



Full wwPDB EM Validation Report ⓘ

May 25, 2025 – 08:42 PM EDT

PDB ID : 7USX / pdb_00007usx
EMDB ID : EMD-26742
Title : Structure of Contracted C. elegans TMC-1 complex
Authors : Jeong, H.; Clark, S.; Gouaux, E.
Deposited on : 2022-04-26
Resolution : 3.09 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.dev118
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0rc1
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) : 2.43.1

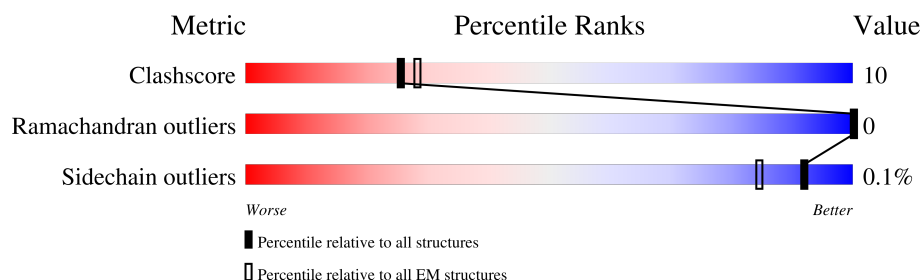
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.09 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 ≥ 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	1285	<div> <div>5%</div> <div>39%</div> <div>8%</div> <div>53%</div> </div>
1	B	1285	<div> <div>5%</div> <div>38%</div> <div>9%</div> <div>53%</div> </div>
2	C	201	<div> <div>5%</div> <div>66%</div> <div>26%</div> <div>8%</div> </div>
2	E	201	<div> <div>5%</div> <div>64%</div> <div>27%</div> <div>8%</div> </div>
3	D	117	<div> <div>6%</div> <div>32%</div> <div>7%</div> <div>61%</div> </div>
3	F	117	<div> <div>6%</div> <div>31%</div> <div>8%</div> <div>61%</div> </div>

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 14240 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 Transmembrane channel-like protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	605	Total	C	N	O	S	0	0
			4883	3215	818	823	27		
1	B	605	Total	C	N	O	S	0	0
			4883	3215	818	823	27		

- Molecule 2 is a protein called CALMyrin (Calcium and Integrin Binding protein) homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	184	Total	C	N	O	S	0	0
			1536	978	256	295	7		
2	E	184	Total	C	N	O	S	0	0
			1536	978	256	295	7		

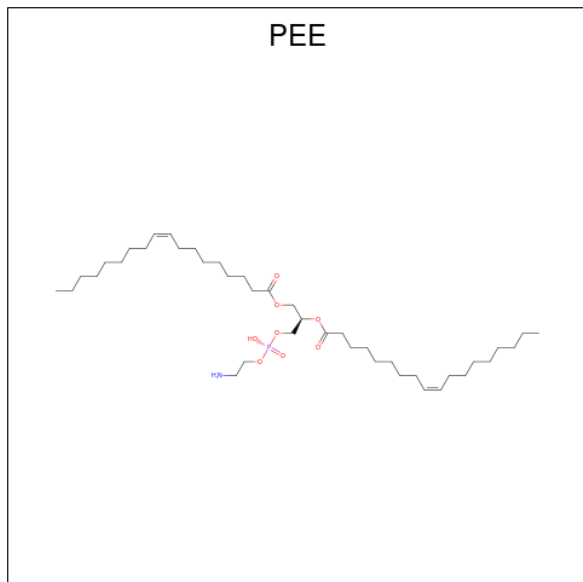
- Molecule 3 is a protein called Transmembrane inner ear expressed protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	46	Total	C	N	O	S	0	0
			353	234	64	50	5		
3	F	46	Total	C	N	O	S	0	0
			353	234	64	50	5		

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

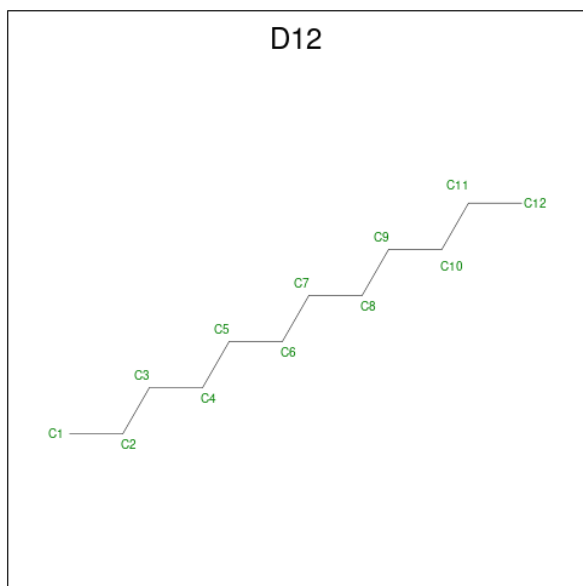
Mol	Chain	Residues	Atoms		AltConf
4	A	2	Total	Ca	0
			2	2	
4	B	2	Total	Ca	0
			2	2	
4	C	2	Total	Ca	0
			2	2	
4	E	2	Total	Ca	0
			2	2	

- Molecule 5 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
5	A	1	42	32	1	8	1	0
5	B	1	42	32	1	8	1	0

- Molecule 6 is DODECANE (CCD ID: D12) (formula: $C_{12}H_{26}$) (labeled as "Ligand of Interest" by depositor).



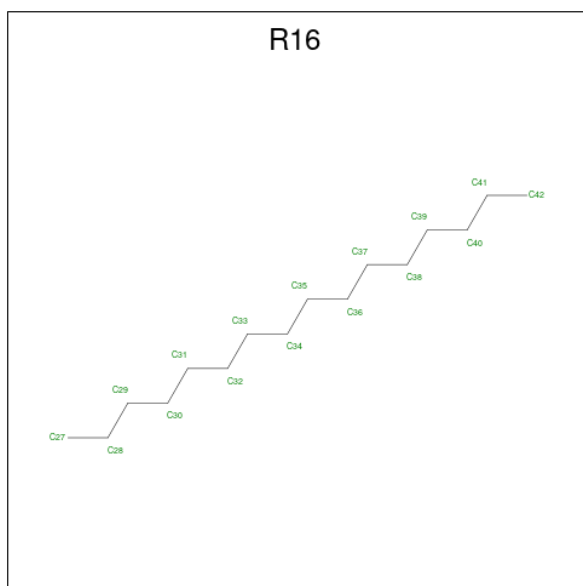
Mol	Chain	Residues	Atoms	AltConf
6	A	1	Total C 9 9	0
6	A	1	Total C 12 12	0
6	A	1	Total C 8 8	0
6	A	1	Total C 9 9	0
6	A	1	Total C 12 12	0
6	A	1	Total C 7 7	0
6	A	1	Total C 12 12	0
6	A	1	Total C 9 9	0
6	A	1	Total C 12 12	0
6	A	1	Total C 7 7	0
6	A	1	Total C 9 9	0
6	A	1	Total C 10 10	0
6	B	1	Total C 9 9	0
6	B	1	Total C 12 12	0
6	B	1	Total C 8 8	0
6	B	1	Total C 9 9	0
6	B	1	Total C 12 12	0
6	B	1	Total C 7 7	0
6	B	1	Total C 12 12	0
6	B	1	Total C 9 9	0
6	B	1	Total C 12 12	0
6	B	1	Total C 7 7	0

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Mol	Chain	Residues	Atoms	AltConf
6	B	1	Total C 9 9	0
6	B	1	Total C 10 10	0
6	D	1	Total C 11 11	0
6	D	1	Total C 12 12	0
6	F	1	Total C 11 11	0
6	F	1	Total C 12 12	0

- Molecule 7 is HEXADECANE (CCD ID: R16) (formula: $C_{16}H_{34}$) (labeled as "Ligand of Interest" by depositor).



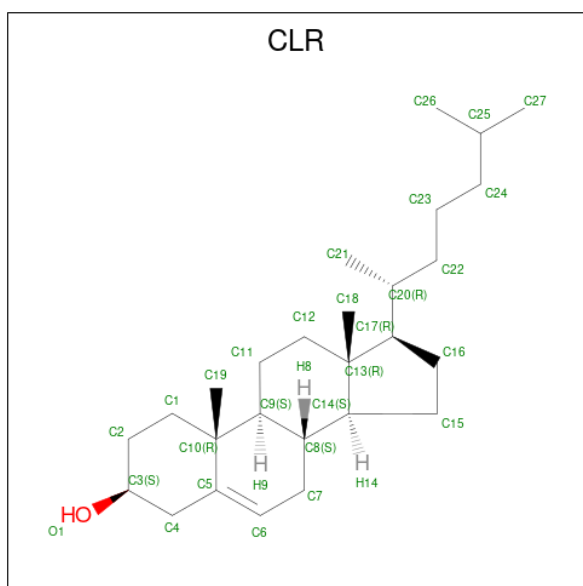
Mol	Chain	Residues	Atoms	AltConf
7	A	1	Total C 16 16	0
7	A	1	Total C 14 14	0
7	A	1	Total C 16 16	0
7	A	1	Total C 16 16	0
7	B	1	Total C 16 16	0

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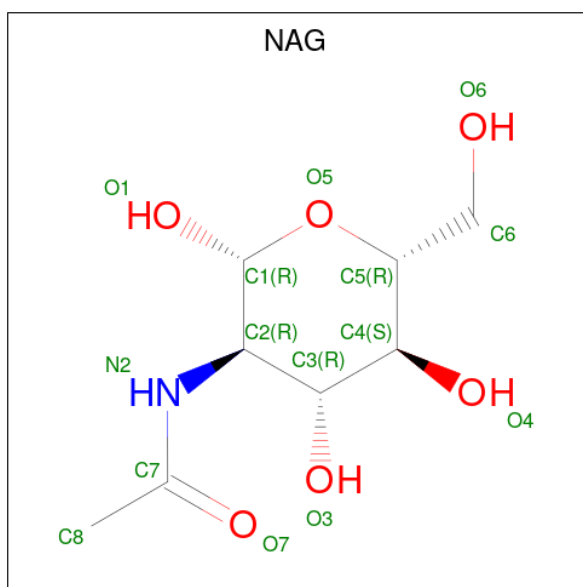
Mol	Chain	Residues	Atoms		AltConf
7	B	1	Total	C	0
			14	14	
7	B	1	Total	C	0
			16	16	
7	B	1	Total	C	0
			16	16	

- Molecule 8 is CHOLESTEROL (CCD ID: CLR) (formula: $C_{27}H_{46}O$) (labeled as "Ligand of Interest" by depositor).



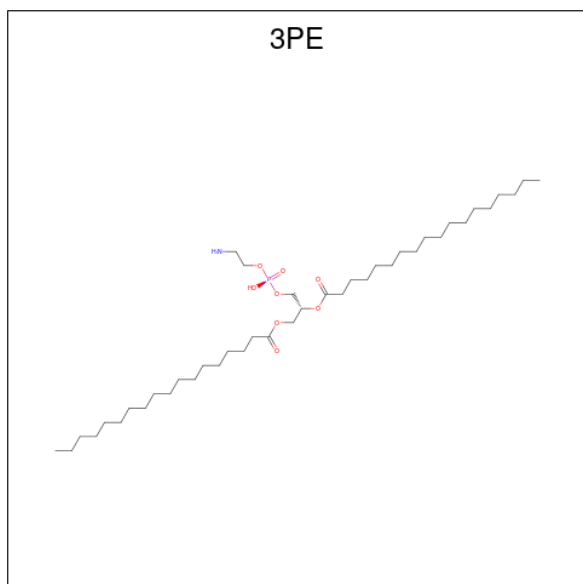
Mol	Chain	Residues	Atoms			AltConf
8	A	1	Total	C	O	0
			28	27	1	
8	B	1	Total	C	O	0
			28	27	1	

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
9	A	1	Total	C	N	O	0
			14	8	1	5	
9	B	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 10 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$) (labeled as "Ligand of Interest" by depositor).



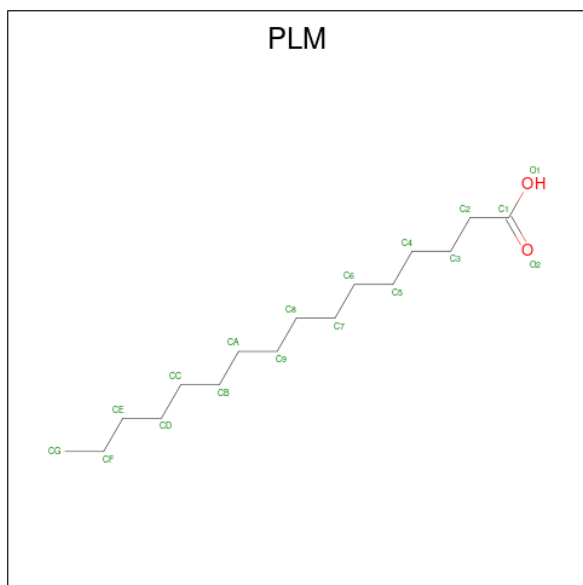
Mol	Chain	Residues	Atoms					AltConf
10	D	1	Total	C	N	O	P	0
			35	25	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
10	F	1	Total	C	N	O	P	0
			35	25	1	8	1	

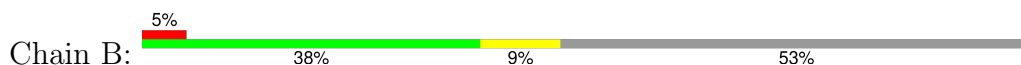
- Molecule 11 is PALMITIC ACID (CCD ID: PLM) (formula: $C_{16}H_{32}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
11	D	1	Total	C	O	0
			14	13	1	
11	D	1	Total	C	O	0
			10	9	1	
11	F	1	Total	C	O	0
			14	13	1	
11	F	1	Total	C	O	0
			10	9	1	

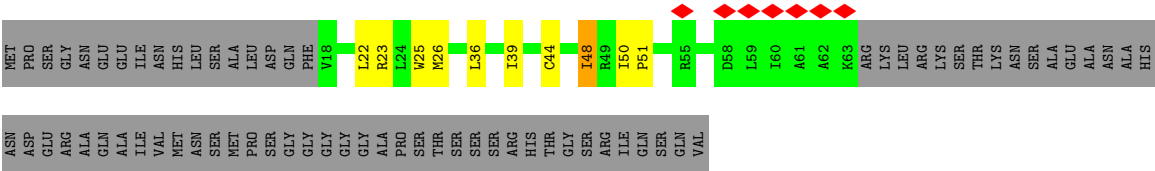
SER	SER	ILE	PRO	LYS	TTR	ASP
	SER	HIS	ILE	LYS	GLN	GLN
	PRO	ARG	THR	THR	GLY	LEU
	GLY	TYR	SER	SER	ILE	MET
	ARG	ASN	LYS	SER	LYS	ILE
	GLN	ILE	LYS	PHE	HIS	LYS
	ASN	ASN	VAL	ASP	PRO	SER
	LYS	GLU	PHE	ASP	VAL	PHE
	LYS	GLU	MET	THR	HIS	GLN
	ALA	ASN	PRO	PRO	PRO	GLY
SER	PRO	THR	GLU	PRO	PRO	GLN
	ASP	THR	THR	ASP	ASN	MET
	PRO	THR	GLU	GLU	THR	GLN
	LEU	GLU	GLU	PRO	ASN	MET
	VAL	GLU	SER	SER	ASN	THR
	VAL	GLU	ALA	ARG	ARG	GLN
	ARG	ALA	ALA	ALA	ARG	GLN
	ALA	PRO	ALA	ALA	ARG	GLN
	PRO	GLU	LEU	LEU	SER	ILE
	PRO	ARG	SER	ARG	SER	THR
GLN	VAL	SER	SER	LYS	TYR	THR
	VAL	VAL	GLU	LYS	ASN	SER
	GLN	GLN	GLN	ASN	SER	CYS
	PHE	PHE	LYS	LYS	PHE	SER
	ASP	PHE	ARG	SER	VAL	GLN
	GLU	ILE	ILE	SER	SER	ILE
	ASP	ILE	THR	THR	LEU	SER
	PRO	VAL	PRO	PRO	TYR	ARG
	PRO	SER	SER	MET	GLU	SER
	ARG	SER	PRO	LEU	HIS	ALA
ASP	GLN	THR	THR	LEU	THR	ILE
	ASP	LYS	LYS	LYS	ASP	VAL
		ILE	THR	THR	ASP	GLN
		ILE	THR	THR	ASP	ALA
		VAL	VAL	LYS	LYS	THR
		THR	VAL	THR	ASN	GLU
		GLU	GLU	GLU	GLY	LEU
		ALA	GLY	GLY	ILE	LEU
		GLN	LYS	LYS	GLY	ARG
		HIS	SER	SER	GLU	THR

- Molecule 1: Transmembrane channel-like protein 1



MET	GLN	ASP	GLY	MET
	GLN	ASP	GLY	
	ALA	GLN	ASP	
	ALA	ARG	GLY	
	ARG	GLU	THR	
	ARG	ASP	THR	
	ALA	ASP	THR	
	SER	GLU	THR	
	LEU	GLU	THR	
	ARG	GLY	THR	
LYS	ASN	ASN	THR	LYS
	LYS	PRO	THR	
	GLU	LEU	THR	
	LYS	THR	THR	
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, POINT, POINT, POINT	Depositor
Number of particles used	140559, 140559, 140559, 140559	Depositor
Resolution determination method	FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION, PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50.00	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	61.397	Depositor
Minimum map value	-38.792	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	5	Depositor
Map size (\AA)	335.6, 335.6, 335.6	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.839, 0.839, 0.839	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: D12, 3PE, CLR, CA, NAG, PLM, R16, PEE

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	0.14	0/5006	0.31	0/6790
1	B	0.14	0/5006	0.32	0/6790
2	C	0.12	0/1569	0.30	0/2111
2	E	0.11	0/1569	0.28	0/2111
3	D	0.15	0/357	0.32	0/482
3	F	0.15	0/357	0.32	0/482
All	All	0.14	0/13864	0.31	0/18766

There are no bond length outliers.

There are no bond angle outliers.

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	4883	0	4948	97	0
1	B	4883	0	4948	104	0
2	C	1536	0	1484	42	0
2	E	1536	0	1484	43	0
3	D	353	0	398	7	0
3	F	353	0	398	9	0
4	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	E	2	0	0	0	0
5	A	42	0	58	6	0
5	B	42	0	58	5	0
6	A	116	0	232	3	0
6	B	116	0	232	2	0
6	D	23	0	47	1	0
6	F	23	0	47	2	0
7	A	62	0	129	5	0
7	B	62	0	129	5	0
8	A	28	0	46	3	0
8	B	28	0	46	4	0
9	A	14	0	13	0	0
9	B	14	0	13	0	0
10	D	35	0	44	6	0
10	F	35	0	44	6	0
11	D	24	0	36	4	0
11	F	24	0	36	3	0
All	All	14240	0	14870	293	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 10.

