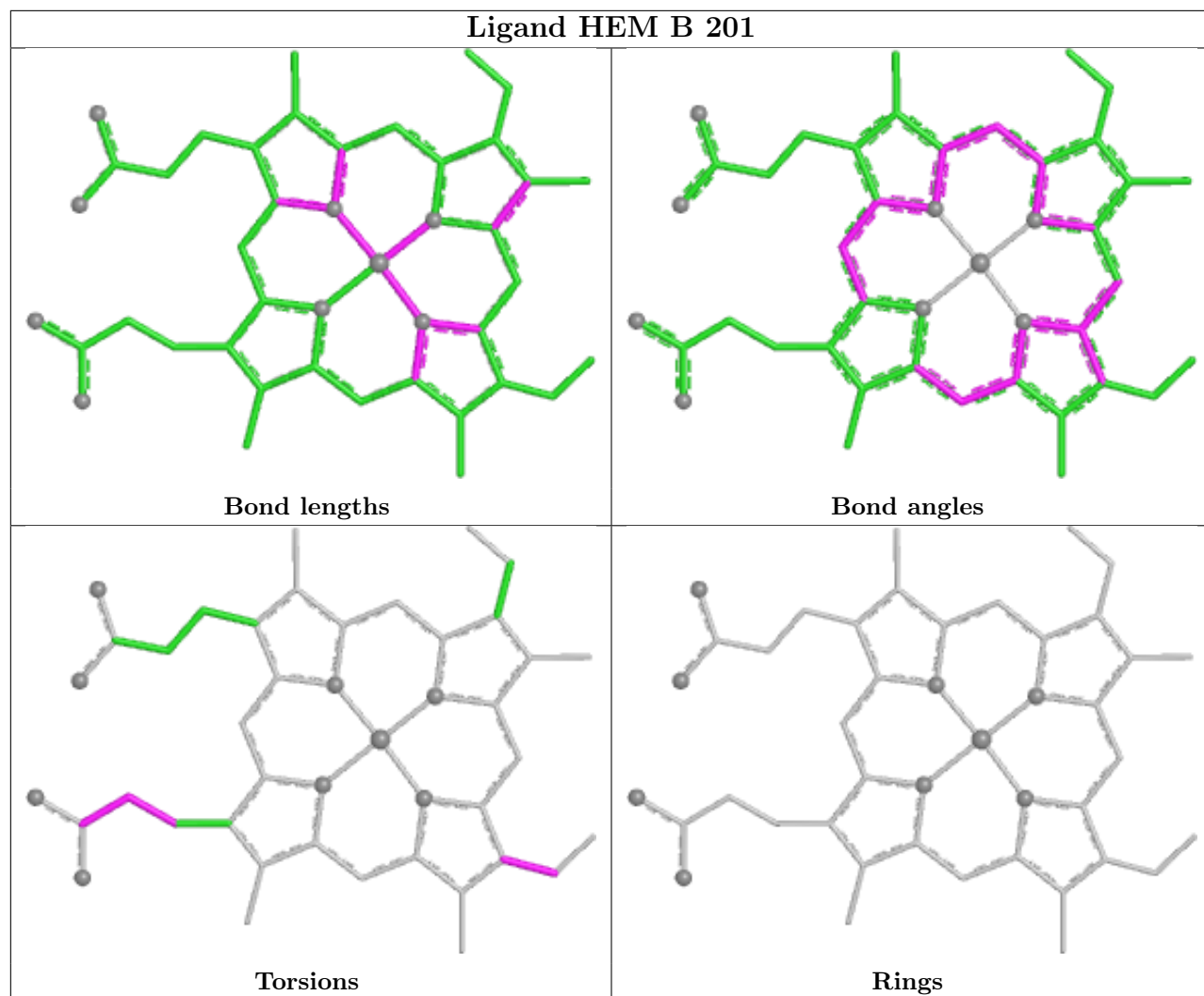


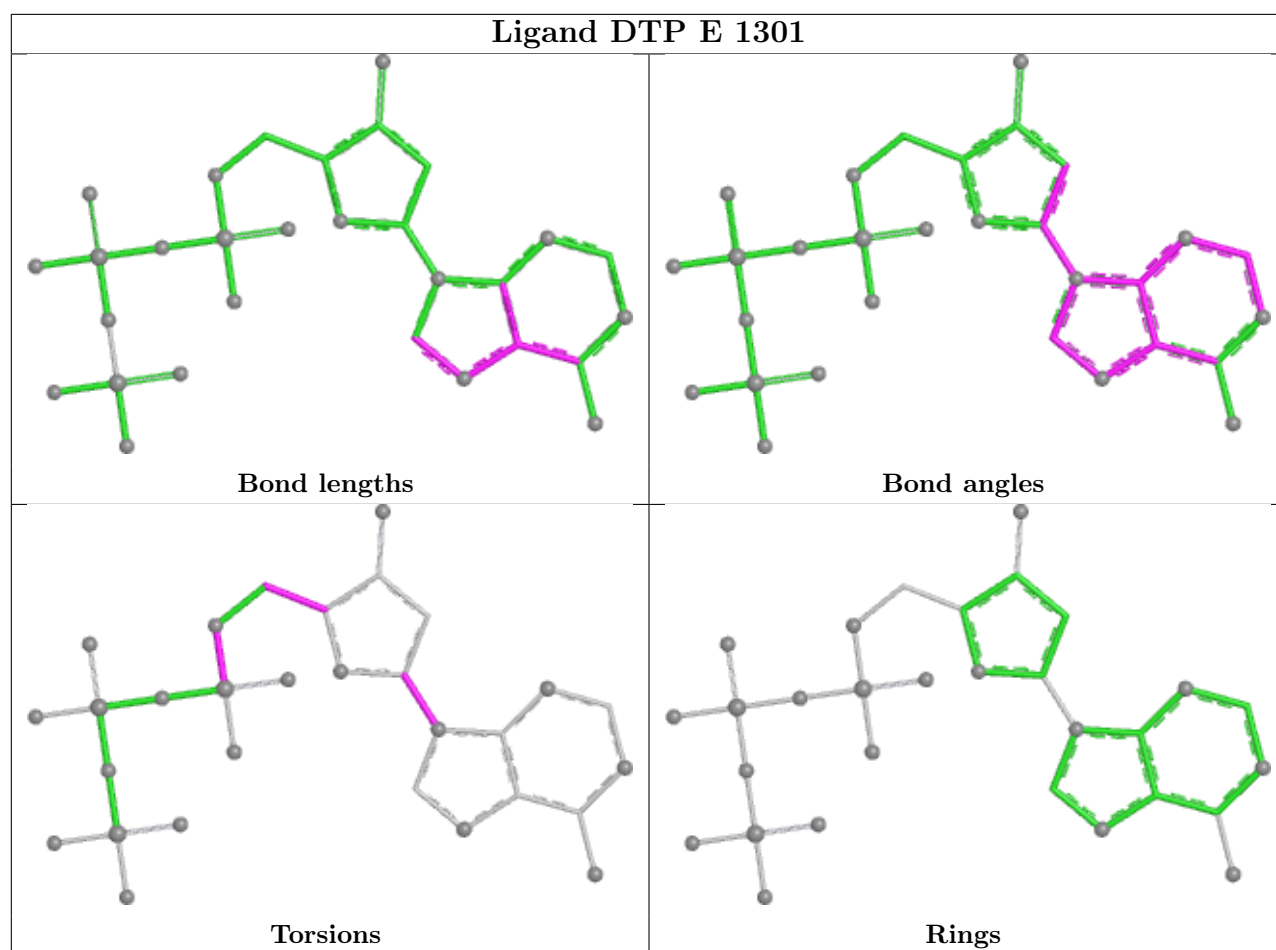












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

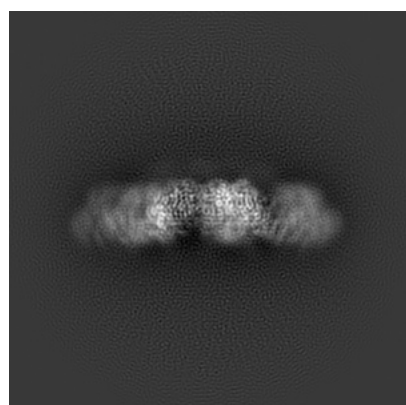
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6480. These allow visual inspection of the internal detail of the map and identification of artifacts.

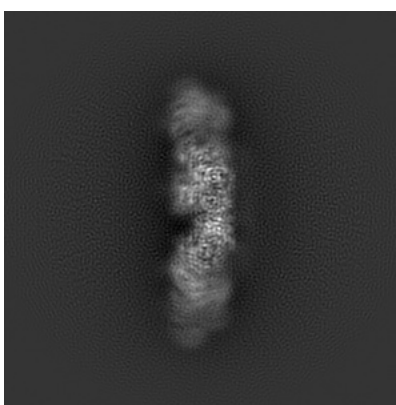
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

