



Full wwPDB EM Validation Report ⓘ

Apr 5, 2026 – 10:45 PM UTC

PDB ID : 9VUB / pdb_00009vub
EMDB ID : EMD-65358
Title : channel C complex with 3
Authors : Jiang, D.H.; Ma, B.
Deposited on : 2025-07-12
Resolution : 3.35 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

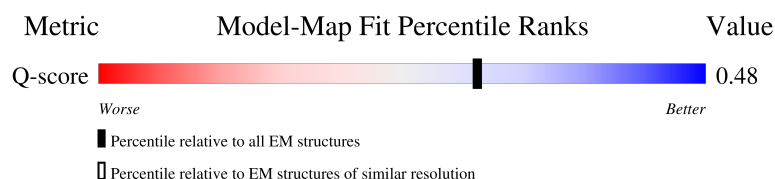
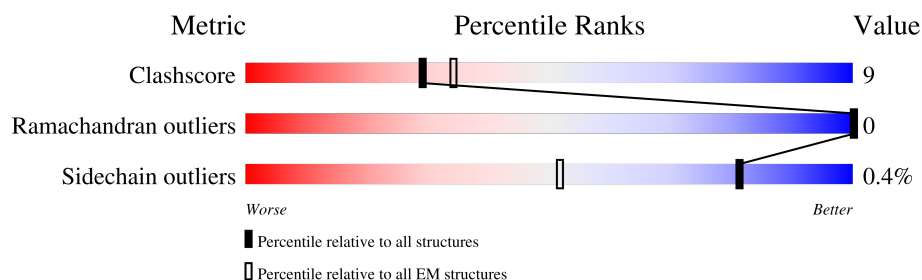
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 3.35 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14390 (2.85 - 3.85)

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

Mol	Chain	Length	Quality of chain
1	A	579	 5% 56% 9% 35%
1	B	579	 5% 55% 10% 35%
1	C	579	 5% 54% 11% 35%
1	D	579	 5% 57% 8% 35%

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Mol	Chain	Length	Quality of chain
2	E	149	<div><div></div><div>30%</div><div>74%</div><div>22%</div><div></div><div>.</div></div>
2	F	149	<div><div></div><div>21%</div><div>68%</div><div>28%</div><div></div><div>.</div></div>
2	G	149	<div><div></div><div>23%</div><div>66%</div><div>30%</div><div></div><div>.</div></div>
2	H	149	<div><div></div><div>23%</div><div>75%</div><div>20%</div><div></div><div>.</div><div>.</div></div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 16807 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Small conductance calcium-activated potassium channel protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	376	Total	C	N	O	S	0	0
			2930	1907	503	498	22		
1	A	377	Total	C	N	O	S	0	0
			2952	1917	510	503	22		
1	B	377	Total	C	N	O	S	0	0
			2928	1902	506	499	21		
1	D	377	Total	C	N	O	S	0	0
			2949	1915	510	503	21		

- Molecule 2 is a protein called Calmodulin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	143	Total	C	N	O	S	0	0
			1021	627	171	216	7		
2	H	143	Total	C	N	O	S	0	0
			1044	639	175	223	7		
2	E	143	Total	C	N	O	S	0	0
			1037	635	169	225	8		
2	F	143	Total	C	N	O	S	0	0
			1028	629	171	221	7		

- Molecule 3 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylammonio)ethyl phosphate (CCD ID: POV) (formula: C₄₂H₈₂NO₈P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
3	C	1	Total	C	O		0
			10	8	2		
3	C	1	Total	C	O		0
			16	14	2		
3	C	1	Total	C	O		0
			13	11	2		
3	C	1	Total	C	O		0
			14	12	2		
3	C	1	Total	C	O		0
			11	9	2		
3	C	1	Total	C	O	P	0
			33	24	8	1	
3	C	1	Total	C	O	P	0
			25	18	6	1	
3	A	1	Total	C	O		0
			20	18	2		
3	A	1	Total	C	O		0
			10	8	2		
3	A	1	Total	C	O		0
			20	18	2		
3	A	1	Total	C	O		0
			16	14	2		
3	A	1	Total	C	O		0
			13	11	2		
3	A	1	Total	C	O		0
			14	12	2		
3	A	1	Total	C	O		0
			14	12	2		

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Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	O	P	0
			33	24	8	1	
3	A	1	Total	C	O	P	0
			25	18	6	1	
3	A	1	Total	C	O		0
			11	9	2		
3	B	1	Total	C	O		0
			20	18	2		
3	B	1	Total	C	O		0
			10	8	2		
3	B	1	Total	C	O		0
			16	14	2		
3	B	1	Total	C	O		0
			13	11	2		
3	B	1	Total	C	O	P	0
			27	20	6	1	
3	B	1	Total	C	O		0
			11	9	2		
3	B	1	Total	C	O	P	0
			33	24	8	1	
3	D	1	Total	C	O		0
			20	18	2		
3	D	1	Total	C	O		0
			11	9	2		
3	D	1	Total	C	O		0
			16	14	2		
3	D	1	Total	C	O		0
			13	11	2		
3	D	1	Total	C	O		0
			14	12	2		
3	D	1	Total	C	O	P	0
			33	24	8	1	
3	D	1	Total	C	O		0
			11	9	2		
3	D	1	Total	C	O	P	0
			25	18	6	1	

- Molecule 4 is CHOLESTEROL (CCD ID: CLR) (formula: C₂₇H₄₆O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
4	C	1	Total	C	O	0
			28	27	1	
4	C	1	Total	C	O	0
			28	27	1	
4	A	1	Total	C	O	0
			28	27	1	
4	A	1	Total	C	O	0
			28	27	1	
4	B	1	Total	C	O	0
			28	27	1	
4	B	1	Total	C	O	0
			28	27	1	
4	D	1	Total	C	O	0
			28	27	1	
4	D	1	Total	C	O	0
			28	27	1	

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

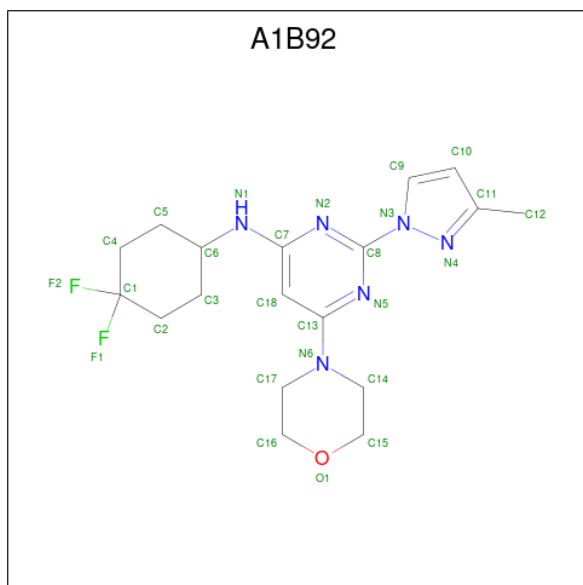
Mol	Chain	Residues	Atoms		AltConf
5	G	3	Total	Ca	0
			3	3	
5	H	3	Total	Ca	0
			3	3	
5	E	3	Total	Ca	0
			3	3	

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Mol	Chain	Residues	Atoms		AltConf
5	F	3	Total	Ca	0
			3	3	

- Molecule 6 is Rimtuzalcap (CCD ID: A1B92) (formula: C₁₈H₂₄F₂N₆O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
6	G	1	Total	C	F	N	O	0
			27	18	2	6	1	
6	H	1	Total	C	F	N	O	0
			27	18	2	6	1	
6	E	1	Total	C	F	N	O	0
			27	18	2	6	1	
6	B	1	Total	C	F	N	O	0
			27	18	2	6	1	

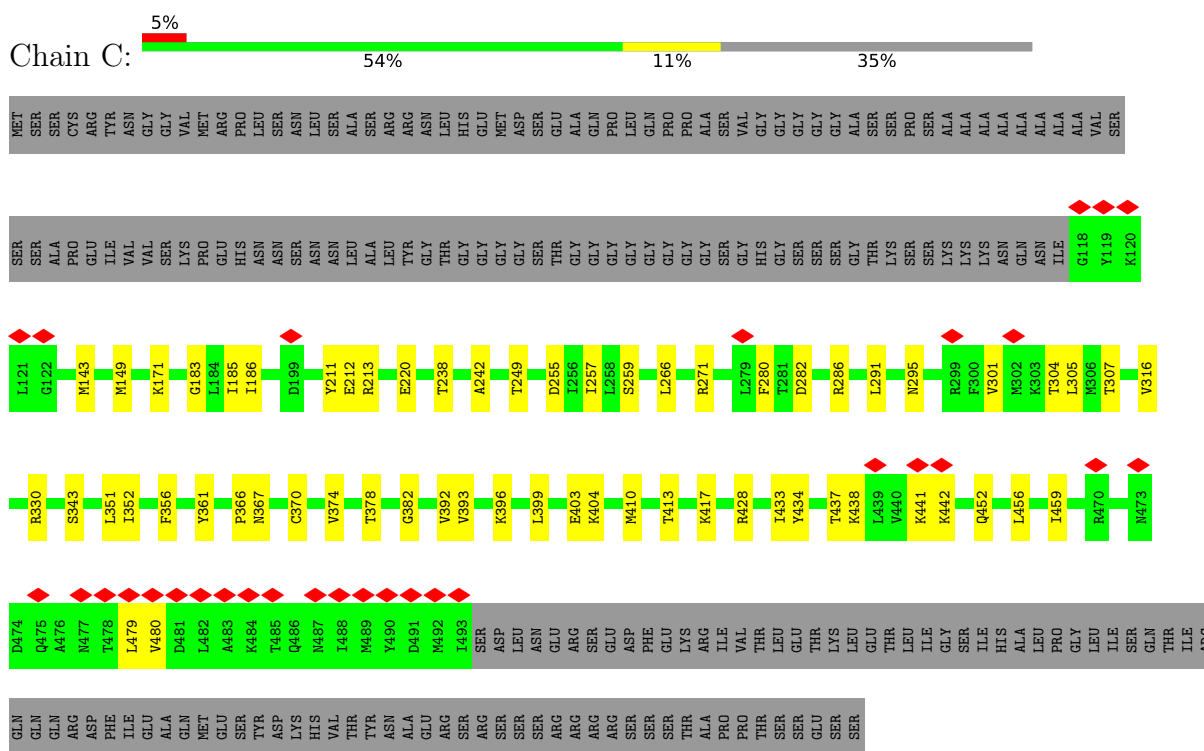
- Molecule 7 is POTASSIUM ION (CCD ID: K) (formula: K) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
7	A	3	Total	K	0
			3	3	

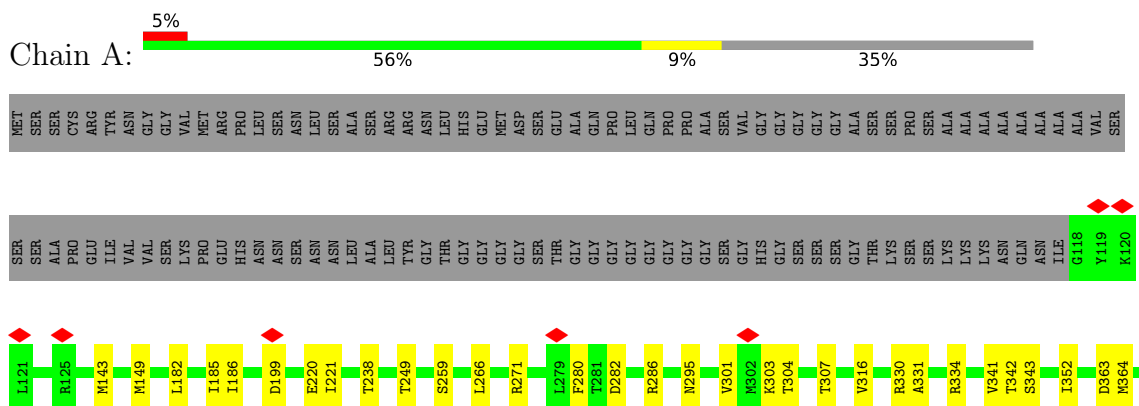
3 Residue-property plots

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.

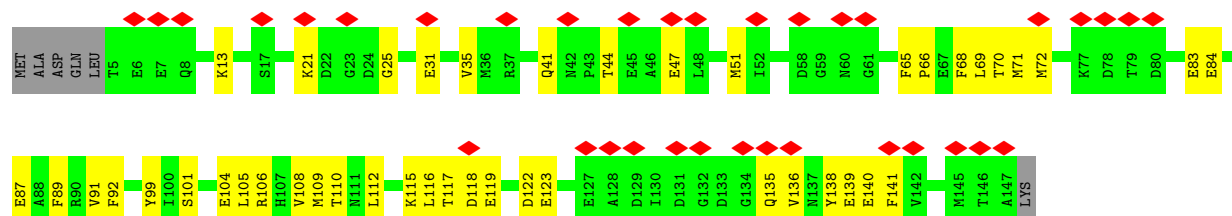
- Molecule 1: Small conductance calcium-activated potassium channel protein 2



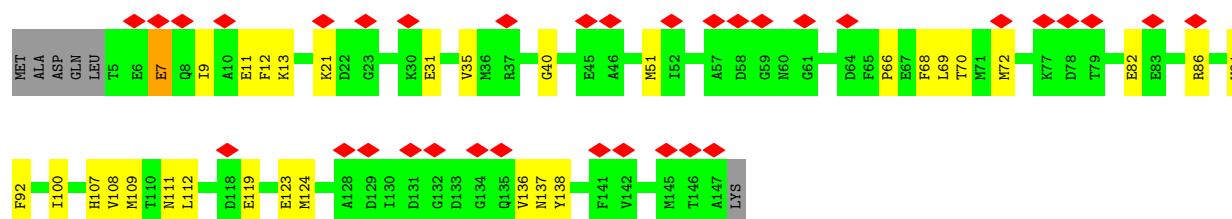
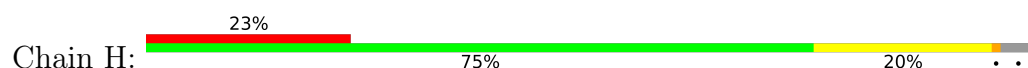
- Molecule 1: Small conductance calcium-activated potassium channel protein 2



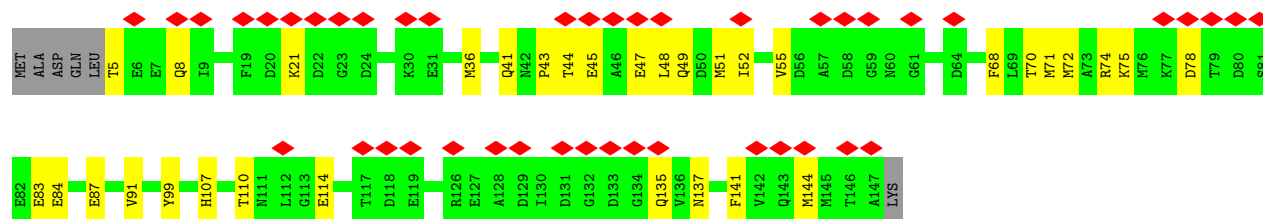
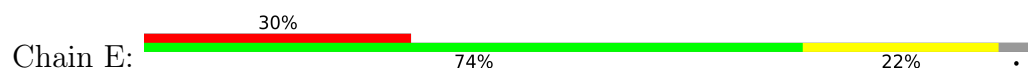
- Molecule 2: Calmodulin-1



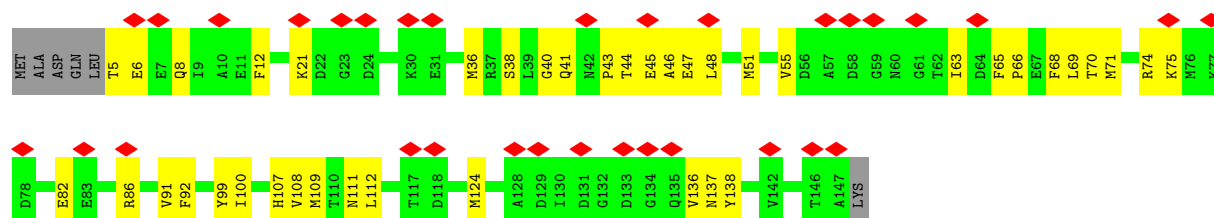
- Molecule 2: Calmodulin-1



- Molecule 2: Calmodulin-1



- Molecule 2: Calmodulin-1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	55003	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.668	Depositor
Minimum map value	-0.357	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.127	Depositor
Map size (Å)	272.0, 272.0, 272.0	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.85, 0.85, 0.85	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: A1B92, CLR, POV, K, 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	0.19	0/3011	0.33	0/4079
1	B	0.23	0/2987	0.39	0/4051
1	C	0.32	0/2989	0.46	0/4052
1	D	0.20	0/3008	0.35	0/4076
2	E	0.26	0/1047	0.51	0/1413
2	F	0.24	0/1038	0.43	0/1403
2	G	0.32	0/1032	0.59	1/1395 (0.1%)
2	H	0.23	0/1054	0.39	0/1422
All	All	0.25	0/16166	0.41	1/21891 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	25	GLY	N-CA-C	-5.86	107.15	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	2952	0	3024	46	0
1	B	2928	0	2974	53	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2930	0	3001	54	0
1	D	2949	0	3017	40	0
2	E	1037	0	910	31	0
2	F	1028	0	895	33	0
2	G	1021	0	879	35	0
2	H	1044	0	922	22	0
3	A	176	0	231	8	0
3	B	130	0	169	6	0
3	C	122	0	147	2	0
3	D	143	0	182	4	0
4	A	56	0	92	5	0
4	B	56	0	92	15	0
4	C	56	0	92	9	0
4	D	56	0	92	8	0
5	E	3	0	0	0	0
5	F	3	0	0	0	0
5	G	3	0	0	0	0
5	H	3	0	0	0	0
6	B	27	0	0	0	0
6	E	27	0	0	5	0
6	G	27	0	0	0	0
6	H	27	0	0	2	0
7	A	3	0	0	0	0
All	All	16807	0	16719	312	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 9.

