



# wwPDB EM Validation Summary Report ⓘ

Nov 11, 2024 – 08:45 AM JST

PDB ID : 3JBT  
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 : 4RSZ, 3J2T

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

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

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<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
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The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev113  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

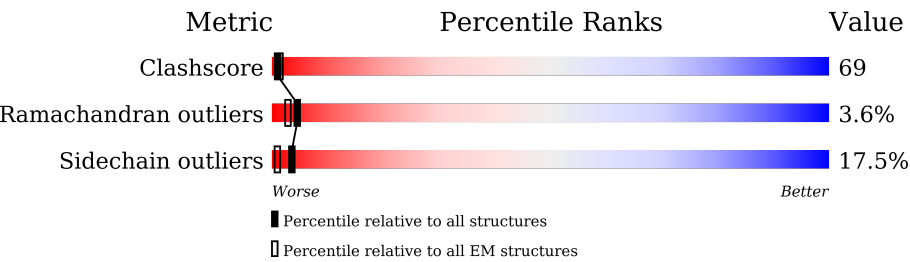


# 1 Overall quality at a glance i

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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

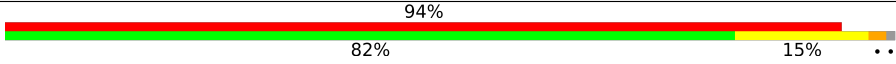
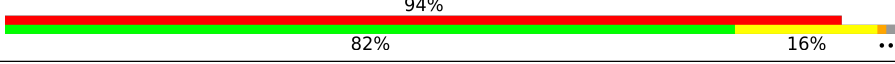
The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey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

Mol	Chain	Length	Quality of chain
1	A	1260	<div><div>50%</div><div><div>32%</div><div>45%</div><div>13%</div><div>•</div><div>9%</div></div></div>
1	C	1260	<div><div>50%</div><div><div>31%</div><div>45%</div><div>13%</div><div>•</div><div>9%</div></div></div>
1	E	1260	<div><div>50%</div><div><div>32%</div><div>45%</div><div>13%</div><div>•</div><div>9%</div></div></div>
1	G	1260	<div><div>50%</div><div><div>32%</div><div>45%</div><div>13%</div><div>•</div><div>9%</div></div></div>
1	I	1260	<div><div>50%</div><div><div>32%</div><div>45%</div><div>13%</div><div>•</div><div>9%</div></div></div>
1	K	1260	<div><div>50%</div><div><div>32%</div><div>45%</div><div>13%</div><div>•</div><div>9%</div></div></div>
1	M	1260	<div><div>50%</div><div><div>32%</div><div>45%</div><div>13%</div><div>•</div><div>9%</div></div></div>
2	B	105	<div><div>94%</div><div><div>82%</div><div>15%</div><div>••</div></div></div>

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Mol	Chain	Length	Quality of chain
2	D	105	
2	F	105	
2	H	105	
2	J	105	
2	L	105	
2	N	105	



## 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	C	N	O	S	
			823	524	144	151	4	0
2	D	104	Total	C	N	O	S	
			823	524	144	151	4	0
2	F	104	Total	C	N	O	S	
			823	524	144	151	4	0
2	H	104	Total	C	N	O	S	
			823	524	144	151	4	0
2	J	104	Total	C	N	O	S	
			823	524	144	151	4	0
2	L	104	Total	C	N	O	S	
			823	524	144	151	4	0

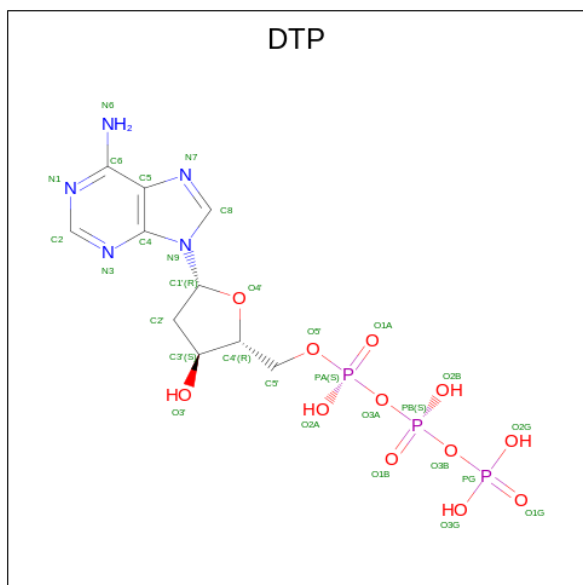
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Mol	Chain	Residues	Atoms					AltConf	Trace
2	N	104	Total	C	N	O	S	0	0
			823	524	144	151	4		

- Molecule 3 is 2'-DEOXYADENOSINE 5'-TRIPHOSPHATE (three-letter code: 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 (three-letter code: 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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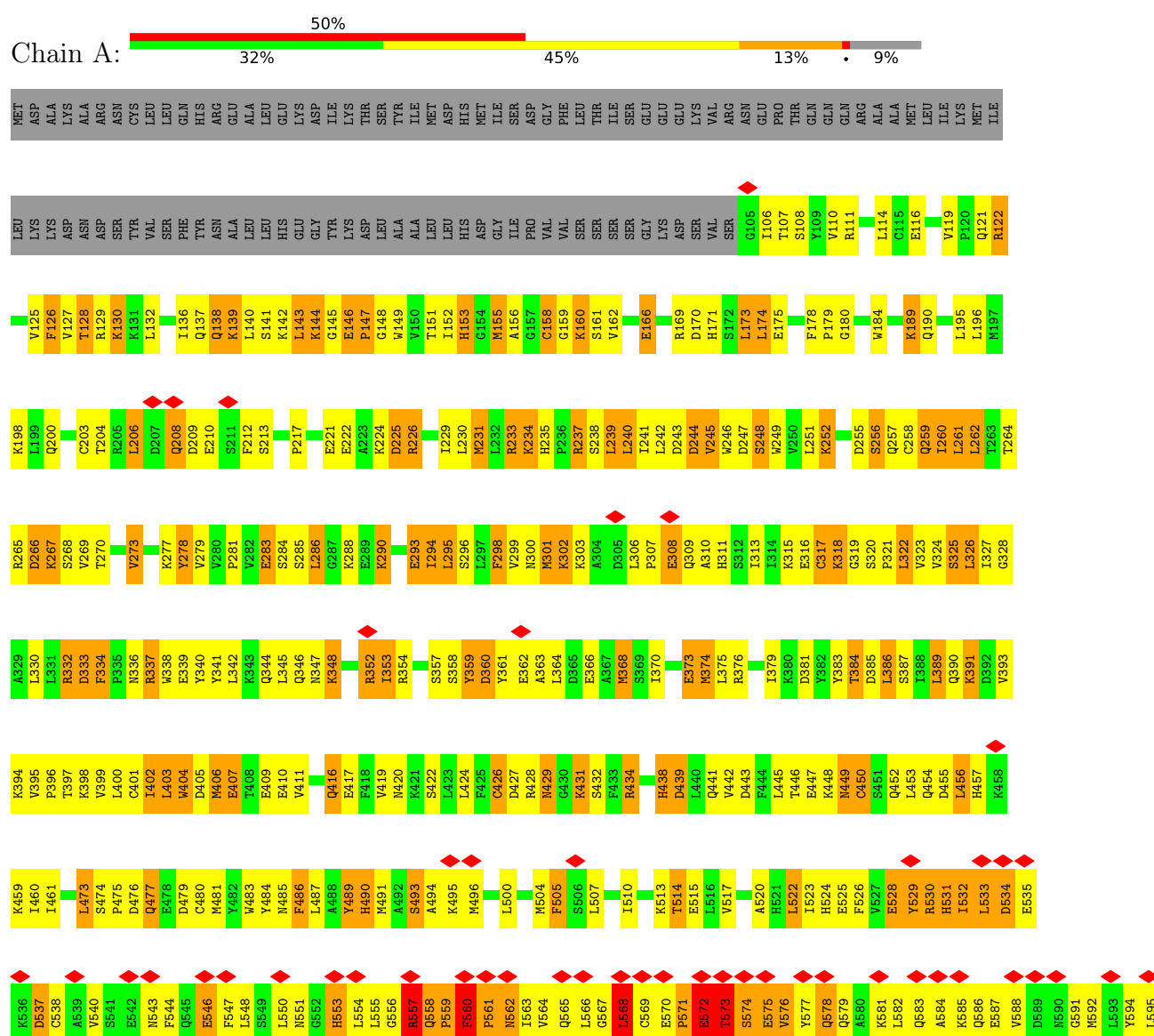
Mol	Chain	Residues	Atoms					AltConf
5	L	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
5	N	1	Total	C	Fe	N	O	0
			43	34	1	4	4	



### 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









S900	T837	E777	A717	H656	L595	E535	K458	V993	G328	T264	K198	L125	LEU
S901	G838	R778	T718	E657	E596	K536	K459	K394	A329	R265	L199	V126	LYS
D902	H839	K779	G719	D658	W597	D537	L460	V996	L331	K267	Q200	F127	LYS
D903	H840	S780	S720	D659	W598	C538	L461	P396	R332	C203	C203	T128	ASP
Q904	S841	T781	S721	V660	N599	V540	L473	T397	D333	T270	R206	R129	ASN
T905	T842	W882	D722	L661	K600	S541	S474	K398	F334	V273	K131	T204	ASP
I906	T843	W783	G723	C662	G601	S542	P475	V999	P335	L207	L132	R129	SER
L908	Q844	K784	F724	C663	E602	E542	D476	C401	R337	Q208	I136	K131	TRR
W909	Y845	Q785	L725	D664	M603	N543	Q477	L402	R338	Q209	I136	L132	VAL
E910	K846	F786	T726	F665	T604	F544	D479	L403	E339	D209	I136	I136	PHE
T911	D847	F787	L727	S666	N605	Q645	D479	W404	E339	D210	Q137	Q137	TRR
E912	F848	W788	L728	T667	N606	E546	N481	D406	Y341	S211	Q138	Q138	ASN
K913	S849	W789	D729	D668	S607	F547	Y482	E407	K343	F212	L140	L140	ALA
L914	P850	D790	L730	D669	R608	S549	Y483	E408	V282	Q214	S213	S213	LEU
C915	N852	E791	W731	R670	L609	L550	Y484	E409	E283	K142	K142	K142	HIS
K916	H853	D792	Q732	F671	N610	N551	N485	E410	Q344	S284	L143	L143	GLU
N917	L854	F793	K733	A673	V611	D552	N487	E411	Q346	S285	K144	K144	GLY
S918	A855	Q794	T674	T674	P613	H553	L488	Q416	K347	L286	G145	G145	TRR
E919	W856	E795	C675	C675	H614	H555	A492	Q417	E221	E222	P217	P217	LYS
W920	V857	D796	S676	S676	T615	R557	A493	E417	E222	K288	E222	E222	ASP
N921	A858	F797	W737	D678	D616	L554	H490	F418	E224	K224	V149	V149	ALA
L922	L859	E798	D678	K679	A617	P559	N491	Y419	E289	K290	V150	V150	ALA
K923	S860	W799	K679	W618	V618	F560	N496	N420	E293	D225	T151	T151	LEU
Q924	Q861	I800	H680	H619	H620	N562	L500	Q426	I294	R226	I152	I152	LEU
E925	Y862	W801	V681	H620	C622	T563	L500	D427	I229	H153	H153	H153	HIS
V926	G863	C802	K682	A621	C622	N564	N504	R428	S296	G154	G154	G154	ASP
D927	W864	C803	W684	C622	C622	N564	F505	N429	S296	M231	M231	M231	GLY
V928	E865	C804	N685	N685	N685	N566	S506	Q430	F298	L232	L232	L232	ILE
W929	L866	S805	S745	S686	E625	G567	L507	K431	V299	R233	C158	C158	PRO
V930	W867	W806	V746	W746	D626	G567	L507	Q432	M301	H235	K160	K160	VAL
Q931	N868	S807	W747	W747	Q627	G567	L507	F433	K302	P236	S161	S161	SER
E932	T869	D808	H748	H748	Q628	C569	T510	R434	A304	R237	S238	S238	SER
N933	D870	D809	G749	G749	T630	E570	K513	H438	D305	S239	E166	E166	GLY
E934	S871	C810	W750	A631	T630	P571	T514	D439	L306	I241	R169	R169	LYS
V935	H872	A811	F751	H693	E572	E572	E515	L440	E308	D243	D170	D170	ASP
K936	S873	B812	S752	T694	S632	T573	L516	Q441	A310	D244	H171	H171	VAL
V937	K874	B813	F753	W695	C633	S574	V517	V442	H311	W245	L173	L173	SER
L938	W875	M814	D754	D696	G634	E575	A520	F444	I313	D247	L174	L174	SER
A939	A876	W815	D755	E697	A635	W576	L522	T446	I314	W249	E175	E175	GLY
W940	D877	A816	K756	H698	D636	Q578	H524	E447	E316	V250	F178	F178	ASP
D941	C878	A817	L757	S699	K637	Q579	E525	K448	C317	L251	P179	P179	SER
H942	R879	K818	L758	E700	L639	A580	V527	C450	T384	K252	G180	G180	VAL
I943	C880	N819	A759	Q701	Q640	K581	E528	Q452	G319	D255	W184	W184	SER
R944	H881	K820	S760	W702	V641	L582	Y529	L453	S320	S256	C115	C115	GLY
R945	L882	B821	C761	W703	F642	Q583	R530	Q454	L322	Q257	E116	E116	ASP
L946	S883	C762	S762	C704	K643	A584	H531	D455	C258	Q258	Q190	Q190	LYS
Q947	W884	L823	A763	C705	E645	K585	Q586	L456	L389	V260	L195	L195	VAL
L948	V885	R824	D764	T646	E647	E587	L533	H457	K391	L262	M197	M197	SER
H949	R886	D825	G765	F707	E648	W588	D534		D255	T263			
N950	G887	T826	T766	T766	K649	D589			S256				
Q951	W888	H827	L767	W708	L650	N590			Q257				
R952	M889	T828	K768	W709	L651	N592			C258				
T953	F890	L769	L769	S710	L651	N592			Q259				
Q954	S893	C829	L769	S711	L653	N593			L261				
E955	D893	Q830	D771	H712	L653	N593			L261				
L956	G894	L831	D772	H713	L654	N594			L262				
D957	S895	L832	A772	L714	L654	N594			L262				
Y958	W958	L833	T773	L715	L655	N594			L262				
L959	T899	B836	H776	L716	L655	N594			L262				







HIS	K1200	T1140	D1080	S1020	T960	S900	H839	K779	G719	D658	W597	D537	I460
	W1201	L1141	F1081	S1021	E961	S901	H840	S780	S720	E959	I598	C538	I461
	W1202	L1142	V1082	S1022	A962	D902	S841	I781	S721	V660	N599	A539	L473
	N1203	A1143	C1083	D1023	Q963	D903	T842	N782	D722	L661	K600	V540	P475
	W1204	T1144	H1084	D1024	V964	Q904	T843	N783	C723	C862	K601	S541	D476
	V1205	G1145	Q1085	A1025	S965	T905	Q844	I783	F724	C863	M602	E542	Q477
	T1206	D1146	G1086	E1026	C966	R907	Y845	K784	L725	A664	I603	N543	E478
	G1207	D1147	T1087	I1027	C967	R908	C846	Q785	L726	F665	T604	F544	D479
	E1208	M1148	V1088	Q1028	C968	Y909	D847	F786	K727	S666	N605	Q546	C480
	S1209	G1149	L1089	V1029	L969	E910	F848	F787	L728	T667	L606	E545	M481
	S1210	E1150	S1090	W1030	S970	T911	S849	M789	W728	D668	S607	F547	Y482
	Q1211	I1151	C1091	N1031	P971	K912	P850	L788	D729	D669	R608	S549	M483
	T1212	R1152	D1092	W1032	H972	K913	Q851	L790	W730	R670	L609	L550	Y484
	F1213	I1153	I1093	Q1033	L973	V914	H853	E791	W731	F671	L509	N551	M485
	W1214	W1154	S1094	Q1034	Q974	C915	L854	F793	K733	A673	V610	G552	F486
	N1215	N1155	H1095	D1035	Y975	C916	A855	Q794	E734	T674	R612	H553	L487
	G1217	V1156	D1096	K1036	I976	N917	V856	E795	C735	S676	P613	L554	A488
	T1218	S1157	A1097	C1037	A977	S918	W857	D796	R736	D678	H614	L555	Y489
	N1219	M1158	T1098	I1038	F978	A919	A858	M797	W737	K679	T615	L556	H490
	L1220	G1159	K1099	F1039	G979	V920	L859	E798	T738	Q558	A617	P559	M491
	K1221	E1160	F1100	L1040	D980	L922	S860	W799	W739	K680	V618	F560	A494
	K1222	L1161	S1101	R1041	E981	K923	Q861	I800	F740	W681	Y619	K495	A492
	I1223	L1162	S1102	G1042	N982	Q924	Y862	V801	G741	K682	H620	P561	M496
	H1224	H1163	T1103	H1043	G983	Q925	C863	K802	H742	I683	A621	N562	L500
	V1225	L1164	S1104	Q1044	A984	E925	V864	C803	T743	W884	I563	I563	M504
	P1227	C1165	A1105	E1045	I985	V926	E865	C904	N744	N685	A621	Q565	F505
	D1228	A1166	D1106	T1046	E986	D927	L866	S905	S745	L566	G567	L566	S506
	F1229	P1167	K1107	V1047	I987	V928	W867	W806	V746	L568	I510	L568	L507
	T1231	L1168	T1108	K1048	L988	V929	N868	S907	W747	G889	Q622	C569	I510
	W1232	S1169	A1109	D1049	E989	F930	T869	A808	H748	E990	Q628	E570	K513
	Y1233	E1170	K1110	F1050	L990	Q931	D870	L691	R629	L691	I630	P571	T514
	T1234	E1171	I1111	R1051	V991	E932	S871	D609	I630	V692	A631	E572	E515
	V1235	G1172	W1112	L1052	N992	N933	S872	G810	H693	H693	S632	T573	L516
	D1236	A1174	S1113	N993	N993	E934	K874	A811	T694	T694	C633	S574	V517
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	T1246	L1183	L1123	S1062	H1002	R944	L882	C761	Q641	Q641	Q583	Y529	R530
	L1247	C1184	R1124	F1063	K1003	R945	S883	S762	F642	F642	A584	H531	H531
	E1248	F1185	G1125	D1064	K1004	L946	W884	A763	C704	C704	K643	K585	I532
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	GLU	P1187	N1127	T1066	V1006	L948	H886	G765	T646	T646	G647	E587	D534
	HIS	D1188	G1128	V1067	W1007	I949	C887	T766	G647	G647	E587	V588	E535
	HIS	G1189	C1129	K1068	H1008	N950	W888	L767	E587	E587	E587	D589	K536
	HIS	K1190	V1130	V1069	I1009	C951	N889	S710	K649	K649	N590	G591	G591
	HIS	L1191	R1131	W1070	Q1010	R952	T828	S711	L651	L651	M592	M592	M592
	HIS	L1192	C1132	I1071	F1011	T953	S829	H712	E593	E593	L593	L593	L593
	HIS	L1193	S1133	I1072	T1012	Q955	G854	H713	I653	I653	Y594	Y594	Y594
	HIS	S1194	A1134	I1073	A1013	Q956	S895	L714	K654	K654	E596	E596	E596
	HIS	A1195	F1135	T1074	D1014	I956	S896	T773	A655	A655	H656	H656	H656
	HIS	G1196	G1075	M1076	K1016	D957	F897	A717	E596	E596	E596	E596	E596
	HIS	G1197	K1077	K1077	T1017	L958	L898	A717	E596	E596	E596	E596	E596
	HIS	Y1198	D1138	E1078	L1018	L959	T899	E596	E596	E596	E596	E596	E596
	HIS	I1199	S1139	K1079	I1019			E596	E596	E596	E596	E596	E596