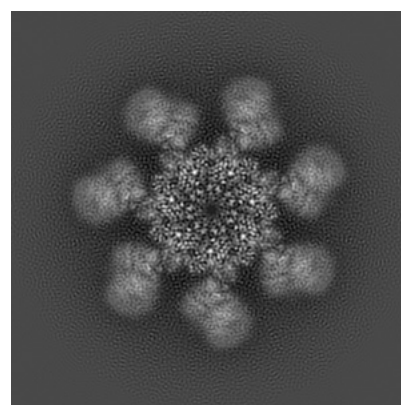
6.1.1 Primary map



X



Y



Z

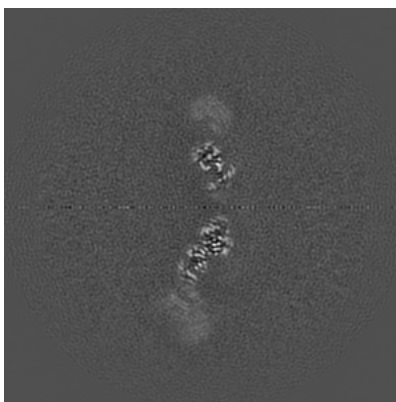
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

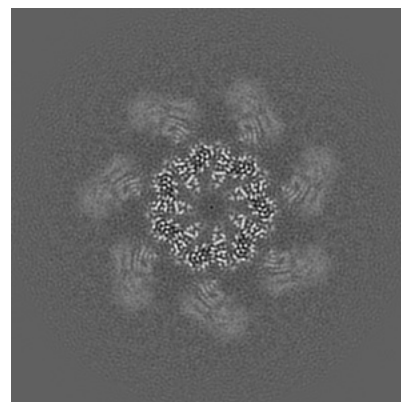
6.2.1 Primary map



X Index: 160



Y Index: 160

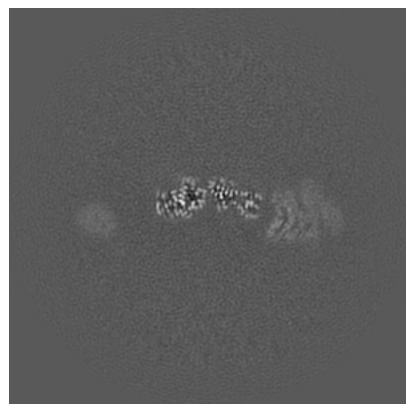


Z Index: 160

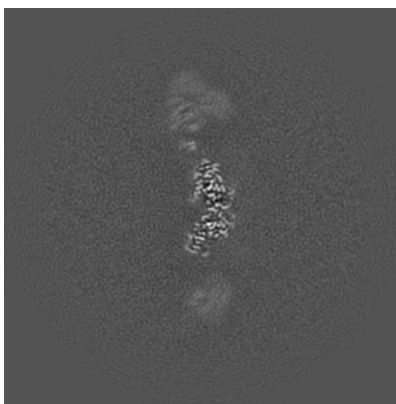
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

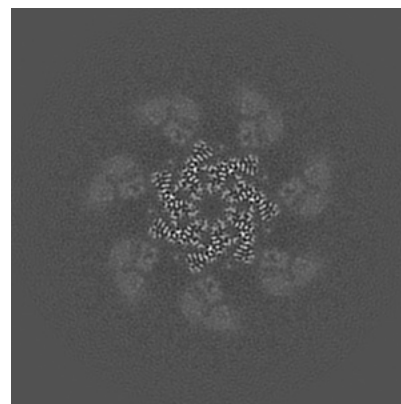
6.3.1 Primary map



X Index: 185



Y Index: 190

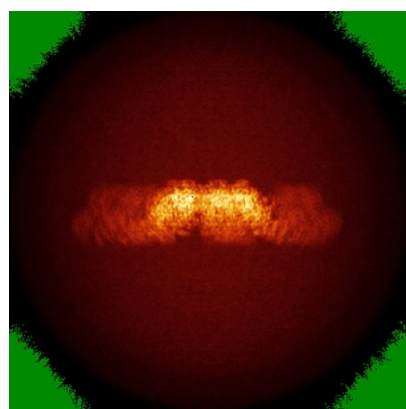


Z Index: 164

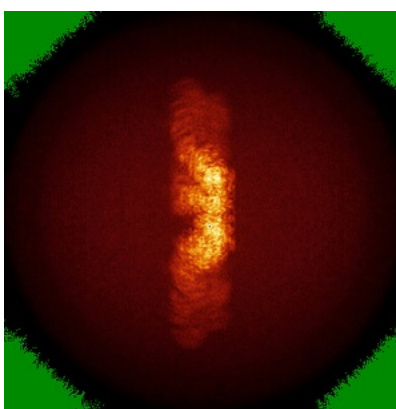
The images above show the largest variance slices of the map in three orthogonal directions.