All (312) 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)
2:E:51:MET:HE3	6:E:204:A1B92:C18	1.73	1.17
1:A:186:ILE:HD11	1:A:221:ILE:HD11	1.29	1.15
1:A:186:ILE:CD1	1:A:221:ILE:HD11	2.00	0.91
2:E:51:MET:HE3	6:E:204:A1B92:C7	2.07	0.84
1:A:399:LEU:HD11	1:B:303:LYS:HB3	1.60	0.82
1:B:183:GLY:O	1:B:186:ILE:HG22	1.80	0.82
1:D:183:GLY:O	1:D:186:ILE:HG22	1.80	0.82
1:B:206:ARG:CD	1:D:449:ARG:NH1	2.43	0.82
1:A:186:ILE:HD11	1:A:221:ILE:CD1	2.10	0.80
1:B:206:ARG:HD2	1:D:449:ARG:NH1	1.95	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:392:VAL:HG12	1:C:396:LYS:HE3	1.65	0.78
1:C:183:GLY:O	1:C:186:ILE:HG22	1.83	0.78
2:E:70:THR:O	2:E:74:ARG:HG2	1.84	0.76
1:C:211:TYR:HB2	3:A:604:POV:H28	1.67	0.75
2:G:65:PHE:CZ	2:G:69:LEU:HD21	2.21	0.75
1:C:370:CYS:HB2	4:C:605:CLR:H11	1.68	0.75
2:H:12:PHE:HB3	2:H:68:PHE:HE1	1.50	0.74
1:C:257:ILE:HG12	4:C:605:CLR:H6	1.68	0.74
1:A:399:LEU:CD1	1:B:303:LYS:HB3	2.18	0.73
1:A:303:LYS:HB3	1:D:399:LEU:HD11	1.68	0.73
1:B:260:ILE:HG21	4:B:605:CLR:H122	1.70	0.73
2:G:68:PHE:O	2:G:72:MET:HG2	1.90	0.72
2:G:108:VAL:HG23	2:G:112:LEU:HD12	1.74	0.70
2:E:5:THR:HG23	2:E:8:GLN:H	1.56	0.70
2:F:75:LYS:HE3	1:B:291:LEU:HD21	1.75	0.69
3:B:606:POV:H21A	4:B:607:CLR:H181	1.74	0.69
1:B:316:VAL:HG12	4:B:607:CLR:H72	1.76	0.68
1:A:282:ASP:O	1:A:286:ARG:HG2	1.95	0.67
2:E:141:PHE:HA	2:E:144:MET:HE3	1.77	0.67
2:H:68:PHE:CE2	2:H:72:MET:HE2	2.30	0.67
1:D:282:ASP:O	1:D:286:ARG:HG2	1.95	0.66
1:A:303:LYS:HB3	1:D:399:LEU:CD1	2.26	0.65
2:E:43:PRO:HG2	2:E:48:LEU:HG	1.78	0.64
3:A:606:POV:H28	3:A:606:POV:H24	1.80	0.63
2:G:92:PHE:CE2	2:G:108:VAL:HG21	2.33	0.63
1:B:370:CYS:HB2	4:B:605:CLR:H11	1.82	0.62
1:A:454:LYS:HE3	3:A:604:POV:O21	2.00	0.62
1:D:433:ILE:O	1:D:437:THR:HG22	1.99	0.62
2:F:65:PHE:CZ	2:F:69:LEU:HD11	2.35	0.62
1:C:437:THR:HG23	1:C:438:LYS:HG2	1.80	0.62
3:C:608:POV:H23	3:C:608:POV:H32	1.82	0.61
2:G:47:GLU:O	2:G:51:MET:HG3	1.99	0.61
1:C:316:VAL:HG12	4:C:606:CLR:H72	1.83	0.61
1:B:260:ILE:HD12	4:B:605:CLR:H9	1.82	0.61
1:D:410:MET:O	1:D:413:THR:HG22	2.02	0.60
2:G:106:ARG:HH21	2:G:122:ASP:HA	1.67	0.60
2:H:31:GLU:O	2:H:35:VAL:HG23	2.02	0.60
1:B:206:ARG:HD2	1:D:449:ARG:HH11	1.65	0.60
1:C:257:ILE:HG23	4:C:605:CLR:H6	1.84	0.60
1:C:459:ILE:HD13	2:E:84:GLU:HG3	1.84	0.60
1:C:410:MET:O	1:C:413:THR:HG22	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:410:MET:O	1:B:413:THR:HG22	2.02	0.60
2:G:31:GLU:O	2:G:35:VAL:HG23	2.02	0.59
1:A:410:MET:O	1:A:413:THR:HG22	2.02	0.59
1:C:211:TYR:CE1	3:A:604:POV:H24A	2.37	0.59
1:C:480:VAL:HG22	2:H:40:GLY:HA2	1.85	0.59
2:F:55:VAL:CG1	2:F:63:ILE:HD11	2.32	0.59
2:F:5:THR:HG23	2:F:8:GLN:H	1.68	0.58
3:D:601:POV:H28	3:D:601:POV:H24	1.85	0.58
2:H:109:MET:HG3	2:H:124:MET:HE1	1.85	0.58
1:B:261:PRO:HG3	4:B:605:CLR:H151	1.84	0.58
2:E:43:PRO:HG2	2:E:48:LEU:CG	2.33	0.58
2:E:51:MET:CE	6:E:204:A1B92:C7	2.79	0.58
1:C:434:TYR:CE1	1:C:438:LYS:HG3	2.39	0.58
1:A:433:ILE:O	1:A:437:THR:HG22	2.04	0.58
2:H:12:PHE:HB3	2:H:68:PHE:CE1	2.36	0.57
2:G:106:ARG:NH2	2:G:122:ASP:HA	2.19	0.57
2:F:108:VAL:HG23	2:F:112:LEU:HD12	1.85	0.57
1:A:398:GLU:O	1:B:303:LYS:NZ	2.35	0.57
1:A:432:LEU:HB3	1:A:451:HIS:CD2	2.39	0.57
2:H:108:VAL:HG23	2:H:112:LEU:HD12	1.85	0.57
1:D:316:VAL:HG12	4:D:608:CLR:H72	1.86	0.57
1:C:171:LYS:NZ	1:C:255:ASP:OD2	2.37	0.57
2:F:36:MET:SD	2:F:43:PRO:HG3	2.45	0.56
1:A:341:VAL:HG23	1:A:342:THR:N	2.21	0.55
2:F:47:GLU:O	2:F:51:MET:HG3	2.07	0.55
1:D:149:MET:SD	1:D:259:SER:OG	2.65	0.55
2:G:99:TYR:HB3	2:G:135:GLN:CB	2.37	0.54
1:A:149:MET:SD	1:A:259:SER:OG	2.65	0.54
2:G:41:GLN:O	2:G:41:GLN:HG3	2.08	0.54
2:G:44:THR:HB	2:G:47:GLU:HG2	1.90	0.54
1:B:220:GLU:OE1	1:B:271:ARG:NH2	2.36	0.54
2:F:55:VAL:HG11	2:F:63:ILE:CD1	2.37	0.54
1:C:149:MET:SD	1:C:259:SER:OG	2.65	0.54
1:B:316:VAL:HG11	3:B:606:POV:H21B	1.89	0.54
1:C:399:LEU:HG	1:D:303:LYS:HD3	1.90	0.54
2:G:66:PRO:O	2:G:70:THR:HG23	2.08	0.53
1:B:149:MET:SD	1:B:259:SER:OG	2.65	0.53
1:D:143:MET:HE1	1:D:266:LEU:HD23	1.90	0.53
1:D:279:LEU:HD22	1:D:280:PHE:CZ	2.43	0.53
1:C:143:MET:HE1	1:C:266:LEU:HD23	1.90	0.53
1:A:404:LYS:HD2	1:A:479:LEU:HD11	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:370:CYS:CB	4:D:606:CLR:H11	2.39	0.53
1:D:404:LYS:HD2	1:D:479:LEU:HD11	1.91	0.53
1:C:220:GLU:OE1	1:C:271:ARG:NH2	2.36	0.53
1:C:404:LYS:HD2	1:C:479:LEU:HD21	1.89	0.53
2:H:9:ILE:HG12	2:H:69:LEU:HD11	1.90	0.53
2:H:68:PHE:CZ	2:H:72:MET:HE2	2.44	0.53
1:C:212:GLU:H	1:C:212:GLU:CD	2.17	0.52
1:C:242:ALA:O	1:B:363:ASP:OD2	2.27	0.52
1:C:370:CYS:HB2	4:C:605:CLR:C1	2.37	0.52
2:H:51:MET:HE3	6:H:204:A1B92:C13	2.39	0.52
2:E:99:TYR:CE2	2:E:137:ASN:HB2	2.44	0.52
1:B:143:MET:HE1	1:B:266:LEU:HD23	1.90	0.52
2:E:44:THR:HG22	2:E:45:GLU:N	2.25	0.52
1:A:143:MET:HE1	1:A:266:LEU:HD23	1.90	0.52
2:G:117:THR:O	2:G:118:ASP:C	2.51	0.52
2:E:51:MET:HE3	6:E:204:A1B92:C13	2.36	0.52
2:F:45:GLU:HA	2:F:48:LEU:HD12	1.92	0.52
2:E:49:GLN:HA	2:E:49:GLN:NE2	2.25	0.51
2:F:12:PHE:HB3	2:F:68:PHE:HE2	1.75	0.51
2:F:41:GLN:O	2:F:43:PRO:HD3	2.10	0.51
1:D:370:CYS:HB2	4:D:606:CLR:H11	1.91	0.51
1:C:183:GLY:O	1:C:186:ILE:CG2	2.56	0.51
1:A:295:ASN:OD1	1:A:295:ASN:N	2.43	0.51
1:B:206:ARG:HD3	1:D:449:ARG:NH1	2.26	0.51
1:B:370:CYS:SG	4:B:605:CLR:H112	2.51	0.51
1:B:428:ARG:O	1:B:432:LEU:HG	2.11	0.51
2:G:65:PHE:O	2:G:69:LEU:HG	2.11	0.51
2:F:55:VAL:CG1	2:F:63:ILE:CD1	2.88	0.51
2:F:44:THR:HG22	2:F:46:ALA:H	1.76	0.51
2:E:78:ASP:HB3	1:A:199:ASP:OD1	2.11	0.50
3:A:609:POV:H25A	1:B:384:GLY:HA3	1.93	0.50
2:E:36:MET:HB3	2:E:41:GLN:HG3	1.94	0.50
2:F:69:LEU:O	2:F:70:THR:C	2.55	0.50
1:B:316:VAL:CG1	4:B:607:CLR:H72	2.40	0.50
1:B:400:THR:OG1	1:B:403:GLU:HG3	2.11	0.50
1:C:351:LEU:HD11	1:C:361:TYR:HD1	1.77	0.50
2:G:99:TYR:HA	2:G:136:VAL:O	2.11	0.50
1:A:220:GLU:OE1	1:A:271:ARG:NH2	2.36	0.50
2:G:119:GLU:O	2:G:123:GLU:HG2	2.12	0.49
2:F:65:PHE:O	2:F:68:PHE:HB3	2.13	0.49
1:B:315:LEU:O	1:B:319:ILE:HG12	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:ARG:HG3	1:A:343:SER:O	2.12	0.49
1:B:260:ILE:HB	1:B:261:PRO:HD3	1.94	0.49
1:B:370:CYS:SG	4:B:605:CLR:H11	2.53	0.49
3:B:606:POV:H21A	4:B:607:CLR:C18	2.40	0.49
2:G:138:TYR:HA	2:G:141:PHE:CD2	2.48	0.49
1:A:428:ARG:O	1:A:432:LEU:HG	2.13	0.49
1:A:433:ILE:HG12	1:A:451:HIS:HB3	1.95	0.48
1:B:330:ARG:HG3	1:B:343:SER:O	2.14	0.48
1:D:279:LEU:HD22	1:D:280:PHE:CE1	2.49	0.48
1:C:282:ASP:O	1:C:286:ARG:HG2	2.13	0.48
1:C:392:VAL:O	1:C:396:LYS:HG3	2.14	0.48
1:A:480:VAL:O	1:A:481:ASP:C	2.54	0.48
1:B:171:LYS:NZ	1:B:255:ASP:OD2	2.37	0.48
2:G:92:PHE:HE1	1:A:420:LYS:HD2	1.77	0.48
2:F:100:ILE:CG2	2:F:136:VAL:HB	2.43	0.48
1:D:238:THR:HG22	1:D:249:THR:HG22	1.96	0.48
1:A:316:VAL:HG12	4:A:614:CLR:H72	1.96	0.48
1:A:429:GLU:O	1:A:433:ILE:HG13	2.14	0.48
1:A:454:LYS:CE	3:A:604:POV:O21	2.62	0.48
1:D:220:GLU:OE1	1:D:271:ARG:NH2	2.36	0.48
1:A:304:THR:HA	1:A:307:THR:HG22	1.96	0.48
1:A:370:CYS:HB2	4:A:611:CLR:H192	1.95	0.47
1:A:182:LEU:O	1:A:186:ILE:HG12	2.14	0.47
1:A:370:CYS:HB2	4:A:611:CLR:C19	2.44	0.47
2:H:66:PRO:O	2:H:70:THR:HG23	2.14	0.47
2:E:48:LEU:O	2:E:52:ILE:HG12	2.14	0.47
1:C:295:ASN:OD1	1:C:295:ASN:N	2.43	0.47
1:B:204:ASP:OD2	1:B:206:ARG:HD2	2.14	0.47
1:C:238:THR:HG22	1:C:249:THR:HG22	1.96	0.47
2:E:49:GLN:HA	2:E:49:GLN:HE21	1.78	0.47
2:E:72:MET:HE1	6:E:204:A1B92:C2	2.44	0.47
2:E:83:GLU:O	2:E:87:GLU:HG2	2.15	0.47
1:A:238:THR:HG22	1:A:249:THR:HG22	1.96	0.47
1:B:304:THR:HA	1:B:307:THR:HG22	1.96	0.47
1:B:238:THR:HG22	1:B:249:THR:HG22	1.96	0.47
1:D:155:LEU:HB3	1:D:160:TYR:CE2	2.50	0.47
1:C:304:THR:HA	1:C:307:THR:HG22	1.97	0.46
2:G:105:LEU:O	2:G:109:MET:HG2	2.15	0.46
2:E:107:HIS:HA	2:E:110:THR:HG22	1.97	0.46
2:E:47:GLU:O	2:E:51:MET:HG3	2.15	0.46
1:D:330:ARG:HG3	1:D:343:SER:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:356:PHE:CZ	1:C:382:GLY:HA2	2.50	0.46
2:G:84:GLU:HG3	1:A:459:ILE:HD13	1.98	0.46
2:H:100:ILE:CG2	2:H:136:VAL:HB	2.46	0.46
1:B:280:PHE:CZ	1:B:301:VAL:HG13	2.50	0.46
1:C:393:VAL:HA	1:C:396:LYS:HD2	1.97	0.46
2:E:87:GLU:O	2:E:91:VAL:HG23	2.16	0.46
2:G:138:TYR:HA	2:G:141:PHE:HD2	1.81	0.46
2:F:12:PHE:HB3	2:F:68:PHE:CE2	2.51	0.46
4:A:611:CLR:H222	4:A:611:CLR:H162	1.71	0.45
2:H:7:GLU:O	2:H:11:GLU:HG3	2.16	0.45
3:B:609:POV:H211	3:B:609:POV:H28A	1.59	0.45
2:G:21:LYS:H	2:G:21:LYS:HG2	1.60	0.45
2:E:68:PHE:CE1	2:E:72:MET:HE3	2.51	0.45
3:A:610:POV:H211	3:A:610:POV:H28A	1.59	0.45
3:A:612:POV:H211	3:A:612:POV:H28A	1.59	0.45
1:C:280:PHE:CZ	1:C:301:VAL:HG13	2.51	0.45
2:G:47:GLU:HB3	2:G:51:MET:HE3	1.99	0.45
2:E:55:VAL:HG23	2:E:71:MET:HB2	1.98	0.45
2:F:55:VAL:HG11	2:F:63:ILE:HD11	1.96	0.45
2:F:109:MET:HE2	2:F:124:MET:HE1	1.99	0.45
1:A:331:ALA:HA	1:A:334:ARG:HD3	1.99	0.45
1:C:404:LYS:HB2	1:C:404:LYS:HE3	1.74	0.45
2:H:119:GLU:O	2:H:123:GLU:HG2	2.17	0.45
4:B:607:CLR:H222	4:B:607:CLR:H162	1.74	0.45
1:C:351:LEU:HD21	1:C:366:PRO:HD3	1.99	0.45
2:F:21:LYS:HE2	2:F:21:LYS:HB3	1.84	0.45
1:B:370:CYS:CB	4:B:605:CLR:H11	2.47	0.45
1:C:433:ILE:HD11	1:C:452:GLN:HA	1.99	0.45
2:F:66:PRO:O	2:F:70:THR:HG23	2.16	0.45
1:A:280:PHE:CE2	1:A:301:VAL:HG22	2.52	0.45
2:G:83:GLU:O	2:G:87:GLU:HG2	2.17	0.44
1:D:155:LEU:HB3	1:D:160:TYR:HE2	1.82	0.44
1:D:433:ILE:HD11	1:D:452:GLN:HA	1.99	0.44
1:C:212:GLU:O	1:C:213:ARG:C	2.60	0.44
2:G:105:LEU:HD22	2:G:136:VAL:HG21	1.98	0.44
2:E:99:TYR:CD2	2:E:135:GLN:HB3	2.53	0.44
2:F:21:LYS:H	2:F:21:LYS:HG2	1.60	0.44
1:B:341:VAL:HG13	1:B:342:THR:H	1.83	0.44
1:B:438:LYS:HE3	1:B:438:LYS:HB3	1.85	0.44
2:E:68:PHE:O	2:E:72:MET:HG2	2.18	0.44
1:D:320:SER:HB2	4:D:608:CLR:H6	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:607:POV:H28A	3:D:607:POV:H211	1.61	0.44
1:C:185:ILE:HD13	1:C:185:ILE:HA	1.90	0.44
2:F:107:HIS:O	2:F:111:ASN:HB2	2.18	0.44
1:B:331:ALA:HA	1:B:334:ARG:HD3	1.99	0.44
1:D:320:SER:CB	4:D:608:CLR:H6	2.48	0.44
2:H:107:HIS:O	2:H:111:ASN:HB2	2.18	0.44
2:F:82:GLU:O	2:F:86:ARG:HG3	2.18	0.44
1:A:185:ILE:HD13	1:A:185:ILE:HA	1.90	0.44
1:C:212:GLU:HG2	1:C:213:ARG:H	1.82	0.43
2:H:82:GLU:O	2:H:86:ARG:HG3	2.18	0.43
1:C:257:ILE:HG12	4:C:605:CLR:C6	2.43	0.43
1:C:291:LEU:HD11	2:G:71:MET:HE2	2.00	0.43
1:D:331:ALA:HA	1:D:334:ARG:HD3	1.99	0.43
2:F:55:VAL:HG11	2:F:63:ILE:HD13	2.01	0.43
1:B:291:LEU:HD23	1:B:291:LEU:HA	1.86	0.43
4:B:605:CLR:H222	4:B:605:CLR:H162	1.77	0.43
2:F:70:THR:O	2:F:74:ARG:HG3	2.17	0.43
1:D:370:CYS:HB2	4:D:606:CLR:C1	2.49	0.43
2:H:21:LYS:HE2	2:H:21:LYS:HB3	1.83	0.43
1:A:428:ARG:HE	1:A:432:LEU:HD11	1.83	0.43
1:B:433:ILE:O	1:B:437:THR:HG22	2.18	0.43
1:A:479:LEU:O	1:A:480:VAL:C	2.62	0.43
1:B:316:VAL:CG1	3:B:606:POV:H21B	2.48	0.43
1:D:457:GLN:HE22	3:D:601:POV:H25A	1.83	0.43
1:C:280:PHE:HE1	1:C:304:THR:HG21	1.84	0.43
2:G:68:PHE:CZ	2:G:72:MET:HE3	2.54	0.43
2:F:65:PHE:CE1	2:F:69:LEU:HD11	2.53	0.43
1:B:282:ASP:O	1:B:286:ARG:HG2	2.18	0.43
2:E:21:LYS:HE2	2:E:21:LYS:HB3	1.84	0.43
1:C:330:ARG:HG3	1:C:343:SER:O	2.19	0.42
1:C:403:GLU:HB3	1:D:300:PHE:HE1	1.84	0.42
1:A:428:ARG:NE	1:A:432:LEU:HD11	2.34	0.42
1:D:437:THR:HG23	1:D:438:LYS:HG2	2.01	0.42
4:C:605:CLR:H222	4:C:605:CLR:H162	1.80	0.42
2:G:116:LEU:HD21	1:A:432:LEU:HD21	2.01	0.42
2:E:68:PHE:CZ	2:E:72:MET:HE3	2.54	0.42
1:A:352:ILE:HG23	1:A:378:THR:HG21	2.01	0.42
1:D:352:ILE:HG23	1:D:378:THR:HG21	2.01	0.42
1:C:428:ARG:NH1	2:E:114:GLU:HG3	2.35	0.42
1:C:452:GLN:O	1:C:456:LEU:HG	2.19	0.42
2:G:109:MET:O	2:G:115:LYS:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:441:LYS:HG3	1:C:442:LYS:N	2.34	0.42
2:F:99:TYR:CE1	2:F:137:ASN:HB2	2.54	0.42
1:B:183:GLY:O	1:B:186:ILE:CG2	2.61	0.42
1:C:434:TYR:CD1	1:C:438:LYS:HG3	2.54	0.42
2:G:139:GLU:O	2:G:140:GLU:C	2.63	0.42
1:D:473:ASN:O	1:D:474:ASP:C	2.61	0.42
4:D:608:CLR:H8	4:D:608:CLR:H182	1.81	0.42
1:C:291:LEU:HD23	1:C:291:LEU:HA	1.86	0.42
1:B:202:ALA:HB1	1:B:207:ILE:HD12	2.02	0.42
1:B:480:VAL:O	1:B:481:ASP:C	2.61	0.42
2:G:101:SER:HB3	2:G:104:GLU:HB3	2.01	0.42
2:F:137:ASN:ND2	2:F:138:TYR:H	2.18	0.42
1:A:437:THR:HG23	1:A:438:LYS:HG2	2.01	0.42
1:B:429:GLU:O	1:B:433:ILE:HG13	2.20	0.42
1:B:320:SER:CB	4:B:607:CLR:H41	2.49	0.41
1:C:305:LEU:HD23	1:C:305:LEU:HA	1.93	0.41
1:C:370:CYS:O	1:C:374:VAL:HG23	2.20	0.41
1:C:417:LYS:HE3	1:C:417:LYS:HB2	1.70	0.41
2:H:137:ASN:ND2	2:H:138:TYR:H	2.18	0.41
2:F:69:LEU:C	2:F:71:MET:N	2.76	0.41
1:C:257:ILE:CG1	4:C:605:CLR:H6	2.45	0.41
1:B:352:ILE:HG23	1:B:378:THR:HG21	2.01	0.41
1:B:437:THR:HG23	1:B:438:LYS:HG2	2.01	0.41
2:H:13:LYS:HD2	2:H:13:LYS:HA	1.85	0.41
1:A:363:ASP:OD2	1:B:242:ALA:O	2.38	0.41
2:H:91:VAL:HG12	2:H:92:PHE:CD1	2.56	0.41
1:A:341:VAL:HG23	1:A:342:THR:H	1.85	0.41
1:B:186:ILE:HG23	1:B:187:VAL:N	2.36	0.41
2:H:51:MET:HE3	6:H:204:A1B92:C18	2.50	0.41
2:F:38:SER:C	2:F:40:GLY:H	2.29	0.41
4:A:611:CLR:H182	4:A:611:CLR:H8	1.78	0.41
3:B:606:POV:H22A	3:B:606:POV:H25	1.91	0.41
2:F:36:MET:HG2	2:F:41:GLN:O	2.20	0.41
1:C:242:ALA:HB2	1:C:367:ASN:OD1	2.20	0.41
4:C:606:CLR:H8	4:C:606:CLR:H182	1.81	0.41
2:G:106:ARG:O	2:G:110:THR:HG22	2.20	0.41
1:A:466:LYS:HB3	1:A:466:LYS:HE2	1.87	0.41
1:D:295:ASN:OD1	1:D:295:ASN:N	2.43	0.41
2:G:91:VAL:HG12	2:G:92:PHE:CD1	2.56	0.41
1:D:183:GLY:O	1:D:186:ILE:CG2	2.62	0.41
1:D:479:LEU:O	1:D:480:VAL:C	2.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:606:CLR:H193	4:D:606:CLR:H111	1.79	0.41
3:C:604:POV:H211	3:C:604:POV:H28A	1.68	0.40
2:H:11:GLU:O	2:H:12:PHE:C	2.63	0.40
2:F:91:VAL:HG12	2:F:92:PHE:CD1	2.56	0.40
1:B:432:LEU:HB3	1:B:451:HIS:CD2	2.56	0.40
1:D:185:ILE:HD13	1:D:185:ILE:HA	1.90	0.40
1:C:352:ILE:HG23	1:C:378:THR:HG21	2.03	0.40
2:G:13:LYS:HE2	2:G:13:LYS:HB2	1.89	0.40
2:G:89:PHE:HB2	2:G:141:PHE:CZ	2.57	0.40
2:E:71:MET:O	2:E:75:LYS:HG2	2.21	0.40
2:E:43:PRO:HB3	2:E:47:GLU:CD	2.46	0.40
1:D:155:LEU:HD23	1:D:155:LEU:HA	1.93	0.40
1:B:320:SER:HB3	4:B:607:CLR:H41	2.02	0.40
1:D:186:ILE:HG23	1:D:187:VAL:N	2.36	0.40
3:D:605:POV:H211	3:D:605:POV:H28A	1.72	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	375/579 (65%)	359 (96%)	16 (4%)	0	100	100
1	B	375/579 (65%)	362 (96%)	13 (4%)	0	100	100
1	C	374/579 (65%)	368 (98%)	6 (2%)	0	100	100
1	D	375/579 (65%)	364 (97%)	11 (3%)	0	100	100
2	E	141/149 (95%)	138 (98%)	3 (2%)	0	100	100
2	F	141/149 (95%)	134 (95%)	7 (5%)	0	100	100
2	G	141/149 (95%)	132 (94%)	9 (6%)	0	100	100
2	H	141/149 (95%)	136 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2063/2912 (71%)	1993 (97%)	70 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	309/486 (64%)	308 (100%)	1 (0%)	86	84
1	B	302/486 (62%)	301 (100%)	1 (0%)	86	84
1	C	306/486 (63%)	306 (100%)	0	100	100
1	D	308/486 (63%)	306 (99%)	2 (1%)	78	79
2	E	99/127 (78%)	99 (100%)	0	100	100
2	F	96/127 (76%)	95 (99%)	1 (1%)	68	74
2	G	93/127 (73%)	93 (100%)	0	100	100
2	H	99/127 (78%)	98 (99%)	1 (1%)	68	74
All	All	1612/2452 (66%)	1606 (100%)	6 (0%)	81	82

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	7	GLU
2	F	6	GLU
1	A	364	MET
1	B	364	MET
1	D	341	VAL
1	D	364	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	336	HIS

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Mol	Chain	Res	Type
1	C	405	HIS
1	C	457	GLN
1	C	475	GLN
1	C	477	ASN
2	G	41	GLN
2	H	137	ASN
2	E	41	GLN
2	E	49	GLN
2	E	111	ASN
2	E	137	ASN
2	F	41	GLN
2	F	137	ASN
1	A	336	HIS
1	A	338	GLN
1	B	336	HIS
1	B	414	GLN
1	D	336	HIS
1	D	339	GLN
1	D	451	HIS
1	D	457	GLN

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 59 ligands modelled in this entry, 15 are monoatomic - leaving 44 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
3	POV	B	609	-	32,32,51	1.17	2 (6%)	35,37,59	1.31	4 (11%)
3	POV	D	605	-	13,13,51	1.28	1 (7%)	13,13,59	1.09	0
4	CLR	C	605	-	31,31,31	0.87	2 (6%)	48,48,48	1.48	8 (16%)
3	POV	C	608	-	32,32,51	1.17	2 (6%)	35,37,59	1.27	4 (11%)
6	A1B92	E	204	-	30,30,30	2.85	11 (36%)	41,43,43	2.38	15 (36%)
3	POV	A	607	-	15,15,51	1.19	1 (6%)	15,15,59	1.00	0
3	POV	A	606	-	19,19,51	1.06	1 (5%)	19,19,59	0.92	1 (5%)
3	POV	A	610	-	13,13,51	1.28	1 (7%)	13,13,59	1.10	1 (7%)
3	POV	A	613	-	24,24,51	1.02	1 (4%)	27,27,59	1.06	2 (7%)
3	POV	C	603	-	12,12,51	1.34	1 (8%)	12,12,59	1.15	1 (8%)
4	CLR	A	611	-	31,31,31	0.85	2 (6%)	48,48,48	1.49	9 (18%)
4	CLR	A	614	-	31,31,31	0.84	1 (3%)	48,48,48	1.43	8 (16%)
3	POV	C	601	-	9,9,51	1.52	1 (11%)	9,9,59	1.18	1 (11%)
4	CLR	D	608	-	31,31,31	0.83	1 (3%)	48,48,48	1.43	8 (16%)
6	A1B92	B	610	-	30,30,30	2.85	11 (36%)	41,43,43	2.38	16 (39%)
3	POV	D	603	-	15,15,51	1.19	1 (6%)	15,15,59	1.00	0
4	CLR	C	606	-	31,31,31	0.84	2 (6%)	48,48,48	1.43	7 (14%)
3	POV	A	605	-	9,9,51	1.53	1 (11%)	9,9,59	1.18	1 (11%)
6	A1B92	G	204	-	30,30,30	2.85	11 (36%)	41,43,43	2.37	14 (34%)
3	POV	A	615	-	10,10,51	1.45	1 (10%)	10,10,59	1.17	1 (10%)
3	POV	D	609	-	10,10,51	1.45	1 (10%)	10,10,59	1.16	1 (10%)
4	CLR	D	606	-	31,31,31	0.86	2 (6%)	48,48,48	1.45	8 (16%)
3	POV	D	601	-	19,19,51	1.07	1 (5%)	19,19,59	0.91	0
3	POV	D	604	-	12,12,51	1.34	1 (8%)	12,12,59	1.15	1 (8%)
3	POV	B	601	-	19,19,51	1.05	1 (5%)	19,19,59	0.94	1 (5%)
3	POV	C	602	-	15,15,51	1.19	1 (6%)	15,15,59	1.00	1 (6%)
3	POV	A	604	-	19,19,51	1.06	1 (5%)	19,19,59	0.95	1 (5%)
3	POV	C	607	-	10,10,51	1.44	1 (10%)	10,10,59	1.15	0
3	POV	A	608	-	12,12,51	1.34	1 (8%)	12,12,59	1.15	1 (8%)
4	CLR	B	605	-	31,31,31	0.87	2 (6%)	48,48,48	1.47	8 (16%)
3	POV	D	607	-	32,32,51	1.18	2 (6%)	35,37,59	1.31	4 (11%)
3	POV	C	609	-	24,24,51	1.02	1 (4%)	27,27,59	1.05	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	POV	A	609	-	13,13,51	1.28	1 (7%)	13,13,59	1.12	1 (7%)
3	POV	B	602	-	9,9,51	1.52	1 (11%)	9,9,59	1.19	1 (11%)
3	POV	B	603	-	15,15,51	1.19	1 (6%)	15,15,59	1.00	0
3	POV	D	602	-	10,10,51	1.45	1 (10%)	10,10,59	1.16	1 (10%)
3	POV	B	608	-	10,10,51	1.45	1 (10%)	10,10,59	1.15	0
3	POV	C	604	-	13,13,51	1.28	1 (7%)	13,13,59	1.09	0
4	CLR	B	607	-	31,31,31	0.83	1 (3%)	48,48,48	1.53	9 (18%)
3	POV	A	612	-	32,32,51	1.17	2 (6%)	35,37,59	1.31	4 (11%)
6	A1B92	H	204	-	30,30,30	2.85	11 (36%)	41,43,43	2.37	14 (34%)
3	POV	B	606	-	26,26,51	0.97	1 (3%)	29,29,59	1.02	2 (6%)
3	POV	D	610	-	24,24,51	1.01	1 (4%)	27,27,59	1.04	2 (7%)
3	POV	B	604	-	12,12,51	1.34	1 (8%)	12,12,59	1.15	1 (8%)