All (293) 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:C:102:PHE:CE2	2:C:106:LEU:HD11	1.80	1.16
2:E:102:PHE:CE2	2:E:106:LEU:HD11	1.95	1.00
1:A:716:THR:HG23	1:A:718:PRO:HD2	1.46	0.98
1:B:716:THR:HG23	1:B:718:PRO:HD2	1.46	0.96
1:A:713:ILE:HA	1:A:716:THR:HG22	1.50	0.94
1:B:713:ILE:HA	1:B:716:THR:HG22	1.50	0.93
1:A:716:THR:HG23	1:A:718:PRO:CD	2.04	0.88
1:B:716:THR:HG23	1:B:718:PRO:CD	2.04	0.86
2:C:102:PHE:CE2	2:C:106:LEU:CD1	2.61	0.84
1:B:440:TYR:CD1	1:B:738:MET:CE	2.61	0.83
1:B:440:TYR:CD1	1:B:738:MET:HE1	2.15	0.82
1:A:440:TYR:CD1	1:A:738:MET:HE1	2.15	0.81
1:A:440:TYR:CD1	1:A:738:MET:CE	2.63	0.81
1:A:372:TYR:HD1	7:A:1313:R16:H281	1.46	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:440:TYR:HD1	1:B:738:MET:CE	1.96	0.78
1:B:713:ILE:HA	1:B:716:THR:CG2	2.15	0.77
1:A:713:ILE:HA	1:A:716:THR:CG2	2.14	0.77
1:A:440:TYR:HD1	1:A:738:MET:CE	1.98	0.77
1:B:372:TYR:HD1	7:B:1313:R16:H281	1.49	0.76
1:A:716:THR:CG2	1:A:718:PRO:HD2	2.15	0.76
2:C:102:PHE:CZ	2:C:106:LEU:HD11	2.21	0.76
1:B:716:THR:CG2	1:B:718:PRO:HD2	2.15	0.75
1:B:737:GLY:HA3	1:B:795:TRP:CD1	2.23	0.74
1:B:411:ASP:OD1	1:B:428:HIS:CE1	2.44	0.69
1:A:411:ASP:OD1	1:A:428:HIS:CE1	2.45	0.69
1:A:440:TYR:HD1	1:A:738:MET:HE1	1.56	0.69
1:B:94:ARG:NH2	2:E:29:GLN:O	2.25	0.69
1:A:94:ARG:NH2	2:C:29:GLN:O	2.25	0.69
1:B:780:ARG:HE	1:B:783:ARG:HG2	1.59	0.67
1:A:780:ARG:HE	1:A:783:ARG:HG2	1.59	0.67
2:C:180:PHE:CZ	2:C:184:GLU:OE1	2.47	0.66
1:A:737:GLY:HA3	1:A:795:TRP:CD1	2.29	0.66
1:B:440:TYR:CE1	1:B:738:MET:CE	2.79	0.66
1:A:683:ASP:OD2	1:A:756:LYS:NZ	2.25	0.65
1:B:298:LYS:O	2:E:189:ARG:NH1	2.31	0.64
1:A:196:GLU:OE2	1:A:215:LYS:NZ	2.29	0.63
3:F:44:CYS:O	10:F:201:3PE:H121	1.97	0.63
1:B:683:ASP:OD2	1:B:756:LYS:NZ	2.25	0.63
1:A:440:TYR:CE1	1:A:738:MET:CE	2.81	0.62
1:B:814:ARG:NH2	1:B:822:TYR:O	2.33	0.62
1:A:814:ARG:NH2	1:A:822:TYR:O	2.32	0.61
1:B:701:TRP:HB2	7:B:1315:R16:H291	1.82	0.61
1:A:701:TRP:HB2	7:A:1315:R16:H291	1.82	0.61
1:B:440:TYR:CE1	1:B:738:MET:HE1	2.35	0.61
1:A:272:THR:HG21	8:A:1308:CLR:H242	1.83	0.60
2:C:87:ARG:NH1	2:C:90:GLU:OE1	2.34	0.60
2:C:102:PHE:HE2	2:C:106:LEU:HD11	1.59	0.60
2:E:87:ARG:NH1	2:E:90:GLU:OE1	2.34	0.60
2:E:102:PHE:CE2	2:E:106:LEU:CD1	2.79	0.60
1:A:440:TYR:CE1	1:A:738:MET:HE1	2.36	0.60
1:A:298:LYS:O	2:C:189:ARG:NH1	2.34	0.60
1:B:272:THR:HG21	8:B:1308:CLR:H242	1.83	0.59
1:B:149:LEU:O	5:B:1303:PEE:H61	2.03	0.59
1:A:307:LYS:HE3	1:A:332:LYS:HD2	1.85	0.59
1:B:233:HIS:NE2	1:B:393:ASN:HB2	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:713:ILE:CA	1:A:716:THR:HG22	2.30	0.58
1:A:233:HIS:NE2	1:A:393:ASN:HB2	2.18	0.58
1:B:440:TYR:CE1	1:B:738:MET:HE2	2.39	0.58
1:A:296:GLY:HA2	2:C:189:ARG:HA	1.84	0.58
1:B:162:HIS:HB3	1:B:769:MET:HE1	1.86	0.58
2:E:62:ARG:HA	2:E:65:ILE:HG12	1.86	0.58
2:E:186:VAL:HG13	2:E:187:VAL:HG13	1.86	0.58
2:E:41:ARG:NH1	2:E:201:ILE:OXT	2.37	0.58
2:E:150:THR:HG22	2:E:153:GLU:H	1.68	0.58
1:A:372:TYR:CD1	7:A:1313:R16:H281	2.35	0.57
2:C:164:GLU:HB3	2:C:165:ARG:HH12	1.69	0.57
1:A:162:HIS:HB3	1:A:769:MET:HE1	1.86	0.57
1:B:296:GLY:HA2	2:E:189:ARG:HA	1.84	0.57
2:C:186:VAL:HG13	2:C:187:VAL:HG13	1.86	0.57
1:B:96:GLN:O	1:B:103:LYS:NZ	2.33	0.57
2:C:142:LEU:HD23	2:C:163:ILE:HG23	1.86	0.57
2:C:41:ARG:NH1	2:C:201:ILE:OXT	2.38	0.57
1:A:363:ILE:HG21	1:A:431:ARG:HD3	1.87	0.57
1:B:870:SER:HA	1:B:873:ARG:HG2	1.87	0.56
1:A:780:ARG:NH2	2:C:192:ASP:OD2	2.38	0.56
1:B:780:ARG:NH2	2:E:192:ASP:OD2	2.38	0.56
1:A:870:SER:HA	1:A:873:ARG:HG2	1.88	0.56
2:E:142:LEU:HD23	2:E:163:ILE:HG23	1.87	0.56
10:F:201:3PE:H342	10:F:201:3PE:H261	1.88	0.56
10:D:201:3PE:H342	10:D:201:3PE:H261	1.88	0.55
1:B:196:GLU:OE2	1:B:215:LYS:NZ	2.29	0.55
2:C:62:ARG:HA	2:C:65:ILE:HG12	1.87	0.55
1:A:440:TYR:CE1	1:A:738:MET:HE2	2.41	0.55
2:E:95:ASP:N	2:E:95:ASP:OD1	2.37	0.55
2:C:164:GLU:HB3	2:C:165:ARG:NH1	2.22	0.55
2:E:63:PRO:O	2:E:101:SER:OG	2.22	0.55
1:A:239:ARG:NH2	1:A:240:TYR:OH	2.39	0.55
1:A:188:ALA:HB2	1:A:273:ILE:HD11	1.88	0.55
1:B:307:LYS:HE3	1:B:332:LYS:HD2	1.88	0.55
1:B:149:LEU:HB3	5:B:1303:PEE:H60	1.88	0.55
1:A:420:HIS:HB3	1:A:423:THR:HG22	1.89	0.55
1:B:420:HIS:HB3	1:B:423:THR:HG22	1.89	0.55
1:B:239:ARG:NH2	1:B:240:TYR:OH	2.39	0.54
1:B:440:TYR:HD1	1:B:738:MET:HE1	1.56	0.54
3:D:22:LEU:O	3:D:26:MET:HE1	2.07	0.54
2:E:28:TYR:O	2:E:32:THR:OG1	2.25	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:22:LEU:O	3:F:26:MET:HE1	2.08	0.54
1:A:431:ARG:HG2	6:A:1310:D12:H32	1.89	0.54
1:B:188:ALA:HB2	1:B:273:ILE:HD11	1.88	0.54
2:C:95:ASP:OD1	2:C:95:ASP:N	2.41	0.54
2:E:57:ASN:O	2:E:62:ARG:NH1	2.41	0.54
2:E:102:PHE:CZ	2:E:106:LEU:HD11	2.41	0.54
1:B:713:ILE:CA	1:B:716:THR:HG22	2.31	0.54
1:B:431:ARG:HG2	6:B:1310:D12:H32	1.88	0.54
1:A:96:GLN:O	1:A:103:LYS:NZ	2.32	0.53
1:A:740:TRP:HA	1:A:743:LEU:HD23	1.90	0.53
3:F:36:LEU:HD21	10:F:201:3PE:H361	1.91	0.53
3:D:36:LEU:HD21	10:D:201:3PE:H361	1.91	0.53
1:B:95:CYS:O	2:E:119:GLN:NE2	2.41	0.53
1:B:740:TRP:HA	1:B:743:LEU:HD23	1.90	0.53
1:B:260:TYR:CE1	8:B:1308:CLR:H72	2.44	0.52
1:B:395:VAL:HG13	1:B:396:PRO:HD3	1.90	0.52
3:D:44:CYS:O	10:D:201:3PE:H121	2.09	0.52
1:A:711:TRP:HE1	1:A:716:THR:HG21	1.74	0.52
1:B:363:ILE:HG21	1:B:431:ARG:HD3	1.90	0.52
1:A:395:VAL:HG13	1:A:396:PRO:HD3	1.90	0.52
1:B:711:TRP:HE1	1:B:716:THR:HG21	1.75	0.52
1:B:258:ILE:HG21	6:B:1309:D12:H72	1.92	0.52
1:B:372:TYR:CD1	7:B:1313:R16:H281	2.37	0.52
1:B:710:CYS:HB2	1:B:711:TRP:HE3	1.75	0.52
1:A:411:ASP:OD1	1:A:428:HIS:CD2	2.63	0.52
1:B:174:LEU:HD13	1:B:732:ILE:HD12	1.92	0.52
2:C:57:ASN:OD1	2:C:62:ARG:NH1	2.33	0.52
2:E:179:ASN:OD1	2:E:182:GLU:HG3	2.09	0.52
1:A:710:CYS:HB2	1:A:711:TRP:HE3	1.75	0.51
1:A:870:SER:O	1:A:873:ARG:HG2	2.10	0.51
2:C:57:ASN:O	2:C:62:ARG:NH1	2.43	0.51
1:B:737:GLY:HA3	1:B:795:TRP:NE1	2.25	0.51
1:B:870:SER:O	1:B:873:ARG:HG2	2.10	0.51
2:C:122:LEU:HD11	2:C:188:SER:HB2	1.91	0.51
1:A:258:ILE:HG21	6:A:1309:D12:H72	1.92	0.51
1:A:174:LEU:HD13	1:A:732:ILE:HD12	1.92	0.51
2:C:28:TYR:O	2:C:32:THR:OG1	2.26	0.51
1:B:411:ASP:OD1	1:B:428:HIS:CD2	2.62	0.51
3:D:25:TRP:NE1	3:D:26:MET:HE2	2.25	0.51
2:E:122:LEU:HD11	2:E:188:SER:HB2	1.93	0.51
1:B:411:ASP:OD1	1:B:428:HIS:NE2	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:150:THR:HG22	2:C:153:GLU:H	1.75	0.50
2:E:119:GLN:HG3	2:E:120:LEU:N	2.27	0.50
3:F:25:TRP:NE1	3:F:26:MET:HE2	2.27	0.50
1:A:411:ASP:OD1	1:A:428:HIS:NE2	2.45	0.50
1:B:132:ARG:HD2	1:B:136:ARG:NH2	2.27	0.50
2:E:23:GLU:CD	2:E:23:GLU:H	2.20	0.50
2:E:57:ASN:OD1	2:E:62:ARG:NH1	2.32	0.50
6:F:203:D12:H62	11:F:204:PLM:H42	1.94	0.50
1:B:671:ILE:O	1:B:675:GLU:HG2	2.12	0.49
1:B:299:ALA:HB2	2:E:189:ARG:HB2	1.94	0.49
2:C:23:GLU:CD	2:C:23:GLU:H	2.20	0.49
1:A:149:LEU:O	5:A:1303:PEE:H61	2.12	0.49
6:D:203:D12:H62	11:D:204:PLM:H42	1.95	0.49
1:B:179:PHE:HB2	5:B:1303:PEE:H8	1.93	0.49
1:B:243:LEU:HA	1:B:748:LEU:HB2	1.95	0.49
2:E:35:THR:O	2:E:39:ILE:HG12	2.13	0.48
1:A:299:ALA:HB2	2:C:189:ARG:HB2	1.94	0.48
2:C:35:THR:O	2:C:39:ILE:HG12	2.13	0.48
1:A:132:ARG:HD2	1:A:136:ARG:NH2	2.28	0.48
1:A:716:THR:HG23	1:A:718:PRO:HD3	1.93	0.48
1:A:179:PHE:HB2	5:A:1303:PEE:H8	1.95	0.48
1:B:440:TYR:CD1	1:B:738:MET:HE2	2.48	0.48
1:A:671:ILE:O	1:A:675:GLU:HG2	2.13	0.48
1:A:243:LEU:HA	1:A:748:LEU:HB2	1.95	0.48
5:A:1303:PEE:H16	5:A:1303:PEE:H21	1.68	0.48
1:B:132:ARG:O	1:B:136:ARG:HG2	2.14	0.48
1:B:677:VAL:HG22	1:B:749:LEU:HD13	1.96	0.48
2:C:179:ASN:OD1	2:C:182:GLU:HG3	2.14	0.48
1:A:677:VAL:HG22	1:A:749:LEU:HD13	1.96	0.47
1:A:132:ARG:O	1:A:136:ARG:HG2	2.13	0.47
1:B:207:ARG:NH2	1:B:249:SER:OG	2.47	0.47
1:A:207:ARG:NH2	1:A:249:SER:OG	2.47	0.47
1:A:303:ILE:O	1:A:307:LYS:HG3	2.15	0.47
1:A:838:ASP:HB3	1:A:841:VAL:HG12	1.97	0.47
1:B:308:LEU:HD23	2:E:145:MET:HE1	1.97	0.47
1:A:268:MET:HB3	8:A:1308:CLR:H213	1.97	0.47
1:B:122:SER:OG	1:B:123:ARG:N	2.48	0.46
1:A:149:LEU:HB3	5:A:1303:PEE:H60	1.98	0.46
1:A:122:SER:OG	1:A:123:ARG:N	2.49	0.46
1:A:711:TRP:NE1	1:A:716:THR:HG21	2.30	0.46
1:B:112:LYS:HA	1:B:112:LYS:HD3	1.69	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:687:THR:HG21	1:B:760:LEU:HD11	1.98	0.46
2:C:156:ASP:OD1	2:C:156:ASP:N	2.46	0.46
1:B:303:ILE:O	1:B:307:LYS:HG3	2.15	0.46
1:A:337:ILE:HA	1:A:340:ILE:HG22	1.98	0.46
1:B:711:TRP:NE1	1:B:716:THR:HG21	2.31	0.46
1:B:783:ARG:O	2:E:191:PRO:HB2	2.16	0.46
1:A:229:ALA:O	1:A:233:HIS:ND1	2.31	0.45
1:A:159:ILE:HA	1:A:769:MET:HE3	1.97	0.45
1:B:159:ILE:HA	1:B:769:MET:HE3	1.97	0.45
1:B:710:CYS:HB2	1:B:711:TRP:CE3	2.52	0.45
1:B:238:LEU:O	1:B:241:SER:OG	2.26	0.45
1:B:378:VAL:HG11	1:B:446:ALA:HB1	1.99	0.45
2:E:156:ASP:OD1	2:E:156:ASP:N	2.46	0.45
1:B:838:ASP:HB3	1:B:841:VAL:HG12	1.97	0.45
2:E:67:THR:HG21	2:E:99:ASN:HB3	1.97	0.45
1:A:112:LYS:HA	1:A:112:LYS:HD3	1.69	0.45
1:A:260:TYR:CE1	8:A:1308:CLR:H72	2.52	0.45
1:A:334:ARG:O	1:A:337:ILE:HG13	2.17	0.45
1:B:716:THR:HG23	1:B:718:PRO:HD3	1.93	0.45
2:C:63:PRO:O	2:C:101:SER:OG	2.29	0.45
3:F:44:CYS:O	10:F:201:3PE:C12	2.62	0.45
1:A:710:CYS:HB2	1:A:711:TRP:CE3	2.51	0.44
1:A:687:THR:HG21	1:A:760:LEU:HD11	1.98	0.44
3:D:50:ILE:HB	3:D:51:PRO:HD3	1.99	0.44
2:E:180:PHE:CZ	2:E:184:GLU:OE1	2.70	0.44
1:A:737:GLY:HA3	1:A:795:TRP:HD1	1.78	0.44
2:C:112:PHE:HB3	2:C:199:ILE:HB	1.99	0.44
1:A:308:LEU:HD23	2:C:145:MET:HE1	1.98	0.44
1:A:861:LEU:HD13	1:B:861:LEU:HD13	1.99	0.44
2:C:171:ASP:HA	2:C:182:GLU:OE1	2.18	0.44
7:A:1307:R16:H332	7:A:1307:R16:H302	1.78	0.44
2:C:184:GLU:O	2:C:188:SER:HB3	2.16	0.44
1:B:870:SER:HA	1:B:873:ARG:CD	2.48	0.44
2:E:155:SER:HB2	2:E:158:GLU:HG3	1.99	0.44
1:B:92:LYS:O	1:B:92:LYS:HG2	2.17	0.44
1:A:123:ARG:HH12	1:A:126:LEU:HD13	1.83	0.44
1:B:302:TYR:HA	2:E:169:GLU:OE1	2.18	0.44
2:C:123:LYS:HE3	2:C:123:LYS:HB2	1.75	0.44
1:A:783:ARG:O	2:C:191:PRO:HB2	2.17	0.43
1:B:203:ALA:HB1	1:B:207:ARG:HB3	2.00	0.43
2:E:45:ARG:NH1	2:E:78:GLU:OE2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:76:MET:HE1	2:E:109:PHE:HZ	1.83	0.43
3:F:50:ILE:HB	3:F:51:PRO:HD3	1.99	0.43
1:B:724:LYS:HB3	1:B:727:GLU:OE2	2.18	0.43
11:D:204:PLM:H51	11:D:204:PLM:H21	1.83	0.43
1:B:376:PHE:CD1	1:B:376:PHE:C	2.97	0.43
1:B:737:GLY:HA3	1:B:795:TRP:HD1	1.81	0.43
2:C:167:ILE:HD13	2:C:167:ILE:HA	1.91	0.43
1:A:409:ILE:O	1:A:413:ILE:HG13	2.18	0.43
1:A:692:LEU:HD11	10:D:201:3PE:H282	2.01	0.43
1:B:123:ARG:HH12	1:B:126:LEU:HD13	1.83	0.43
1:B:363:ILE:HD13	1:B:431:ARG:CD	2.49	0.43
1:A:870:SER:HA	1:A:873:ARG:CD	2.48	0.43
1:B:337:ILE:HA	1:B:340:ILE:HG22	1.99	0.43
1:B:376:PHE:HE1	1:B:380:LYS:HD3	1.83	0.43
2:E:40:ILE:HD13	2:E:40:ILE:HA	1.92	0.43
1:A:724:LYS:HB3	1:A:727:GLU:OE2	2.19	0.43
1:B:692:LEU:HD11	10:F:201:3PE:H282	2.00	0.43
2:C:66:THR:O	2:C:101:SER:OG	2.36	0.42
2:E:184:GLU:O	2:E:188:SER:HB3	2.18	0.42
3:F:48:ILE:H	3:F:48:ILE:HG13	1.55	0.42
2:E:67:THR:CG2	2:E:99:ASN:HB3	2.48	0.42
1:B:268:MET:HB3	8:B:1308:CLR:H213	2.02	0.42
3:F:39:ILE:CG2	11:F:205:PLM:H22	2.50	0.42
10:F:201:3PE:H221	11:F:205:PLM:H21	2.01	0.42
1:A:146:LYS:HG3	5:A:1303:PEE:H22	2.01	0.42
1:A:378:VAL:HG11	1:A:446:ALA:HB1	2.01	0.42
1:A:749:LEU:HB3	1:A:750:PRO:HD3	2.02	0.42
1:B:797:LEU:HA	1:B:800:THR:HG22	2.02	0.42
2:E:22:ARG:HD3	2:E:22:ARG:HA	1.83	0.42
2:E:167:ILE:HD13	2:E:167:ILE:HA	1.89	0.42
1:B:214:ARG:HG3	1:B:215:LYS:HG3	2.01	0.42
1:A:203:ALA:HB1	1:A:207:ARG:HB3	2.01	0.42
1:A:214:ARG:HG3	1:A:215:LYS:HG3	2.01	0.42
1:A:302:TYR:HA	2:C:169:GLU:OE1	2.19	0.42
1:B:149:LEU:O	5:B:1303:PEE:C37	2.66	0.42
1:B:749:LEU:HB3	1:B:750:PRO:HD3	2.02	0.42
3:D:39:ILE:CG2	11:D:205:PLM:H22	2.50	0.42
1:A:797:LEU:HA	1:A:800:THR:HG22	2.02	0.42
1:B:165:SER:OG	1:B:313:ASP:OD2	2.35	0.42
1:B:363:ILE:HD13	1:B:431:ARG:HD3	2.02	0.42
7:B:1307:R16:H302	7:B:1307:R16:H332	1.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:D:201:3PE:H221	11:D:205:PLM:H21	2.02	0.42
2:C:155:SER:HB2	2:C:158:GLU:HG3	2.02	0.41
3:F:23:ARG:HH12	6:F:202:D12:H21	1.86	0.41
1:B:242:PRO:HG2	7:B:1307:R16:H352	2.03	0.41
1:B:313:ASP:OD1	1:B:315:THR:OG1	2.39	0.41
2:E:112:PHE:HB3	2:E:199:ILE:HB	2.01	0.41
1:A:313:ASP:OD1	1:A:315:THR:OG1	2.37	0.41
1:A:160:GLU:OE1	2:C:200:ARG:NE	2.38	0.41
1:A:376:PHE:CD1	1:A:376:PHE:C	2.98	0.41
1:B:100:MET:HG2	2:E:107:ASP:OD2	2.21	0.41
1:B:227:GLU:C	1:B:229:ALA:H	2.29	0.41
1:B:411:ASP:OD1	1:B:428:HIS:CG	2.74	0.41
2:C:49:LEU:HD23	2:C:49:LEU:HA	1.90	0.41
2:E:73:VAL:HG21	2:E:100:LEU:HD12	2.03	0.41
2:E:171:ASP:HA	2:E:182:GLU:OE1	2.21	0.41
1:A:363:ILE:HD13	1:A:431:ARG:CD	2.51	0.41
1:A:411:ASP:OD1	1:A:428:HIS:CG	2.74	0.41
1:A:716:THR:HG23	1:A:717:PHE:N	2.36	0.41
1:B:716:THR:HG23	1:B:717:PHE:N	2.35	0.41
1:B:146:LYS:HG3	5:B:1303:PEE:H22	2.02	0.41
1:B:185:THR:O	1:B:189:LEU:HB2	2.21	0.41
1:B:208:PHE:O	1:B:212:LYS:HB2	2.21	0.41
1:B:444:ILE:HD13	1:B:802:PRO:HG3	2.03	0.41
2:C:94:GLU:HG2	2:C:96:GLY:H	1.85	0.41
3:D:44:CYS:O	10:D:201:3PE:C12	2.69	0.41
1:A:149:LEU:O	5:A:1303:PEE:C37	2.69	0.41
1:A:208:PHE:O	1:A:212:LYS:HB2	2.20	0.40
1:A:842:LEU:HD23	1:A:842:LEU:HA	1.91	0.40
1:A:242:PRO:HG2	7:A:1307:R16:H352	2.03	0.40
1:A:227:GLU:C	1:A:229:ALA:H	2.29	0.40
6:A:1310:D12:H12	6:A:1310:D12:H41	1.87	0.40
1:B:261:ALA:H	8:B:1308:CLR:H6	1.87	0.40
2:C:22:ARG:O	2:C:25:LEU:N	2.54	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	601/1285 (47%)	578 (96%)	23 (4%)	0	100	100
1	B	601/1285 (47%)	579 (96%)	22 (4%)	0	100	100
2	C	182/201 (90%)	176 (97%)	6 (3%)	0	100	100
2	E	182/201 (90%)	176 (97%)	6 (3%)	0	100	100
3	D	44/117 (38%)	42 (96%)	2 (4%)	0	100	100
3	F	44/117 (38%)	41 (93%)	3 (7%)	0	100	100
All	All	1654/3206 (52%)	1592 (96%)	62 (4%)	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	519/1150 (45%)	519 (100%)	0	100	100
1	B	519/1150 (45%)	519 (100%)	0	100	100
2	C	171/185 (92%)	171 (100%)	0	100	100
2	E	171/185 (92%)	170 (99%)	1 (1%)	84	91
3	D	37/96 (38%)	37 (100%)	0	100	100
3	F	37/96 (38%)	36 (97%)	1 (3%)	40	67
All	All	1454/2862 (51%)	1452 (100%)	2 (0%)	92	97