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

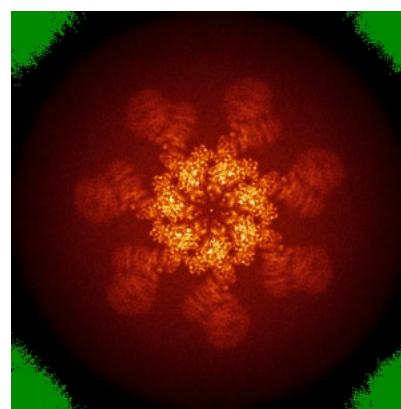
6.4.1 Primary map



X



Y

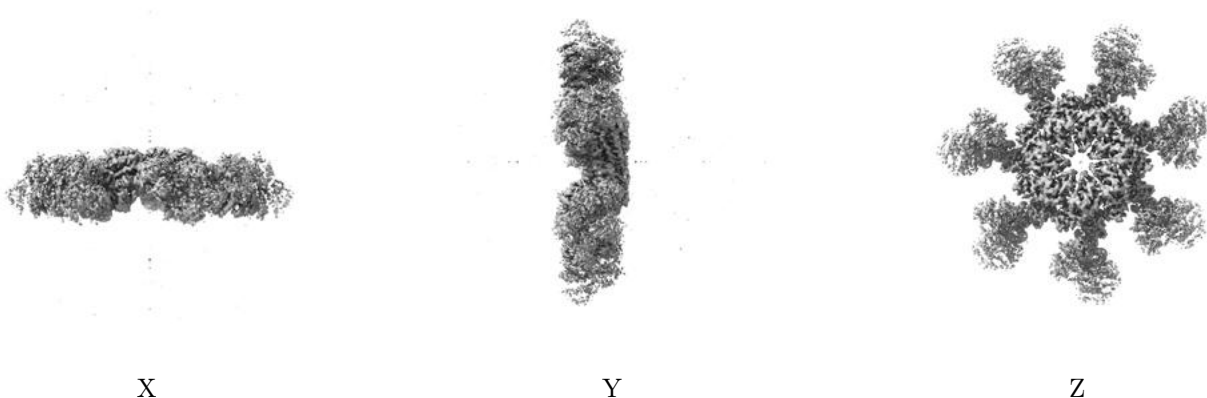


Z

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

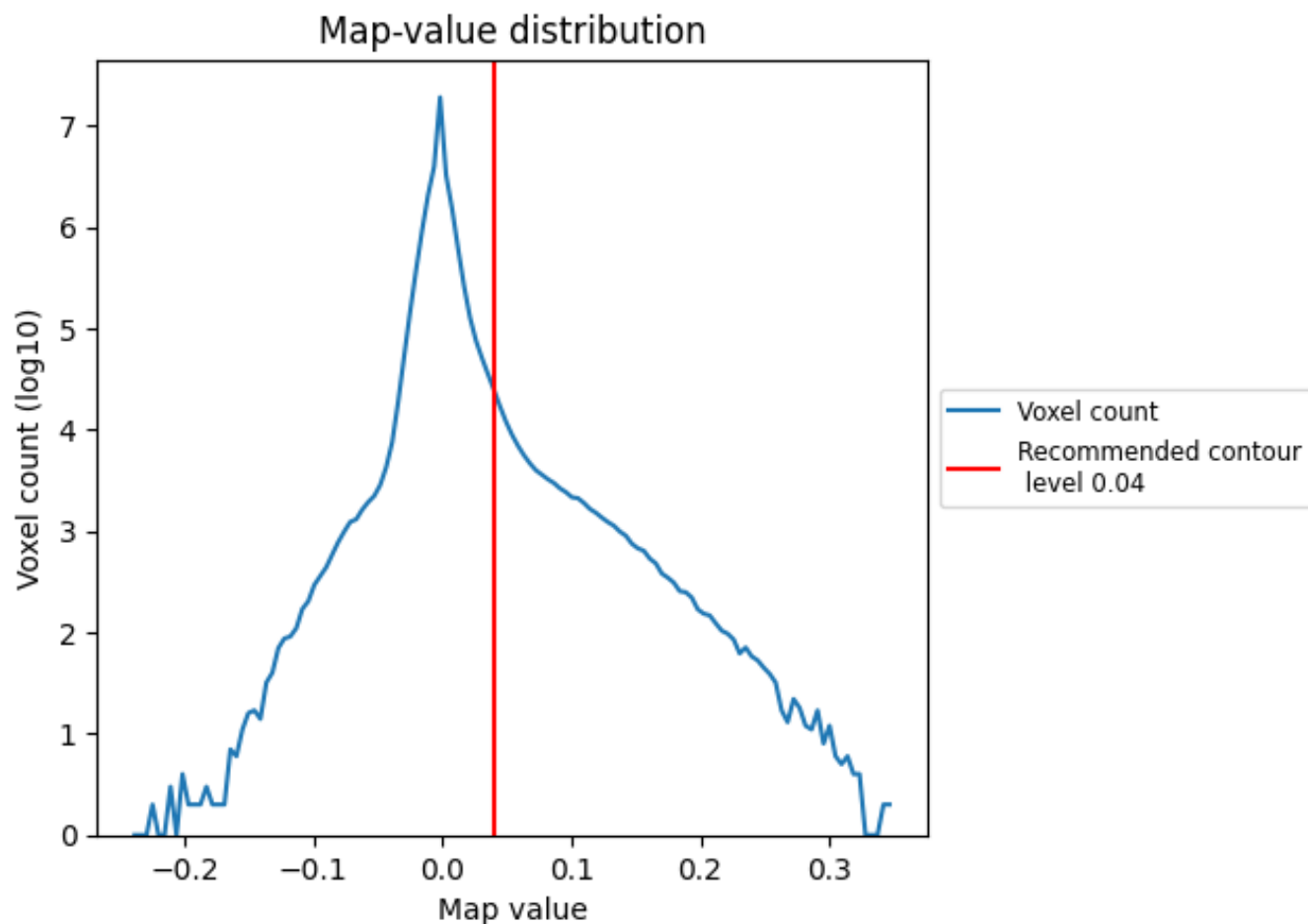
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

