



## Full wwPDB EM Validation Report ⓘ

Oct 6, 2024 – 11:21 AM EDT

PDB ID : 8SI6  
EMDB ID : EMD-40500  
Title : Cryo-EM structure of TRPM7 in MSP2N2 nanodisc in complex with agonist  
naltriben in closed state  
Authors : Nadezhdin, K.D.; Neuberger, A.; Sobolevsky, A.I.  
Deposited on : 2023-04-14  
Resolution : 2.44 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

---

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

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

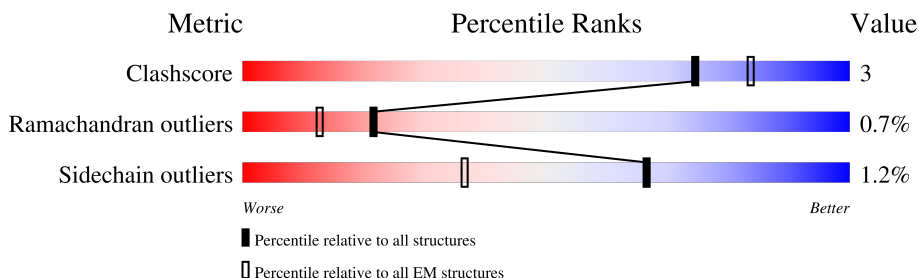
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.44 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	1279	<div> <div>48%</div> <div> <div></div> <div>79%</div> <div>7%</div> <div>13%</div> </div> </div>
1	B	1279	<div> <div>48%</div> <div> <div></div> <div>79%</div> <div>7%</div> <div>13%</div> </div> </div>
1	C	1279	<div> <div>48%</div> <div> <div></div> <div>79%</div> <div>7%</div> <div>13%</div> </div> </div>
1	D	1279	<div> <div>48%</div> <div> <div></div> <div>79%</div> <div>7%</div> <div>13%</div> </div> </div>

2 Entry composition [i](#)

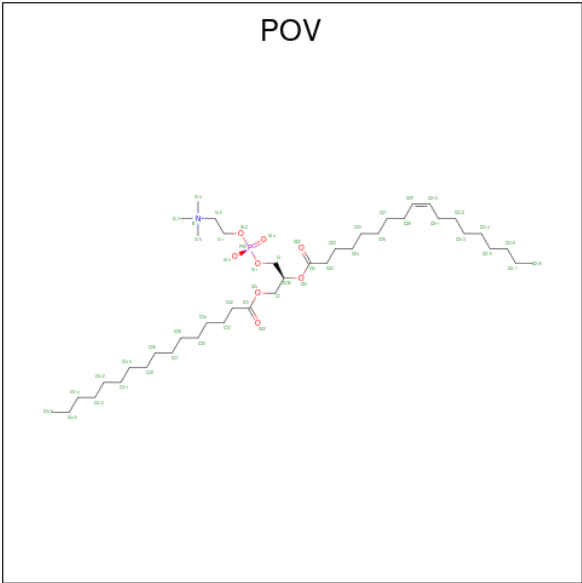
There are 6 unique types of molecules in this entry. The entry contains 79305 atoms, of which 40656 are hydrogens and 0 are deuteriums.

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 Transient receptor potential cation channel subfamily M member 7.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	1107	Total 18006	5813	9060	1493	1580	60	0	0
1	B	1107	Total 18006	5813	9060	1493	1580	60	0	0
1	C	1107	Total 18006	5813	9060	1493	1580	60	0	0
1	D	1107	Total 18006	5813	9060	1493	1580	60	0	0

- Molecule 2 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylamm onio)ethyl phosphate (three-letter code: POV) (formula: C<sub>42</sub>H<sub>82</sub>NO<sub>8</sub>P).



Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
2	A	1	Total 134	42	82	1	8	1	0
2	A	1	Total 134	42	82	1	8	1	0

Continued on next page...

*Continued from previous page...*

Mol	Chain	Residues	Atoms						AltConf
2	A	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
2	A	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
2	A	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
2	A	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
2	A	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
2	A	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
2	A	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
2	A	1	Total 82	C 25	H 49	N 1	O 6	P 1	0
2	A	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
2	A	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
2	A	1	Total 44	C 15	H 29				0
2	A	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
2	B	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
2	B	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
2	B	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
2	B	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
2	B	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
2	B	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
2	B	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
2	B	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
2	B	1	Total 82	C 25	H 49	N 1	O 6	P 1	0

*Continued on next page...*

*Continued from previous page...*

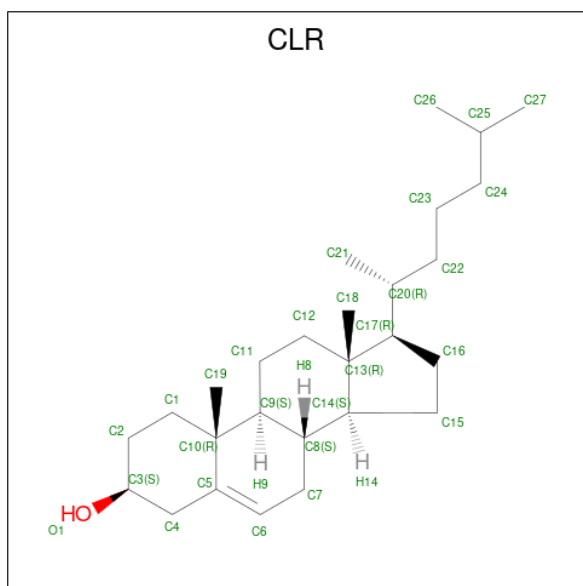
Mol	Chain	Residues	Atoms						AltConf
2	B	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
2	B	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
2	B	1	Total    C    H 44    15    29						0
2	C	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
2	C	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
2	C	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
2	C	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
2	C	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
2	C	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
2	C	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
2	C	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
2	C	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
2	C	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
2	C	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
2	C	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
2	C	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
2	C	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
2	C	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
2	C	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
2	C	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
2	C	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
2	C	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
2	C	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
2	C	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
2	C	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
2	C	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
2	C	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
2	C	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
2	C	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
2	C	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
2	C	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
2	C	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
2	C	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
2	C	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
2	C	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
2	C	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
2	C	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
2	C	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
2	C	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
2	C	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
2	C	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
2	C	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
2	C	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
2	C	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
2	C	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
2	C	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
2	C	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
2	C	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
2	C	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
2	C	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
2	C	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
2	C	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
2	C	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
2	C	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
2	C	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
2	C	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
2	C	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
2	C	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
2	C	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
2	C	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
2	C	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
2	C	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
2	C	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
2	C	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
2	C	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
2	C	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
2	C	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
2	C	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
2	C	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
2	C	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
2	C	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
2	C	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
2	C	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
2	C	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
2	C	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
2	C	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
2	C	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
2	C	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
2	C	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
2	C	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
2									

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms						AltConf
2	D	1	Total	C	H	N	O	P	0
			134	42	82	1	8	1	
2	D	1	Total	C	H	N	O	P	0
			134	42	82	1	8	1	
2	D	1	Total	C	H	N	O	P	0
			134	42	82	1	8	1	
2	D	1	Total	C	H	N	O	P	0
			134	42	82	1	8	1	
2	D	1	Total	C	H	N	O	P	0
			134	42	82	1	8	1	
2	D	1	Total	C	H	N	O	P	0
			82	25	49	1	6	1	
2	D	1	Total	C	H	N	O	P	0
			134	42	82	1	8	1	

- Molecule 3 is CHOLESTEROL (three-letter code: CLR) (formula:  $C_{27}H_{46}O$ ).



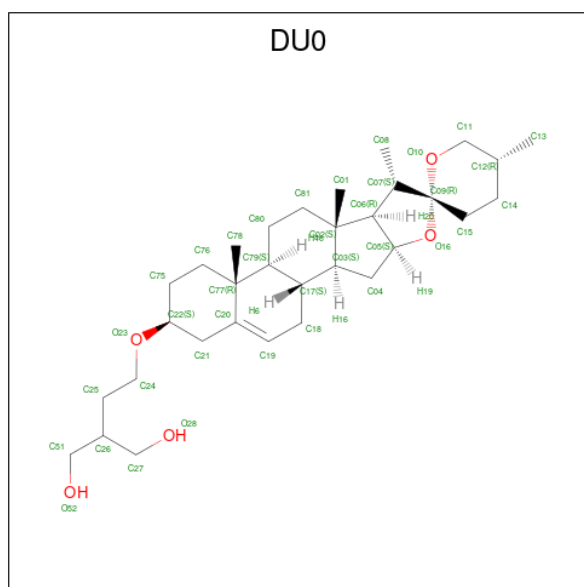
Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	H	O	0
			74	27	46	1	
3	B	1	Total	C	H	O	0
			74	27	46	1	
3	C	1	Total	C	H	O	0
			74	27	46	1	

Continued on next page...

Continued from previous page...

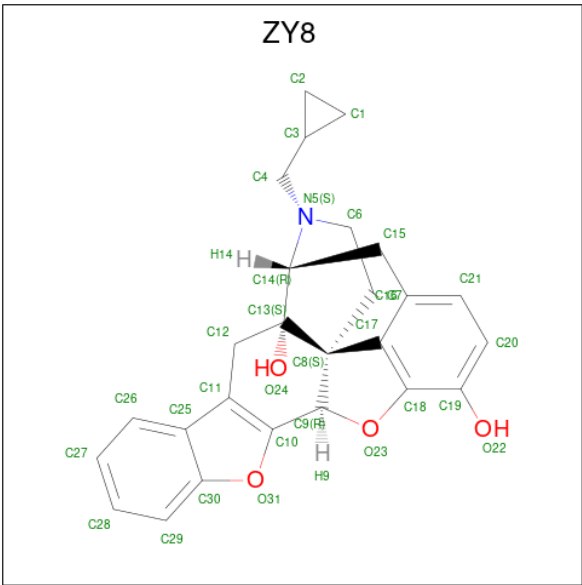
Mol	Chain	Residues	Atoms				AltConf
3	D	1	Total	C	H	O	0
			74	27	46	1	

- Molecule 4 is 2-[2-[(1 {S},2 {S},4 {S},5' {R},6 {R},7 {S},8 {R},9 {S},12 {S},13 {R},16 {S})-5',7,9,13-tetramethylspiro[5-oxapentacyclo[10.8.0.0<sup>2,9</sup>.0<sup>4,8</sup>.0<sup>13,18</sup>]]icos-18-ene-6,2'-oxane]-16-yl]oxyethyl]propane-1,3-diol (three-letter code: DU0) (formula: C<sub>32</sub>H<sub>52</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	H	O	0
			89	32	52	5	
4	B	1	Total	C	H	O	0
			89	32	52	5	
4	C	1	Total	C	H	O	0
			89	32	52	5	
4	D	1	Total	C	H	O	0
			89	32	52	5	

- Molecule 5 is (4bS,8R,8aS,14bR)-7-(cyclopropylmethyl)-5,6,7,8,9,14b-hexahydro-8aH-4,8-methanobis[1]benzofuro[3,2-e:2',3'-g]isoquinoline-1,8a-diol (three-letter code: ZY8) (formula: C<sub>26</sub>H<sub>25</sub>NO<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	H	N	O	0
			57	26	26	1	4	
5	B	1	Total	C	H	N	O	0
			57	26	26	1	4	
5	C	1	Total	C	H	N	O	0
			57	26	26	1	4	
5	D	1	Total	C	H	N	O	0
			57	26	26	1	4	

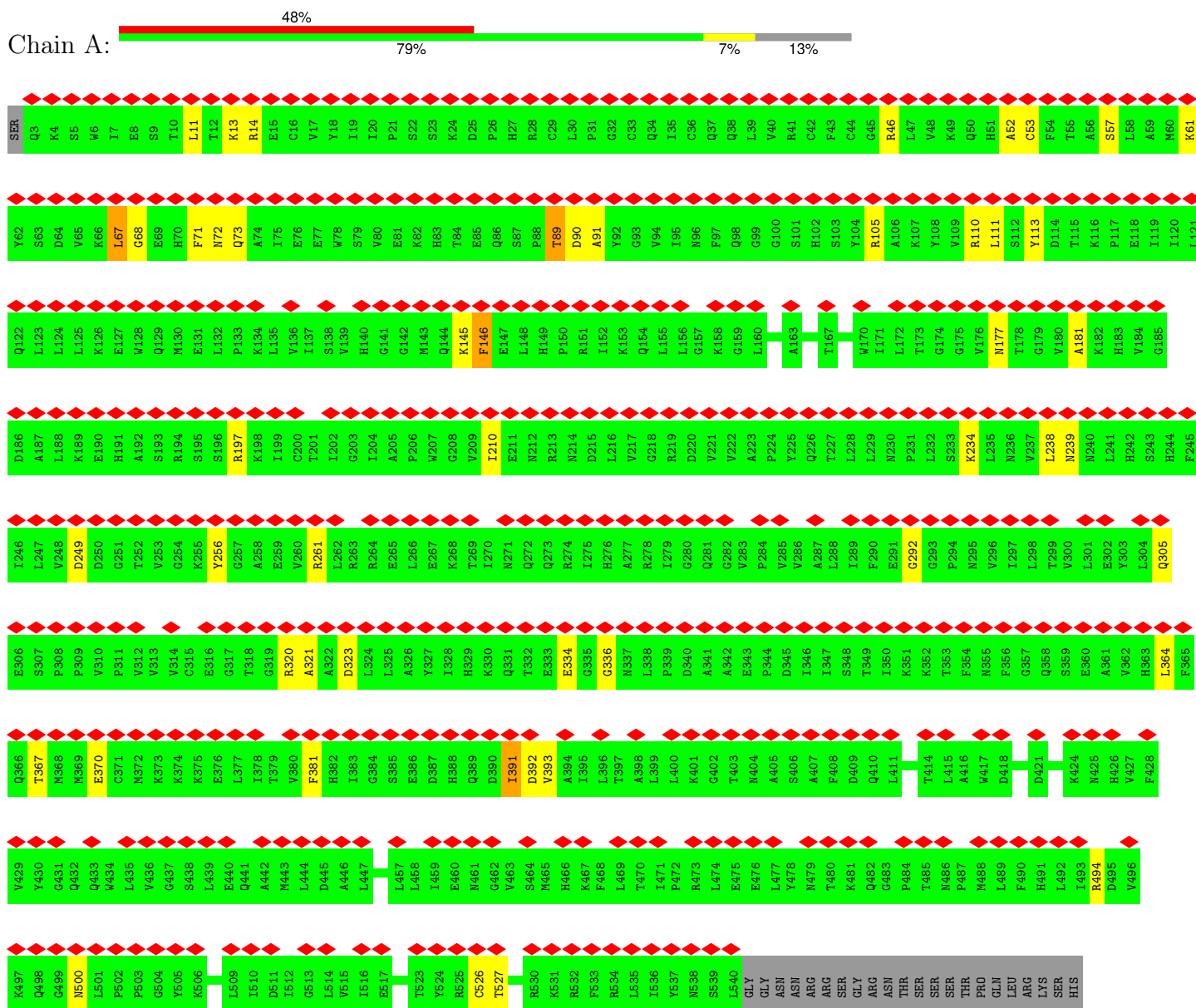
- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

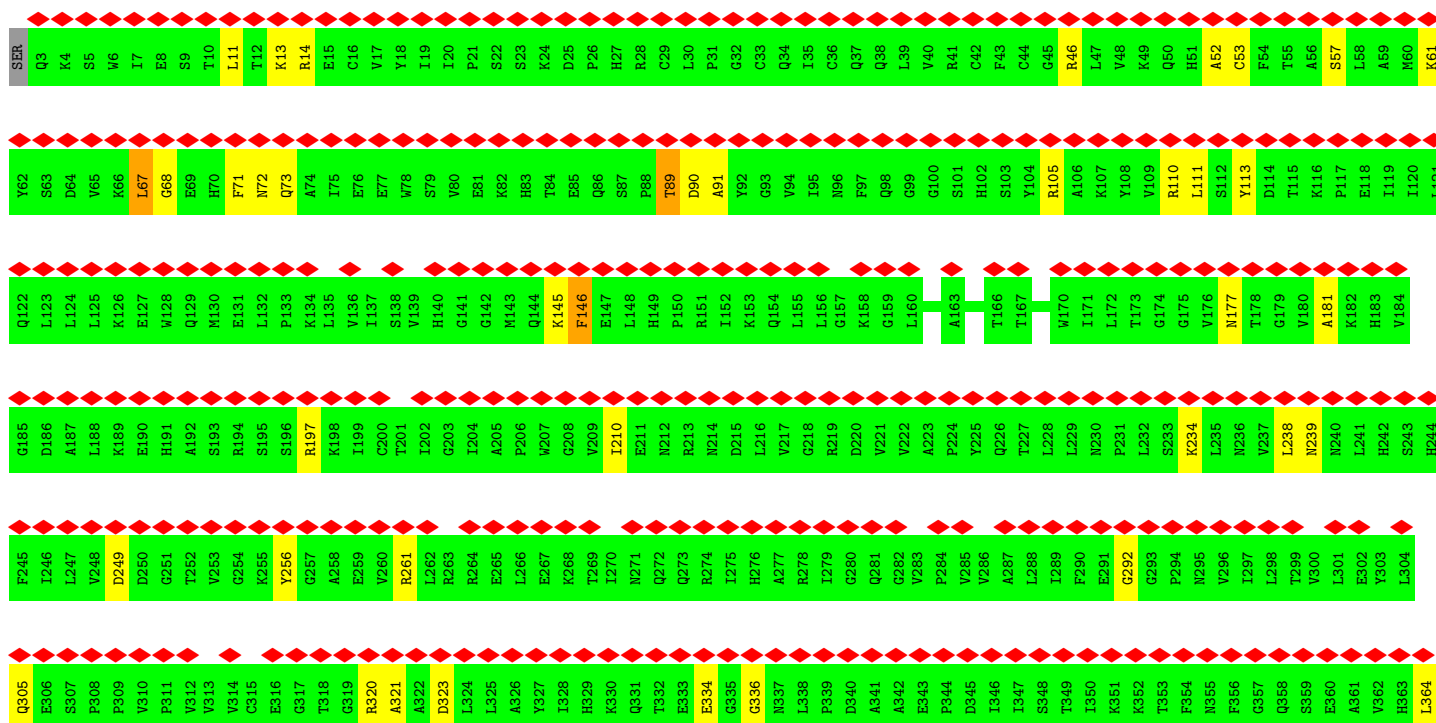
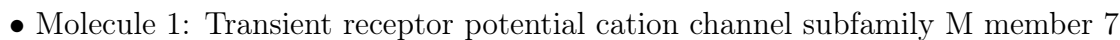
Mol	Chain	Residues	Atoms		AltConf
6	C	1	Total	Ca	0
			1	1	

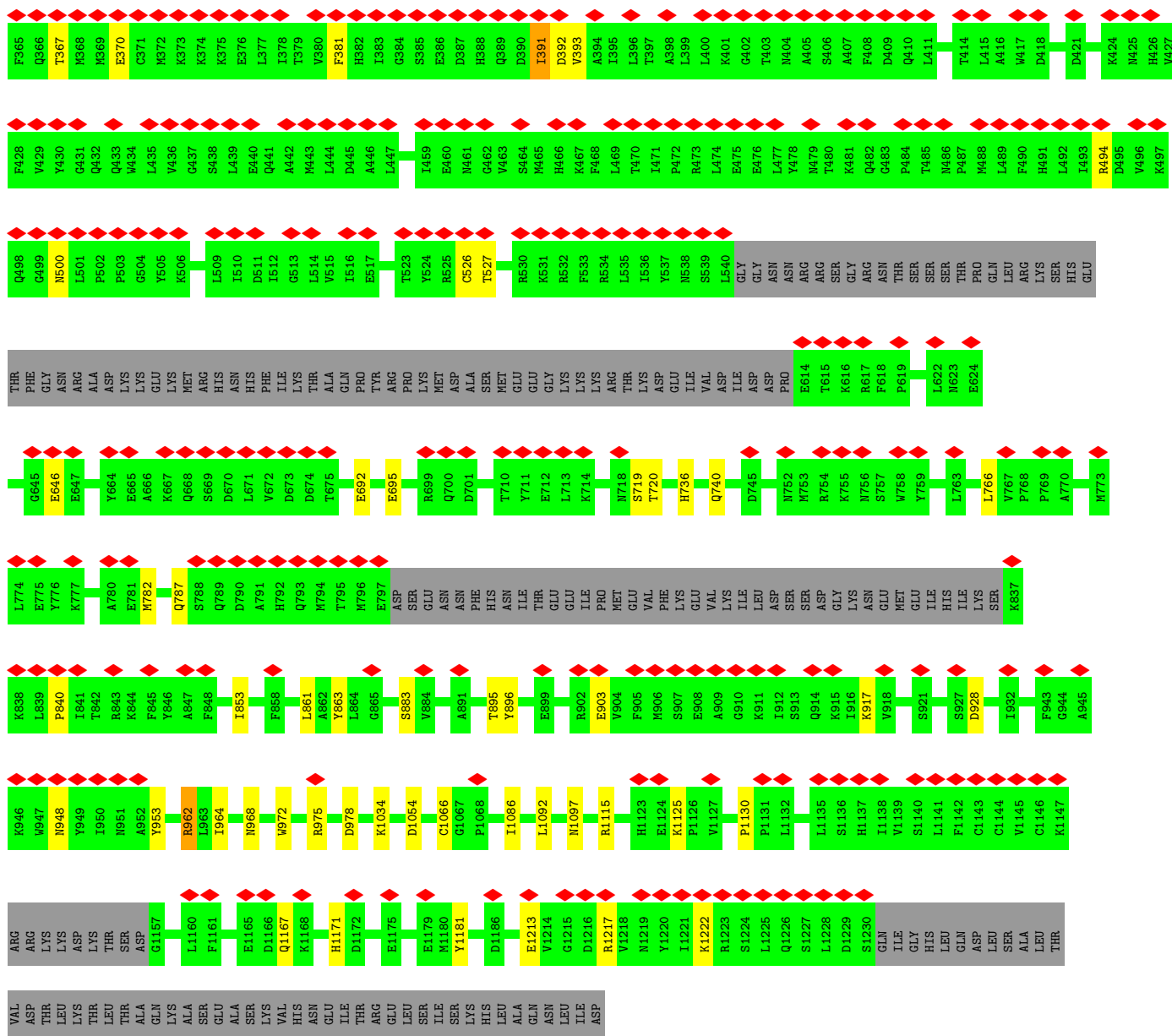
### 3 Residue-property plots

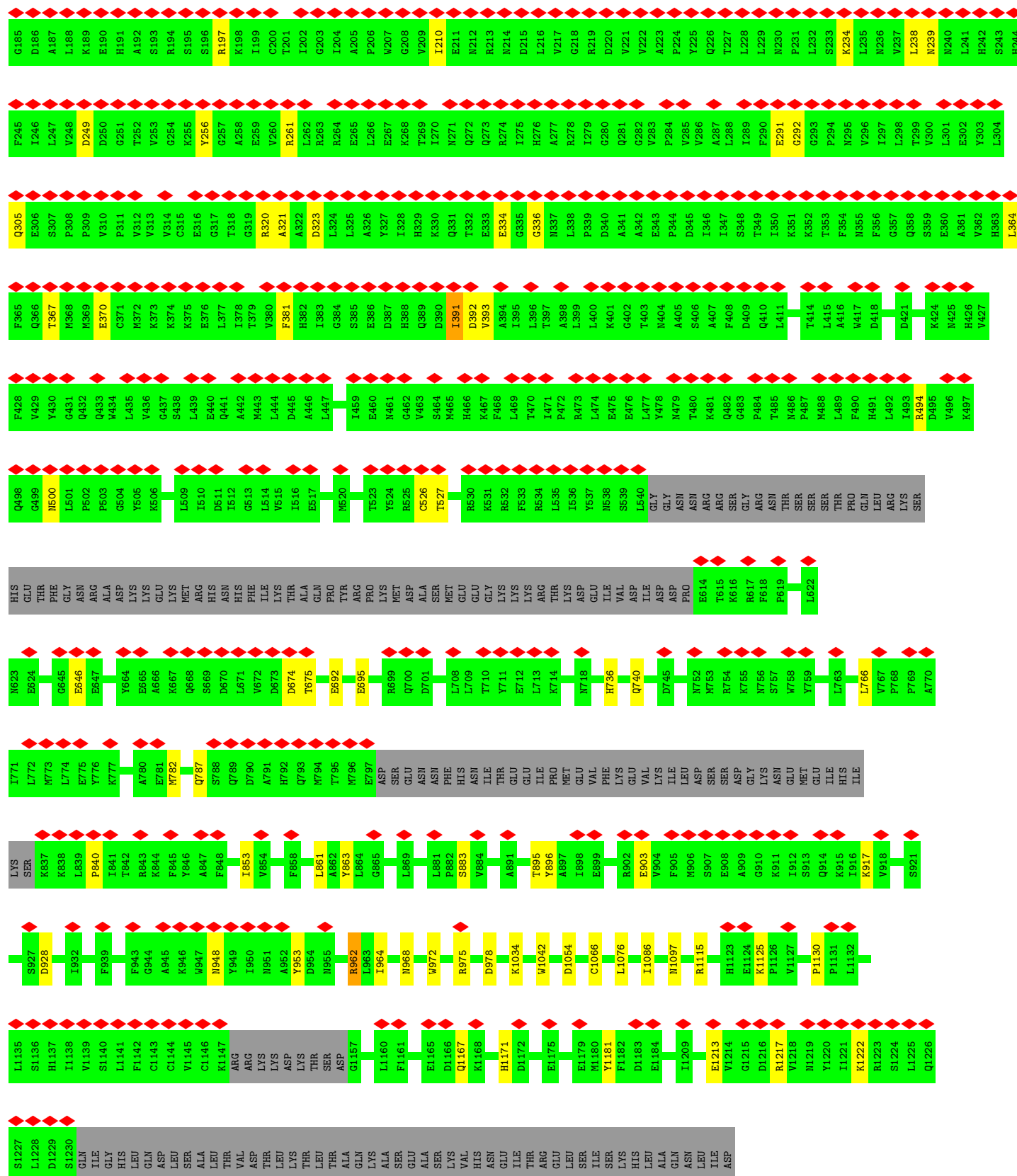
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

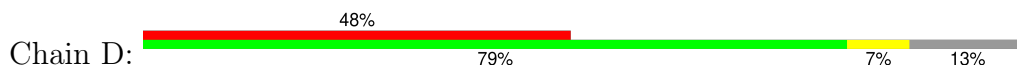
- Molecule 1: Transient receptor potential cation channel subfamily M member 7



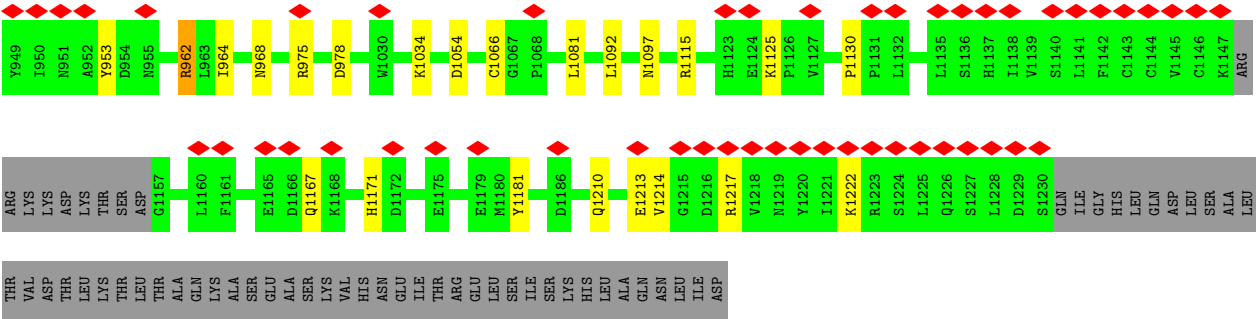








SER	Q3	K4	S5	W6	I7	E8	S9	T10	L11	T12	K13	R14	E15	C16	V17	I18	Y19	I20	P21	S22	S23	K24	D25	P26	H27	R28	C29	L30	P31	G32	C33	Q34	I35	C36	Q37	Q38	L39	V40	R41	C42	F43	C44	G45	R46	L47	V48	K49	Q50	H51	A52	C53	F54	T55	A56	S57	L58	A59	M60	K61
Y62	S63	D64	V65	K66	L67	G68	E69	H70	F71	N72	Q73	A74	I75	E76	E77	W78	S79	V80	E81	K82	H83	T84	E85	Q86	S87	P88	T89	D90	A91	Y92	G93	V94	I95	N96	F97	Q98	G99	G100	S101	H102	S103	Y104	R105	A106	I107	Y108	V109	R110	H111	S112	Y113	T114	T115	K116	P117	E118	A119	I120	L121
Q122	L123	L124	L125	K126	E127	W128	Q129	M130	E131	L132	P133	K134	I135	V136	I137	S138	V139	H140	G141	G142	M143	Q144	K145	F146	E147	L148	H149	P150	R151	I152	K153	Q154	L155	L156	G157	K158	G159	L160	A163	T166	T167	W170	I171	L172	T173	G174	G175	V176	N177	T178	G179	V180	A181	K182	H183	V184			
G185	D186	A187	L188	K189	E190	H191	A192	S193	R194	S195	S196	R197	K198	I199	C200	T201	L202	G203	L204	A205	P206	W207	K208	V209	L210	E211	N212	R213	N214	D215	L216	V217	G218	R219	D220	V221	V222	A223	Y225	Q226	T227	L228	L229	N230	P231	L232	S233	K234	L235	N236	V237	L238	N239	L241	H242	S243	H244		
F245	T246	L247	V248	D249	D250	G251	T252	G253	G254	K255	Y256	G257	A258	E259	V260	R261	L262	R263	R264	E265	L266	E267	K268	T269	L270	N271	Q272	Q273	R274	L275	H276	A277	R278	L279	G280	Q281	G282	P283	P284	V285	V286	A287	L288	T289	F290	E291	G292	G293	P294	N295	V296	T297	L298	T299	V300	L301	E302	Y303	L304
Q305	E306	S307	P308	P309	V310	P311	V312	V313	V314	C315	E316	G317	T318	G319	R320	A321	A322	D323	L324	L325	A326	V327	L328	H329	K330	Q331	D332	E333	E334	G335	G336	N337	L338	P339	D340	A341	A342	E343	P344	D345	L346	L347	S348	T349	K351	K352	T353	F354	N355	F356	G357	Q358	S359	E360	A361	V362	H363	L364	
F365	Q366	T367	K368	K369	E370	C371	K372	K373	K374	K375	E376	L377	T378	T379	V380	F381	H382	L383	G384	S385	E386	D387	H388	Q389	D390	O391	D392	V393	A394	L395	L396	T397	A398	L399	L400	K401	G402	T403	M404	A405	S406	A407	F408	D409	Q410	L411	L415	A416	W417	D418	A421	K424	M425	H426	V427	F428			
V429	Y430	G431	Q432	Q433	W434	L435	V436	G437	S438	L439	E440	Q441	M442	M443	L444	D445	A446	L447	I449	E450	N461	G462	V463	S464	M465	H466	K467	F468	L469	T470	L471	P472	R473	L474	E475	E476	L477	Y478	M479	T480	K481	Q482	G483	P484	T485	M486	P487	M488	L489	F490	H491	L492	L493	R494	D495	V496	K497	Q498	
G499	N500	L501	P502	P503	G504	Y505	L509	I510	D511	I512	G513	L514	V515	I516	E517	T523	Y524	R525	C526	T527	V528	T529	R530	K531	R532	F533	L534	L535	L536	Y537	N538	S539	L540	GLY	GLY	ASN	ARG	ASN	ARG	ARG	SER	GLY	ARG	ARG	ASN	THR	SER	SER	THR	PRO	GLN	LEU	ARG	LYS	SER	HIS	GLU		
THR	PHE	GLY	ASN	ARG	ALA	ASP	LYS	GLU	LYS	MET	ARG	HIS	ASN	PHE	ILE	LYS	THR	ALA	GLN	PRO	TYR	ARG	PRO	LYS	MET	ASN	ASP	ALA	SER	MET	ASN	GLU	GLY	LYS	LYS	ARG	MET	THR	VAL	GLU	ILE	VAL	ASP	ASP	ASN	PRO	E614	T615	K616	R617	F618	P619	L622	N623	E624				
G645	Y646	E647	Y664	E665	A666	K667	Q668	S669	D670	L671	V672	D673	D674	T675	E692	E695	R699	Q700	D701	T710	Y711	E712	L713	K714	N718	H736	Q740	D745	N752	M753	R754	K755	N756	S757	W758	Y759	L763	L766	V767	P768	P769	A770	I771	L772	M773	L774													
E775	Y776	K777	T778	K779	A780	E781	M782	Q787	S788	Q789	D790	A791	H792	Q793	M794	T795	M796	E797	ASP	SER	GLU	ASN	ASN	PHE	HIS	ASN	ILE	THR	GLU	ILE	PRO	MET	GLU	VAL	PHE	LYS	GLU	VAL	LYS	ILE	ASP	LEU	ASP	SER	ASP	GLY	LYS	ASN	GLU	MET	GLU	ILE	ILE	K837					
K838	L839	P840	I841	T842	R843	K844	F845	Y846	A847	F848	I853	F858	L861	G865	S883	Y884	A891	T895	Y896	E899	R902	E903	V904	F905	M906	S907	E908	A909	G910	K911	I912	S913	Q914	K915	V918	S921	S927	D928	I932	F943	G944	A945	K946	W947	N948														



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	96984	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	58	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.839	Depositor
Minimum map value	-1.124	Depositor
Average map value	0.010	Depositor
Map value standard deviation	0.070	Depositor
Recommended contour level	0.26	Depositor
Map size ( $\text{\AA}$ )	249.0, 249.0, 249.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.83, 0.83, 0.83	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CLR, ZY8, DU0, POV, CA

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	0.48	0/9162	0.59	0/12409
1	B	0.48	0/9162	0.59	0/12409
1	C	0.48	0/9162	0.59	0/12409
1	D	0.48	0/9162	0.59	0/12409
All	All	0.48	0/36648	0.59	0/49636

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	B	0	5
1	C	0	5
1	D	0	5
All	All	0	20

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	145	LYS	Peptide
1	A	146	PHE	Peptide
1	A	256	TYR	Peptide
1	A	52	ALA	Peptide
1	A	67	LEU	Peptide

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
1	B	145	LYS	Peptide
1	B	146	PHE	Peptide
1	B	256	TYR	Peptide
1	B	52	ALA	Peptide
1	B	67	LEU	Peptide
1	C	145	LYS	Peptide
1	C	146	PHE	Peptide
1	C	256	TYR	Peptide
1	C	52	ALA	Peptide
1	C	67	LEU	Peptide
1	D	145	LYS	Peptide
1	D	146	PHE	Peptide
1	D	256	TYR	Peptide
1	D	52	ALA	Peptide
1	D	67	LEU	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8946	9060	9056	48	0
1	B	8946	9060	9056	48	0
1	C	8946	9060	9056	50	0
1	D	8946	9060	9056	49	0
2	A	672	1062	1056	23	0
2	B	568	898	892	20	0
2	C	620	980	974	21	0
2	D	620	980	974	22	0
3	A	28	46	46	1	0
3	B	28	46	46	1	0
3	C	28	46	46	1	0
3	D	28	46	46	1	0
4	A	37	52	0	0	0
4	B	37	52	0	0	0
4	C	37	52	0	0	0
4	D	37	52	0	0	0
5	A	31	26	0	1	0
5	B	31	26	0	1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	31	26	0	1	0
5	D	31	26	0	1	0
6	C	1	0	0	0	0
All	All	38649	40656	40304	234	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 3.