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
3	POV	B	609	-	-	6/34/34/55	-
3	POV	D	605	-	-	2/11/11/55	-
4	CLR	C	605	-	-	2/10/68/68	0/4/4/4
3	POV	C	608	-	-	4/34/34/55	-
6	A1B92	E	204	-	-	6/12/32/32	0/4/4/4
3	POV	A	607	-	-	2/13/13/55	-
3	POV	A	606	-	-	4/17/17/55	-
3	POV	A	610	-	-	2/11/11/55	-
3	POV	A	613	-	-	0/23/23/55	-
3	POV	C	603	-	-	2/10/10/55	-
4	CLR	A	611	-	-	3/10/68/68	0/4/4/4
4	CLR	A	614	-	-	0/10/68/68	0/4/4/4
3	POV	C	601	-	-	2/7/7/55	-
4	CLR	D	608	-	-	0/10/68/68	0/4/4/4
6	A1B92	B	610	-	-	6/12/32/32	0/4/4/4
3	POV	D	603	-	-	2/13/13/55	-
4	CLR	C	606	-	-	0/10/68/68	0/4/4/4
3	POV	A	605	-	-	2/7/7/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	A1B92	G	204	-	-	6/12/32/32	0/4/4/4
3	POV	A	615	-	-	2/8/8/55	-
3	POV	D	609	-	-	2/8/8/55	-
4	CLR	D	606	-	-	2/10/68/68	0/4/4/4
3	POV	D	601	-	-	4/17/17/55	-
3	POV	D	604	-	-	2/10/10/55	-
3	POV	B	601	-	-	2/17/17/55	-
3	POV	C	602	-	-	2/13/13/55	-
3	POV	A	604	-	-	2/17/17/55	-
3	POV	C	607	-	-	2/8/8/55	-
3	POV	A	608	-	-	2/10/10/55	-
4	CLR	B	605	-	-	1/10/68/68	0/4/4/4
3	POV	D	607	-	-	5/34/34/55	-
3	POV	C	609	-	-	1/23/23/55	-
3	POV	A	609	-	-	3/11/11/55	-
3	POV	B	602	-	-	2/7/7/55	-
3	POV	B	603	-	-	2/13/13/55	-
3	POV	D	602	-	-	2/8/8/55	-
3	POV	B	608	-	-	2/8/8/55	-
3	POV	C	604	-	-	2/11/11/55	-
4	CLR	B	607	-	-	3/10/68/68	0/4/4/4
3	POV	A	612	-	-	6/34/34/55	-
6	A1B92	H	204	-	-	6/12/32/32	0/4/4/4
3	POV	B	606	-	-	2/25/25/55	-
3	POV	D	610	-	-	3/23/23/55	-
3	POV	B	604	-	-	2/10/10/55	-

All (93) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	204	A1B92	C8-N2	7.03	1.47	1.34
6	H	204	A1B92	C8-N2	7.02	1.47	1.34
6	E	204	A1B92	C8-N2	7.01	1.47	1.34
6	B	610	A1B92	C8-N2	6.98	1.47	1.34
6	G	204	A1B92	C8-N5	6.53	1.46	1.34
6	H	204	A1B92	C8-N5	6.51	1.46	1.34
6	E	204	A1B92	C8-N5	6.51	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	610	A1B92	C8-N5	6.50	1.46	1.34
6	H	204	A1B92	C18-C13	6.15	1.48	1.39
6	B	610	A1B92	C18-C13	6.14	1.48	1.39
6	G	204	A1B92	C18-C13	6.12	1.48	1.39
6	E	204	A1B92	C18-C13	6.10	1.48	1.39
6	E	204	A1B92	C13-N5	5.82	1.43	1.34
6	G	204	A1B92	C13-N5	5.77	1.43	1.34
6	B	610	A1B92	C13-N5	5.77	1.43	1.34
6	H	204	A1B92	C13-N5	5.75	1.43	1.34
6	B	610	A1B92	C7-N2	4.90	1.44	1.34
6	G	204	A1B92	C7-N2	4.90	1.44	1.34
6	H	204	A1B92	C7-N2	4.87	1.44	1.34
6	E	204	A1B92	C7-N2	4.85	1.44	1.34
3	B	604	POV	O21-C21	4.56	1.45	1.30
3	D	604	POV	O21-C21	4.56	1.45	1.30
3	A	608	POV	O21-C21	4.56	1.45	1.30
3	A	615	POV	O21-C21	4.56	1.45	1.30
3	D	601	POV	O21-C21	4.56	1.45	1.30
3	C	602	POV	O21-C21	4.55	1.45	1.30
3	A	604	POV	O21-C21	4.55	1.45	1.30
3	D	602	POV	O21-C21	4.55	1.45	1.30
3	B	608	POV	O21-C21	4.55	1.45	1.30
3	B	603	POV	O21-C21	4.55	1.45	1.30
3	C	603	POV	O21-C21	4.54	1.45	1.30
3	D	605	POV	O21-C21	4.54	1.45	1.30
3	D	609	POV	O21-C21	4.54	1.45	1.30
3	A	606	POV	O21-C21	4.54	1.45	1.30
3	C	601	POV	O21-C21	4.53	1.45	1.30
3	A	605	POV	O21-C21	4.53	1.45	1.30
3	A	610	POV	O21-C21	4.53	1.45	1.30
3	C	607	POV	O21-C21	4.53	1.45	1.30
3	D	603	POV	O21-C21	4.52	1.45	1.30
3	A	607	POV	O21-C21	4.52	1.45	1.30
3	A	609	POV	O21-C21	4.52	1.45	1.30
3	C	604	POV	O21-C21	4.52	1.45	1.30
3	B	601	POV	O21-C21	4.51	1.45	1.30
3	B	602	POV	O21-C21	4.51	1.45	1.30
3	C	609	POV	O21-C21	4.29	1.45	1.33
3	A	613	POV	O21-C21	4.28	1.45	1.33
3	C	608	POV	O31-C31	4.25	1.45	1.33
3	B	609	POV	O31-C31	4.25	1.45	1.33
3	D	610	POV	O21-C21	4.25	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	606	POV	O21-C21	4.23	1.45	1.33
3	D	607	POV	O31-C31	4.22	1.45	1.33
3	A	612	POV	O31-C31	4.22	1.45	1.33
3	D	607	POV	O21-C21	4.09	1.45	1.34
3	B	609	POV	O21-C21	4.06	1.45	1.34
3	C	608	POV	O21-C21	4.06	1.45	1.34
3	A	612	POV	O21-C21	4.02	1.45	1.34
6	G	204	A1B92	C18-C7	3.53	1.48	1.39
6	H	204	A1B92	C18-C7	3.53	1.48	1.39
6	E	204	A1B92	C18-C7	3.53	1.48	1.39
6	B	610	A1B92	C18-C7	3.51	1.48	1.39
6	H	204	A1B92	C7-N1	3.45	1.44	1.37
6	G	204	A1B92	C7-N1	3.43	1.44	1.37
6	B	610	A1B92	C7-N1	3.42	1.44	1.37
6	E	204	A1B92	C7-N1	3.39	1.44	1.37
6	E	204	A1B92	C9-N3	-2.60	1.32	1.35
6	B	610	A1B92	C9-N3	-2.59	1.32	1.35
6	H	204	A1B92	C9-N3	-2.56	1.32	1.35
6	G	204	A1B92	C9-N3	-2.55	1.32	1.35
6	E	204	A1B92	C13-N6	2.46	1.43	1.37
6	B	610	A1B92	C13-N6	2.43	1.43	1.37
6	G	204	A1B92	C13-N6	2.42	1.43	1.37
6	H	204	A1B92	C13-N6	2.42	1.43	1.37
6	E	204	A1B92	C8-N3	2.23	1.44	1.40
6	B	610	A1B92	C8-N3	2.22	1.44	1.40
4	C	605	CLR	C10-C9	-2.21	1.52	1.56
4	B	605	CLR	C10-C9	-2.20	1.52	1.56
6	H	204	A1B92	C8-N3	2.19	1.44	1.40
6	G	204	A1B92	C8-N3	2.18	1.44	1.40
4	A	611	CLR	C13-C14	-2.16	1.51	1.55
4	D	606	CLR	C13-C14	-2.16	1.51	1.55
4	C	605	CLR	C13-C14	-2.13	1.51	1.55
4	D	606	CLR	C10-C9	-2.12	1.52	1.56
4	B	605	CLR	C13-C14	-2.11	1.51	1.55
6	H	204	A1B92	C10-C11	-2.11	1.35	1.40
6	E	204	A1B92	C10-C11	-2.10	1.35	1.40
4	A	614	CLR	C13-C14	-2.09	1.51	1.55
6	G	204	A1B92	C10-C11	-2.09	1.35	1.40
4	A	611	CLR	C10-C9	-2.08	1.52	1.56
4	B	607	CLR	C13-C14	-2.08	1.51	1.55
6	B	610	A1B92	C10-C11	-2.07	1.35	1.40
4	D	608	CLR	C13-C14	-2.07	1.51	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	606	CLR	C13-C14	-2.06	1.51	1.55
4	C	606	CLR	C10-C9	-2.02	1.52	1.56

All (164) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	204	A1B92	C11-N4-N3	4.96	107.17	104.66
6	B	610	A1B92	C11-N4-N3	4.93	107.16	104.66
6	G	204	A1B92	C11-N4-N3	4.90	107.15	104.66
6	E	204	A1B92	C11-N4-N3	4.87	107.13	104.66
6	H	204	A1B92	C10-C11-N4	-4.82	108.65	111.05
6	G	204	A1B92	C8-N3-N4	4.82	125.17	121.49
6	E	204	A1B92	C3-C2-C1	-4.82	108.08	110.75
6	E	204	A1B92	C10-C11-N4	-4.82	108.65	111.05
6	B	610	A1B92	C10-C11-N4	-4.81	108.66	111.05
6	B	610	A1B92	C8-N3-N4	4.77	125.13	121.49
6	G	204	A1B92	C10-C11-N4	-4.77	108.67	111.05
6	B	610	A1B92	C3-C2-C1	-4.74	108.12	110.75
6	H	204	A1B92	C8-N3-N4	4.69	125.07	121.49
6	E	204	A1B92	C8-N3-N4	4.69	125.06	121.49
6	G	204	A1B92	C3-C2-C1	-4.67	108.16	110.75
6	H	204	A1B92	C3-C2-C1	-4.54	108.24	110.75
6	E	204	A1B92	C12-C11-N4	4.37	125.75	120.24
6	B	610	A1B92	C12-C11-N4	4.35	125.72	120.24
6	H	204	A1B92	C12-C11-N4	4.32	125.69	120.24
6	G	204	A1B92	C12-C11-N4	4.32	125.68	120.24
6	G	204	A1B92	N2-C8-N3	4.16	121.94	115.90
6	H	204	A1B92	N2-C8-N3	4.14	121.91	115.90
3	C	608	POV	O21-C21-C22	4.08	120.32	111.48
6	B	610	A1B92	N2-C8-N3	4.05	121.78	115.90
6	E	204	A1B92	N2-C8-N3	4.04	121.77	115.90
3	A	612	POV	O21-C21-C22	4.04	120.22	111.48
3	B	609	POV	O21-C21-C22	4.03	120.19	111.48
4	C	605	CLR	C13-C17-C20	-4.02	113.28	119.50
3	D	607	POV	O21-C21-C22	4.01	120.15	111.48
4	D	606	CLR	C13-C17-C20	-3.95	113.39	119.50
4	A	611	CLR	C13-C17-C20	-3.93	113.43	119.50
6	G	204	A1B92	N5-C8-N2	-3.90	119.34	126.27
6	B	610	A1B92	N5-C8-N2	-3.89	119.36	126.27
6	H	204	A1B92	N5-C8-N2	-3.87	119.39	126.27
6	E	204	A1B92	N5-C8-N2	-3.86	119.40	126.27
4	A	611	CLR	C13-C14-C8	-3.86	108.93	114.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	607	CLR	C13-C17-C20	-3.84	113.56	119.50
4	B	605	CLR	C13-C17-C20	-3.83	113.58	119.50
6	H	204	A1B92	C9-C10-C11	3.80	108.15	105.83
6	E	204	A1B92	C9-C10-C11	3.76	108.13	105.83
6	G	204	A1B92	C9-C10-C11	3.70	108.09	105.83
4	C	605	CLR	C13-C14-C8	-3.67	109.21	114.41
6	B	610	A1B92	C9-C10-C11	3.67	108.07	105.83
4	B	605	CLR	C13-C14-C8	-3.60	109.30	114.41
4	D	608	CLR	C13-C14-C8	-3.60	109.31	114.41
4	A	614	CLR	C13-C17-C20	-3.59	113.95	119.50
4	D	606	CLR	C13-C14-C8	-3.57	109.34	114.41
4	C	606	CLR	C13-C17-C20	-3.57	113.98	119.50
4	A	614	CLR	C13-C14-C8	-3.56	109.36	114.41
4	D	608	CLR	C13-C17-C20	-3.56	114.00	119.50
4	C	606	CLR	C13-C14-C8	-3.55	109.37	114.41
4	B	607	CLR	C8-C7-C6	-3.53	107.87	112.76
4	A	611	CLR	C17-C13-C14	3.47	104.08	100.10
4	B	607	CLR	C13-C14-C8	-3.39	109.60	114.41
4	C	605	CLR	C17-C13-C14	3.31	103.90	100.10
4	D	606	CLR	C17-C13-C14	3.29	103.88	100.10
4	B	605	CLR	C17-C13-C14	3.29	103.88	100.10
4	D	606	CLR	C11-C12-C13	-3.20	107.34	112.74
6	G	204	A1B92	C9-N3-N4	-3.20	108.92	111.66
6	H	204	A1B92	C9-N3-N4	-3.17	108.94	111.66
4	C	605	CLR	C11-C12-C13	-3.17	107.40	112.74
6	E	204	A1B92	C9-N3-N4	-3.12	108.98	111.66
6	B	610	A1B92	C9-N3-N4	-3.12	108.99	111.66
4	B	607	CLR	C11-C12-C13	-3.10	107.51	112.74
4	D	608	CLR	C17-C13-C14	3.04	103.58	100.10
4	B	605	CLR	C11-C12-C13	-3.03	107.63	112.74
4	C	606	CLR	C17-C13-C14	3.02	103.57	100.10
4	A	614	CLR	C17-C13-C14	3.01	103.55	100.10
4	B	607	CLR	C17-C13-C14	2.99	103.53	100.10
4	A	611	CLR	C8-C7-C6	-2.95	108.67	112.76
4	A	611	CLR	C11-C12-C13	-2.95	107.77	112.74
4	C	606	CLR	C8-C7-C6	-2.93	108.70	112.76
4	D	608	CLR	C8-C7-C6	-2.89	108.75	112.76
4	A	614	CLR	C8-C7-C6	-2.88	108.77	112.76
4	C	605	CLR	C8-C7-C6	-2.86	108.80	112.76
6	H	204	A1B92	C2-C1-C4	-2.86	111.49	114.33
4	D	608	CLR	C11-C12-C13	-2.86	107.92	112.74
4	A	614	CLR	C11-C12-C13	-2.86	107.92	112.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	606	CLR	C11-C12-C13	-2.85	107.93	112.74
6	G	204	A1B92	C2-C1-C4	-2.84	111.52	114.33
3	D	607	POV	C2-O21-C21	-2.84	111.01	117.80
6	E	204	A1B92	C2-C1-C4	-2.83	111.52	114.33
6	B	610	A1B92	C2-C1-C4	-2.81	111.54	114.33
3	A	612	POV	C2-O21-C21	-2.80	111.11	117.80
4	B	605	CLR	C8-C7-C6	-2.79	108.89	112.76
3	B	609	POV	C2-O21-C21	-2.77	111.17	117.80
3	A	613	POV	O21-C21-C22	2.76	120.24	111.83
3	C	609	POV	O21-C21-C22	2.72	120.13	111.83
3	D	610	POV	O21-C21-C22	2.70	120.08	111.83
3	B	609	POV	O31-C31-C32	2.67	119.97	111.83
3	B	606	POV	O21-C21-C22	2.66	119.95	111.83
4	B	607	CLR	C3-C4-C5	-2.65	107.83	112.05
3	A	612	POV	O31-C31-C32	2.65	119.93	111.83
4	B	605	CLR	C11-C9-C10	-2.65	109.82	113.08
4	D	606	CLR	C11-C9-C10	-2.64	109.83	113.08
4	C	605	CLR	C11-C9-C10	-2.63	109.84	113.08
3	D	607	POV	O31-C31-C32	2.63	119.84	111.83
4	D	608	CLR	C11-C9-C10	-2.52	109.98	113.08
4	C	606	CLR	C11-C9-C10	-2.51	109.99	113.08
4	A	611	CLR	C11-C9-C10	-2.51	110.00	113.08
6	E	204	A1B92	C12-C11-C10	-2.49	125.60	128.51
6	B	610	A1B92	C8-N5-C13	2.48	119.91	115.02
4	A	614	CLR	C11-C9-C10	-2.47	110.03	113.08
6	B	610	A1B92	C12-C11-C10	-2.47	125.62	128.51
6	G	204	A1B92	C8-N5-C13	2.46	119.88	115.02
6	H	204	A1B92	C8-N5-C13	2.46	119.87	115.02
6	E	204	A1B92	C8-N5-C13	2.46	119.87	115.02
6	G	204	A1B92	C12-C11-C10	-2.45	125.64	128.51
3	C	608	POV	O31-C31-C32	2.44	119.26	111.83
4	D	606	CLR	C8-C7-C6	-2.43	109.39	112.76
6	H	204	A1B92	C12-C11-C10	-2.43	125.66	128.51
6	G	204	A1B92	C17-N6-C14	-2.37	106.24	111.57
6	H	204	A1B92	C17-N6-C14	-2.36	106.26	111.57
3	A	612	POV	O13-P-O14	2.36	120.02	110.83
3	C	608	POV	O13-P-O14	2.35	120.01	110.83
3	B	606	POV	O13-P-O14	2.35	120.01	110.83
3	C	609	POV	O13-P-O14	2.34	119.97	110.83
3	D	610	POV	O13-P-O14	2.34	119.95	110.83
3	A	613	POV	O13-P-O14	2.34	119.95	110.83
3	D	607	POV	O13-P-O14	2.33	119.93	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	610	A1B92	C17-N6-C14	-2.33	106.32	111.57
3	B	609	POV	O13-P-O14	2.32	119.89	110.83
6	E	204	A1B92	C17-N6-C14	-2.32	106.35	111.57
4	B	607	CLR	C11-C9-C10	-2.32	110.23	113.08
4	C	606	CLR	C3-C4-C5	-2.30	108.38	112.05
3	C	608	POV	C2-O21-C21	-2.29	112.32	117.80
4	A	611	CLR	C3-C4-C5	-2.27	108.44	112.05
6	E	204	A1B92	C7-C18-C13	2.25	118.44	116.64
4	D	608	CLR	C3-C4-C5	-2.24	108.48	112.05
4	A	614	CLR	C3-C4-C5	-2.21	108.53	112.05
4	B	605	CLR	C3-C4-C5	-2.20	108.55	112.05
6	B	610	A1B92	C7-C18-C13	2.20	118.40	116.64
4	D	606	CLR	C3-C4-C5	-2.20	108.55	112.05
4	C	605	CLR	C3-C4-C5	-2.19	108.56	112.05
3	B	604	POV	O21-C21-C22	2.17	120.86	114.00
3	A	608	POV	O21-C21-C22	2.17	120.86	114.00
6	H	204	A1B92	C7-C18-C13	2.17	118.38	116.64
3	D	604	POV	O21-C21-C22	2.17	120.84	114.00
4	B	607	CLR	C2-C3-C4	-2.16	107.25	110.29
6	G	204	A1B92	C7-C18-C13	2.16	118.37	116.64
3	C	603	POV	O21-C21-C22	2.16	120.81	114.00
4	B	607	CLR	C4-C5-C10	2.13	119.15	116.42
4	B	605	CLR	C19-C10-C9	-2.13	109.27	111.66
6	B	610	A1B92	C5-C4-C1	-2.11	109.58	110.75
4	A	611	CLR	C19-C10-C9	-2.11	109.29	111.66
3	A	609	POV	C23-C22-C21	-2.08	109.07	114.51
3	A	615	POV	C23-C22-C21	-2.07	109.10	114.51
3	A	605	POV	C23-C22-C21	-2.06	109.12	114.51
3	B	602	POV	C23-C22-C21	-2.06	109.12	114.51
4	A	611	CLR	C9-C10-C5	2.06	112.66	109.65
3	D	609	POV	C23-C22-C21	-2.05	109.15	114.51
4	C	605	CLR	C19-C10-C9	-2.05	109.36	111.66
4	D	606	CLR	C19-C10-C9	-2.04	109.37	111.66
6	B	610	A1B92	N5-C8-N3	2.04	118.86	115.90
3	A	606	POV	C23-C22-C21	-2.03	109.22	114.51
3	C	602	POV	C23-C22-C21	-2.02	109.23	114.51
4	D	608	CLR	C19-C10-C9	-2.02	109.39	111.66
6	E	204	A1B92	N5-C8-N3	2.02	118.83	115.90
3	C	601	POV	C23-C22-C21	-2.01	109.26	114.51
4	A	614	CLR	C19-C10-C9	-2.01	109.40	111.66
3	A	604	POV	C23-C22-C21	-2.01	109.27	114.51
3	D	602	POV	C23-C22-C21	-2.01	109.27	114.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	601	POV	C23-C22-C21	-2.00	109.28	114.51
3	A	610	POV	C23-C22-C21	-2.00	109.29	114.51

There are no chirality outliers.

All (115) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	608	POV	O22-C21-O21-C2
6	G	204	A1B92	C18-C13-N6-C14
6	G	204	A1B92	N5-C13-N6-C14
6	H	204	A1B92	C18-C13-N6-C14
6	H	204	A1B92	N5-C13-N6-C14
6	E	204	A1B92	C18-C13-N6-C14
6	E	204	A1B92	N5-C13-N6-C14
6	B	610	A1B92	C18-C13-N6-C14
6	B	610	A1B92	N5-C13-N6-C14
3	C	608	POV	C22-C21-O21-C2
3	B	609	POV	C32-C31-O31-C3
3	B	609	POV	O32-C31-O31-C3
3	A	612	POV	C32-C31-O31-C3
6	G	204	A1B92	N2-C8-N3-C9
6	G	204	A1B92	N5-C8-N3-C9
6	H	204	A1B92	N2-C8-N3-C9
6	H	204	A1B92	N5-C8-N3-C9
6	E	204	A1B92	N5-C8-N3-C9
6	B	610	A1B92	N5-C8-N3-C9
3	D	607	POV	C22-C21-O21-C2
3	A	612	POV	O32-C31-O31-C3
3	D	607	POV	O22-C21-O21-C2
3	A	612	POV	C22-C21-O21-C2
6	E	204	A1B92	N2-C8-N3-C9
6	B	610	A1B92	N2-C8-N3-C9
3	B	606	POV	C22-C21-O21-C2
3	A	612	POV	O22-C21-O21-C2
3	B	606	POV	O22-C21-O21-C2
6	G	204	A1B92	N2-C8-N3-N4
6	G	204	A1B92	N5-C8-N3-N4
6	H	204	A1B92	N2-C8-N3-N4
6	H	204	A1B92	N5-C8-N3-N4
6	E	204	A1B92	N2-C8-N3-N4
6	E	204	A1B92	N5-C8-N3-N4
6	B	610	A1B92	N2-C8-N3-N4

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Mol	Chain	Res	Type	Atoms
6	B	610	A1B92	N5-C8-N3-N4
3	D	601	POV	C25-C26-C27-C28
3	D	610	POV	O11-C1-C2-O21
3	B	609	POV	C2-C1-O11-P
3	C	608	POV	C1-C2-C3-O31
4	A	611	CLR	C13-C17-C20-C21
3	B	609	POV	C1-O11-P-O14
4	A	611	CLR	C13-C17-C20-C22
3	A	612	POV	C2-C1-O11-P
3	A	606	POV	C25-C26-C27-C28
3	D	607	POV	C2-C1-O11-P
3	D	601	POV	C27-C28-C29-C210
3	A	608	POV	O22-C21-C22-C23
3	B	604	POV	O22-C21-C22-C23
4	A	611	CLR	C16-C17-C20-C22
4	B	607	CLR	C13-C17-C20-C21
3	C	603	POV	O22-C21-C22-C23
3	A	607	POV	O22-C21-C22-C23
3	B	603	POV	O22-C21-C22-C23
3	D	604	POV	O22-C21-C22-C23
3	D	603	POV	O22-C21-C22-C23
3	B	604	POV	O21-C21-C22-C23
3	A	606	POV	C27-C28-C29-C210
3	B	601	POV	O22-C21-C22-C23
3	C	601	POV	O22-C21-C22-C23
3	C	607	POV	O22-C21-C22-C23
3	A	608	POV	O21-C21-C22-C23
3	B	608	POV	O22-C21-C22-C23
3	D	601	POV	O22-C21-C22-C23
4	B	607	CLR	C13-C17-C20-C22
3	C	603	POV	O21-C21-C22-C23
3	C	604	POV	O22-C21-C22-C23
3	D	602	POV	O22-C21-C22-C23
3	D	604	POV	O21-C21-C22-C23
3	D	605	POV	O22-C21-C22-C23
3	D	609	POV	O22-C21-C22-C23
3	B	609	POV	O22-C21-O21-C2
3	C	602	POV	O22-C21-C22-C23
3	A	610	POV	O22-C21-C22-C23
3	B	602	POV	O22-C21-C22-C23
3	C	608	POV	O21-C2-C3-O31
3	A	604	POV	O22-C21-C22-C23