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	150	THR
3	F	48	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	144	ASN
1	A	420	HIS
1	A	731	HIS
1	A	839	GLN
1	B	224	HIS
1	B	420	HIS
1	B	439	ASN
1	B	731	HIS
1	B	839	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 56 ligands modelled in this entry, 8 are monoatomic - leaving 48 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
7	R16	B	1313	-	15,15,15	0.29	0	14,14,14	0.88	0
7	R16	A	1312	-	13,13,15	0.28	0	12,12,14	0.86	0
10	3PE	D	201	-	34,34,50	1.04	4 (11%)	37,39,55	1.18	2 (5%)
11	PLM	F	204	3	12,13,17	0.27	0	11,12,17	0.84	0
9	NAG	A	1321	1	14,14,15	0.28	0	17,19,21	0.55	0
6	D12	A	1311	-	6,6,11	0.30	0	5,5,10	0.68	0
6	D12	A	1310	-	11,11,11	0.28	0	10,10,10	0.85	0
7	R16	A	1307	-	15,15,15	0.28	0	14,14,14	0.86	0
11	PLM	F	205	3	8,9,17	0.41	0	7,8,17	1.07	0
6	D12	B	1320	-	9,9,11	0.30	0	8,8,10	0.81	0
6	D12	A	1317	-	11,11,11	0.29	0	10,10,10	0.81	0
6	D12	F	202	-	10,10,11	0.29	0	9,9,10	0.84	0
6	D12	A	1318	-	6,6,11	0.32	0	5,5,10	0.68	0
6	D12	B	1311	-	6,6,11	0.31	0	5,5,10	0.68	0
6	D12	B	1310	-	11,11,11	0.29	0	10,10,10	0.86	0
6	D12	B	1317	-	11,11,11	0.29	0	10,10,10	0.81	0
6	D12	A	1305	-	11,11,11	0.28	0	10,10,10	0.85	0
6	D12	B	1305	-	11,11,11	0.28	0	10,10,10	0.85	0
6	D12	B	1319	-	8,8,11	0.30	0	7,7,10	0.76	0
11	PLM	D	204	3	12,13,17	0.27	0	11,12,17	0.84	0
7	R16	A	1315	-	15,15,15	0.28	0	14,14,14	0.88	0
6	D12	B	1318	-	6,6,11	0.32	0	5,5,10	0.68	0
6	D12	A	1319	-	8,8,11	0.31	0	7,7,10	0.77	0
6	D12	A	1316	-	8,8,11	0.30	0	7,7,10	0.76	0
6	D12	A	1320	-	9,9,11	0.29	0	8,8,10	0.81	0
11	PLM	D	205	3	8,9,17	0.42	0	7,8,17	1.07	0
6	D12	A	1306	-	7,7,11	0.28	0	6,6,10	0.79	0
8	CLR	B	1308	-	31,31,31	0.39	0	48,48,48	0.73	0
10	3PE	F	201	-	34,34,50	1.04	4 (11%)	37,39,55	1.18	2 (5%)
6	D12	D	203	-	11,11,11	0.29	0	10,10,10	0.83	0
5	PEE	A	1303	-	41,41,50	1.28	6 (14%)	44,46,55	1.21	6 (13%)
6	D12	A	1309	-	8,8,11	0.29	0	7,7,10	0.79	0
7	R16	B	1307	-	15,15,15	0.28	0	14,14,14	0.86	0
6	D12	B	1306	-	7,7,11	0.28	0	6,6,10	0.79	0
6	D12	D	202	-	10,10,11	0.29	0	9,9,10	0.84	0
7	R16	B	1312	-	13,13,15	0.28	0	12,12,14	0.86	0
6	D12	B	1314	-	11,11,11	0.28	0	10,10,10	0.87	0
6	D12	B	1309	-	8,8,11	0.30	0	7,7,10	0.79	0
6	D12	A	1314	-	11,11,11	0.28	0	10,10,10	0.86	0
6	D12	F	203	-	11,11,11	0.29	0	10,10,10	0.83	0
9	NAG	B	1321	1	14,14,15	0.28	0	17,19,21	0.55	0
5	PEE	B	1303	-	41,41,50	1.28	6 (14%)	44,46,55	1.21	6 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	R16	B	1315	-	15,15,15	0.28	0	14,14,14	0.88	0
6	D12	A	1304	-	8,8,11	0.30	0	7,7,10	0.79	0
7	R16	A	1313	-	15,15,15	0.29	0	14,14,14	0.87	0
6	D12	B	1316	-	8,8,11	0.30	0	7,7,10	0.76	0
8	CLR	A	1308	-	31,31,31	0.39	0	48,48,48	0.70	0
6	D12	B	1304	-	8,8,11	0.30	0	7,7,10	0.79	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
7	R16	B	1313	-	-	1/13/13/13	-
7	R16	A	1312	-	-	4/11/11/13	-
10	3PE	D	201	-	-	15/38/38/54	-
11	PLM	F	204	3	-	4/11/11/15	-
9	NAG	A	1321	1	-	4/6/23/26	0/1/1/1
6	D12	A	1311	-	-	0/4/4/9	-
6	D12	A	1310	-	-	0/9/9/9	-
7	R16	A	1307	-	-	3/13/13/13	-
11	PLM	F	205	3	-	1/7/7/15	-
6	D12	B	1320	-	-	0/7/7/9	-
6	D12	A	1317	-	-	2/9/9/9	-
6	D12	F	202	-	-	0/8/8/9	-
6	D12	A	1318	-	-	0/4/4/9	-
6	D12	B	1311	-	-	0/4/4/9	-
6	D12	B	1310	-	-	0/9/9/9	-
6	D12	B	1317	-	-	2/9/9/9	-
6	D12	A	1305	-	-	0/9/9/9	-
6	D12	B	1305	-	-	0/9/9/9	-
6	D12	B	1319	-	-	0/6/6/9	-
11	PLM	D	204	3	-	4/11/11/15	-
7	R16	A	1315	-	-	0/13/13/13	-
6	D12	B	1318	-	-	0/4/4/9	-
6	D12	A	1319	-	-	0/6/6/9	-
6	D12	A	1316	-	-	1/6/6/9	-
6	D12	A	1320	-	-	0/7/7/9	-
11	PLM	D	205	3	-	1/7/7/15	-
6	D12	A	1306	-	-	1/5/5/9	-
8	CLR	B	1308	-	-	3/10/68/68	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	3PE	F	201	-	-	15/38/38/54	-
6	D12	D	203	-	-	1/9/9/9	-
5	PEE	A	1303	-	-	24/45/45/54	-
6	D12	A	1309	-	-	0/6/6/9	-
7	R16	B	1307	-	-	3/13/13/13	-
6	D12	B	1306	-	-	1/5/5/9	-
6	D12	D	202	-	-	0/8/8/9	-
7	R16	B	1312	-	-	4/11/11/13	-
6	D12	B	1314	-	-	0/9/9/9	-
6	D12	B	1309	-	-	0/6/6/9	-
6	D12	A	1314	-	-	0/9/9/9	-
6	D12	F	203	-	-	1/9/9/9	-
9	NAG	B	1321	1	-	4/6/23/26	0/1/1/1
5	PEE	B	1303	-	-	24/45/45/54	-
7	R16	B	1315	-	-	0/13/13/13	-
6	D12	A	1304	-	-	0/6/6/9	-
7	R16	A	1313	-	-	1/13/13/13	-
6	D12	B	1316	-	-	1/6/6/9	-
8	CLR	A	1308	-	-	3/10/68/68	0/4/4/4
6	D12	B	1304	-	-	0/6/6/9	-

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1303	PEE	C39-C38	3.79	1.53	1.31
5	A	1303	PEE	C39-C38	3.79	1.53	1.31
5	A	1303	PEE	C18-C19	3.77	1.53	1.31
5	B	1303	PEE	C18-C19	3.76	1.53	1.31
5	A	1303	PEE	O2-C2	-2.70	1.40	1.46
5	B	1303	PEE	O2-C2	-2.68	1.40	1.46
10	D	201	3PE	O21-C2	-2.67	1.40	1.46
10	F	201	3PE	O21-C2	-2.67	1.40	1.46
10	D	201	3PE	O31-C31	2.38	1.40	1.33
5	B	1303	PEE	O3-C30	2.35	1.40	1.33
10	F	201	3PE	O31-C31	2.35	1.40	1.33
5	A	1303	PEE	O3-C30	2.35	1.40	1.33
5	A	1303	PEE	O3-C3	-2.28	1.40	1.45
5	B	1303	PEE	O3-C3	-2.27	1.40	1.45
10	D	201	3PE	O31-C3	-2.20	1.40	1.45
10	F	201	3PE	O31-C3	-2.20	1.40	1.45
5	B	1303	PEE	O2-C10	2.19	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1303	PEE	O2-C10	2.18	1.40	1.34
10	F	201	3PE	O21-C21	2.13	1.40	1.34
10	D	201	3PE	O21-C21	2.11	1.40	1.34

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	D	201	3PE	O21-C21-C22	4.04	120.22	111.48
10	F	201	3PE	O21-C21-C22	4.04	120.22	111.48
5	A	1303	PEE	O2-C10-C11	3.79	119.68	111.48
5	B	1303	PEE	O2-C10-C11	3.79	119.67	111.48
10	F	201	3PE	O31-C31-C32	2.80	120.38	111.83
10	D	201	3PE	O31-C31-C32	2.79	120.33	111.83
5	A	1303	PEE	O3-C30-C31	2.74	120.19	111.83
5	B	1303	PEE	O3-C30-C31	2.74	120.17	111.83
5	B	1303	PEE	C37-C38-C39	-2.08	109.26	124.83
5	A	1303	PEE	C37-C38-C39	-2.07	109.29	124.83
5	B	1303	PEE	C17-C18-C19	-2.05	109.48	124.83
5	A	1303	PEE	C17-C18-C19	-2.04	109.54	124.83
5	B	1303	PEE	C40-C39-C38	-2.04	109.55	124.83
5	A	1303	PEE	C40-C39-C38	-2.04	109.56	124.83
5	B	1303	PEE	C20-C19-C18	-2.03	109.65	124.83
5	A	1303	PEE	C20-C19-C18	-2.02	109.68	124.83

There are no chirality outliers.

All (128) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1303	PEE	C4-O4P-P-O3P
5	A	1303	PEE	C4-O4P-P-O1P
5	A	1303	PEE	O4P-C4-C5-N
5	B	1303	PEE	C4-O4P-P-O3P
5	B	1303	PEE	C4-O4P-P-O1P
5	B	1303	PEE	O4P-C4-C5-N
9	A	1321	NAG	C3-C2-N2-C7
9	A	1321	NAG	C8-C7-N2-C2
9	A	1321	NAG	O7-C7-N2-C2
9	B	1321	NAG	C3-C2-N2-C7
9	B	1321	NAG	C8-C7-N2-C2
9	B	1321	NAG	O7-C7-N2-C2
10	D	201	3PE	C1-O11-P-O12
10	D	201	3PE	C1-O11-P-O13

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Mol	Chain	Res	Type	Atoms
10	D	201	3PE	C1-O11-P-O14
10	D	201	3PE	C11-O13-P-O11
10	D	201	3PE	C11-O13-P-O12
10	F	201	3PE	C1-O11-P-O12
10	F	201	3PE	C1-O11-P-O13
10	F	201	3PE	C1-O11-P-O14
10	F	201	3PE	C11-O13-P-O11
10	F	201	3PE	C11-O13-P-O12
5	A	1303	PEE	O5-C30-O3-C3
5	B	1303	PEE	O5-C30-O3-C3
5	A	1303	PEE	C31-C30-O3-C3
5	B	1303	PEE	C31-C30-O3-C3
5	A	1303	PEE	C17-C18-C19-C20
5	B	1303	PEE	C17-C18-C19-C20
8	A	1308	CLR	C17-C20-C22-C23
8	B	1308	CLR	C17-C20-C22-C23
10	D	201	3PE	C21-C22-C23-C24
10	D	201	3PE	C31-C32-C33-C34
10	F	201	3PE	C21-C22-C23-C24
10	F	201	3PE	C31-C32-C33-C34
5	A	1303	PEE	C37-C38-C39-C40
5	B	1303	PEE	C37-C38-C39-C40
8	A	1308	CLR	C21-C20-C22-C23
8	B	1308	CLR	C21-C20-C22-C23
7	A	1312	R16	C36-C37-C38-C39
7	B	1312	R16	C36-C37-C38-C39
7	A	1312	R16	C34-C35-C36-C37
7	B	1312	R16	C34-C35-C36-C37
10	D	201	3PE	C23-C24-C25-C26
10	F	201	3PE	C23-C24-C25-C26
6	B	1317	D12	C6-C7-C8-C9
6	A	1317	D12	C6-C7-C8-C9
9	A	1321	NAG	O5-C5-C6-O6
9	B	1321	NAG	O5-C5-C6-O6
5	A	1303	PEE	O2-C2-C3-O3
5	B	1303	PEE	O2-C2-C3-O3
10	D	201	3PE	C33-C34-C35-C36
10	F	201	3PE	C33-C34-C35-C36
5	A	1303	PEE	C35-C36-C37-C38
5	B	1303	PEE	C35-C36-C37-C38
6	A	1316	D12	C3-C4-C5-C6
10	F	201	3PE	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
10	D	201	3PE	C32-C33-C34-C35
6	B	1316	D12	C3-C4-C5-C6
7	A	1307	R16	C36-C37-C38-C39
7	B	1307	R16	C36-C37-C38-C39
5	A	1303	PEE	C34-C35-C36-C37
5	B	1303	PEE	C31-C32-C33-C34
5	A	1303	PEE	C31-C32-C33-C34
5	A	1303	PEE	C1-C2-C3-O3
5	B	1303	PEE	C1-C2-C3-O3
6	A	1306	D12	C2-C3-C4-C5
6	B	1306	D12	C2-C3-C4-C5
5	A	1303	PEE	C11-C10-O2-C2
7	A	1307	R16	C31-C32-C33-C34
5	B	1303	PEE	C14-C15-C16-C17
7	B	1307	R16	C31-C32-C33-C34
11	F	204	PLM	C6-C7-C8-C9
11	D	204	PLM	C6-C7-C8-C9
5	A	1303	PEE	C12-C13-C14-C15
5	B	1303	PEE	C34-C35-C36-C37
5	A	1303	PEE	O3P-C1-C2-O2
5	B	1303	PEE	O3P-C1-C2-O2
10	D	201	3PE	O11-C1-C2-O21
10	F	201	3PE	O11-C1-C2-O21
5	B	1303	PEE	C11-C10-O2-C2
5	A	1303	PEE	C14-C15-C16-C17
5	B	1303	PEE	C12-C13-C14-C15
11	D	204	PLM	C8-C9-CA-CB
11	F	204	PLM	C8-C9-CA-CB
5	A	1303	PEE	O3P-C1-C2-C3
5	B	1303	PEE	O3P-C1-C2-C3
10	D	201	3PE	O11-C1-C2-C3
10	F	201	3PE	O11-C1-C2-C3
5	A	1303	PEE	O4-C10-O2-C2
5	B	1303	PEE	O4-C10-O2-C2
10	D	201	3PE	C1-C2-C3-O31
10	F	201	3PE	C1-C2-C3-O31
5	A	1303	PEE	C1-O3P-P-O1P
5	A	1303	PEE	C4-O4P-P-O2P
5	B	1303	PEE	C1-O3P-P-O1P
5	B	1303	PEE	C4-O4P-P-O2P
6	A	1317	D12	C2-C3-C4-C5
6	B	1317	D12	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
8	B	1308	CLR	C20-C22-C23-C24
10	D	201	3PE	C37-C38-C39-C3A
7	A	1313	R16	C32-C33-C34-C35
7	B	1313	R16	C32-C33-C34-C35
8	A	1308	CLR	C20-C22-C23-C24
10	F	201	3PE	C37-C38-C39-C3A
5	A	1303	PEE	C11-C12-C13-C14
5	B	1303	PEE	C11-C12-C13-C14
11	D	204	PLM	C7-C8-C9-CA
11	F	204	PLM	C7-C8-C9-CA
5	A	1303	PEE	C38-C39-C40-C41
5	B	1303	PEE	C38-C39-C40-C41
10	F	201	3PE	O21-C2-C3-O31
10	D	201	3PE	O21-C2-C3-O31
5	A	1303	PEE	C36-C37-C38-C39
6	F	203	D12	C6-C7-C8-C9
5	B	1303	PEE	C36-C37-C38-C39
7	B	1312	R16	C32-C33-C34-C35
7	A	1312	R16	C32-C33-C34-C35
6	D	203	D12	C6-C7-C8-C9
5	A	1303	PEE	C16-C17-C18-C19
5	B	1303	PEE	C16-C17-C18-C19
11	F	205	PLM	C6-C7-C8-C9
11	D	204	PLM	C1-C2-C3-C4
11	F	204	PLM	C1-C2-C3-C4
11	D	205	PLM	C6-C7-C8-C9
7	B	1307	R16	C37-C38-C39-C40
7	A	1307	R16	C37-C38-C39-C40
7	A	1312	R16	C33-C34-C35-C36
7	B	1312	R16	C33-C34-C35-C36

There are no ring outliers.

23 monomers are involved in 51 short contacts:

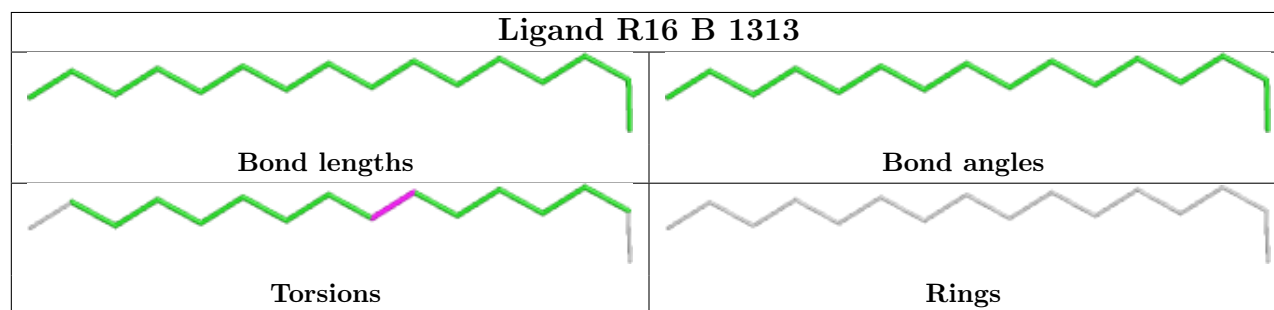
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	1313	R16	2	0
10	D	201	3PE	6	0
11	F	204	PLM	1	0
6	A	1310	D12	2	0
7	A	1307	R16	2	0
11	F	205	PLM	2	0
6	F	202	D12	1	0