All (234) 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:B:903:GLU:OE2	1:B:1125:LYS:NZ	2.16	0.79
1:C:903:GLU:OE2	1:C:1125:LYS:NZ	2.16	0.79
1:A:903:GLU:OE2	1:A:1125:LYS:NZ	2.16	0.78
1:D:903:GLU:OE2	1:D:1125:LYS:NZ	2.16	0.78
1:A:895:THR:OG1	1:A:1130:PRO:O	2.05	0.75
1:D:895:THR:OG1	1:D:1130:PRO:O	2.05	0.74
1:B:895:THR:OG1	1:B:1130:PRO:O	2.05	0.74
1:C:692:GLU:OE1	1:C:1181:TYR:OH	2.05	0.74
1:A:692:GLU:OE1	1:A:1181:TYR:OH	2.05	0.73
1:D:692:GLU:OE1	1:D:1181:TYR:OH	2.05	0.73
1:A:978:ASP:OD1	5:A:1314:ZY8:O24	2.07	0.73
1:D:978:ASP:OD1	5:D:1316:ZY8:O24	2.07	0.73
1:C:895:THR:OG1	1:C:1130:PRO:O	2.05	0.73
1:B:978:ASP:OD1	5:B:1313:ZY8:O24	2.07	0.72
1:C:978:ASP:OD1	5:C:1314:ZY8:O24	2.07	0.72
1:D:953:TYR:OH	1:D:962:ARG:NH2	2.23	0.72
1:B:692:GLU:OE1	1:B:1181:TYR:OH	2.05	0.72
1:B:953:TYR:OH	1:B:962:ARG:NH2	2.23	0.72
1:A:953:TYR:OH	1:A:962:ARG:NH2	2.23	0.72
1:C:953:TYR:OH	1:C:962:ARG:NH2	2.23	0.71
1:A:14:ARG:NH1	1:A:249:ASP:O	2.26	0.69
1:D:14:ARG:NH1	1:D:249:ASP:O	2.26	0.68
1:B:14:ARG:NH1	1:B:249:ASP:O	2.26	0.68
1:C:14:ARG:NH1	1:C:249:ASP:O	2.26	0.68
1:B:1034:LYS:NZ	1:C:1054:ASP:OD2	2.24	0.66
1:C:695:GLU:OE1	1:C:736:HIS:NE2	2.26	0.66
1:D:695:GLU:OE1	1:D:736:HIS:NE2	2.26	0.65
2:B:1302:POV:H21J	2:C:1301:POV:H31G	1.79	0.64
2:C:1303:POV:H21J	2:D:1303:POV:H31G	1.79	0.64
1:B:695:GLU:OE1	1:B:736:HIS:NE2	2.26	0.64

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1317:POV:H31G	2:D:1305:POV:H21J	1.78	0.63
1:A:695:GLU:OE1	1:A:736:HIS:NE2	2.26	0.63
2:A:1302:POV:H21J	2:A:1306:POV:H31G	1.79	0.63
1:A:782:MET:SD	1:A:787:GLN:NE2	2.72	0.63
1:D:782:MET:SD	1:D:787:GLN:NE2	2.72	0.63
1:C:782:MET:SD	1:C:787:GLN:NE2	2.72	0.62
1:B:782:MET:SD	1:B:787:GLN:NE2	2.72	0.62
2:C:1310:POV:H13B	2:C:1311:POV:H14	1.83	0.61
2:A:1315:POV:O11	2:A:1315:POV:H15A	2.01	0.61
1:C:181:ALA:O	1:C:239:ASN:ND2	2.34	0.61
1:D:181:ALA:O	1:D:239:ASN:ND2	2.34	0.61
1:A:181:ALA:O	1:A:239:ASN:ND2	2.34	0.61
2:B:1309:POV:H13B	2:B:1310:POV:H14	1.83	0.61
2:D:1301:POV:O11	2:D:1301:POV:H15A	2.01	0.61
2:D:1312:POV:H13B	2:D:1313:POV:H14	1.83	0.60
2:A:1310:POV:H13B	2:A:1311:POV:H14	1.83	0.60
1:B:181:ALA:O	1:B:239:ASN:ND2	2.34	0.60
2:C:1315:POV:O11	2:C:1315:POV:H15A	2.01	0.60
2:B:1314:POV:O11	2:B:1314:POV:H15A	2.02	0.59
1:C:861:LEU:HD22	2:C:1312:POV:H316	1.85	0.59
1:A:861:LEU:HD22	2:A:1312:POV:H316	1.84	0.59
1:D:861:LEU:HD22	2:D:1314:POV:H316	1.84	0.59
1:B:53:CYS:O	1:B:57:SER:N	2.36	0.58
1:C:53:CYS:O	1:C:57:SER:N	2.36	0.58
1:B:113:TYR:O	1:B:261:ARG:NH2	2.36	0.58
1:A:53:CYS:O	1:A:57:SER:N	2.36	0.58
1:D:53:CYS:O	1:D:57:SER:N	2.36	0.58
2:D:1312:POV:C13	2:D:1313:POV:H14	2.35	0.57
1:D:113:TYR:O	1:D:261:ARG:NH2	2.36	0.57
2:A:1310:POV:C13	2:A:1311:POV:H14	2.35	0.57
1:C:1034:LYS:NZ	1:D:1054:ASP:OD2	2.34	0.57
1:D:1167:GLN:O	1:D:1171:HIS:ND1	2.30	0.57
1:A:1167:GLN:O	1:A:1171:HIS:ND1	2.30	0.57
1:B:861:LEU:HD22	2:B:1311:POV:H316	1.86	0.57
2:B:1309:POV:C13	2:B:1310:POV:H14	2.35	0.56
1:B:646:GLU:OE2	1:C:105:ARG:NH2	2.38	0.56
2:C:1310:POV:C13	2:C:1311:POV:H14	2.35	0.56
1:A:113:TYR:O	1:A:261:ARG:NH2	2.36	0.55
1:B:1092:LEU:HD21	1:C:1086:ILE:HG23	1.87	0.55
1:B:1167:GLN:O	1:B:1171:HIS:ND1	2.30	0.55
1:C:113:TYR:O	1:C:261:ARG:NH2	2.36	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1213:GLU:OE1	1:A:1217:ARG:NH1	2.41	0.54
1:C:1097:ASN:ND2	1:D:1097:ASN:OD1	2.40	0.54
1:D:1213:GLU:OE1	1:D:1217:ARG:NH1	2.41	0.54
1:B:964:ILE:HG23	2:B:1307:POV:H21H	1.89	0.54
1:B:1213:GLU:OE1	1:B:1217:ARG:NH1	2.41	0.54
1:C:1213:GLU:OE1	1:C:1217:ARG:NH1	2.41	0.54
1:A:964:ILE:HG23	2:A:1308:POV:H21H	1.90	0.53
1:C:964:ILE:HG23	2:C:1308:POV:H21H	1.89	0.53
1:C:740:GLN:OE1	1:C:1115:ARG:NH1	2.42	0.53
1:C:853:ILE:HD12	2:C:1315:POV:H13	1.90	0.53
1:D:964:ILE:HG23	2:D:1310:POV:H21H	1.90	0.53
1:A:1034:LYS:NZ	1:B:1054:ASP:OD2	2.37	0.53
1:D:740:GLN:OE1	1:D:1115:ARG:NH1	2.42	0.53
2:C:1307:POV:O13	2:C:1307:POV:H13A	2.09	0.53
1:A:320:ARG:O	1:A:323:ASP:N	2.42	0.53
2:D:1309:POV:O13	2:D:1309:POV:H13A	2.09	0.52
1:B:320:ARG:O	1:B:323:ASP:N	2.42	0.52
1:A:740:GLN:OE1	1:A:1115:ARG:NH1	2.42	0.52
2:A:1307:POV:O13	2:A:1307:POV:H13A	2.09	0.52
1:B:1097:ASN:ND2	1:C:1097:ASN:OD1	2.44	0.51
1:D:320:ARG:O	1:D:323:ASP:N	2.42	0.51
2:B:1306:POV:O13	2:B:1306:POV:H13A	2.09	0.51
1:A:853:ILE:HD12	2:A:1315:POV:H13	1.91	0.51
1:C:1167:GLN:O	1:C:1171:HIS:ND1	2.30	0.51
1:B:292:GLY:O	1:B:320:ARG:NE	2.43	0.50
1:B:766:LEU:HD11	2:B:1314:POV:H21J	1.92	0.50
2:B:1305:POV:C312	2:B:1305:POV:H218	2.42	0.50
2:A:1305:POV:H218	2:A:1305:POV:C312	2.41	0.50
1:C:320:ARG:O	1:C:323:ASP:N	2.42	0.50
1:D:528:TYR:OH	1:D:624:GLU:OE1	2.11	0.50
1:A:105:ARG:NH2	1:D:646:GLU:OE2	2.45	0.50
1:A:1054:ASP:OD2	1:D:1034:LYS:NZ	2.35	0.50
2:D:1308:POV:H218	2:D:1308:POV:C312	2.41	0.50
1:A:1097:ASN:ND2	1:B:1097:ASN:OD1	2.44	0.50
2:C:1306:POV:H218	2:C:1306:POV:C312	2.41	0.50
1:C:766:LEU:HD11	2:C:1315:POV:H21J	1.95	0.49
1:D:1066:CYS:SG	2:D:1303:POV:H15A	2.53	0.49
1:B:740:GLN:OE1	1:B:1115:ARG:NH1	2.42	0.49
1:D:766:LEU:HD11	2:D:1301:POV:H21J	1.94	0.49
1:A:1097:ASN:OD1	1:D:1097:ASN:ND2	2.47	0.48
1:D:853:ILE:HD12	2:D:1301:POV:H13	1.95	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:LEU:O	1:A:367:THR:OG1	2.24	0.48
1:C:646:GLU:OE2	1:D:105:ARG:NH2	2.47	0.48
1:C:334:GLU:O	1:C:336:GLY:N	2.45	0.47
1:A:646:GLU:OE2	1:B:105:ARG:NH2	2.48	0.47
1:A:766:LEU:HD11	2:A:1315:POV:H21J	1.95	0.47
1:B:883:SER:HB3	2:B:1311:POV:H13	1.96	0.47
1:A:292:GLY:O	1:A:320:ARG:NE	2.43	0.47
1:B:853:ILE:HD12	2:B:1314:POV:H13	1.96	0.47
1:C:896:TYR:OH	1:C:975:ARG:NH1	2.46	0.47
1:D:292:GLY:O	1:D:320:ARG:NE	2.43	0.47
1:A:1086:ILE:HG23	1:D:1092:LEU:HD21	1.97	0.47
1:D:883:SER:HB3	2:D:1314:POV:H13	1.96	0.46
1:C:883:SER:HB3	2:C:1312:POV:H13	1.96	0.46
1:A:883:SER:CB	2:A:1312:POV:H13	2.45	0.46
1:A:883:SER:HB3	2:A:1312:POV:H13	1.96	0.46
1:B:392:ASP:OD1	1:B:393:VAL:N	2.49	0.46
1:B:883:SER:CB	2:B:1311:POV:H13	2.45	0.46
1:C:392:ASP:OD1	1:C:393:VAL:N	2.49	0.46
1:C:883:SER:CB	2:C:1312:POV:H13	2.45	0.46
1:C:89:THR:HG22	1:C:91:ALA:H	1.81	0.46
1:D:392:ASP:OD1	1:D:393:VAL:N	2.49	0.46
1:D:883:SER:CB	2:D:1314:POV:H13	2.45	0.46
1:A:392:ASP:OD1	1:A:393:VAL:N	2.49	0.46
1:A:89:THR:HG22	1:A:91:ALA:H	1.81	0.45
1:B:11:LEU:HD12	1:B:111:LEU:HB3	1.98	0.45
1:B:89:THR:HG22	1:B:91:ALA:H	1.81	0.45
1:C:292:GLY:O	1:C:320:ARG:NE	2.43	0.45
1:B:364:LEU:O	1:B:367:THR:OG1	2.24	0.45
2:C:1312:POV:H31H	2:C:1315:POV:H21H	1.98	0.45
1:D:142:GLY:N	1:D:291:GLU:O	2.45	0.45
1:B:71:PHE:O	1:B:73:GLN:N	2.50	0.45
1:C:11:LEU:HD12	1:C:111:LEU:HB3	1.98	0.45
1:A:71:PHE:O	1:A:73:GLN:N	2.50	0.45
1:A:334:GLU:O	1:A:336:GLY:N	2.45	0.45
1:B:13:LYS:HD2	1:B:90:ASP:HB2	1.99	0.45
1:A:896:TYR:OH	1:A:975:ARG:NH1	2.46	0.44
1:C:71:PHE:O	1:C:73:GLN:N	2.50	0.44
1:D:11:LEU:HD12	1:D:111:LEU:HB3	1.98	0.44
1:D:13:LYS:HD2	1:D:90:ASP:HB2	1.99	0.44
1:D:896:TYR:OH	1:D:975:ARG:NH1	2.46	0.44
1:B:863:TYR:OH	1:B:972:TRP:O	2.29	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:210:ILE:HD11	1:C:238:LEU:HG	2.00	0.44
1:D:89:THR:HG22	1:D:91:ALA:H	1.81	0.44
1:D:71:PHE:O	1:D:73:GLN:N	2.50	0.44
1:A:863:TYR:OH	1:A:972:TRP:O	2.29	0.44
2:A:1310:POV:O12	2:A:1310:POV:H13A	2.18	0.44
1:A:11:LEU:HD12	1:A:111:LEU:HB3	1.98	0.44
2:D:1301:POV:H21H	2:D:1314:POV:C316	2.48	0.44
1:A:13:LYS:HD2	1:A:90:ASP:HB2	1.99	0.44
1:D:210:ILE:HD11	1:D:238:LEU:HG	2.00	0.44
1:C:896:TYR:OH	1:C:975:ARG:NH2	2.49	0.43
1:A:210:ILE:HD11	1:A:238:LEU:HG	2.00	0.43
1:A:928:ASP:OD1	1:A:975:ARG:NH2	2.51	0.43
1:C:13:LYS:HD2	1:C:90:ASP:HB2	1.99	0.43
1:D:928:ASP:OD1	1:D:975:ARG:NH2	2.51	0.43
2:C:1310:POV:O12	2:C:1310:POV:H13A	2.18	0.43
1:C:863:TYR:OH	1:C:972:TRP:O	2.29	0.43
2:A:1312:POV:H31H	2:A:1315:POV:H21H	2.01	0.43
2:D:1312:POV:H13A	2:D:1312:POV:O12	2.18	0.43
1:A:896:TYR:OH	1:A:975:ARG:NH2	2.49	0.43
1:C:928:ASP:OD1	1:C:975:ARG:NH2	2.51	0.43
1:B:928:ASP:OD1	1:B:975:ARG:NH2	2.51	0.43
2:A:1312:POV:C316	2:A:1315:POV:H21H	2.48	0.43
1:D:1210:GLN:O	1:D:1214:VAL:N	2.42	0.43
3:C:1305:CLR:H221	3:C:1305:CLR:H263	2.01	0.43
1:D:305:GLN:NE2	1:D:370:GLU:OE1	2.52	0.43
3:D:1307:CLR:H221	3:D:1307:CLR:H263	2.01	0.43
2:A:1306:POV:H15A	1:B:1066:CYS:SG	2.58	0.42
2:A:1317:POV:H31G	2:D:1305:POV:C218	2.49	0.42
1:B:210:ILE:HD11	1:B:238:LEU:HG	2.00	0.42
1:B:305:GLN:NE2	1:B:370:GLU:OE1	2.52	0.42
1:B:896:TYR:OH	1:B:975:ARG:NH1	2.46	0.42
3:B:1304:CLR:H221	3:B:1304:CLR:H263	2.01	0.42
2:C:1312:POV:C316	2:C:1315:POV:H21H	2.49	0.42
2:B:1311:POV:C316	2:B:1314:POV:H21H	2.49	0.42
2:C:1306:POV:H218	2:C:1306:POV:H31C	2.00	0.42
2:A:1305:POV:H218	2:A:1305:POV:H31C	2.00	0.42
1:C:364:LEU:O	1:C:367:THR:OG1	2.24	0.42
1:A:305:GLN:NE2	1:A:370:GLU:OE1	2.52	0.42
2:B:1311:POV:H31H	2:B:1314:POV:H21H	2.01	0.42
1:D:896:TYR:OH	1:D:975:ARG:NH2	2.49	0.42
2:B:1309:POV:O12	2:B:1309:POV:H13A	2.18	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:305:GLN:NE2	1:C:370:GLU:OE1	2.52	0.42
1:A:719:SER:OG	1:A:720:THR:N	2.52	0.42
2:D:1308:POV:H218	2:D:1308:POV:H31C	2.00	0.42
3:A:1304:CLR:H263	3:A:1304:CLR:H221	2.02	0.42
2:B:1306:POV:H13A	2:B:1306:POV:P	2.60	0.42
2:B:1305:POV:H218	2:B:1305:POV:H31C	2.01	0.42
2:A:1307:POV:H13A	2:A:1307:POV:P	2.60	0.41
1:D:334:GLU:O	1:D:336:GLY:N	2.45	0.41
1:A:1210:GLN:O	1:A:1214:VAL:N	2.42	0.41
1:C:1042:TRP:HZ3	1:D:1081:LEU:HD12	1.84	0.41
1:B:896:TYR:OH	1:B:975:ARG:NH2	2.49	0.41
1:C:142:GLY:N	1:C:291:GLU:O	2.45	0.41
2:C:1307:POV:H13A	2:C:1307:POV:P	2.60	0.41
1:B:719:SER:OG	1:B:720:THR:N	2.52	0.41
1:B:381:PHE:CE2	1:B:391:ILE:HD11	2.56	0.41
2:B:1301:POV:H31G	1:C:1076:LEU:HD22	2.03	0.41
2:A:1303:POV:H15B	2:A:1303:POV:O14	2.21	0.41
1:A:381:PHE:CE2	1:A:391:ILE:HD11	2.56	0.41
1:A:917:LYS:HE2	2:A:1308:POV:H14B	2.03	0.41
1:A:1092:LEU:HD21	1:B:1086:ILE:HG23	2.02	0.41
1:B:334:GLU:O	1:B:336:GLY:N	2.45	0.41
1:B:917:LYS:HE2	2:B:1307:POV:H14B	2.03	0.41
2:B:1303:POV:H15B	2:B:1303:POV:O14	2.21	0.41
1:C:381:PHE:CE2	1:C:391:ILE:HD11	2.56	0.41
2:D:1301:POV:H21H	2:D:1314:POV:H31H	2.03	0.41
2:D:1309:POV:H13A	2:D:1309:POV:P	2.60	0.41
2:D:1306:POV:H15B	2:D:1306:POV:O14	2.21	0.41
2:A:1310:POV:H13A	2:A:1311:POV:H15	2.04	0.40
1:C:674:ASP:O	1:C:675:THR:OG1	2.36	0.40
2:D:1312:POV:H13A	2:D:1313:POV:H15	2.04	0.40
1:A:526:CYS:SG	1:A:527:THR:N	2.95	0.40
1:C:1066:CYS:SG	2:C:1301:POV:H15A	2.61	0.40
2:C:1304:POV:H15B	2:C:1304:POV:O14	2.21	0.40
1:B:526:CYS:SG	1:B:527:THR:N	2.95	0.40
1:C:526:CYS:SG	1:C:527:THR:N	2.95	0.40
1:D:240:ASN:OD1	1:D:241:LEU:N	2.55	0.40
1:D:364:LEU:O	1:D:367:THR:OG1	2.24	0.40
1:D:526:CYS:SG	1:D:527:THR:N	2.95	0.40
1:C:917:LYS:HE2	2:C:1308:POV:H14B	2.03	0.40
1:D:381:PHE:CE2	1:D:391:ILE:HD11	2.56	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1099/1279 (86%)	1009 (92%)	82 (8%)	8 (1%)	19	22
1	B	1099/1279 (86%)	1008 (92%)	83 (8%)	8 (1%)	19	22
1	C	1099/1279 (86%)	1009 (92%)	82 (8%)	8 (1%)	19	22
1	D	1099/1279 (86%)	1008 (92%)	83 (8%)	8 (1%)	19	22
All	All	4396/5116 (86%)	4034 (92%)	330 (8%)	32 (1%)	21	22

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	67	LEU
1	A	146	PHE
1	B	67	LEU
1	B	146	PHE
1	C	67	LEU
1	C	146	PHE
1	D	67	LEU
1	D	146	PHE
1	A	72	ASN
1	B	72	ASN
1	C	72	ASN
1	D	72	ASN
1	A	321	ALA
1	A	391	ILE
1	B	321	ALA
1	B	391	ILE
1	C	321	ALA
1	C	391	ILE
1	D	321	ALA
1	D	391	ILE
1	A	89	THR
1	B	89	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	68	GLY
1	B	68	GLY
1	C	68	GLY
1	C	89	THR
1	D	68	GLY
1	D	89	THR
1	B	840	PRO
1	C	840	PRO
1	D	840	PRO
1	A	840	PRO

### 5.3.2 Protein sidechains [i](#)

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	981/1138 (86%)	969 (99%)	12 (1%)	67	79
1	B	981/1138 (86%)	969 (99%)	12 (1%)	67	79
1	C	981/1138 (86%)	969 (99%)	12 (1%)	67	79
1	D	981/1138 (86%)	969 (99%)	12 (1%)	67	79
All	All	3924/4552 (86%)	3876 (99%)	48 (1%)	66	79

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	ARG
1	A	61	LYS
1	A	110	ARG
1	A	177	ASN
1	A	197	ARG
1	A	234	LYS
1	A	494	ARG
1	A	500	ASN
1	A	948	ASN
1	A	962	ARG
1	A	968	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	1222	LYS
1	B	46	ARG
1	B	61	LYS
1	B	110	ARG
1	B	177	ASN
1	B	197	ARG
1	B	234	LYS
1	B	494	ARG
1	B	500	ASN
1	B	948	ASN
1	B	962	ARG
1	B	968	ASN
1	B	1222	LYS
1	C	46	ARG
1	C	61	LYS
1	C	110	ARG
1	C	177	ASN
1	C	197	ARG
1	C	234	LYS
1	C	494	ARG
1	C	500	ASN
1	C	948	ASN
1	C	962	ARG
1	C	968	ASN
1	C	1222	LYS
1	D	46	ARG
1	D	61	LYS
1	D	110	ARG
1	D	177	ASN
1	D	197	ARG
1	D	234	LYS
1	D	494	ARG
1	D	500	ASN
1	D	948	ASN
1	D	962	ARG
1	D	968	ASN
1	D	1222	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	500	ASN
1	A	955	ASN
1	B	3	GLN
1	B	276	HIS
1	B	500	ASN
1	B	955	ASN
1	B	1098	ASN
1	C	3	GLN
1	C	98	GLN
1	C	276	HIS
1	C	500	ASN
1	C	955	ASN
1	D	3	GLN
1	D	276	HIS
1	D	500	ASN
1	D	955	ASN

### 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 65 ligands modelled in this entry, 1 is monoatomic - leaving 64 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
2	POV	C	1302	-	51,51,51	0.34	0	57,59,59	0.38	0
2	POV	B	1308	-	51,51,51	0.35	0	57,59,59	0.50	0
2	POV	A	1316	-	14,14,51	1.01	1 (7%)	13,13,59	0.58	0
2	POV	D	1301	-	51,51,51	0.37	0	57,59,59	0.49	0
5	ZY8	B	1313	-	34,38,38	1.17	4 (11%)	49,63,63	1.31	6 (12%)
2	POV	B	1305	-	51,51,51	0.32	0	57,59,59	0.37	0
2	POV	C	1306	-	51,51,51	0.32	0	57,59,59	0.37	0
4	DU0	B	1312	-	42,42,42	0.22	0	64,66,66	0.34	0
2	POV	B	1301	-	51,51,51	0.33	0	57,59,59	0.38	0
2	POV	D	1304	-	51,51,51	0.33	0	57,59,59	0.37	0
2	POV	D	1313	-	32,32,51	0.41	0	37,38,59	0.37	0
2	POV	A	1310	-	51,51,51	0.32	0	57,59,59	0.40	0
2	POV	B	1314	-	51,51,51	0.36	0	57,59,59	0.49	0
2	POV	A	1303	-	51,51,51	0.38	0	57,59,59	0.65	1 (1%)
2	POV	B	1307	-	51,51,51	0.37	0	57,59,59	0.46	0
2	POV	A	1306	-	51,51,51	0.31	0	57,59,59	0.37	0
2	POV	B	1310	-	32,32,51	0.41	0	37,38,59	0.37	0
2	POV	B	1315	-	14,14,51	1.01	1 (7%)	13,13,59	0.59	0
2	POV	C	1308	-	51,51,51	0.37	0	57,59,59	0.46	0
2	POV	C	1307	-	51,51,51	0.33	0	57,59,59	0.48	0
2	POV	A	1308	-	51,51,51	0.37	0	57,59,59	0.46	0
2	POV	C	1303	-	51,51,51	0.38	0	57,59,59	0.53	1 (1%)
2	POV	C	1304	-	51,51,51	0.38	0	57,59,59	0.64	1 (1%)
2	POV	B	1309	-	51,51,51	0.32	0	57,59,59	0.40	0
2	POV	C	1301	-	51,51,51	0.31	0	57,59,59	0.38	0
2	POV	B	1306	-	51,51,51	0.33	0	57,59,59	0.49	0
2	POV	C	1316	-	14,14,51	1.01	1 (7%)	13,13,59	0.58	0
2	POV	D	1308	-	51,51,51	0.32	0	57,59,59	0.37	0
5	ZY8	D	1316	-	34,38,38	1.17	4 (11%)	49,63,63	1.32	5 (10%)
2	POV	A	1305	-	51,51,51	0.32	0	57,59,59	0.37	0
2	POV	D	1305	-	51,51,51	0.37	0	57,59,59	0.53	1 (1%)
2	POV	C	1310	-	51,51,51	0.32	0	57,59,59	0.40	0
2	POV	C	1315	-	51,51,51	0.37	0	57,59,59	0.48	0
3	CLR	D	1307	-	31,31,31	0.20	0	48,48,48	0.35	0
2	POV	B	1303	-	51,51,51	0.38	0	57,59,59	0.65	1 (1%)
3	CLR	A	1304	-	31,31,31	0.20	0	48,48,48	0.35	0
3	CLR	C	1305	-	31,31,31	0.20	0	48,48,48	0.35	0
4	DU0	A	1313	-	42,42,42	0.21	0	64,66,66	0.34	0
2	POV	D	1303	-	51,51,51	0.30	0	57,59,59	0.37	0
2	POV	C	1309	-	51,51,51	0.35	0	57,59,59	0.50	0
2	POV	A	1315	-	51,51,51	0.37	0	57,59,59	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	POV	D	1312	-	51,51,51	0.32	0	57,59,59	0.40	0
2	POV	B	1311	-	51,51,51	0.31	0	57,59,59	0.39	0
2	POV	A	1302	-	51,51,51	0.37	0	57,59,59	0.53	1 (1%)
2	POV	A	1309	-	51,51,51	0.35	0	57,59,59	0.50	0
2	POV	D	1309	-	51,51,51	0.33	0	57,59,59	0.49	0
2	POV	D	1314	-	51,51,51	0.31	0	57,59,59	0.39	0
3	CLR	B	1304	-	31,31,31	0.20	0	48,48,48	0.35	0
2	POV	C	1311	-	32,32,51	0.41	0	37,38,59	0.37	0
2	POV	C	1312	-	51,51,51	0.31	0	57,59,59	0.39	0
5	ZY8	A	1314	-	34,38,38	1.17	4 (11%)	49,63,63	1.32	6 (12%)
5	ZY8	C	1314	-	34,38,38	1.17	4 (11%)	49,63,63	1.33	6 (12%)
2	POV	B	1302	-	51,51,51	0.37	0	57,59,59	0.54	1 (1%)
2	POV	D	1310	-	51,51,51	0.37	0	57,59,59	0.46	0
4	DU0	D	1315	-	42,42,42	0.22	0	64,66,66	0.34	0
2	POV	A	1301	-	51,51,51	0.33	0	57,59,59	0.38	0
2	POV	D	1302	-	14,14,51	1.01	1 (7%)	13,13,59	0.58	0
2	POV	D	1311	-	51,51,51	0.35	0	57,59,59	0.50	0
2	POV	A	1311	-	32,32,51	0.41	0	37,38,59	0.37	0
2	POV	D	1306	-	51,51,51	0.38	0	57,59,59	0.64	1 (1%)
2	POV	A	1312	-	51,51,51	0.31	0	57,59,59	0.39	0
4	DU0	C	1313	-	42,42,42	0.24	0	64,66,66	0.36	0
2	POV	A	1307	-	51,51,51	0.32	0	57,59,59	0.48	0
2	POV	A	1317	-	51,51,51	0.31	0	57,59,59	0.37	0

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
2	POV	C	1302	-	-	26/55/55/55	-
2	POV	B	1308	-	-	21/55/55/55	-
2	POV	A	1316	-	-	6/12/12/55	-
2	POV	D	1301	-	-	23/55/55/55	-
5	ZY8	B	1313	-	-	2/4/60/60	0/1/8/8
2	POV	B	1305	-	-	23/55/55/55	-
2	POV	C	1306	-	-	24/55/55/55	-
4	DU0	B	1312	-	-	3/10/98/98	0/6/6/6
2	POV	B	1301	-	-	26/55/55/55	-

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	POV	D	1304	-	-	26/55/55/55	-
2	POV	D	1313	-	-	13/33/33/55	-
2	POV	A	1310	-	-	20/55/55/55	-
2	POV	B	1314	-	-	24/55/55/55	-
2	POV	A	1303	-	-	25/55/55/55	-
2	POV	B	1307	-	-	20/55/55/55	-
2	POV	A	1306	-	-	20/55/55/55	-
2	POV	B	1310	-	-	13/33/33/55	-
2	POV	B	1315	-	-	6/12/12/55	-
2	POV	C	1308	-	-	20/55/55/55	-
2	POV	C	1307	-	-	27/55/55/55	-
2	POV	A	1308	-	-	20/55/55/55	-
2	POV	C	1303	-	-	24/55/55/55	-
2	POV	C	1304	-	-	25/55/55/55	-
2	POV	B	1309	-	-	20/55/55/55	-
2	POV	C	1301	-	-	18/55/55/55	-
2	POV	B	1306	-	-	27/55/55/55	-
2	POV	C	1316	-	-	6/12/12/55	-
2	POV	D	1308	-	-	24/55/55/55	-
5	ZY8	D	1316	-	-	2/4/60/60	0/1/8/8
2	POV	A	1305	-	-	24/55/55/55	-
2	POV	D	1305	-	-	24/55/55/55	-
2	POV	C	1310	-	-	20/55/55/55	-
2	POV	C	1315	-	-	23/55/55/55	-
3	CLR	D	1307	-	-	4/10/68/68	0/4/4/4
2	POV	B	1303	-	-	25/55/55/55	-
3	CLR	A	1304	-	-	4/10/68/68	0/4/4/4
3	CLR	C	1305	-	-	4/10/68/68	0/4/4/4
4	DU0	A	1313	-	-	3/10/98/98	0/6/6/6
2	POV	D	1303	-	-	20/55/55/55	-
2	POV	C	1309	-	-	21/55/55/55	-
2	POV	A	1315	-	-	24/55/55/55	-
2	POV	D	1312	-	-	20/55/55/55	-
2	POV	B	1311	-	-	23/55/55/55	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	POV	A	1302	-	-	24/55/55/55	-
2	POV	A	1309	-	-	21/55/55/55	-
2	POV	D	1309	-	-	27/55/55/55	-
2	POV	D	1314	-	-	23/55/55/55	-
3	CLR	B	1304	-	-	4/10/68/68	0/4/4/4
2	POV	C	1311	-	-	13/33/33/55	-
2	POV	C	1312	-	-	23/55/55/55	-
5	ZY8	A	1314	-	-	2/4/60/60	0/1/8/8
5	ZY8	C	1314	-	-	2/4/60/60	0/1/8/8
2	POV	B	1302	-	-	24/55/55/55	-
2	POV	D	1310	-	-	20/55/55/55	-
4	DU0	D	1315	-	-	3/10/98/98	0/6/6/6
2	POV	A	1301	-	-	26/55/55/55	-
2	POV	D	1302	-	-	6/12/12/55	-
2	POV	D	1311	-	-	21/55/55/55	-
2	POV	A	1311	-	-	13/33/33/55	-
2	POV	D	1306	-	-	25/55/55/55	-
2	POV	A	1312	-	-	23/55/55/55	-
4	DU0	C	1313	-	-	3/10/98/98	0/6/6/6
2	POV	A	1307	-	-	27/55/55/55	-
2	POV	A	1317	-	-	19/55/55/55	-

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1314	ZY8	C14-N5	4.37	1.52	1.48
5	A	1314	ZY8	C14-N5	4.35	1.52	1.48
5	B	1313	ZY8	C14-N5	4.34	1.52	1.48
5	D	1316	ZY8	C14-N5	4.32	1.52	1.48
2	D	1302	POV	C29-C210	3.62	1.52	1.31
2	A	1316	POV	C29-C210	3.62	1.52	1.31
2	B	1315	POV	C29-C210	3.62	1.52	1.31
2	C	1316	POV	C29-C210	3.62	1.52	1.31
5	D	1316	ZY8	C4-N5	2.28	1.51	1.47
5	C	1314	ZY8	C4-N5	2.24	1.51	1.47
5	A	1314	ZY8	C4-N5	2.22	1.51	1.47
5	B	1313	ZY8	C4-N5	2.21	1.51	1.47

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1313	ZY8	C25-C30	-2.18	1.38	1.43
5	C	1314	ZY8	C25-C30	-2.15	1.38	1.43
5	A	1314	ZY8	C25-C30	-2.14	1.38	1.43
5	D	1316	ZY8	C25-C30	-2.14	1.38	1.43
5	C	1314	ZY8	C6-N5	2.07	1.51	1.47
5	A	1314	ZY8	C6-N5	2.05	1.50	1.47
5	D	1316	ZY8	C6-N5	2.02	1.50	1.47
5	B	1313	ZY8	C6-N5	2.00	1.50	1.47

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1314	ZY8	C13-C14-N5	4.23	109.40	105.41
5	A	1314	ZY8	C13-C14-N5	4.21	109.38	105.41
5	D	1316	ZY8	C13-C14-N5	4.18	109.36	105.41
5	A	1314	ZY8	C15-C14-N5	-4.18	111.16	115.63
5	B	1313	ZY8	C13-C14-N5	4.18	109.35	105.41
5	C	1314	ZY8	C15-C14-N5	-4.18	111.17	115.63
5	D	1316	ZY8	C15-C14-N5	-4.16	111.19	115.63
5	B	1313	ZY8	C15-C14-N5	-4.13	111.22	115.63
2	B	1303	POV	C2-O21-C21	3.00	124.98	117.80
2	A	1303	POV	C2-O21-C21	3.00	124.98	117.80
2	C	1304	POV	C2-O21-C21	2.99	124.96	117.80
2	D	1306	POV	C2-O21-C21	2.99	124.95	117.80
5	A	1314	ZY8	C26-C25-C30	-2.98	118.49	120.38
5	D	1316	ZY8	C26-C25-C30	-2.97	118.50	120.38
5	D	1316	ZY8	O24-C13-C8	2.92	115.49	109.64
5	B	1313	ZY8	O24-C13-C8	2.90	115.46	109.64
5	C	1314	ZY8	C26-C25-C30	-2.90	118.55	120.38
5	A	1314	ZY8	O24-C13-C8	2.89	115.42	109.64
5	C	1314	ZY8	O24-C13-C8	2.88	115.41	109.64
5	B	1313	ZY8	C26-C25-C30	-2.86	118.57	120.38
2	D	1305	POV	C2-O21-C21	2.39	123.52	117.80
2	A	1302	POV	C2-O21-C21	2.38	123.49	117.80
2	C	1303	POV	C2-O21-C21	2.37	123.48	117.80
2	B	1302	POV	C2-O21-C21	2.37	123.47	117.80
5	C	1314	ZY8	O24-C13-C14	2.21	109.38	107.82
5	A	1314	ZY8	O24-C13-C14	2.15	109.34	107.82
5	D	1316	ZY8	O24-C13-C14	2.15	109.34	107.82
5	B	1313	ZY8	O24-C13-C14	2.08	109.29	107.82
5	B	1313	ZY8	C7-C6-N5	2.02	113.89	111.00
5	A	1314	ZY8	C7-C6-N5	2.02	113.88	111.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1314	ZY8	C6-C7-C8	2.00	113.77	111.62

There are no chirality outliers.