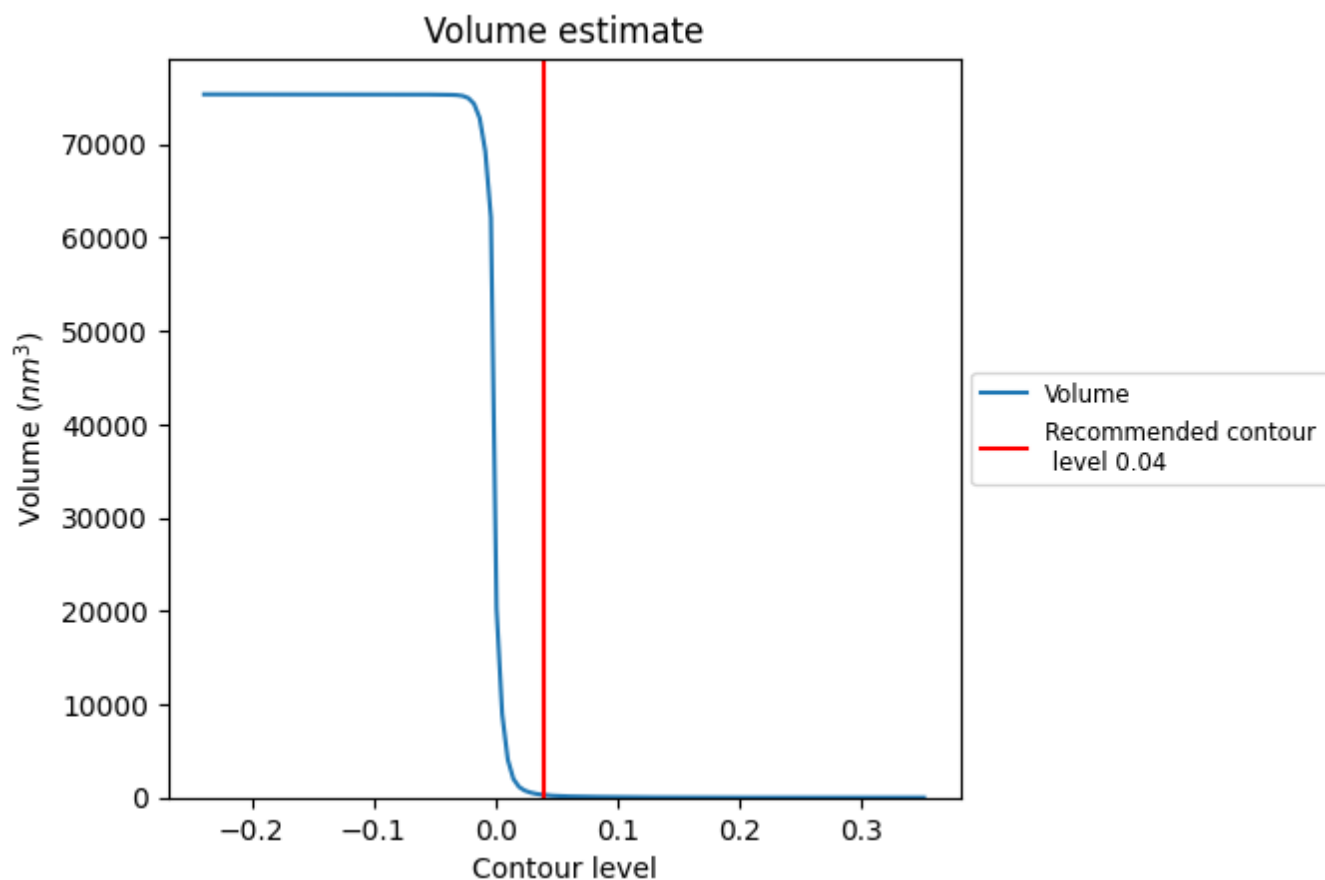
This section contains the results of statistical analysis of the map.