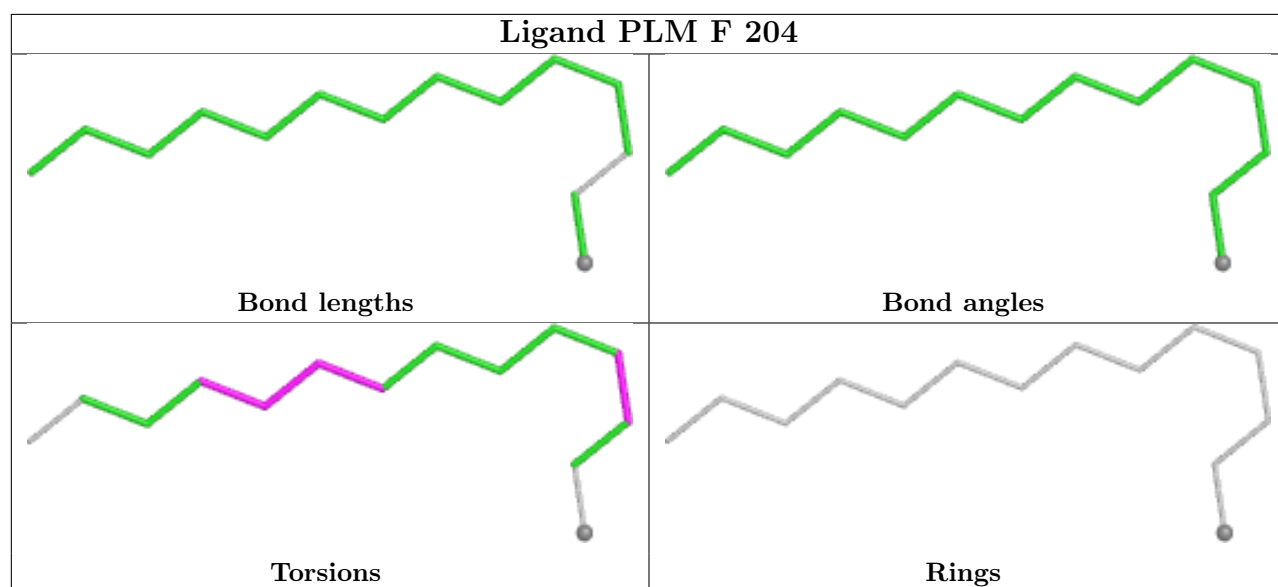
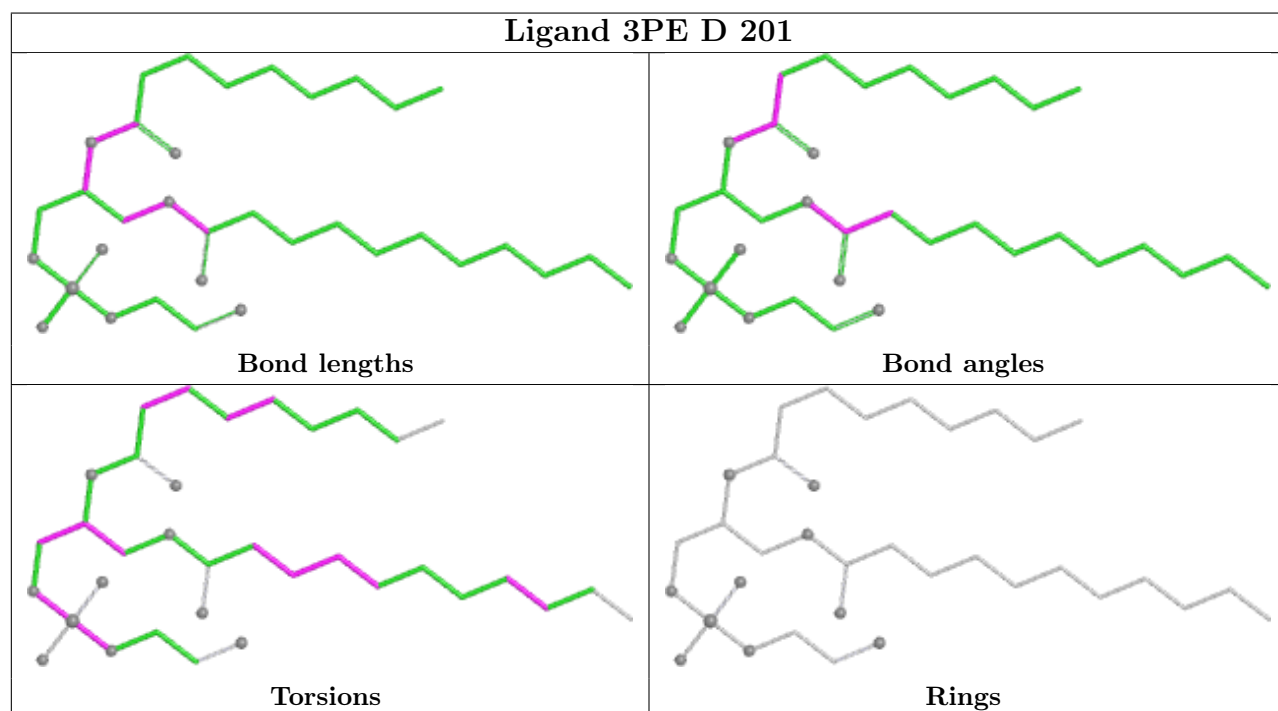
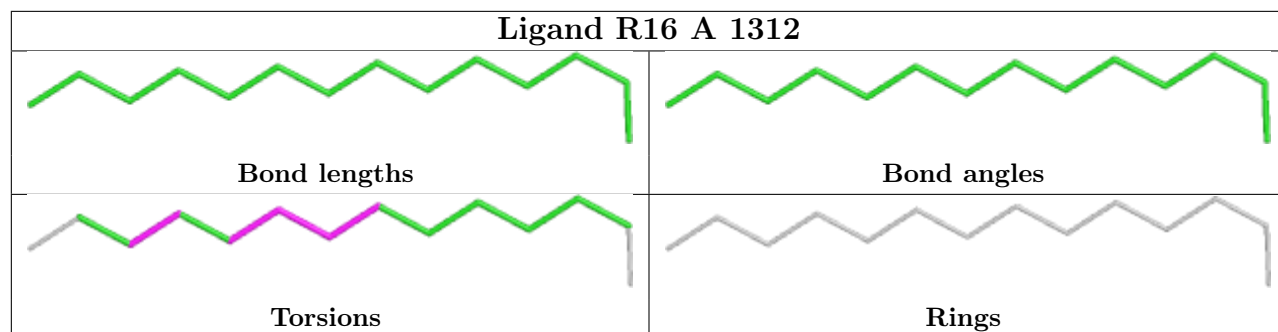
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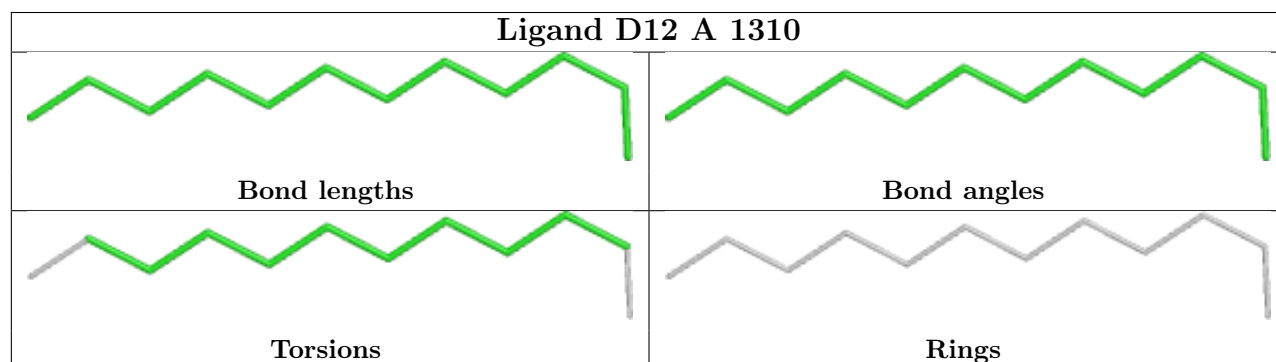
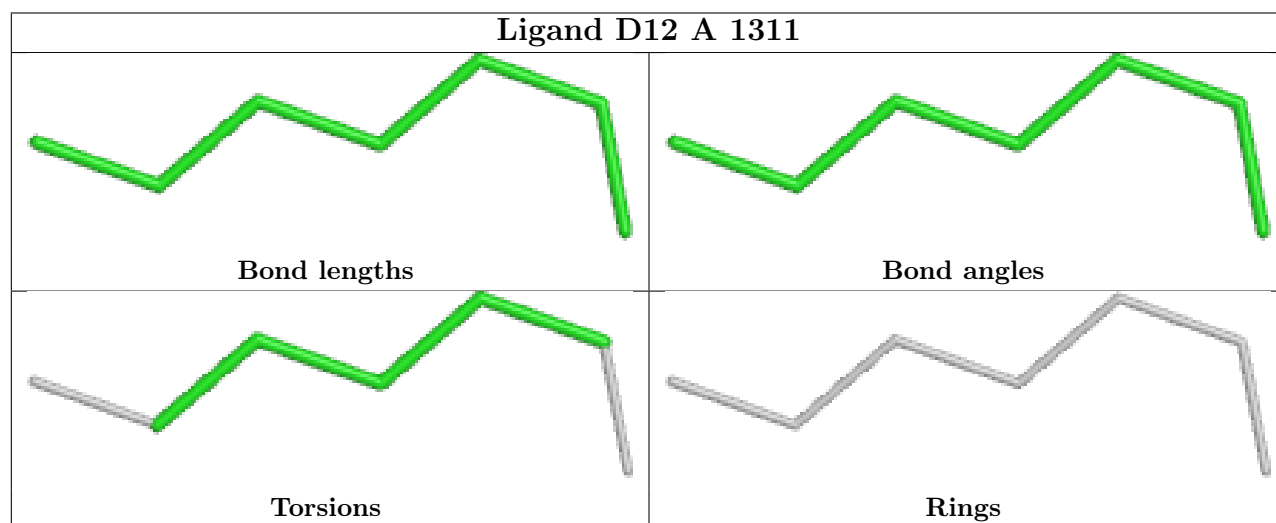
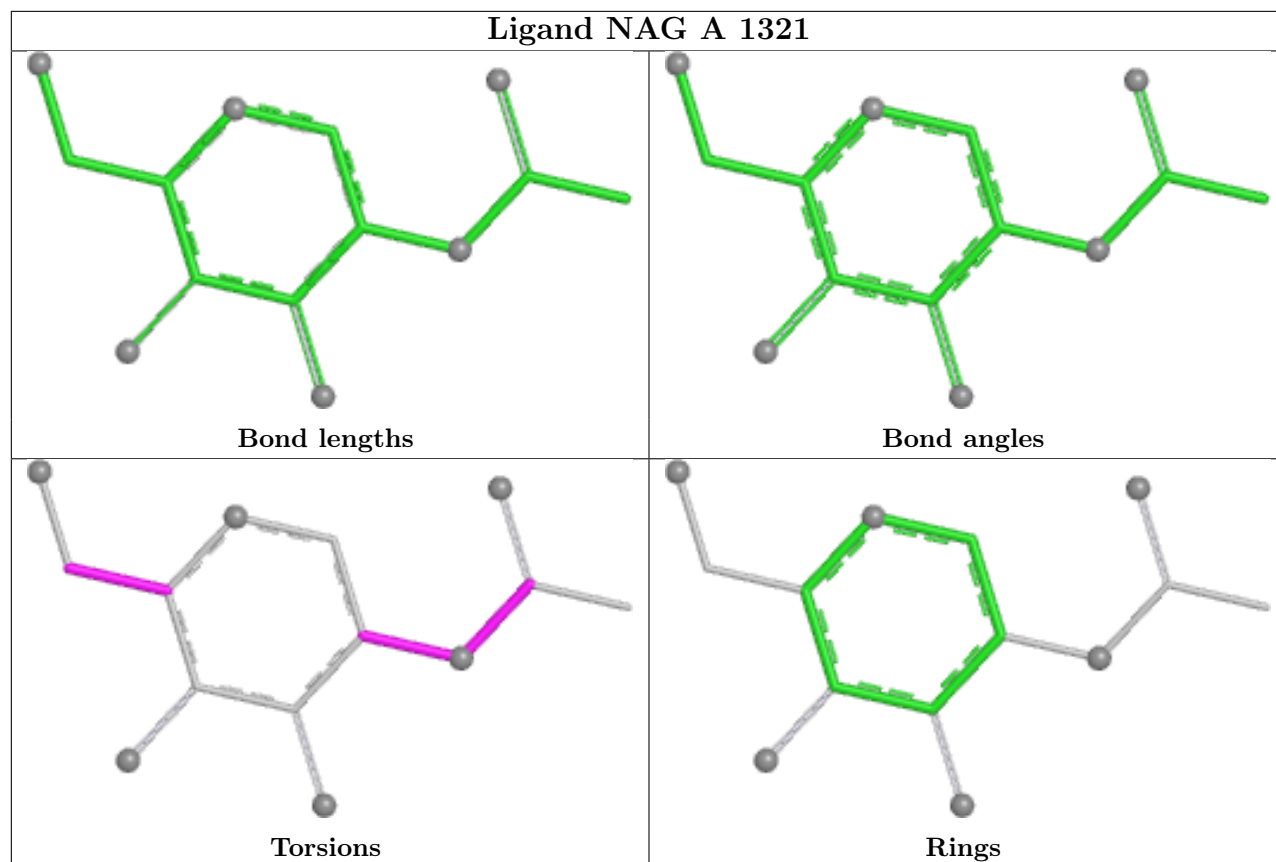
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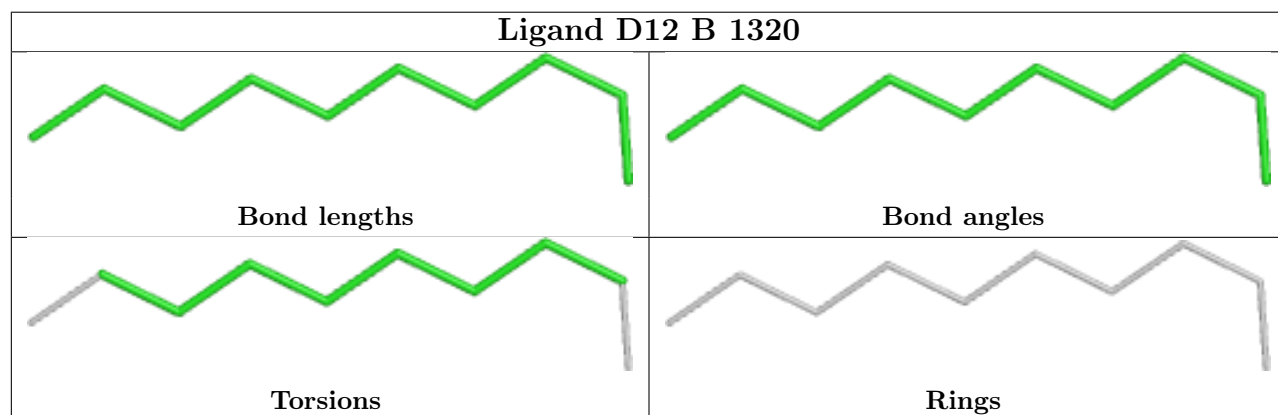
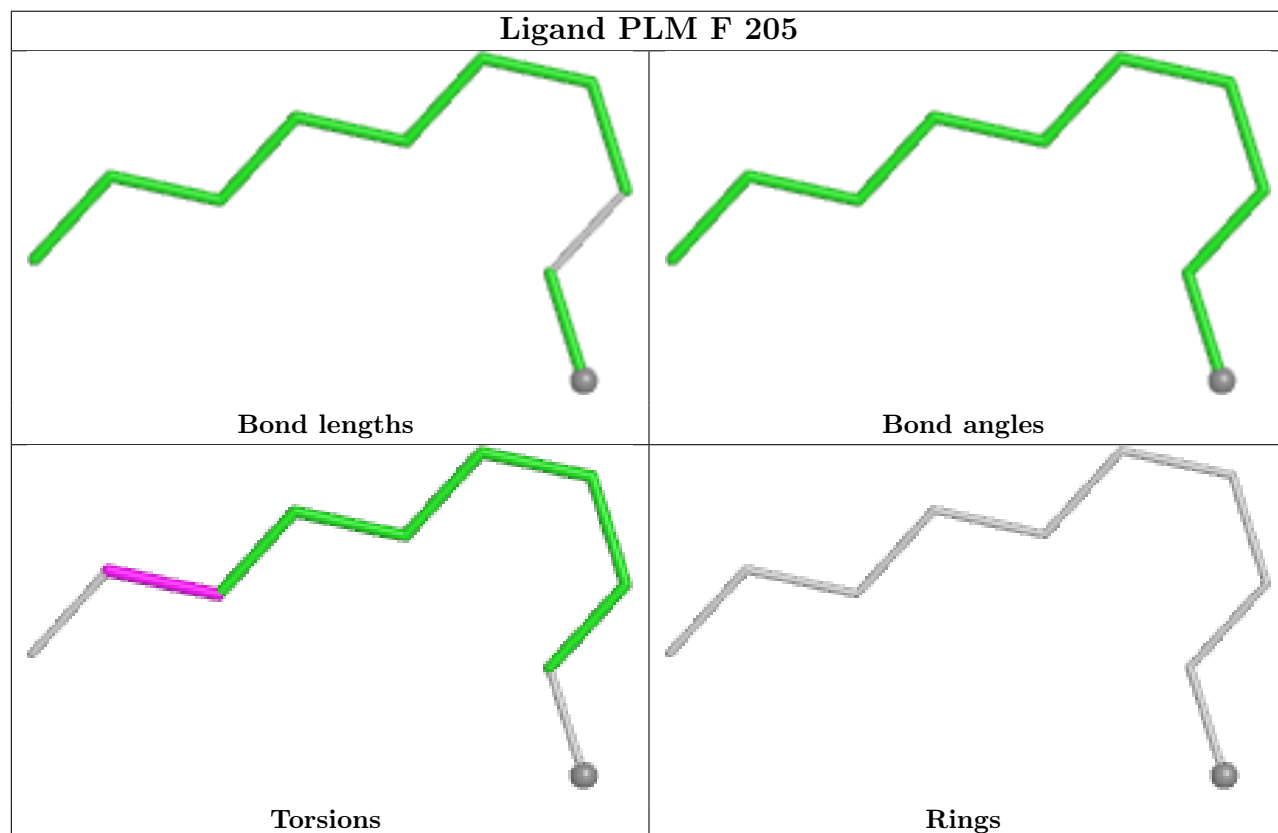
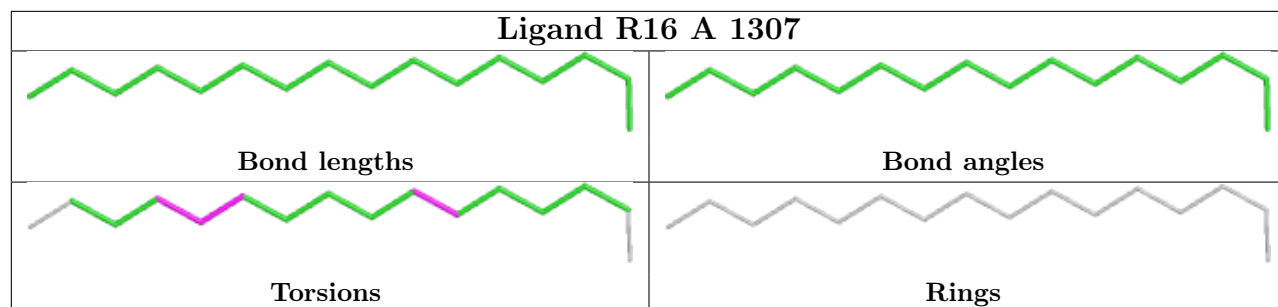
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	1310	D12	1	0
11	D	204	PLM	2	0
7	A	1315	R16	1	0
11	D	205	PLM	2	0
8	B	1308	CLR	4	0
10	F	201	3PE	6	0
6	D	203	D12	1	0
5	A	1303	PEE	6	0
6	A	1309	D12	1	0
7	B	1307	R16	2	0
6	B	1309	D12	1	0
6	F	203	D12	1	0
5	B	1303	PEE	5	0
7	B	1315	R16	1	0
7	A	1313	R16	2	0
8	A	1308	CLR	3	0

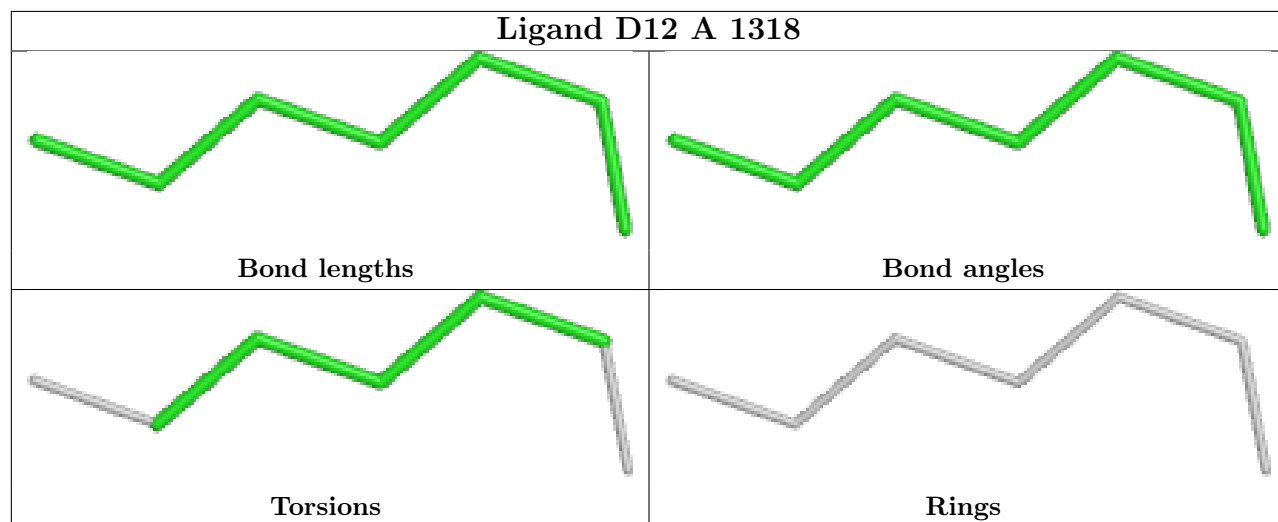
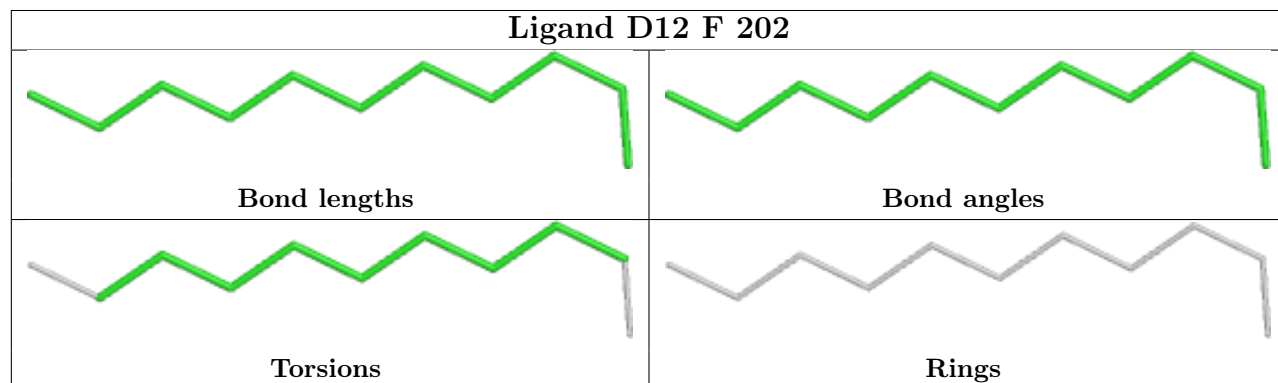
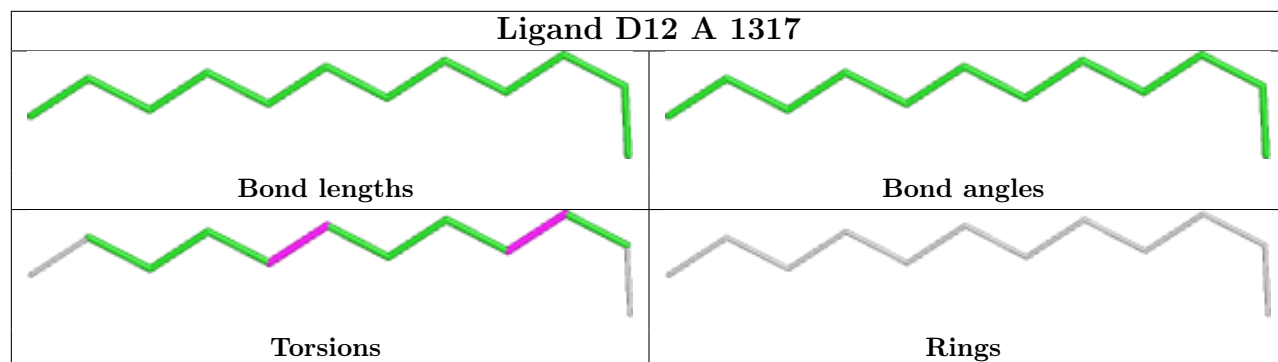
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