## ● Molecule 1: Apoptotic protease-activating factor 1



MET	ASP	ALA	LYS	ALA	ARG	ASN	CYS	LEU	LEU	GLN	HIS	GLN	LEU	ARG	GLU	ALA	LEU	LEU	LYS	ASP	ILE	LEU	MET	ASP	HIS	MET	ILE	SER	THR	THR	ILE	SER	SER	GLU	GLU	LYS	LYS	VAL	ARG	ASN	GLU	PRO	THR	THR	GLN	GLN	ARG	ALA	ALA	MET	LEU	ILE	LYS	MET	LYS	ILE																																																																																																																																																																																																																																																																																																																																																																																																																	
K198	L199	Q200	C203	T204	R205	L206	D207	Q208	D209	E210	S211	F212	S213	Q214	P217	E221	E222	A223	K224	D225	R226	E229	S230	M231	L232	R233	K234	H235	P236	R237	S238	L239	L240	L241	L242	D243	D244	V245	W246	D247	S248	W249	V250	L251	K252	D255	S256	Q257	C258	Q259	L260	L261	L262	T263	T264	R265	K267	V268	T270	V273	K277	Y278	Y279	V280	P281	E282	S284	S285	L286	K288	E289	K290	E293	I294	L295	S296	L297	F298	V299	N300	K301	K302	K303	A304	D305	L306	P307	E308	Q309	A310	H311	S312	I313	I314	K315	E316	C317	K318	G319	S320	P321	L322	V323	L324	S325	K326	I327	G328	A329	L330	R331	R332	D333	F334	P335	N336	R337	W338	E339	Y340	Y341	K342	Q343	Q344	L345	Q346	N347	K348	R352	I353	R354	S357	L358	Y359	D360	Y361	E362	A363	M364	D365	E366	A367	M368	S369	I370	E373	M374	L375	R376	I379	K380	D381	Y382	Y383	T384	M449	C450	S451	Q452	L453	Q454	D455	I456	H457	K458	K459	I460	L461	L473	D476	Q477	E478	C480	M481	Y482	W483	Y484	N485	F486	L487	H488	A489	H490	M491	A492	S493	A494	K495	M496	L500	M504	F505	S506	G507	L507	T510	K513	T514	E515	L516	V517	A520	H521	L522	I523	H524	E525	F526	V527	E528	Y529	H530	H531	I532	E533	L534	E535	K536	D537	C538	A539	V540	S541	E542	N543	Q544	Q545	E546	F547	L548	S549	L550	N551	Q552	H553	L554	L555	G556	R557	Q558	P559	F560	P561	N562	I563	V564	Q565	L566	G567	L568	C569	E570	F571	I572	E573	S574	E575	V576	Y577	Q578	Q579	A580	K581	L582	Q583	A584	K585	Q586	E587	V588	D589	N590	G591	M592	L593	Y594	L595	E596	W597	I598	R599	K600	K601	N602	I603	T604	N605	L606	S607	R608	L609	V610	R612	P613	H614	T615	D616	A617	V618	Y619	H620	A621	C622	E625	D626	G627	Q628	R629	I630	A631	S632	C633	G634	A635	D636	K637	T638	L639	Q640	V641	F642	K643	A644	E645	T646	G647	E648	K649	L650	L651	E652	I653	K654	A655	H656	E657	D658	E659	V660	L661	C662	C663	A664	F665	S666	T667	D668	D669	R670	F671	L672	A673	T674	C675	S676	V677	D678	K679	K680	V681	K682	L683	W684	N685	S686	G689	E690	L691	V692	H693	T694	V695	D696	E697	H698	S699	E700	Q701	V702	N703	C704	C705	A763	D764	G765	T766	L767	K768	W769	W770	D771	A772	L773	S774	A775	W776	E777	R778	K779	S780	I781	N782	L783	K784	Q785	F786	L787	L788	N789	L790	E791	D792	P793	Q794	E795	D796	W797	E798	W799	I800	V801	K802	C803	C804	S805	H806	S807	H808	D809	C810	N811	R812	L813	H814	V815	A816	A817	K818	N819	K820	L821	F822	L823	F824	D825	T826	S827	T828	S829	Q830	L831	L832	C833	E834	I835	H836	T837

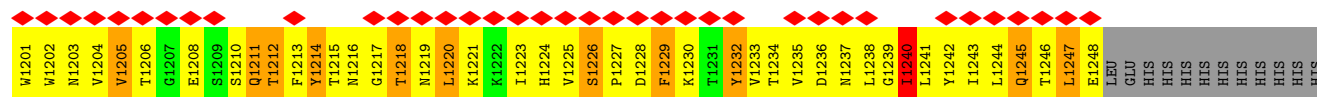




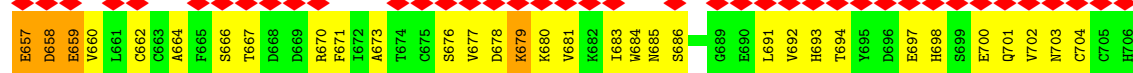
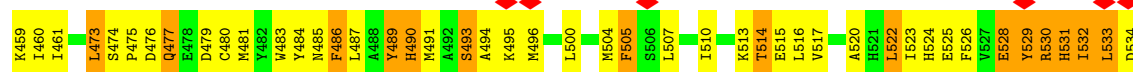
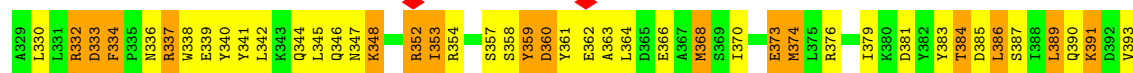
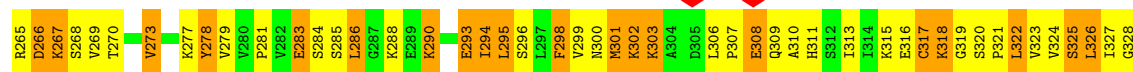
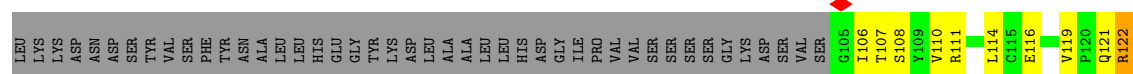
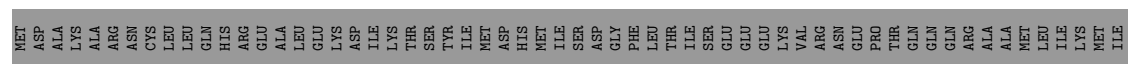


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S1021	S1022	D1023	D1024	A1025	E1026	I1027	Q1028	V1029	W1030	N1031	W1032	Q1033	L1034	D1035	K1036	C1037	I1038	F1039	L1040	R1041	G1042	H1043	Q1044	A1045	T1046	V1047	K1048	D1049	F1050	R1051	L1052	L1053	K1054	N1055	S1056	R1057	L1058	L1059	S1060	W1061	S1062	F1063	D1064	G1065	T1066	V1067	K1068	V1069	W1070	N1071	C1132	S1133	A1134	F1135	S1136	V1137	D1138	S1139	T1140
E961	A962	Q963	V964	S965	C966	C967	C968	L969	S970	P971	H972	L973	Q974	Y975	I976	A977	F978	G979	D980	E981	N982	G983	A984	I985	E986	I987	L988	E989	L990	V991	N992	N993	R994	V995	F996	Q997	S998	R999	F1000	Q1001	H1002	K1003	K1004	T1005	V1006	W1007	H1008	I1009	Q1010	F1011	T1012	A1013	D1014	E1015	K1016	T1017	L1018	I1019	D1020
S901	D902	D903	Q904	T905	I906	R907	L908	W909	E910	T911	K912	K913	V914	C915	K916	N917	S918	A919	V920	N921	L922	K923	Q924	E925	V926	D927	V928	V929	F930	Q931	E932	N933	E934	V935	N936	V937	L938	A939	V940	D941	H942	I943	R944	R945	L946	Q947	L948	I949	N950	C951	R952	T953	G954	Q955	I956	F957	Y958	L959	T960
S841	T842	I843	Q844	Y845	C846	D847	F848	S849	P850	Q851	N852	H853	L854	A855	V856	V857	A858	L859	S860	Q861	Y862	C863	V864	E865	L866	W867	N868	T869	D870	S871	R872	S873	K874	W875	A876	D877	C878	R879	C880	H881	L882	S883	W884	V885	H886	C887	W888	H889	F890	S891	P892	D893	C894	S895	S896	F897	L898	T899	S900
I781	N782	V783	K784	Q785	F786	F787	L788	N789	L790	E791	D792	F793	Q794	E795	D796	N797	E798	V799	T800	W801	K802	C803	C804	S805	W806	S807	A808	D809	G810	A811	R812	I813	W814	W815	A816	A817	K818	N819	K820	I821	F822	L823	F824	D825	I826	H827	T828	S829	C830	L831	L832	Q833	E834	I835	H836	T837	C838	H839	H840
S721	D722	C723	F724	L725	K726	L727	W728	D729	L730	N731	Q732	F733	E734	C735	R736	N737	T738	W739	F740	G741	H742	T743	N744	S745	V746	N747	H748	C749	R750	F751	S752	P753	D754	D755	F756	L757	L758	A759	S760	C761	S762	A763	D764	G765	T766	L767	K768	L769	W770	D771	A772	T773	S774	A775	N776	E777	K778	K779	S780
V660	L661	C662	C663	A664	F665	S666	D668	D669	R670	F671	L672	A673	T674	C675	S676	D678	K679	K680	V681	H682	L683	W684	N685	S686	G689	E690	L691	V692	H693	T694	Y695	D696	E697	H698	S699	E700	Q701	V702	N703	C704	K643	A644	E645	T646	G647	E648	K649	L650	L651	E652	K654	A655	H656	E657	D658	E659			
N599	K600	K601	N602	T603	T604	N605	L606	S607	R608	L609	V610	G611	R612	P613	H614	T615	D616	A617	V618	Y619	H620	A621	C622	E625	D626	G627	Q628	R629	I630	A631	S632	C633	G634	A635	D636	K637	T638	L639	Q640	V641	F642	K643	A644	E645	T646	G647	E648	K649	L650	L651	E652	K654	A655	H656	E657	D658	E659		
A539	V540	S541	E542	N543	F544	Q545	E546	F547	L548	S549	L550	G551	H553	L554	L555	G556	S557	Q558	P559	F560	P561	N562	L563	V564	Q565	L566	G567	L568	C569	E570	P571	E572	T573	S574	E575	V576	Y577	Q578	Q579	A580	K581	L582	Q583	A584	K585	Q586	E587	V588	D589	N590	G591	L592	L593	Y594	L595	E596	W597	I598	
V395	P396	K397	K398	V399	L400	C401	I402	W338	L403	W404	D405	W406	E407	L342	K343	Q344	L345	E410	V411	Q416	E417	F418	V419	M420	K421	S422	L423	L424	C426	D427	R428	M429	G430	K431	R434	H438	D439	L440	Q441	V442	D443	F444	L445	T446	E447	K448	M449	C450	S451	Q452	L453	Q454	D455	L389	L456	H457	K458	K459	I460