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.

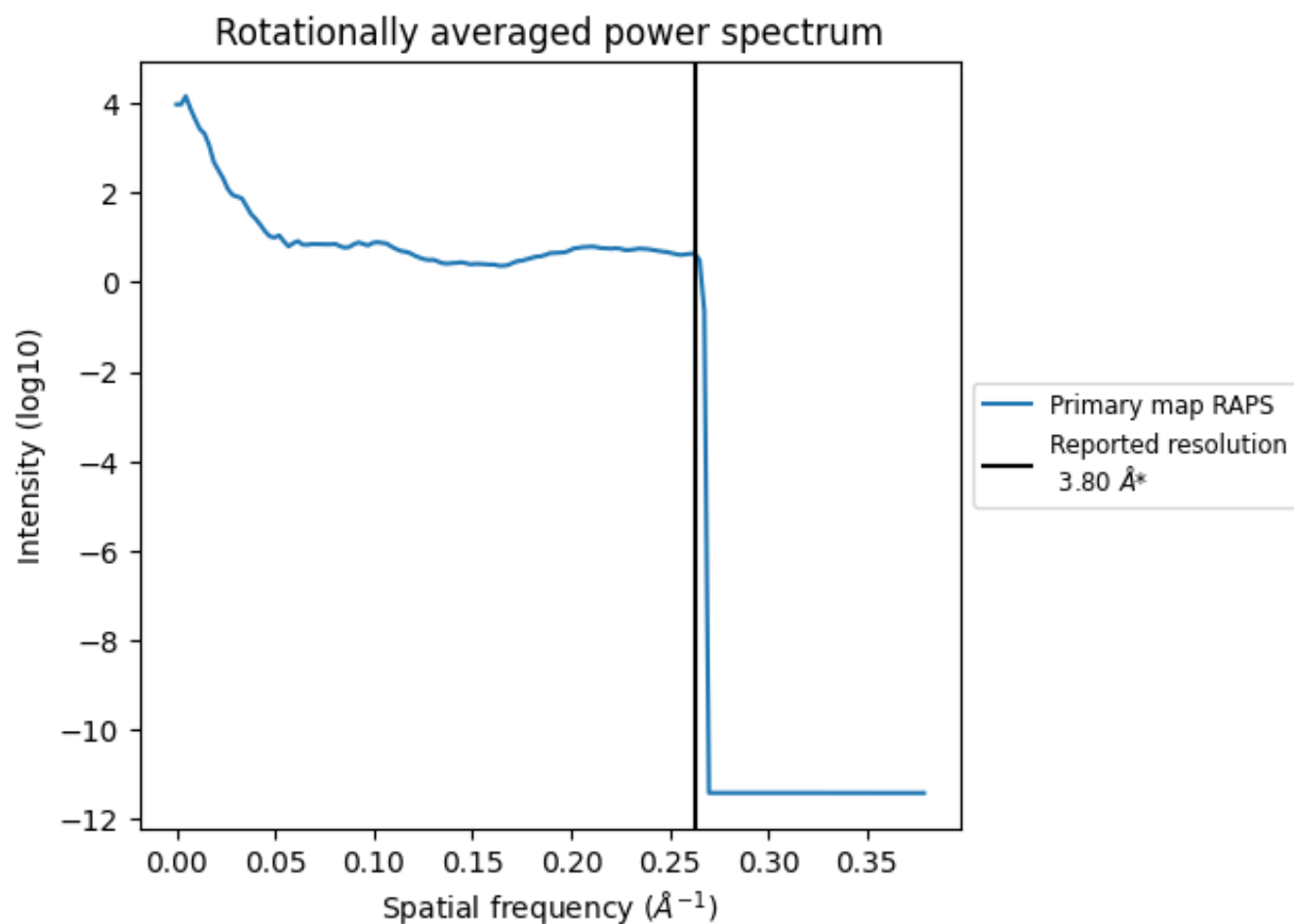
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 276 nm³; this corresponds to an approximate mass of 249 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 0.263 Å⁻¹