All (1122) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1301	POV	C1-O11-P-O12
2	A	1301	POV	C1-O11-P-O13
2	A	1301	POV	C1-O11-P-O14
2	A	1301	POV	C11-O12-P-O11
2	A	1301	POV	C11-O12-P-O13
2	A	1301	POV	C11-O12-P-O14
2	A	1301	POV	O21-C2-C3-O31
2	A	1302	POV	O12-C11-C12-N
2	A	1302	POV	C22-C21-O21-C2
2	A	1302	POV	O22-C21-O21-C2
2	A	1303	POV	C1-O11-P-O12
2	A	1303	POV	C1-O11-P-O14
2	A	1303	POV	C11-O12-P-O11
2	A	1303	POV	C11-O12-P-O13
2	A	1303	POV	C11-O12-P-O14
2	A	1303	POV	O12-C11-C12-N
2	A	1303	POV	C22-C21-O21-C2
2	A	1303	POV	O22-C21-O21-C2
2	A	1303	POV	C32-C31-O31-C3
2	A	1303	POV	O32-C31-O31-C3
2	A	1305	POV	C11-O12-P-O11
2	A	1305	POV	C11-O12-P-O13
2	A	1305	POV	C11-O12-P-O14
2	A	1306	POV	C1-O11-P-O12
2	A	1306	POV	C1-O11-P-O14
2	A	1307	POV	O12-C11-C12-N
2	A	1308	POV	C11-O12-P-O11
2	A	1308	POV	C32-C31-O31-C3
2	A	1308	POV	O32-C31-O31-C3
2	A	1309	POV	C1-O11-P-O12
2	A	1309	POV	C1-O11-P-O13
2	A	1309	POV	C11-O12-P-O14
2	A	1309	POV	C2-C1-O11-P
2	A	1309	POV	C32-C31-O31-C3
2	A	1309	POV	O32-C31-O31-C3
2	A	1310	POV	O21-C2-C3-O31

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
2	A	1310	POV	O12-C11-C12-N
2	A	1311	POV	C1-O11-P-O12
2	A	1311	POV	C1-O11-P-O13
2	A	1311	POV	O11-C1-C2-O21
2	A	1311	POV	O12-C11-C12-N
2	A	1312	POV	C1-O11-P-O14
2	A	1312	POV	C11-O12-P-O14
2	A	1312	POV	O12-C11-C12-N
2	A	1315	POV	C32-C31-O31-C3
2	A	1315	POV	O32-C31-O31-C3
2	A	1317	POV	C1-O11-P-O12
2	A	1317	POV	C1-O11-P-O14
2	B	1301	POV	C1-O11-P-O12
2	B	1301	POV	C1-O11-P-O13
2	B	1301	POV	C1-O11-P-O14
2	B	1301	POV	C11-O12-P-O11
2	B	1301	POV	C11-O12-P-O13
2	B	1301	POV	C11-O12-P-O14
2	B	1301	POV	O21-C2-C3-O31
2	B	1302	POV	O12-C11-C12-N
2	B	1302	POV	C22-C21-O21-C2
2	B	1302	POV	O22-C21-O21-C2
2	B	1303	POV	C1-O11-P-O12
2	B	1303	POV	C1-O11-P-O14
2	B	1303	POV	C11-O12-P-O11
2	B	1303	POV	C11-O12-P-O13
2	B	1303	POV	C11-O12-P-O14
2	B	1303	POV	O12-C11-C12-N
2	B	1303	POV	C22-C21-O21-C2
2	B	1303	POV	O22-C21-O21-C2
2	B	1303	POV	C32-C31-O31-C3
2	B	1303	POV	O32-C31-O31-C3
2	B	1305	POV	C11-O12-P-O11
2	B	1305	POV	C11-O12-P-O13
2	B	1305	POV	C11-O12-P-O14
2	B	1306	POV	O12-C11-C12-N
2	B	1307	POV	C11-O12-P-O11
2	B	1307	POV	C32-C31-O31-C3
2	B	1307	POV	O32-C31-O31-C3
2	B	1308	POV	C1-O11-P-O12
2	B	1308	POV	C1-O11-P-O13
2	B	1308	POV	C11-O12-P-O14

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
2	B	1308	POV	C2-C1-O11-P
2	B	1308	POV	C32-C31-O31-C3
2	B	1308	POV	O32-C31-O31-C3
2	B	1309	POV	O21-C2-C3-O31
2	B	1309	POV	O12-C11-C12-N
2	B	1310	POV	C1-O11-P-O12
2	B	1310	POV	C1-O11-P-O13
2	B	1310	POV	O11-C1-C2-O21
2	B	1310	POV	O12-C11-C12-N
2	B	1311	POV	C1-O11-P-O14
2	B	1311	POV	C11-O12-P-O14
2	B	1311	POV	O12-C11-C12-N
2	B	1314	POV	C32-C31-O31-C3
2	B	1314	POV	O32-C31-O31-C3
2	C	1301	POV	C1-O11-P-O12
2	C	1301	POV	C1-O11-P-O14
2	C	1302	POV	C1-O11-P-O12
2	C	1302	POV	C1-O11-P-O13
2	C	1302	POV	C1-O11-P-O14
2	C	1302	POV	C11-O12-P-O11
2	C	1302	POV	C11-O12-P-O13
2	C	1302	POV	C11-O12-P-O14
2	C	1302	POV	O21-C2-C3-O31
2	C	1303	POV	O12-C11-C12-N
2	C	1303	POV	C22-C21-O21-C2
2	C	1303	POV	O22-C21-O21-C2
2	C	1304	POV	C1-O11-P-O12
2	C	1304	POV	C1-O11-P-O14
2	C	1304	POV	C11-O12-P-O11
2	C	1304	POV	C11-O12-P-O13
2	C	1304	POV	C11-O12-P-O14
2	C	1304	POV	O12-C11-C12-N
2	C	1304	POV	C22-C21-O21-C2
2	C	1304	POV	O22-C21-O21-C2
2	C	1304	POV	C32-C31-O31-C3
2	C	1304	POV	O32-C31-O31-C3
2	C	1306	POV	C11-O12-P-O11
2	C	1306	POV	C11-O12-P-O13
2	C	1306	POV	C11-O12-P-O14
2	C	1307	POV	O12-C11-C12-N
2	C	1308	POV	C11-O12-P-O11
2	C	1308	POV	C32-C31-O31-C3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
2	C	1308	POV	O32-C31-O31-C3
2	C	1309	POV	C1-O11-P-O12
2	C	1309	POV	C1-O11-P-O13
2	C	1309	POV	C11-O12-P-O14
2	C	1309	POV	C2-C1-O11-P
2	C	1309	POV	C32-C31-O31-C3
2	C	1309	POV	O32-C31-O31-C3
2	C	1310	POV	O21-C2-C3-O31
2	C	1310	POV	O12-C11-C12-N
2	C	1311	POV	C1-O11-P-O12
2	C	1311	POV	C1-O11-P-O13
2	C	1311	POV	O11-C1-C2-O21
2	C	1311	POV	O12-C11-C12-N
2	C	1312	POV	C1-O11-P-O14
2	C	1312	POV	C11-O12-P-O14
2	C	1312	POV	O12-C11-C12-N
2	C	1315	POV	C32-C31-O31-C3
2	C	1315	POV	O32-C31-O31-C3
2	D	1301	POV	C32-C31-O31-C3
2	D	1301	POV	O32-C31-O31-C3
2	D	1303	POV	C1-O11-P-O12
2	D	1303	POV	C1-O11-P-O14
2	D	1304	POV	C1-O11-P-O12
2	D	1304	POV	C1-O11-P-O13
2	D	1304	POV	C1-O11-P-O14
2	D	1304	POV	C11-O12-P-O11
2	D	1304	POV	C11-O12-P-O13
2	D	1304	POV	C11-O12-P-O14
2	D	1304	POV	O21-C2-C3-O31
2	D	1305	POV	O12-C11-C12-N
2	D	1305	POV	C22-C21-O21-C2
2	D	1305	POV	O22-C21-O21-C2
2	D	1306	POV	C1-O11-P-O12
2	D	1306	POV	C1-O11-P-O14
2	D	1306	POV	C11-O12-P-O11
2	D	1306	POV	C11-O12-P-O13
2	D	1306	POV	C11-O12-P-O14
2	D	1306	POV	O12-C11-C12-N
2	D	1306	POV	C22-C21-O21-C2
2	D	1306	POV	O22-C21-O21-C2
2	D	1306	POV	C32-C31-O31-C3
2	D	1306	POV	O32-C31-O31-C3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
2	D	1308	POV	C11-O12-P-O11
2	D	1308	POV	C11-O12-P-O13
2	D	1308	POV	C11-O12-P-O14
2	D	1309	POV	O12-C11-C12-N
2	D	1310	POV	C11-O12-P-O11
2	D	1310	POV	C32-C31-O31-C3
2	D	1310	POV	O32-C31-O31-C3
2	D	1311	POV	C1-O11-P-O12
2	D	1311	POV	C1-O11-P-O13
2	D	1311	POV	C11-O12-P-O14
2	D	1311	POV	C2-C1-O11-P
2	D	1311	POV	C32-C31-O31-C3
2	D	1311	POV	O32-C31-O31-C3
2	D	1312	POV	O21-C2-C3-O31
2	D	1312	POV	O12-C11-C12-N
2	D	1313	POV	C1-O11-P-O12
2	D	1313	POV	C1-O11-P-O13
2	D	1313	POV	O11-C1-C2-O21
2	D	1313	POV	O12-C11-C12-N
2	D	1314	POV	C1-O11-P-O14
2	D	1314	POV	C11-O12-P-O14
2	D	1314	POV	O12-C11-C12-N
4	A	1313	DU0	C25-C24-O23-C22
4	B	1312	DU0	C25-C24-O23-C22
4	C	1313	DU0	C25-C24-O23-C22
4	D	1315	DU0	C25-C24-O23-C22
2	A	1310	POV	C32-C33-C34-C35
2	B	1309	POV	C32-C33-C34-C35
2	C	1310	POV	C32-C33-C34-C35
2	D	1312	POV	C32-C33-C34-C35
2	A	1308	POV	C32-C33-C34-C35
2	B	1307	POV	C32-C33-C34-C35
2	C	1308	POV	C32-C33-C34-C35
2	D	1310	POV	C32-C33-C34-C35
2	B	1310	POV	C214-C215-C216-C217
2	C	1311	POV	C214-C215-C216-C217
2	A	1311	POV	C214-C215-C216-C217
2	D	1313	POV	C214-C215-C216-C217
2	C	1301	POV	C31-C32-C33-C34
2	A	1311	POV	C21-C22-C23-C24
2	A	1312	POV	C21-C22-C23-C24
2	A	1317	POV	C31-C32-C33-C34

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
2	B	1307	POV	C21-C22-C23-C24
2	B	1310	POV	C21-C22-C23-C24
2	B	1311	POV	C21-C22-C23-C24
2	C	1308	POV	C21-C22-C23-C24
2	C	1311	POV	C21-C22-C23-C24
2	C	1312	POV	C21-C22-C23-C24
2	D	1310	POV	C21-C22-C23-C24
2	D	1313	POV	C21-C22-C23-C24
2	D	1314	POV	C21-C22-C23-C24
2	A	1306	POV	C2-C1-O11-P
2	A	1317	POV	C2-C1-O11-P
2	C	1301	POV	C2-C1-O11-P
2	D	1303	POV	C2-C1-O11-P
2	A	1306	POV	C31-C32-C33-C34
2	A	1308	POV	C21-C22-C23-C24
2	D	1303	POV	C31-C32-C33-C34
2	A	1306	POV	C37-C38-C39-C310
2	A	1317	POV	C37-C38-C39-C310
2	C	1301	POV	C37-C38-C39-C310
2	D	1303	POV	C37-C38-C39-C310
2	A	1315	POV	C21-C22-C23-C24
2	C	1315	POV	C21-C22-C23-C24
2	D	1301	POV	C21-C22-C23-C24
2	B	1314	POV	C21-C22-C23-C24
2	A	1315	POV	C2-C1-O11-P
2	C	1315	POV	C2-C1-O11-P
2	B	1311	POV	C311-C310-C39-C38
2	D	1314	POV	C311-C310-C39-C38
2	A	1307	POV	C32-C33-C34-C35
2	B	1306	POV	C32-C33-C34-C35
2	C	1307	POV	C32-C33-C34-C35
2	D	1309	POV	C32-C33-C34-C35
2	A	1312	POV	C311-C310-C39-C38
2	B	1305	POV	C23-C24-C25-C26
2	C	1302	POV	C33-C34-C35-C36
2	C	1306	POV	C23-C24-C25-C26
2	C	1312	POV	C311-C310-C39-C38
2	C	1315	POV	C213-C214-C215-C216
2	A	1301	POV	C33-C34-C35-C36
2	A	1301	POV	C34-C35-C36-C37
2	A	1305	POV	C23-C24-C25-C26
2	B	1301	POV	C33-C34-C35-C36

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
2	B	1301	POV	C34-C35-C36-C37
2	C	1302	POV	C34-C35-C36-C37
2	D	1304	POV	C33-C34-C35-C36
2	D	1304	POV	C34-C35-C36-C37
2	D	1308	POV	C23-C24-C25-C26
2	A	1308	POV	C39-C310-C311-C312
2	A	1312	POV	C24-C25-C26-C27
2	B	1307	POV	C39-C310-C311-C312
2	B	1311	POV	C24-C25-C26-C27
2	C	1308	POV	C39-C310-C311-C312
2	C	1312	POV	C24-C25-C26-C27
2	D	1310	POV	C39-C310-C311-C312
2	D	1314	POV	C24-C25-C26-C27
2	C	1310	POV	C25-C26-C27-C28
2	A	1310	POV	C25-C26-C27-C28
2	B	1309	POV	C25-C26-C27-C28
2	D	1312	POV	C25-C26-C27-C28
2	A	1315	POV	C213-C214-C215-C216
2	A	1310	POV	C21-C22-C23-C24
2	C	1310	POV	C21-C22-C23-C24
2	D	1312	POV	C21-C22-C23-C24
2	A	1302	POV	C213-C214-C215-C216
2	B	1302	POV	C213-C214-C215-C216
2	B	1314	POV	C213-C214-C215-C216
2	C	1303	POV	C213-C214-C215-C216
2	D	1303	POV	C25-C26-C27-C28
2	D	1305	POV	C213-C214-C215-C216
2	D	1301	POV	C213-C214-C215-C216
2	B	1311	POV	C310-C311-C312-C313
2	C	1301	POV	C25-C26-C27-C28
2	B	1309	POV	C21-C22-C23-C24
2	A	1317	POV	C25-C26-C27-C28
2	B	1307	POV	C34-C35-C36-C37
2	A	1307	POV	C23-C24-C25-C26
2	A	1308	POV	C34-C35-C36-C37
2	C	1307	POV	C23-C24-C25-C26
2	C	1308	POV	C34-C35-C36-C37
2	D	1309	POV	C23-C24-C25-C26
2	D	1310	POV	C34-C35-C36-C37
2	A	1306	POV	C25-C26-C27-C28
2	A	1312	POV	C33-C34-C35-C36
2	B	1306	POV	C23-C24-C25-C26

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
2	A	1307	POV	C1-C2-C3-O31
2	B	1306	POV	C1-C2-C3-O31
2	C	1307	POV	C1-C2-C3-O31
2	D	1309	POV	C1-C2-C3-O31
2	A	1312	POV	C310-C311-C312-C313
2	A	1312	POV	C214-C215-C216-C217
2	B	1311	POV	C33-C34-C35-C36
2	C	1312	POV	C310-C311-C312-C313
2	C	1312	POV	C214-C215-C216-C217
2	D	1314	POV	C33-C34-C35-C36
2	B	1302	POV	C33-C34-C35-C36
2	B	1311	POV	C214-C215-C216-C217
2	C	1312	POV	C33-C34-C35-C36
2	D	1314	POV	C310-C311-C312-C313
2	D	1314	POV	C214-C215-C216-C217
2	A	1309	POV	C34-C35-C36-C37
2	B	1308	POV	C34-C35-C36-C37
2	C	1303	POV	C33-C34-C35-C36
2	C	1309	POV	C34-C35-C36-C37
2	D	1311	POV	C34-C35-C36-C37
2	A	1302	POV	C33-C34-C35-C36
2	D	1305	POV	C33-C34-C35-C36
2	D	1308	POV	C311-C310-C39-C38
2	A	1305	POV	C311-C310-C39-C38
2	B	1305	POV	C311-C310-C39-C38
2	C	1306	POV	C311-C310-C39-C38
2	A	1311	POV	C23-C24-C25-C26
2	B	1310	POV	C23-C24-C25-C26
2	C	1311	POV	C23-C24-C25-C26
2	D	1313	POV	C23-C24-C25-C26
2	D	1301	POV	C2-C1-O11-P
2	A	1310	POV	C23-C24-C25-C26
2	B	1309	POV	C23-C24-C25-C26
2	C	1310	POV	C23-C24-C25-C26
2	C	1311	POV	C212-C213-C214-C215
2	D	1312	POV	C23-C24-C25-C26
2	D	1313	POV	C212-C213-C214-C215
2	A	1311	POV	C212-C213-C214-C215
2	B	1303	POV	C212-C213-C214-C215
2	B	1310	POV	C212-C213-C214-C215
2	D	1301	POV	C36-C37-C38-C39
2	A	1303	POV	C212-C213-C214-C215

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
2	A	1310	POV	C36-C37-C38-C39
2	A	1315	POV	C36-C37-C38-C39
2	B	1309	POV	C36-C37-C38-C39
2	C	1310	POV	C36-C37-C38-C39
2	D	1306	POV	C212-C213-C214-C215
2	D	1312	POV	C36-C37-C38-C39
3	A	1304	CLR	C21-C20-C22-C23
3	B	1304	CLR	C21-C20-C22-C23
3	C	1305	CLR	C21-C20-C22-C23
3	D	1307	CLR	C21-C20-C22-C23
2	B	1314	POV	C36-C37-C38-C39
2	C	1304	POV	C25-C26-C27-C28
2	A	1303	POV	C25-C26-C27-C28
2	B	1301	POV	C39-C310-C311-C312
2	B	1303	POV	C25-C26-C27-C28
2	B	1314	POV	C35-C36-C37-C38
2	C	1304	POV	C212-C213-C214-C215
2	C	1315	POV	C36-C37-C38-C39
2	D	1304	POV	C39-C310-C311-C312
2	D	1306	POV	C25-C26-C27-C28
2	D	1309	POV	C24-C25-C26-C27
2	A	1301	POV	C39-C310-C311-C312
2	B	1306	POV	C24-C25-C26-C27
2	C	1307	POV	C312-C313-C314-C315
2	C	1315	POV	C310-C311-C312-C313
2	D	1309	POV	C312-C313-C314-C315
2	A	1307	POV	C312-C313-C314-C315
2	C	1302	POV	C39-C310-C311-C312
2	A	1307	POV	C24-C25-C26-C27
2	B	1306	POV	C312-C313-C314-C315
2	B	1314	POV	C310-C311-C312-C313
2	B	1314	POV	C32-C33-C34-C35
2	C	1315	POV	C32-C33-C34-C35
2	D	1301	POV	C35-C36-C37-C38
2	A	1315	POV	C32-C33-C34-C35
2	D	1301	POV	C32-C33-C34-C35
2	A	1302	POV	C21-C22-C23-C24
2	A	1307	POV	C214-C215-C216-C217
2	A	1315	POV	C310-C311-C312-C313
2	D	1301	POV	C310-C311-C312-C313
2	D	1309	POV	C214-C215-C216-C217
2	A	1315	POV	C35-C36-C37-C38

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
2	B	1306	POV	C214-C215-C216-C217
2	C	1307	POV	C214-C215-C216-C217
2	C	1315	POV	C35-C36-C37-C38
2	A	1315	POV	C26-C27-C28-C29
2	C	1315	POV	C26-C27-C28-C29
2	D	1301	POV	C26-C27-C28-C29
2	D	1312	POV	C312-C313-C314-C315
2	A	1310	POV	C312-C313-C314-C315
2	B	1309	POV	C312-C313-C314-C315
2	B	1302	POV	C21-C22-C23-C24
2	D	1305	POV	C21-C22-C23-C24
2	D	1309	POV	C21-C22-C23-C24
2	C	1310	POV	C312-C313-C314-C315
2	C	1316	POV	C211-C210-C29-C28
2	B	1301	POV	C311-C312-C313-C314
2	C	1309	POV	C311-C312-C313-C314
2	D	1304	POV	C311-C312-C313-C314
2	A	1307	POV	C21-C22-C23-C24
2	B	1306	POV	C21-C22-C23-C24
2	C	1303	POV	C21-C22-C23-C24
2	C	1307	POV	C21-C22-C23-C24
2	A	1301	POV	C311-C312-C313-C314
2	A	1309	POV	C311-C312-C313-C314
2	B	1308	POV	C311-C312-C313-C314
2	C	1307	POV	C24-C25-C26-C27
2	D	1311	POV	C311-C312-C313-C314
2	C	1309	POV	C22-C23-C24-C25
2	A	1302	POV	C36-C37-C38-C39
2	A	1309	POV	C22-C23-C24-C25
2	B	1308	POV	C22-C23-C24-C25
2	D	1305	POV	C36-C37-C38-C39
2	D	1311	POV	C22-C23-C24-C25
2	A	1310	POV	C39-C310-C311-C312
2	B	1309	POV	C39-C310-C311-C312
2	C	1310	POV	C39-C310-C311-C312
2	A	1307	POV	C35-C36-C37-C38
2	A	1317	POV	C311-C310-C39-C38
2	B	1306	POV	C35-C36-C37-C38
2	C	1303	POV	C36-C37-C38-C39
2	C	1306	POV	C310-C311-C312-C313
2	D	1309	POV	C35-C36-C37-C38
2	D	1312	POV	C39-C310-C311-C312

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
2	A	1301	POV	C26-C27-C28-C29
2	B	1301	POV	C26-C27-C28-C29
2	C	1307	POV	C26-C27-C28-C29
2	D	1304	POV	C26-C27-C28-C29
2	A	1306	POV	C311-C310-C39-C38
2	B	1305	POV	C310-C311-C312-C313
2	C	1307	POV	C35-C36-C37-C38
2	A	1305	POV	C310-C311-C312-C313
2	A	1309	POV	C37-C38-C39-C310
2	B	1302	POV	C36-C37-C38-C39
2	C	1301	POV	C311-C310-C39-C38
2	C	1302	POV	C311-C312-C313-C314
2	D	1303	POV	C311-C310-C39-C38
2	D	1308	POV	C310-C311-C312-C313
2	B	1308	POV	C37-C38-C39-C310
2	D	1311	POV	C37-C38-C39-C310
2	A	1316	POV	C29-C210-C211-C212
2	B	1306	POV	C29-C210-C211-C212
2	C	1307	POV	C29-C210-C211-C212
2	D	1302	POV	C29-C210-C211-C212
2	D	1309	POV	C29-C210-C211-C212
2	B	1314	POV	C2-C1-O11-P
2	A	1310	POV	C212-C213-C214-C215
2	B	1309	POV	C212-C213-C214-C215
2	C	1309	POV	C37-C38-C39-C310
2	D	1312	POV	C212-C213-C214-C215
2	D	1306	POV	C312-C313-C314-C315
2	A	1303	POV	C312-C313-C314-C315
2	B	1303	POV	C312-C313-C314-C315
2	C	1304	POV	C312-C313-C314-C315
2	C	1310	POV	C212-C213-C214-C215
2	A	1316	POV	C211-C210-C29-C28
2	B	1315	POV	C211-C210-C29-C28
2	D	1302	POV	C211-C210-C29-C28
2	A	1309	POV	C31-C32-C33-C34
2	B	1308	POV	C31-C32-C33-C34
2	C	1309	POV	C31-C32-C33-C34
2	D	1311	POV	C31-C32-C33-C34
2	A	1307	POV	C29-C210-C211-C212
2	B	1315	POV	C29-C210-C211-C212
2	A	1307	POV	C26-C27-C28-C29
2	B	1306	POV	C26-C27-C28-C29

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
2	C	1302	POV	C26-C27-C28-C29
2	D	1309	POV	C26-C27-C28-C29
2	A	1312	POV	C25-C26-C27-C28
2	B	1311	POV	C213-C214-C215-C216
2	B	1311	POV	C25-C26-C27-C28
2	C	1312	POV	C213-C214-C215-C216
2	C	1312	POV	C25-C26-C27-C28
2	D	1314	POV	C25-C26-C27-C28
2	A	1312	POV	C213-C214-C215-C216
2	D	1314	POV	C213-C214-C215-C216
2	C	1302	POV	C36-C37-C38-C39
2	D	1304	POV	C36-C37-C38-C39
2	A	1301	POV	C36-C37-C38-C39
2	B	1301	POV	C36-C37-C38-C39
2	A	1309	POV	C214-C215-C216-C217
2	B	1308	POV	C214-C215-C216-C217
2	D	1311	POV	C214-C215-C216-C217
2	C	1316	POV	C29-C210-C211-C212
2	C	1309	POV	C214-C215-C216-C217
2	D	1305	POV	C211-C212-C213-C214
2	A	1312	POV	C1-C2-C3-O31
2	B	1311	POV	C1-C2-C3-O31
2	C	1303	POV	C1-C2-C3-O31
2	C	1312	POV	C1-C2-C3-O31
2	D	1314	POV	C1-C2-C3-O31
2	A	1302	POV	C211-C212-C213-C214
2	B	1302	POV	C211-C212-C213-C214
2	C	1303	POV	C211-C212-C213-C214
2	A	1311	POV	C210-C211-C212-C213
2	B	1310	POV	C210-C211-C212-C213
2	B	1314	POV	C26-C27-C28-C29
2	C	1311	POV	C210-C211-C212-C213
2	D	1313	POV	C210-C211-C212-C213
3	A	1304	CLR	C23-C24-C25-C27
3	B	1304	CLR	C23-C24-C25-C27
3	C	1305	CLR	C23-C24-C25-C27
3	D	1307	CLR	C23-C24-C25-C27
2	A	1305	POV	C214-C215-C216-C217
2	B	1305	POV	C214-C215-C216-C217
2	C	1306	POV	C214-C215-C216-C217
2	D	1302	POV	C212-C213-C214-C215
2	D	1308	POV	C214-C215-C216-C217

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
2	A	1316	POV	C212-C213-C214-C215
2	B	1315	POV	C212-C213-C214-C215
2	C	1316	POV	C212-C213-C214-C215
2	A	1309	POV	C310-C311-C312-C313
2	B	1308	POV	C310-C311-C312-C313
2	D	1311	POV	C310-C311-C312-C313
2	C	1309	POV	C310-C311-C312-C313
2	A	1305	POV	C210-C211-C212-C213
2	B	1305	POV	C210-C211-C212-C213
2	C	1306	POV	C210-C211-C212-C213
2	D	1308	POV	C210-C211-C212-C213
2	A	1302	POV	O11-C1-C2-O21
2	A	1306	POV	O11-C1-C2-O21
2	A	1317	POV	O11-C1-C2-O21
2	B	1302	POV	O11-C1-C2-O21
2	C	1303	POV	O11-C1-C2-O21
2	D	1303	POV	O11-C1-C2-O21
2	D	1305	POV	O11-C1-C2-O21
2	A	1301	POV	C24-C25-C26-C27
2	A	1306	POV	C35-C36-C37-C38
2	A	1309	POV	C24-C25-C26-C27
2	A	1317	POV	C35-C36-C37-C38
2	C	1301	POV	C35-C36-C37-C38
2	C	1302	POV	C24-C25-C26-C27
2	D	1303	POV	C35-C36-C37-C38
2	D	1311	POV	C24-C25-C26-C27
2	B	1301	POV	C24-C25-C26-C27
2	B	1308	POV	C24-C25-C26-C27
2	C	1309	POV	C24-C25-C26-C27
2	D	1304	POV	C24-C25-C26-C27
2	B	1301	POV	C212-C213-C214-C215
3	A	1304	CLR	C17-C20-C22-C23
3	B	1304	CLR	C17-C20-C22-C23
3	C	1305	CLR	C17-C20-C22-C23
3	D	1307	CLR	C17-C20-C22-C23
2	C	1303	POV	C313-C314-C315-C316
2	D	1305	POV	C313-C314-C315-C316
4	A	1313	DU0	C51-C26-C27-O28
4	B	1312	DU0	C51-C26-C27-O28
4	C	1313	DU0	C51-C26-C27-O28
4	D	1315	DU0	C51-C26-C27-O28
2	A	1302	POV	C313-C314-C315-C316

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
2	B	1302	POV	C313-C314-C315-C316
4	A	1313	DU0	C25-C26-C27-O28
4	B	1312	DU0	C25-C26-C27-O28
4	C	1313	DU0	C25-C26-C27-O28
4	D	1315	DU0	C25-C26-C27-O28
2	C	1301	POV	C23-C24-C25-C26
2	C	1308	POV	C311-C310-C39-C38
2	A	1308	POV	C311-C310-C39-C38
2	B	1307	POV	C311-C310-C39-C38
2	D	1310	POV	C311-C310-C39-C38
2	A	1301	POV	C313-C314-C315-C316
2	A	1305	POV	C32-C33-C34-C35
2	C	1302	POV	C313-C314-C315-C316
2	C	1306	POV	C32-C33-C34-C35
2	A	1317	POV	C23-C24-C25-C26
2	D	1303	POV	C23-C24-C25-C26
2	D	1304	POV	C212-C213-C214-C215
2	A	1306	POV	C23-C24-C25-C26
2	A	1303	POV	C2-C1-O11-P
2	A	1312	POV	C2-C1-O11-P
2	B	1303	POV	C2-C1-O11-P
2	B	1311	POV	C2-C1-O11-P
2	C	1304	POV	C2-C1-O11-P
2	C	1312	POV	C2-C1-O11-P
2	D	1306	POV	C2-C1-O11-P
2	D	1314	POV	C2-C1-O11-P
2	C	1308	POV	C214-C215-C216-C217
2	D	1304	POV	C313-C314-C315-C316
2	B	1305	POV	C32-C33-C34-C35
2	D	1308	POV	C32-C33-C34-C35
2	A	1312	POV	C37-C38-C39-C310
2	A	1308	POV	C214-C215-C216-C217
2	C	1312	POV	C37-C38-C39-C310
2	D	1314	POV	C37-C38-C39-C310
2	A	1302	POV	O11-C1-C2-C3
2	A	1306	POV	O11-C1-C2-C3
2	A	1317	POV	O11-C1-C2-C3
2	B	1302	POV	O11-C1-C2-C3
2	C	1301	POV	O11-C1-C2-C3
2	C	1303	POV	O11-C1-C2-C3
2	D	1303	POV	O11-C1-C2-C3
2	D	1305	POV	O11-C1-C2-C3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
2	B	1307	POV	C214-C215-C216-C217
2	D	1310	POV	C214-C215-C216-C217
2	B	1301	POV	C313-C314-C315-C316
2	B	1302	POV	C215-C216-C217-C218
2	B	1311	POV	C37-C38-C39-C310
2	A	1302	POV	C215-C216-C217-C218
2	C	1303	POV	C215-C216-C217-C218
2	D	1305	POV	C215-C216-C217-C218
2	A	1301	POV	C215-C216-C217-C218
2	C	1302	POV	C215-C216-C217-C218
2	D	1304	POV	C215-C216-C217-C218
2	A	1311	POV	C2-C1-O11-P
2	B	1310	POV	C2-C1-O11-P
2	C	1311	POV	C2-C1-O11-P
2	D	1313	POV	C2-C1-O11-P
2	A	1306	POV	C311-C312-C313-C314
2	A	1317	POV	C311-C312-C313-C314
2	C	1301	POV	C311-C312-C313-C314
2	D	1303	POV	C311-C312-C313-C314
2	A	1301	POV	C1-C2-C3-O31
2	A	1302	POV	C1-C2-C3-O31
2	A	1310	POV	C1-C2-C3-O31
2	B	1301	POV	C1-C2-C3-O31
2	B	1302	POV	C1-C2-C3-O31
2	B	1309	POV	C1-C2-C3-O31
2	C	1302	POV	C1-C2-C3-O31
2	C	1310	POV	C1-C2-C3-O31
2	D	1304	POV	C1-C2-C3-O31
2	D	1305	POV	C1-C2-C3-O31
2	D	1312	POV	C1-C2-C3-O31
2	A	1301	POV	C212-C213-C214-C215
2	A	1305	POV	C35-C36-C37-C38
2	B	1305	POV	C35-C36-C37-C38
2	B	1307	POV	C311-C312-C313-C314
2	D	1308	POV	C35-C36-C37-C38
2	A	1308	POV	C311-C312-C313-C314
2	C	1308	POV	C311-C312-C313-C314
2	C	1306	POV	C35-C36-C37-C38
2	D	1310	POV	C311-C312-C313-C314
2	D	1306	POV	C33-C34-C35-C36
2	C	1301	POV	O11-C1-C2-O21
2	B	1301	POV	C215-C216-C217-C218

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
2	A	1303	POV	C33-C34-C35-C36
2	C	1304	POV	C33-C34-C35-C36
2	A	1305	POV	C313-C314-C315-C316
2	B	1305	POV	C313-C314-C315-C316
2	C	1306	POV	C313-C314-C315-C316
2	B	1303	POV	C33-C34-C35-C36
2	D	1308	POV	C313-C314-C315-C316
2	A	1308	POV	C312-C313-C314-C315
2	B	1307	POV	C312-C313-C314-C315
2	D	1305	POV	C24-C25-C26-C27
2	D	1310	POV	C312-C313-C314-C315
2	A	1302	POV	C24-C25-C26-C27
2	C	1308	POV	C312-C313-C314-C315
2	B	1302	POV	C24-C25-C26-C27
2	C	1303	POV	C24-C25-C26-C27
2	C	1307	POV	C311-C310-C39-C38
2	C	1302	POV	C212-C213-C214-C215
2	C	1306	POV	C24-C25-C26-C27
2	A	1307	POV	C311-C310-C39-C38
2	B	1306	POV	C311-C310-C39-C38
2	D	1309	POV	C311-C310-C39-C38
2	C	1302	POV	C35-C36-C37-C38
2	B	1301	POV	C35-C36-C37-C38
2	C	1315	POV	C37-C38-C39-C310
2	A	1305	POV	O11-C1-C2-C3
2	A	1312	POV	O11-C1-C2-C3
2	B	1311	POV	O11-C1-C2-C3
2	C	1306	POV	O11-C1-C2-C3
2	C	1312	POV	O11-C1-C2-C3
2	D	1308	POV	O11-C1-C2-C3
2	D	1314	POV	O11-C1-C2-C3
3	B	1304	CLR	C23-C24-C25-C26
2	D	1304	POV	C35-C36-C37-C38
2	A	1301	POV	C35-C36-C37-C38
2	D	1310	POV	C215-C216-C217-C218
2	A	1308	POV	C215-C216-C217-C218
2	B	1307	POV	C215-C216-C217-C218
2	A	1310	POV	C35-C36-C37-C38
2	B	1305	POV	C24-C25-C26-C27
2	B	1309	POV	C35-C36-C37-C38
2	C	1311	POV	C22-C23-C24-C25
2	D	1312	POV	C35-C36-C37-C38

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
2	C	1304	POV	C21-C22-C23-C24
2	C	1308	POV	C215-C216-C217-C218
3	A	1304	CLR	C23-C24-C25-C26
3	D	1307	CLR	C23-C24-C25-C26
2	A	1312	POV	C39-C310-C311-C312
2	C	1310	POV	C35-C36-C37-C38
2	C	1315	POV	C211-C212-C213-C214
2	D	1313	POV	C22-C23-C24-C25
2	A	1311	POV	C22-C23-C24-C25
2	B	1310	POV	C22-C23-C24-C25
2	D	1306	POV	C21-C22-C23-C24
2	C	1302	POV	C23-C24-C25-C26
2	A	1315	POV	C37-C38-C39-C310
2	C	1312	POV	C39-C310-C311-C312
2	B	1311	POV	C39-C310-C311-C312
2	D	1314	POV	C39-C310-C311-C312
3	C	1305	CLR	C23-C24-C25-C26
2	A	1303	POV	C21-C22-C23-C24
2	B	1303	POV	C21-C22-C23-C24
2	A	1305	POV	O11-C1-C2-O21
2	A	1309	POV	O11-C1-C2-O21
2	A	1312	POV	O11-C1-C2-O21
2	B	1305	POV	O11-C1-C2-O21
2	B	1308	POV	O11-C1-C2-O21
2	B	1311	POV	O11-C1-C2-O21
2	C	1306	POV	O11-C1-C2-O21
2	C	1309	POV	O11-C1-C2-O21
2	C	1312	POV	O11-C1-C2-O21
2	D	1308	POV	O11-C1-C2-O21
2	D	1311	POV	O11-C1-C2-O21
2	D	1314	POV	O11-C1-C2-O21
2	A	1301	POV	C23-C24-C25-C26
2	A	1305	POV	C24-C25-C26-C27
2	B	1303	POV	C310-C311-C312-C313
2	D	1304	POV	C23-C24-C25-C26
2	D	1308	POV	C24-C25-C26-C27
2	A	1311	POV	C12-C11-O12-P
2	B	1310	POV	C12-C11-O12-P
2	C	1311	POV	C12-C11-O12-P
2	D	1313	POV	C12-C11-O12-P
2	A	1303	POV	C310-C311-C312-C313
2	B	1301	POV	C23-C24-C25-C26