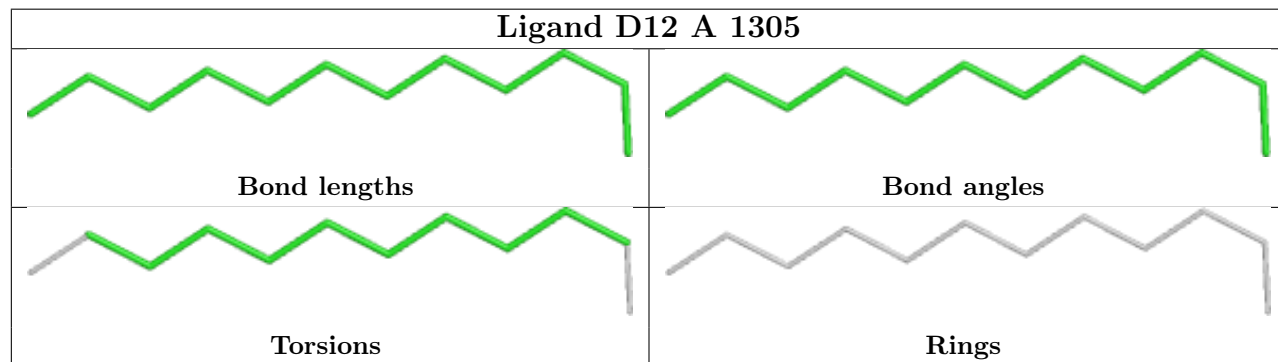
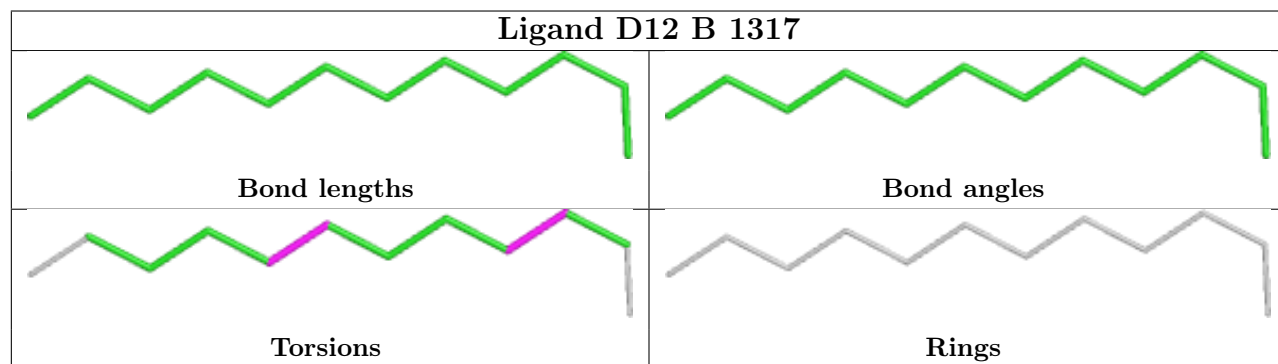
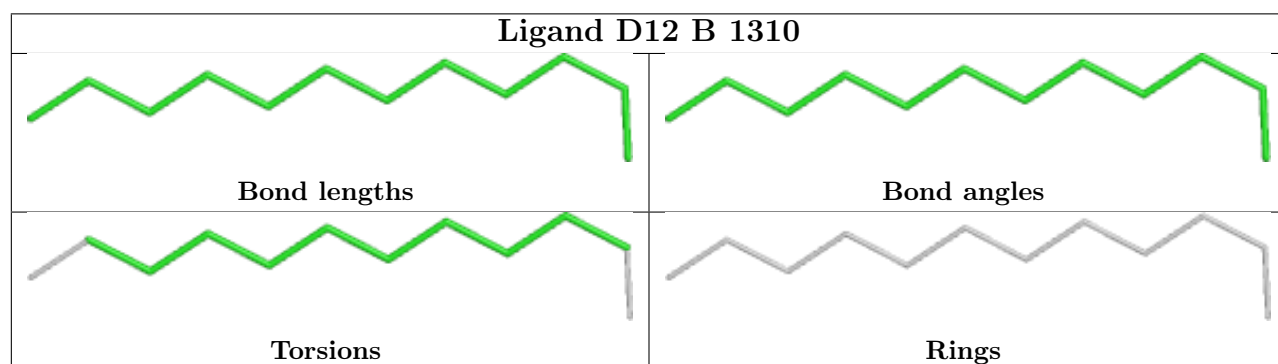
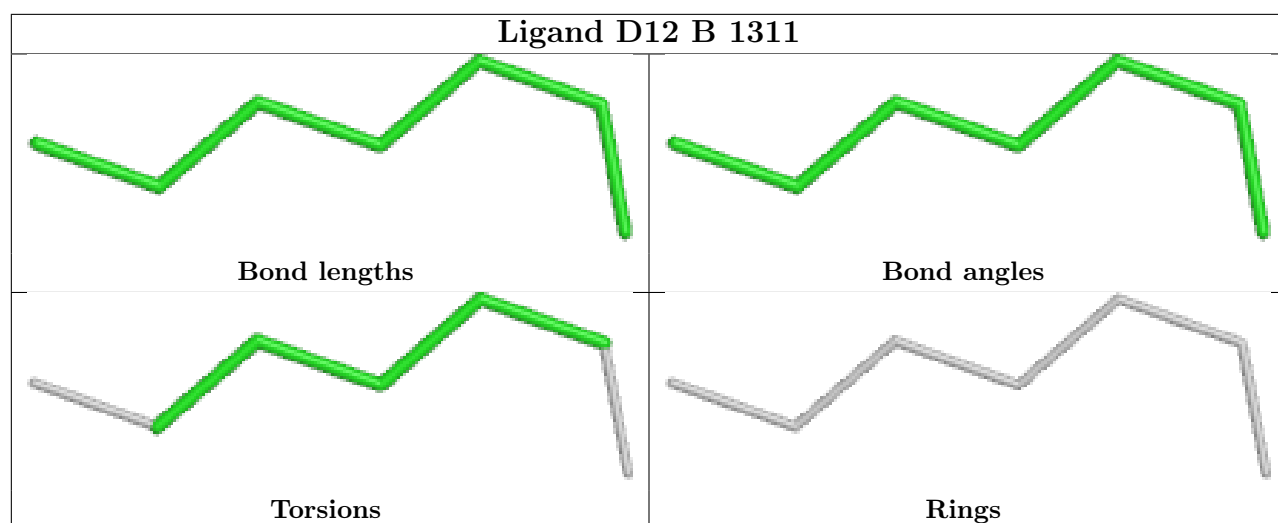


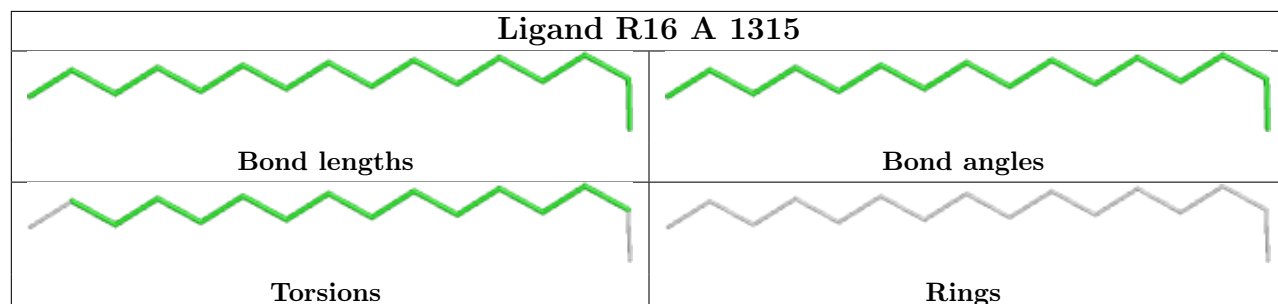
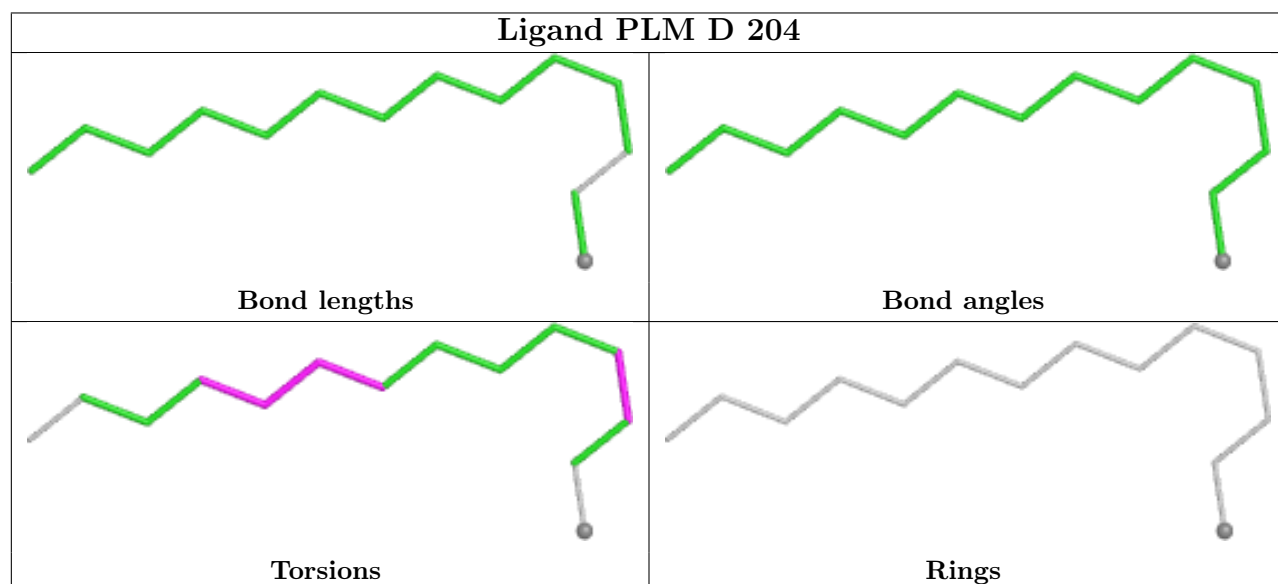
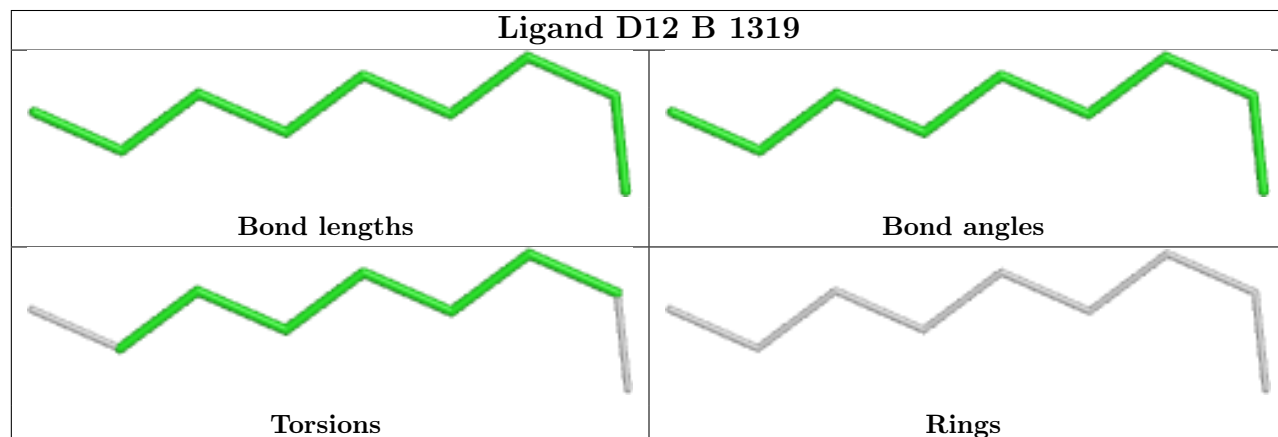
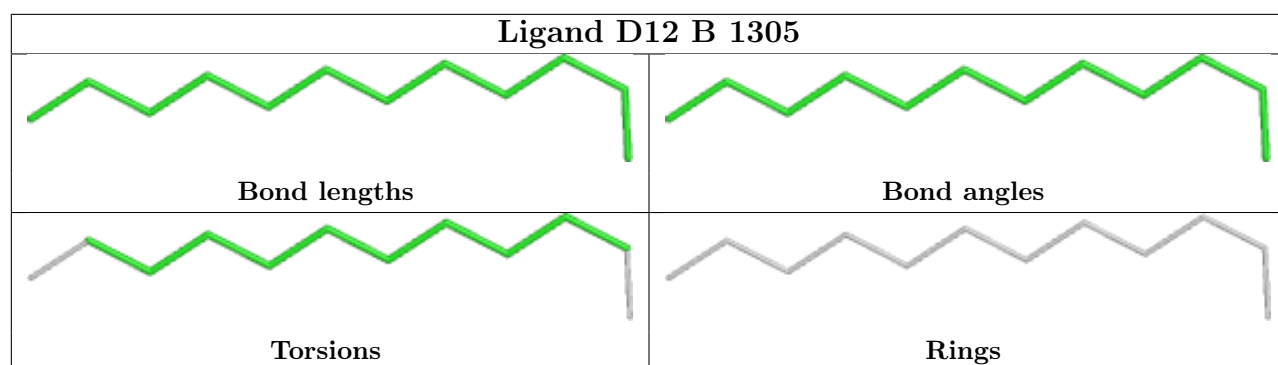


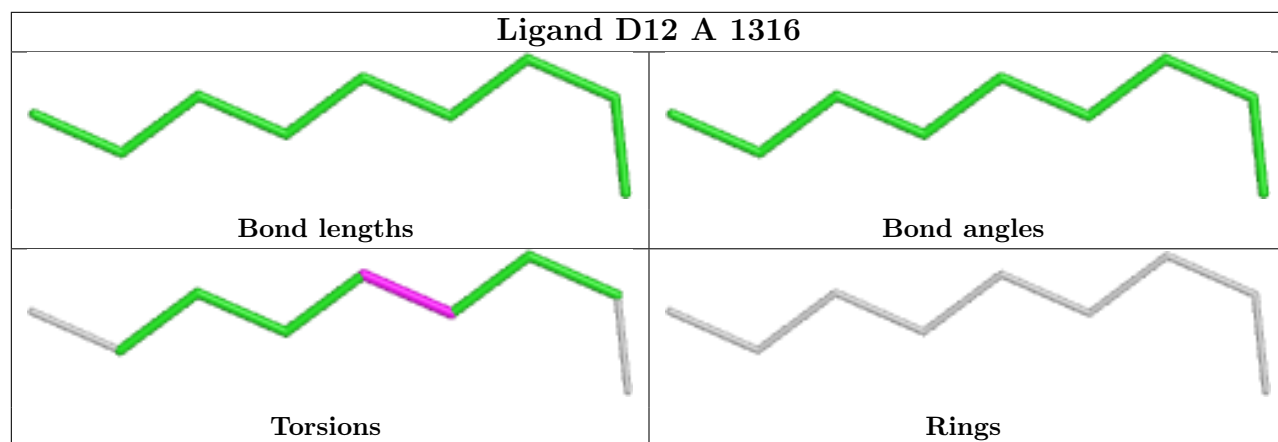
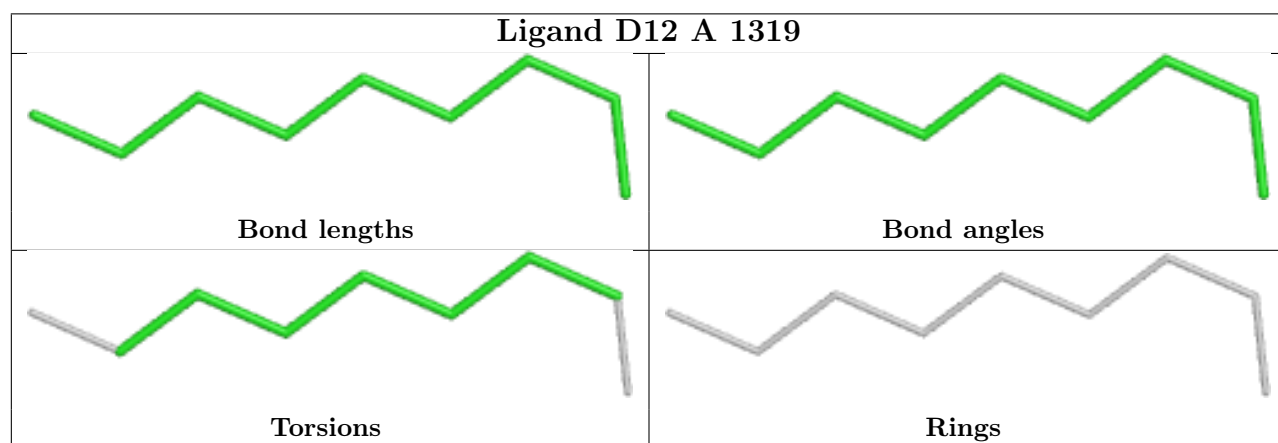
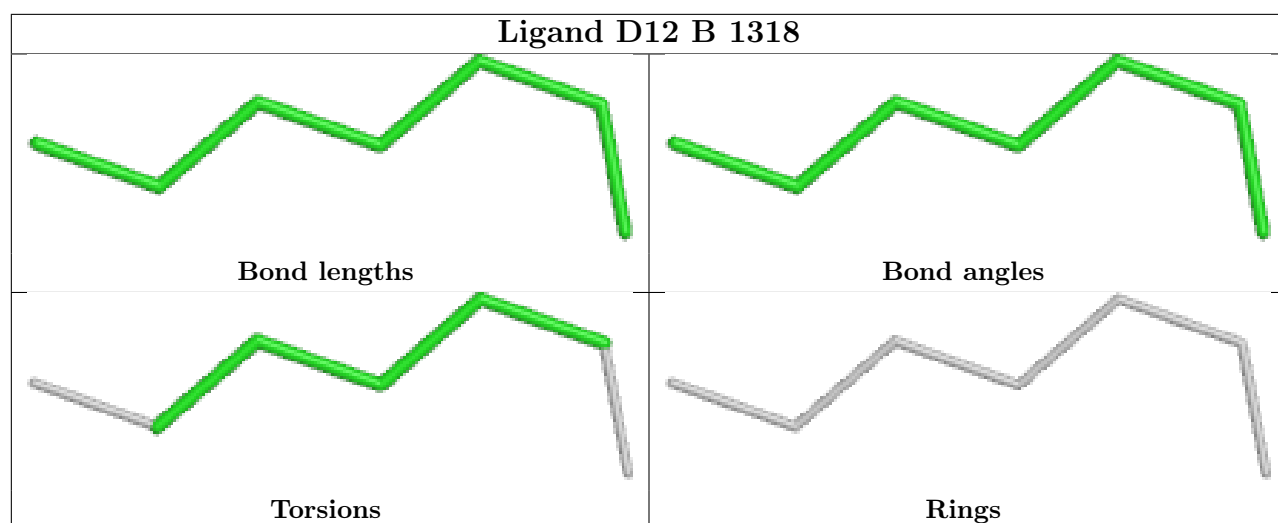