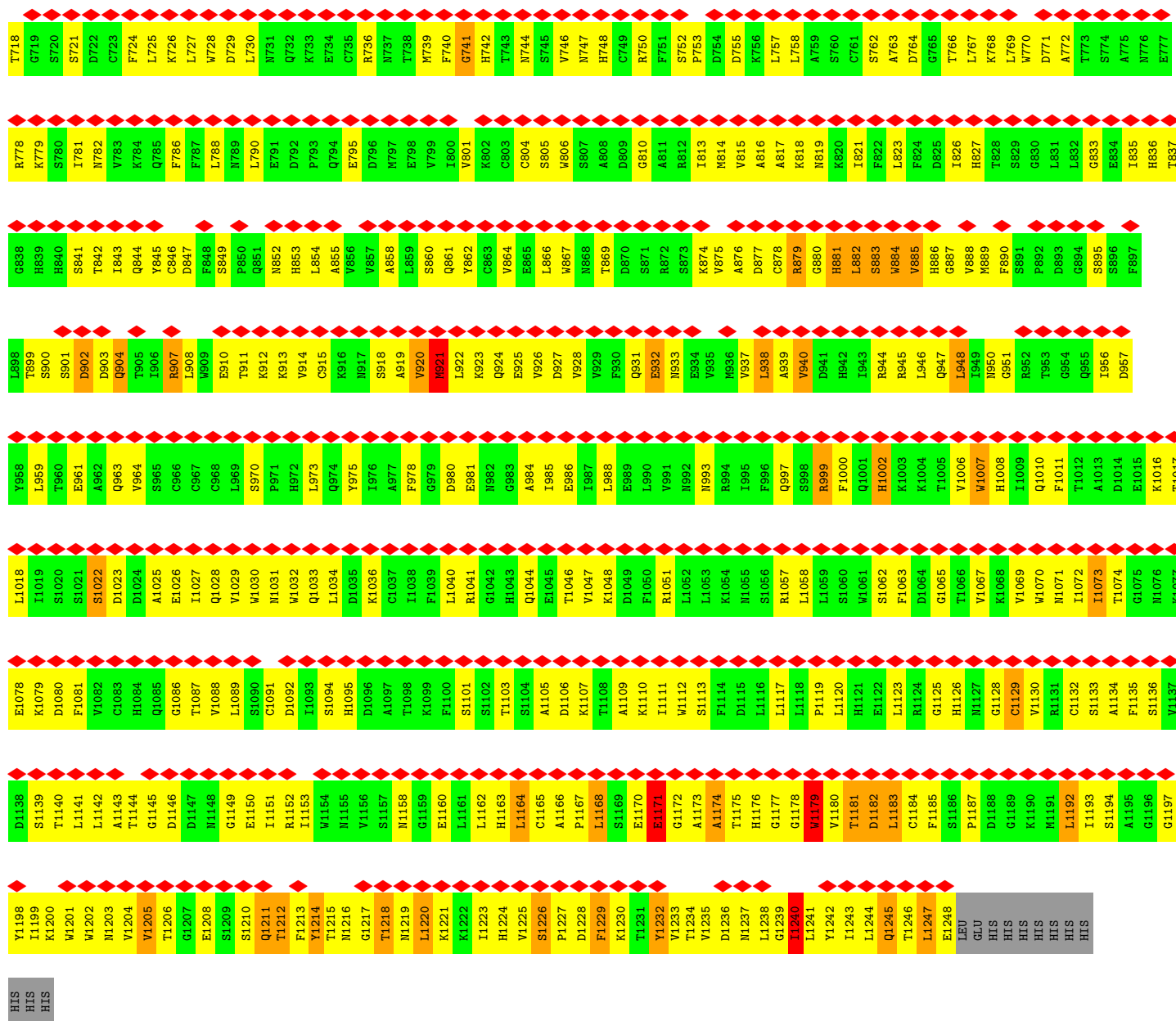




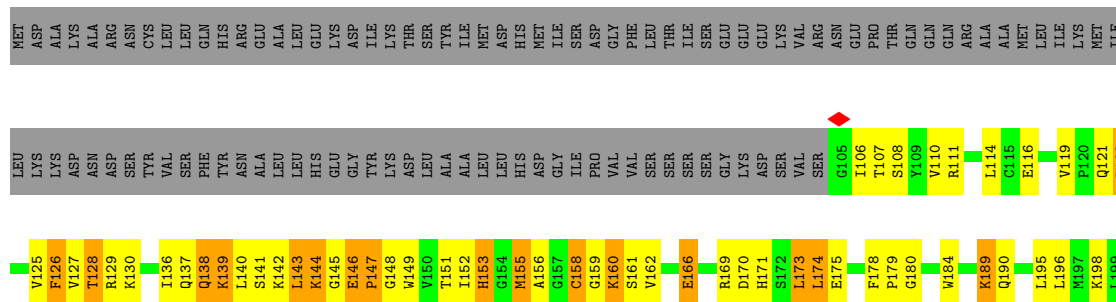
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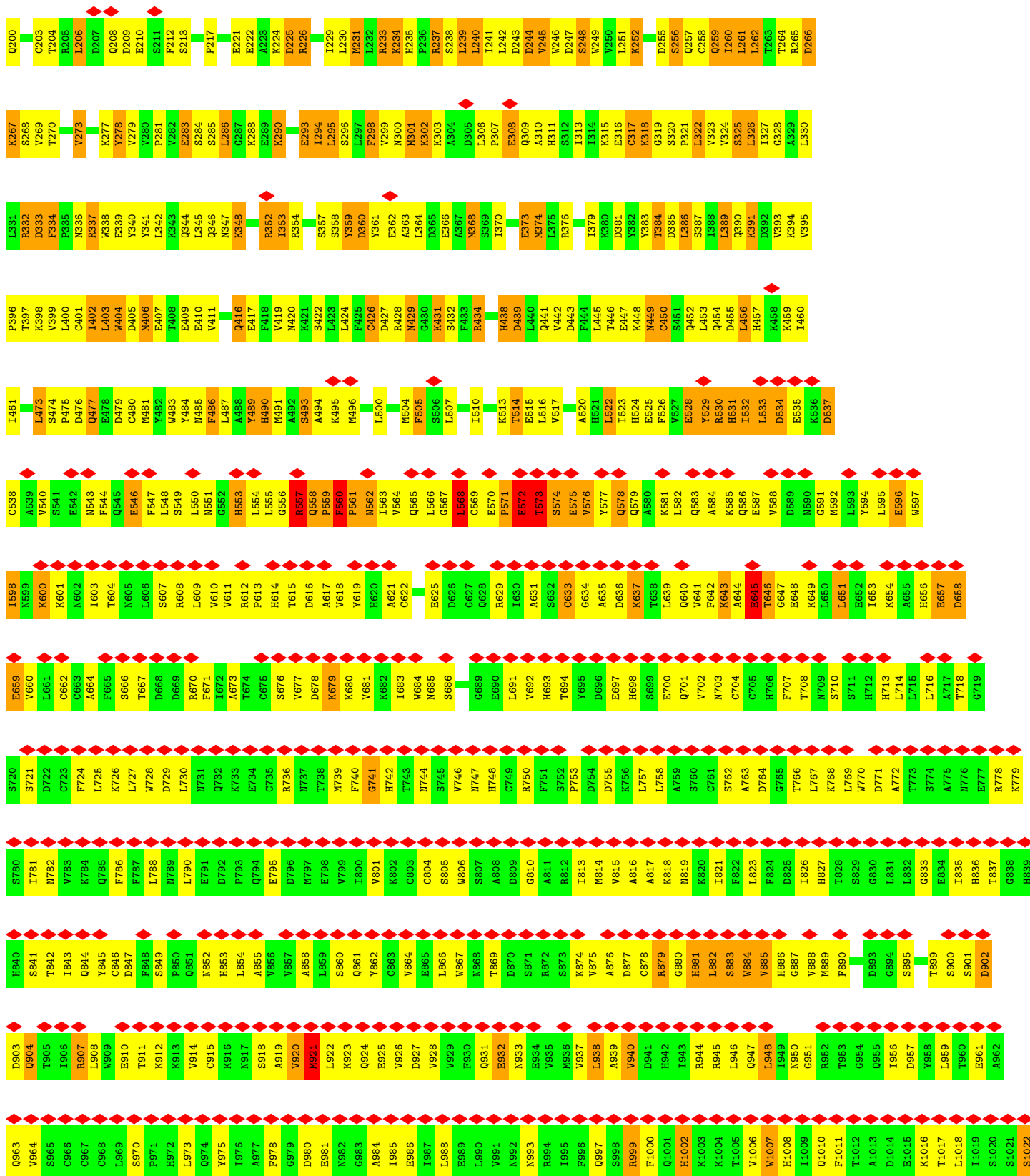




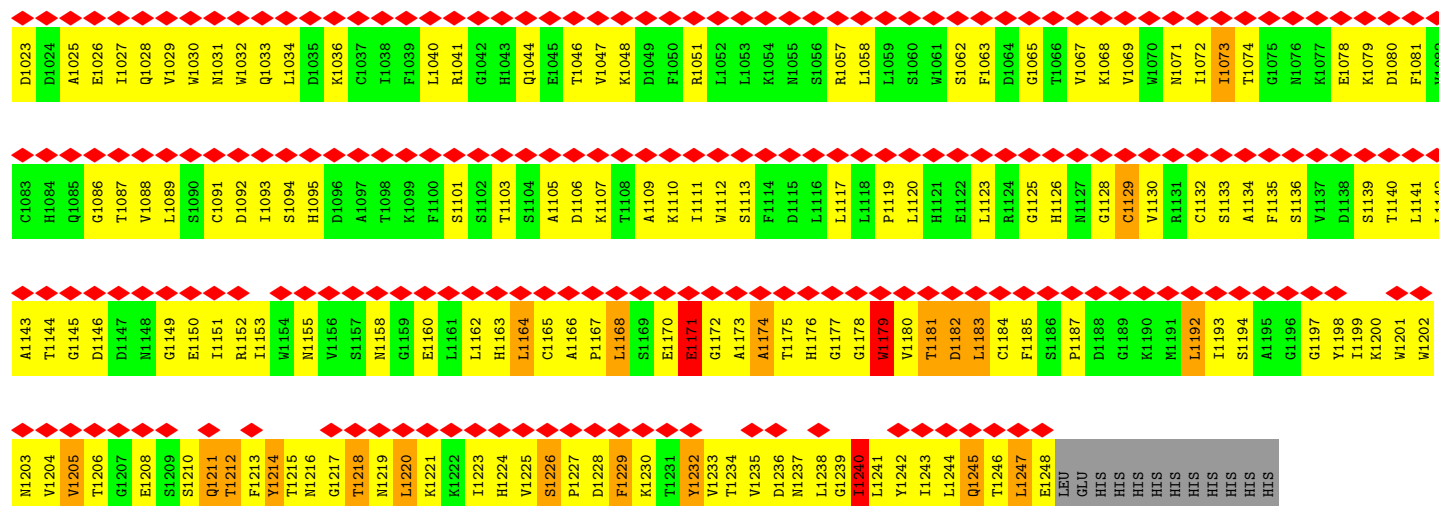
● Molecule 1: Apoptotic protease-activating factor 1



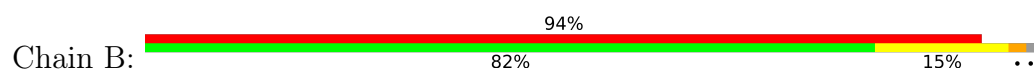




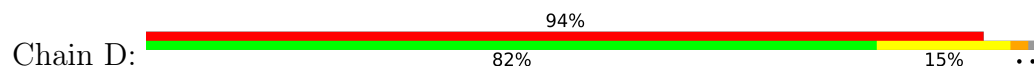




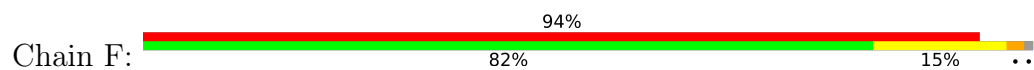
• Molecule 2: Cytochrome c



• Molecule 2: Cytochrome c

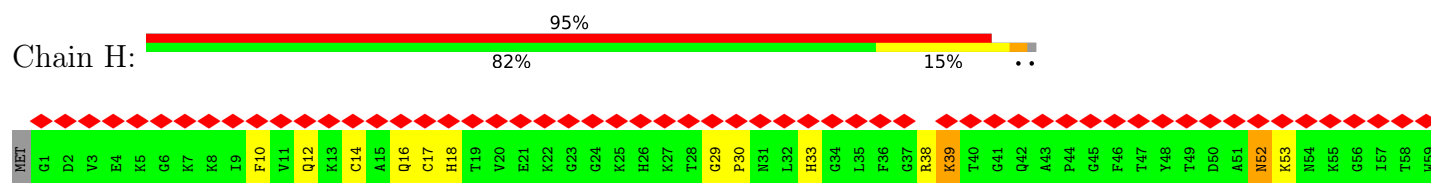


• Molecule 2: Cytochrome c

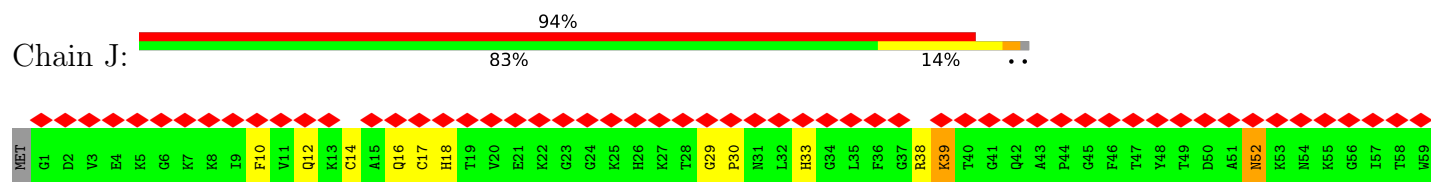


• Molecule 2: Cytochrome c

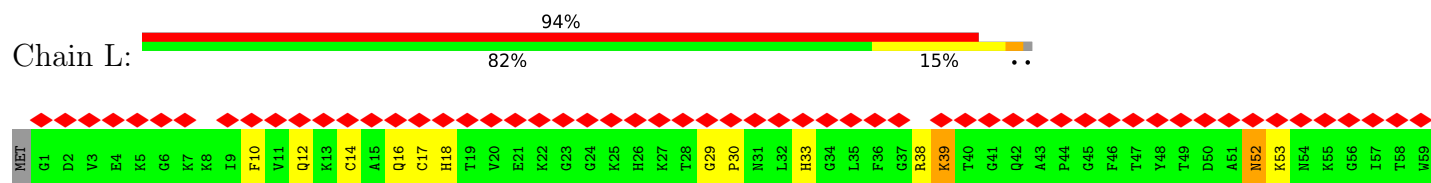




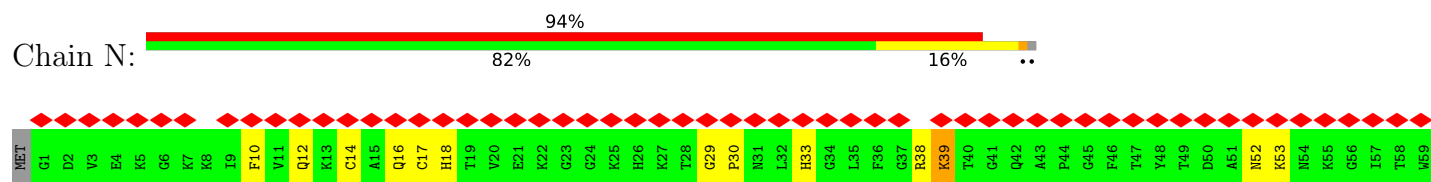
## • Molecule 2: Cytochrome c



## • Molecule 2: Cytochrome c



## • Molecule 2: Cytochrome c





## 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: DTP, MG, HEM

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	0.30	0/9337	0.51	2/12636 (0.0%)
1	C	0.30	0/9337	0.51	2/12636 (0.0%)
1	E	0.30	0/9337	0.51	2/12636 (0.0%)
1	G	0.30	0/9337	0.51	2/12636 (0.0%)
1	I	0.30	0/9337	0.51	2/12636 (0.0%)
1	K	0.30	0/9337	0.51	2/12636 (0.0%)
1	M	0.30	0/9337	0.51	2/12636 (0.0%)
2	B	0.65	0/839	0.73	0/1118
2	D	0.65	0/839	0.73	0/1118
2	F	0.65	0/839	0.73	0/1118
2	H	0.65	0/839	0.73	0/1118
2	J	0.65	0/839	0.73	0/1118
2	L	0.65	0/839	0.73	0/1118
2	N	0.65	0/839	0.73	0/1118
All	All	0.34	0/71232	0.53	14/96278 (0.0%)

There are no bond length outliers.

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	880	GLY	N-CA-C	5.73	127.43	113.10
1	I	880	GLY	N-CA-C	5.73	127.43	113.10
1	K	880	GLY	N-CA-C	5.73	127.43	113.10
1	M	880	GLY	N-CA-C	5.73	127.42	113.10
1	E	880	GLY	N-CA-C	5.72	127.41	113.10

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	1372	0
1	C	9139	0	9005	1371	0
1	E	9139	0	9005	1360	0
1	G	9139	0	9005	1382	0
1	I	9139	0	9005	1358	0
1	K	9139	0	9005	1357	0
1	M	9139	0	9005	1366	0
2	B	823	0	849	31	0
2	D	823	0	849	33	0
2	F	823	0	849	30	0
2	H	823	0	849	34	0
2	J	823	0	849	32	0
2	L	823	0	849	33	0
2	N	823	0	849	31	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	16	0
5	F	43	0	30	14	0
5	H	43	0	30	16	0
5	J	43	0	30	15	0
5	L	43	0	30	15	0
5	N	43	0	30	13	0
All	All	70252	0	69272	9596	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 69.

The worst 5 of 9596 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	21
1	C	1142/1260 (91%)	999 (88%)	98 (9%)	45 (4%)	2	21
1	E	1142/1260 (91%)	999 (88%)	98 (9%)	45 (4%)	2	21
1	G	1142/1260 (91%)	999 (88%)	98 (9%)	45 (4%)	2	21
1	I	1142/1260 (91%)	999 (88%)	98 (9%)	45 (4%)	2	21
1	K	1142/1260 (91%)	999 (88%)	97 (8%)	46 (4%)	2	21
1	M	1142/1260 (91%)	999 (88%)	97 (8%)	46 (4%)	2	21
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	23

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%)	838 (82%)	189 (18%)	1	9
1	C	1027/1131 (91%)	838 (82%)	189 (18%)	1	9
1	E	1027/1131 (91%)	838 (82%)	189 (18%)	1	9
1	G	1027/1131 (91%)	838 (82%)	189 (18%)	1	9
1	I	1027/1131 (91%)	838 (82%)	189 (18%)	1	9
1	K	1027/1131 (91%)	838 (82%)	189 (18%)	1	9
1	M	1027/1131 (91%)	838 (82%)	189 (18%)	1	9
2	B	86/87 (99%)	80 (93%)	6 (7%)	12	37
2	D	86/87 (99%)	80 (93%)	6 (7%)	12	37
2	F	86/87 (99%)	80 (93%)	6 (7%)	12	37
2	H	86/87 (99%)	80 (93%)	6 (7%)	12	37
2	J	86/87 (99%)	81 (94%)	5 (6%)	17	42
2	L	86/87 (99%)	80 (93%)	6 (7%)	12	37
2	N	86/87 (99%)	80 (93%)	6 (7%)	12	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	7791/8526 (91%)	6427 (82%)	1364 (18%)	<b>3</b> <b>10</b>

5 of 1364 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	633	CYS
1	K	1170	GLU
1	I	1171	GLU
1	I	619	TYR
1	K	332	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 208 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	1237	ASN
1	I	1126	HIS
1	M	840	HIS
1	I	138	GLN
1	I	457	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	H	201	2	41,50,50	1.32	6 (14%)	45,82,82	1.73	6 (13%)
5	HEM	J	201	2	41,50,50	1.32	6 (14%)	45,82,82	1.73	6 (13%)
3	DTP	G	1301	4	26,32,32	0.87	1 (3%)	30,50,50	1.56	4 (13%)
3	DTP	I	1301	4	26,32,32	0.86	1 (3%)	30,50,50	1.56	4 (13%)
3	DTP	C	1301	4	26,32,32	0.86	1 (3%)	30,50,50	1.56	4 (13%)
3	DTP	K	1301	4	26,32,32	0.86	1 (3%)	30,50,50	1.56	4 (13%)
5	HEM	B	201	2	41,50,50	1.31	6 (14%)	45,82,82	1.73	6 (13%)
3	DTP	A	1301	4	26,32,32	0.86	1 (3%)	30,50,50	1.56	4 (13%)
5	HEM	F	201	2	41,50,50	1.31	5 (12%)	45,82,82	1.73	6 (13%)
5	HEM	N	201	2	41,50,50	1.31	6 (14%)	45,82,82	1.74	6 (13%)
5	HEM	L	201	2	41,50,50	1.32	6 (14%)	45,82,82	1.73	6 (13%)
3	DTP	E	1301	4	26,32,32	0.87	1 (3%)	30,50,50	1.56	4 (13%)
3	DTP	M	1301	4	26,32,32	0.86	1 (3%)	30,50,50	1.56	4 (13%)
5	HEM	D	201	2	41,50,50	1.31	6 (14%)	45,82,82	1.73	6 (13%)