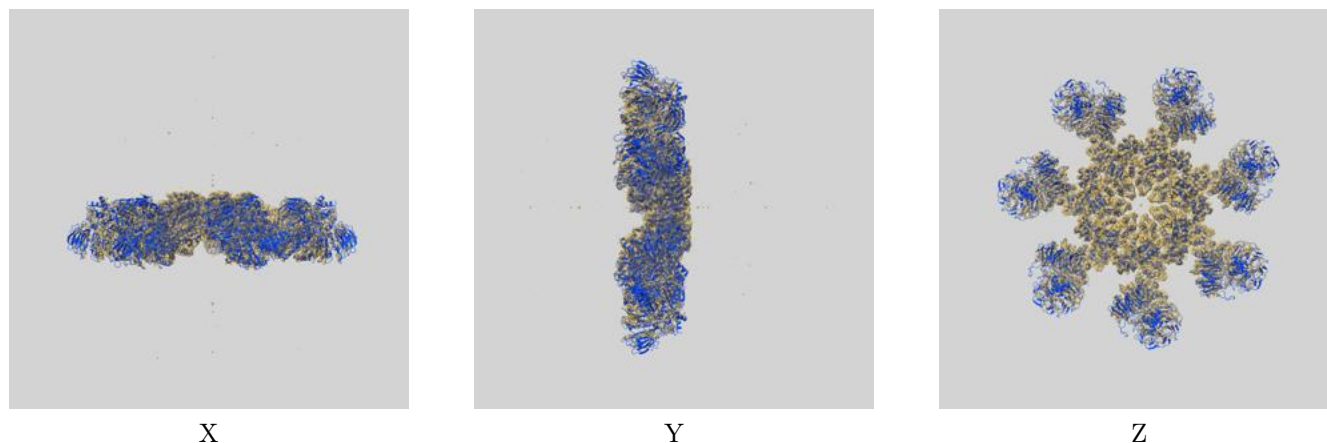
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

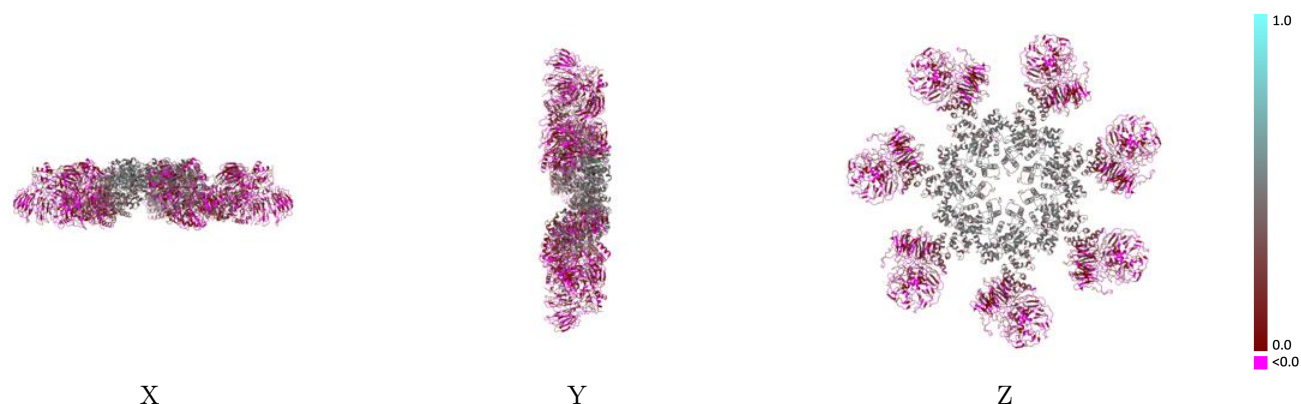
This section contains information regarding the fit between EMDB map EMD-6480 and PDB model 3JBT. Per-residue inclusion information can be found in [section 3](#) on [page 10](#).

9.1 Map-model overlay [i](#)



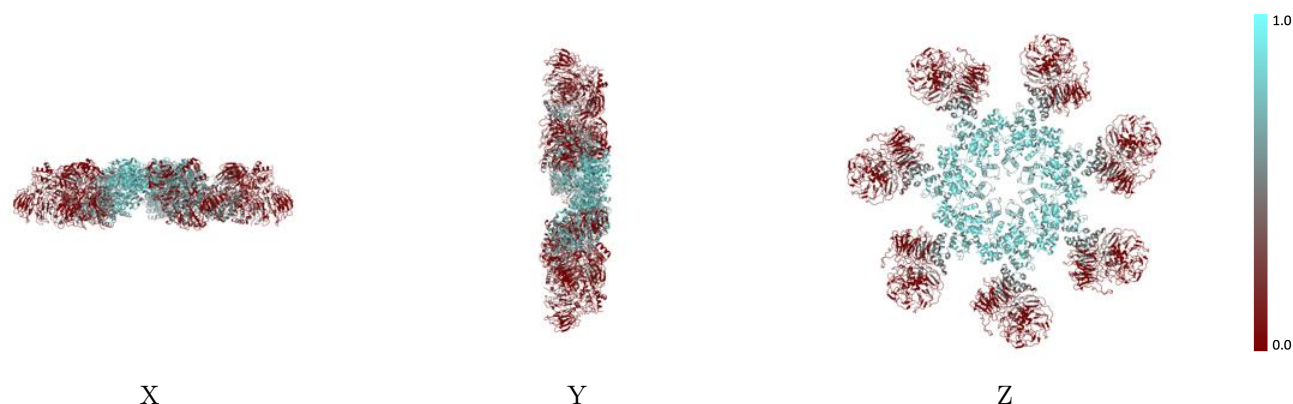
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