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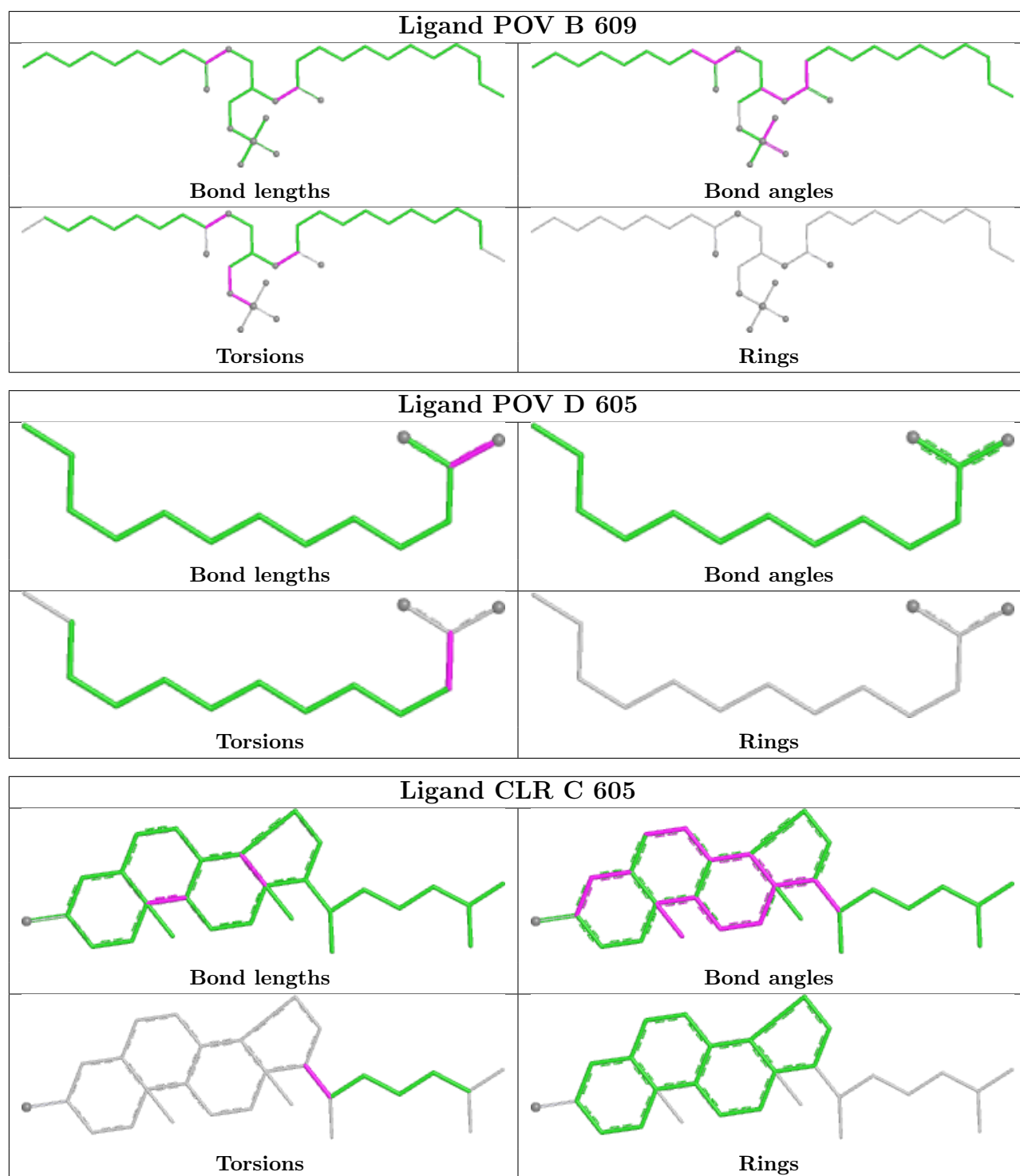
Mol	Chain	Res	Type	Atoms
3	A	605	POV	O22-C21-C22-C23
3	A	606	POV	O22-C21-C22-C23
3	A	615	POV	O22-C21-C22-C23
3	A	609	POV	O22-C21-C22-C23
4	D	606	CLR	C13-C17-C20-C21
3	A	609	POV	O21-C21-C22-C23
3	C	601	POV	O21-C21-C22-C23
3	C	604	POV	O21-C21-C22-C23
3	C	607	POV	O21-C21-C22-C23
3	A	605	POV	O21-C21-C22-C23
3	A	607	POV	O21-C21-C22-C23
3	B	602	POV	O21-C21-C22-C23
3	D	602	POV	O21-C21-C22-C23
4	C	605	CLR	C13-C17-C20-C21
3	A	604	POV	O21-C21-C22-C23
3	A	610	POV	O21-C21-C22-C23
3	A	615	POV	O21-C21-C22-C23
3	B	603	POV	O21-C21-C22-C23
3	B	608	POV	O21-C21-C22-C23
3	D	605	POV	O21-C21-C22-C23
3	D	609	POV	O21-C21-C22-C23
3	B	609	POV	C22-C21-O21-C2
3	C	602	POV	O21-C21-C22-C23
3	A	606	POV	O21-C21-C22-C23
3	A	609	POV	C27-C28-C29-C210
3	D	603	POV	O21-C21-C22-C23
3	B	601	POV	O21-C21-C22-C23
3	C	609	POV	C27-C28-C29-C210
3	A	612	POV	C1-O11-P-O14
3	D	610	POV	C1-O11-P-O14
3	D	601	POV	O21-C21-C22-C23
4	B	607	CLR	C16-C17-C20-C22
3	D	610	POV	C29-C210-C211-C212
4	B	605	CLR	C13-C17-C20-C21
4	D	606	CLR	C13-C17-C20-C22
3	D	607	POV	C32-C31-O31-C3
3	D	607	POV	O32-C31-O31-C3
4	C	605	CLR	C13-C17-C20-C22

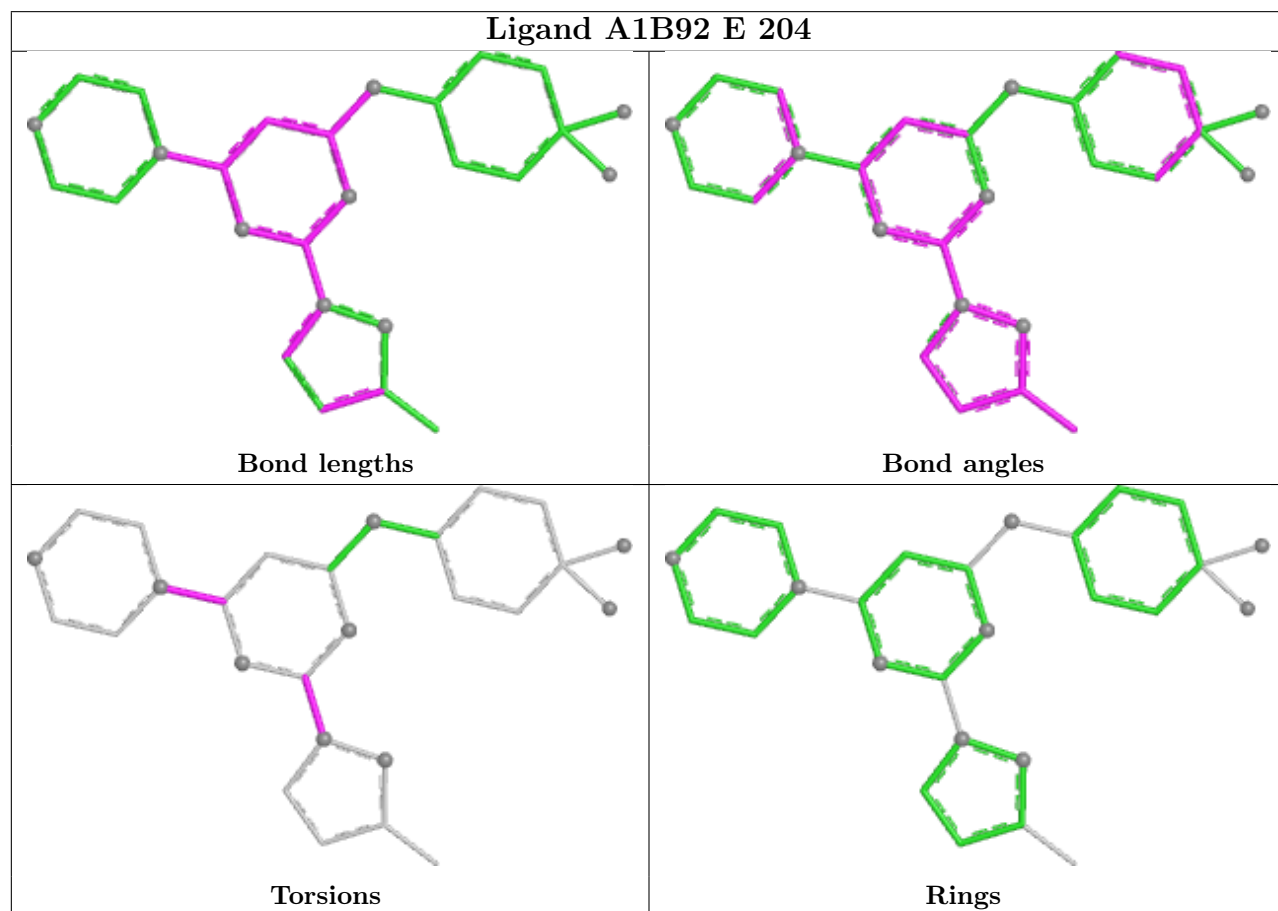
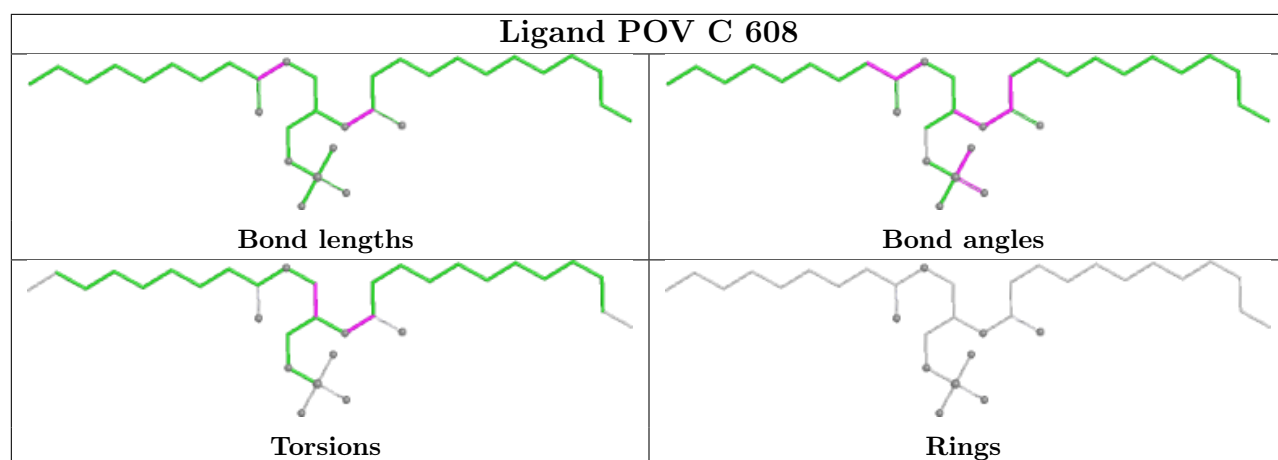
There are no ring outliers.

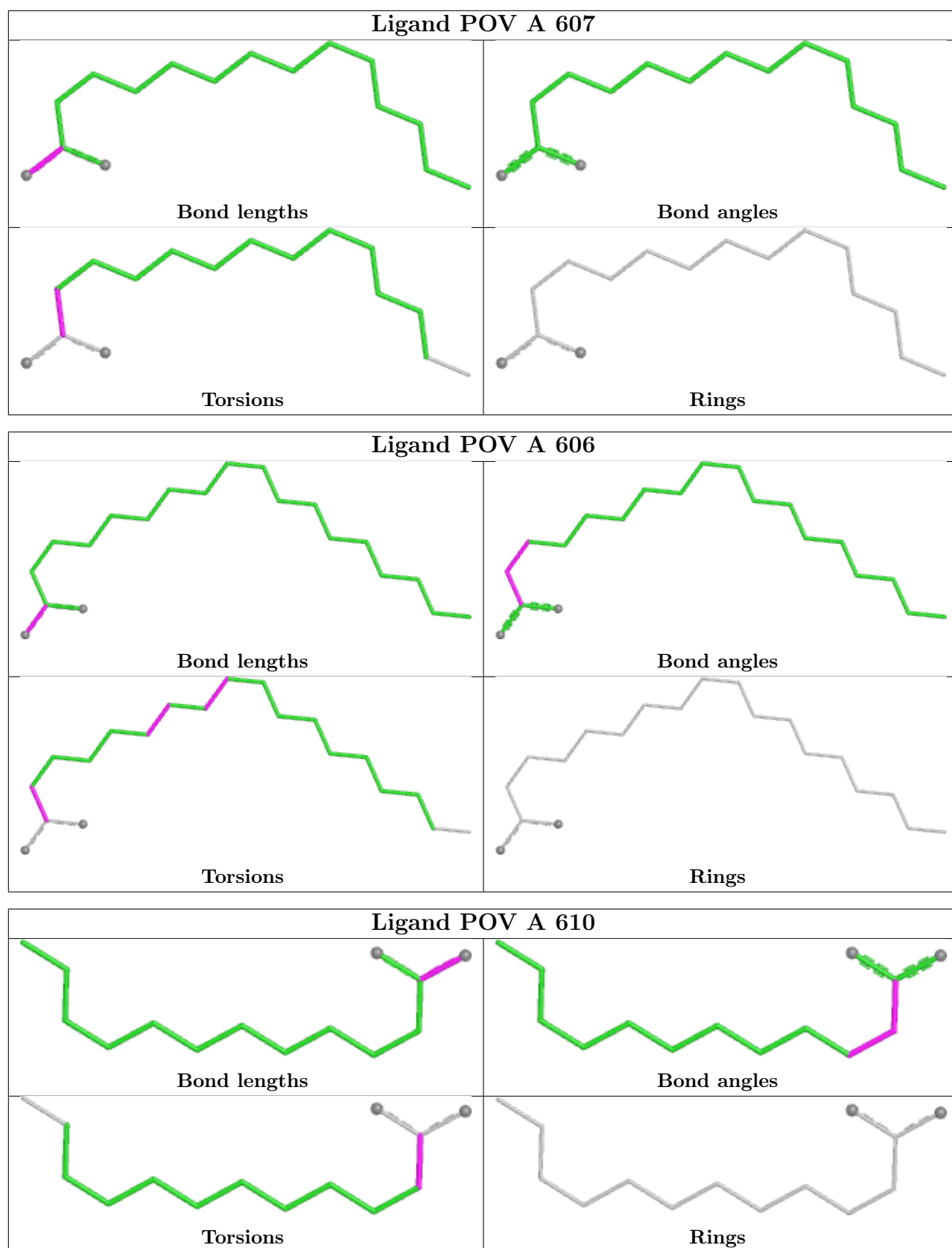
22 monomers are involved in 62 short contacts:

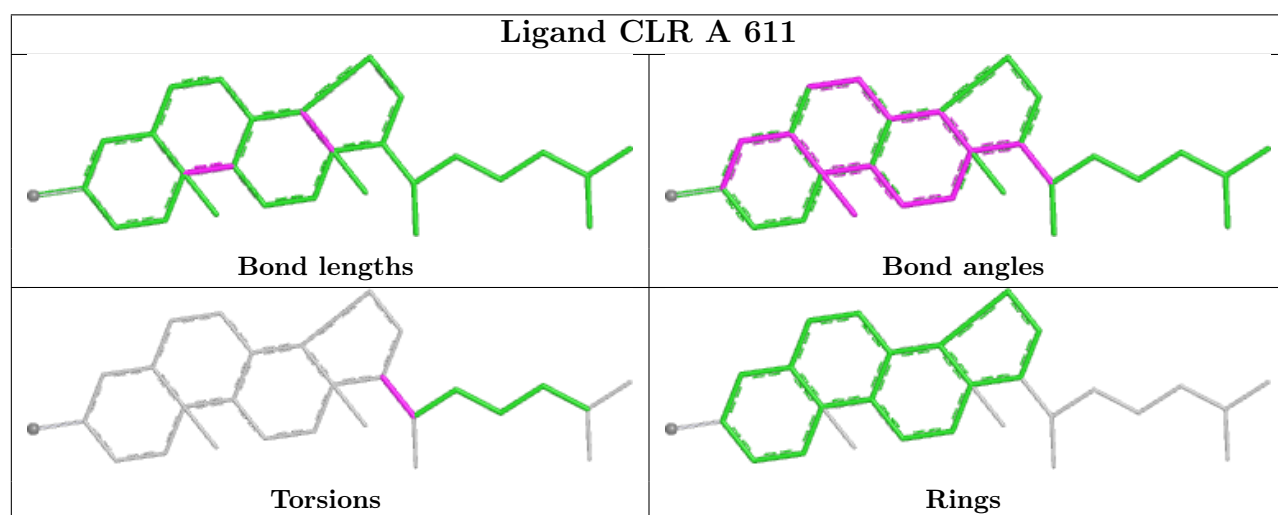
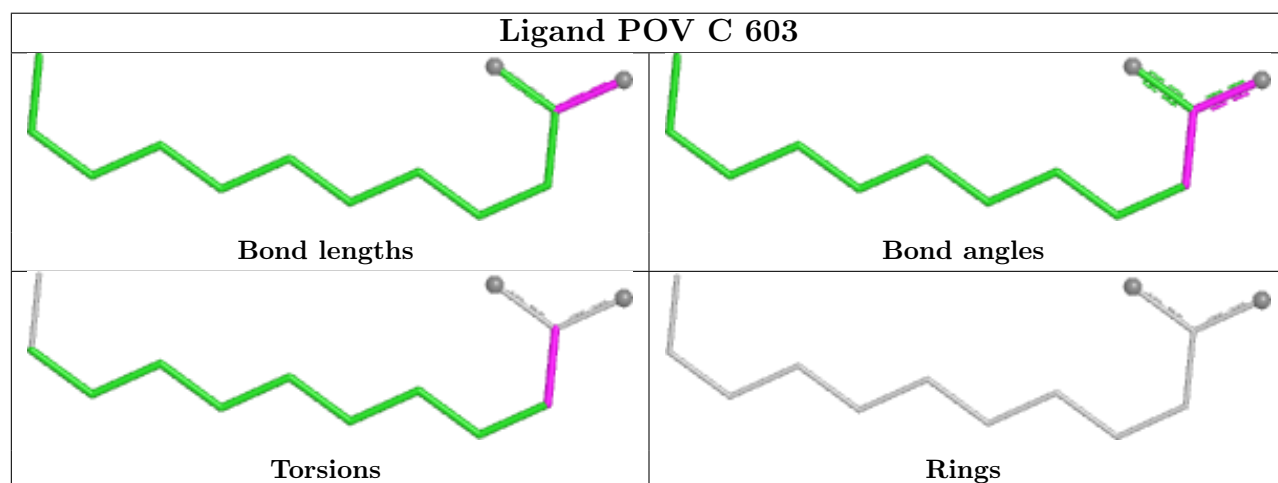
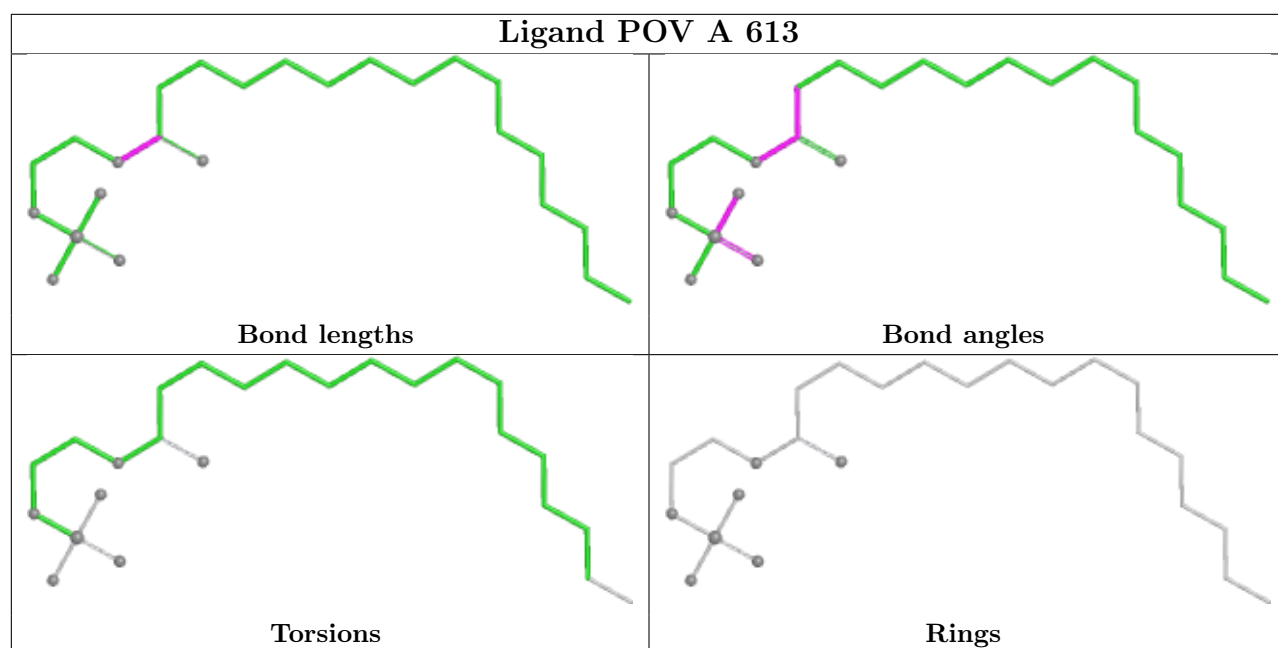
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	609	POV	1	0
3	D	605	POV	1	0
4	C	605	CLR	7	0
3	C	608	POV	1	0
6	E	204	A1B92	5	0
3	A	606	POV	1	0
3	A	610	POV	1	0
4	A	611	CLR	4	0
4	A	614	CLR	1	0
4	D	608	CLR	4	0
4	C	606	CLR	2	0
4	D	606	CLR	4	0
3	D	601	POV	2	0
3	A	604	POV	4	0
4	B	605	CLR	8	0
3	D	607	POV	1	0
3	A	609	POV	1	0
3	C	604	POV	1	0
4	B	607	CLR	7	0
3	A	612	POV	1	0
6	H	204	A1B92	2	0
3	B	606	POV	5	0