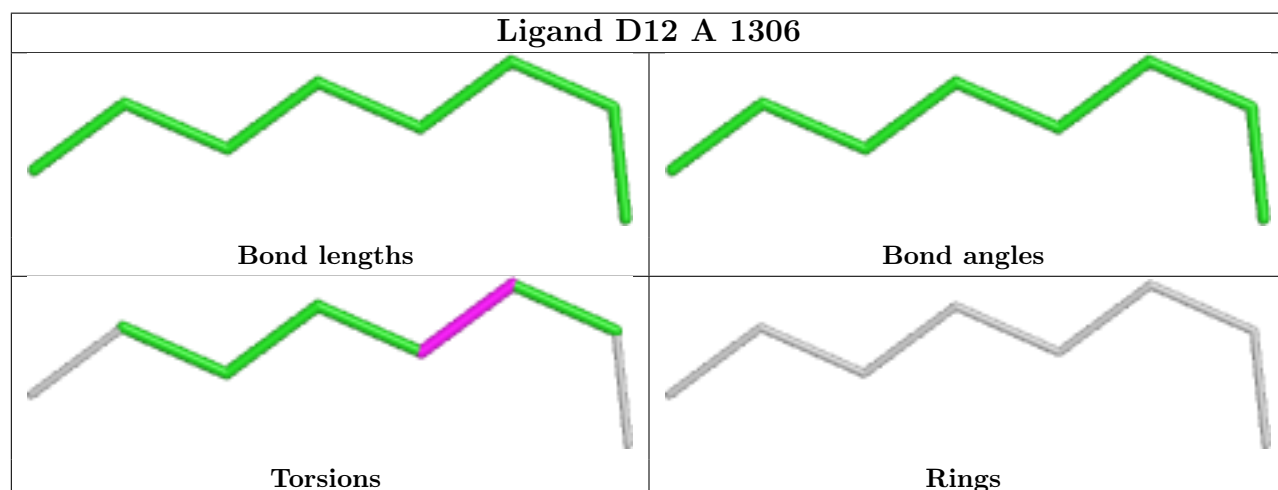
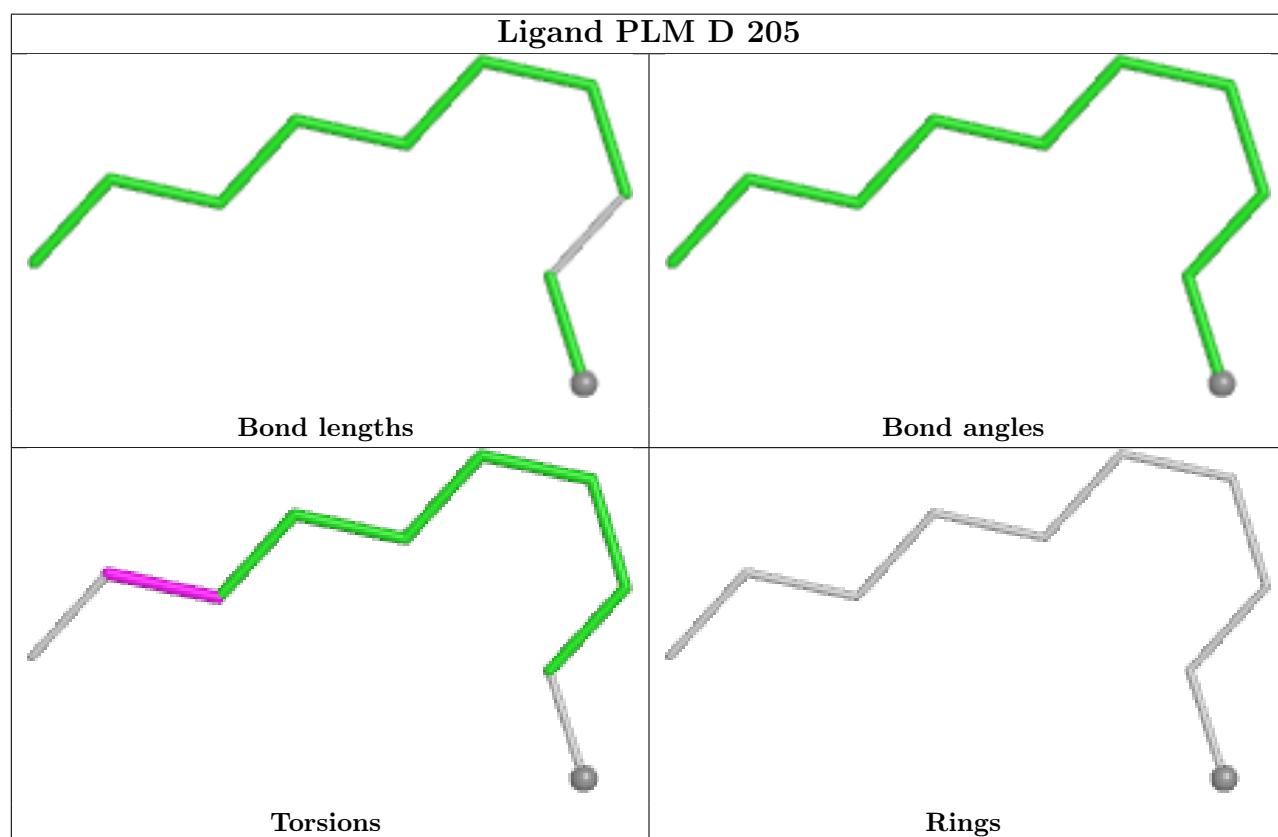
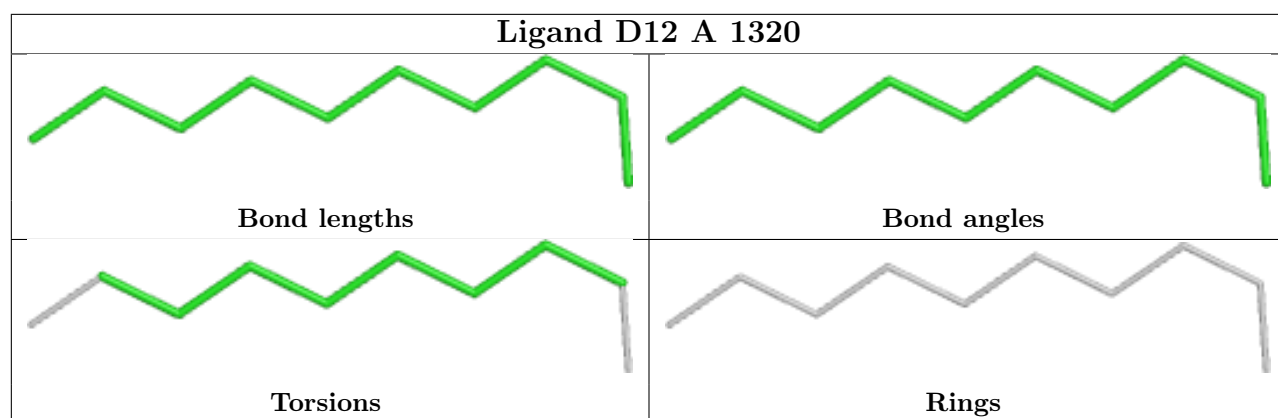


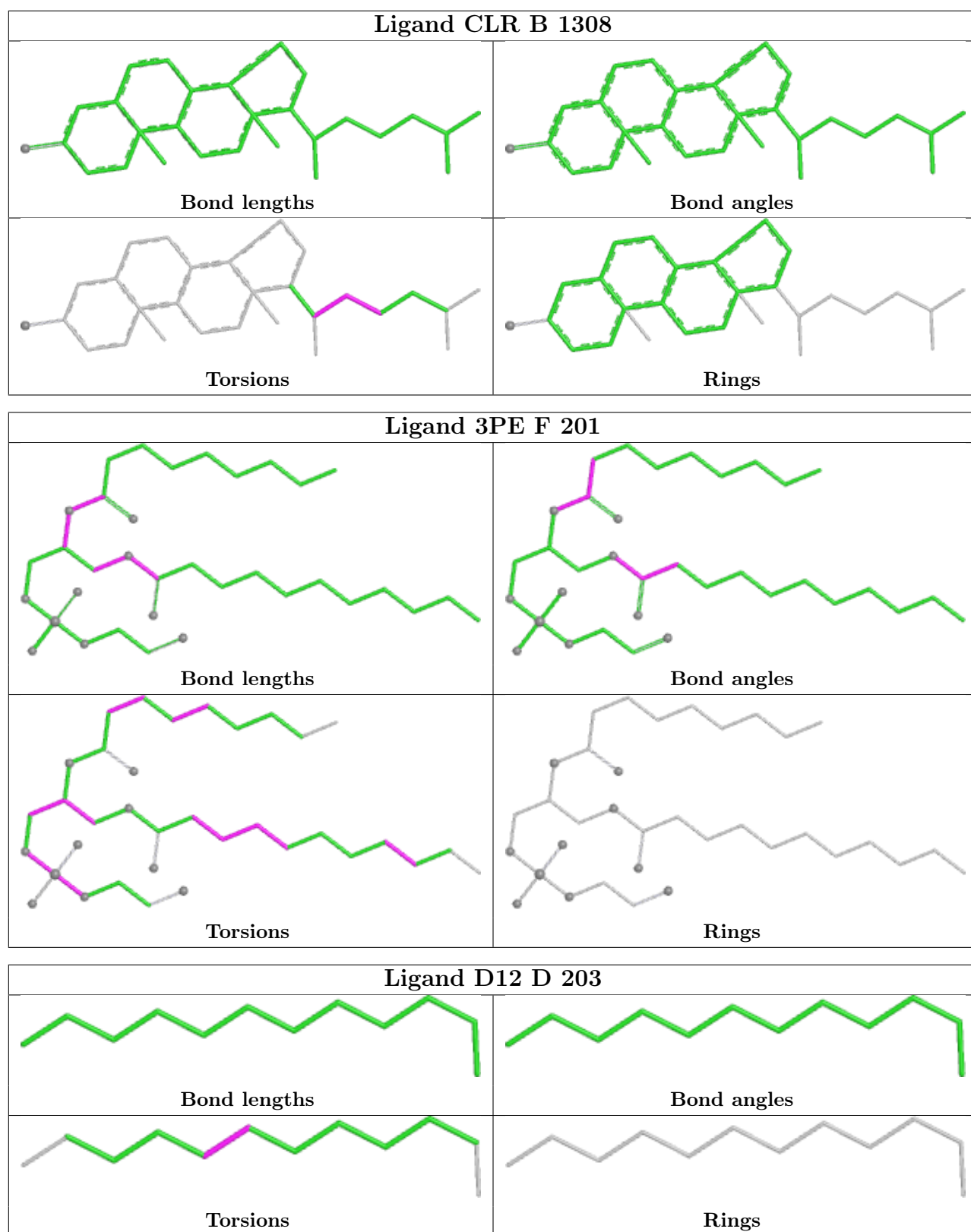


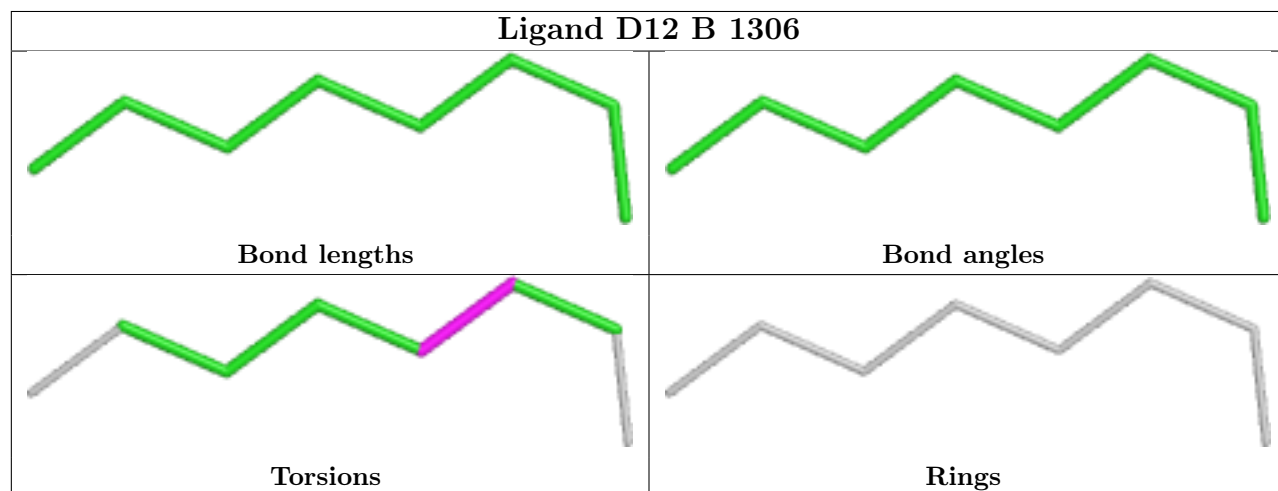
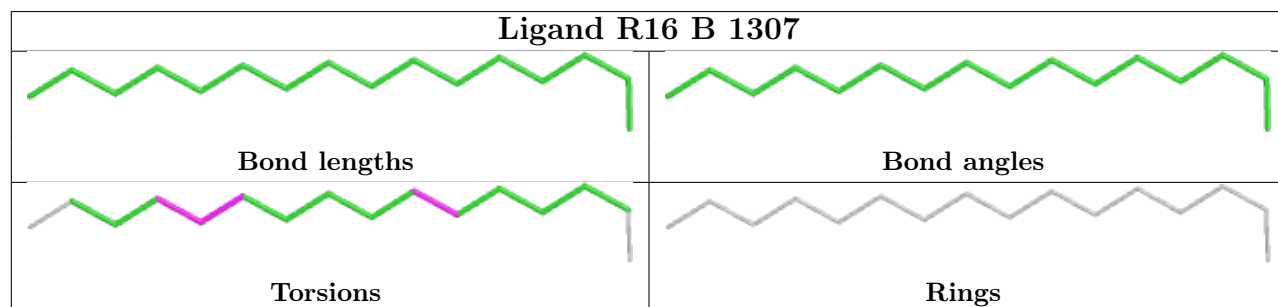
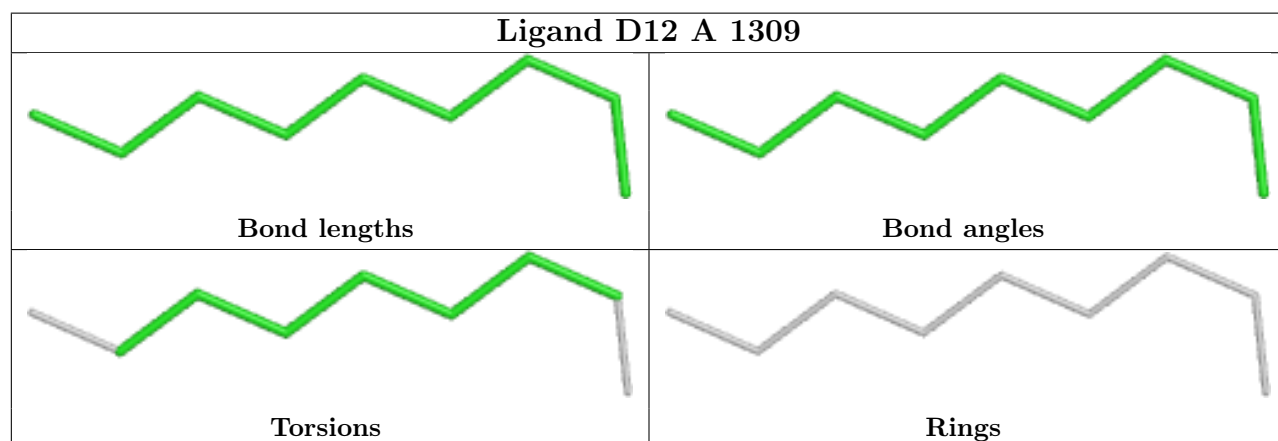
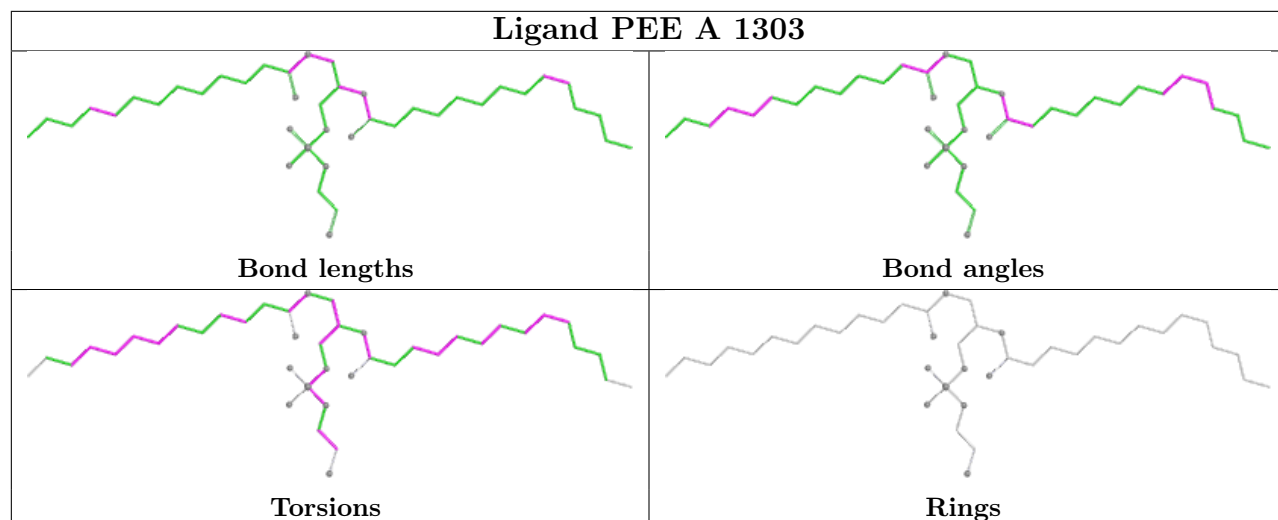


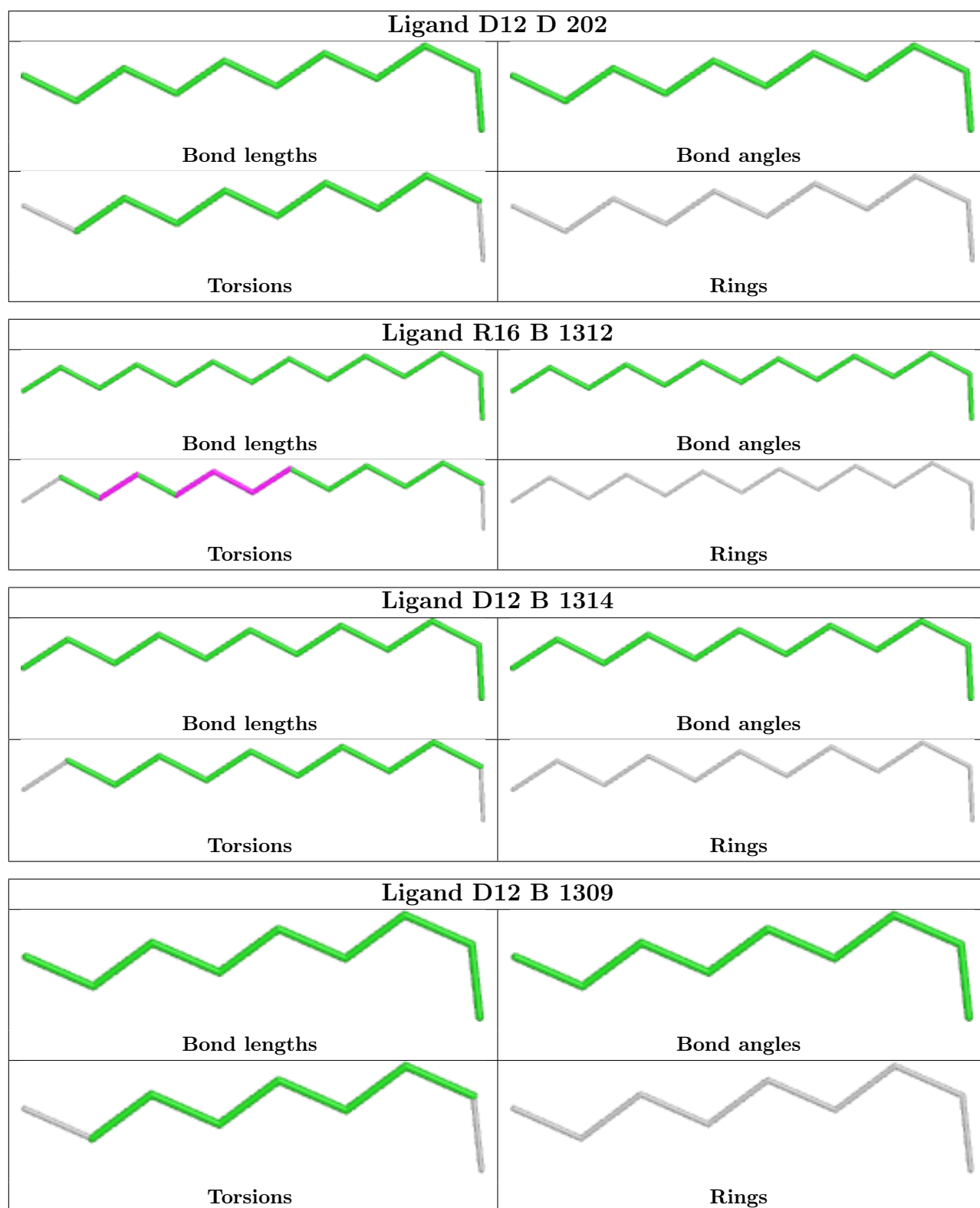


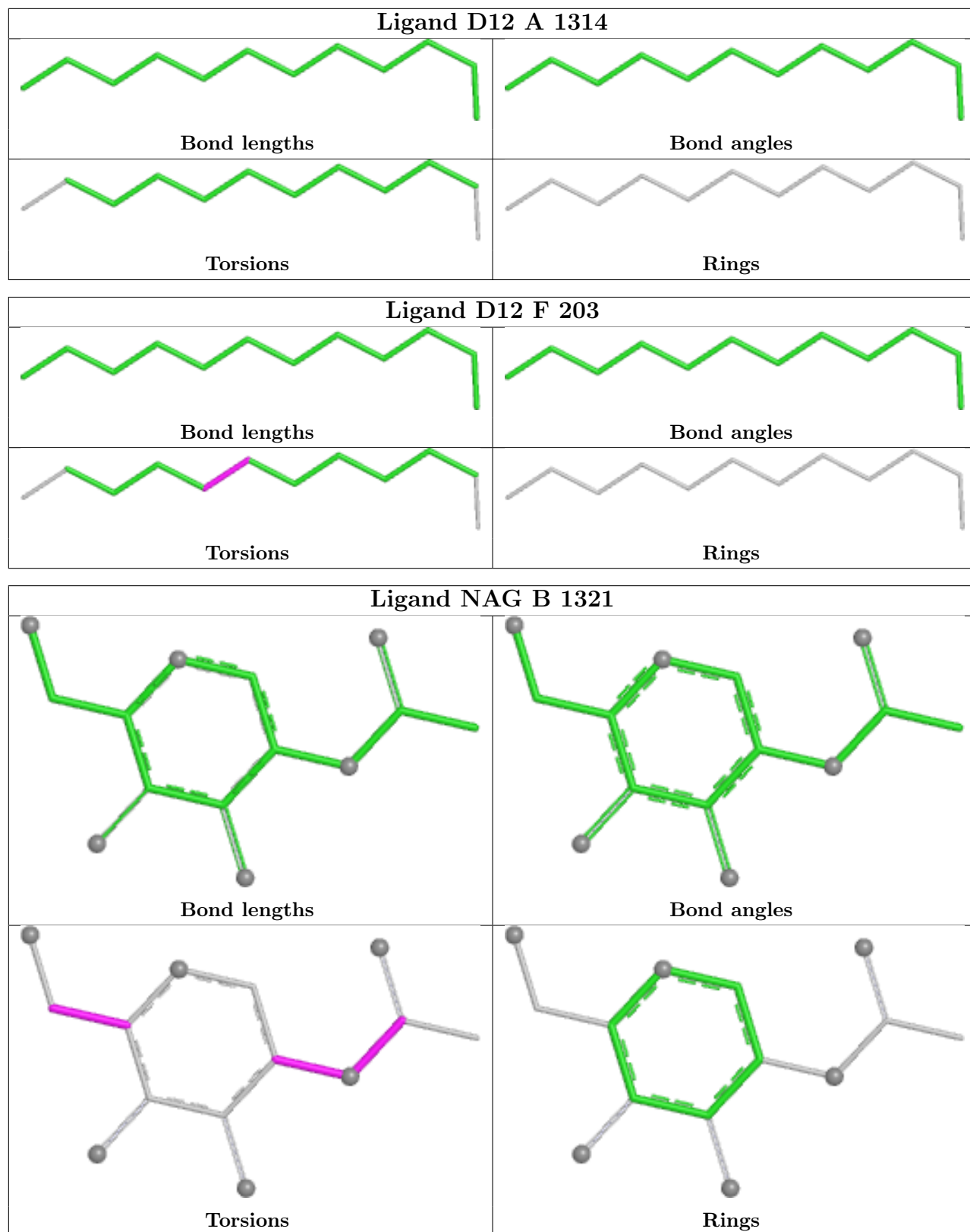


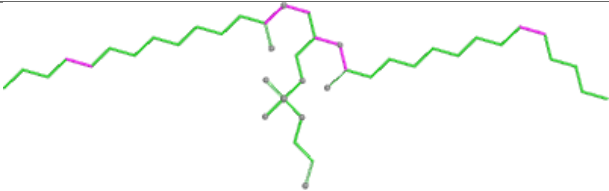
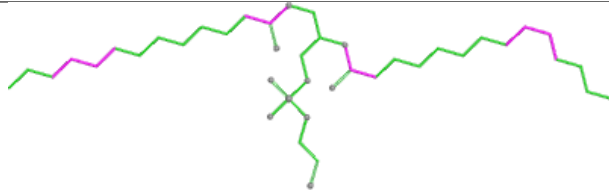
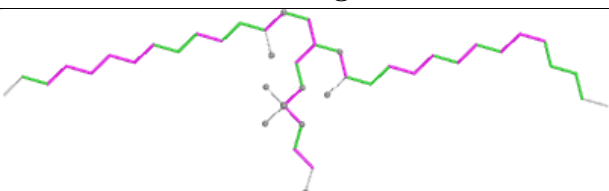
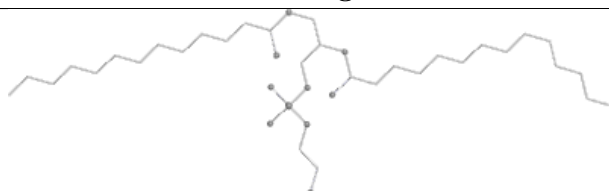