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
2	A	1302	POV	O21-C2-C3-O31
2	A	1312	POV	O21-C2-C3-O31
2	B	1302	POV	O21-C2-C3-O31
2	B	1311	POV	O21-C2-C3-O31
2	C	1303	POV	O21-C2-C3-O31
2	D	1305	POV	O21-C2-C3-O31
2	D	1314	POV	O21-C2-C3-O31
2	D	1306	POV	C310-C311-C312-C313
2	A	1316	POV	C23-C24-C25-C26
2	C	1304	POV	C310-C311-C312-C313
2	C	1316	POV	C23-C24-C25-C26
2	D	1302	POV	C23-C24-C25-C26
2	A	1315	POV	C211-C212-C213-C214
2	B	1314	POV	C211-C212-C213-C214
2	B	1315	POV	C23-C24-C25-C26
2	D	1301	POV	C37-C38-C39-C310
2	A	1305	POV	O12-C11-C12-N
2	B	1305	POV	O12-C11-C12-N
2	C	1306	POV	O12-C11-C12-N
2	D	1308	POV	O12-C11-C12-N
2	D	1301	POV	C211-C212-C213-C214
2	B	1303	POV	C211-C212-C213-C214
2	D	1306	POV	C211-C212-C213-C214
2	A	1303	POV	C211-C212-C213-C214
2	C	1315	POV	C39-C310-C311-C312
2	D	1303	POV	C21-C22-C23-C24
2	C	1304	POV	C211-C212-C213-C214
2	B	1306	POV	C211-C212-C213-C214
2	A	1307	POV	C211-C212-C213-C214
2	D	1309	POV	C211-C212-C213-C214
2	C	1307	POV	C25-C26-C27-C28
2	A	1306	POV	C21-C22-C23-C24
2	A	1317	POV	C21-C22-C23-C24
2	A	1315	POV	C39-C310-C311-C312
2	A	1307	POV	C25-C26-C27-C28
2	B	1314	POV	C27-C28-C29-C210
2	B	1306	POV	C25-C26-C27-C28
2	D	1309	POV	C25-C26-C27-C28
2	A	1310	POV	O11-C1-C2-C3
2	B	1305	POV	O11-C1-C2-C3
2	B	1309	POV	O11-C1-C2-C3
2	C	1310	POV	O11-C1-C2-C3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
2	D	1312	POV	O11-C1-C2-C3
2	A	1310	POV	C310-C311-C312-C313
2	B	1301	POV	C214-C215-C216-C217
2	D	1301	POV	C39-C310-C311-C312
2	D	1312	POV	C310-C311-C312-C313
2	B	1309	POV	C310-C311-C312-C313
2	C	1307	POV	C211-C212-C213-C214
2	C	1310	POV	C310-C311-C312-C313
2	C	1315	POV	C25-C26-C27-C28
2	A	1315	POV	C25-C26-C27-C28
2	B	1302	POV	C25-C26-C27-C28
2	B	1314	POV	C39-C310-C311-C312
2	B	1302	POV	C2-C1-O11-P
2	A	1302	POV	C25-C26-C27-C28
2	D	1305	POV	C25-C26-C27-C28
2	B	1314	POV	C37-C38-C39-C310
2	C	1301	POV	C21-C22-C23-C24
2	D	1301	POV	C25-C26-C27-C28
2	C	1303	POV	C25-C26-C27-C28
2	A	1307	POV	O21-C2-C3-O31
2	B	1306	POV	O21-C2-C3-O31
2	C	1307	POV	O21-C2-C3-O31
2	C	1312	POV	O21-C2-C3-O31
2	D	1309	POV	O21-C2-C3-O31
2	A	1303	POV	C1-C2-C3-O31
2	B	1303	POV	C1-C2-C3-O31
2	C	1304	POV	C1-C2-C3-O31
2	D	1306	POV	C1-C2-C3-O31
2	A	1312	POV	C210-C211-C212-C213
2	B	1301	POV	C210-C211-C212-C213
2	C	1303	POV	C210-C211-C212-C213
2	C	1312	POV	C210-C211-C212-C213
2	A	1303	POV	C29-C210-C211-C212
2	B	1303	POV	C29-C210-C211-C212
2	C	1304	POV	C29-C210-C211-C212
2	C	1315	POV	C27-C28-C29-C210
2	D	1301	POV	C27-C28-C29-C210
2	D	1306	POV	C29-C210-C211-C212
2	B	1314	POV	C25-C26-C27-C28
2	D	1303	POV	C212-C213-C214-C215
2	A	1306	POV	C212-C213-C214-C215
2	C	1306	POV	C25-C26-C27-C28

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
2	C	1301	POV	C212-C213-C214-C215
2	D	1304	POV	C214-C215-C216-C217
2	A	1302	POV	C11-O12-P-O14
2	A	1303	POV	C1-O11-P-O13
2	A	1305	POV	C1-O11-P-O14
2	A	1306	POV	C1-O11-P-O13
2	A	1307	POV	C11-O12-P-O11
2	A	1308	POV	C1-O11-P-O13
2	A	1308	POV	C11-O12-P-O14
2	A	1309	POV	C11-O12-P-O11
2	A	1315	POV	C1-O11-P-O12
2	A	1315	POV	C1-O11-P-O13
2	A	1317	POV	C1-O11-P-O13
2	B	1302	POV	C11-O12-P-O14
2	B	1303	POV	C1-O11-P-O13
2	B	1305	POV	C1-O11-P-O14
2	B	1306	POV	C11-O12-P-O11
2	B	1307	POV	C1-O11-P-O13
2	B	1307	POV	C11-O12-P-O14
2	B	1308	POV	C11-O12-P-O11
2	B	1314	POV	C1-O11-P-O12
2	B	1314	POV	C1-O11-P-O13
2	C	1301	POV	C1-O11-P-O13
2	C	1303	POV	C11-O12-P-O14
2	C	1304	POV	C1-O11-P-O13
2	C	1306	POV	C1-O11-P-O14
2	C	1307	POV	C11-O12-P-O11
2	C	1308	POV	C1-O11-P-O13
2	C	1308	POV	C11-O12-P-O14
2	C	1309	POV	C11-O12-P-O11
2	C	1315	POV	C1-O11-P-O12
2	D	1301	POV	C1-O11-P-O12
2	D	1301	POV	C1-O11-P-O13
2	D	1303	POV	C1-O11-P-O13
2	D	1305	POV	C11-O12-P-O14
2	D	1306	POV	C1-O11-P-O13
2	D	1308	POV	C1-O11-P-O14
2	D	1309	POV	C11-O12-P-O11
2	D	1310	POV	C1-O11-P-O13
2	D	1310	POV	C11-O12-P-O14
2	D	1311	POV	C11-O12-P-O11
2	A	1317	POV	C212-C213-C214-C215

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
2	B	1305	POV	C25-C26-C27-C28
2	C	1316	POV	C213-C214-C215-C216
2	A	1310	POV	O31-C31-C32-C33
2	C	1310	POV	O31-C31-C32-C33
2	A	1315	POV	C27-C28-C29-C210
2	A	1302	POV	C210-C211-C212-C213
2	B	1302	POV	C210-C211-C212-C213
2	B	1311	POV	C210-C211-C212-C213
2	D	1304	POV	C210-C211-C212-C213
2	D	1305	POV	C210-C211-C212-C213
2	D	1314	POV	C210-C211-C212-C213
2	A	1302	POV	C2-C1-O11-P
2	A	1308	POV	C2-C1-O11-P
2	B	1307	POV	C2-C1-O11-P
2	C	1303	POV	C2-C1-O11-P
2	C	1308	POV	C2-C1-O11-P
2	D	1305	POV	C2-C1-O11-P
2	D	1310	POV	C2-C1-O11-P
2	B	1309	POV	O31-C31-C32-C33
2	D	1312	POV	O31-C31-C32-C33
2	C	1308	POV	C1-C2-O21-C21
2	A	1312	POV	O31-C31-C32-C33
2	B	1311	POV	O31-C31-C32-C33
2	D	1314	POV	O31-C31-C32-C33
2	A	1301	POV	C214-C215-C216-C217
2	A	1303	POV	C313-C314-C315-C316
2	C	1304	POV	C313-C314-C315-C316
2	D	1306	POV	C313-C314-C315-C316
2	B	1303	POV	C313-C314-C315-C316
2	C	1302	POV	C214-C215-C216-C217
2	C	1312	POV	O31-C31-C32-C33
2	C	1307	POV	C212-C213-C214-C215
2	A	1305	POV	C25-C26-C27-C28
2	A	1301	POV	C210-C211-C212-C213
2	B	1301	POV	C25-C26-C27-C28
2	A	1316	POV	C213-C214-C215-C216
2	D	1308	POV	C25-C26-C27-C28
2	D	1309	POV	C212-C213-C214-C215
2	B	1315	POV	C213-C214-C215-C216
2	A	1307	POV	C212-C213-C214-C215
2	C	1307	POV	C311-C312-C313-C314
2	B	1306	POV	C311-C312-C313-C314

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
2	B	1306	POV	C212-C213-C214-C215
2	A	1307	POV	C311-C312-C313-C314
2	D	1309	POV	C311-C312-C313-C314
2	D	1304	POV	C25-C26-C27-C28
5	A	1314	ZY8	C2-C3-C4-N5
5	B	1313	ZY8	C2-C3-C4-N5
5	C	1314	ZY8	C1-C3-C4-N5
5	C	1314	ZY8	C2-C3-C4-N5
5	D	1316	ZY8	C2-C3-C4-N5
2	D	1302	POV	C213-C214-C215-C216
2	B	1308	POV	O11-C1-C2-C3
2	B	1307	POV	C212-C213-C214-C215
2	D	1310	POV	C212-C213-C214-C215
2	A	1308	POV	C212-C213-C214-C215
2	A	1301	POV	C25-C26-C27-C28
2	C	1308	POV	C212-C213-C214-C215
2	A	1305	POV	C34-C35-C36-C37
2	C	1315	POV	C29-C210-C211-C212
2	B	1305	POV	C34-C35-C36-C37
2	B	1314	POV	C312-C313-C314-C315
2	C	1302	POV	C25-C26-C27-C28
2	D	1308	POV	C34-C35-C36-C37
2	D	1301	POV	C312-C313-C314-C315
2	C	1315	POV	C312-C313-C314-C315
2	C	1306	POV	C34-C35-C36-C37
2	D	1309	POV	C215-C216-C217-C218
2	A	1315	POV	C312-C313-C314-C315
2	A	1307	POV	C215-C216-C217-C218
2	B	1306	POV	C215-C216-C217-C218
2	C	1307	POV	C215-C216-C217-C218
2	D	1301	POV	C29-C210-C211-C212
2	D	1309	POV	C34-C35-C36-C37
2	A	1307	POV	C34-C35-C36-C37
2	B	1306	POV	C34-C35-C36-C37
2	A	1307	POV	C3-C2-O21-C21
2	A	1308	POV	C1-C2-O21-C21
2	B	1306	POV	C3-C2-O21-C21
2	B	1307	POV	C1-C2-O21-C21
2	C	1307	POV	C3-C2-O21-C21
2	D	1309	POV	C3-C2-O21-C21
2	D	1310	POV	C1-C2-O21-C21
2	C	1302	POV	C210-C211-C212-C213

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
2	C	1307	POV	C34-C35-C36-C37
2	A	1315	POV	C29-C210-C211-C212
2	B	1314	POV	C29-C210-C211-C212
2	B	1311	POV	C22-C23-C24-C25
2	A	1312	POV	C22-C23-C24-C25
2	C	1312	POV	C22-C23-C24-C25
2	A	1303	POV	O11-C1-C2-O21
2	B	1303	POV	O11-C1-C2-O21
2	C	1304	POV	O11-C1-C2-O21
2	D	1306	POV	O11-C1-C2-O21
2	D	1314	POV	C22-C23-C24-C25
2	D	1303	POV	C29-C210-C211-C212
2	B	1306	POV	C2-C1-O11-P
2	A	1309	POV	O11-C1-C2-C3
2	C	1309	POV	O11-C1-C2-C3
2	D	1311	POV	O11-C1-C2-C3
2	A	1306	POV	C29-C210-C211-C212
2	A	1317	POV	C29-C210-C211-C212
2	C	1301	POV	C29-C210-C211-C212
2	A	1317	POV	C213-C214-C215-C216
2	D	1303	POV	C213-C214-C215-C216
2	A	1306	POV	C213-C214-C215-C216
2	C	1301	POV	C213-C214-C215-C216
2	A	1302	POV	C32-C33-C34-C35
2	C	1302	POV	C211-C212-C213-C214
2	B	1309	POV	C311-C312-C313-C314
2	D	1312	POV	C311-C312-C313-C314
5	A	1314	ZY8	C1-C3-C4-N5
5	B	1313	ZY8	C1-C3-C4-N5
5	D	1316	ZY8	C1-C3-C4-N5
2	D	1305	POV	C32-C33-C34-C35
2	C	1310	POV	C311-C312-C313-C314
2	D	1309	POV	C2-C1-O11-P
2	A	1310	POV	C311-C312-C313-C314
2	C	1303	POV	C32-C33-C34-C35
2	C	1309	POV	O21-C21-C22-C23
2	B	1314	POV	C313-C314-C315-C316
2	A	1310	POV	O11-C1-C2-O21
2	B	1309	POV	O11-C1-C2-O21
2	C	1310	POV	O11-C1-C2-O21
2	D	1312	POV	O11-C1-C2-O21
2	C	1315	POV	C313-C314-C315-C316

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
2	D	1301	POV	C313-C314-C315-C316
2	A	1309	POV	O21-C21-C22-C23
2	B	1308	POV	O21-C21-C22-C23
2	A	1301	POV	C211-C212-C213-C214
2	C	1308	POV	C210-C211-C212-C213
2	D	1311	POV	O21-C21-C22-C23
2	C	1309	POV	C211-C212-C213-C214
2	A	1315	POV	C313-C314-C315-C316
2	A	1308	POV	C37-C38-C39-C310
2	D	1310	POV	C37-C38-C39-C310
2	D	1305	POV	C29-C210-C211-C212
2	A	1307	POV	C2-C1-O11-P
2	C	1307	POV	C2-C1-O11-P
2	B	1307	POV	C37-C38-C39-C310
2	C	1308	POV	C37-C38-C39-C310
2	D	1308	POV	C22-C23-C24-C25
2	A	1305	POV	C22-C23-C24-C25
2	A	1308	POV	C210-C211-C212-C213
2	B	1307	POV	C210-C211-C212-C213
2	D	1310	POV	C210-C211-C212-C213
2	D	1311	POV	C211-C212-C213-C214
2	B	1302	POV	C32-C33-C34-C35
2	A	1302	POV	C29-C210-C211-C212
2	A	1306	POV	C27-C28-C29-C210
2	B	1302	POV	C29-C210-C211-C212
2	C	1303	POV	C29-C210-C211-C212
2	A	1309	POV	C211-C212-C213-C214
2	B	1308	POV	C211-C212-C213-C214
2	D	1314	POV	C23-C24-C25-C26
2	A	1305	POV	C3-C2-O21-C21
2	C	1306	POV	C3-C2-O21-C21
2	D	1308	POV	C3-C2-O21-C21
2	B	1311	POV	C23-C24-C25-C26
2	A	1311	POV	C29-C210-C211-C212
2	A	1317	POV	C27-C28-C29-C210
2	B	1310	POV	C29-C210-C211-C212
2	C	1301	POV	C27-C28-C29-C210
2	D	1303	POV	C27-C28-C29-C210
2	D	1313	POV	C29-C210-C211-C212
2	C	1312	POV	C23-C24-C25-C26
2	A	1303	POV	C22-C23-C24-C25
2	A	1312	POV	C23-C24-C25-C26

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
2	B	1305	POV	C22-C23-C24-C25
2	C	1310	POV	C29-C210-C211-C212
2	C	1311	POV	C29-C210-C211-C212
2	B	1301	POV	C211-C212-C213-C214
2	C	1310	POV	C37-C38-C39-C310
2	A	1307	POV	O11-C1-C2-O21
2	C	1307	POV	O11-C1-C2-O21
2	B	1303	POV	C22-C23-C24-C25
2	C	1306	POV	C22-C23-C24-C25
2	A	1310	POV	C37-C38-C39-C310
2	D	1304	POV	C211-C212-C213-C214
2	D	1312	POV	C37-C38-C39-C310
2	B	1309	POV	C37-C38-C39-C310
2	D	1306	POV	C22-C23-C24-C25
2	A	1301	POV	C27-C28-C29-C210
2	A	1310	POV	C29-C210-C211-C212
2	B	1301	POV	C27-C28-C29-C210
2	B	1309	POV	C29-C210-C211-C212
2	D	1312	POV	C29-C210-C211-C212
2	C	1303	POV	O31-C31-C32-C33
2	D	1301	POV	C311-C312-C313-C314
2	B	1302	POV	O31-C31-C32-C33
2	A	1315	POV	C311-C312-C313-C314
2	B	1314	POV	C311-C310-C39-C38
2	B	1303	POV	O21-C2-C3-O31
2	C	1304	POV	O21-C2-C3-O31
2	D	1306	POV	O21-C2-C3-O31
2	C	1307	POV	C213-C214-C215-C216
2	D	1304	POV	C27-C28-C29-C210
2	A	1305	POV	O21-C21-C22-C23
2	B	1305	POV	O21-C21-C22-C23
2	C	1306	POV	O21-C21-C22-C23
2	D	1308	POV	O21-C21-C22-C23
2	C	1304	POV	C22-C23-C24-C25
2	A	1307	POV	C213-C214-C215-C216
2	B	1306	POV	C213-C214-C215-C216
2	D	1309	POV	C213-C214-C215-C216
2	A	1302	POV	O31-C31-C32-C33
2	D	1305	POV	O31-C31-C32-C33
2	D	1301	POV	C311-C310-C39-C38
2	C	1302	POV	C27-C28-C29-C210
2	B	1314	POV	C311-C312-C313-C314

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
2	A	1315	POV	C311-C310-C39-C38
2	B	1302	POV	C37-C38-C39-C310
2	C	1315	POV	C311-C312-C313-C314
2	C	1315	POV	C311-C310-C39-C38
2	B	1301	POV	C31-C32-C33-C34
2	D	1312	POV	C22-C23-C24-C25
2	A	1310	POV	C22-C23-C24-C25
2	B	1306	POV	O11-C1-C2-O21
2	D	1309	POV	O11-C1-C2-O21
2	B	1309	POV	C22-C23-C24-C25
2	C	1312	POV	C211-C212-C213-C214
2	A	1301	POV	C31-C32-C33-C34
2	D	1304	POV	C31-C32-C33-C34
2	B	1311	POV	C211-C212-C213-C214
2	A	1312	POV	C211-C212-C213-C214
2	D	1314	POV	C211-C212-C213-C214
2	C	1307	POV	C22-C23-C24-C25
2	C	1310	POV	C22-C23-C24-C25
2	A	1309	POV	O31-C31-C32-C33
2	B	1308	POV	O31-C31-C32-C33
2	A	1303	POV	O21-C2-C3-O31
2	B	1314	POV	O21-C21-C22-C23
2	C	1309	POV	O31-C31-C32-C33
2	D	1311	POV	O31-C31-C32-C33
2	A	1307	POV	C22-C23-C24-C25
2	B	1306	POV	C39-C310-C311-C312
2	B	1306	POV	C22-C23-C24-C25
2	D	1309	POV	C22-C23-C24-C25
2	C	1315	POV	O21-C21-C22-C23
2	A	1305	POV	C1-C2-O21-C21
2	A	1307	POV	C1-C2-O21-C21
2	B	1305	POV	C1-C2-O21-C21
2	B	1305	POV	C3-C2-O21-C21
2	B	1306	POV	C1-C2-O21-C21
2	C	1306	POV	C1-C2-O21-C21
2	C	1307	POV	C1-C2-O21-C21
2	D	1308	POV	C1-C2-O21-C21
2	D	1309	POV	C1-C2-O21-C21
2	C	1307	POV	C39-C310-C311-C312
2	A	1315	POV	O21-C21-C22-C23
2	A	1302	POV	C37-C38-C39-C310
2	A	1307	POV	C39-C310-C311-C312

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
2	D	1309	POV	C39-C310-C311-C312
2	D	1305	POV	C37-C38-C39-C310
2	A	1306	POV	C33-C34-C35-C36
2	D	1301	POV	O21-C21-C22-C23
2	B	1315	POV	C22-C23-C24-C25
2	C	1302	POV	C31-C32-C33-C34
2	D	1310	POV	O21-C21-C22-C23
2	C	1316	POV	C22-C23-C24-C25
2	D	1302	POV	C22-C23-C24-C25
2	C	1303	POV	C37-C38-C39-C310
2	A	1308	POV	O21-C21-C22-C23
2	B	1307	POV	O21-C21-C22-C23
2	A	1302	POV	O32-C31-C32-C33
2	D	1305	POV	O32-C31-C32-C33
2	A	1316	POV	C22-C23-C24-C25
2	C	1306	POV	O22-C21-C22-C23
2	C	1308	POV	O21-C21-C22-C23
2	B	1305	POV	O22-C21-C22-C23
2	B	1308	POV	O32-C31-C32-C33
2	C	1309	POV	O32-C31-C32-C33
2	D	1308	POV	O22-C21-C22-C23
2	D	1311	POV	O32-C31-C32-C33
2	D	1303	POV	C33-C34-C35-C36
2	A	1305	POV	O22-C21-C22-C23
2	A	1309	POV	O32-C31-C32-C33
2	B	1302	POV	O32-C31-C32-C33
2	C	1303	POV	O32-C31-C32-C33
2	A	1306	POV	O21-C21-C22-C23
2	B	1314	POV	O22-C21-C22-C23
2	A	1317	POV	O21-C21-C22-C23
2	C	1315	POV	C34-C35-C36-C37
2	D	1303	POV	O21-C21-C22-C23
2	A	1315	POV	O22-C21-C22-C23
2	A	1305	POV	O31-C31-C32-C33
2	C	1306	POV	O31-C31-C32-C33
2	D	1308	POV	O31-C31-C32-C33

There are no ring outliers.

49 monomers are involved in 90 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1301	POV	5	0

*Continued on next page...*

*Continued from previous page...*

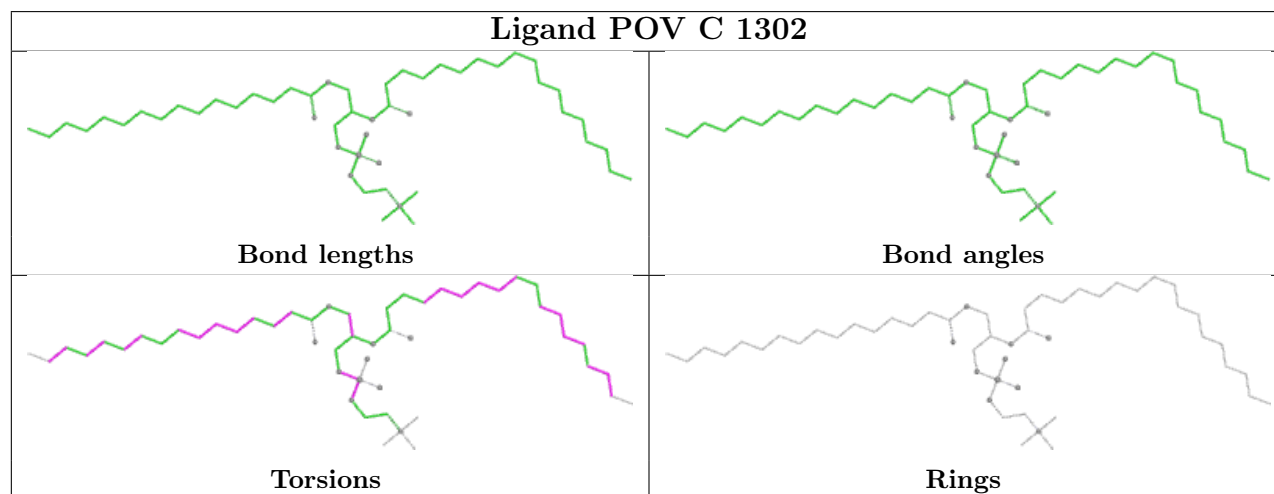
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1313	ZY8	1	0
2	B	1305	POV	2	0
2	C	1306	POV	2	0
2	B	1301	POV	1	0
2	D	1313	POV	3	0
2	A	1310	POV	4	0
2	B	1314	POV	5	0
2	A	1303	POV	1	0
2	B	1307	POV	2	0
2	A	1306	POV	2	0
2	B	1310	POV	2	0
2	C	1308	POV	2	0
2	C	1307	POV	2	0
2	A	1308	POV	2	0
2	C	1303	POV	1	0
2	C	1304	POV	1	0
2	B	1309	POV	3	0
2	C	1301	POV	2	0
2	B	1306	POV	2	0
2	D	1308	POV	2	0
5	D	1316	ZY8	1	0
2	A	1305	POV	2	0
2	D	1305	POV	2	0
2	C	1310	POV	3	0
2	C	1315	POV	5	0
3	D	1307	CLR	1	0
2	B	1303	POV	1	0
3	A	1304	CLR	1	0
3	C	1305	CLR	1	0
2	D	1303	POV	2	0
2	A	1315	POV	5	0
2	D	1312	POV	4	0
2	B	1311	POV	5	0
2	A	1302	POV	1	0
2	D	1309	POV	2	0
2	D	1314	POV	5	0
3	B	1304	CLR	1	0
2	C	1311	POV	2	0
2	C	1312	POV	5	0
5	A	1314	ZY8	1	0
5	C	1314	ZY8	1	0
2	B	1302	POV	1	0

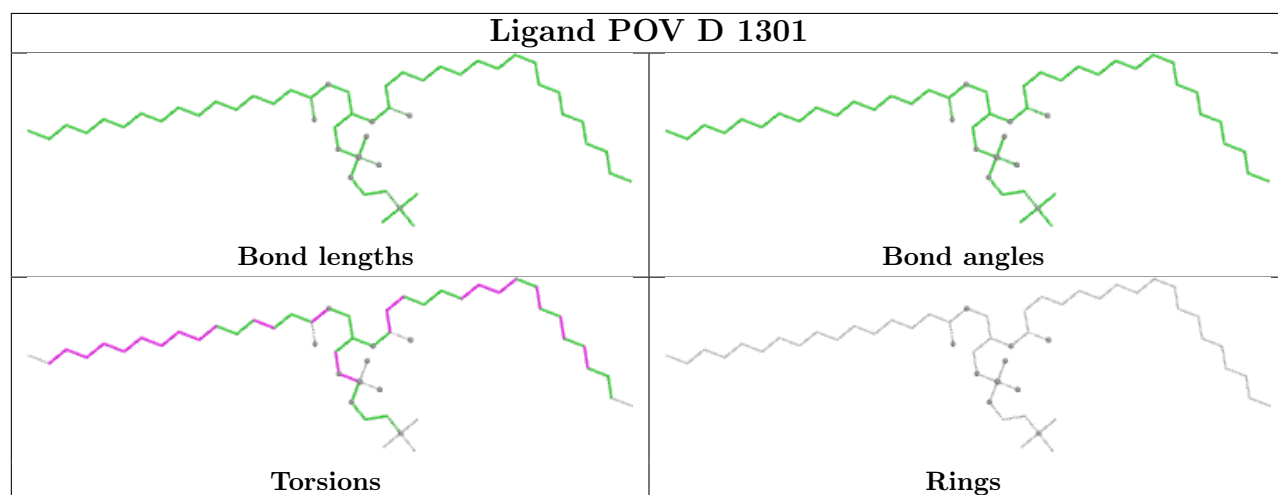
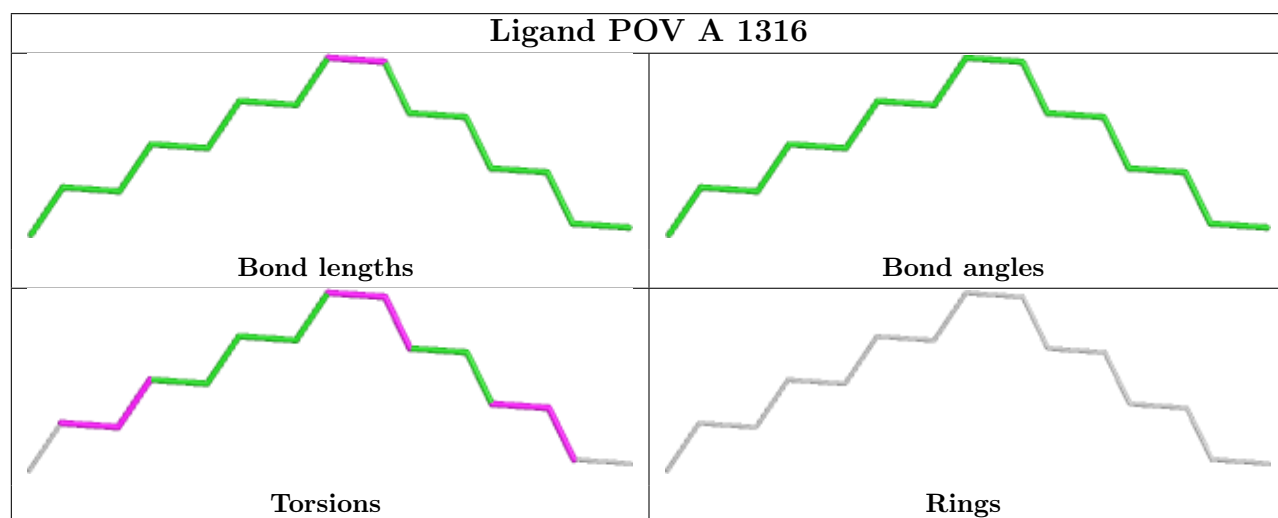
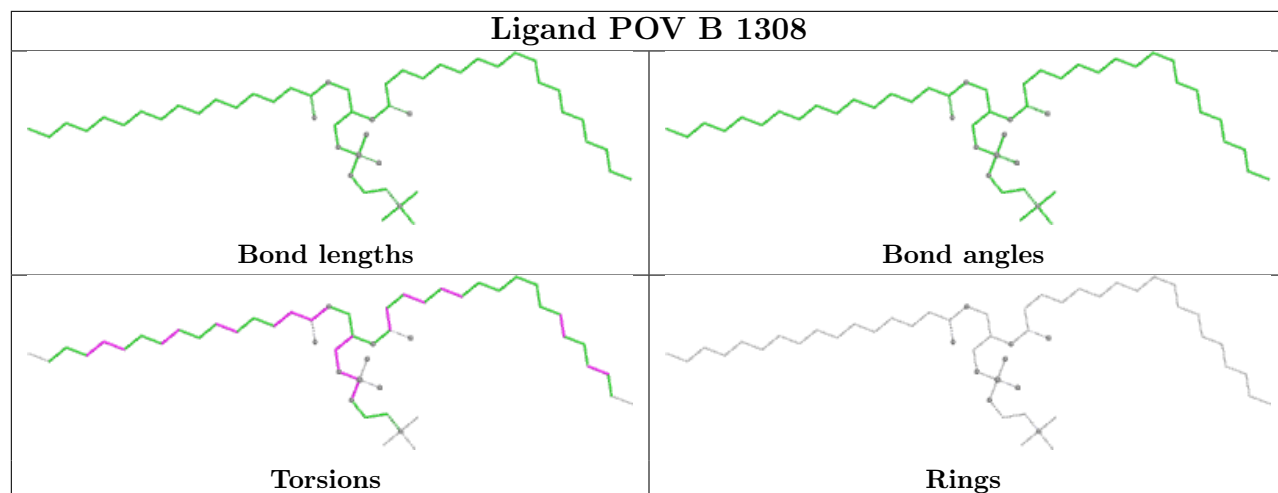
*Continued on next page...*

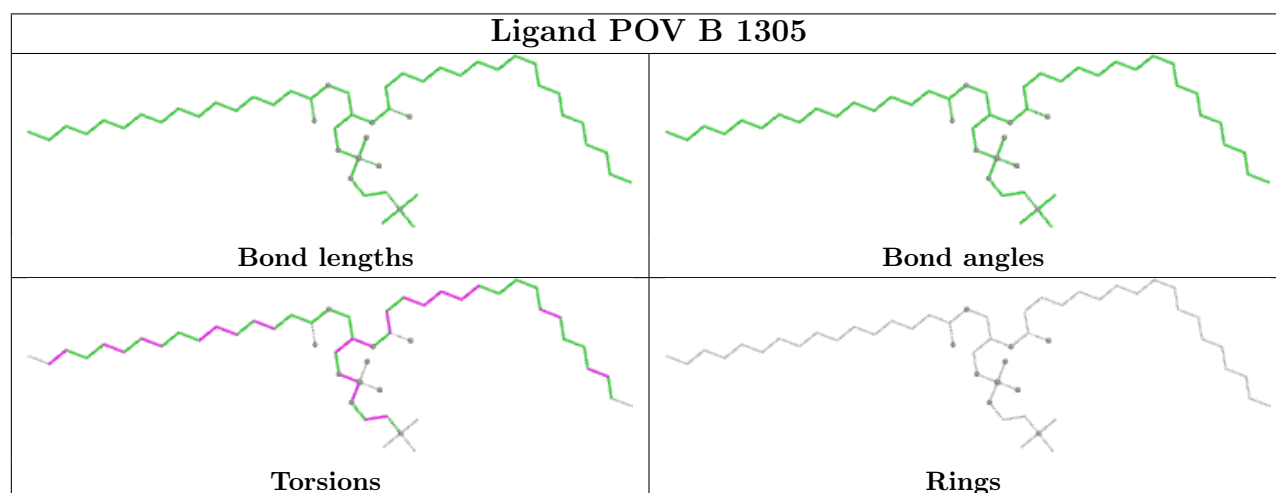
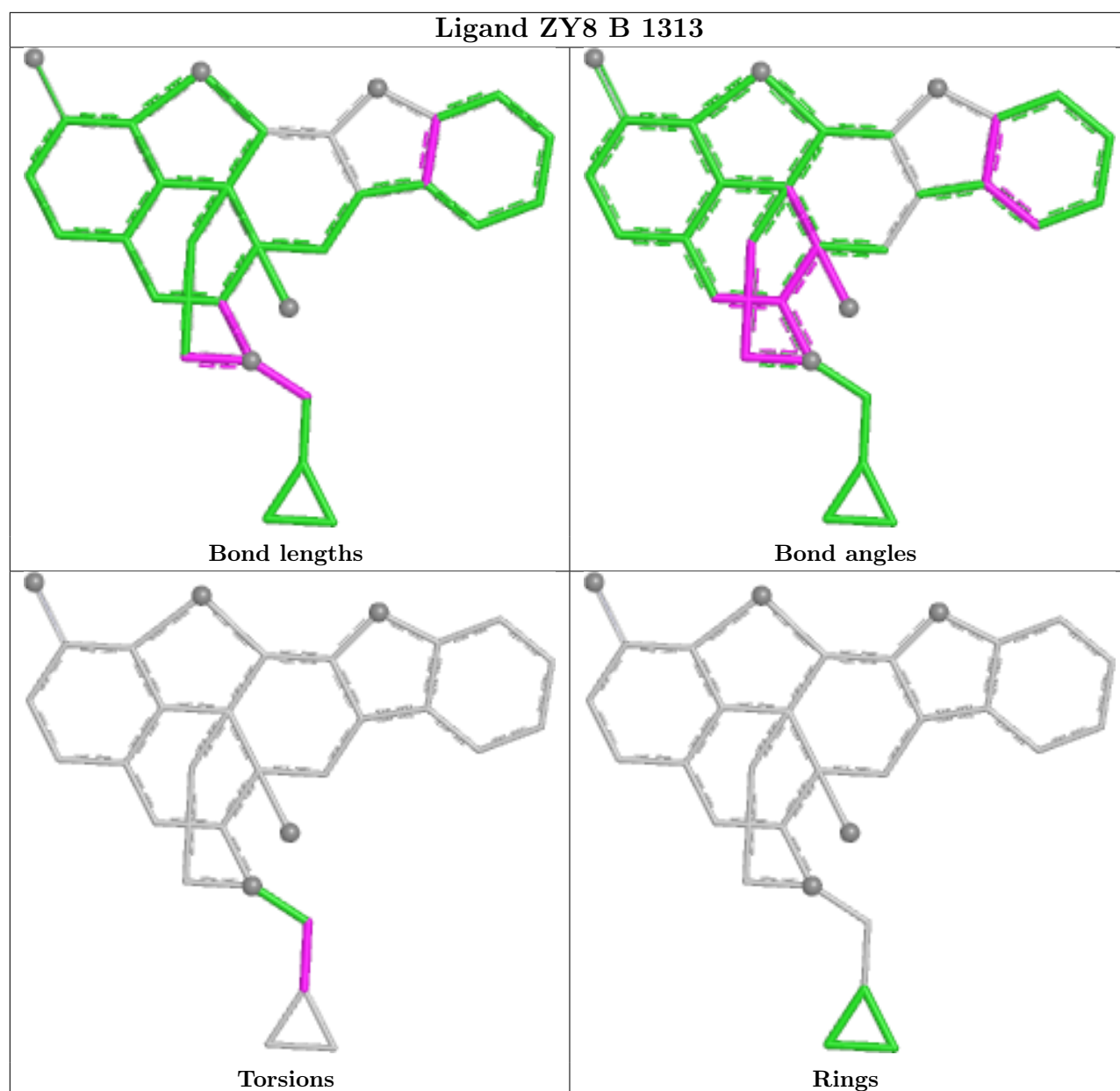
*Continued from previous page...*