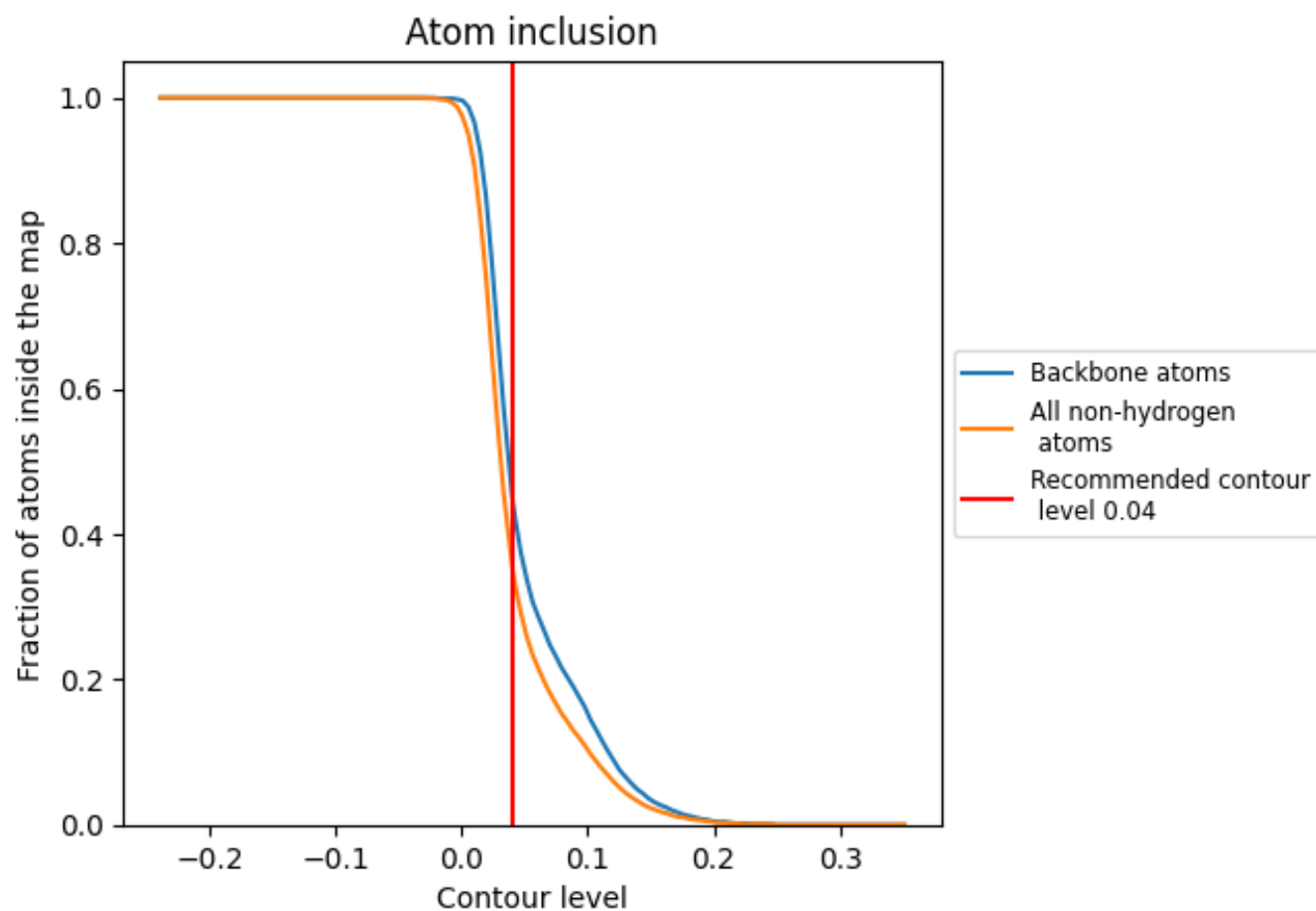
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.4 Atom inclusion [i](#)



At the recommended contour level, 45% of all backbone atoms, 36% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.3550	 0.2010
A	 0.3790	 0.2120
B	 0.0960	 0.0860
C	 0.3780	 0.2120
D	 0.0940	 0.0880
E	 0.3800	 0.2120
F	 0.0990	 0.0840
G	 0.3790	 0.2110
H	 0.0990	 0.0830
I	 0.3780	 0.2110
J	 0.1030	 0.0870
K	 0.3790	 0.2110
L	 0.1010	 0.0900
M	 0.3800	 0.2110
N	 0.0970	 0.0860