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	H	201	2	-	7/12/54/54	-
5	HEM	J	201	2	-	7/12/54/54	-
3	DTP	G	1301	4	-	5/18/34/34	0/3/3/3
3	DTP	I	1301	4	-	5/18/34/34	0/3/3/3
3	DTP	C	1301	4	-	5/18/34/34	0/3/3/3
3	DTP	K	1301	4	-	5/18/34/34	0/3/3/3
5	HEM	B	201	2	-	7/12/54/54	-
3	DTP	A	1301	4	-	5/18/34/34	0/3/3/3
5	HEM	F	201	2	-	7/12/54/54	-
5	HEM	N	201	2	-	7/12/54/54	-
5	HEM	L	201	2	-	7/12/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	DTP	E	1301	4	-	5/18/34/34	0/3/3/3
3	DTP	M	1301	4	-	5/18/34/34	0/3/3/3
5	HEM	D	201	2	-	7/12/54/54	-

The worst 5 of 48 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	J	201	HEM	C1B-NB	-3.40	1.34	1.40
5	H	201	HEM	C1B-NB	-3.38	1.34	1.40
5	L	201	HEM	C1B-NB	-3.37	1.34	1.40
5	N	201	HEM	C1B-NB	-3.37	1.34	1.40
5	F	201	HEM	C1B-NB	-3.35	1.34	1.40

The worst 5 of 70 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	201	HEM	CHC-C4B-NB	4.71	129.54	124.43
5	N	201	HEM	CHC-C4B-NB	4.70	129.53	124.43
5	L	201	HEM	CHC-C4B-NB	4.69	129.52	124.43
5	H	201	HEM	CHC-C4B-NB	4.67	129.51	124.43
5	D	201	HEM	CHC-C4B-NB	4.65	129.49	124.43

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	C	1301	DTP	C5'-O5'-PA-O2A
3	C	1301	DTP	C5'-O5'-PA-O3A
3	E	1301	DTP	C5'-O5'-PA-O2A

There are no ring outliers.

14 monomers are involved in 147 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	201	HEM	16	0
5	J	201	HEM	15	0
3	G	1301	DTP	6	0
3	I	1301	DTP	7	0

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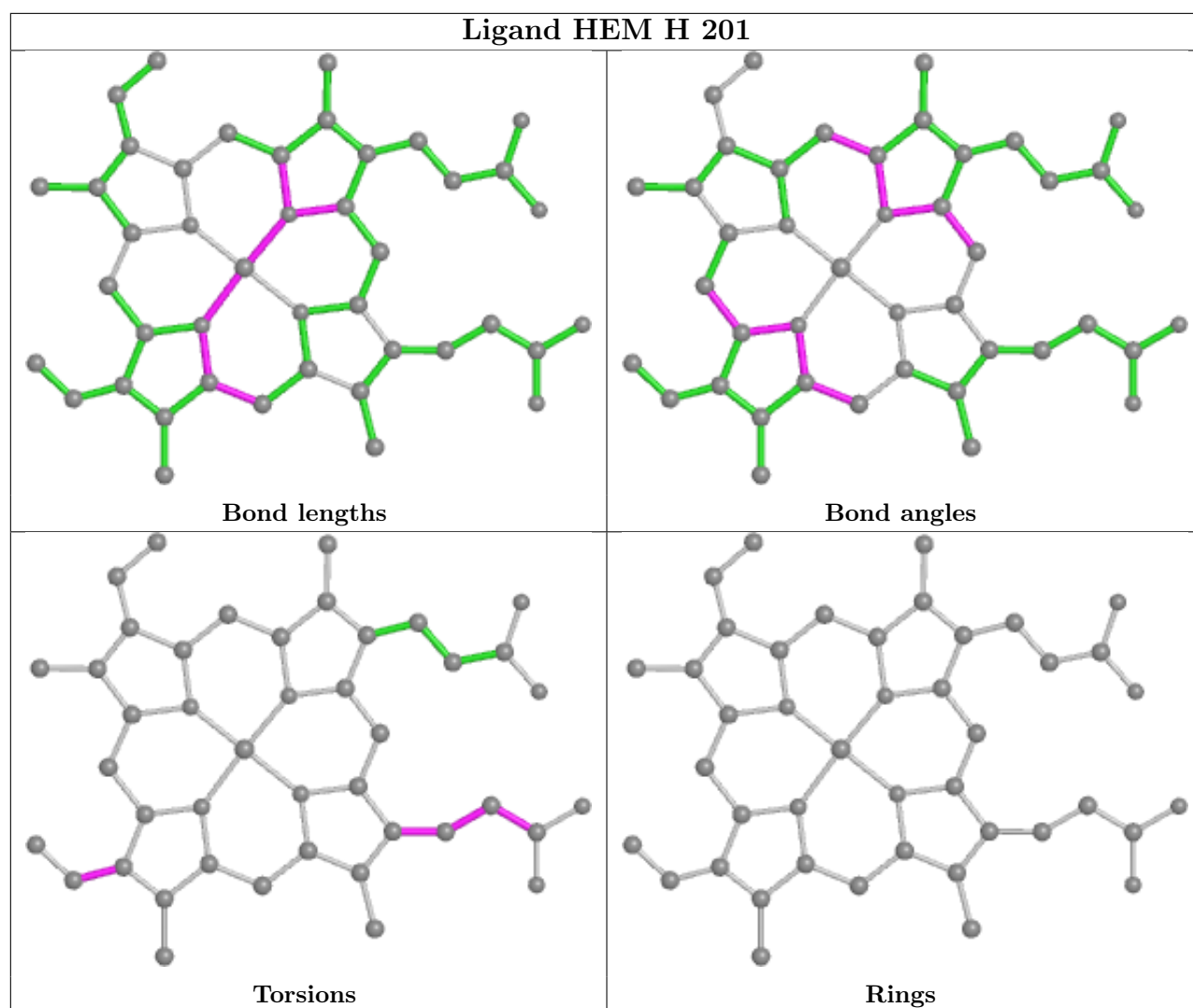


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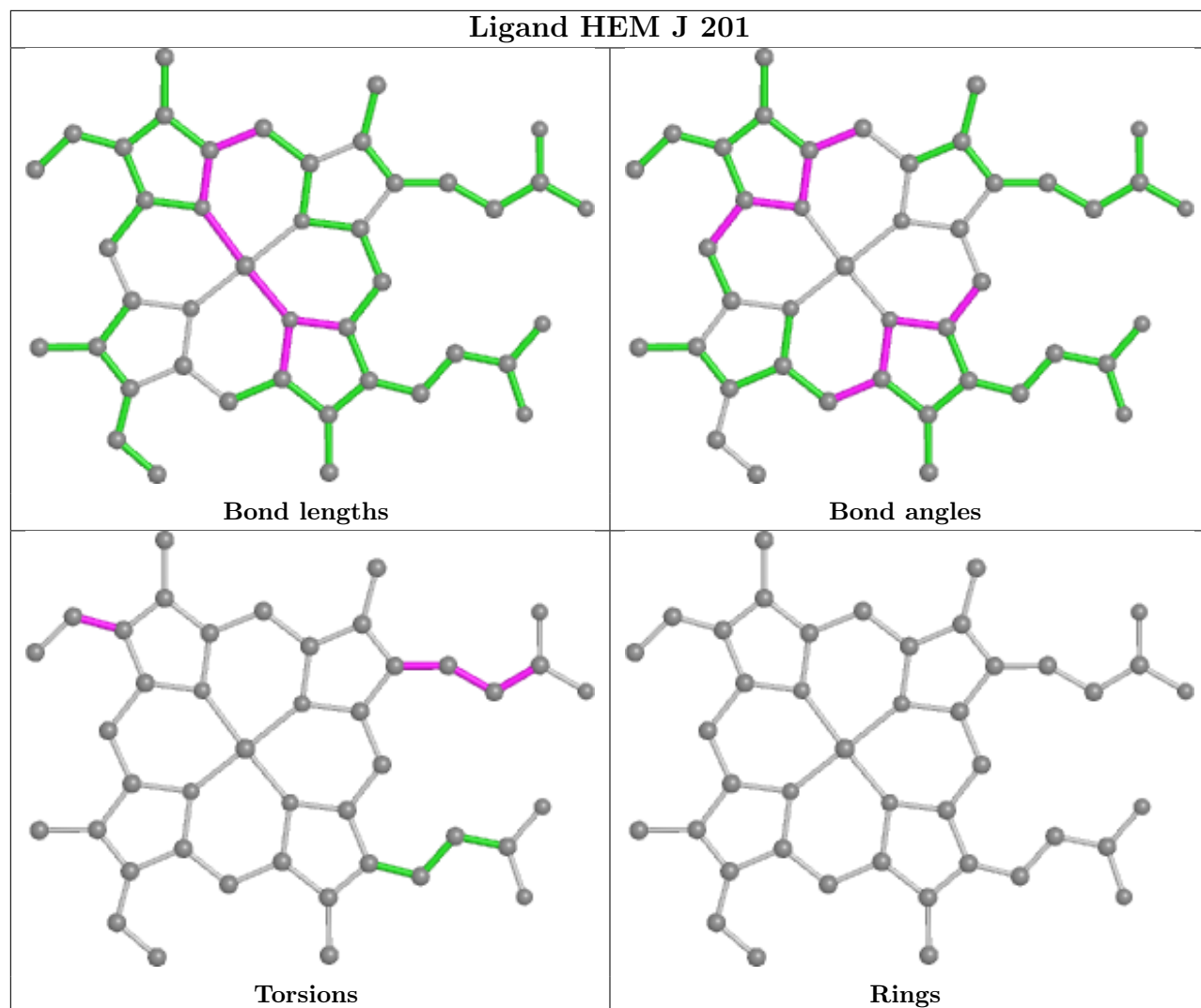
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1301	DTP	6	0
3	K	1301	DTP	6	0
5	B	201	HEM	15	0
3	A	1301	DTP	6	0
5	F	201	HEM	14	0
5	N	201	HEM	13	0
5	L	201	HEM	15	0
3	E	1301	DTP	6	0
3	M	1301	DTP	6	0
5	D	201	HEM	16	0

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.