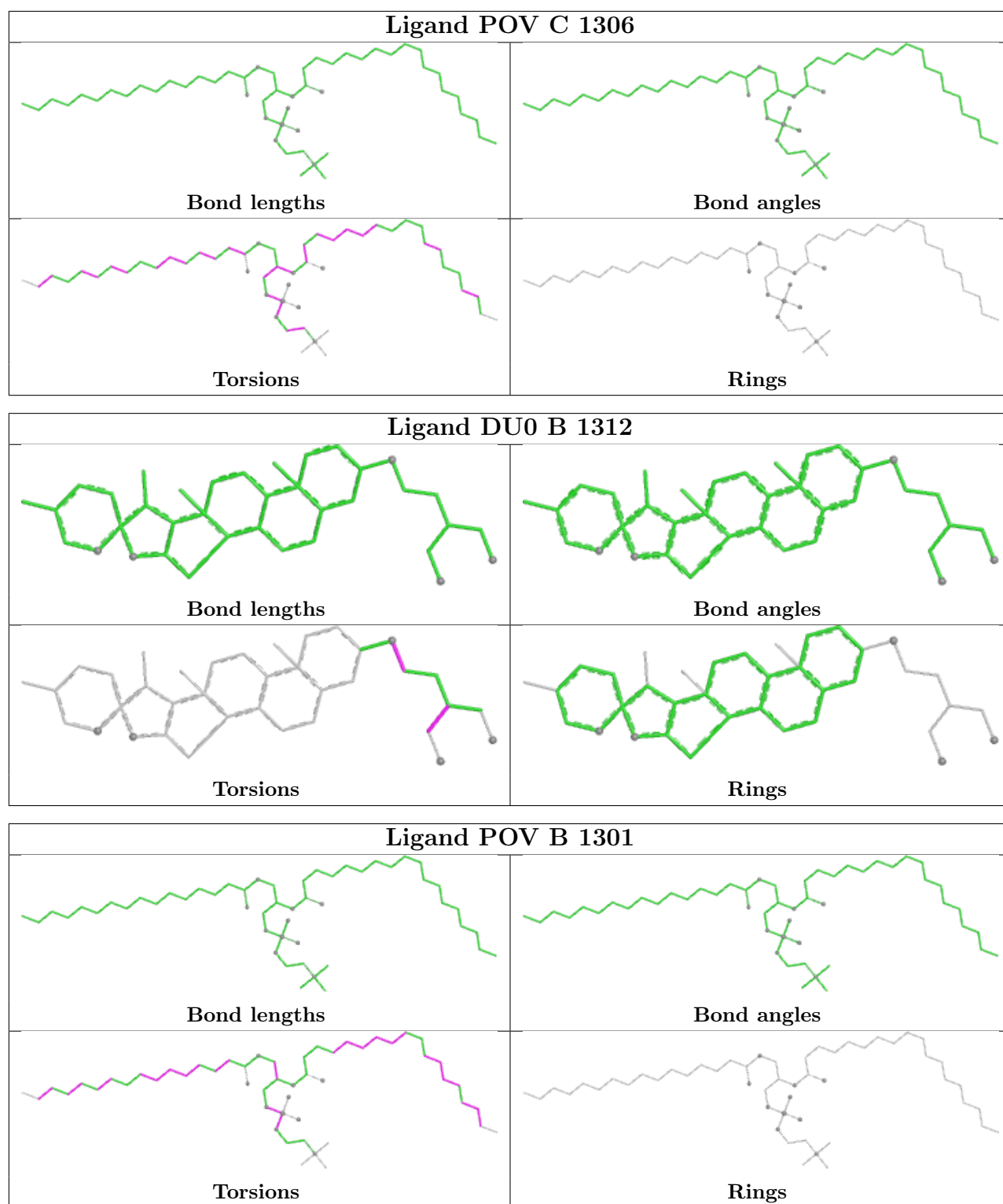
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1310	POV	1	0
2	A	1311	POV	3	0
2	D	1306	POV	1	0
2	A	1312	POV	5	0
2	A	1307	POV	2	0
2	A	1317	POV	2	0

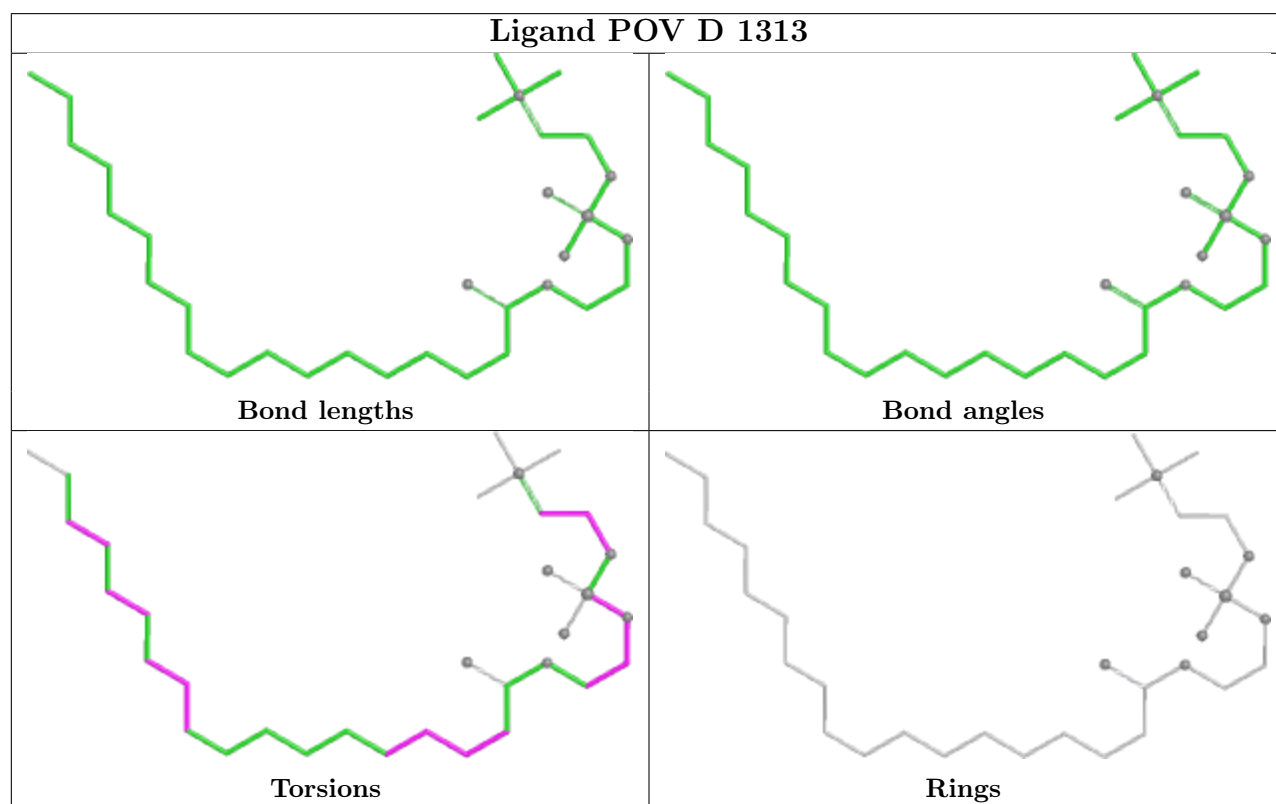
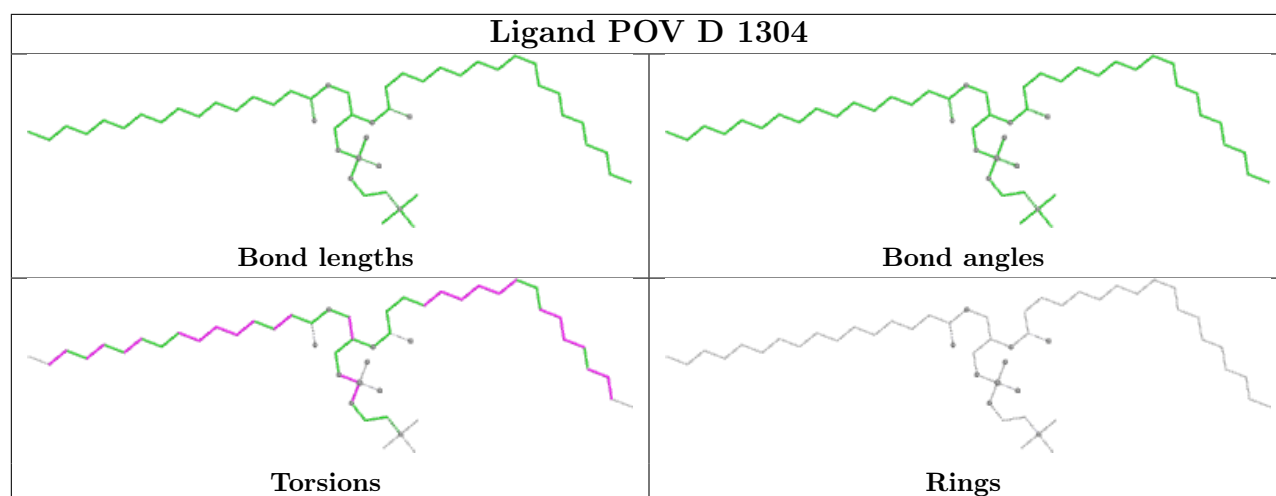
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

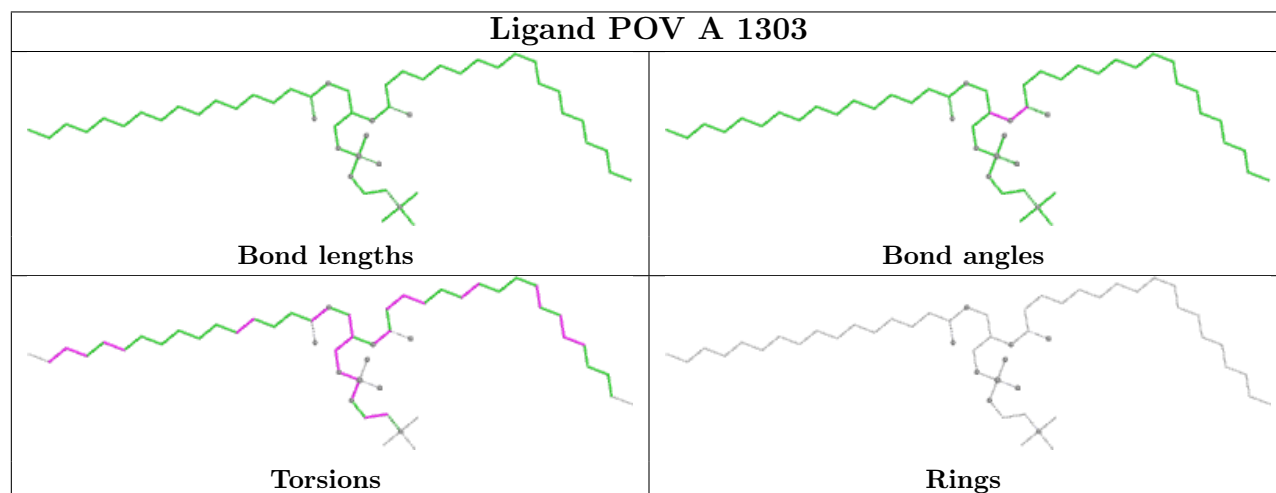
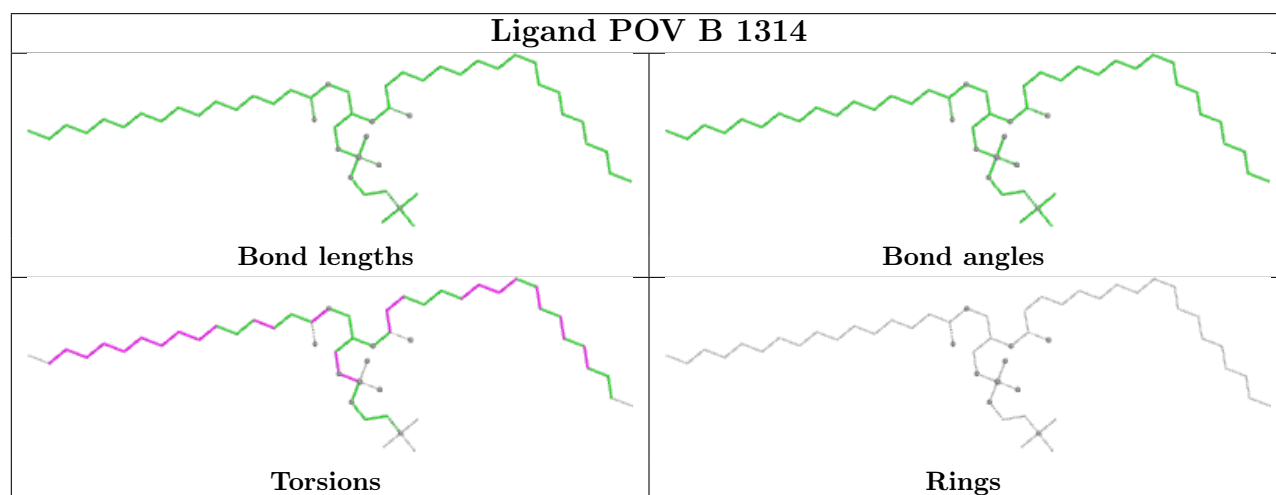
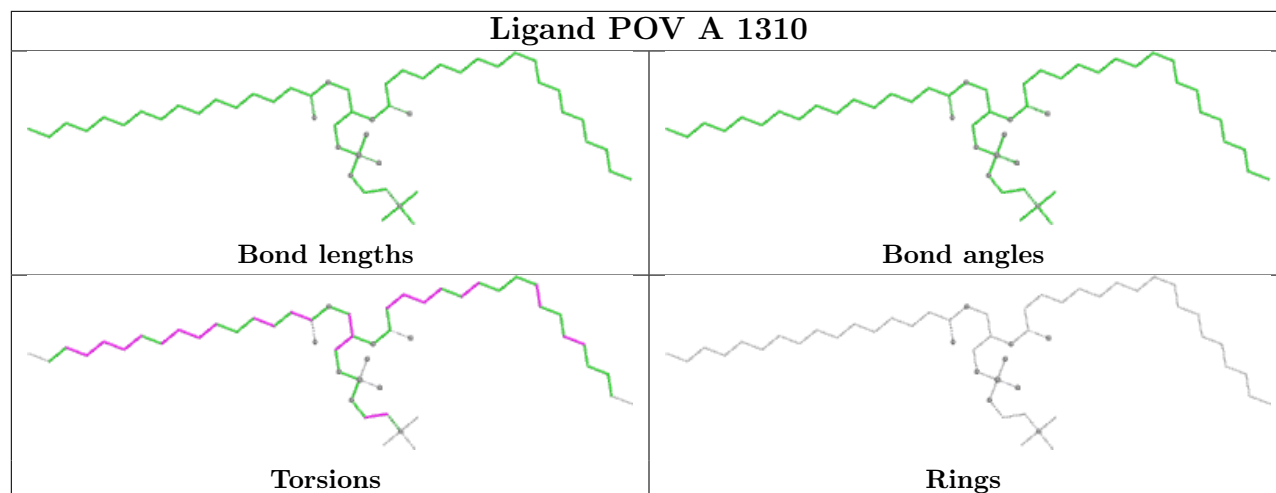


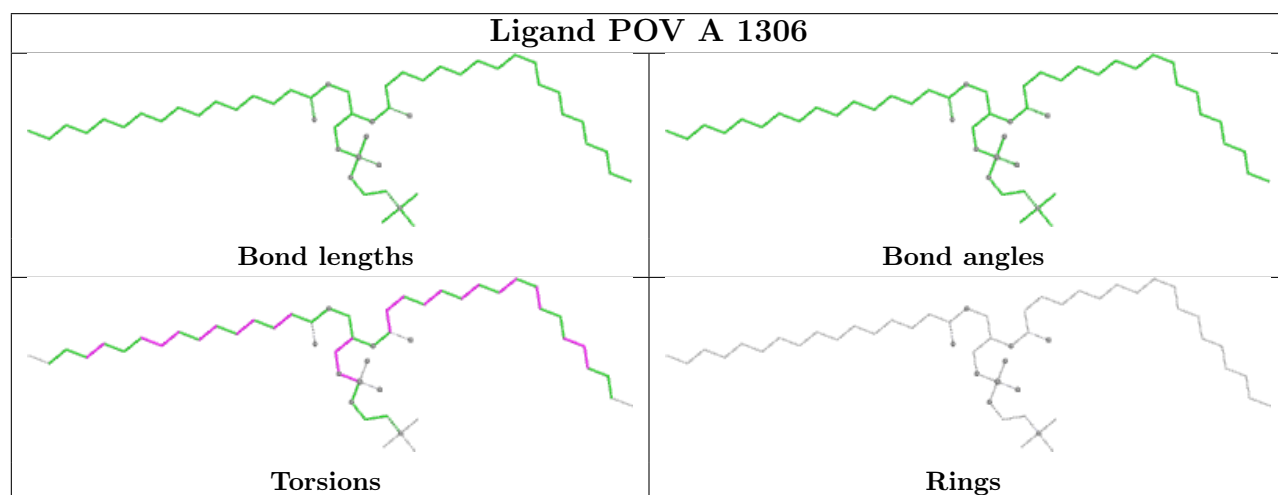
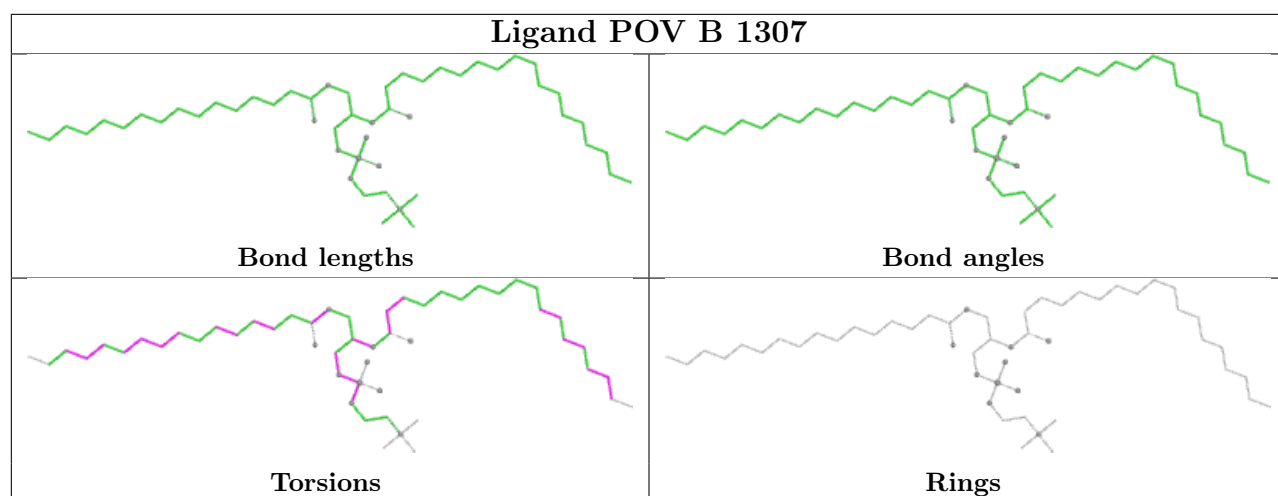


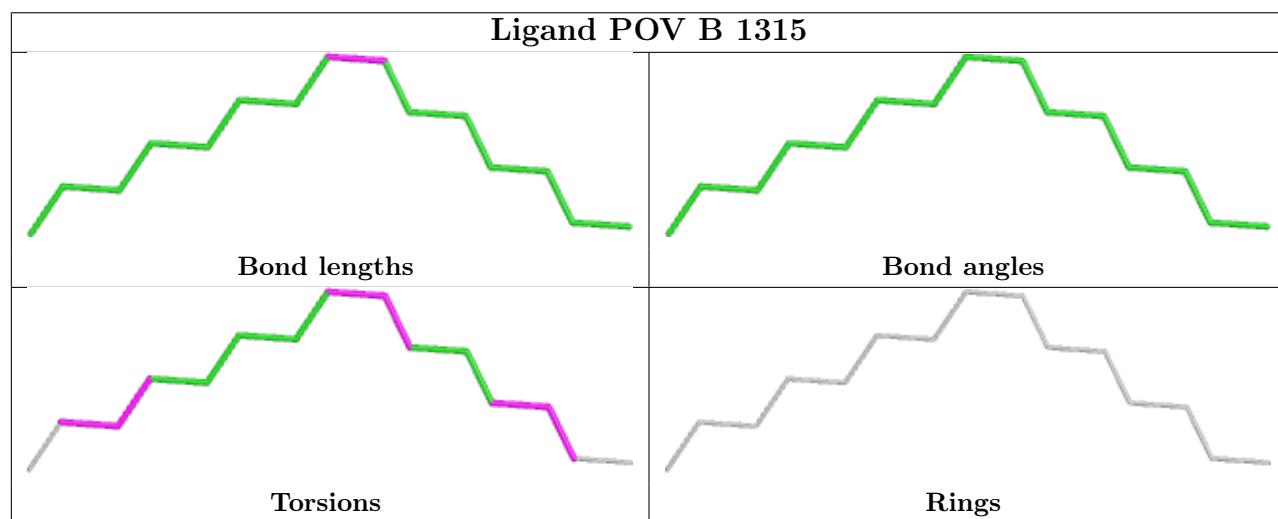
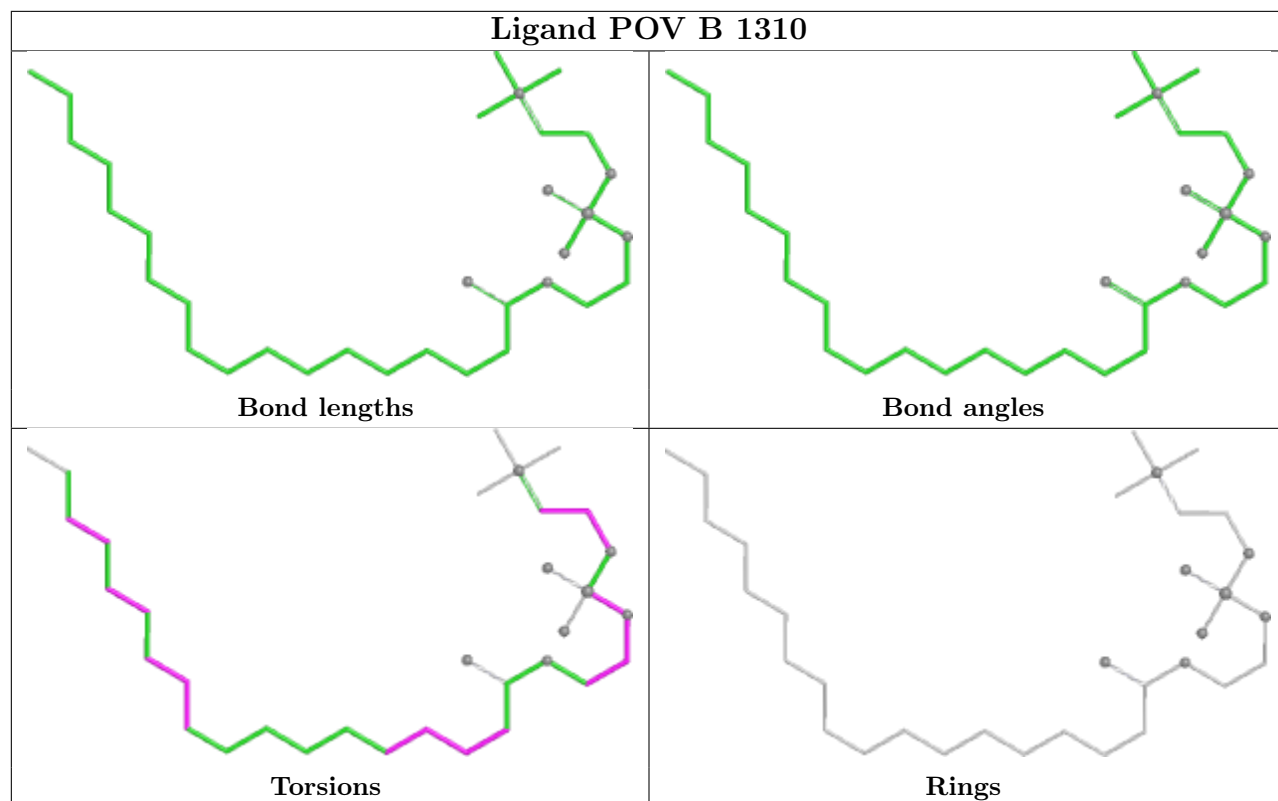


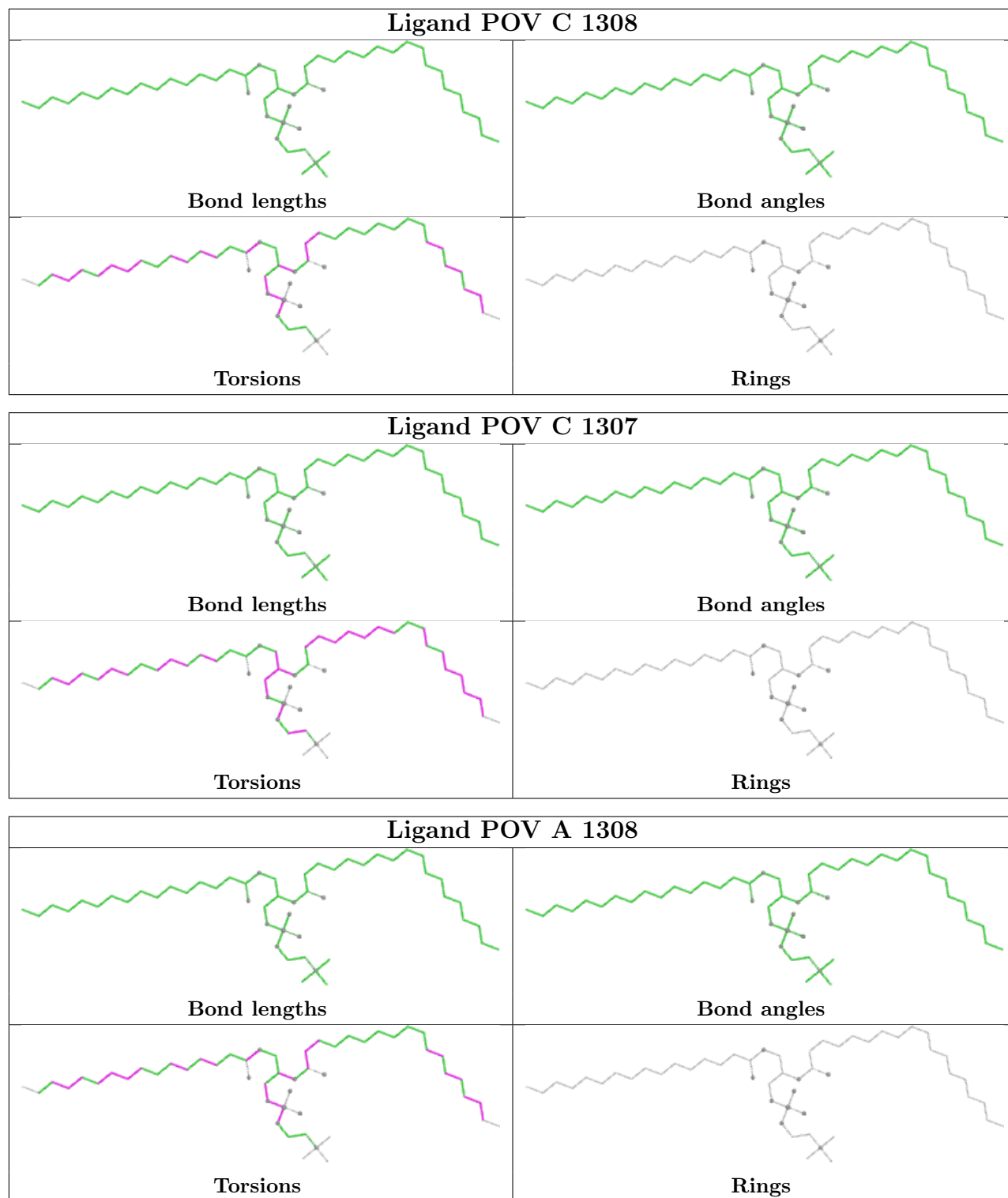


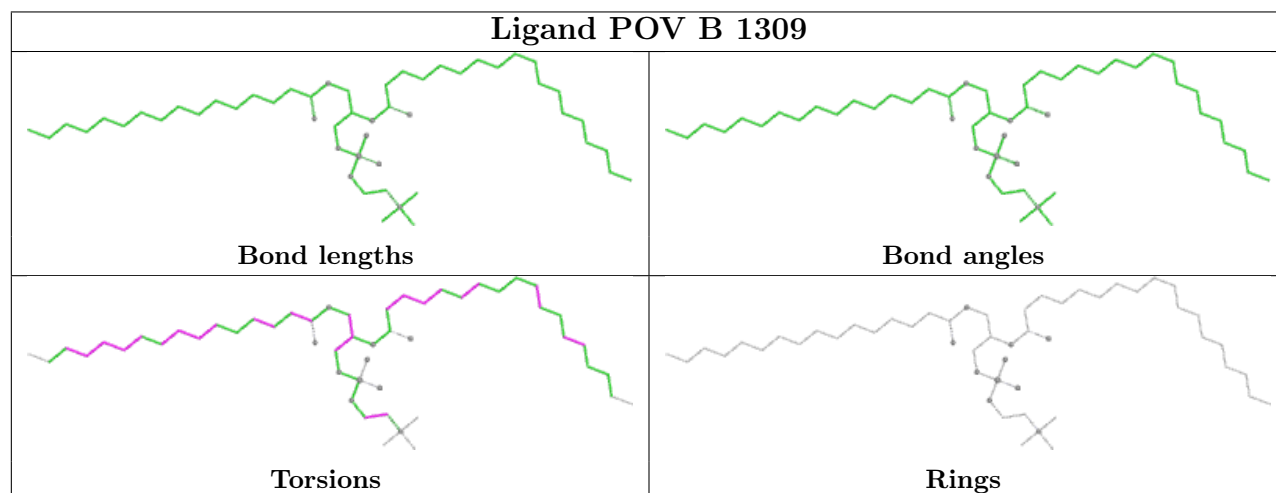
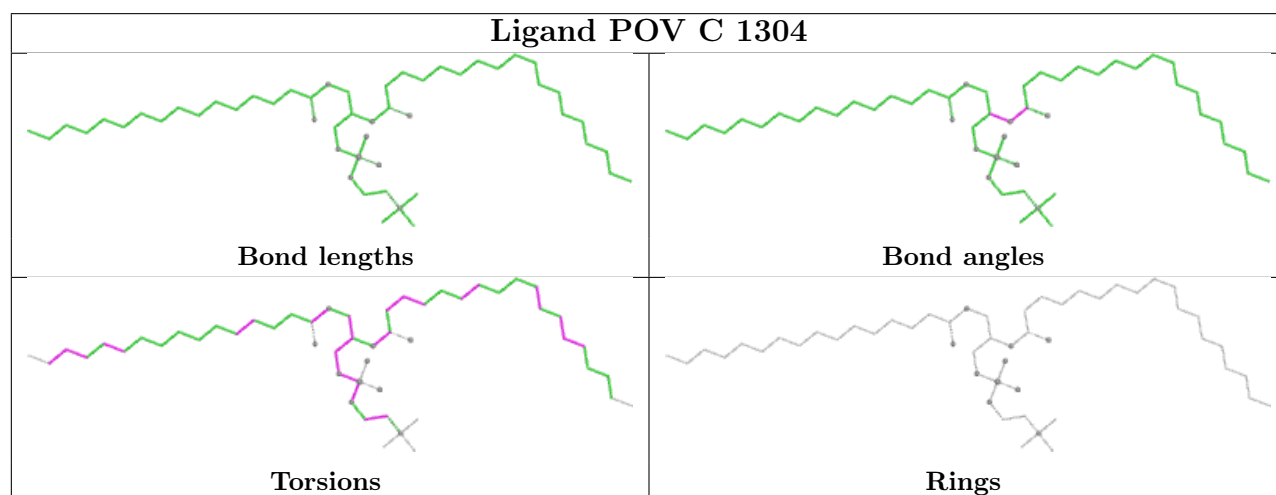
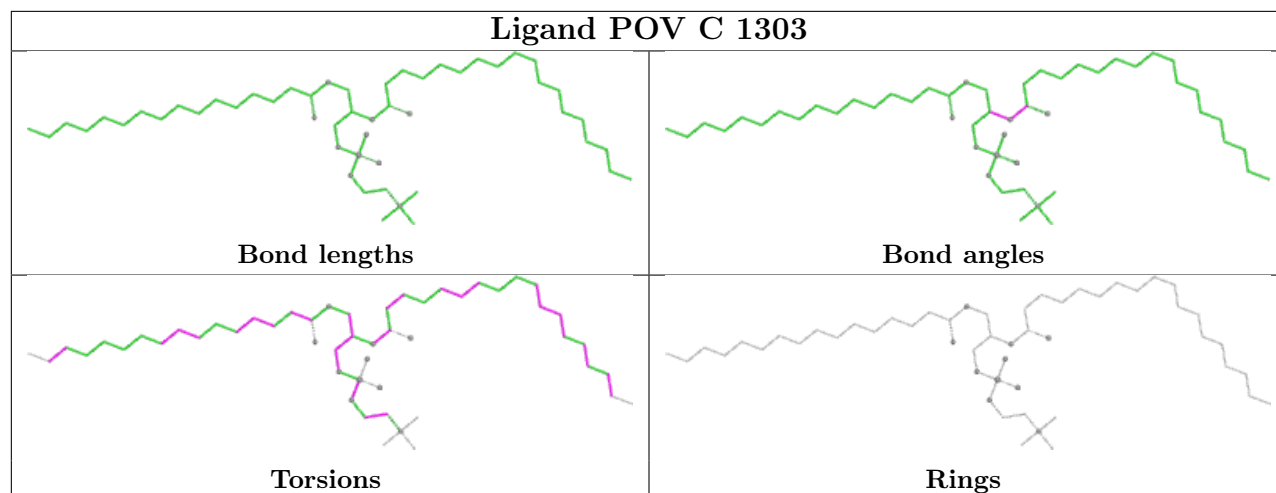


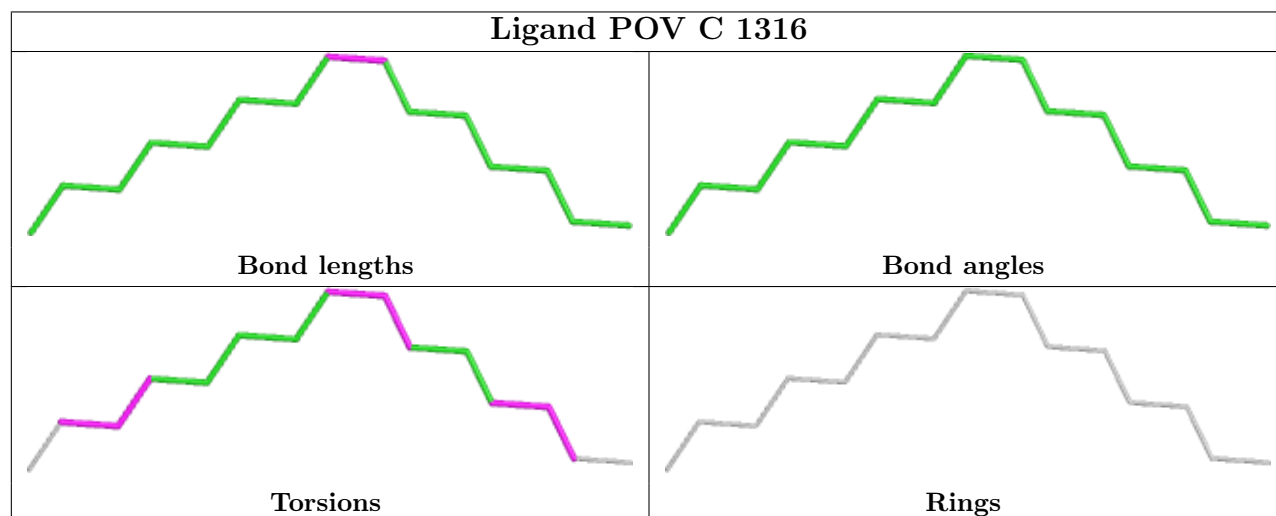
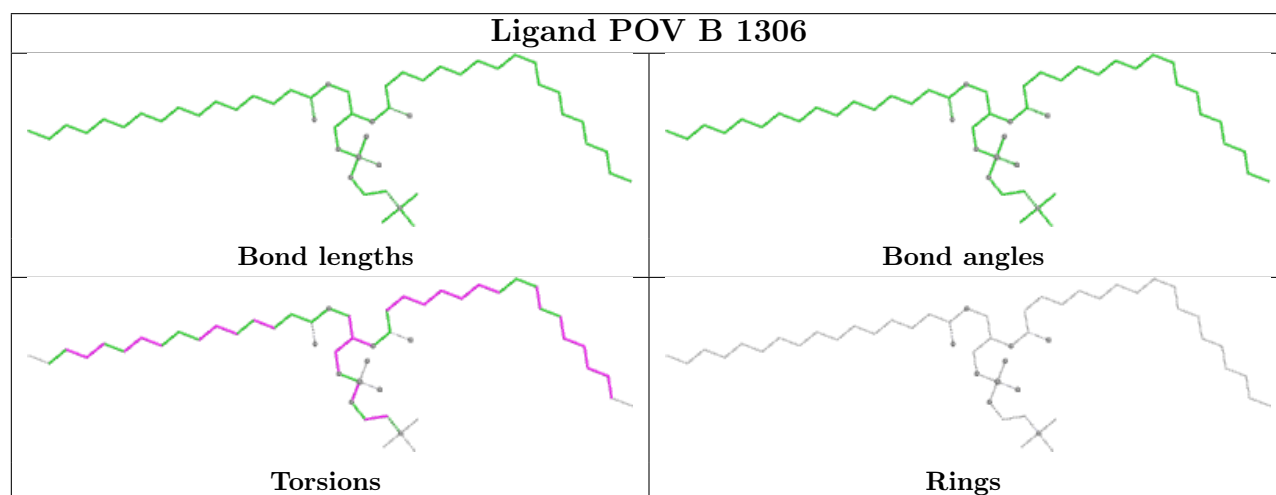
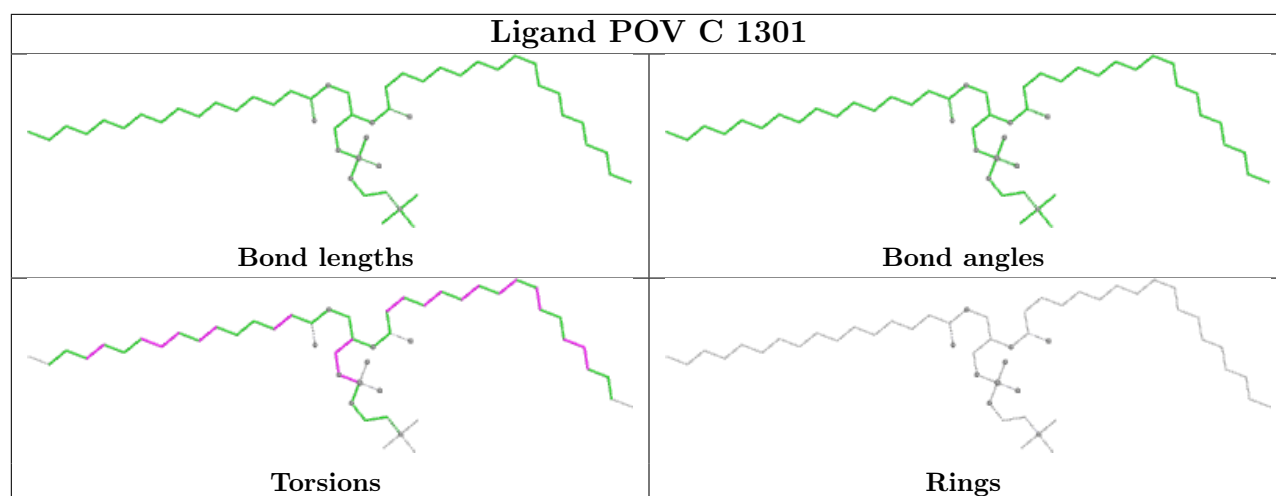