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

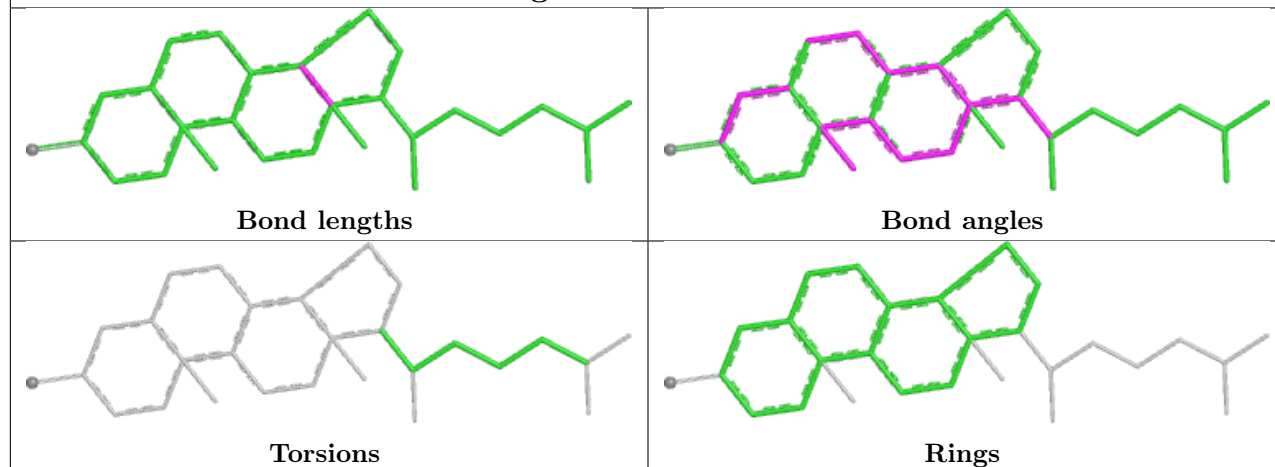




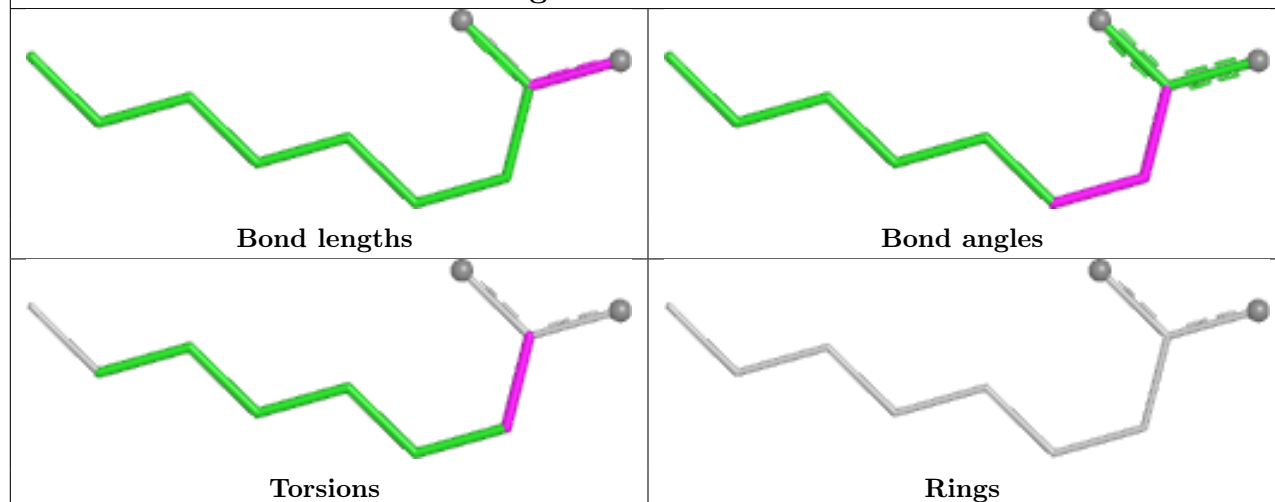




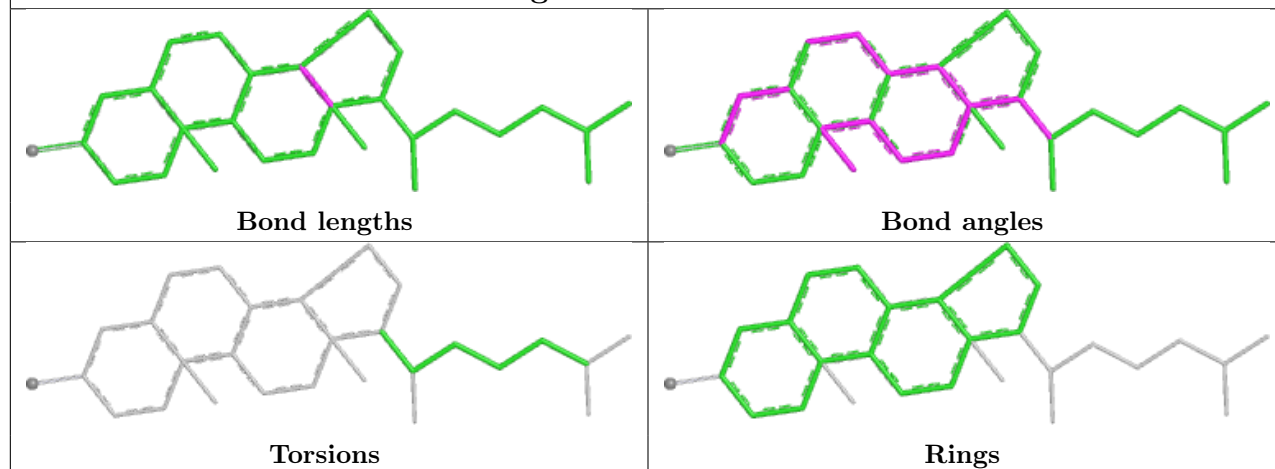
Ligand CLR A 614

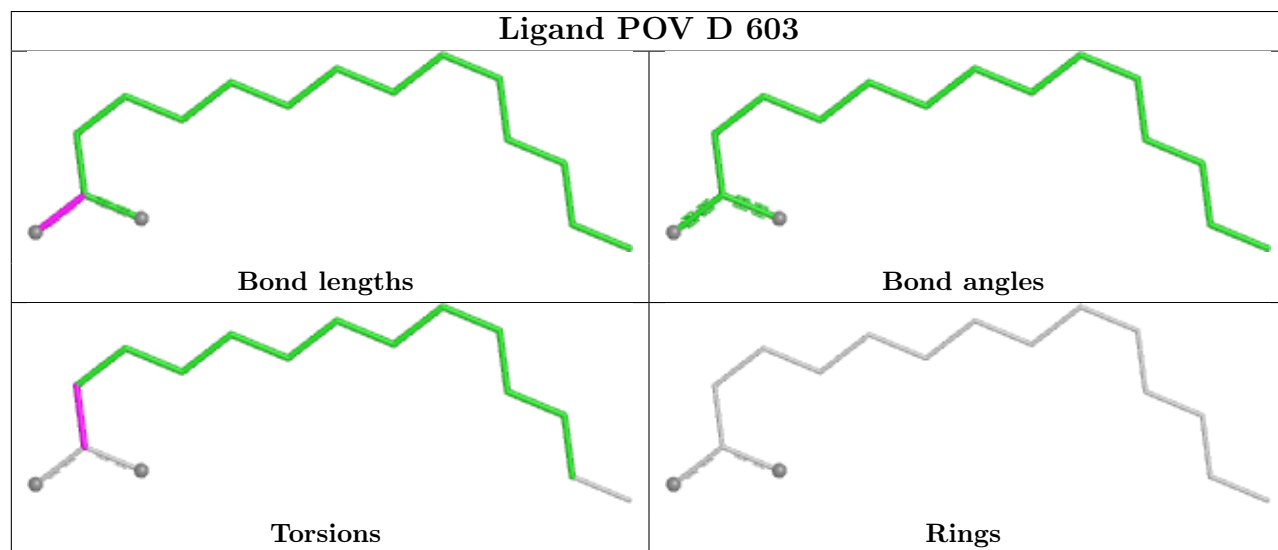
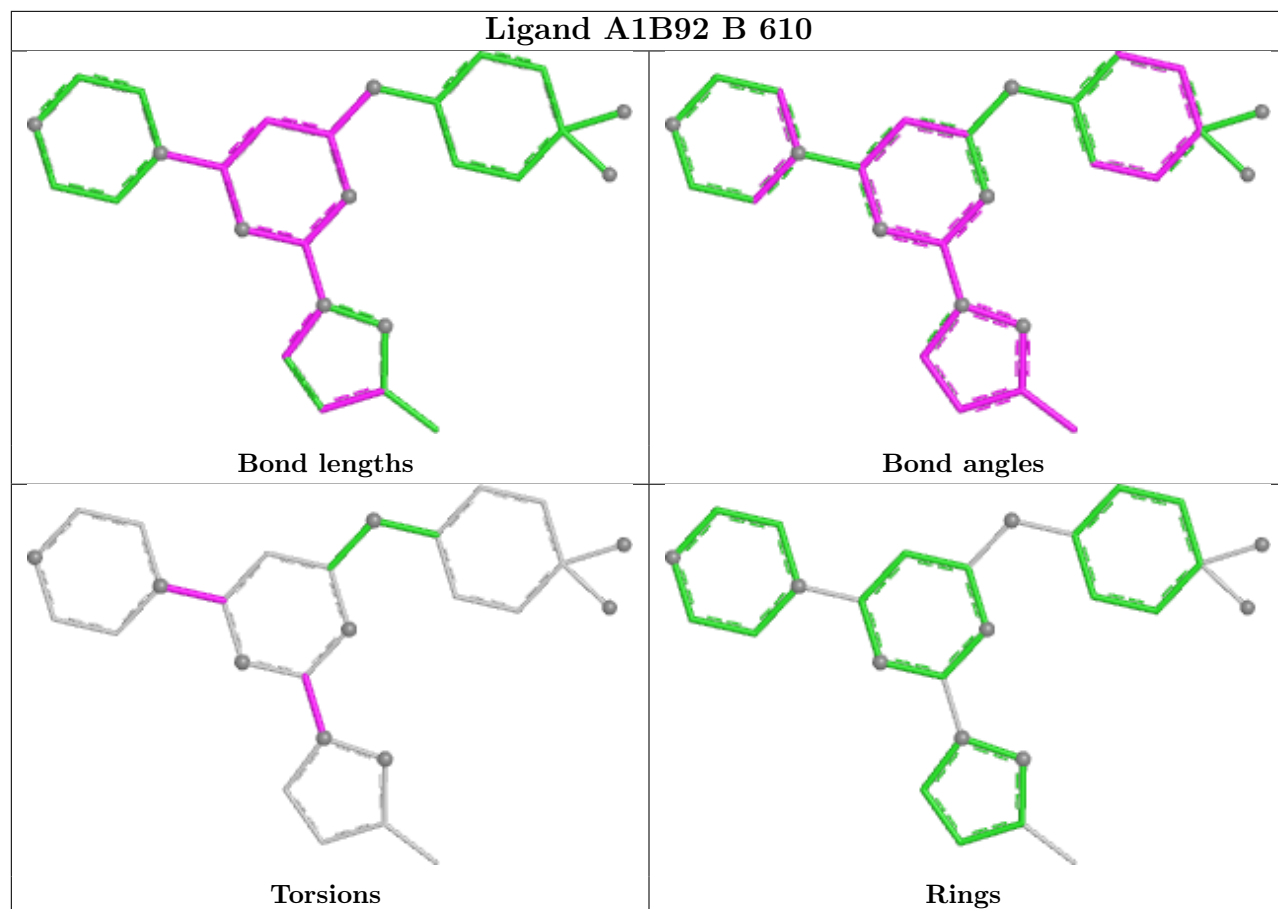


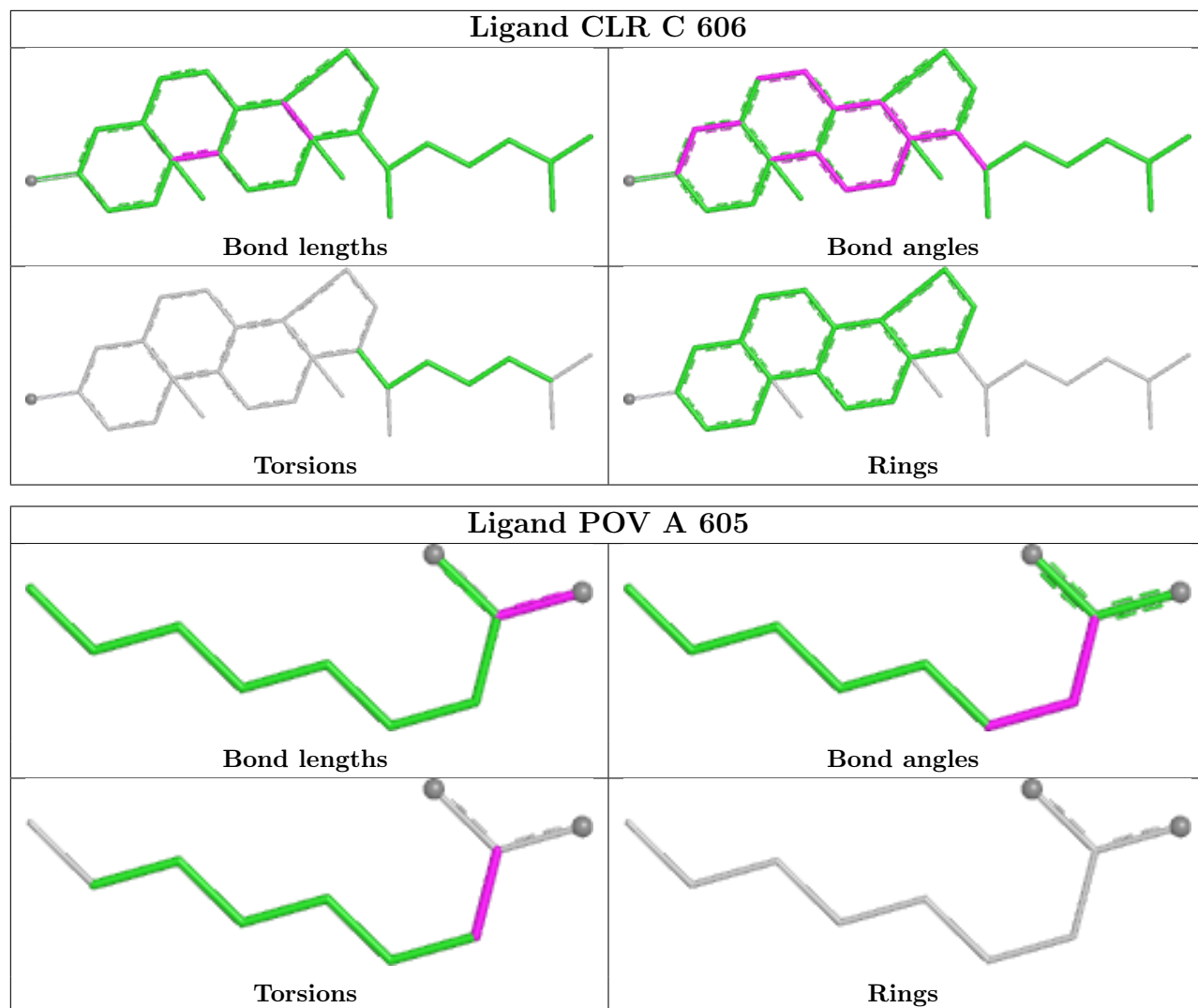
Ligand POV C 601

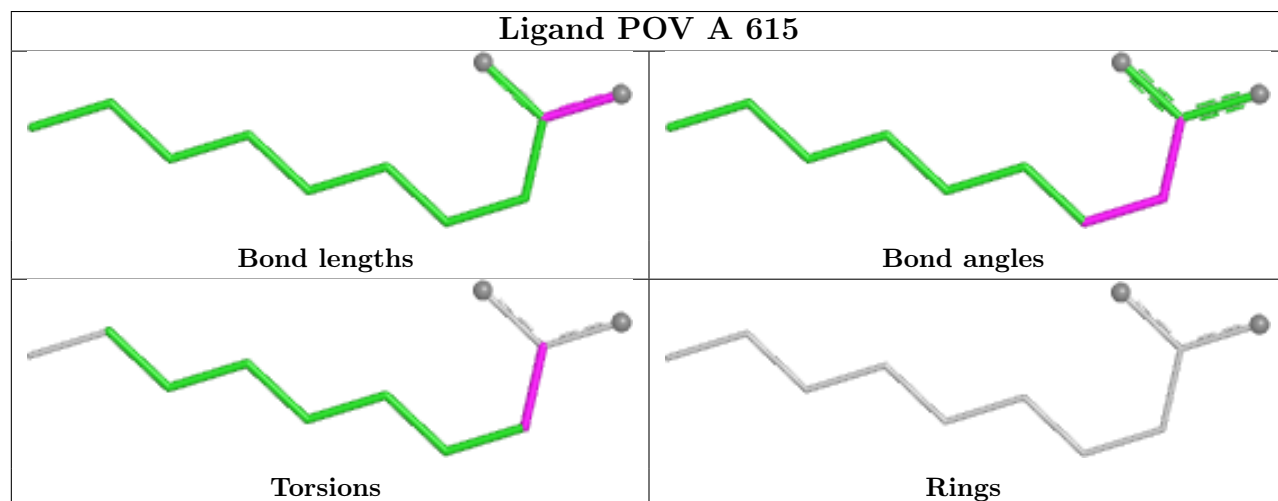
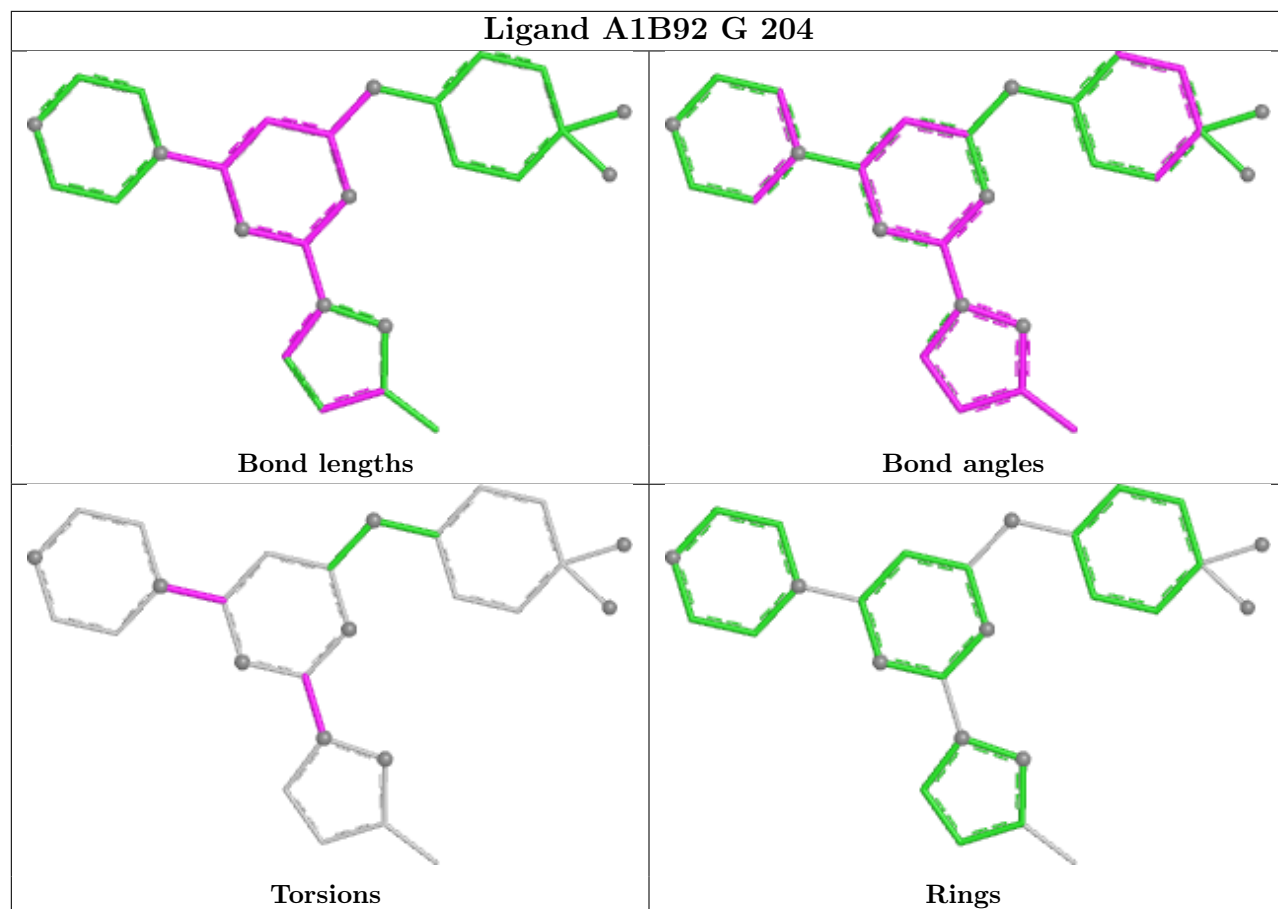


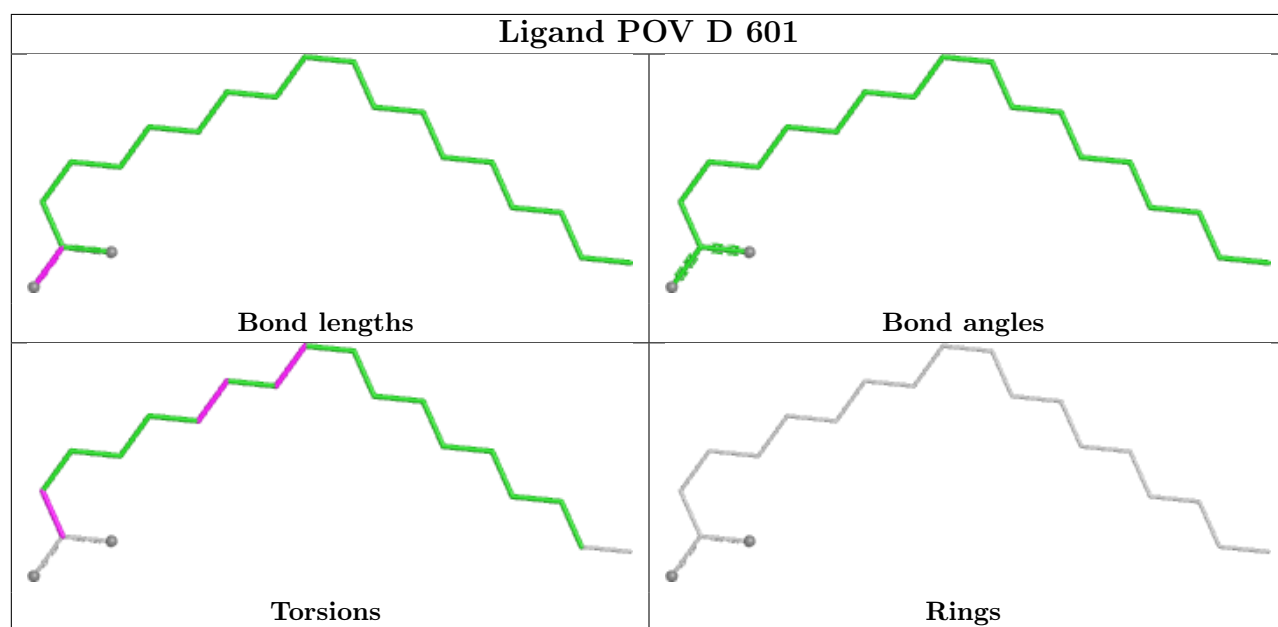
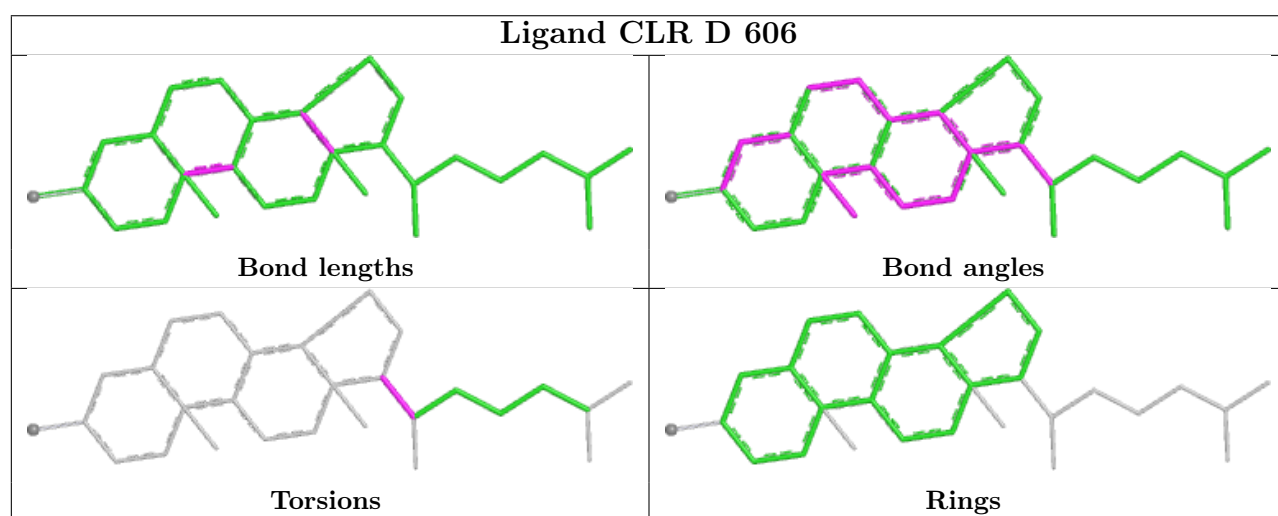
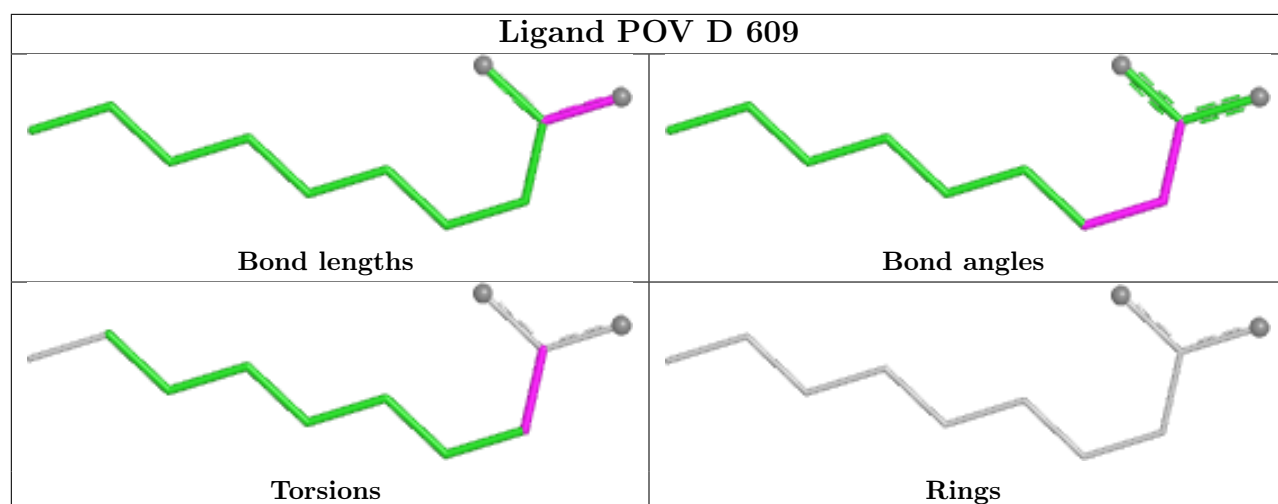
Ligand CLR D 608