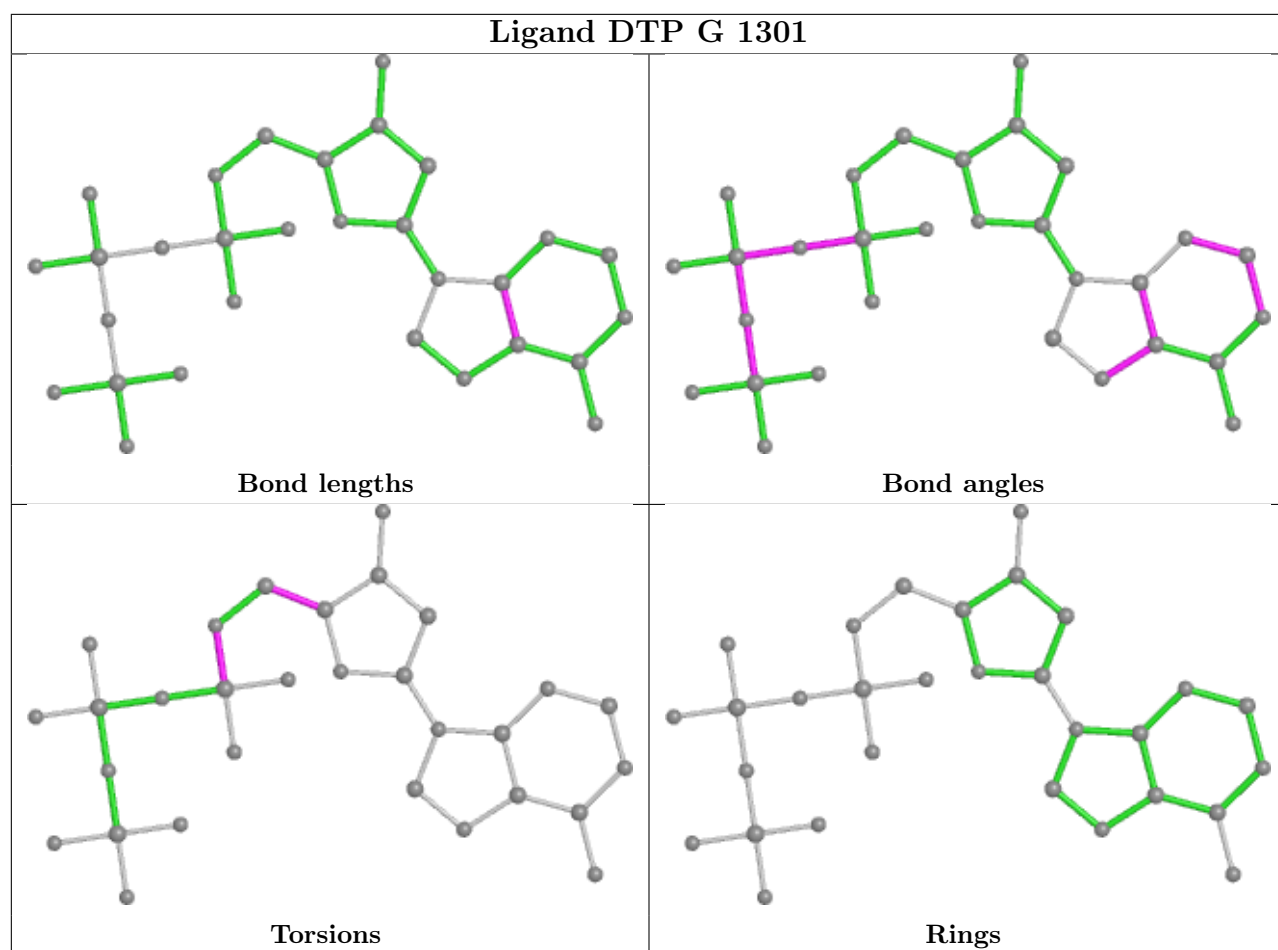




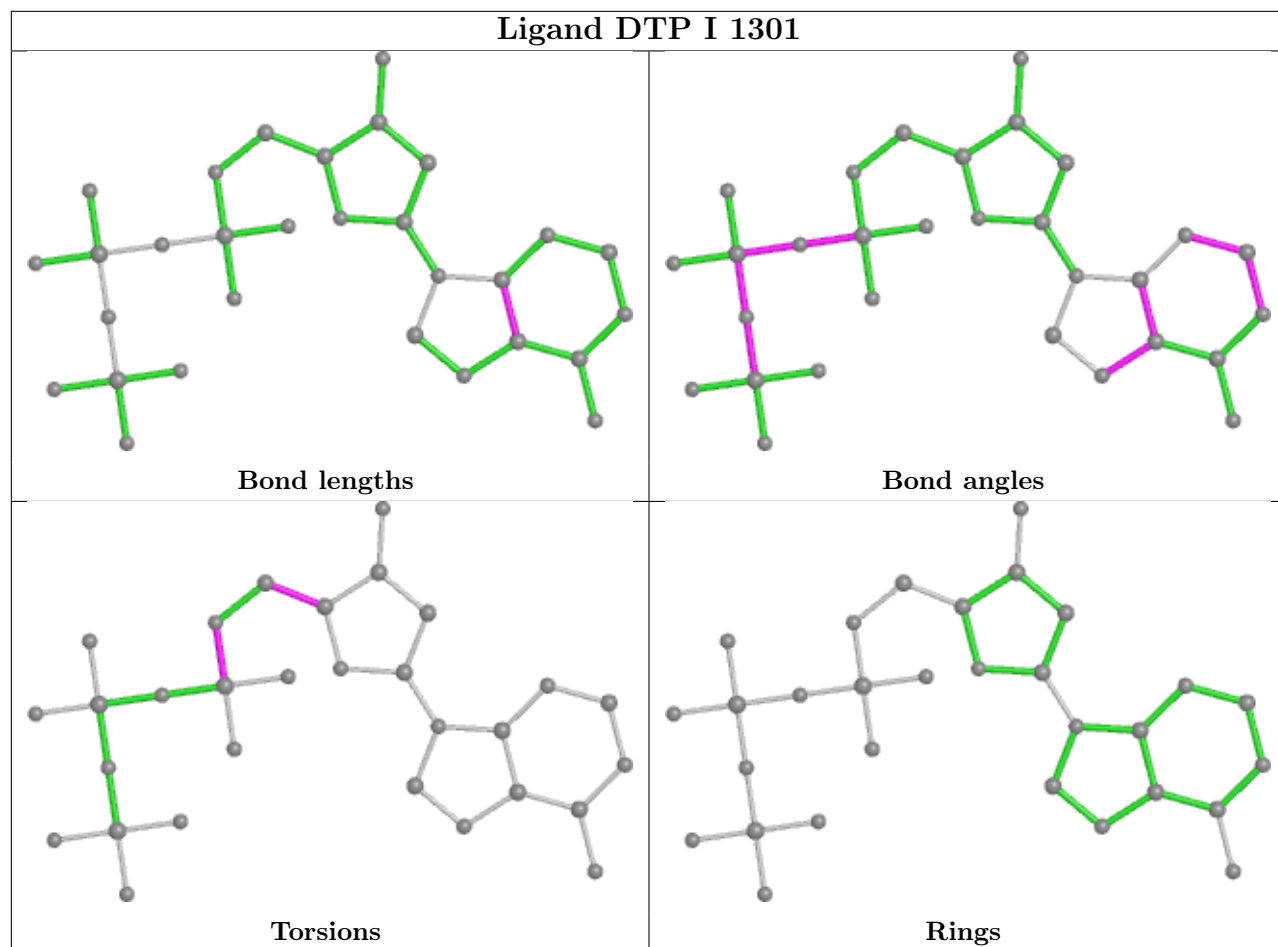




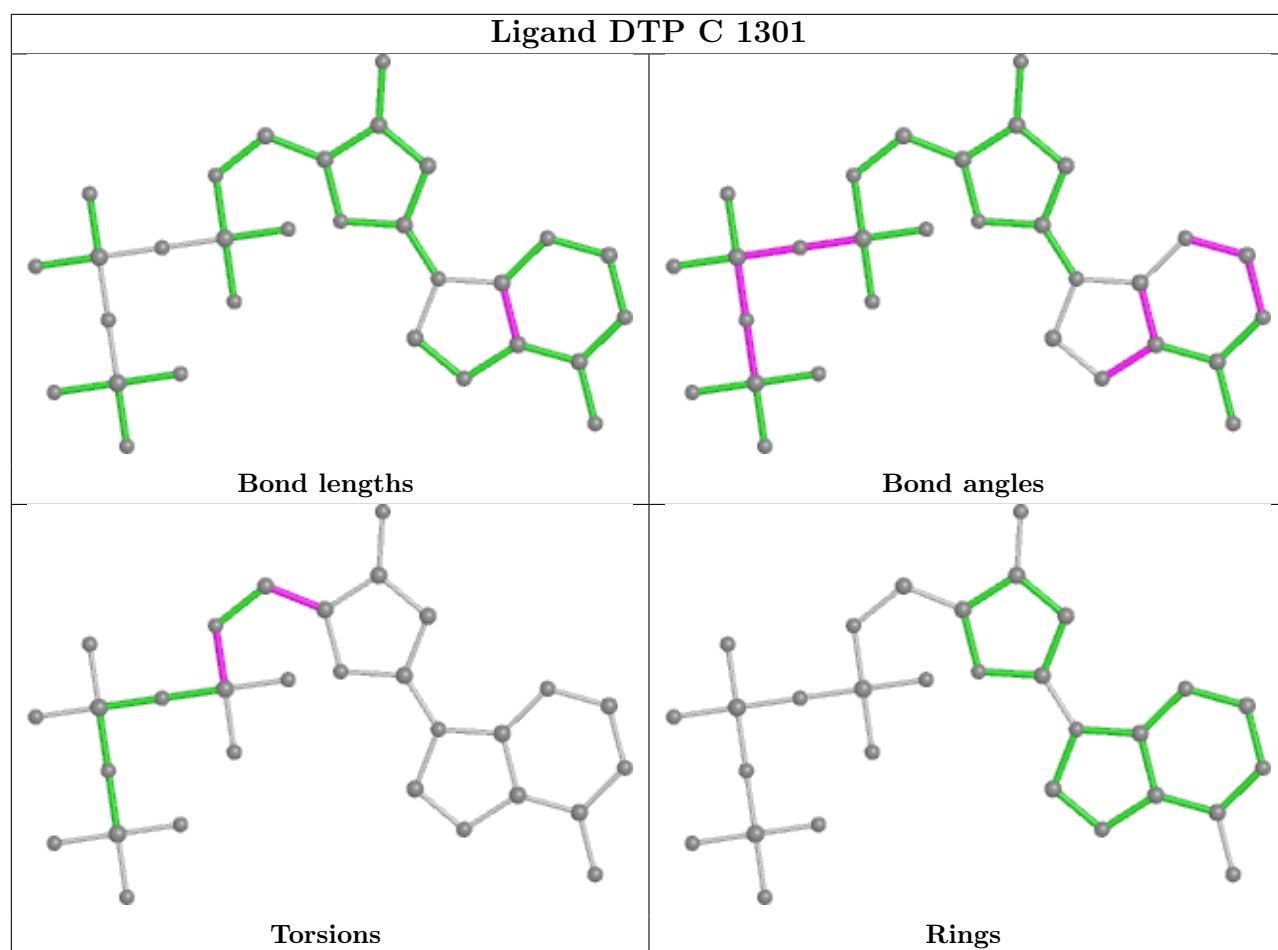




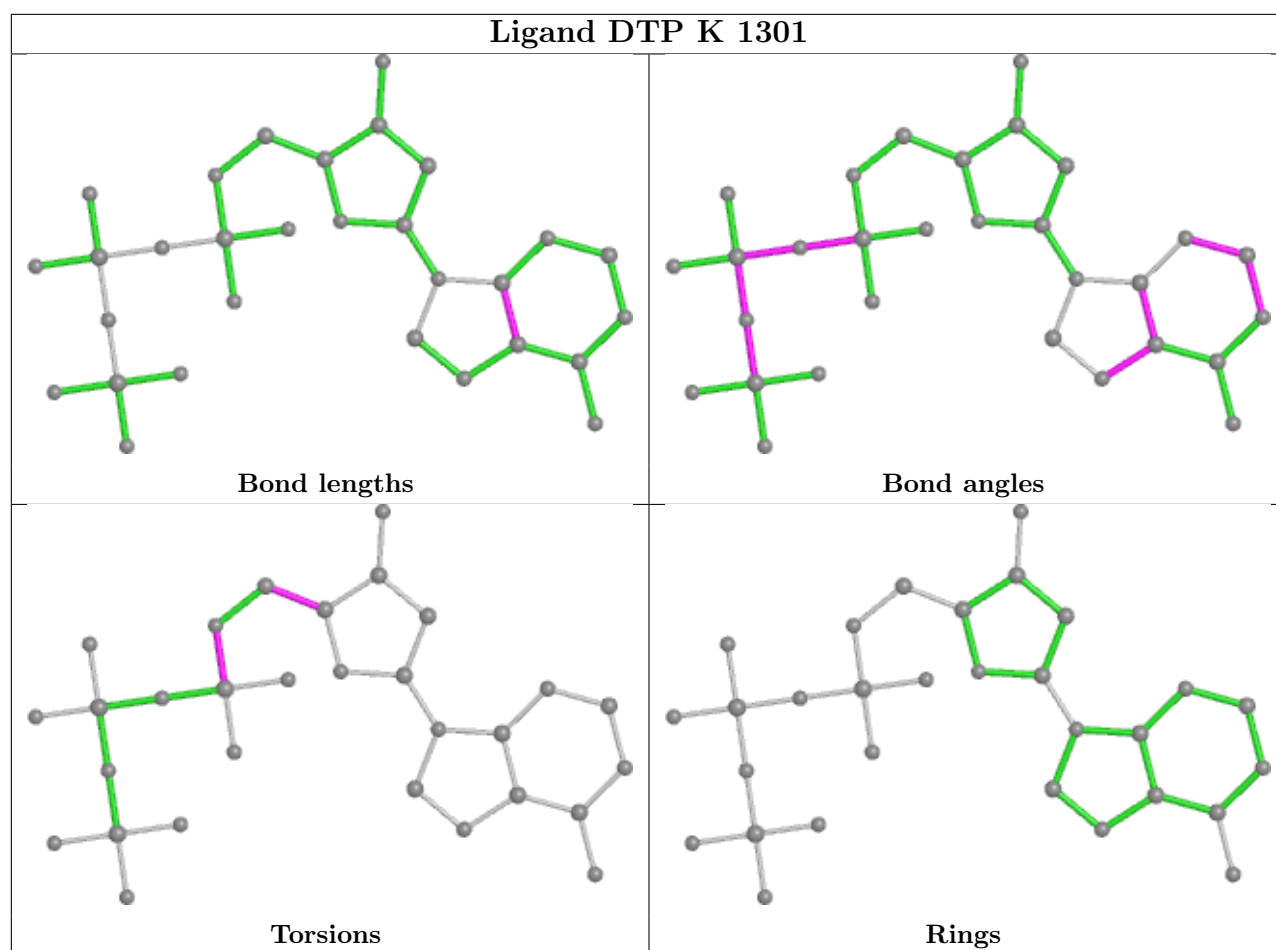




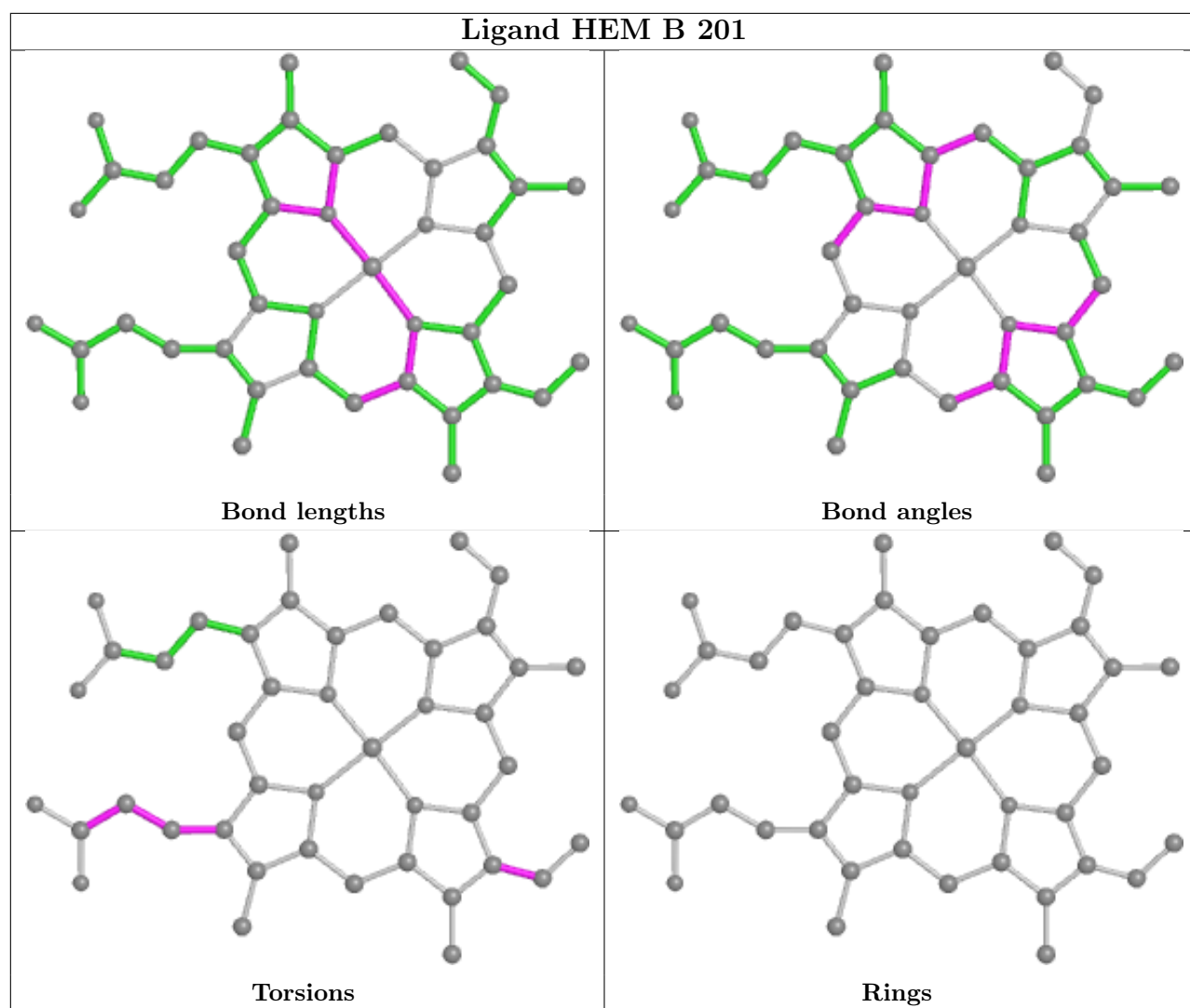




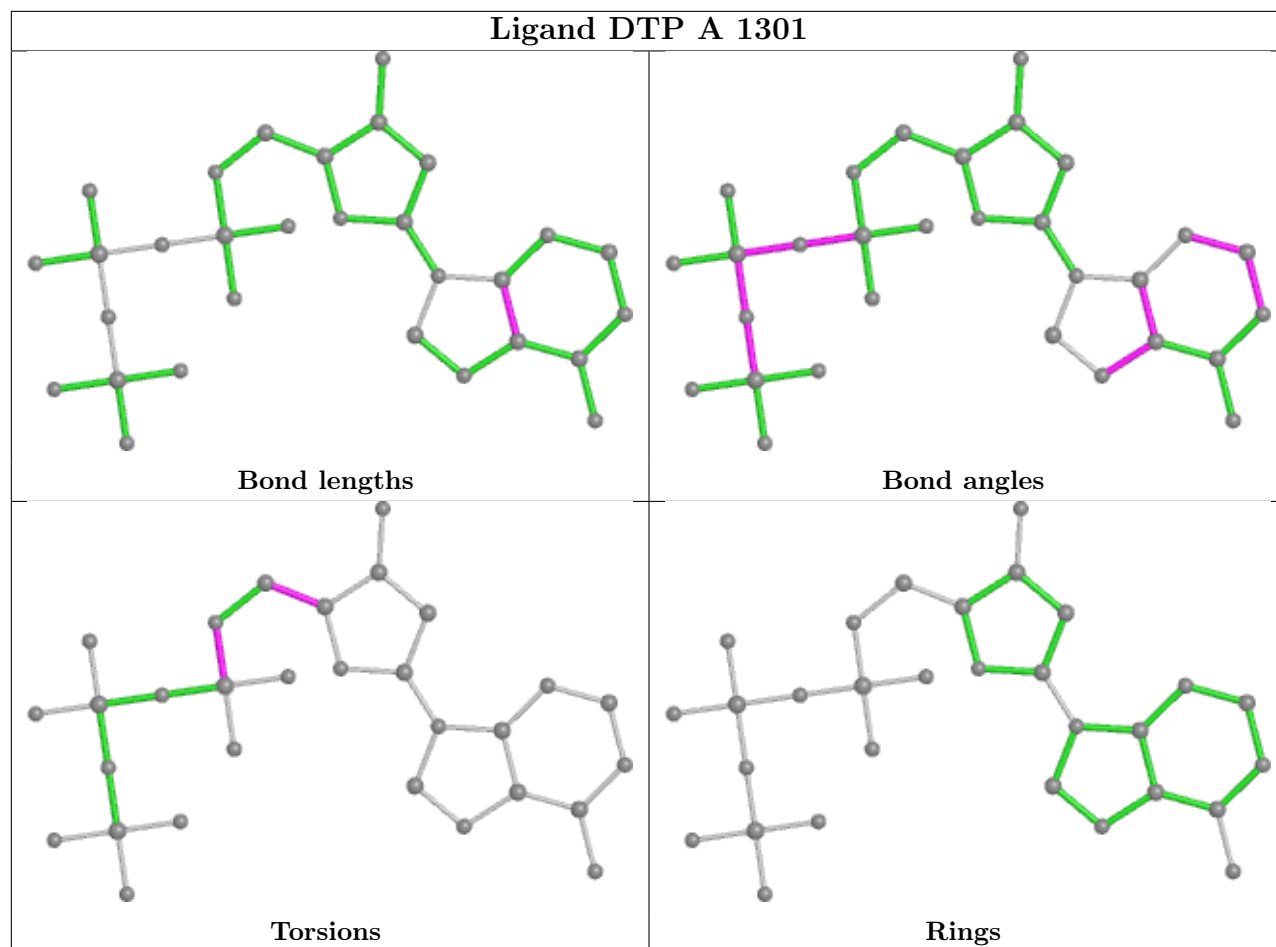




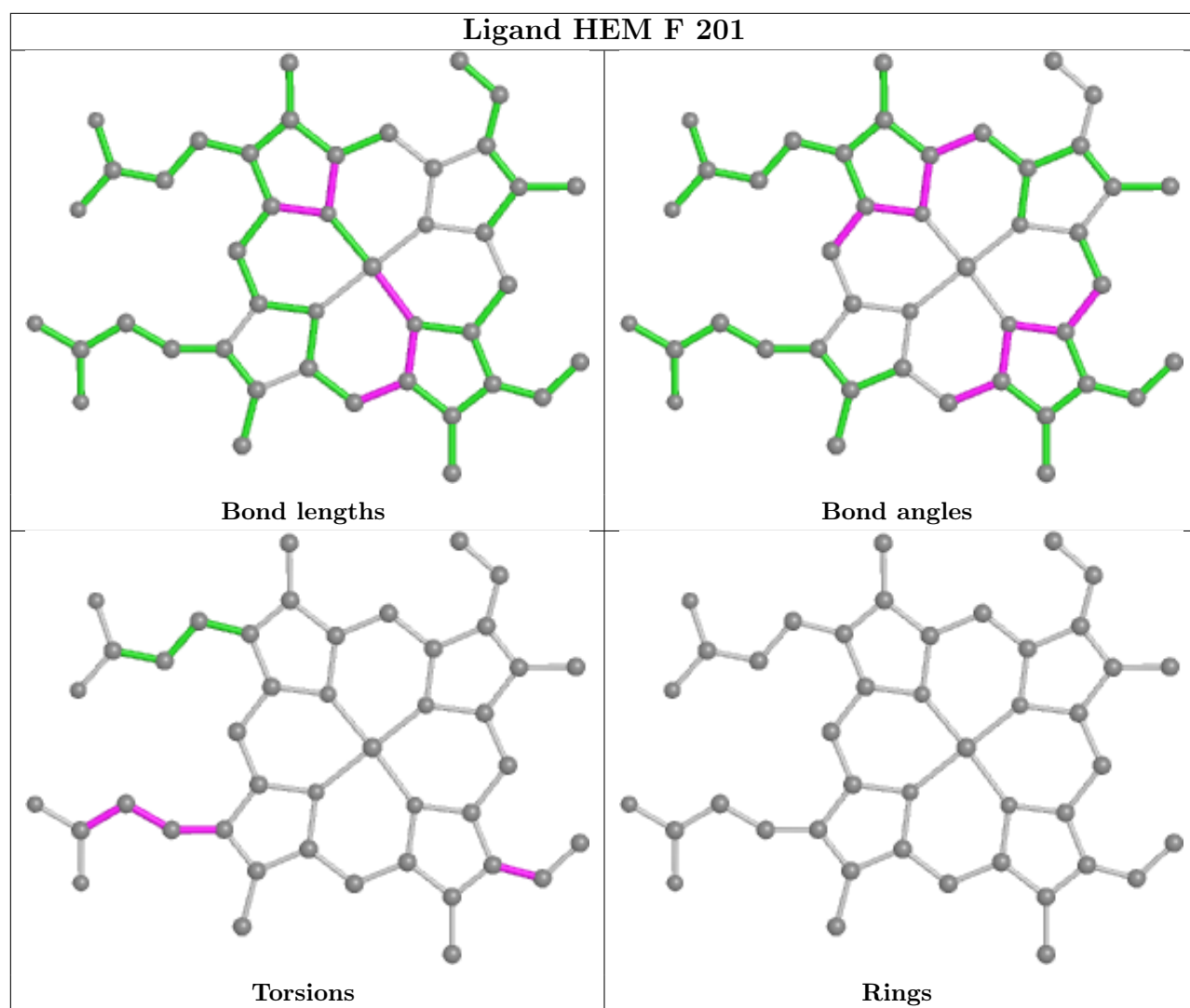




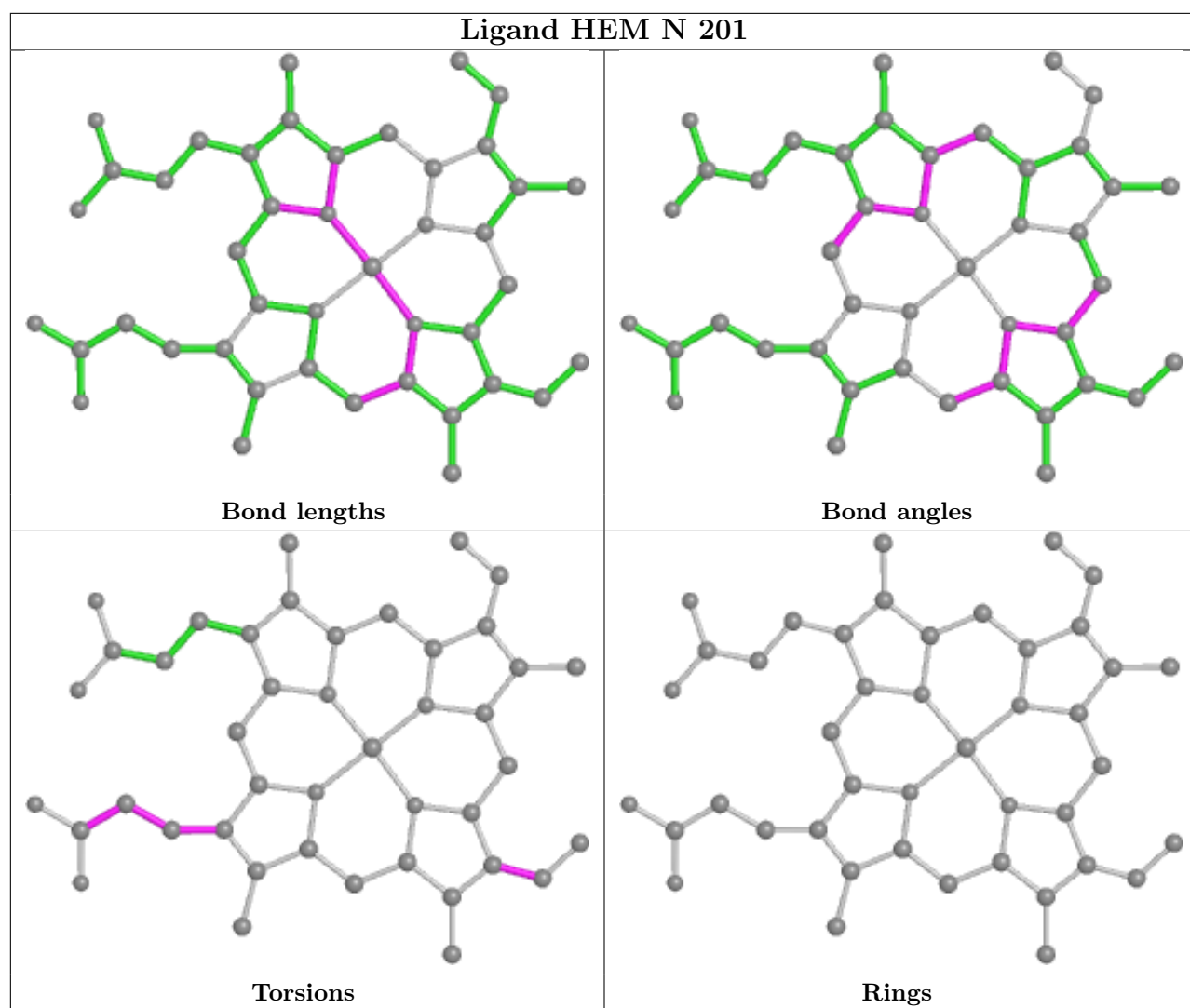




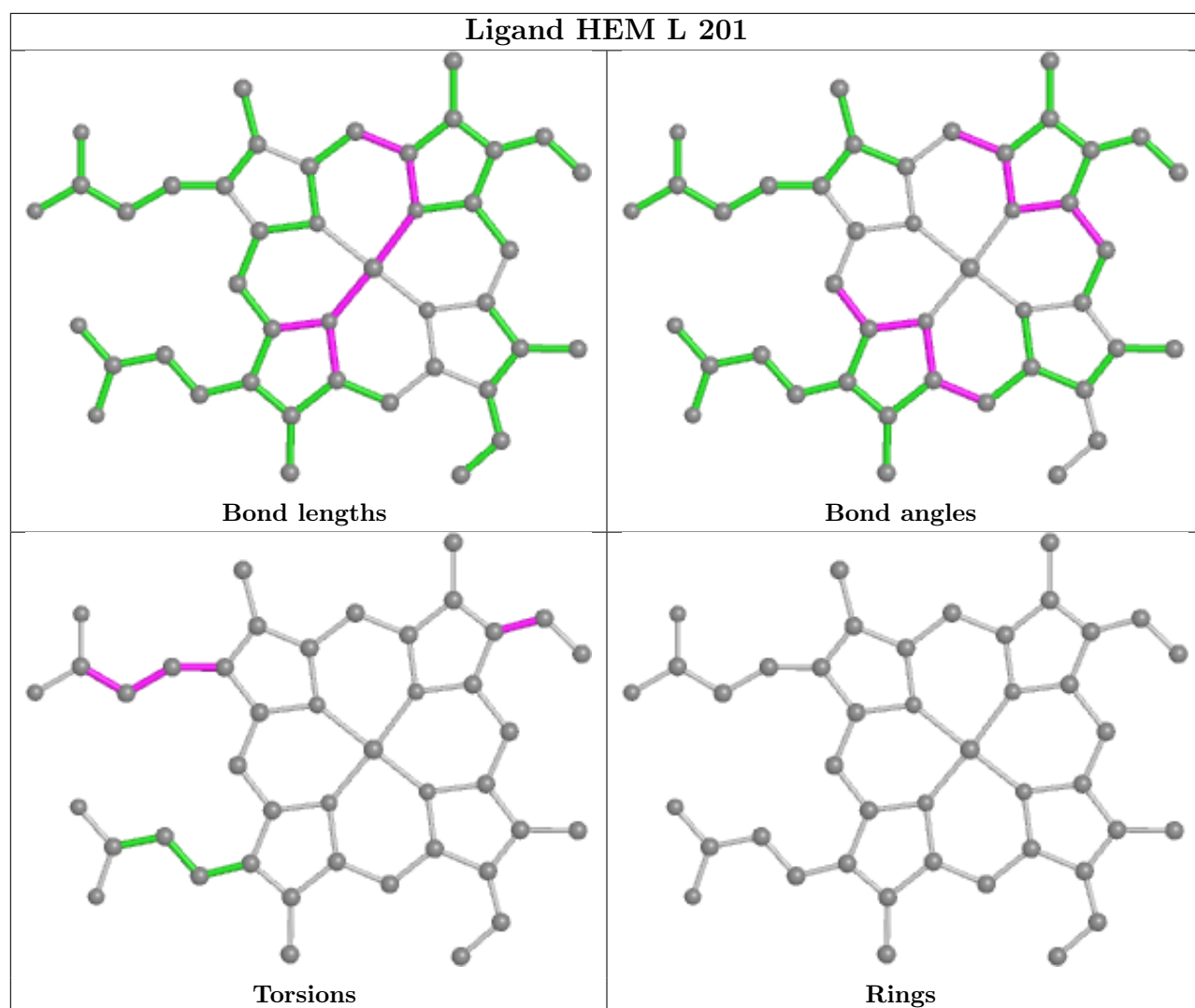




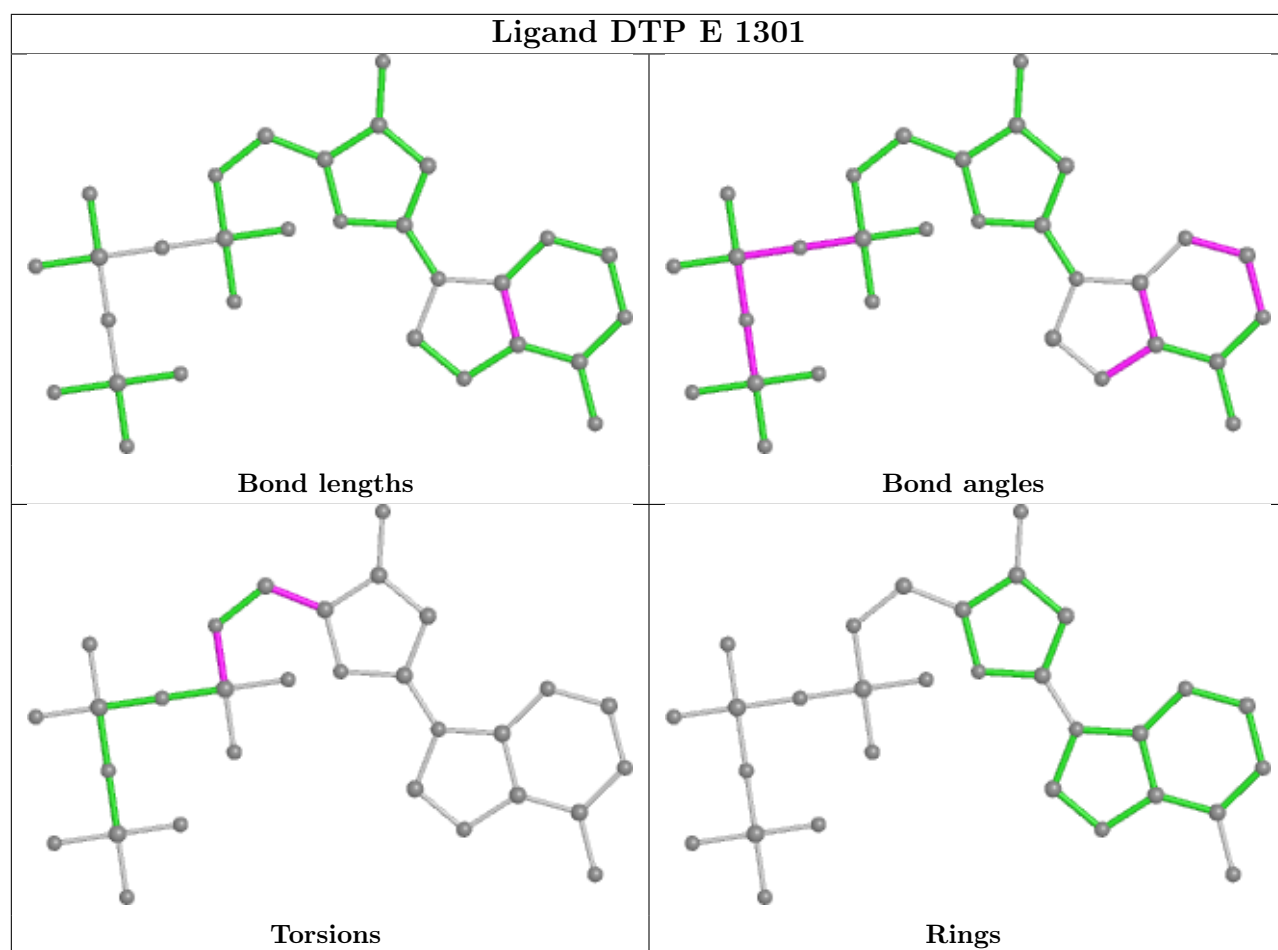




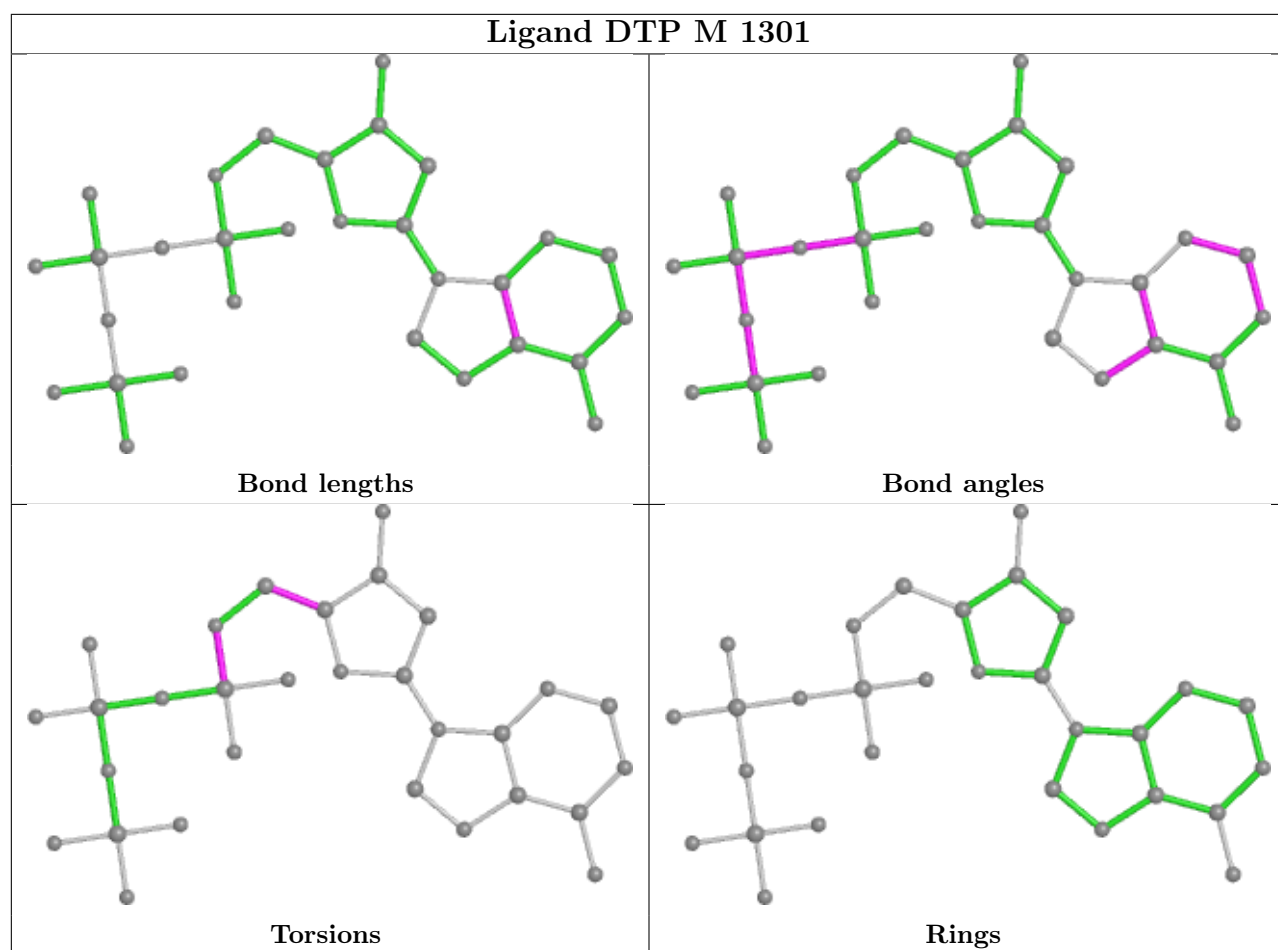




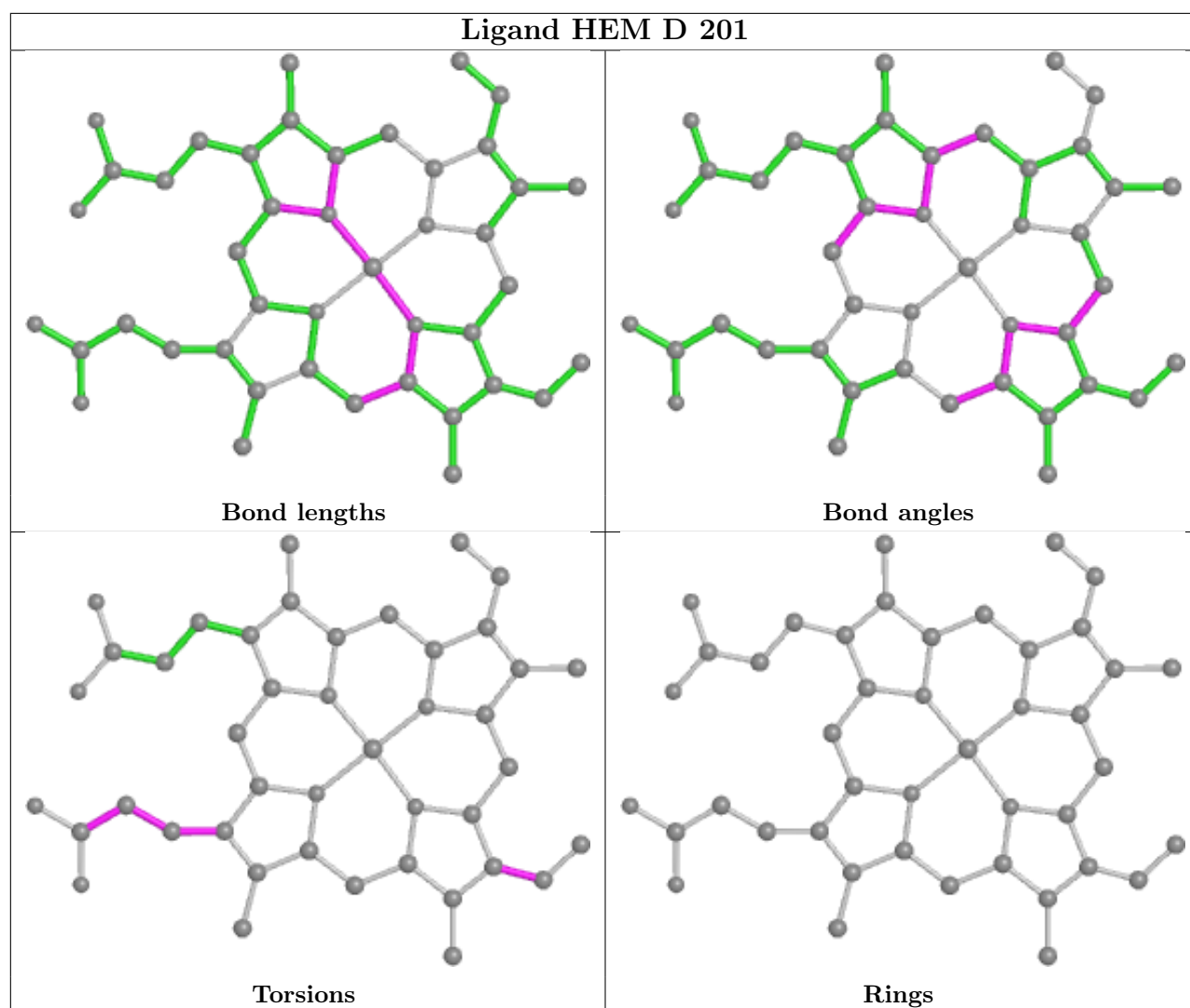












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.



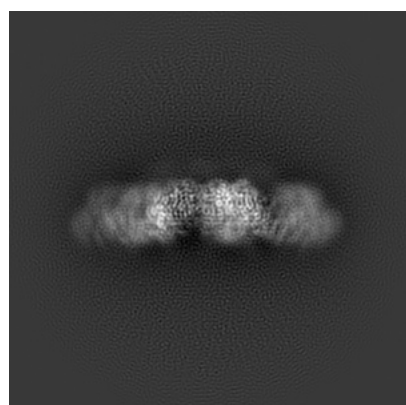