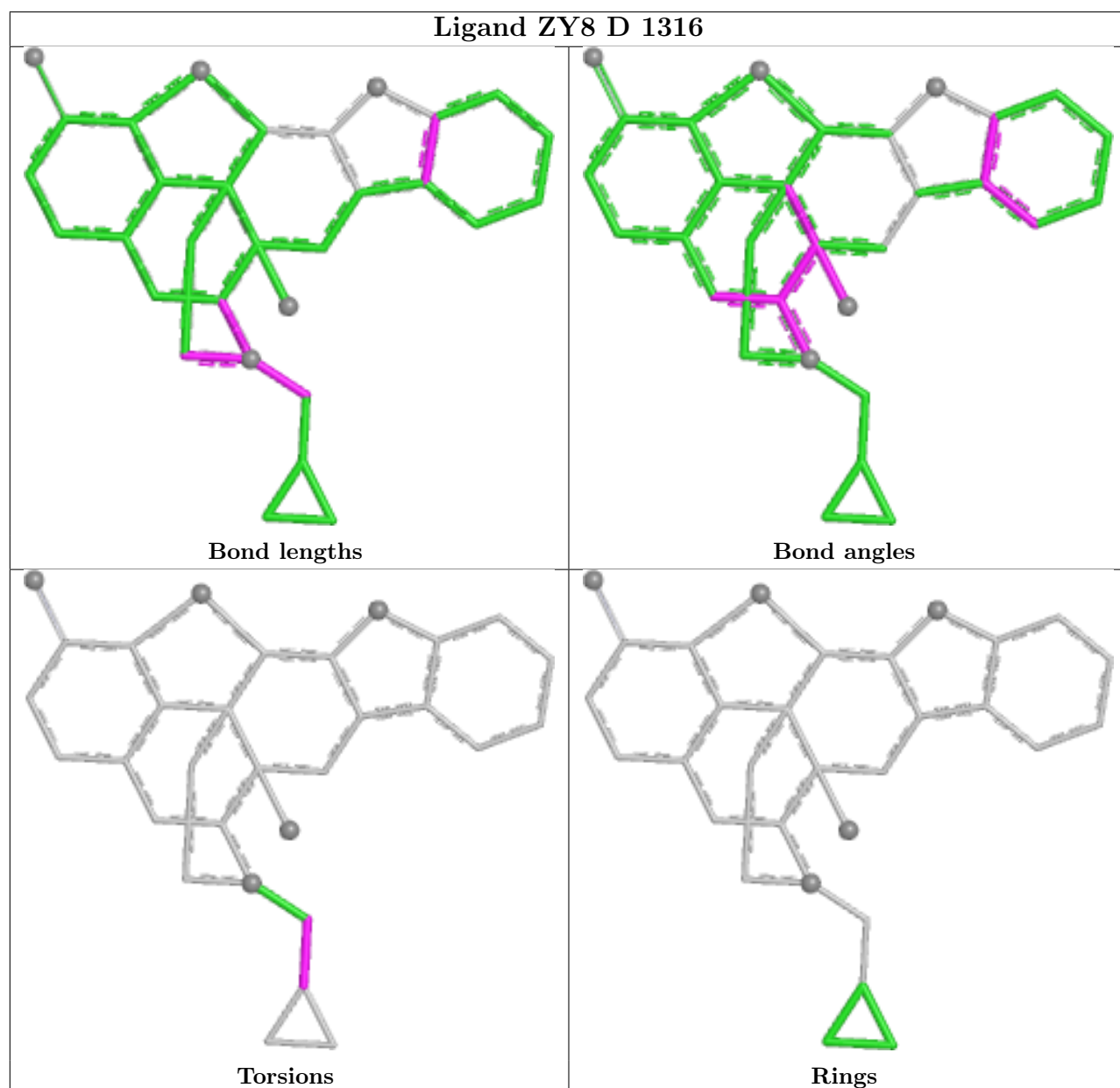
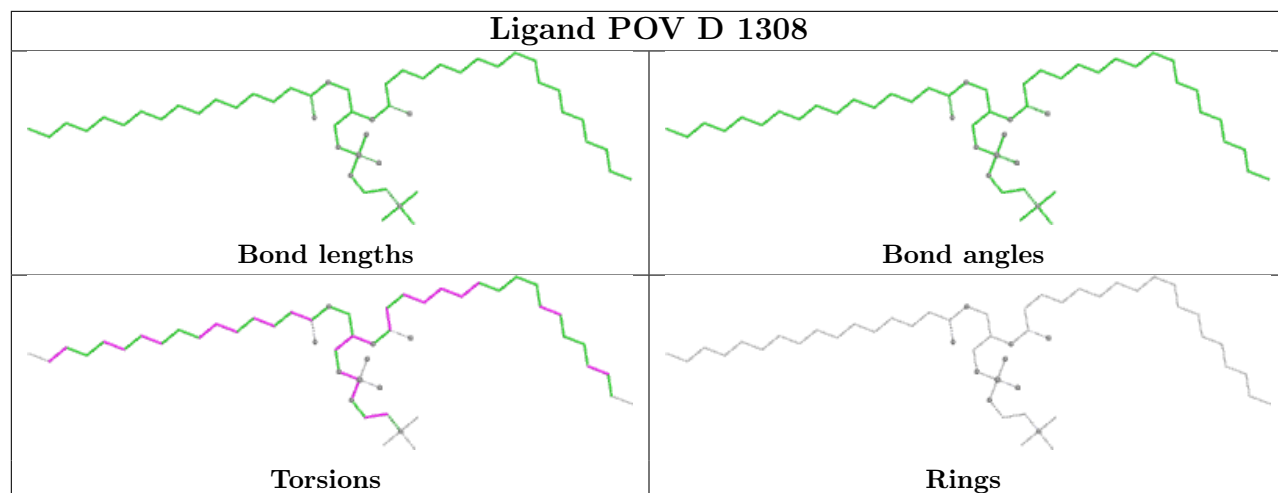


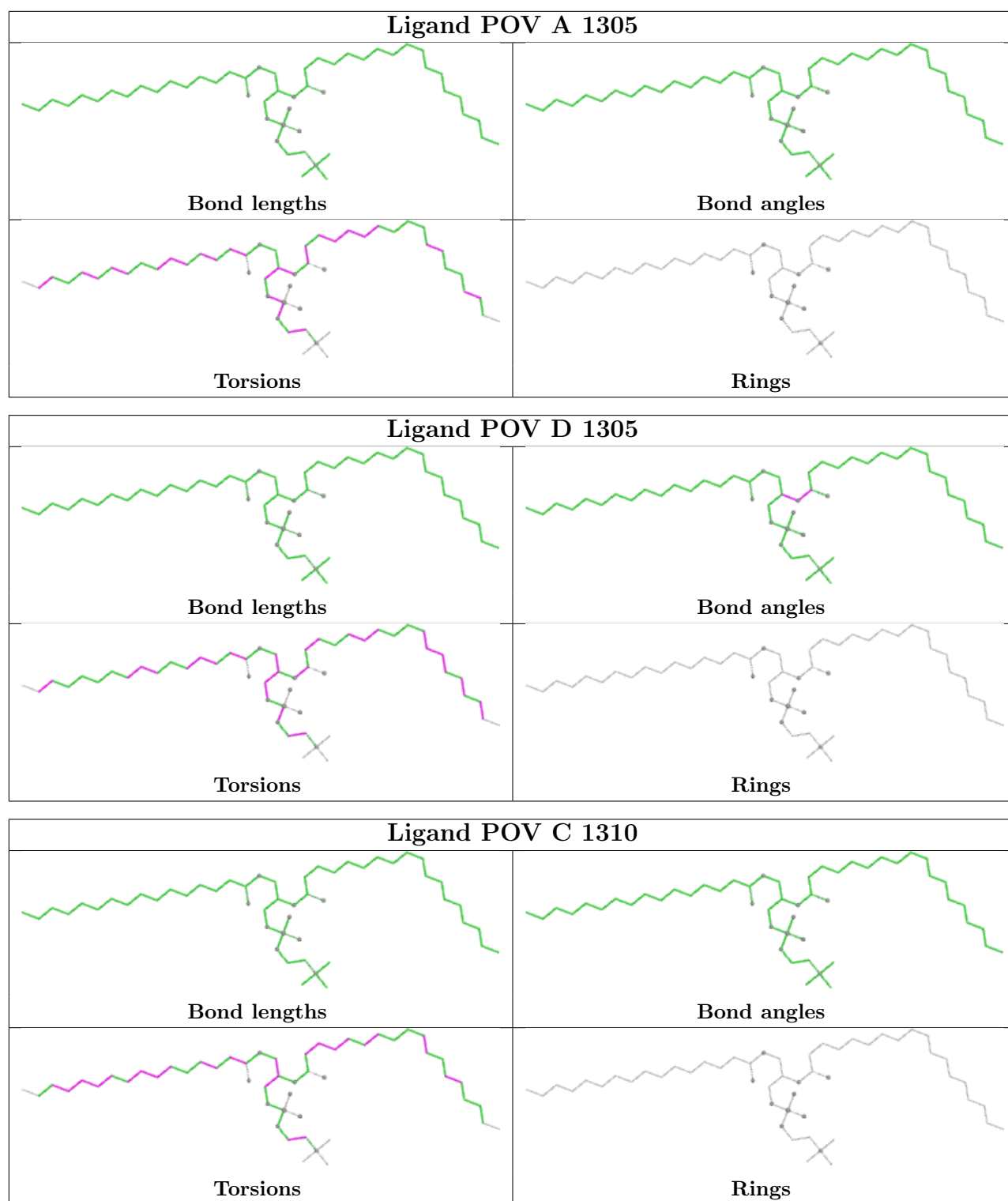


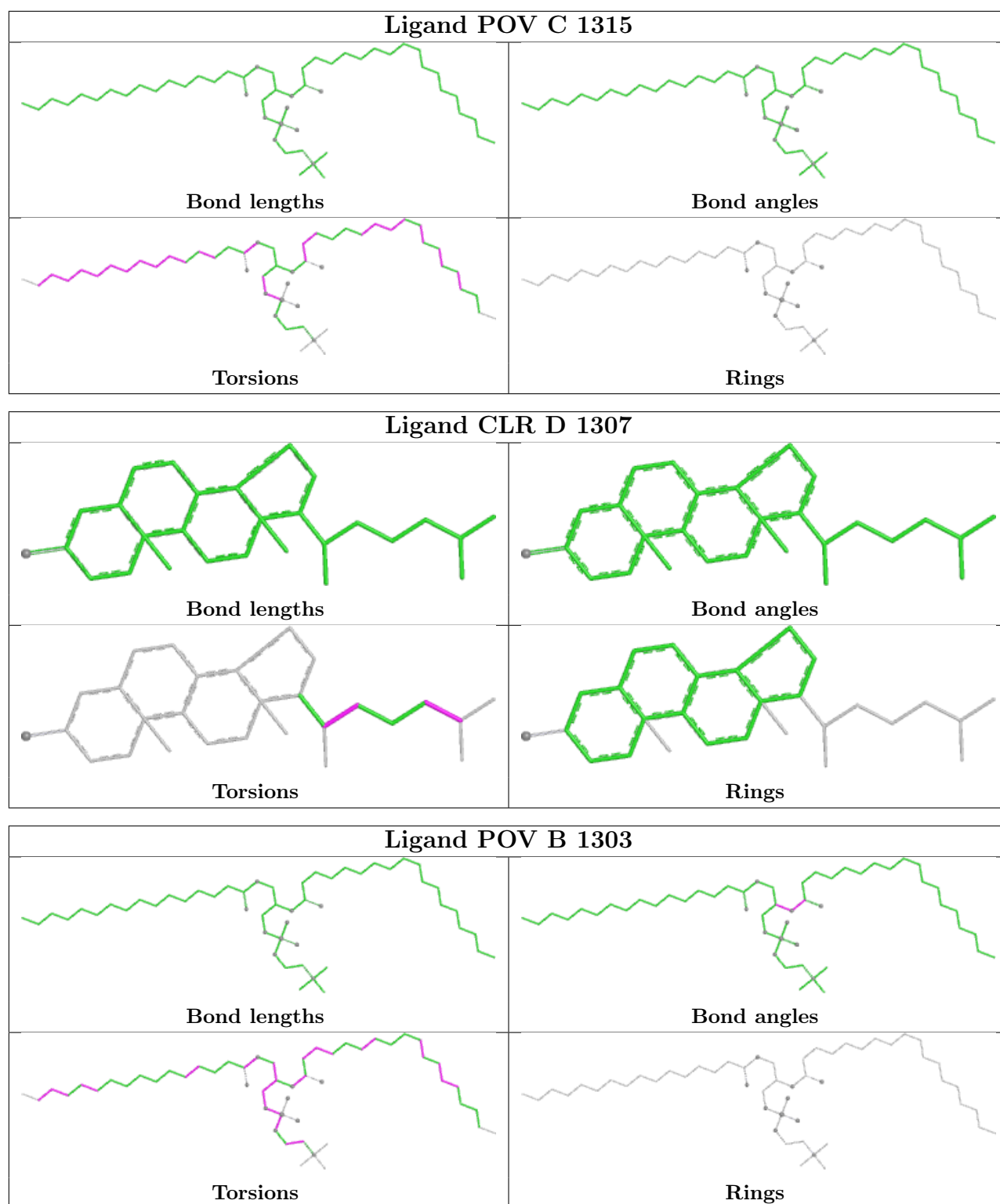


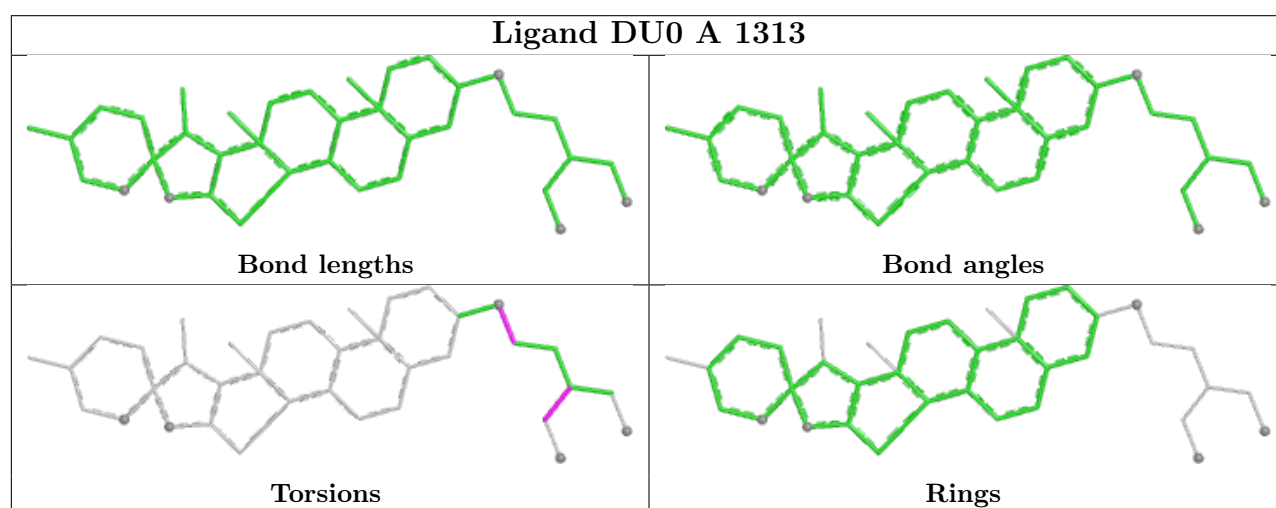
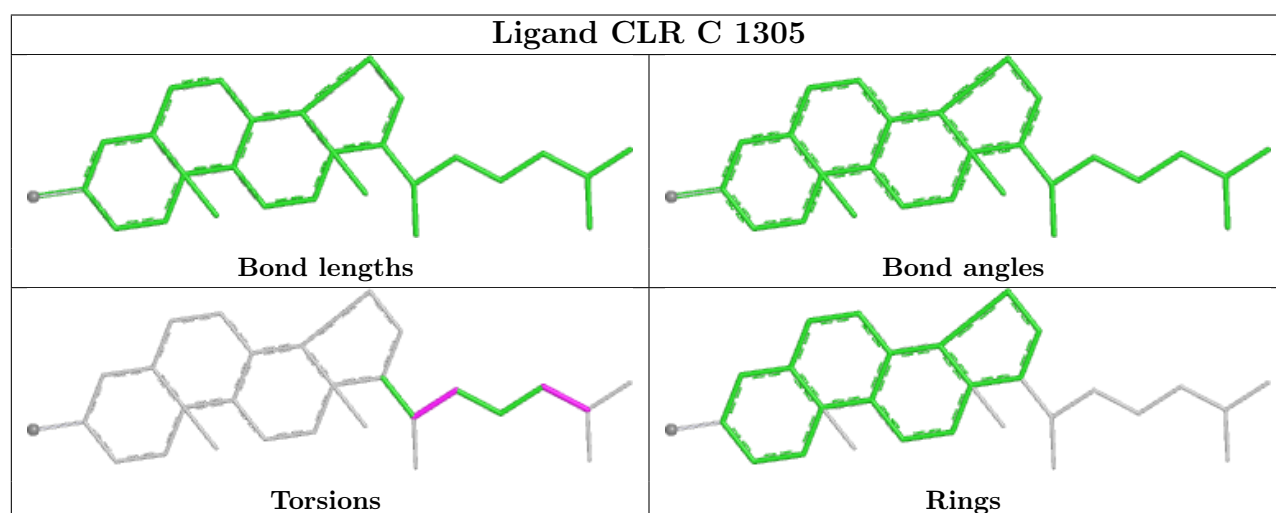
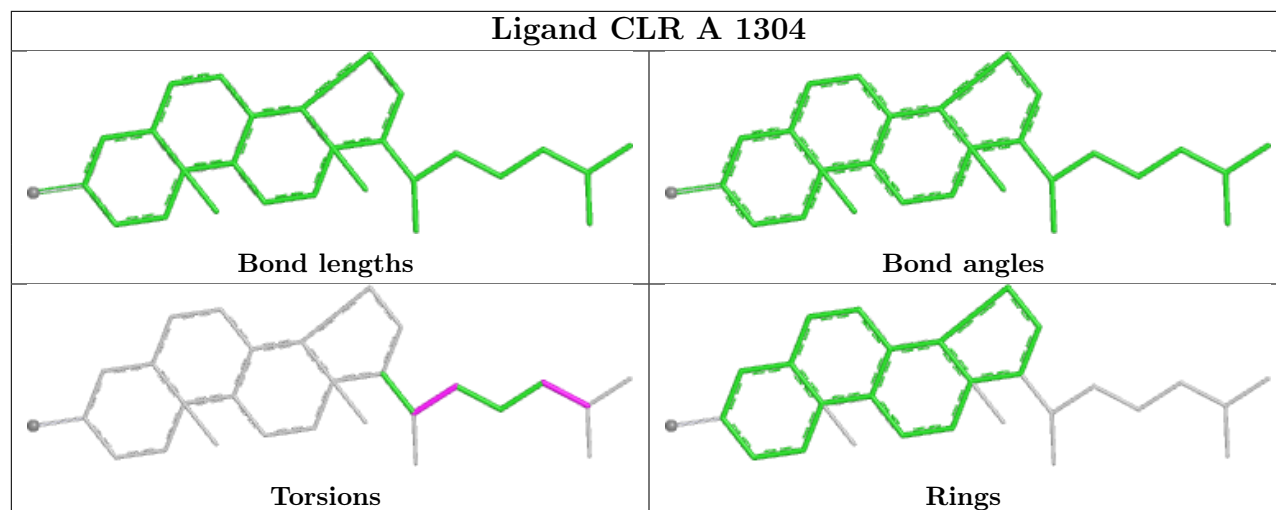


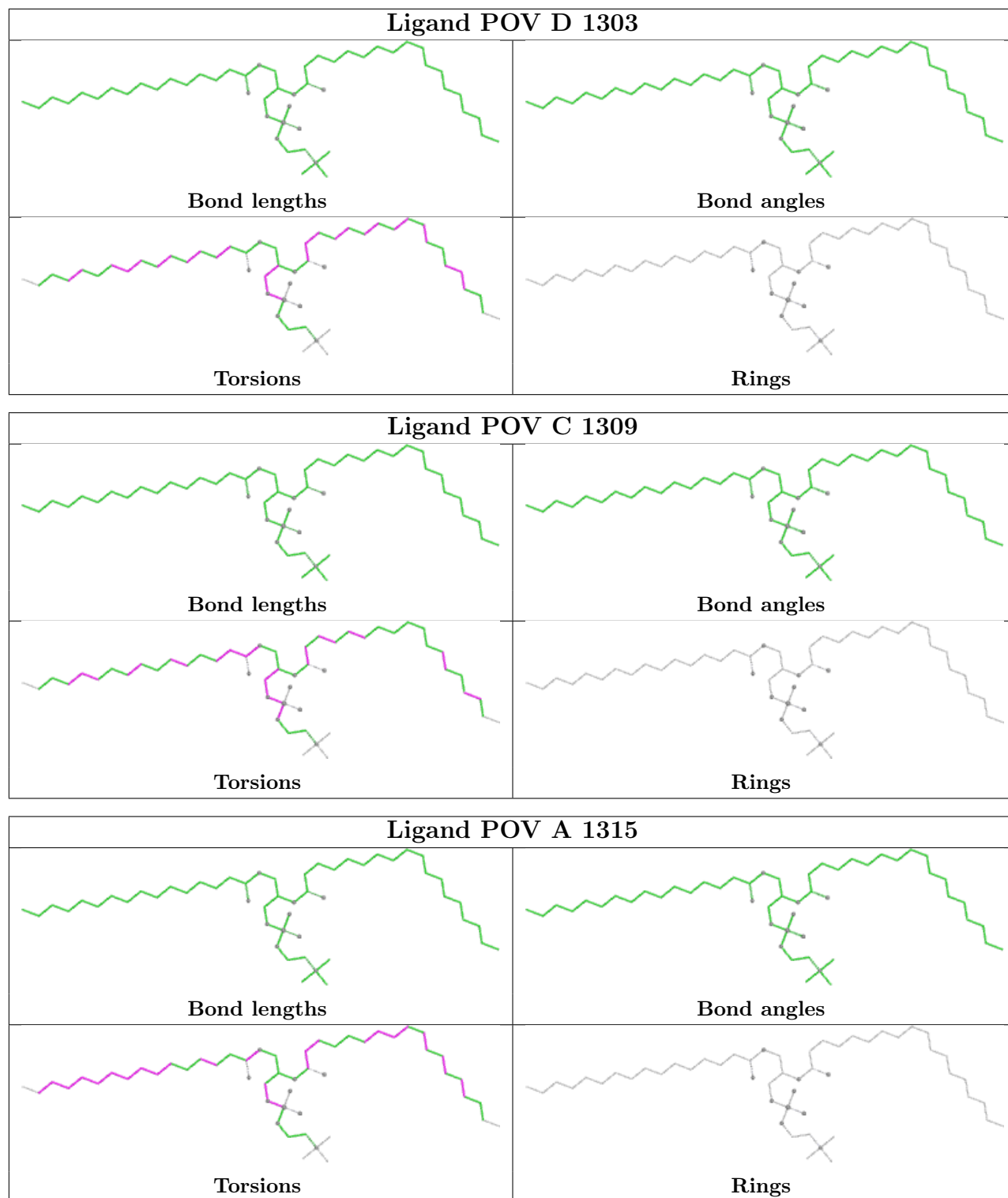


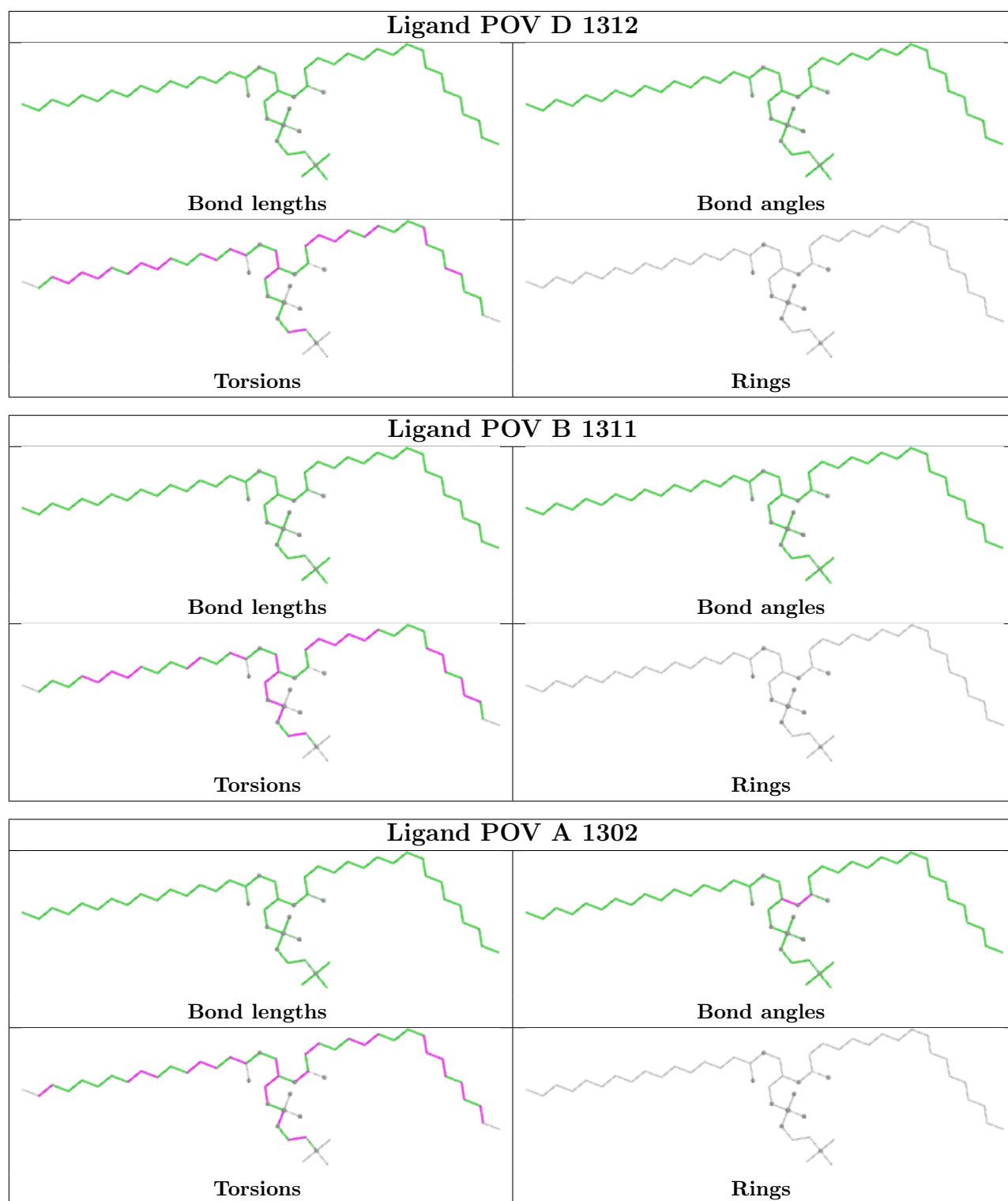


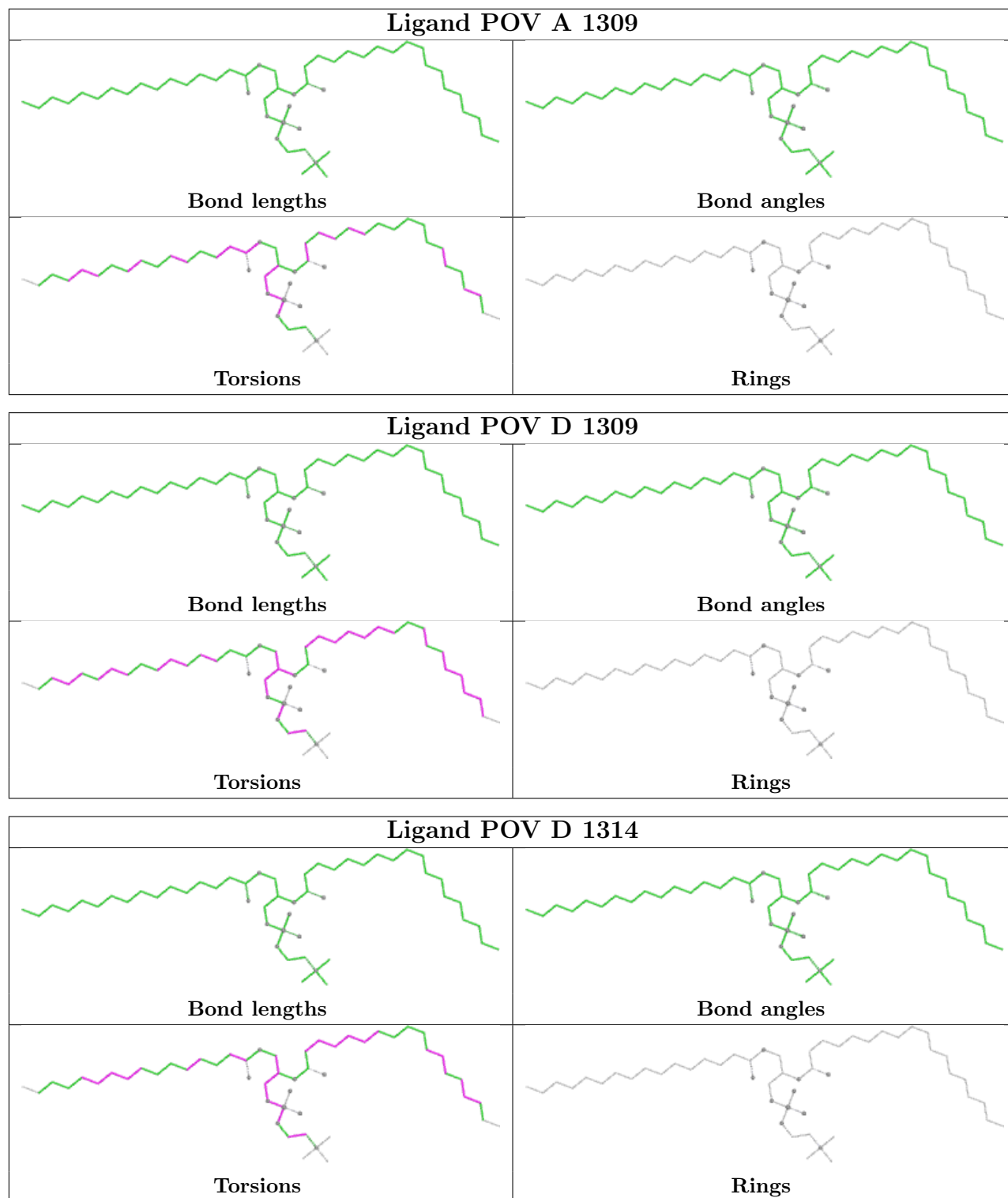


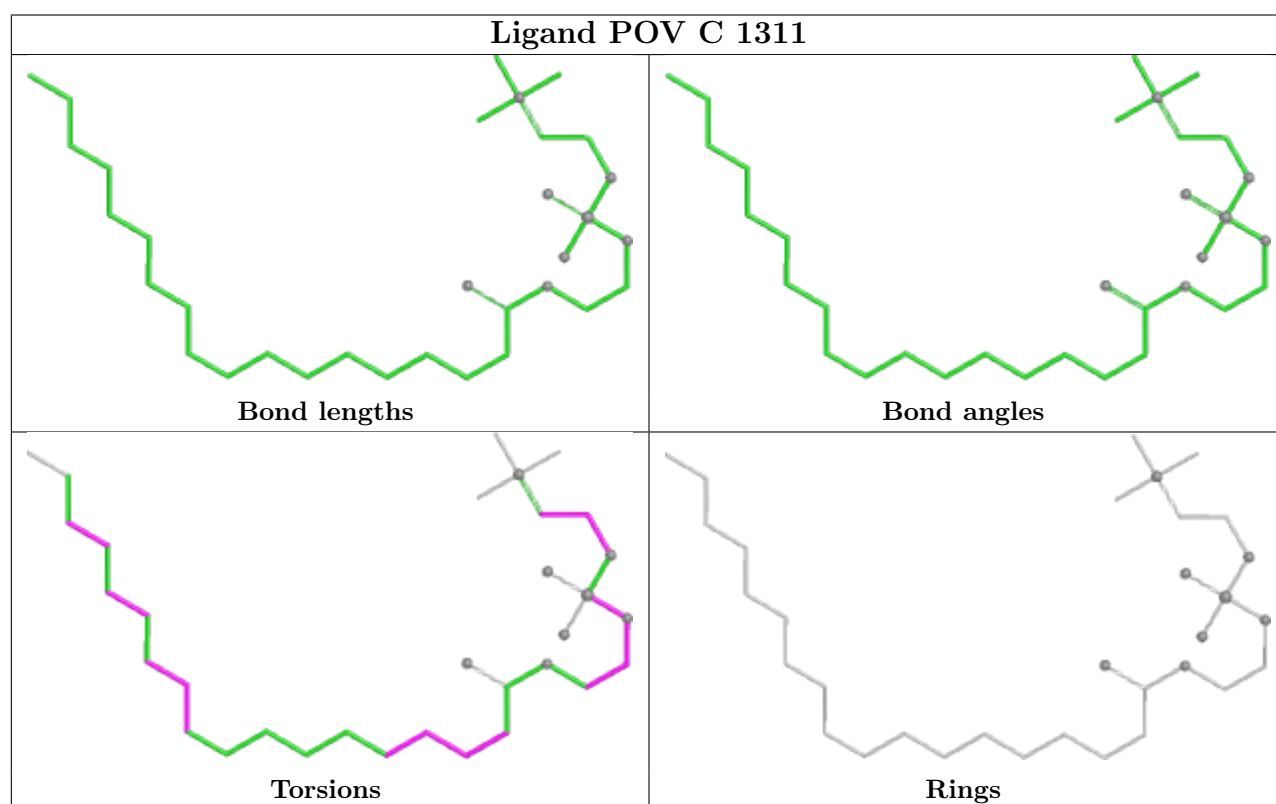
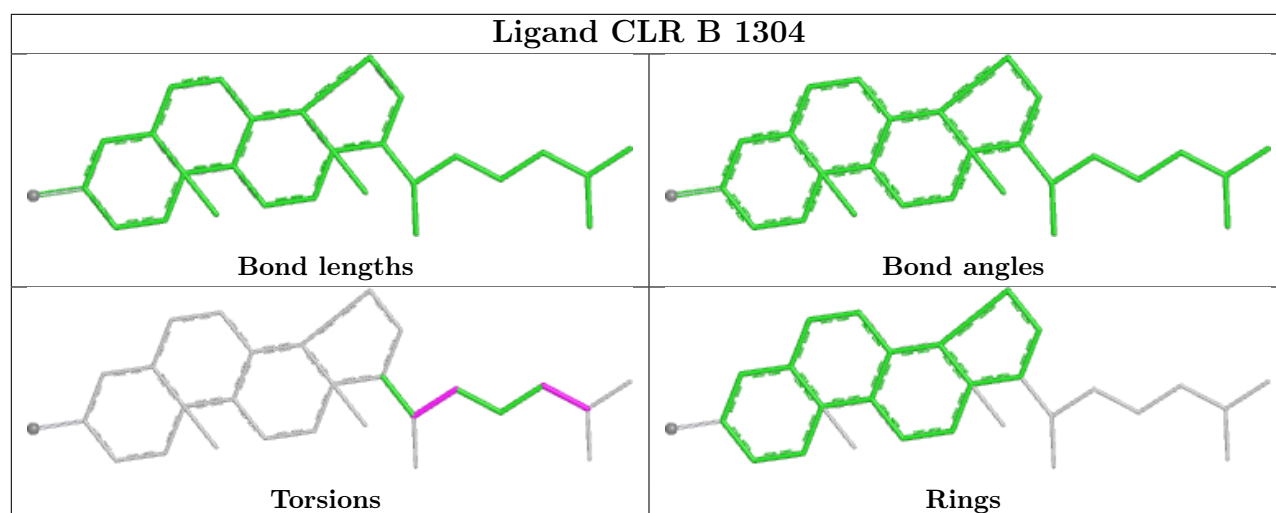