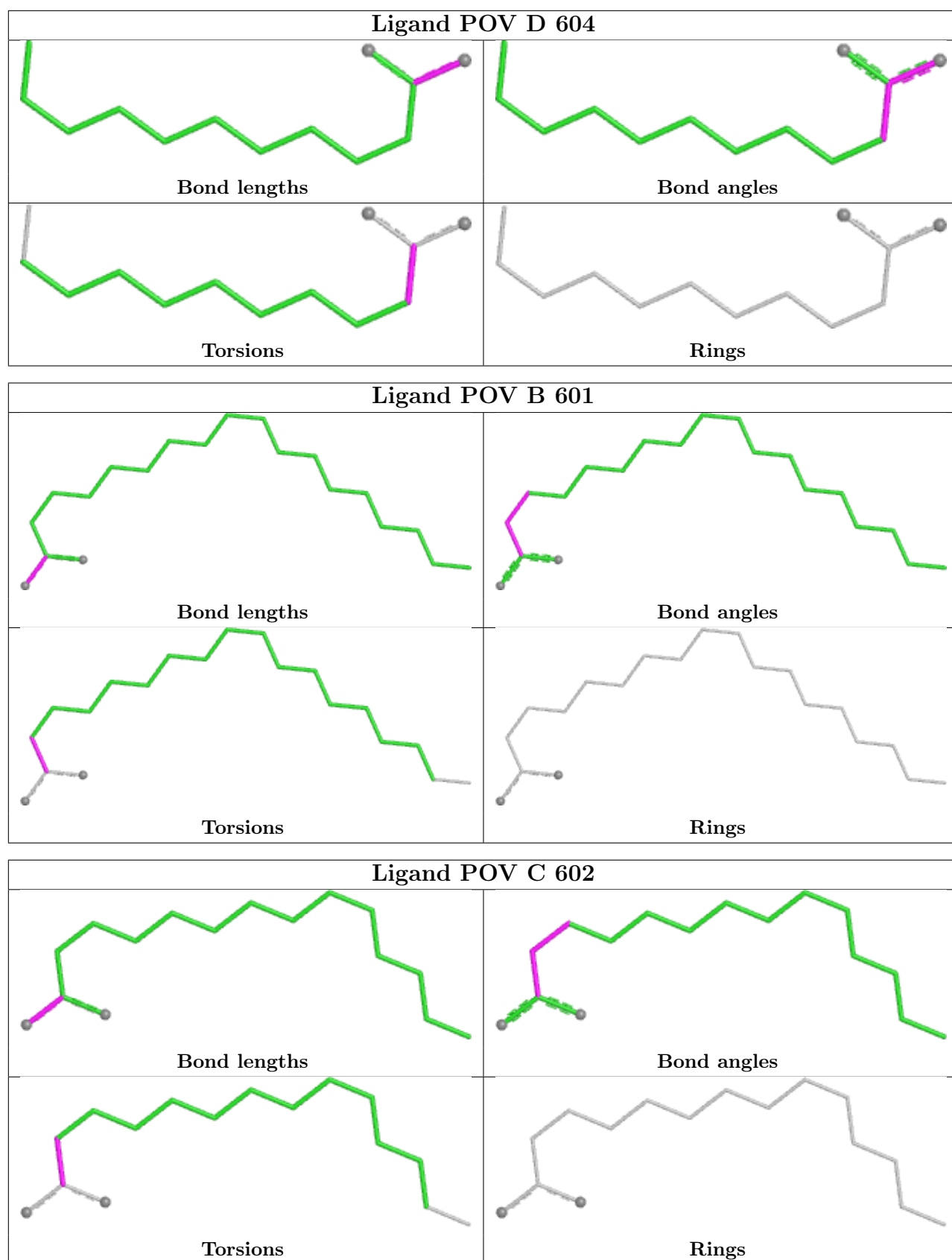


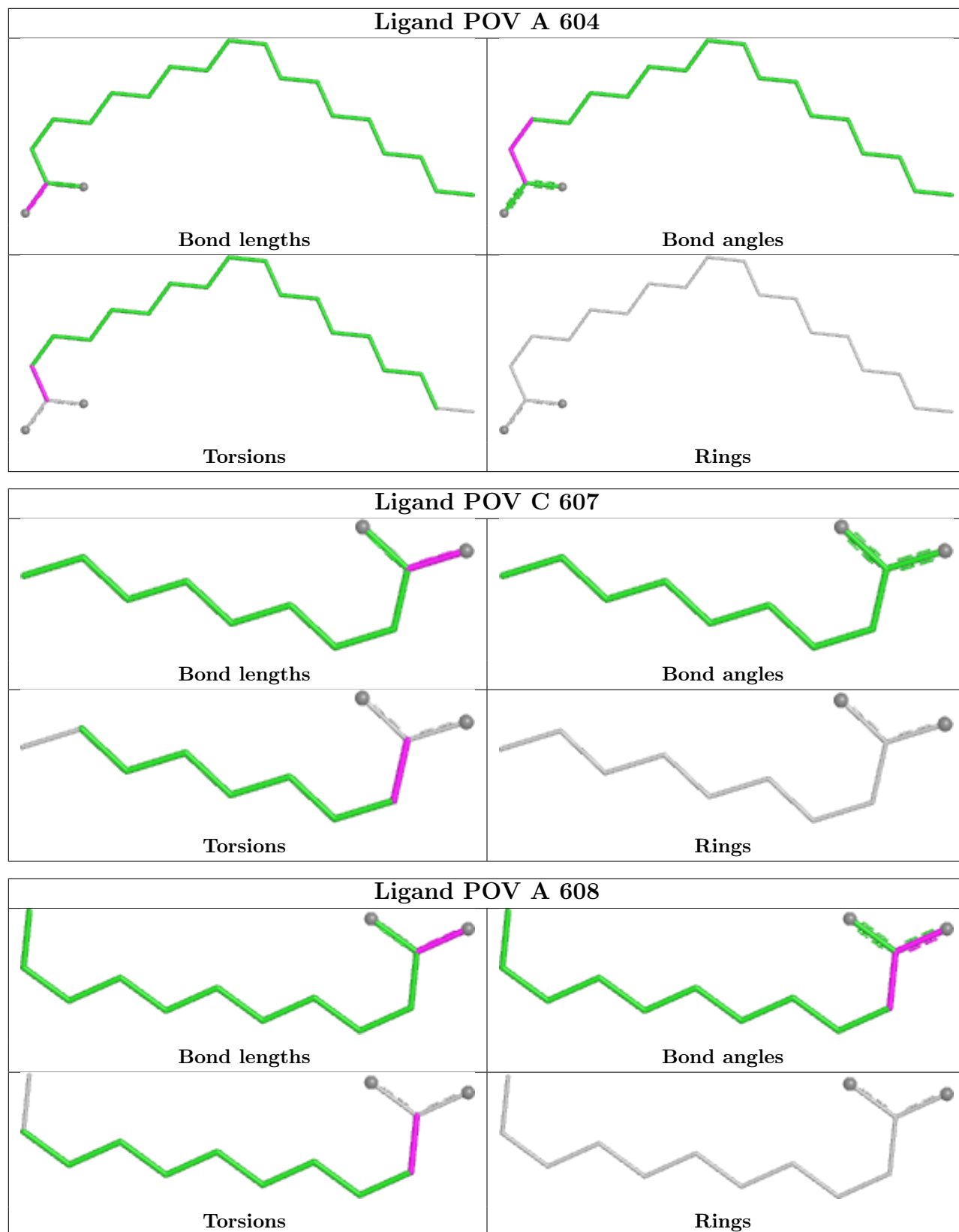


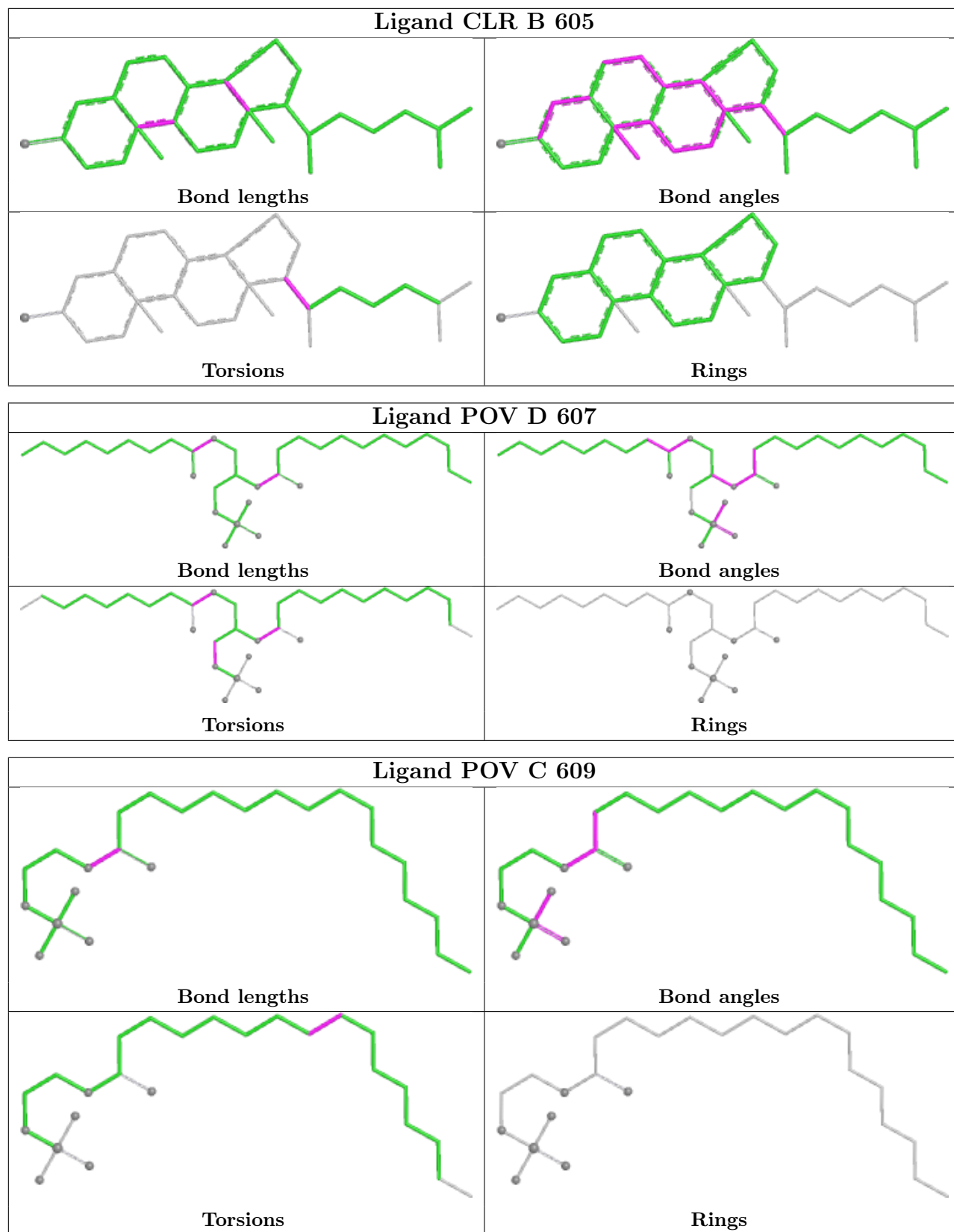


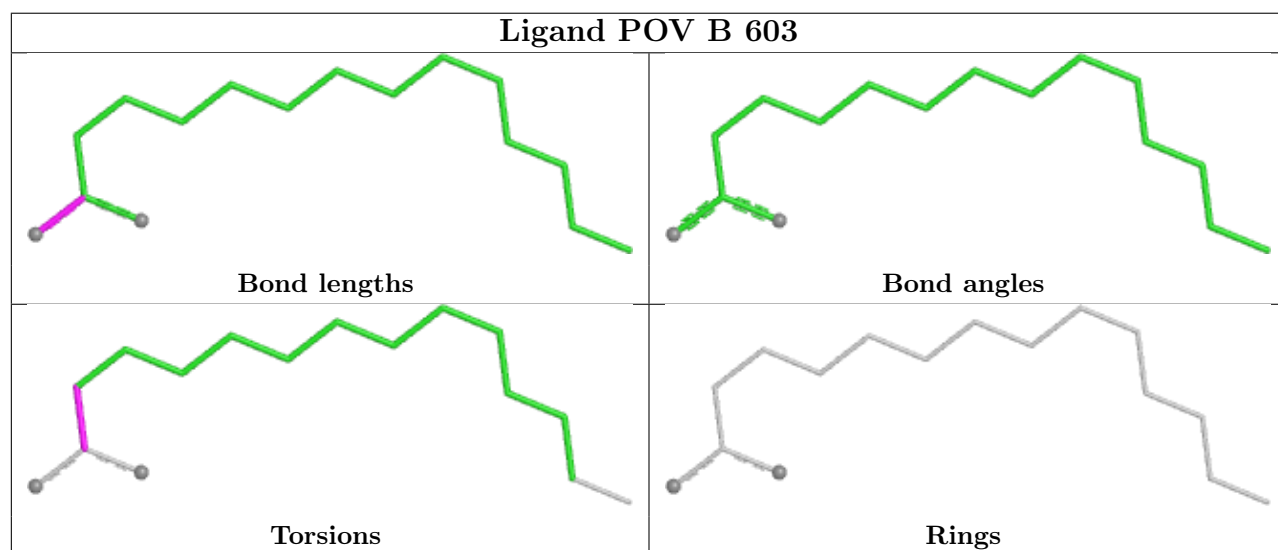
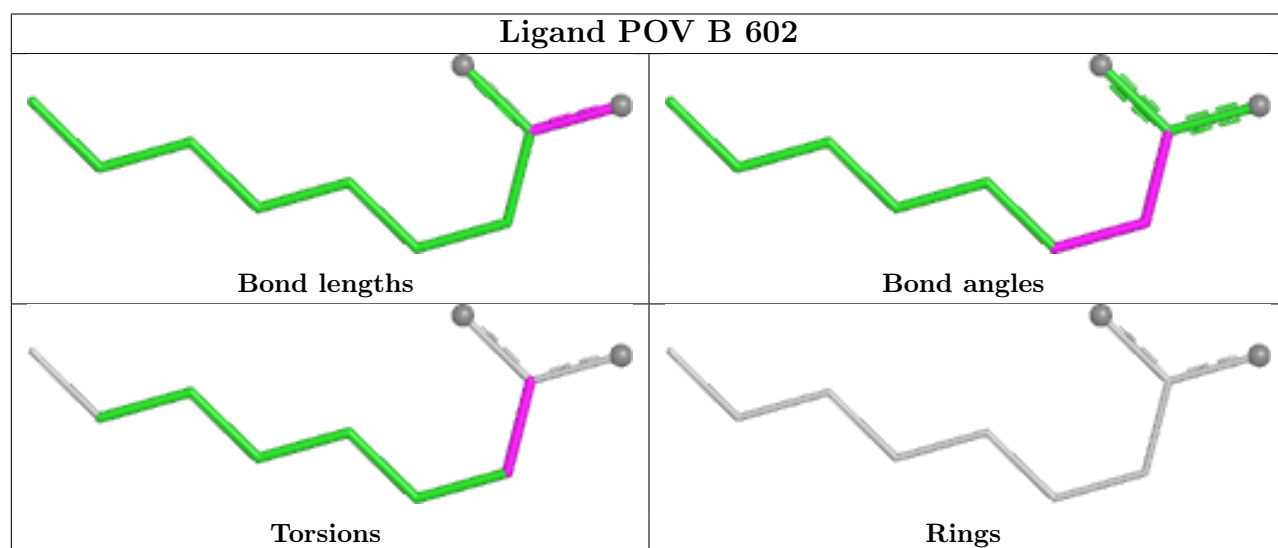
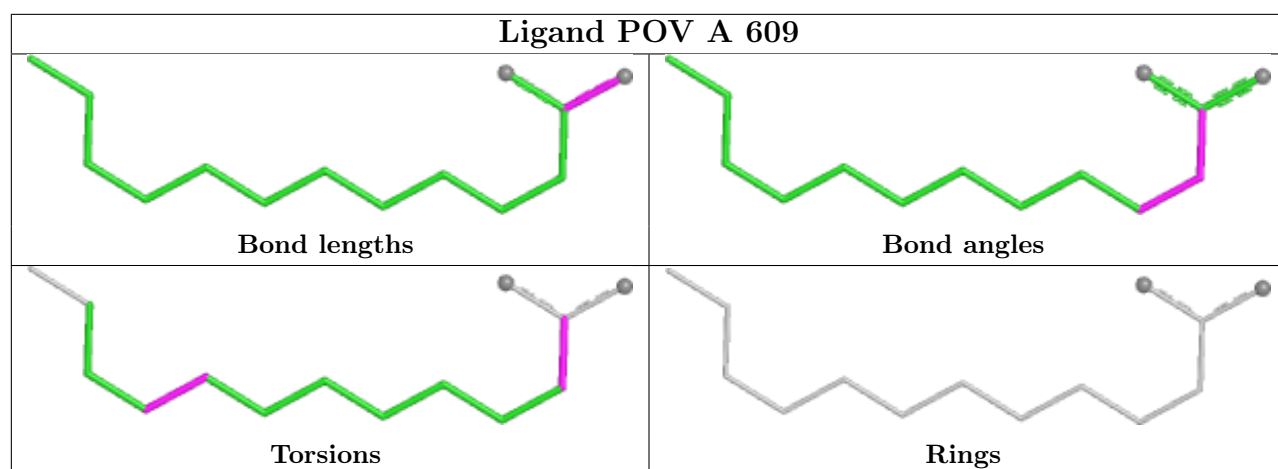


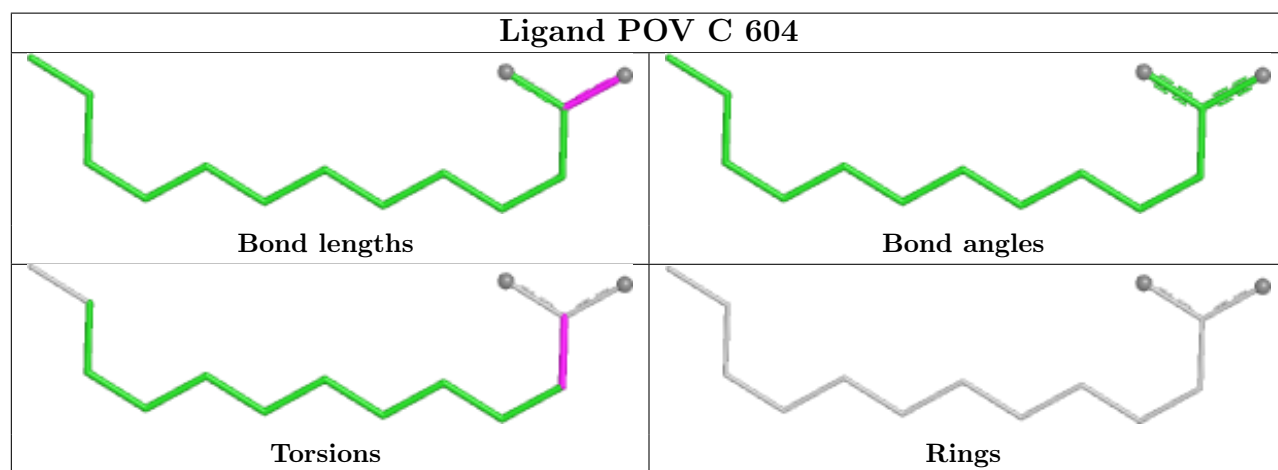
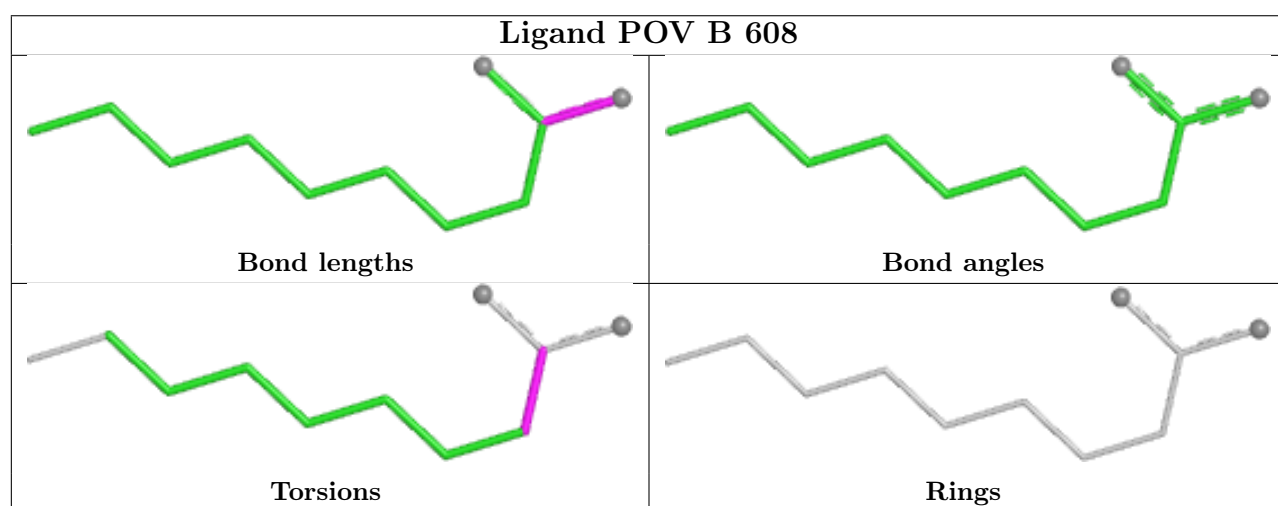
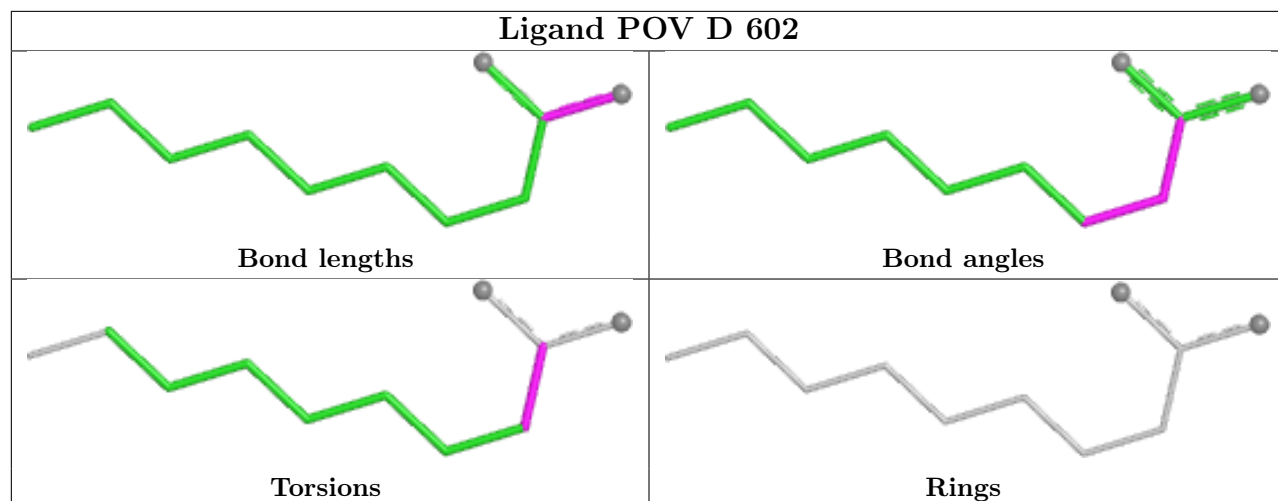