## 6 Map visualisation [i](#)

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.

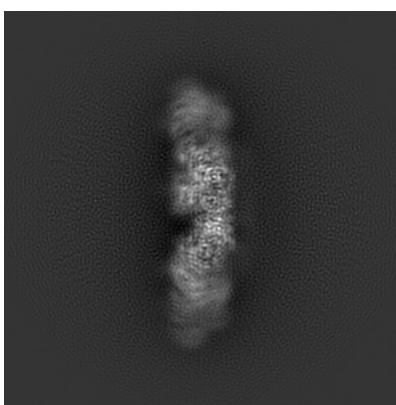
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

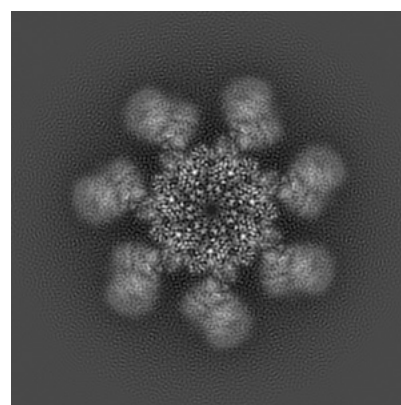
#### 6.1.1 Primary map



X



Y



Z

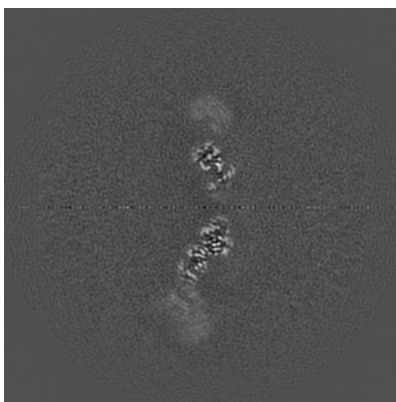
The images above show the map projected in three orthogonal directions.

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

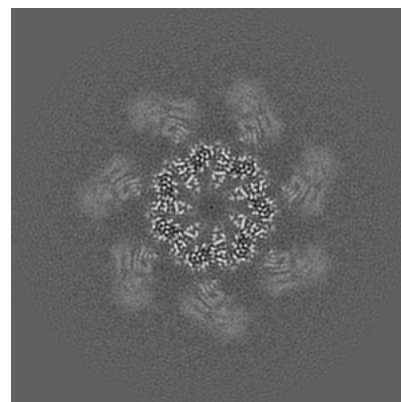
#### 6.2.1 Primary map



X Index: 160



Y Index: 160



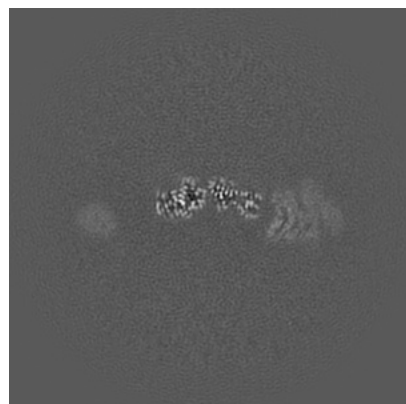
Z Index: 160



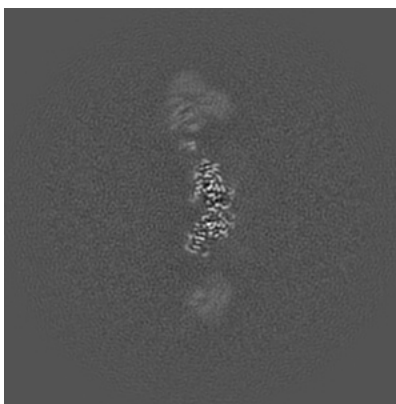
The images above show central slices of the map in three orthogonal directions.