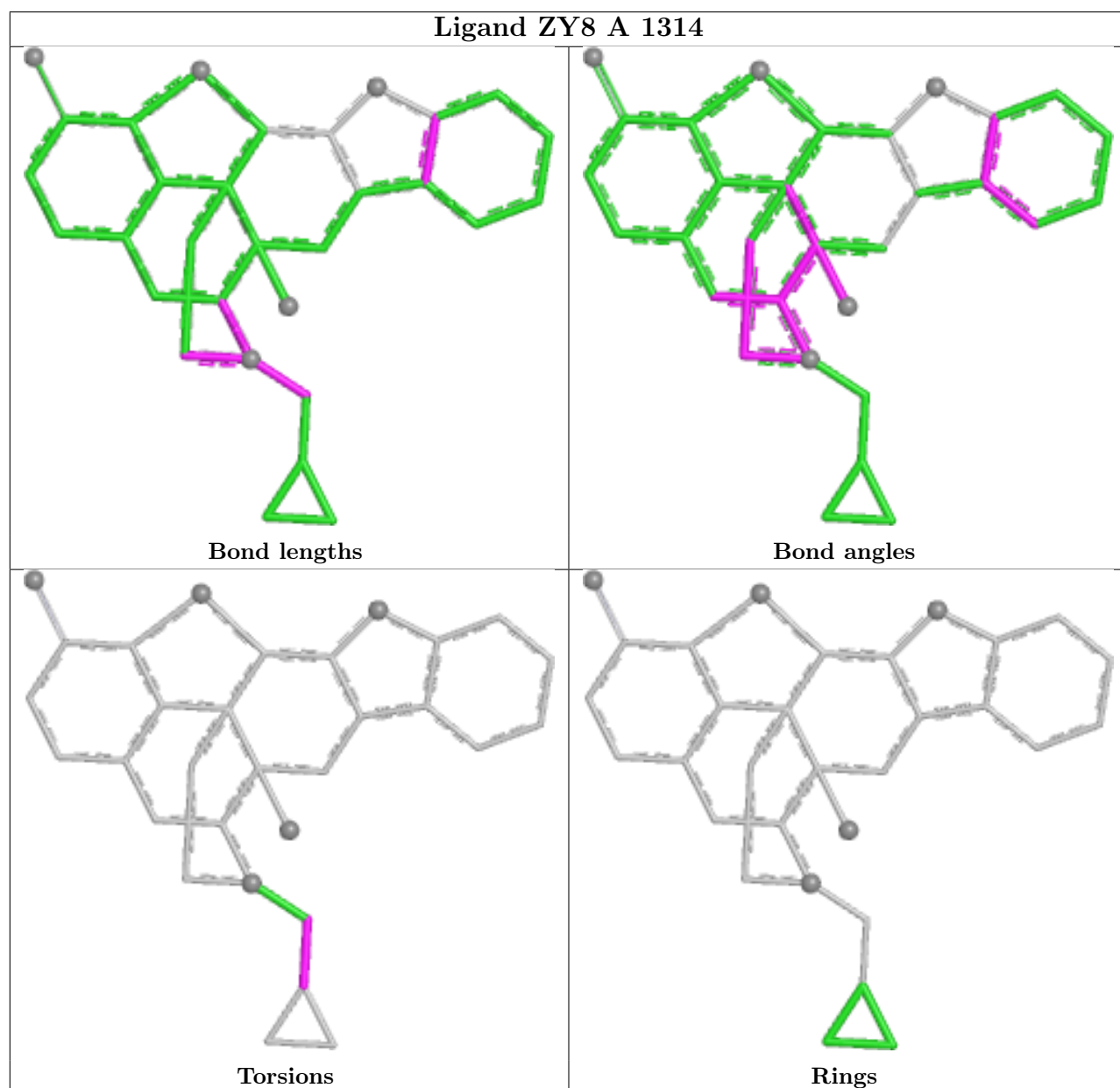
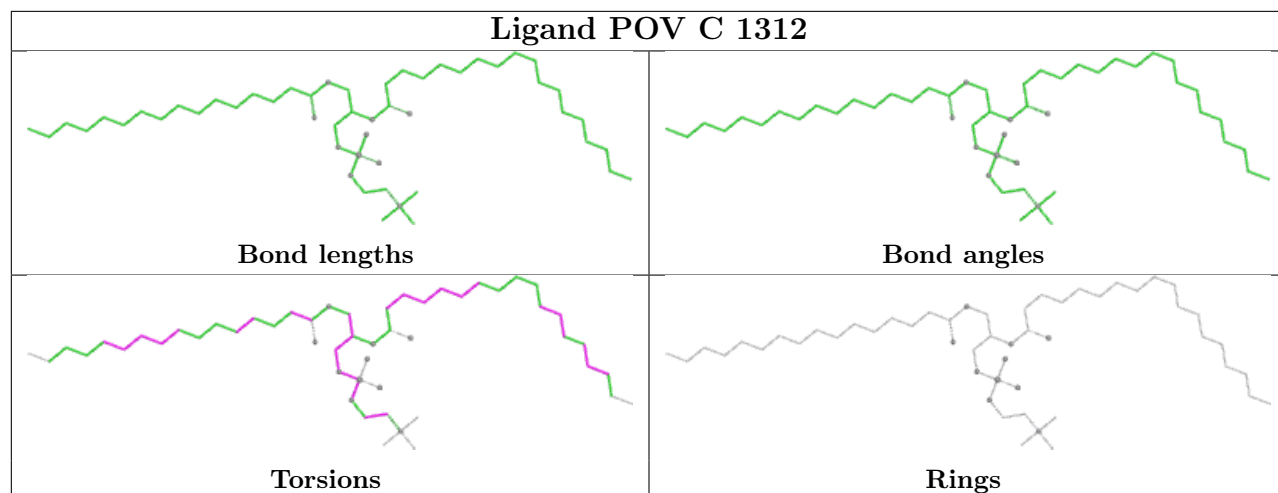


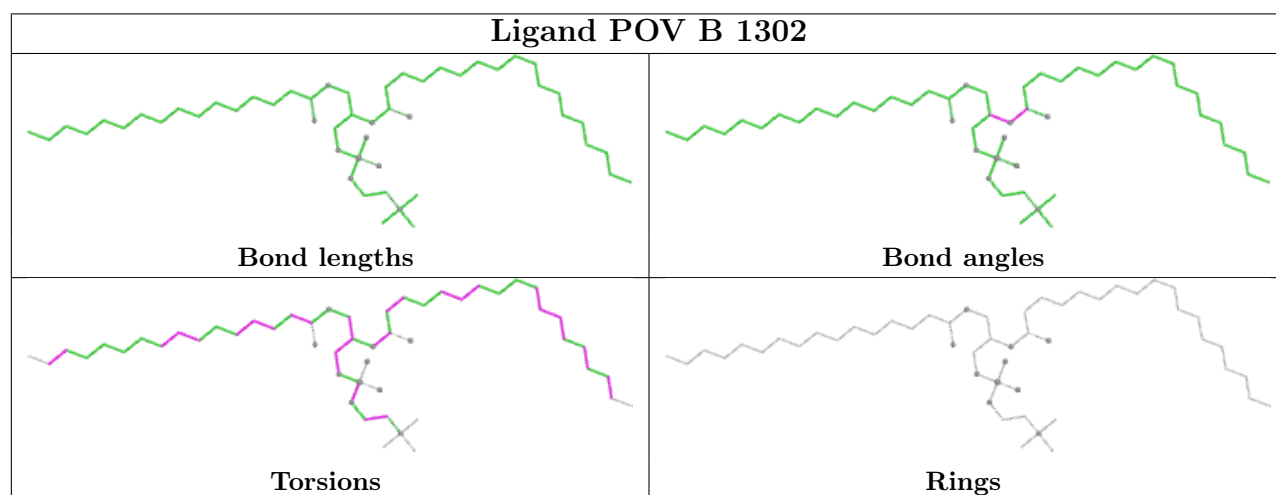
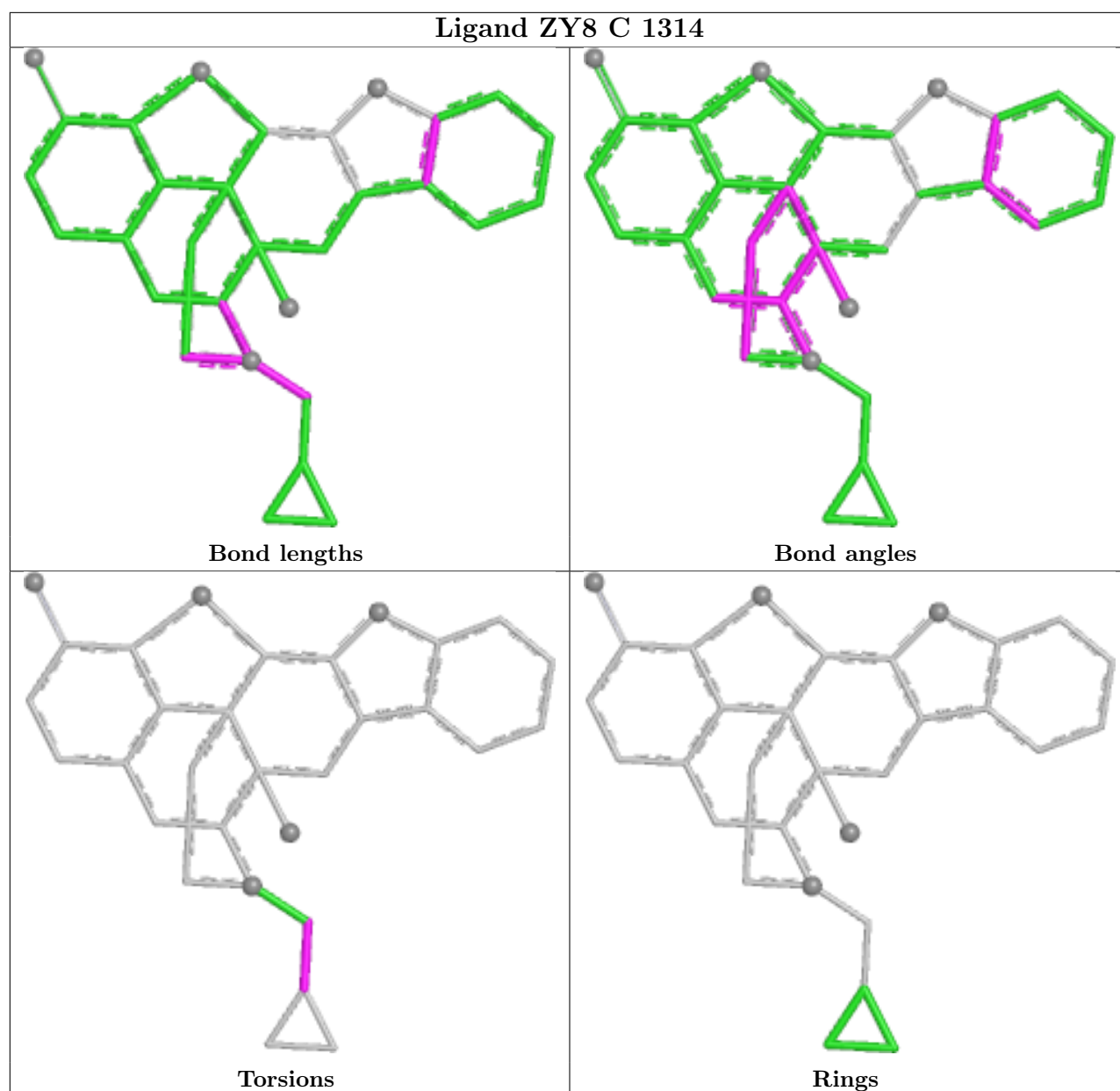


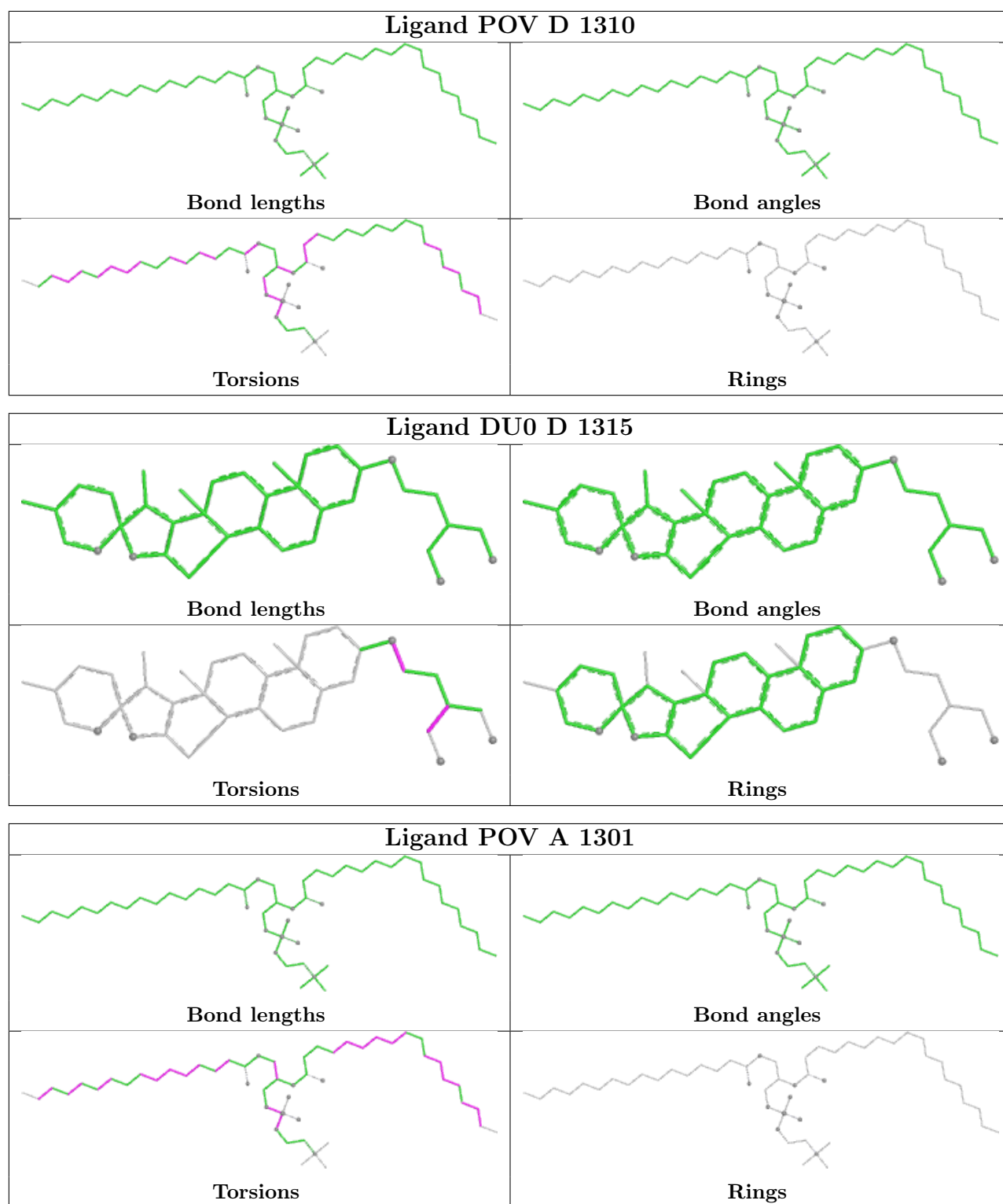


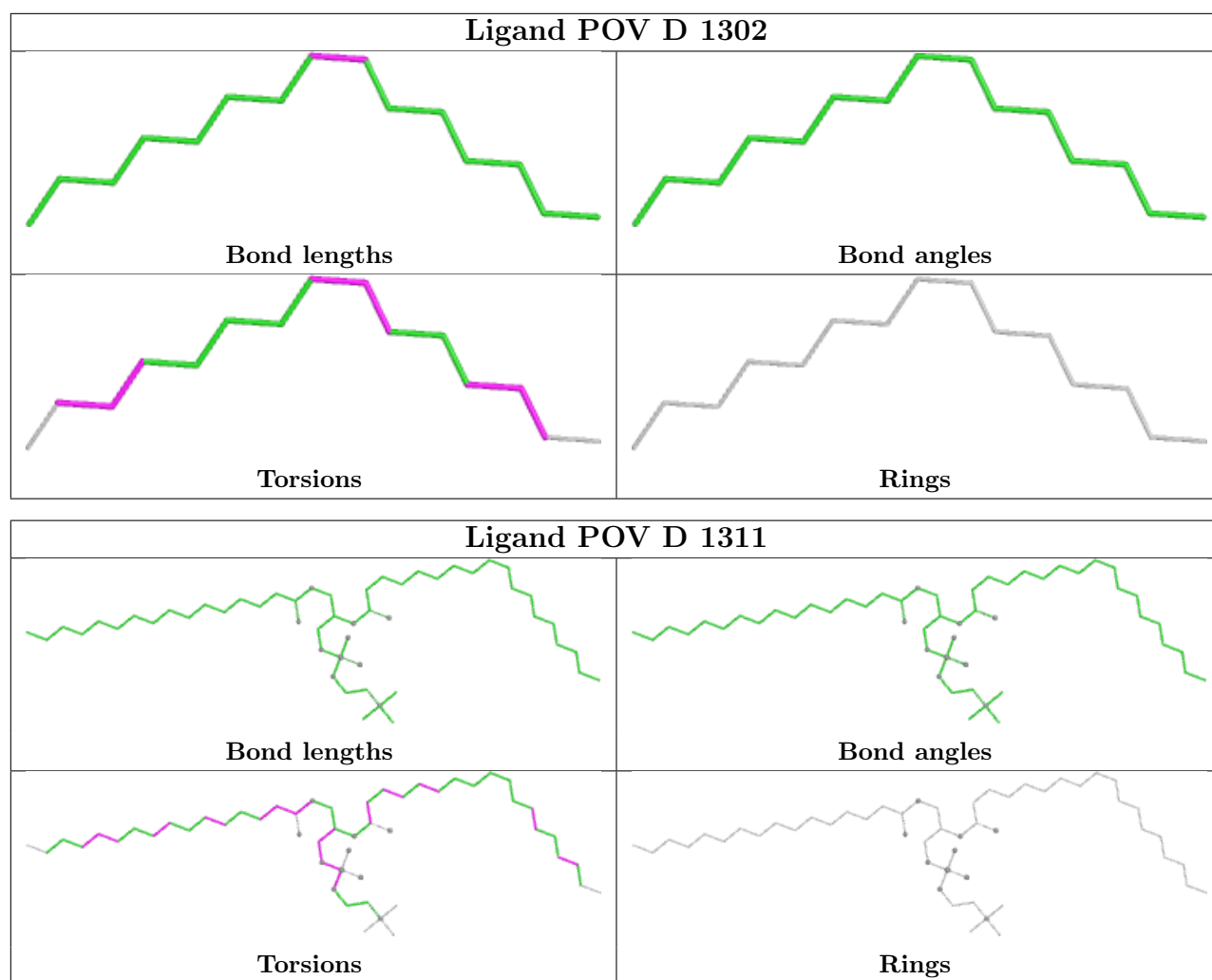


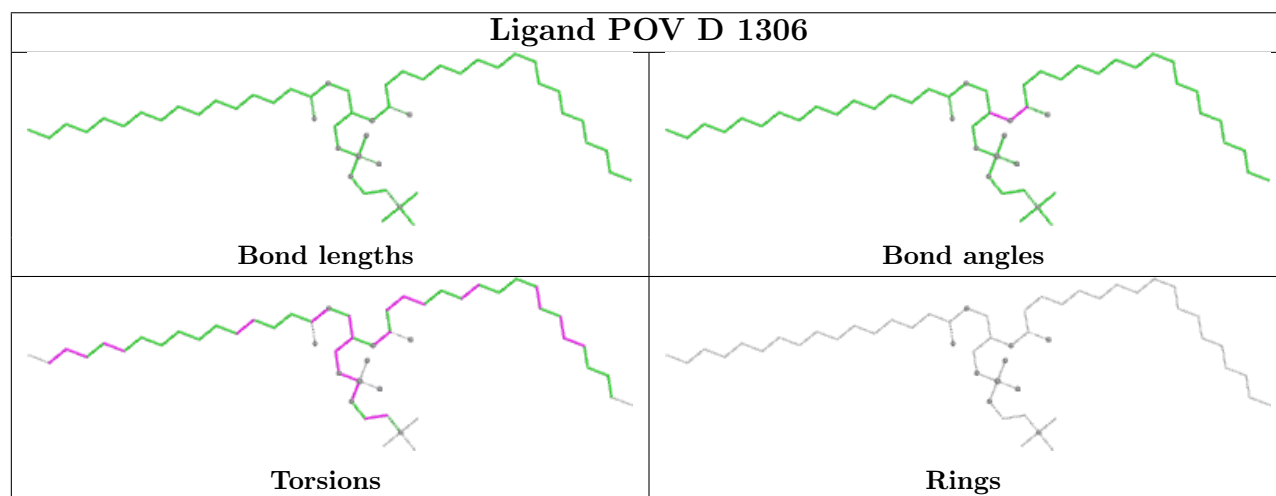
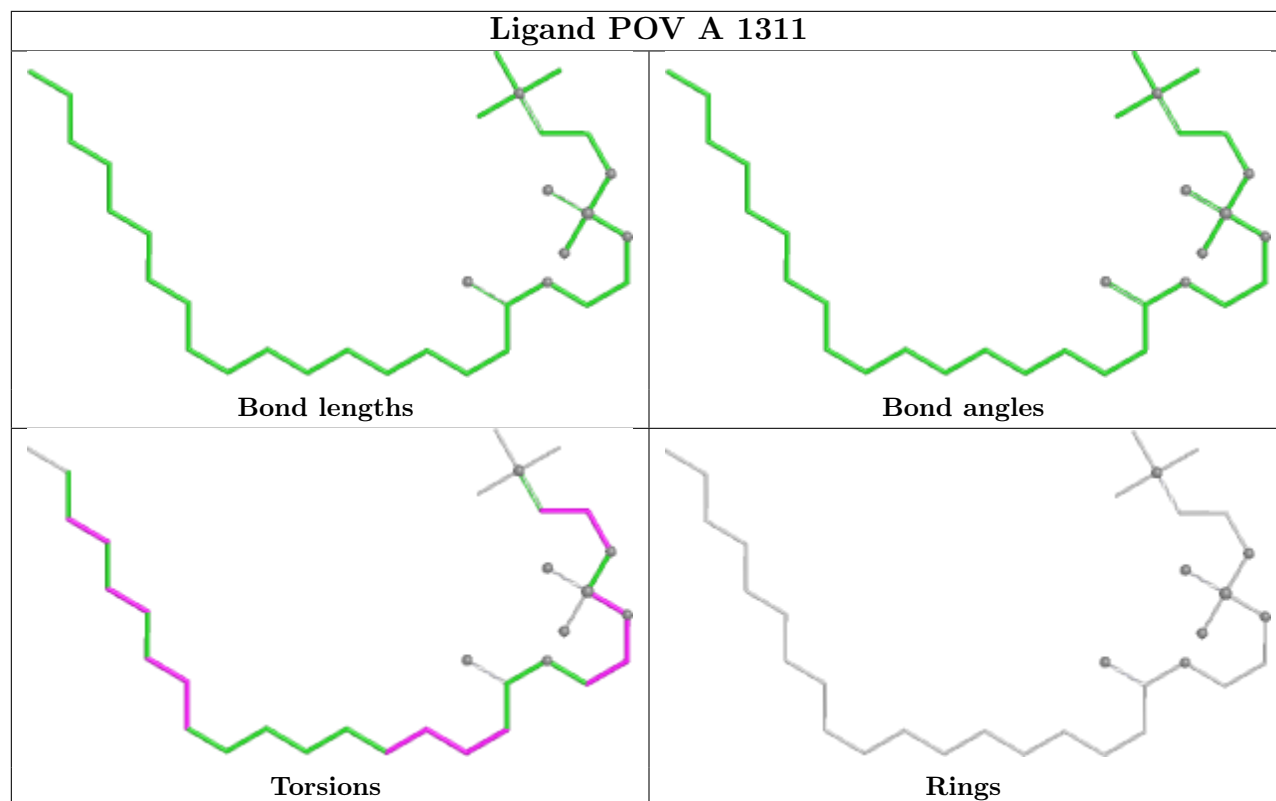


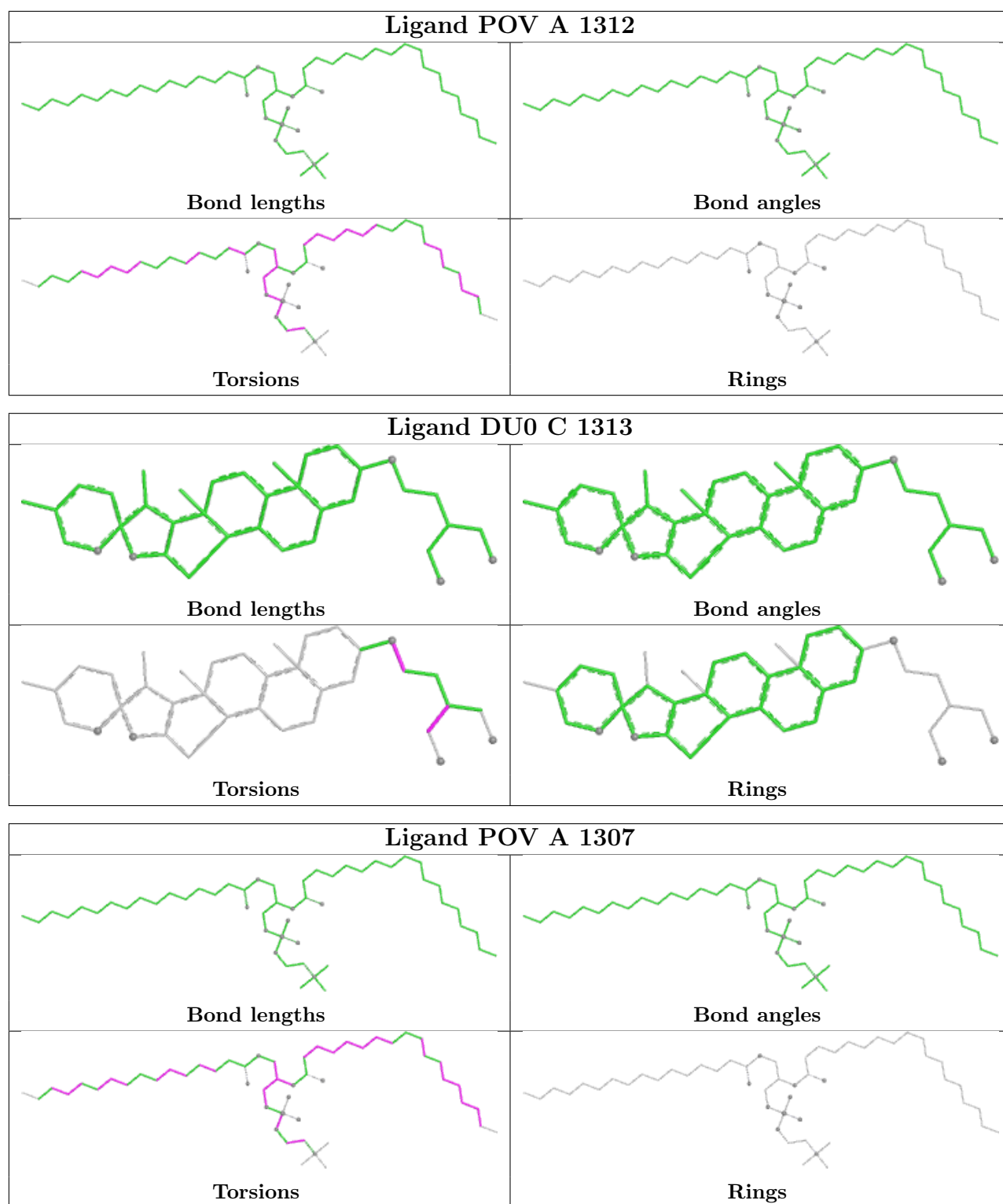


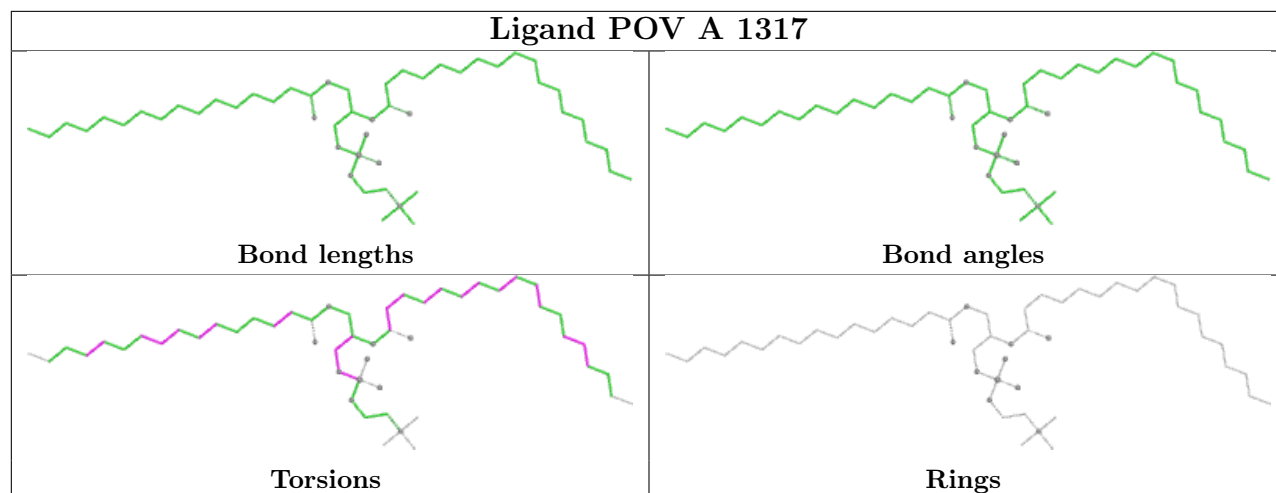












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

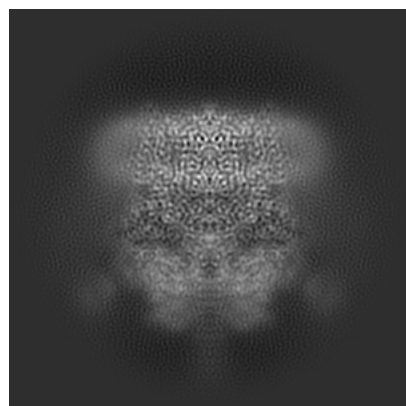
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-40500. These allow visual inspection of the internal detail of the map and identification of artifacts.

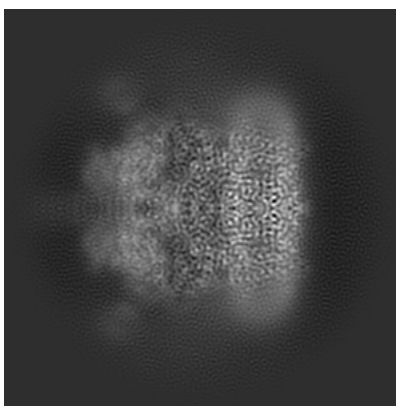
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

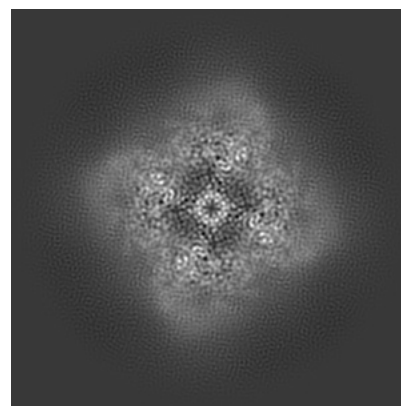
#### 6.1.1 Primary map



X

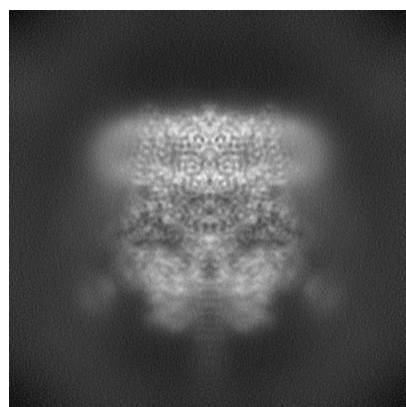


Y

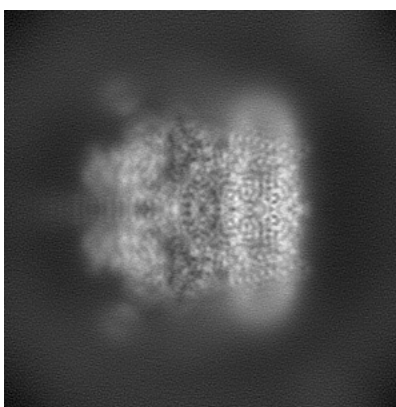


Z

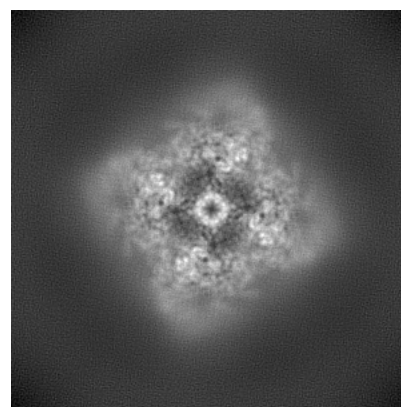
#### 6.1.2 Raw map



X



Y

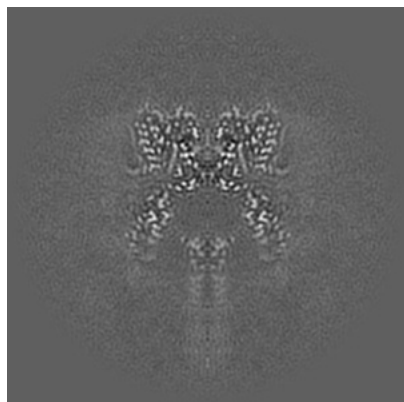


Z

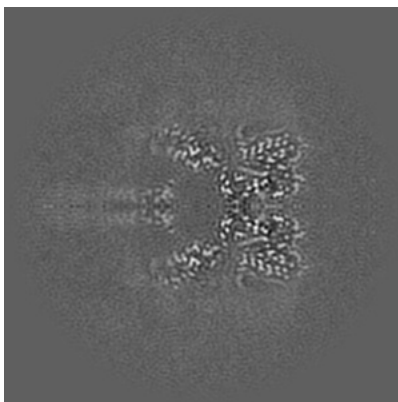
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

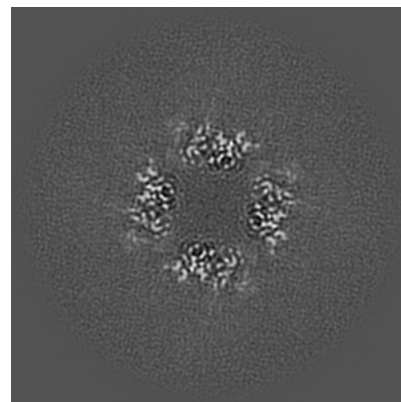
### 6.2.1 Primary map



X Index: 150

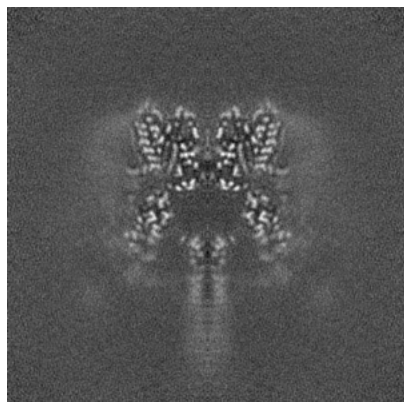


Y Index: 150

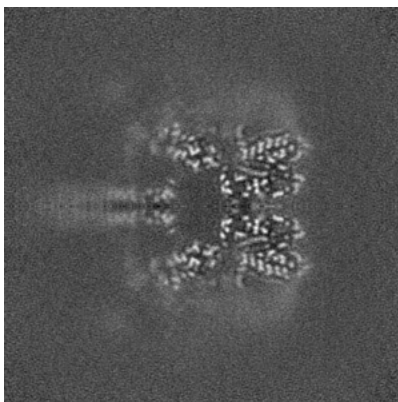


Z Index: 150

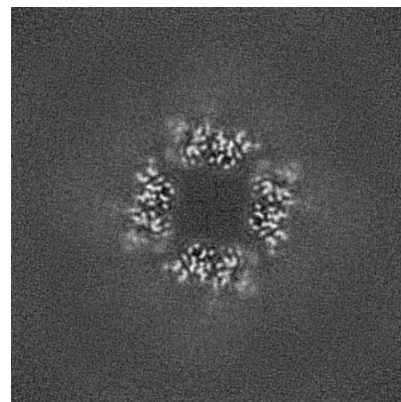
### 6.2.2 Raw map



X Index: 150



Y Index: 150

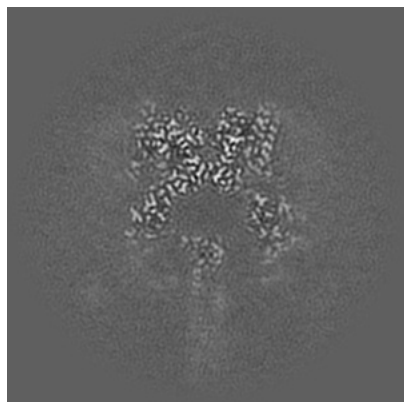


Z Index: 150

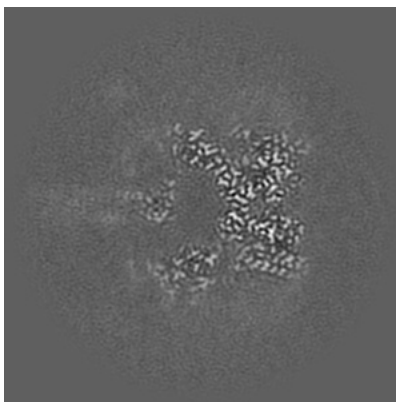
The images above show central slices of the map in three orthogonal directions.