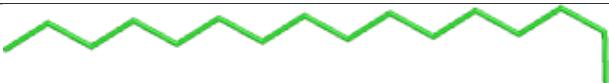
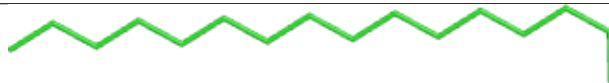
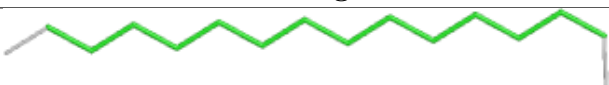
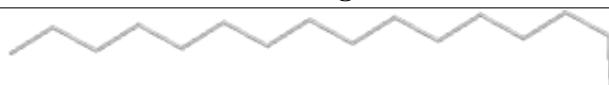


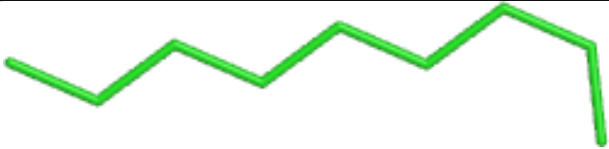
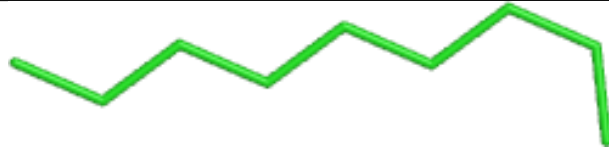

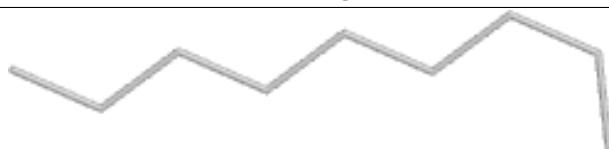


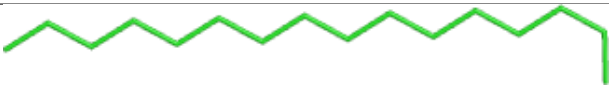
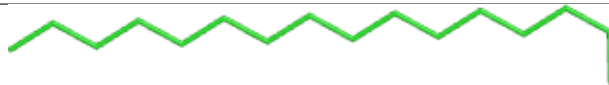
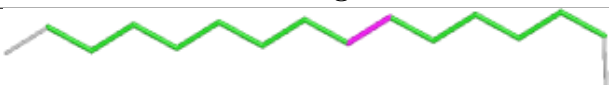
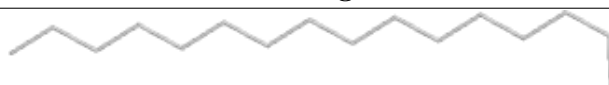


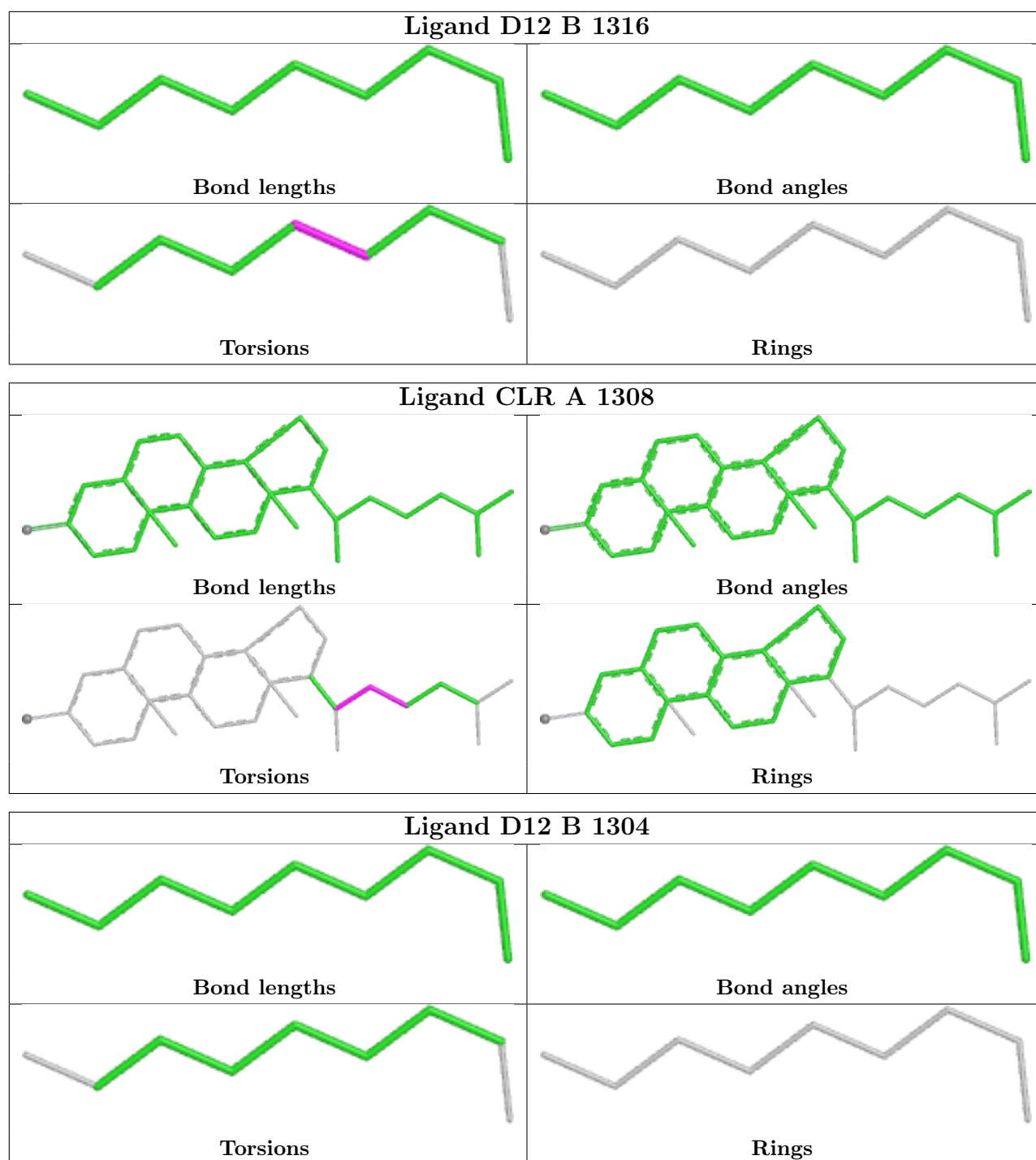


Ligand PEE B 1303	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand R16 B 1315	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand D12 A 1304	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand R16 A 1313	
	
Bond lengths	Bond angles
	
Torsions	Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

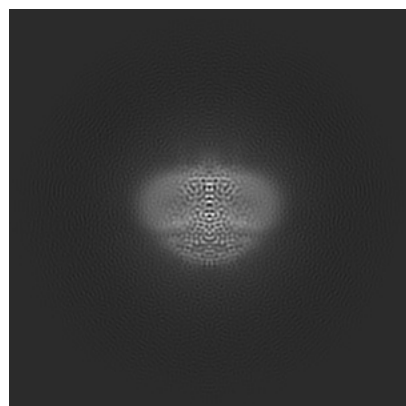
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26742. These allow visual inspection of the internal detail of the map and identification of artifacts.

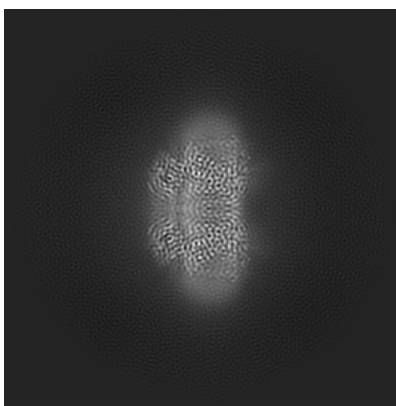
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

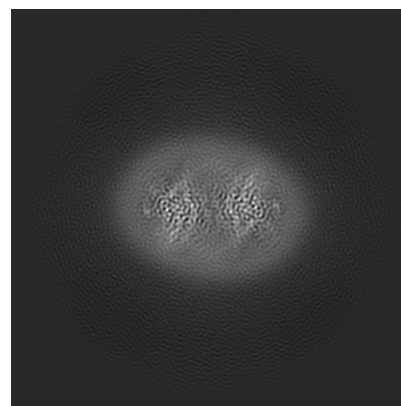
6.1.1 Primary map



X

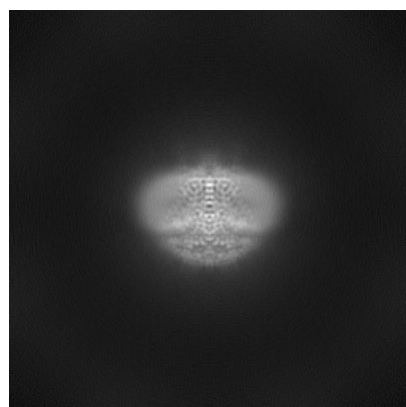


Y

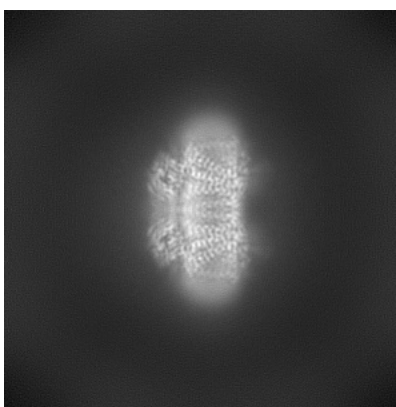


Z

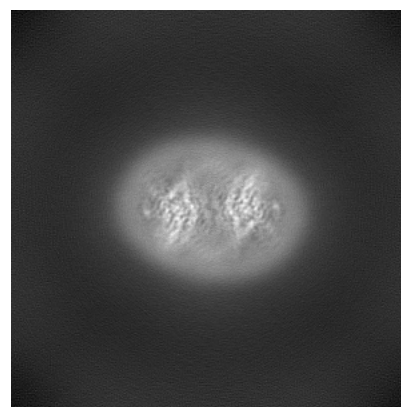
6.1.2 Raw map



X



Y

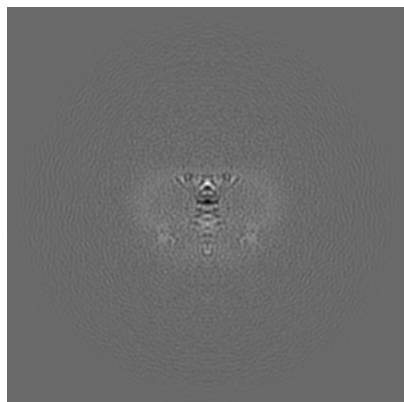


Z

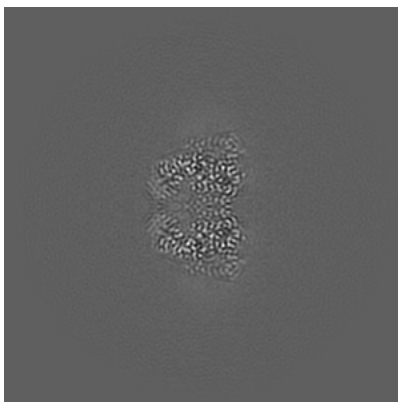
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

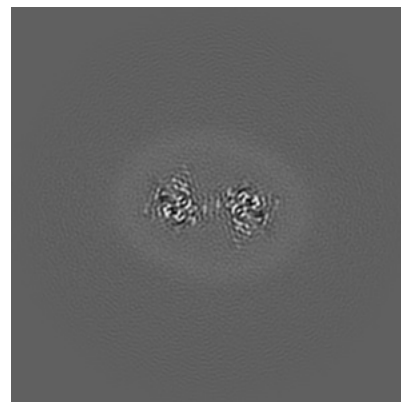
6.2.1 Primary map



X Index: 200

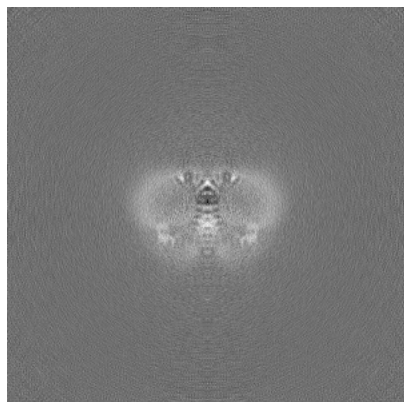


Y Index: 200

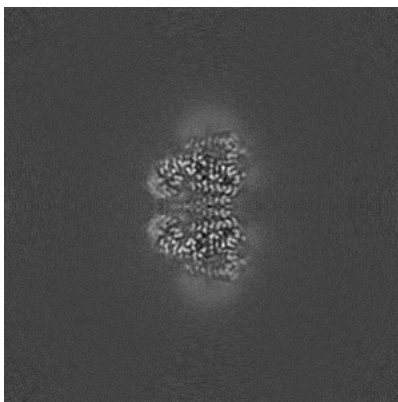


Z Index: 200

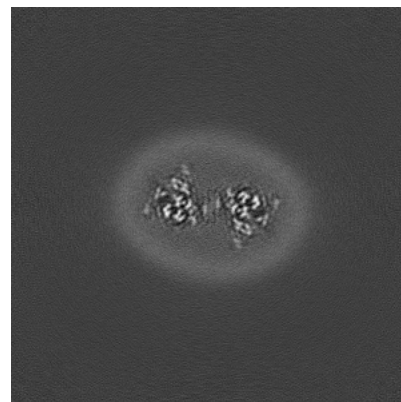
6.2.2 Raw map



X Index: 200



Y Index: 200

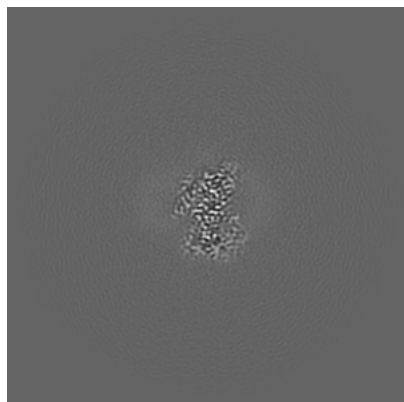


Z Index: 200

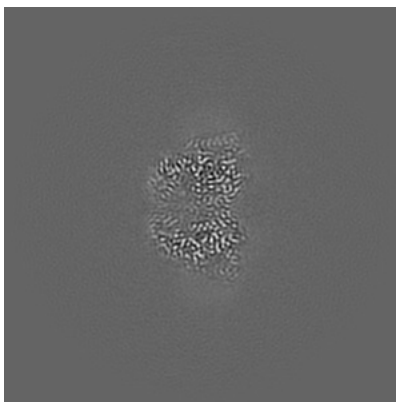
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

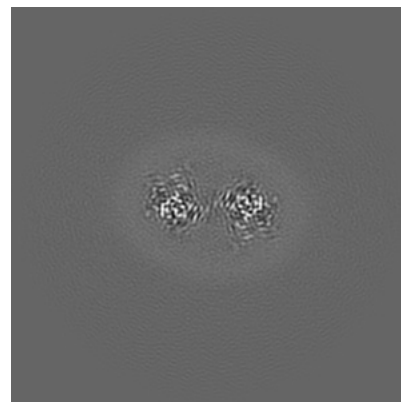
6.3.1 Primary map



X Index: 235

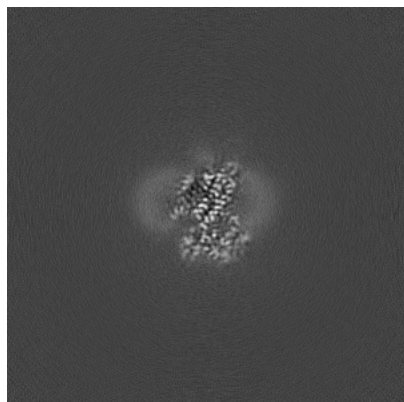


Y Index: 202

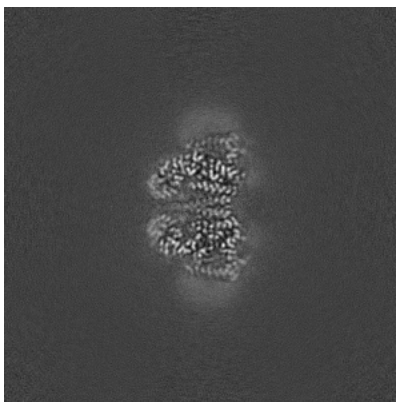


Z Index: 195

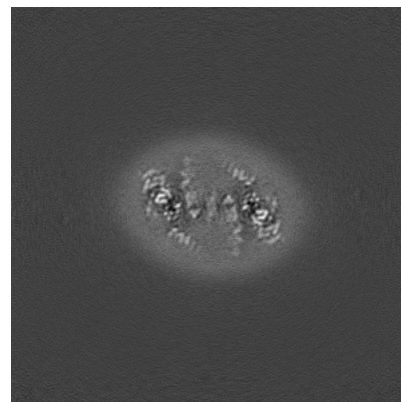
6.3.2 Raw map



X Index: 234



Y Index: 199

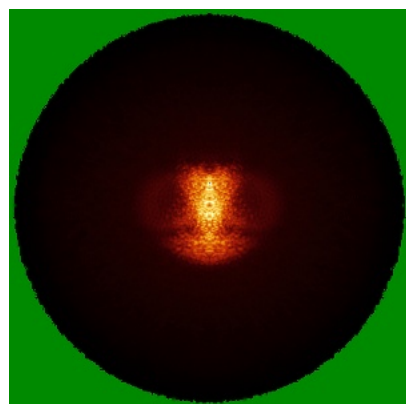


Z Index: 186

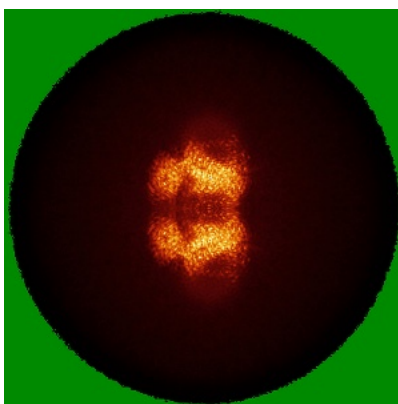
The images above show the largest variance slices of the map in three orthogonal directions.