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

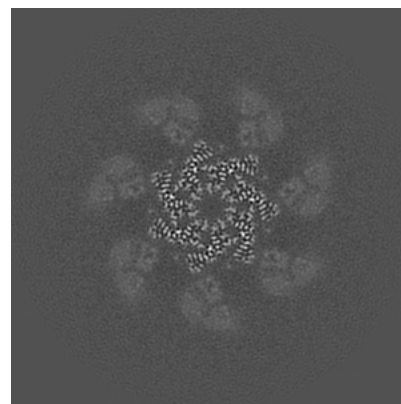
### 6.3.1 Primary map



X Index: 185



Y Index: 190

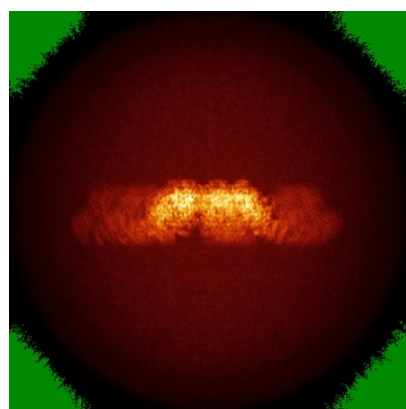


Z Index: 164

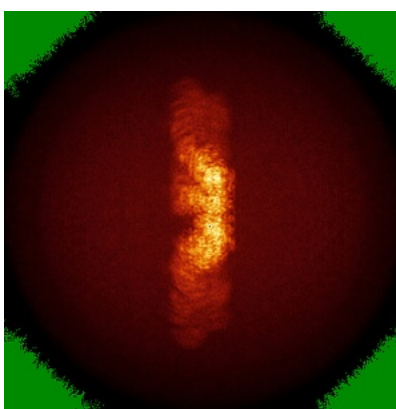
The images above show the largest variance slices of the map in three orthogonal directions.

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

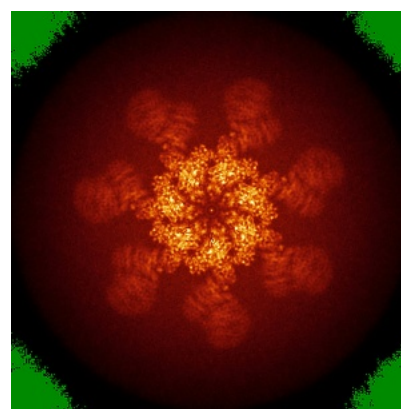
### 6.4.1 Primary map



X



Y



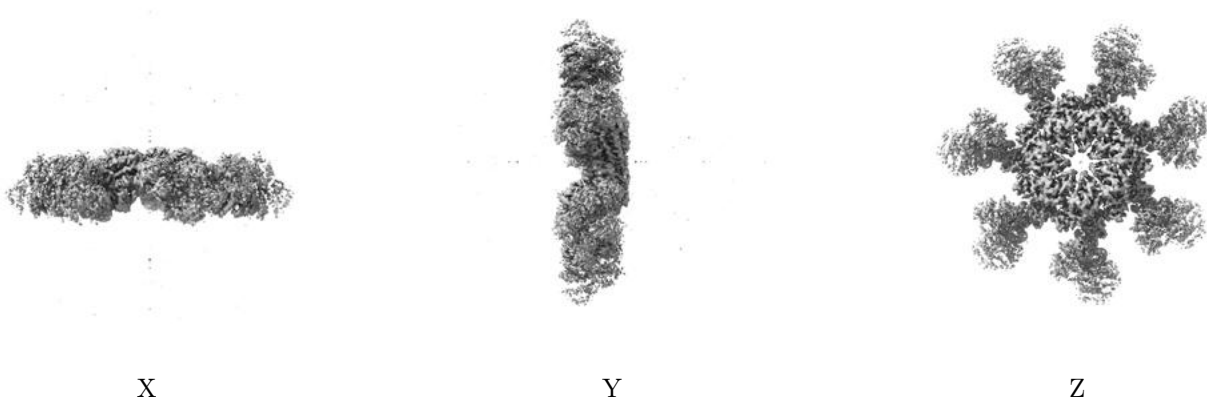
Z

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](#)

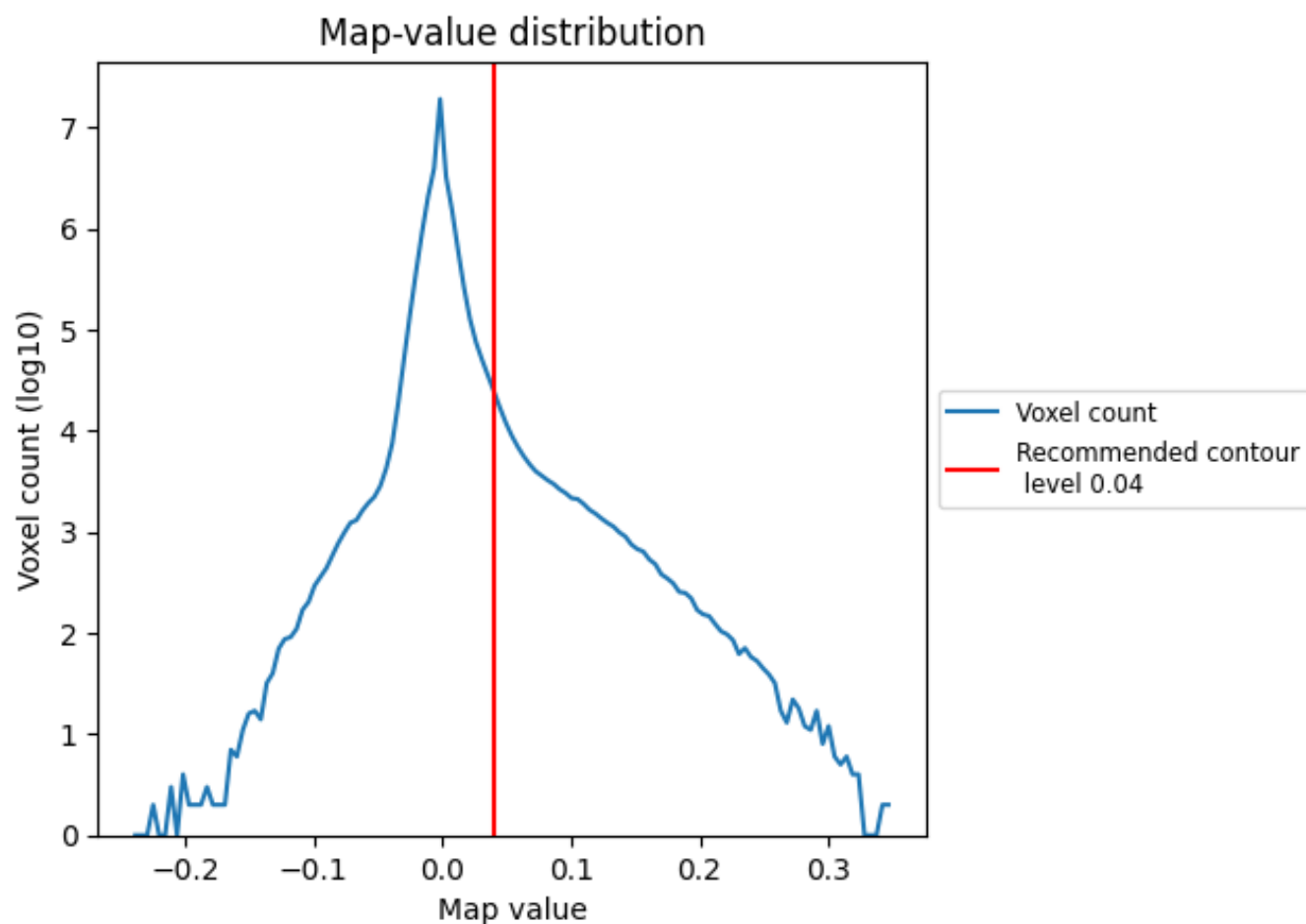
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