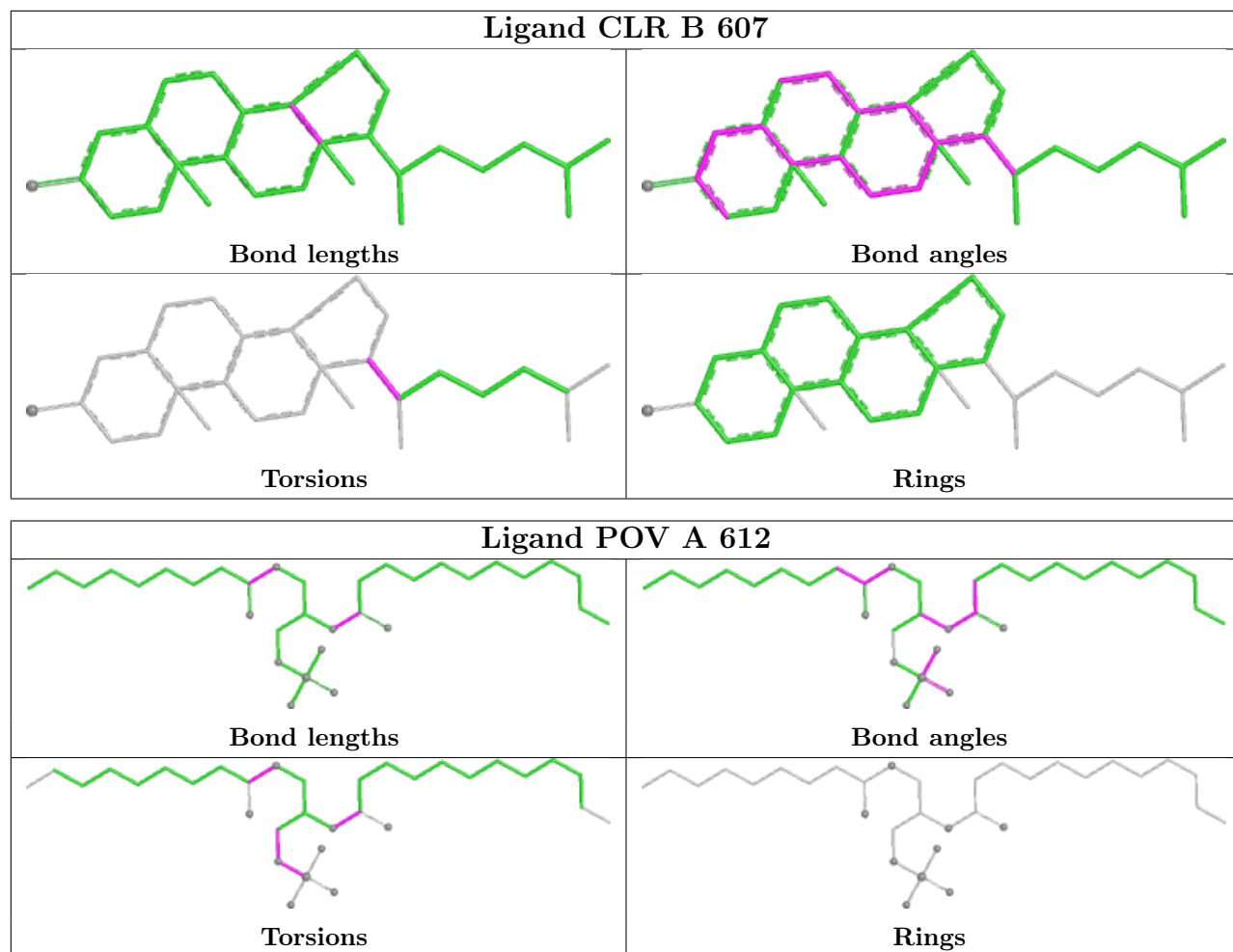


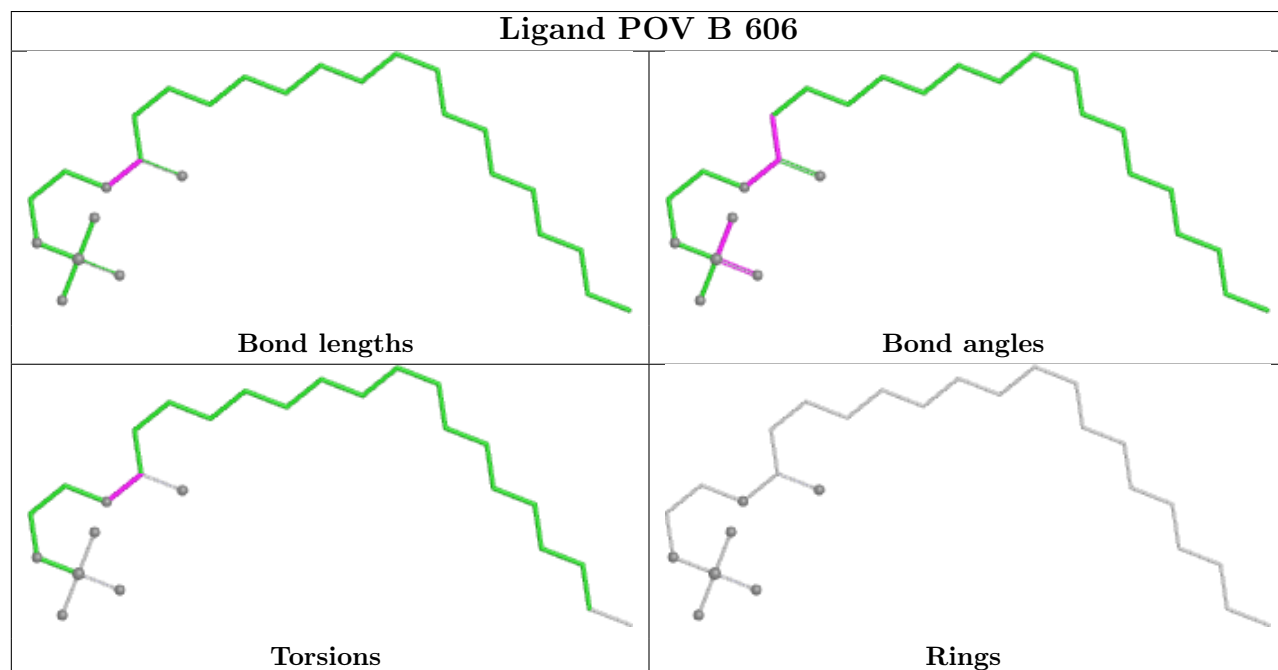
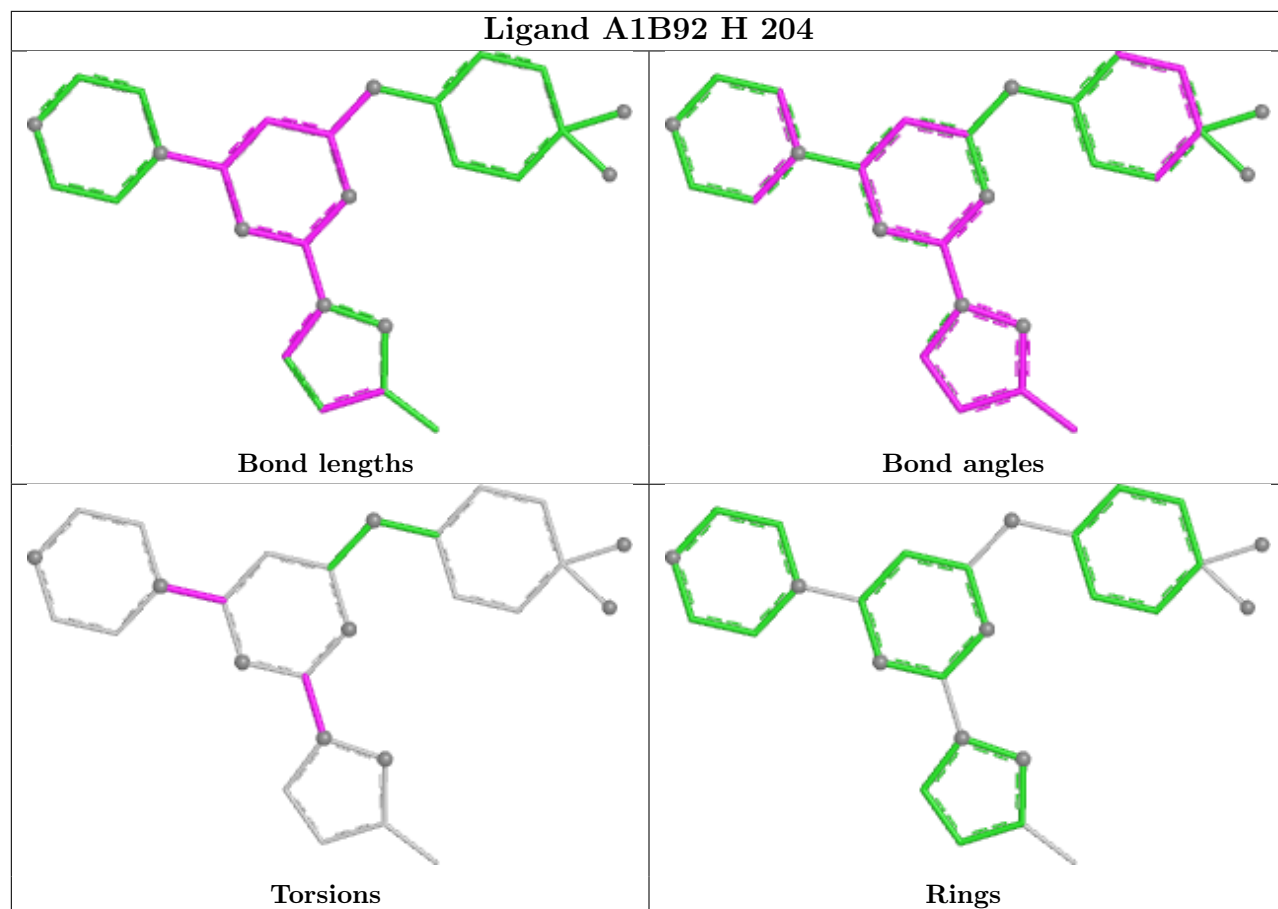


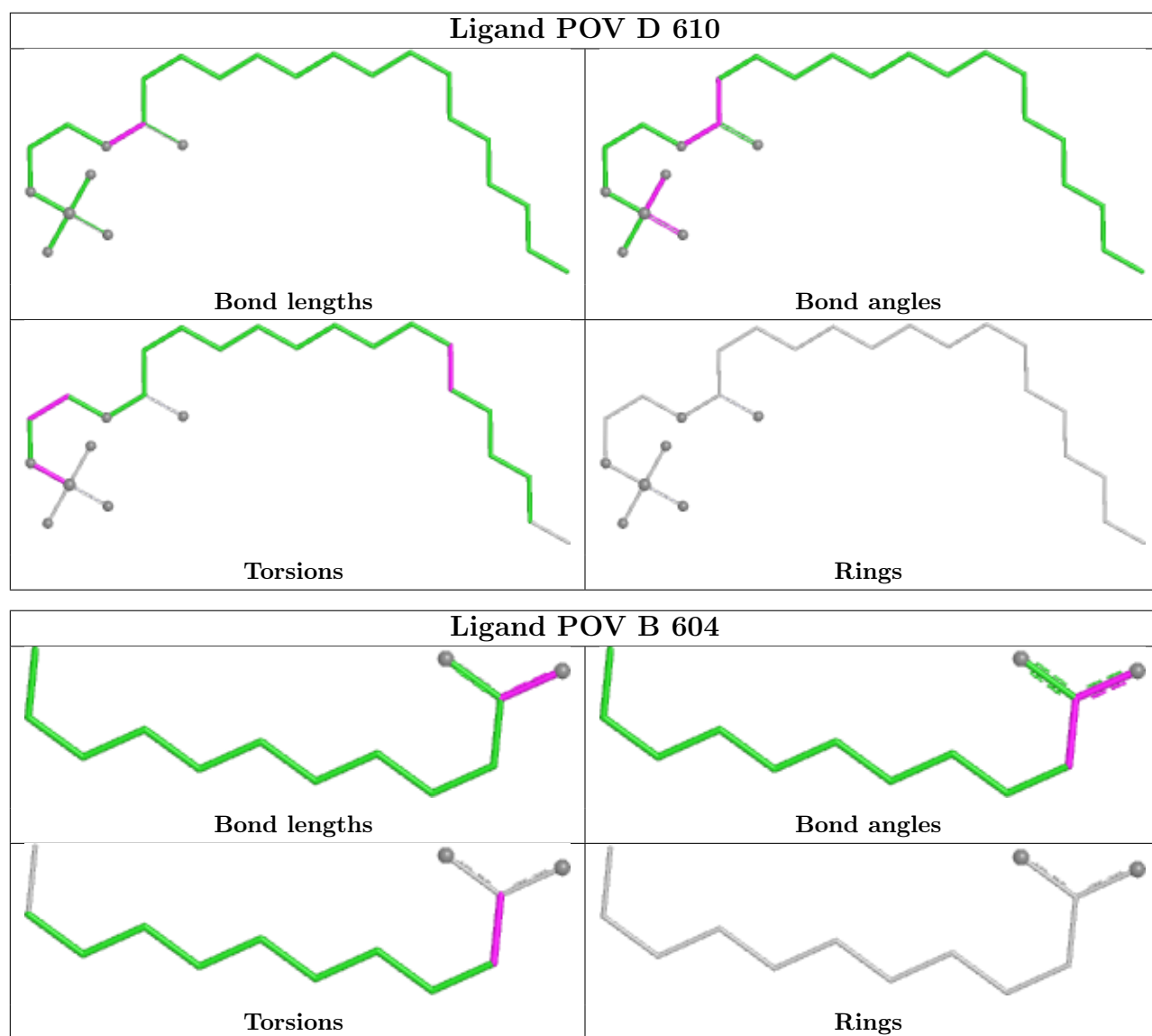












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

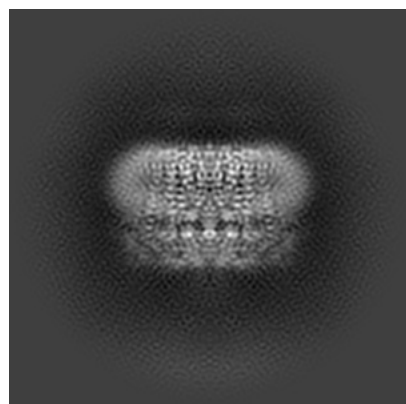
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-65358. These allow visual inspection of the internal detail of the map and identification of artifacts.

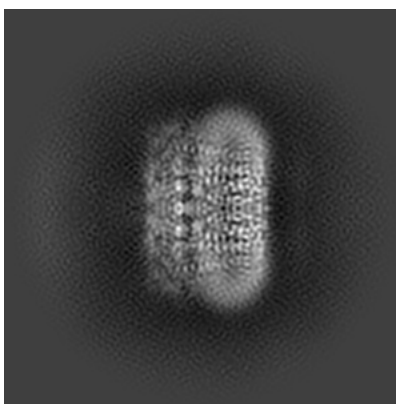
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

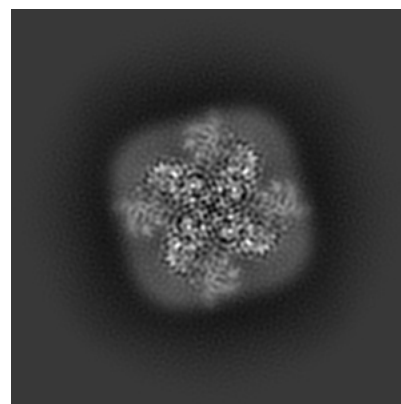
6.1.1 Primary map



X

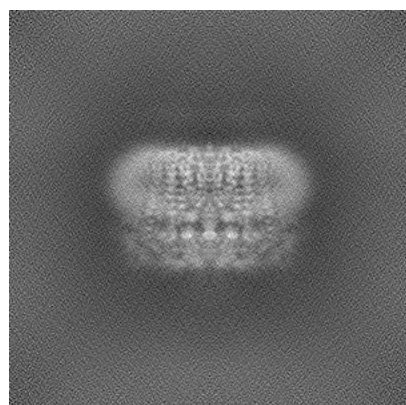


Y

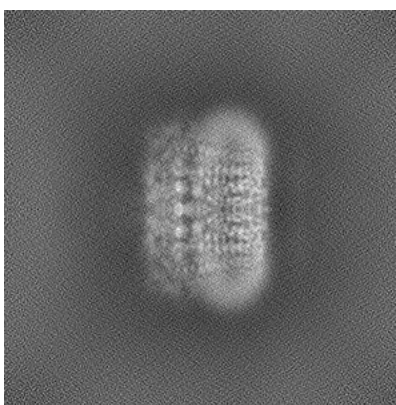


Z

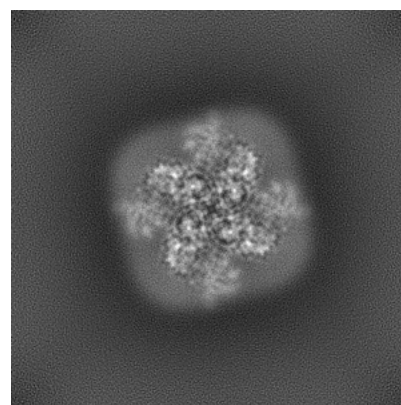
6.1.2 Raw map



X



Y

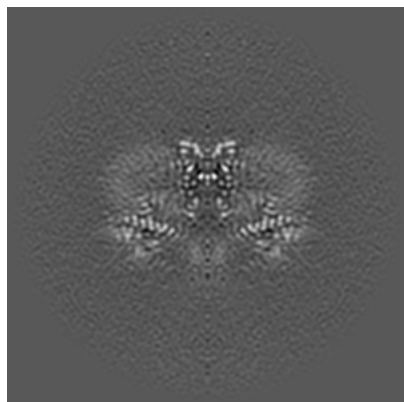


Z

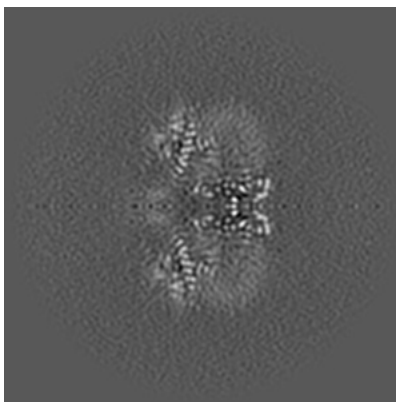
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

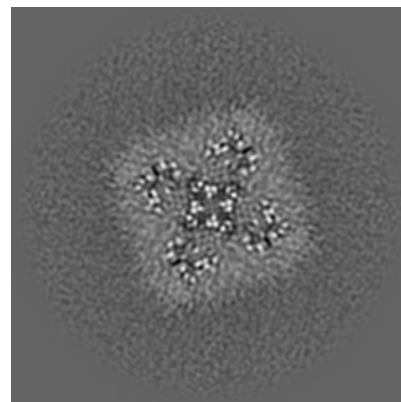
6.2.1 Primary map



X Index: 160

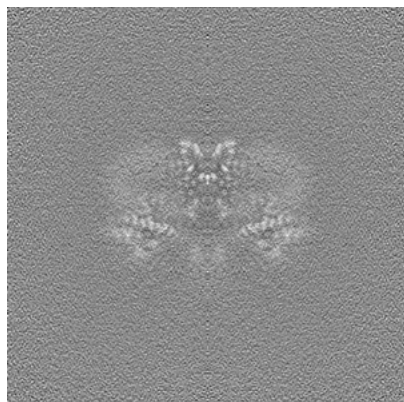


Y Index: 160

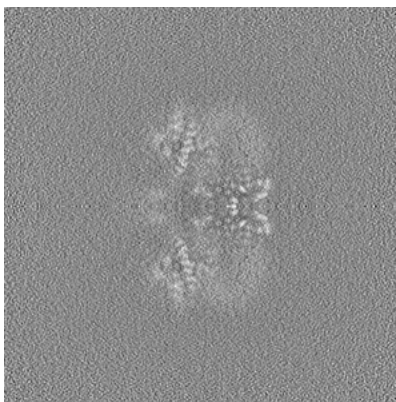


Z Index: 160

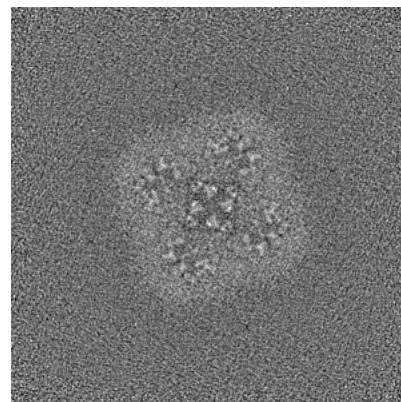
6.2.2 Raw map



X Index: 160



Y Index: 160

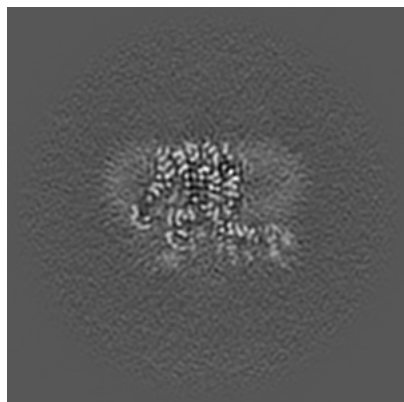


Z Index: 160

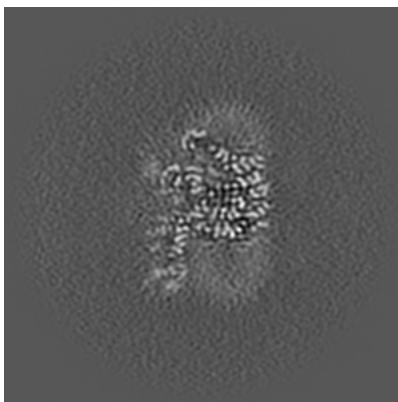
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

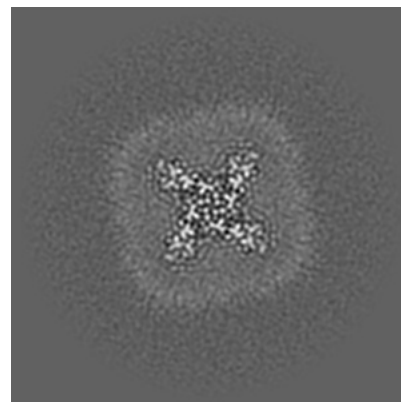
6.3.1 Primary map



X Index: 145

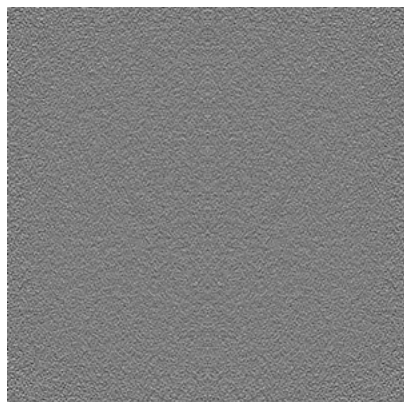


Y Index: 145

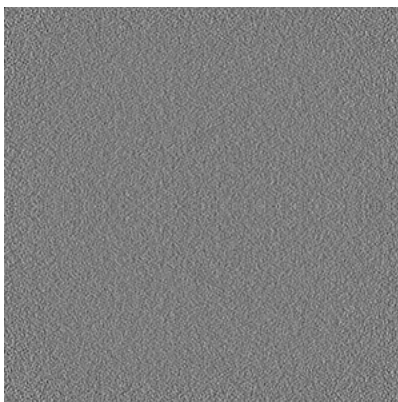


Z Index: 189

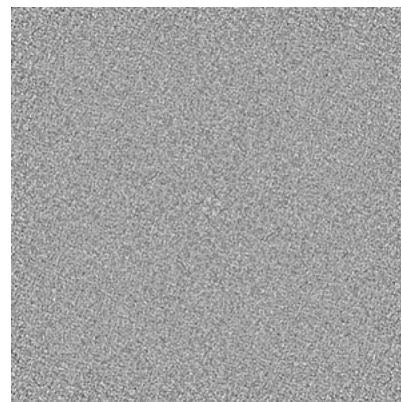
6.3.2 Raw map



X Index: 0



Y Index: 0

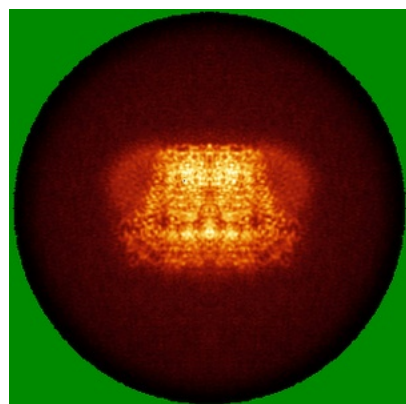


Z Index: 0

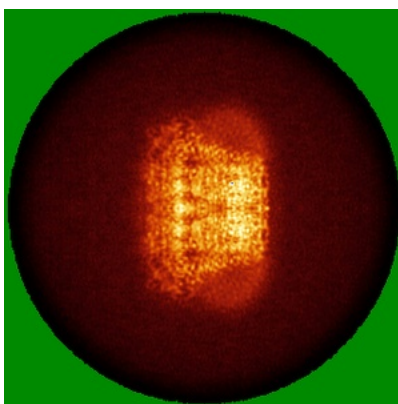
The images above show the largest variance slices of the map in three orthogonal directions.

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

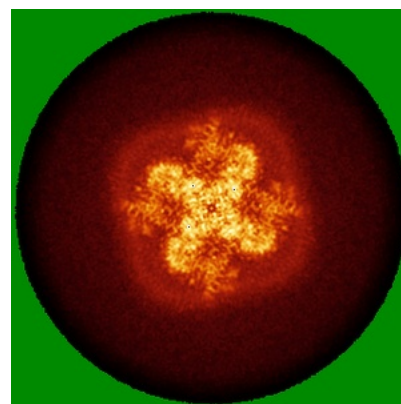
6.4.1 Primary map



X

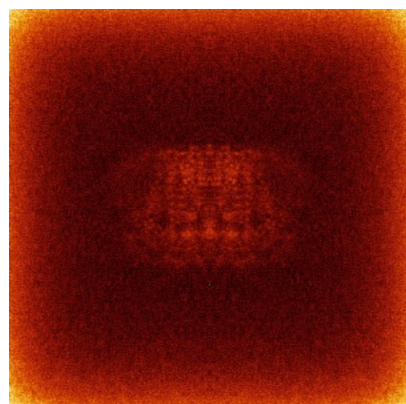


Y

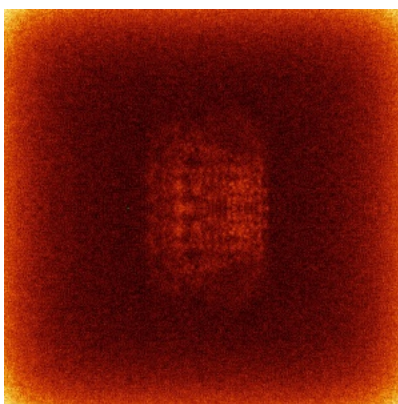


Z

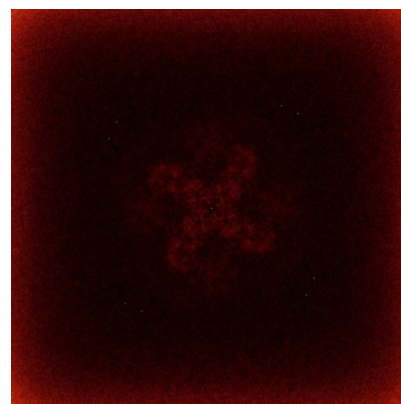
6.4.2 Raw map



X



Y

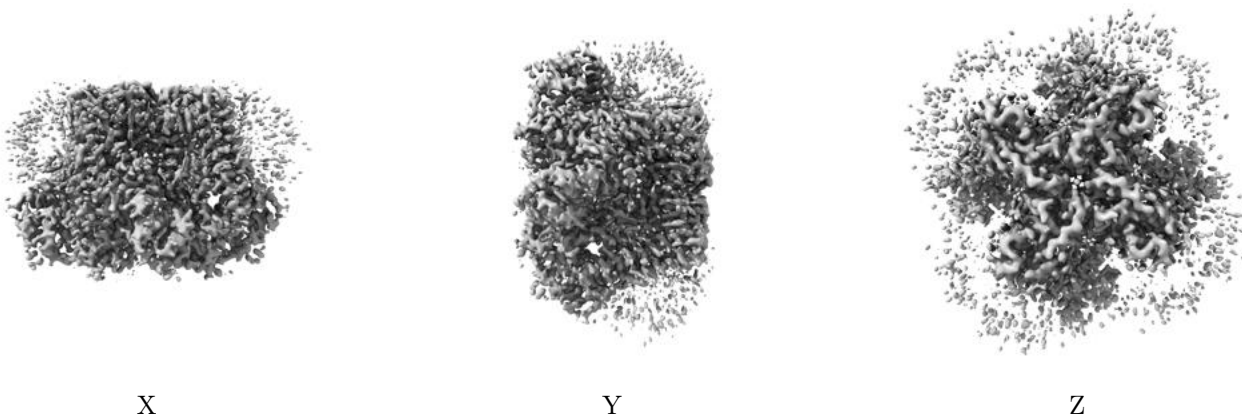


Z

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.

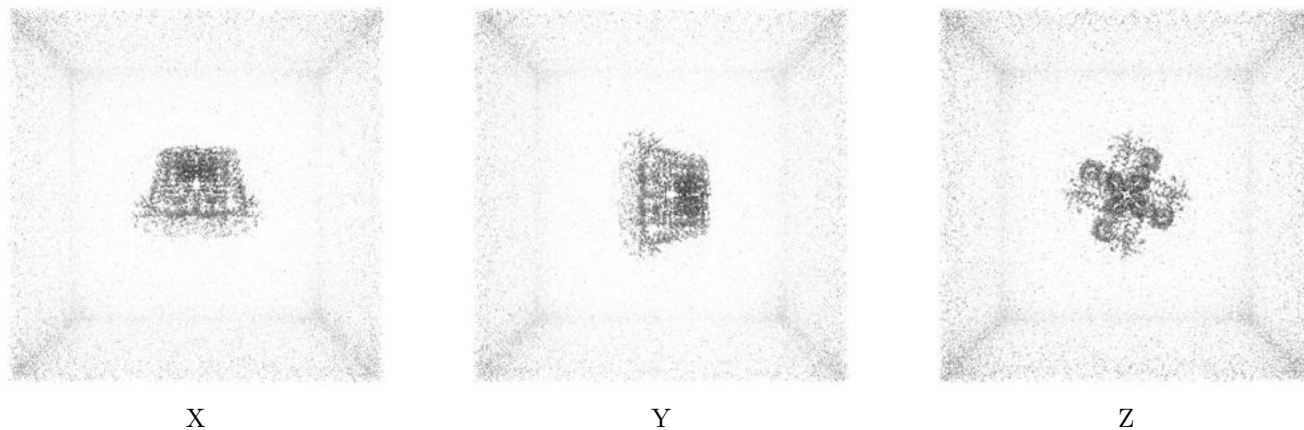
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.127. 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.