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

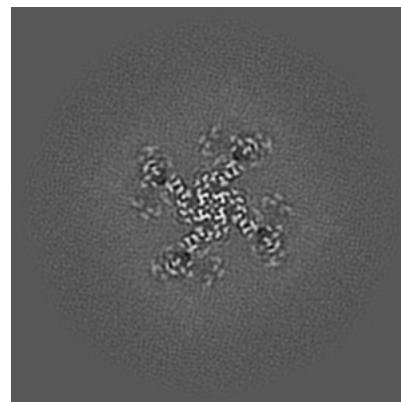
### 6.3.1 Primary map



X Index: 147

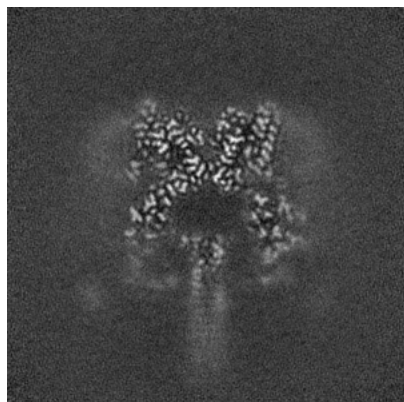


Y Index: 147

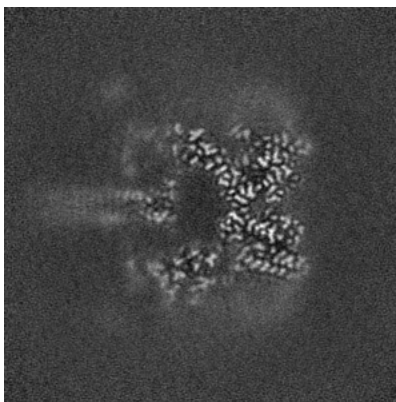


Z Index: 174

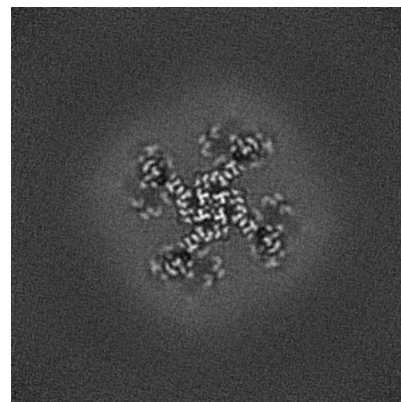
### 6.3.2 Raw map



X Index: 147



Y Index: 147

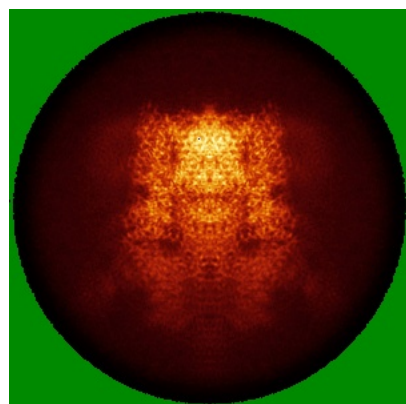


Z Index: 174

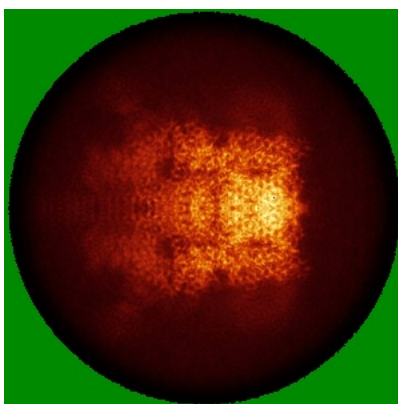
The images above show the largest variance slices of the map in three orthogonal directions.

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

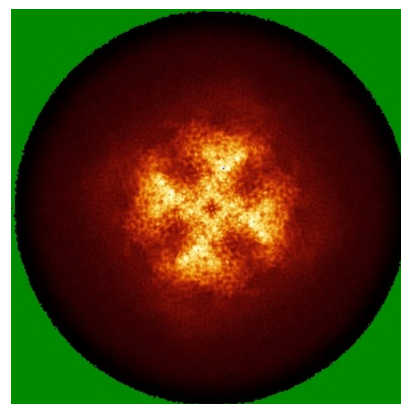
### 6.4.1 Primary map



X

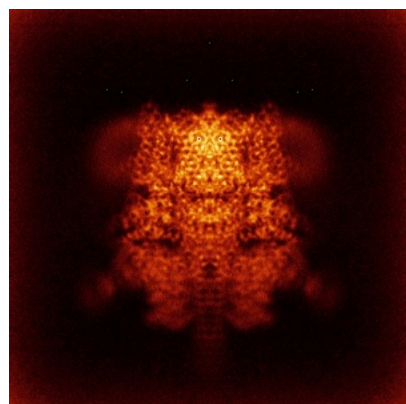


Y

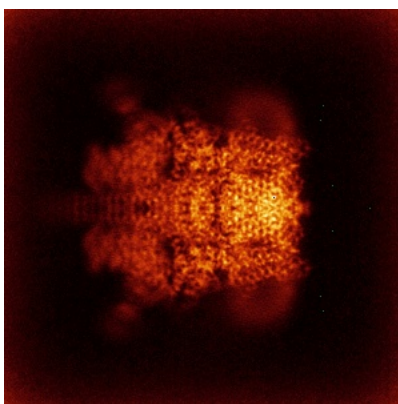


Z

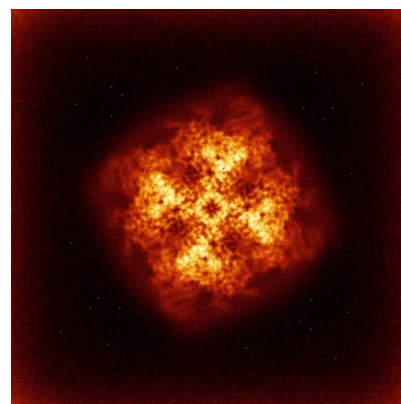
### 6.4.2 Raw map



X



Y

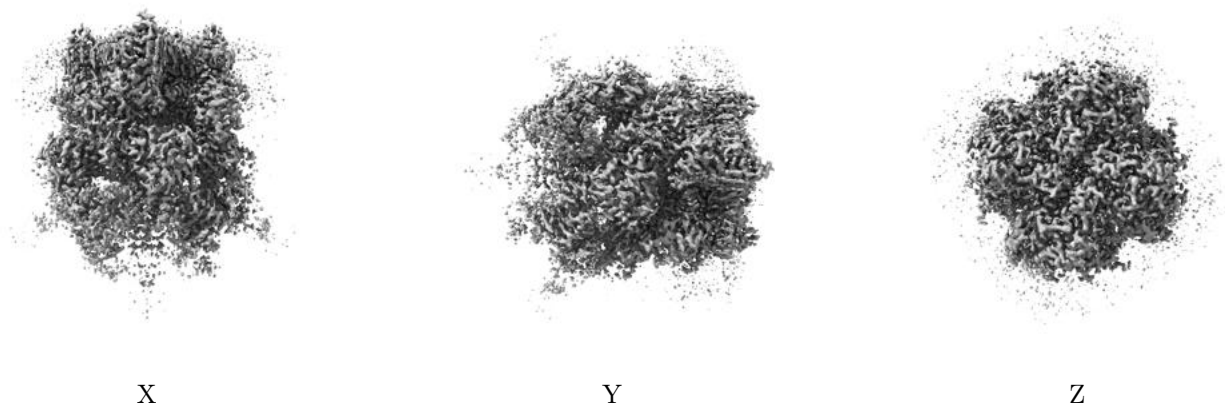


Z

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.

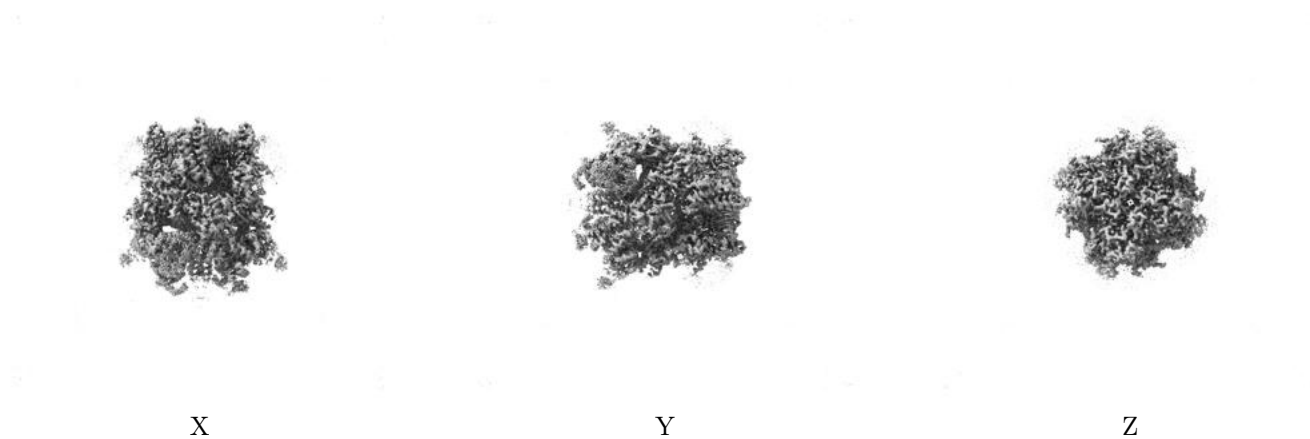
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.26. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

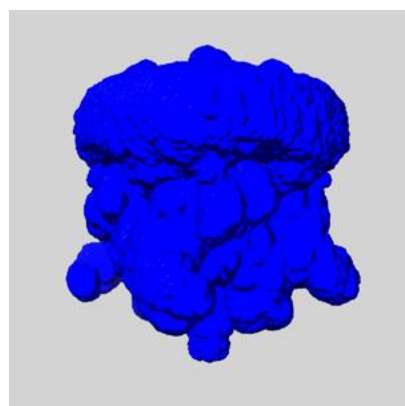
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

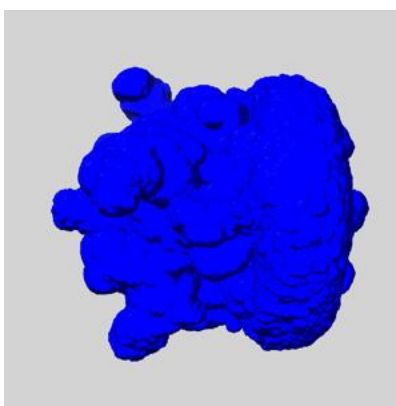
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

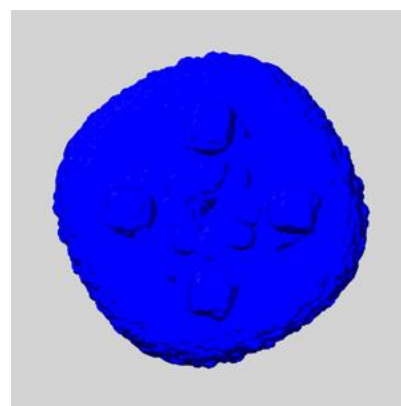
### 6.6.1 emd\_40500\_msk\_1.map [i](#)



X



Y

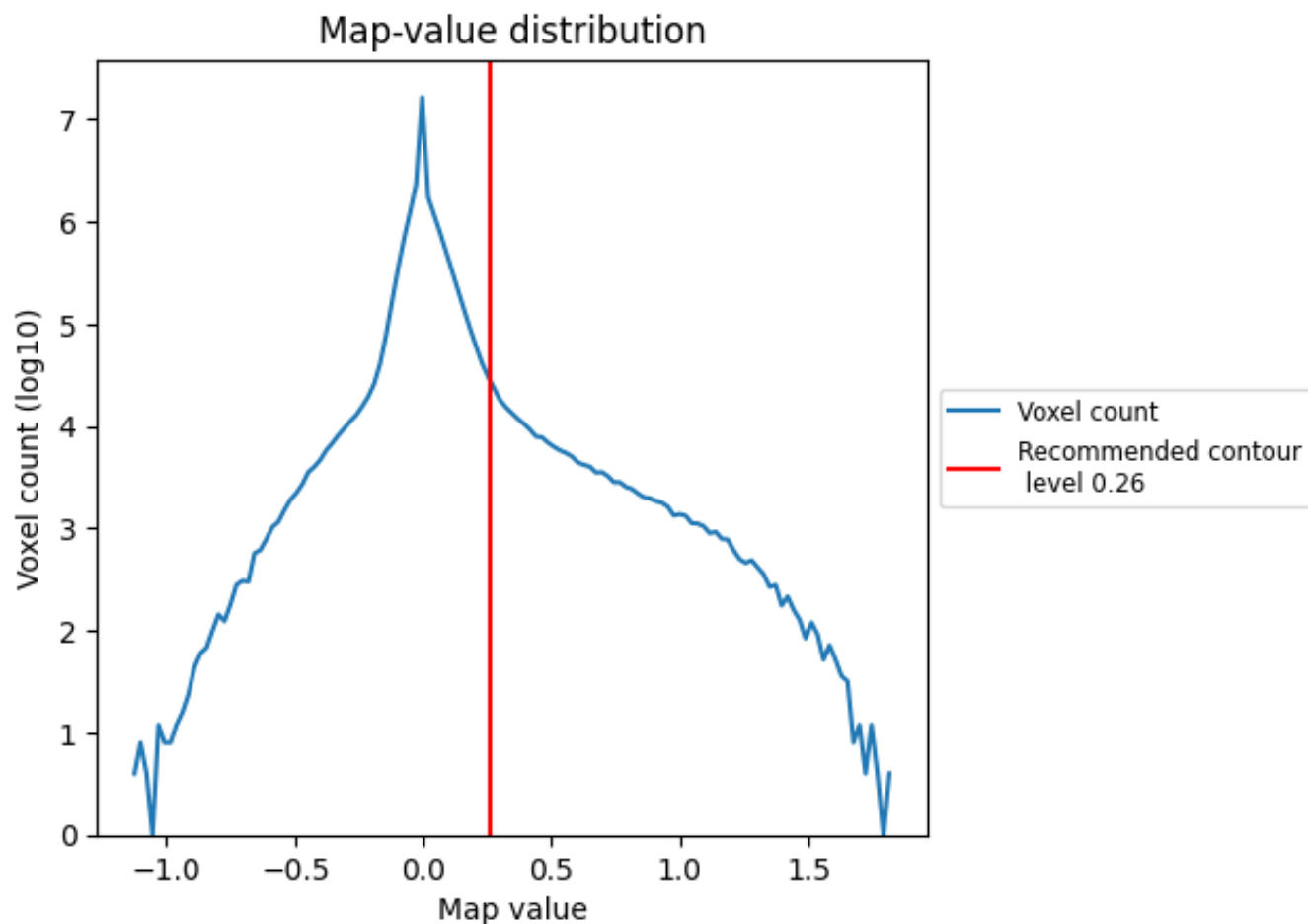


Z

## 7 Map analysis [i](#)

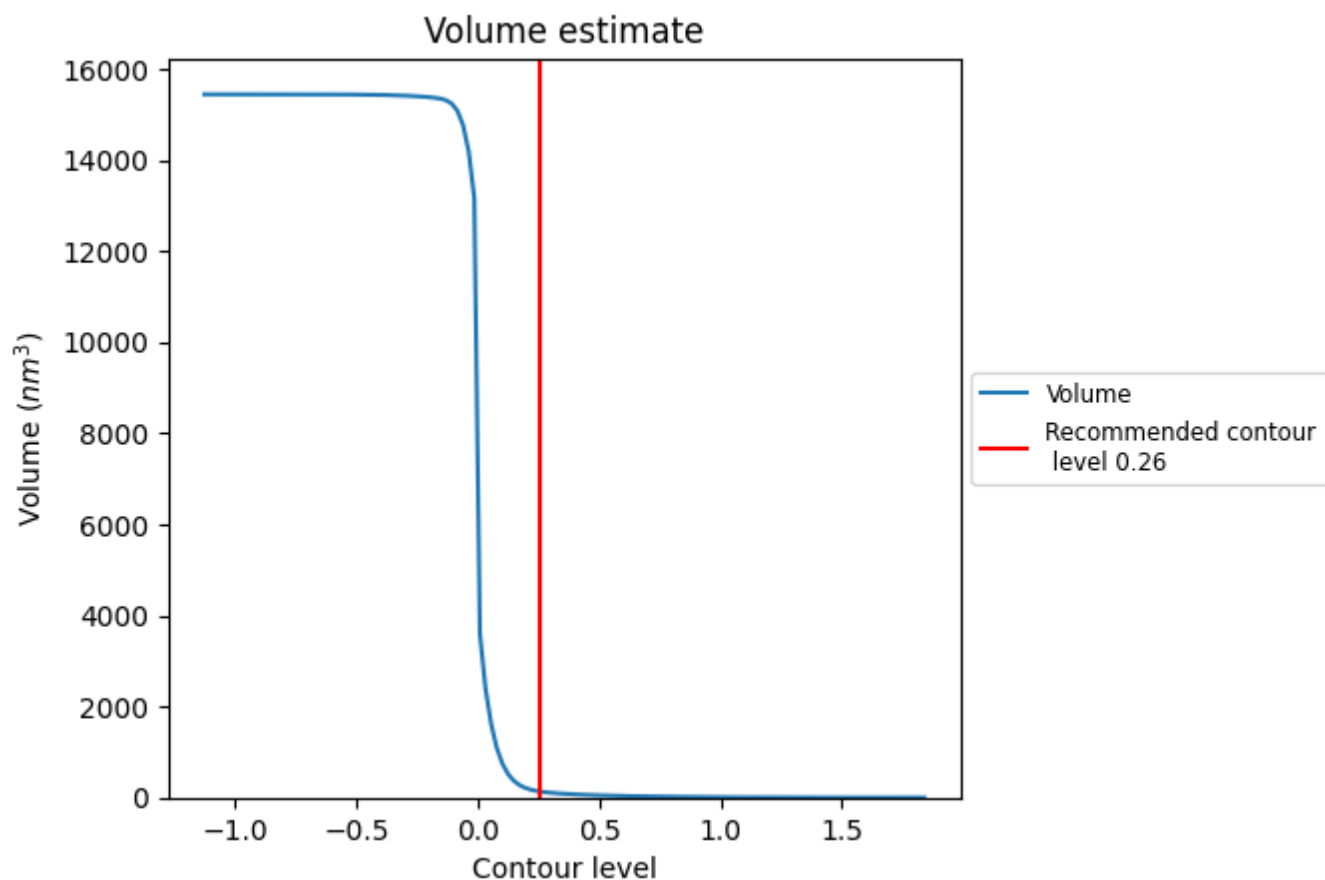
This section contains the results of statistical analysis of the map.

### 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.

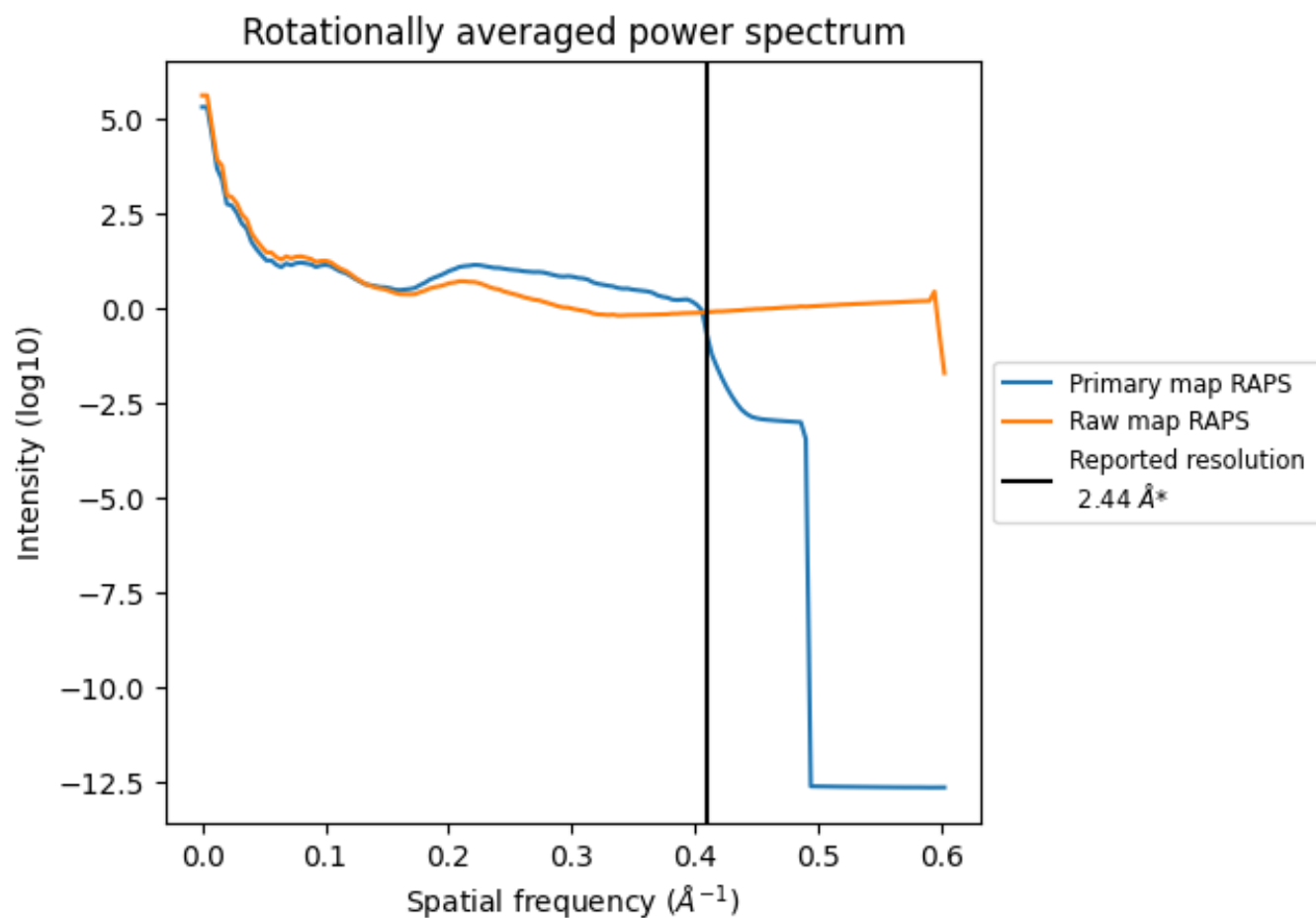
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 131 nm<sup>3</sup>; this corresponds to an approximate mass of 118 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 ⓘ

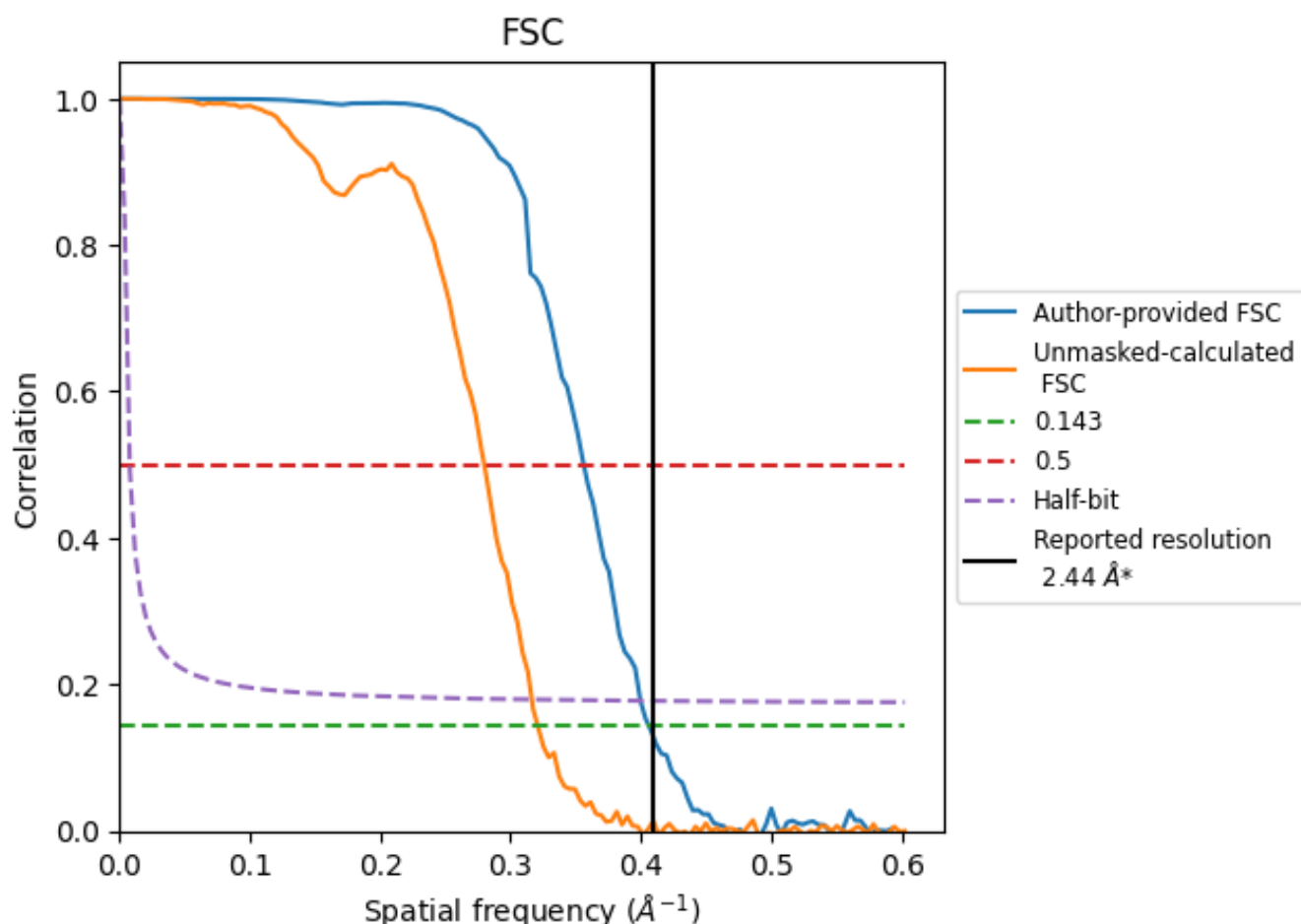


\*Reported resolution corresponds to spatial frequency of 0.410  $\text{\AA}^{-1}$

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.410  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

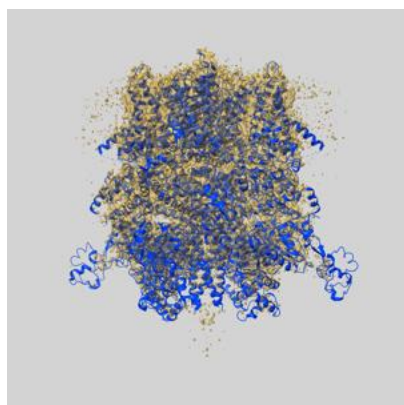
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.44	-	-
Author-provided FSC curve	2.46	2.81	2.50
Unmasked-calculated*	3.12	3.57	3.16

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.12 differs from the reported value 2.44 by more than 10 %

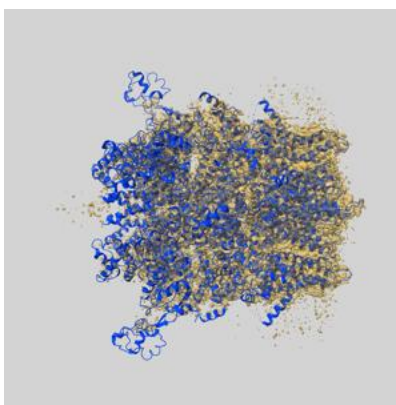
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-40500 and PDB model 8SI6. Per-residue inclusion information can be found in [section 3](#) on [page 9](#).

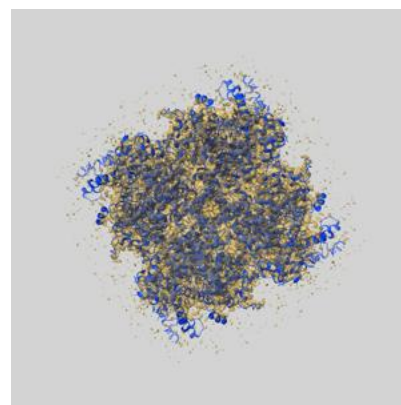
### 9.1 Map-model overlay [i](#)



X



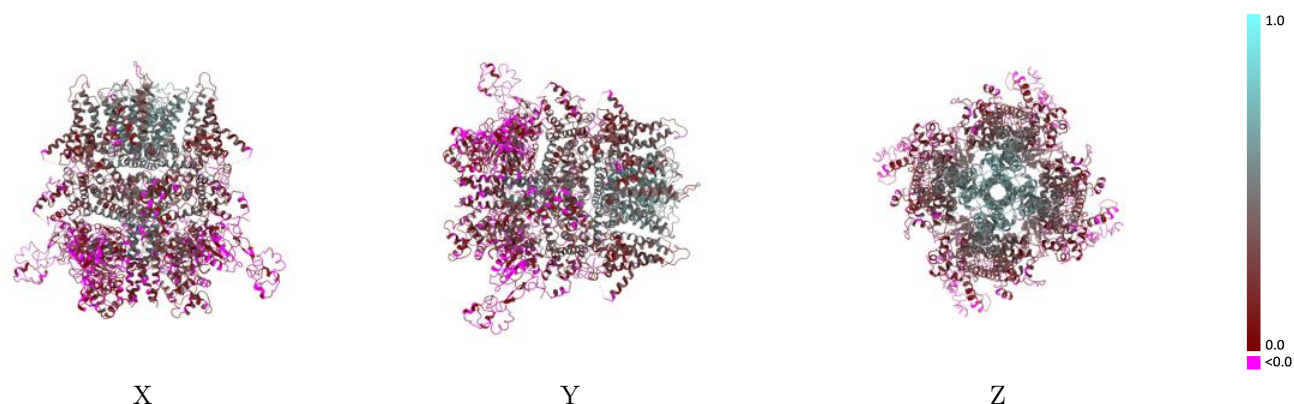
Y



Z

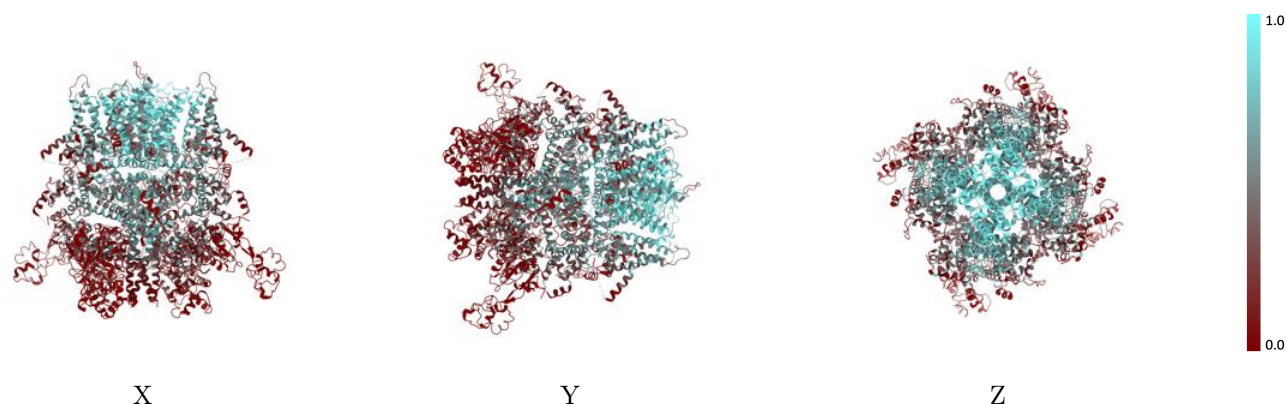
The images above show the 3D surface view of the map at the recommended contour level 0.26 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



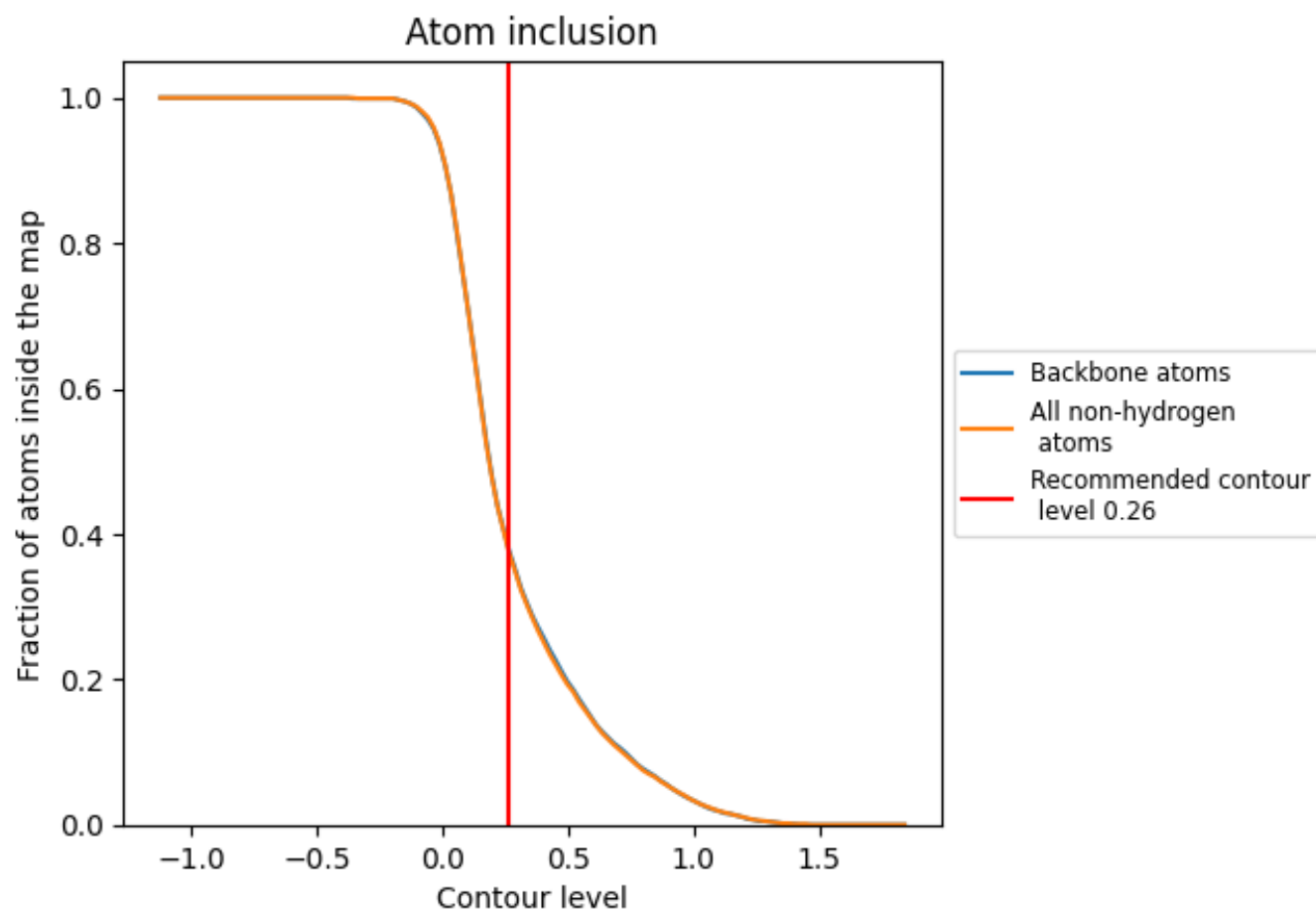
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.26).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 38% of all backbone atoms, 38% 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 (0.26) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.3790	<div></div> 0.2400
A	<div></div> 0.3790	<div></div> 0.2390
B	<div></div> 0.3830	<div></div> 0.2390
C	<div></div> 0.3810	<div></div> 0.2420
D	<div></div> 0.3820	<div></div> 0.2410