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

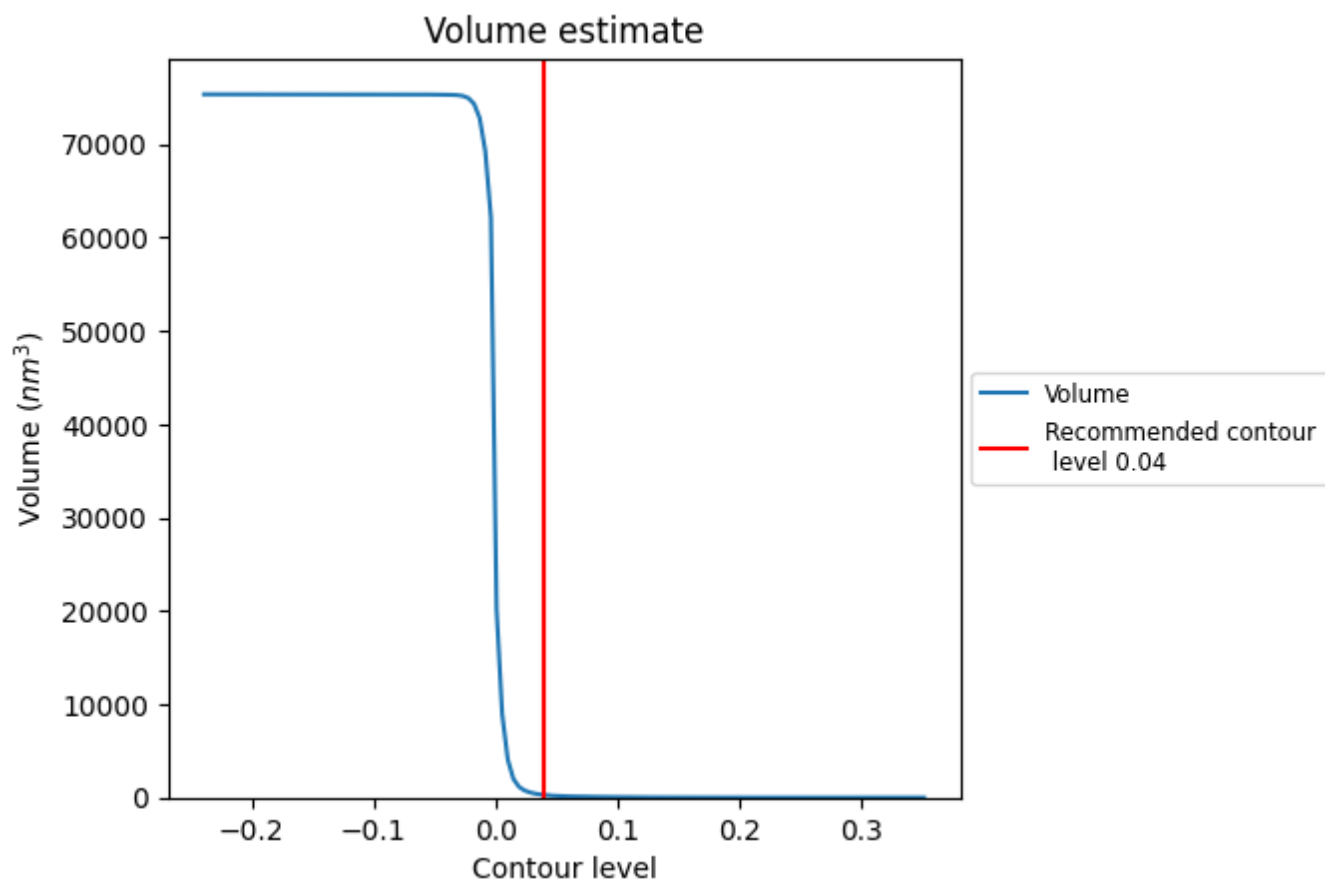
### 7.1 Map-value distribution [i](#)



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](#)

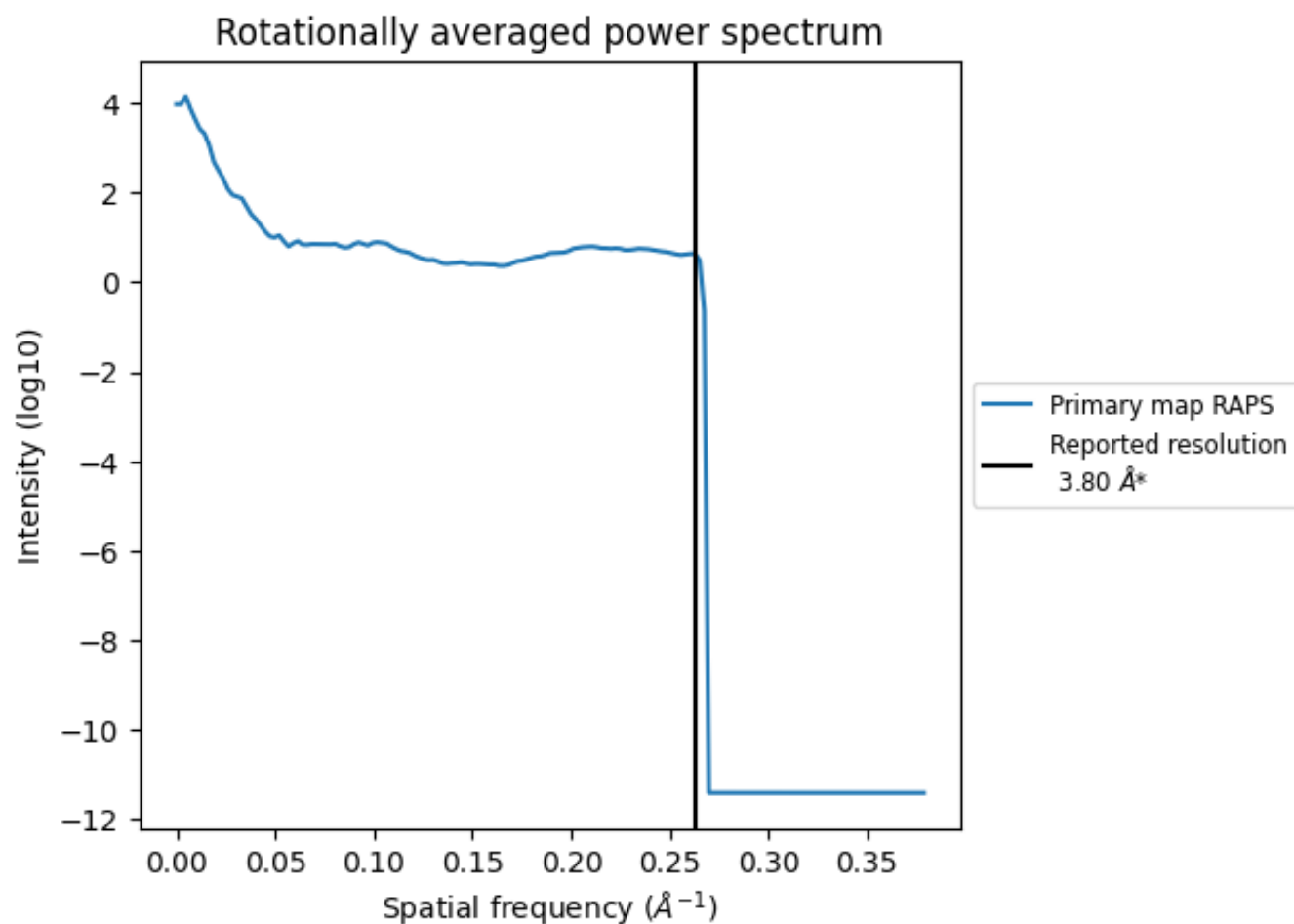


The volume at the recommended contour level is 276 nm<sup>3</sup>; this corresponds to an approximate mass of 249 kDa.

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 [i](#)



\*Reported resolution corresponds to spatial frequency of 0.263  $\text{\AA}^{-1}$



## 8 Fourier-Shell correlation

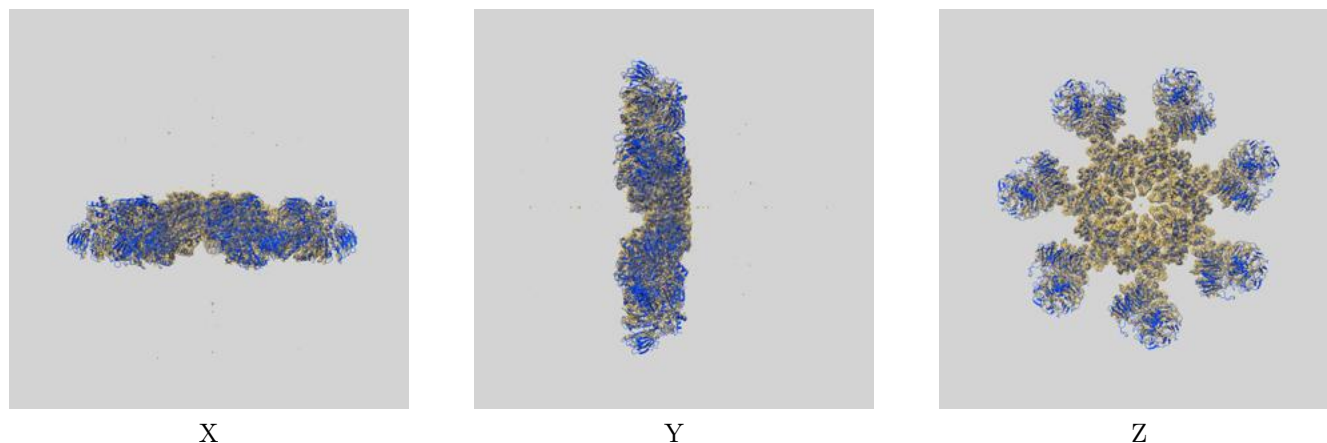
This section was not generated. No FSC curve or half-maps provided.



## 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](#).

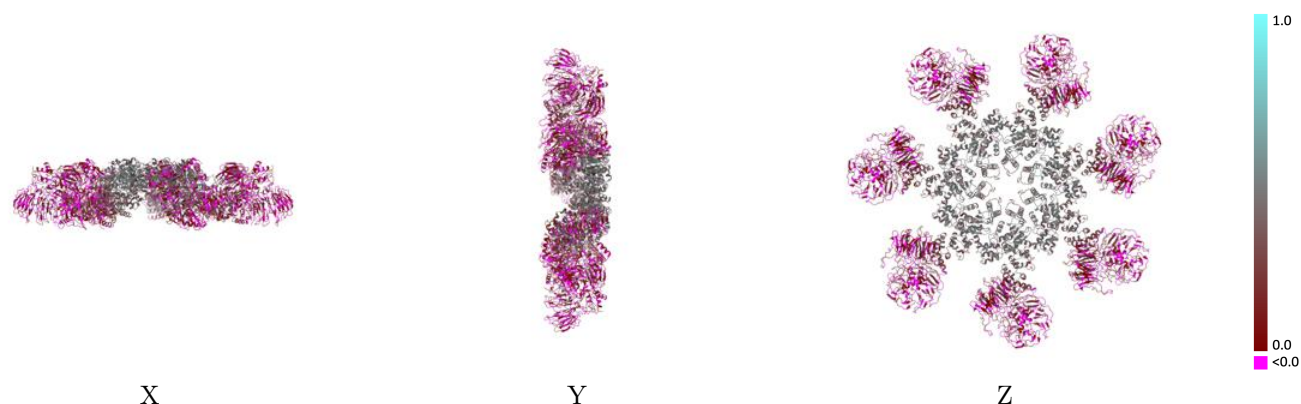
### 9.1 Map-model overlay [i](#)



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.

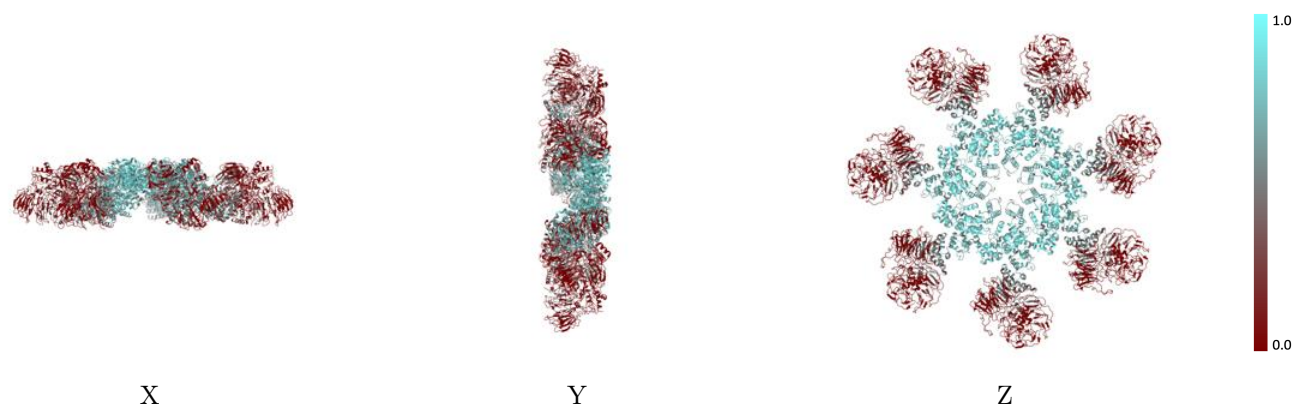


## 9.2 Q-score mapped to coordinate model [i](#)



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.

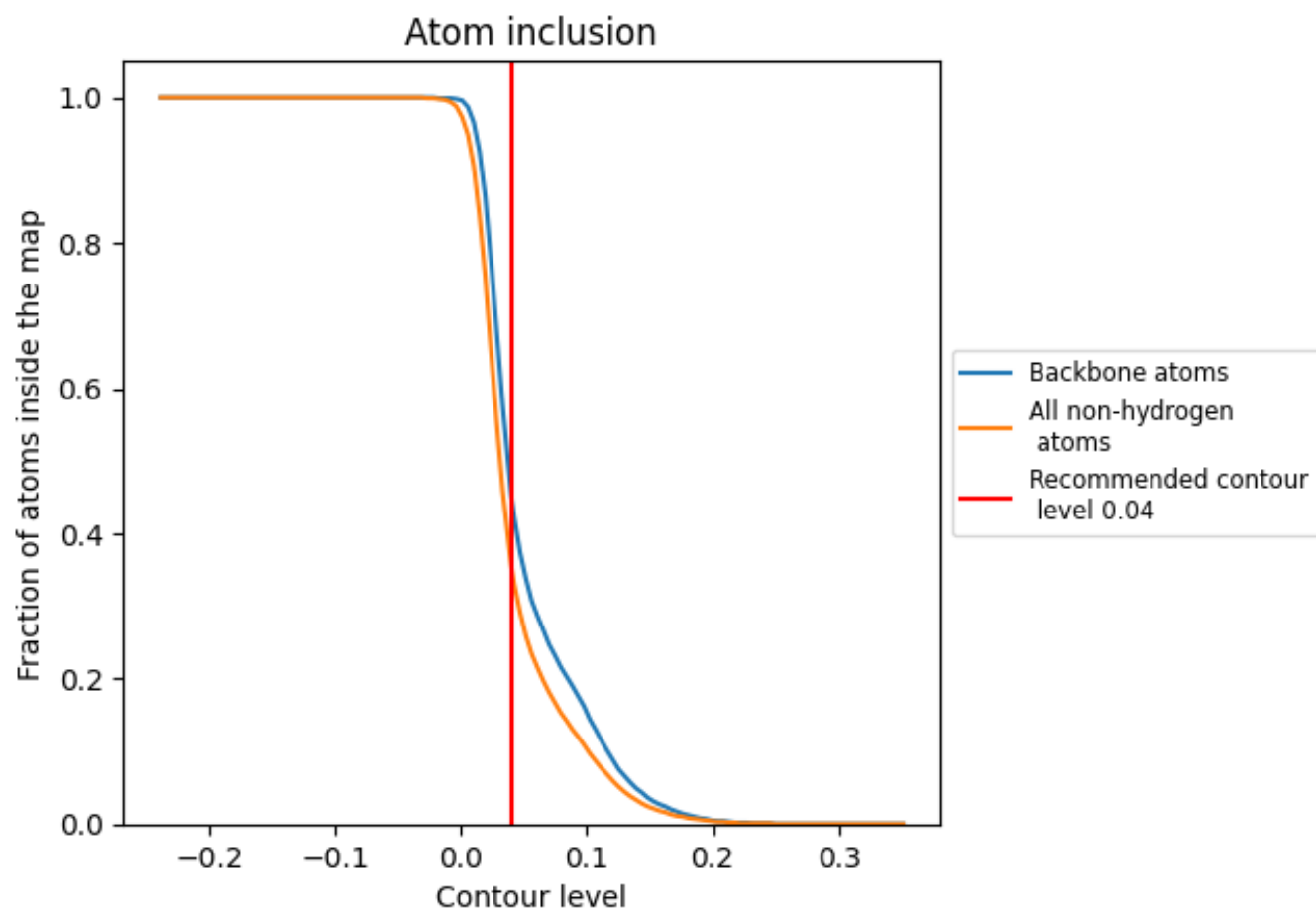
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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	<div></div> 0.3550	<div></div> 0.2010
A	<div></div> 0.3790	<div></div> 0.2120
B	<div></div> 0.0960	<div></div> 0.0860
C	<div></div> 0.3780	<div></div> 0.2120
D	<div></div> 0.0940	<div></div> 0.0880
E	<div></div> 0.3800	<div></div> 0.2120
F	<div></div> 0.0990	<div></div> 0.0840
G	<div></div> 0.3790	<div></div> 0.2110
H	<div></div> 0.0990	<div></div> 0.0830
I	<div></div> 0.3780	<div></div> 0.2110
J	<div></div> 0.1030	<div></div> 0.0870
K	<div></div> 0.3790	<div></div> 0.2110
L	<div></div> 0.1010	<div></div> 0.0900
M	<div></div> 0.3800	<div></div> 0.2110
N	<div></div> 0.0970	<div></div> 0.0860

1.0

0.0

<0.0