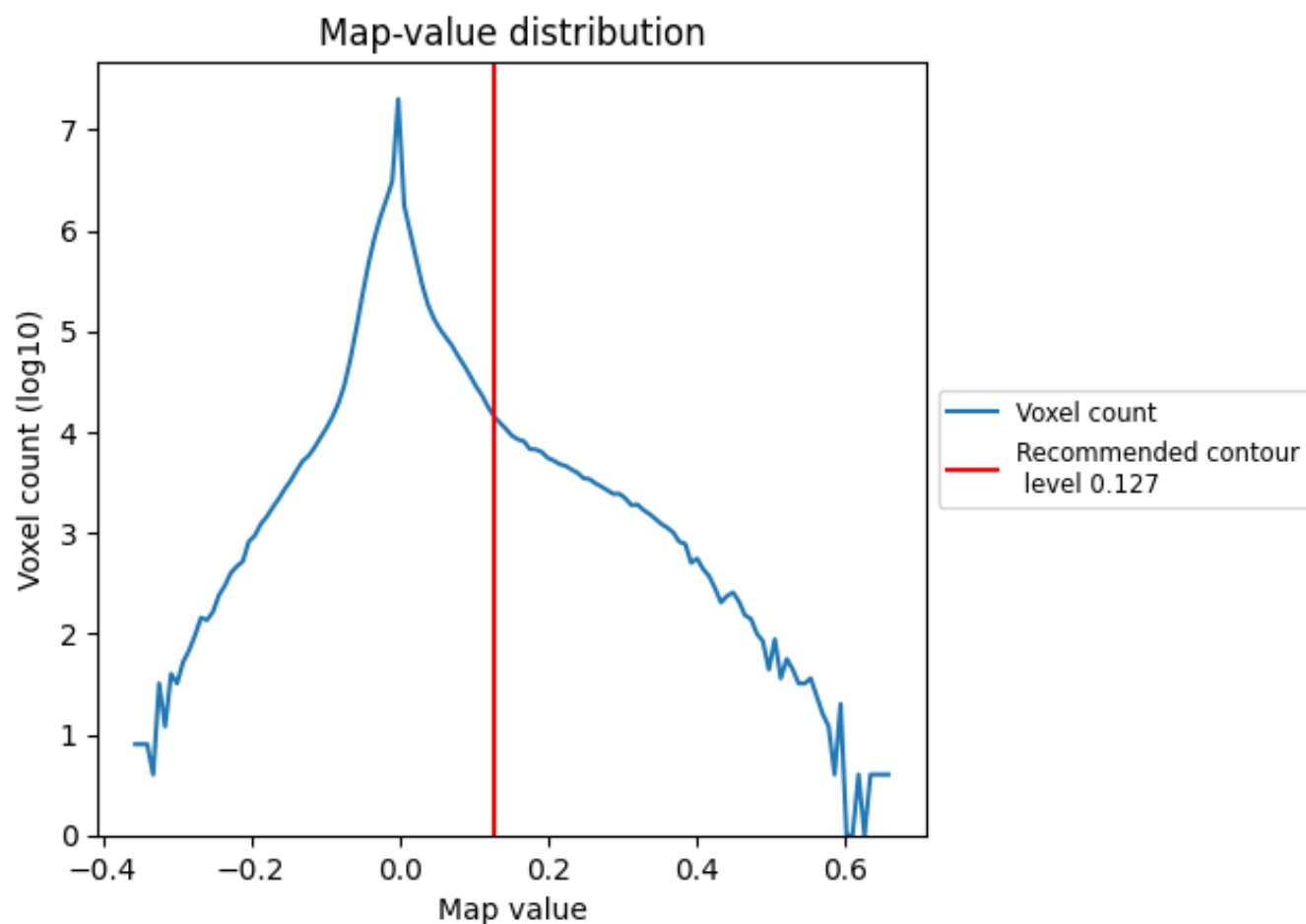
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

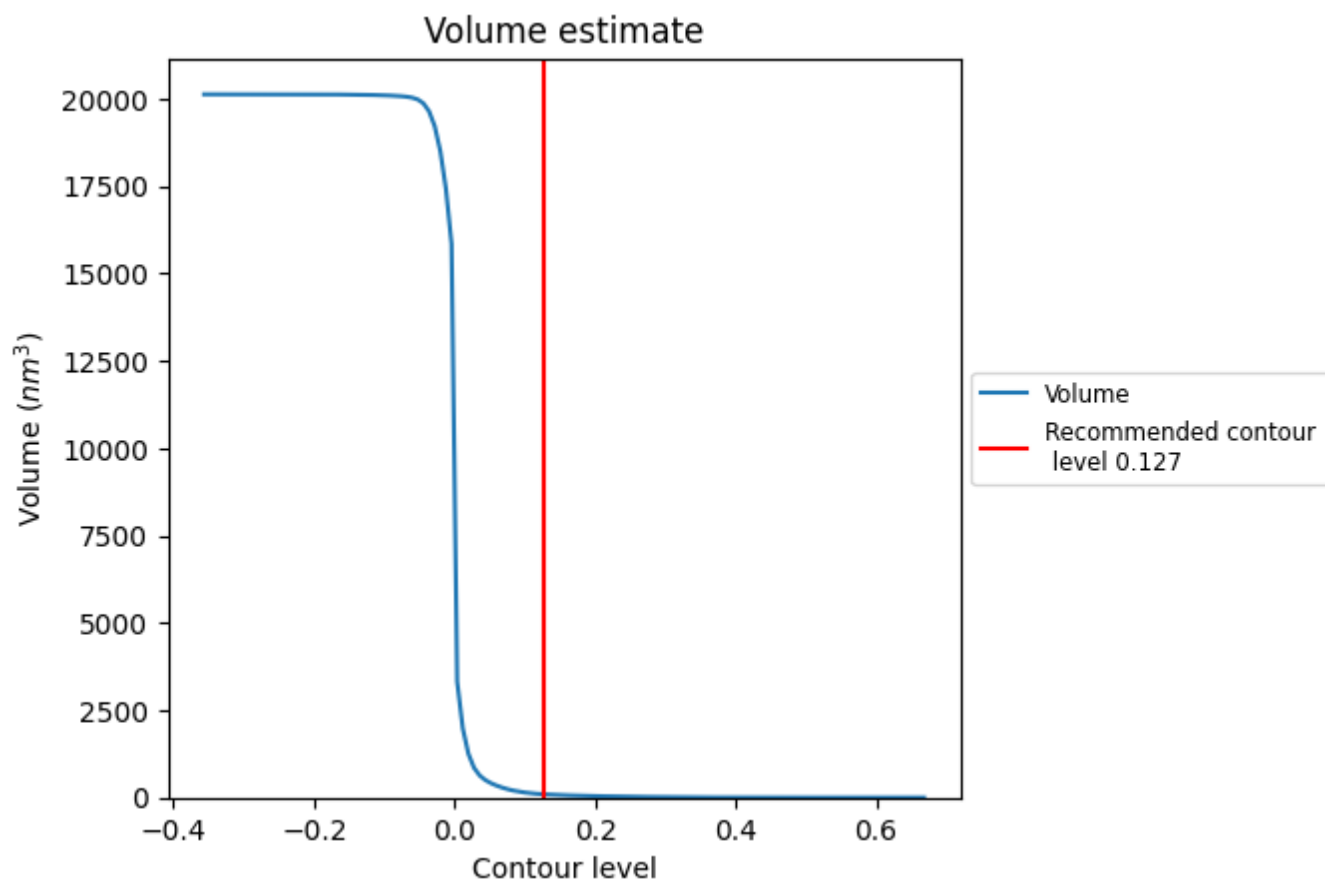
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

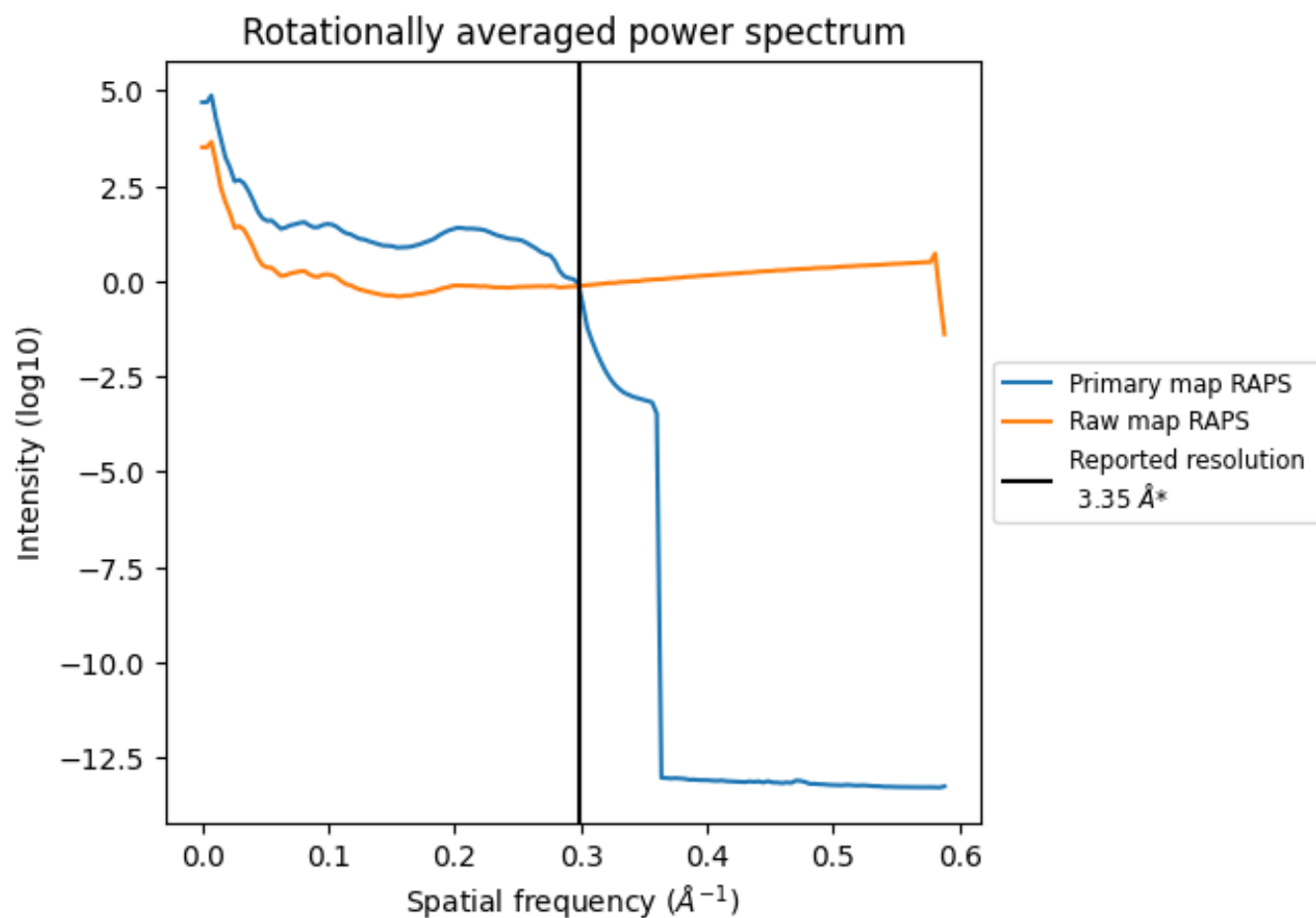
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 94 nm³; this corresponds to an approximate mass of 85 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 ⓘ

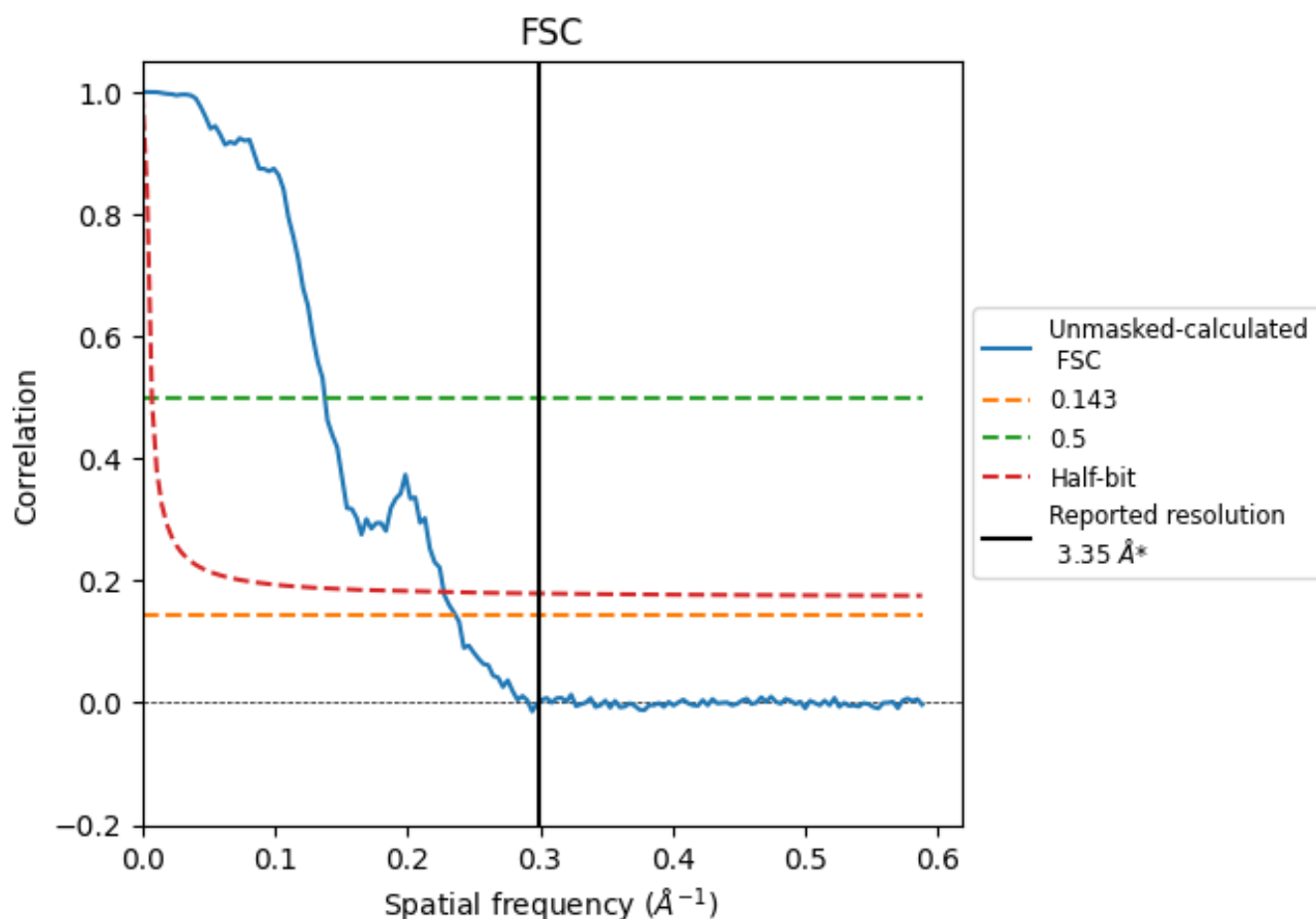


*Reported resolution corresponds to spatial frequency of 0.299 Å⁻¹

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 0.299 \AA^{-1}

8.2 Resolution estimates [i](#)

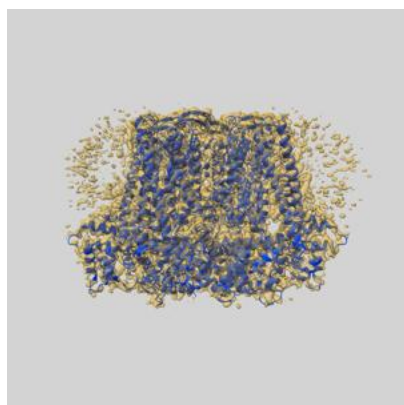
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.35	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.23	7.26	4.40

*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 4.23 differs from the reported value 3.35 by more than 10 %

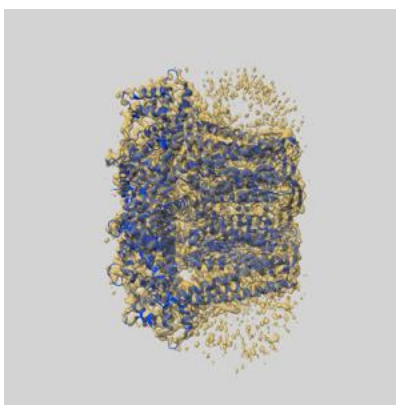
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-65358 and PDB model 9VUB. Per-residue inclusion information can be found in [section 3](#) on [page 9](#).

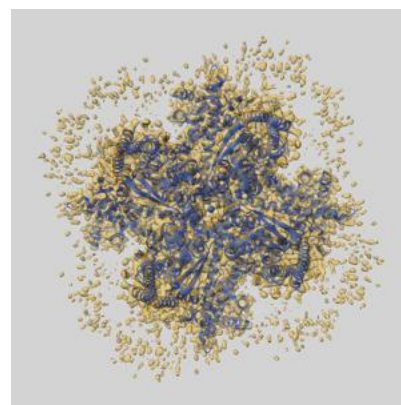
9.1 Map-model overlay [i](#)



X



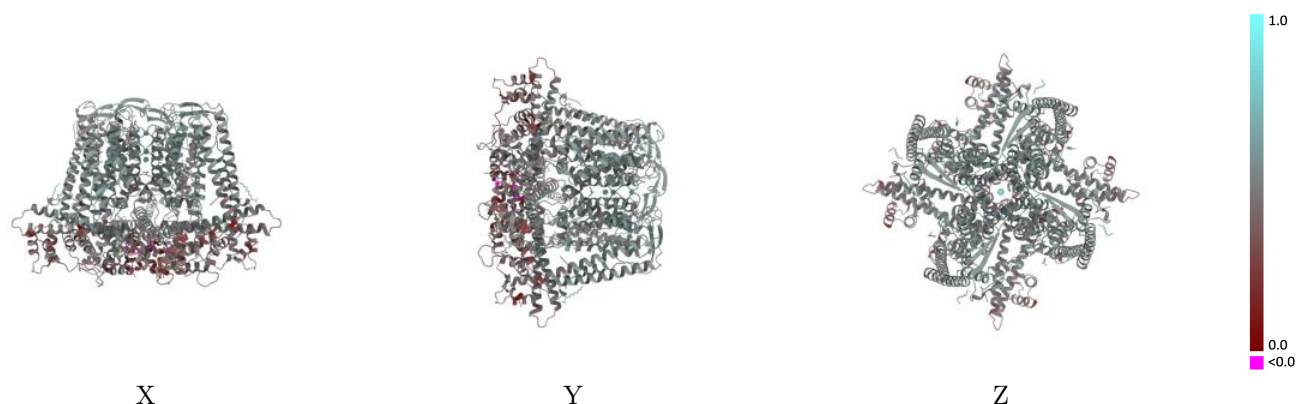
Y



Z

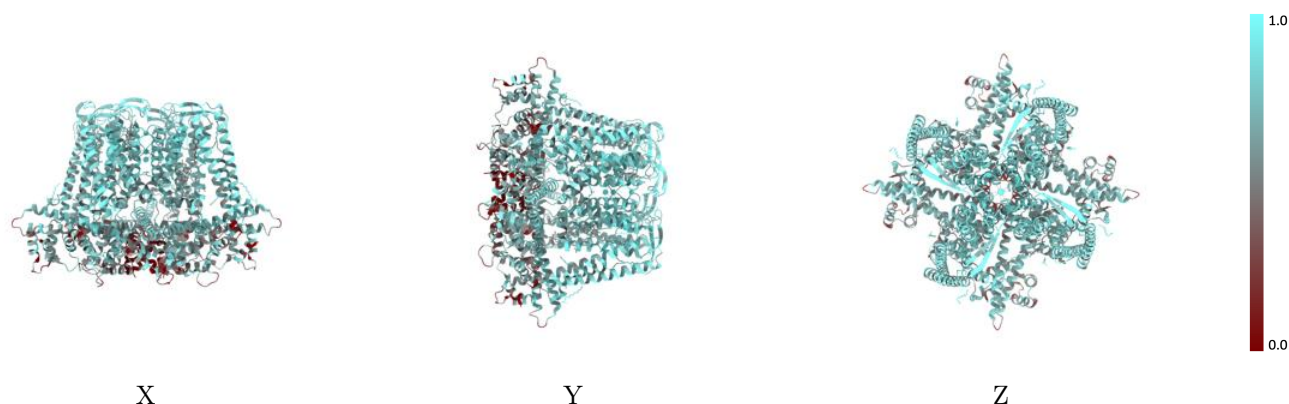
The images above show the 3D surface view of the map at the recommended contour level 0.127 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



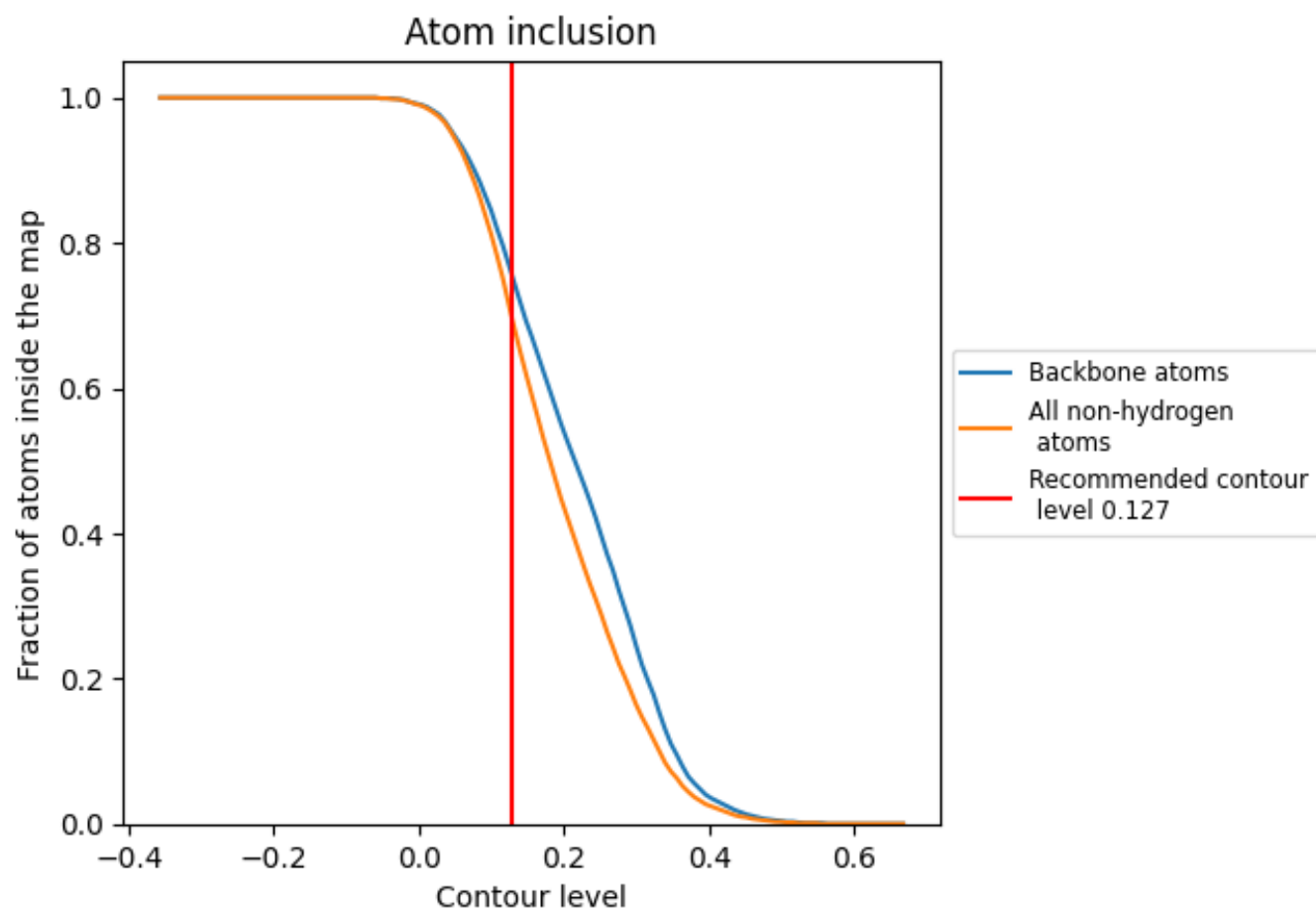
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.127).

9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 70% 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 (0.127) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7020	<div></div> 0.4800
A	<div></div> 0.7480	<div></div> 0.5090
B	<div></div> 0.7510	<div></div> 0.5060
C	<div></div> 0.7460	<div></div> 0.4980
D	<div></div> 0.7540	<div></div> 0.5090
E	<div></div> 0.5370	<div></div> 0.3800
F	<div></div> 0.5700	<div></div> 0.4100
G	<div></div> 0.5600	<div></div> 0.4040
H	<div></div> 0.5760	<div></div> 0.4240

1.0

0.0

<0.0