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

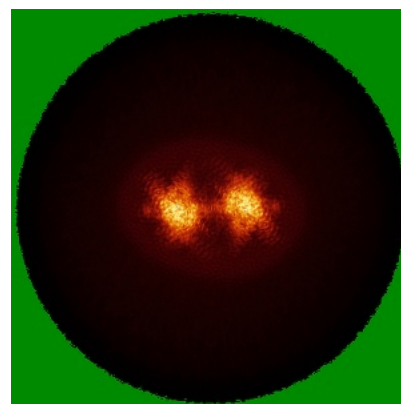
6.4.1 Primary map



X

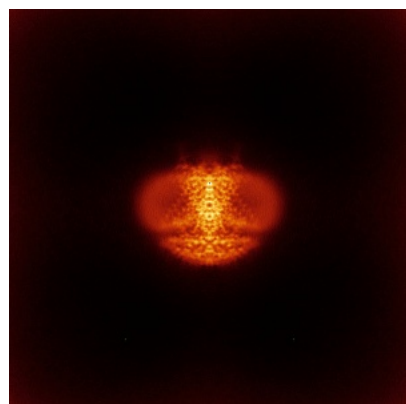


Y

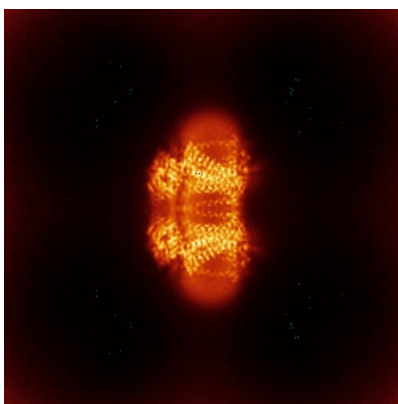


Z

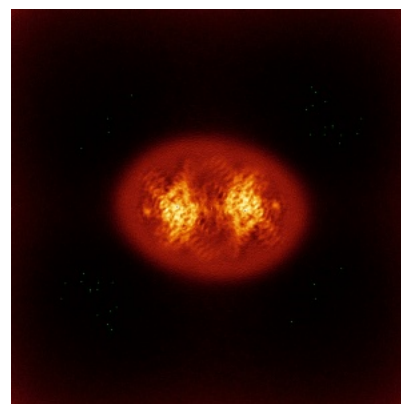
6.4.2 Raw map



X



Y

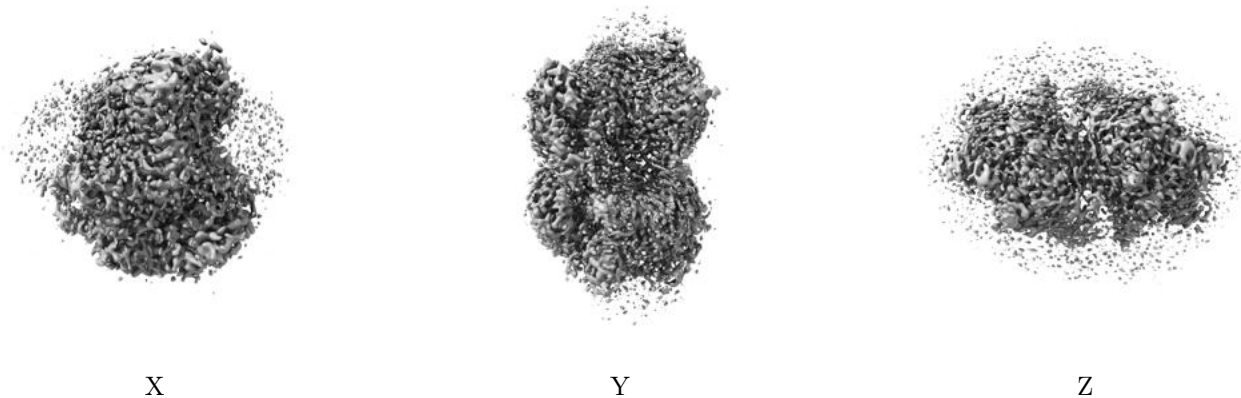


Z

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.

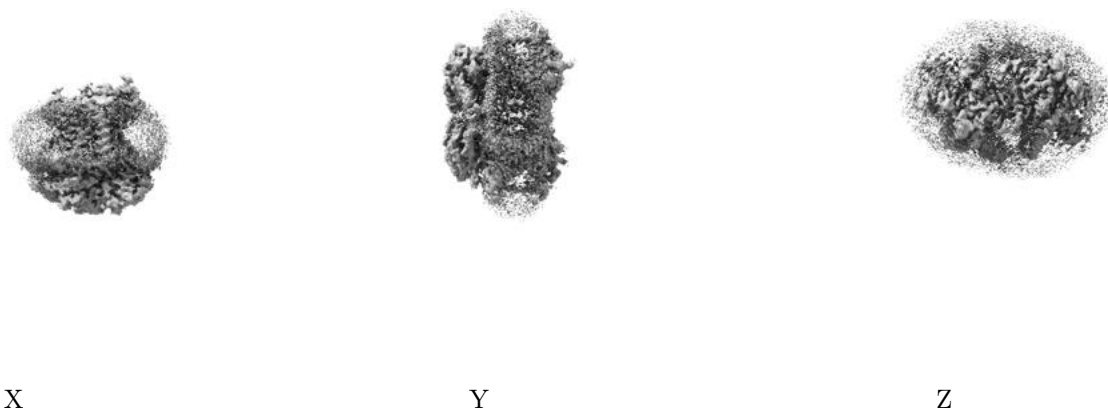
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 5.0. 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.

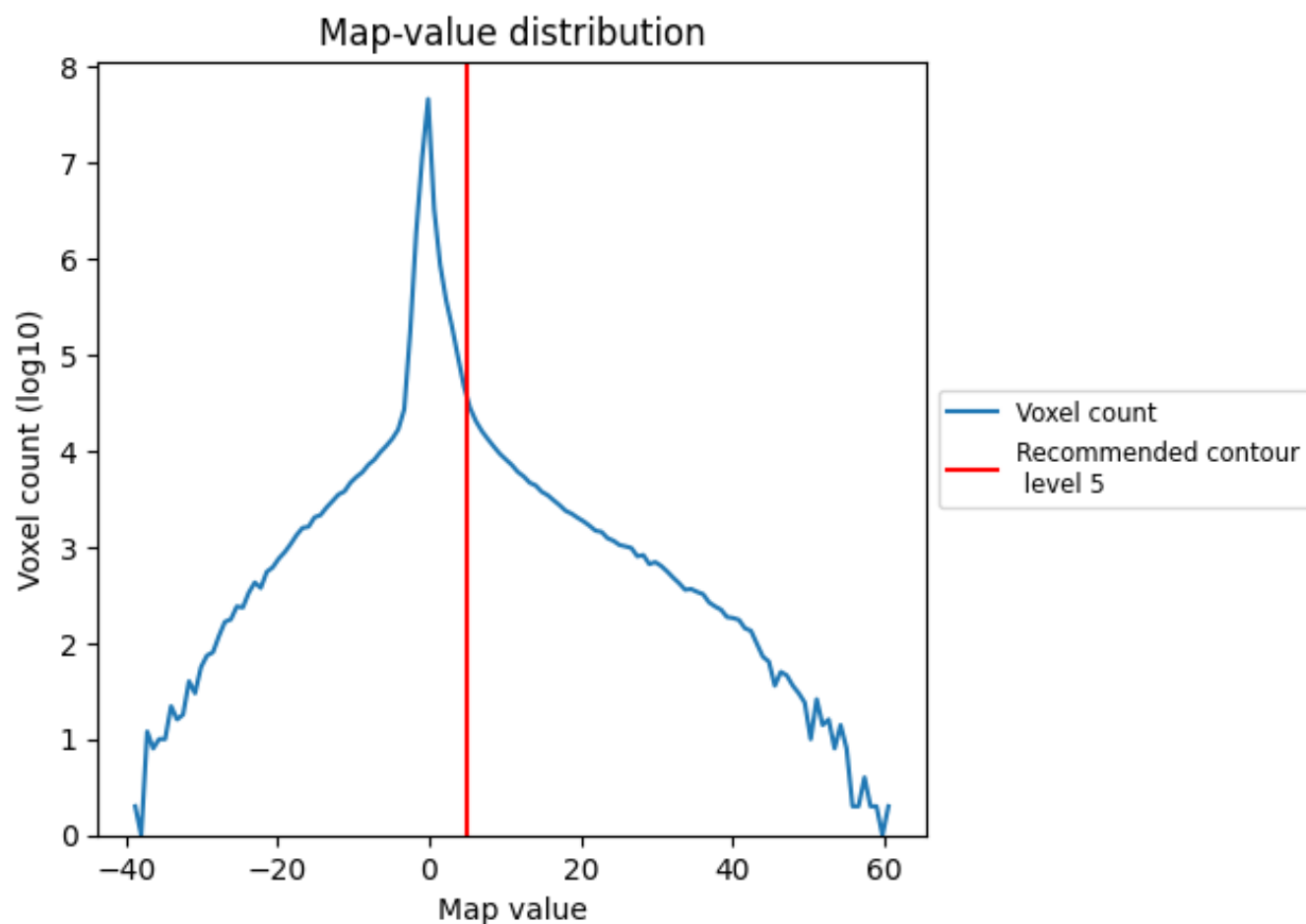
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

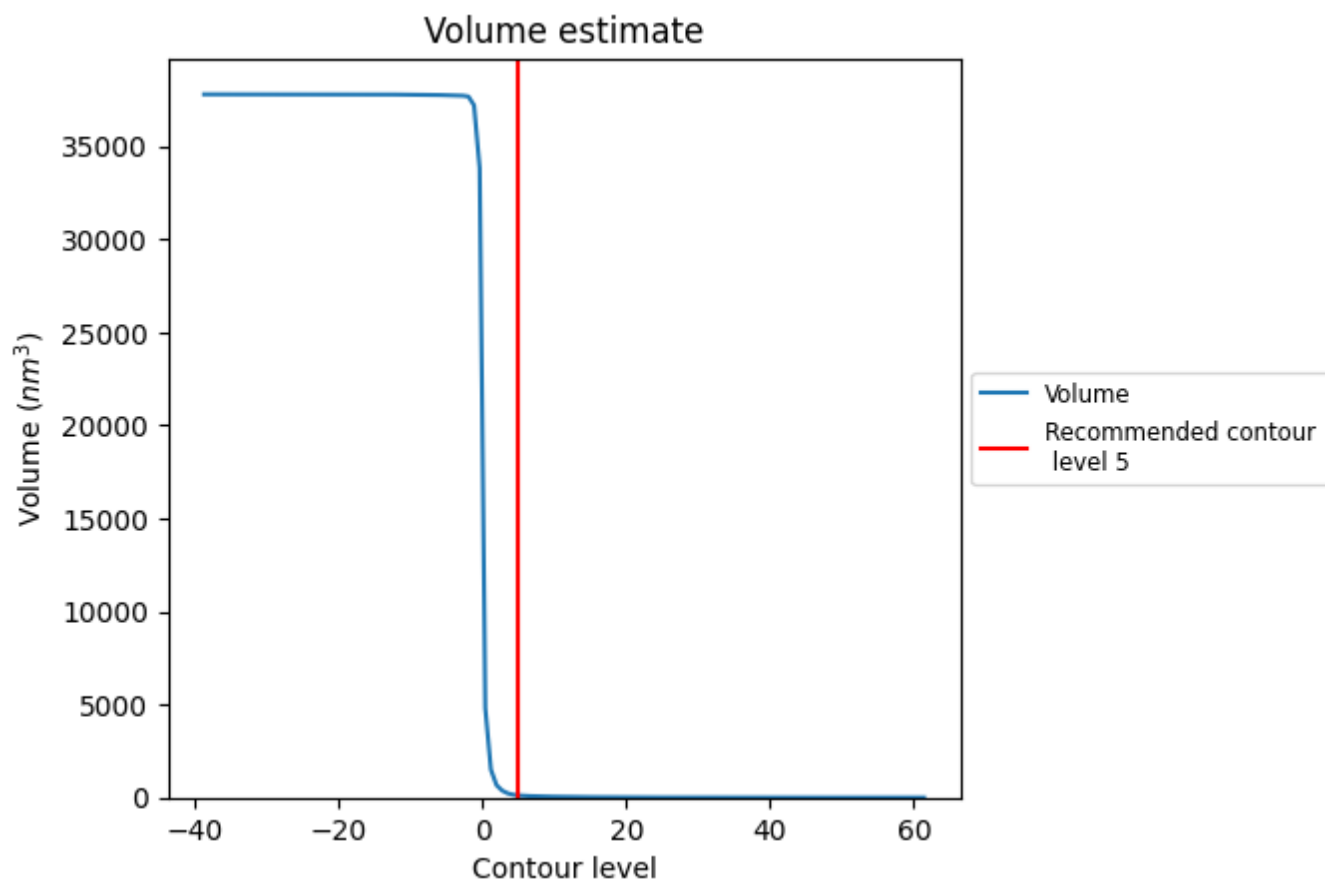
This section contains the results of statistical analysis of the map.

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.

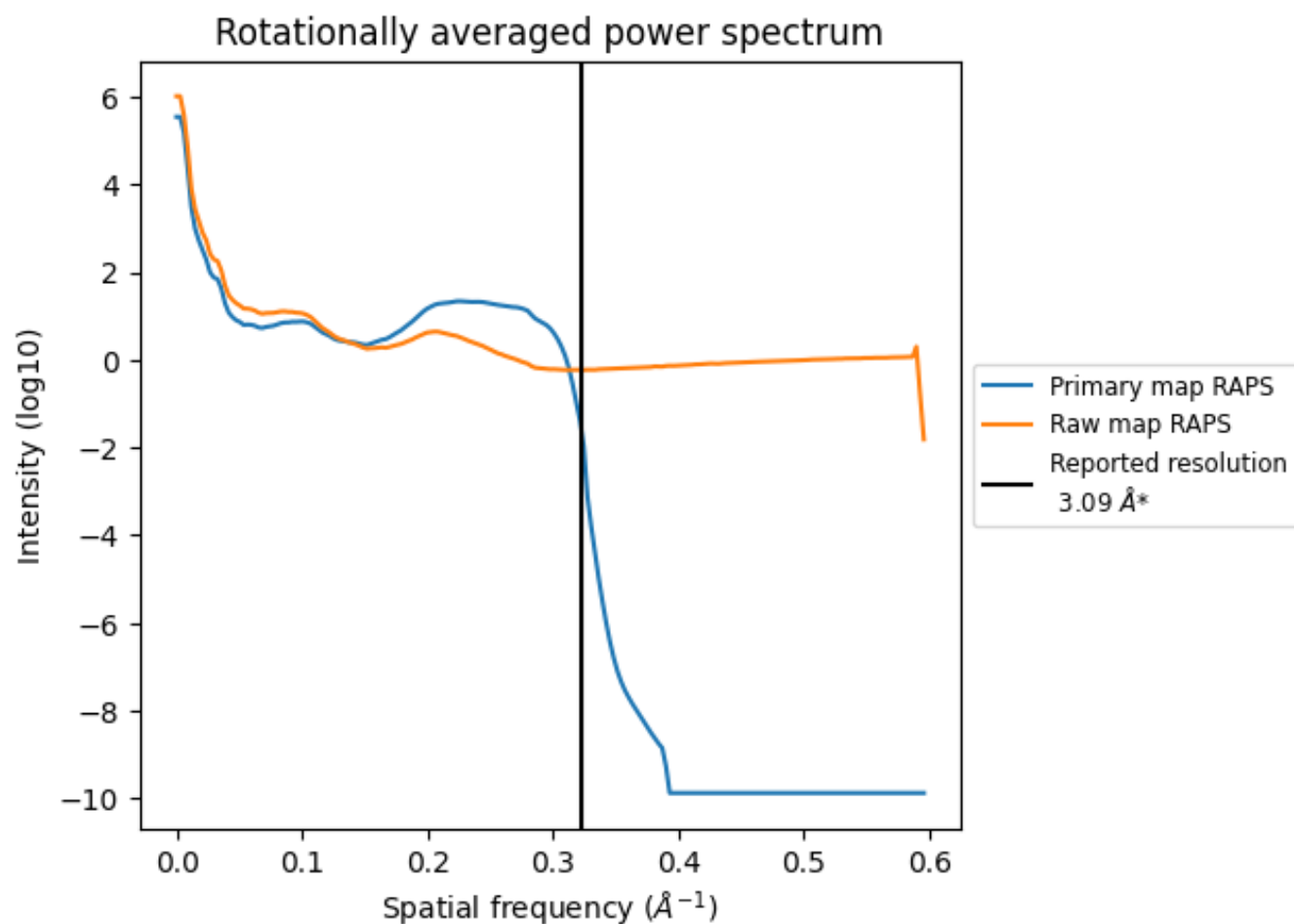
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 114 nm³; this corresponds to an approximate mass of 103 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 ⓘ

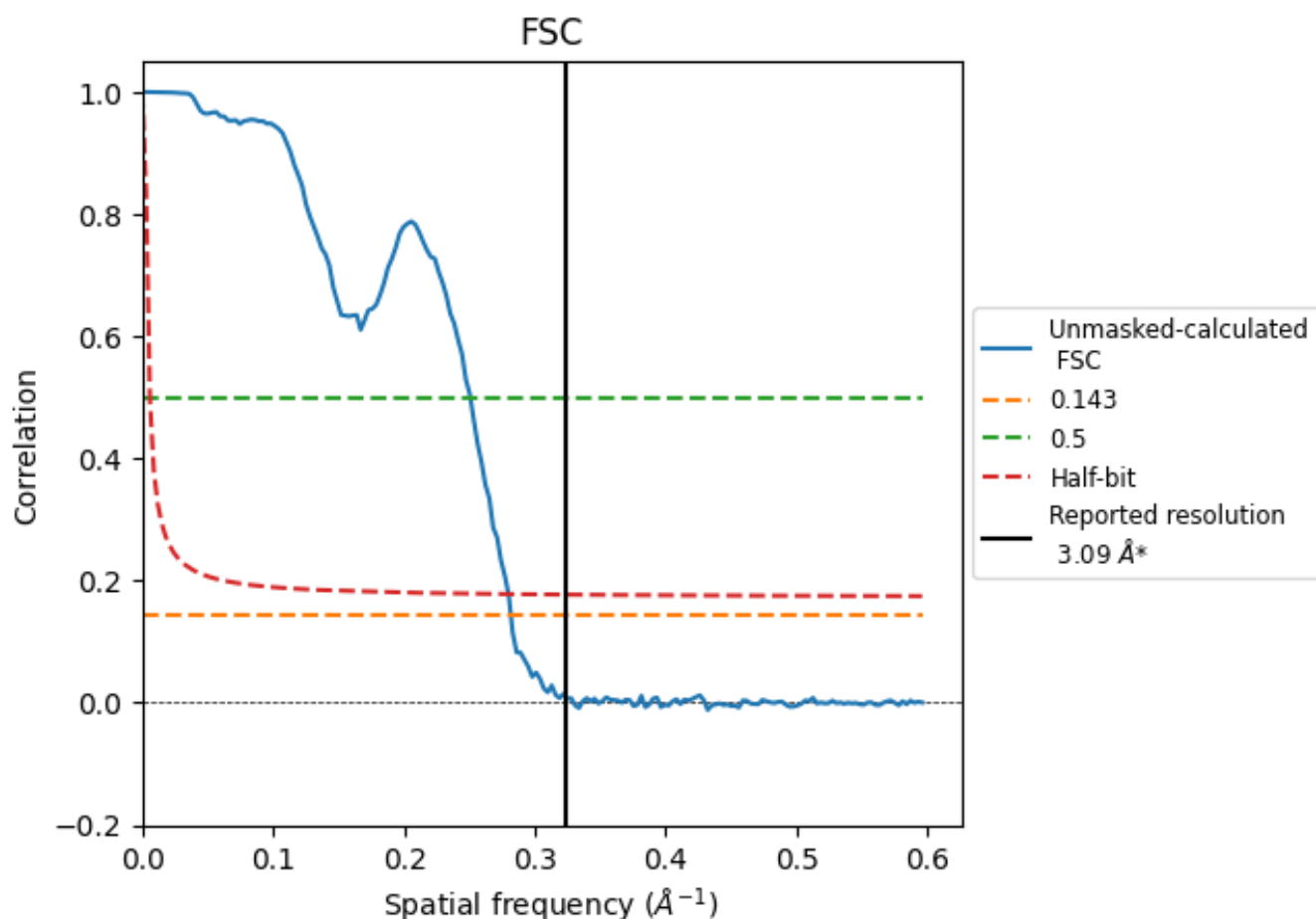


*Reported resolution corresponds to spatial frequency of 0.324 Å⁻¹

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 0.324 \AA^{-1}

8.2 Resolution estimates [i](#)

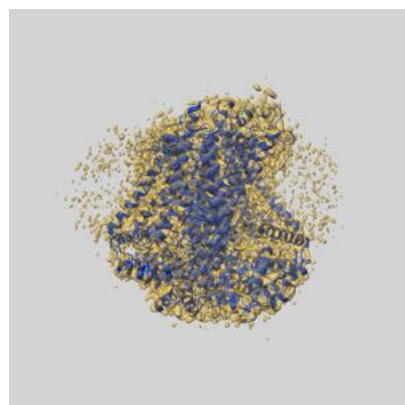
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.55	3.99	3.57

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

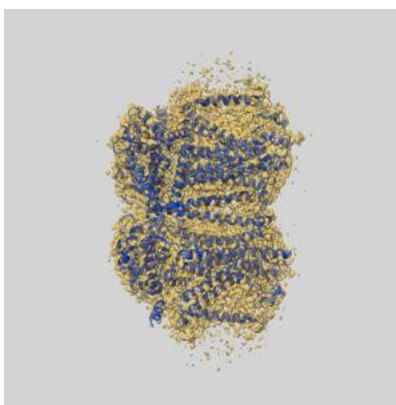
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-26742 and PDB model 7USX. Per-residue inclusion information can be found in section 3 on page 10.

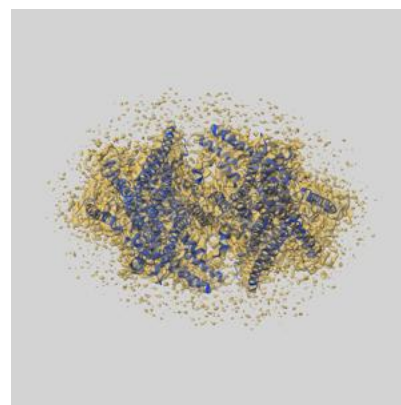
9.1 Map-model overlay [i](#)



X



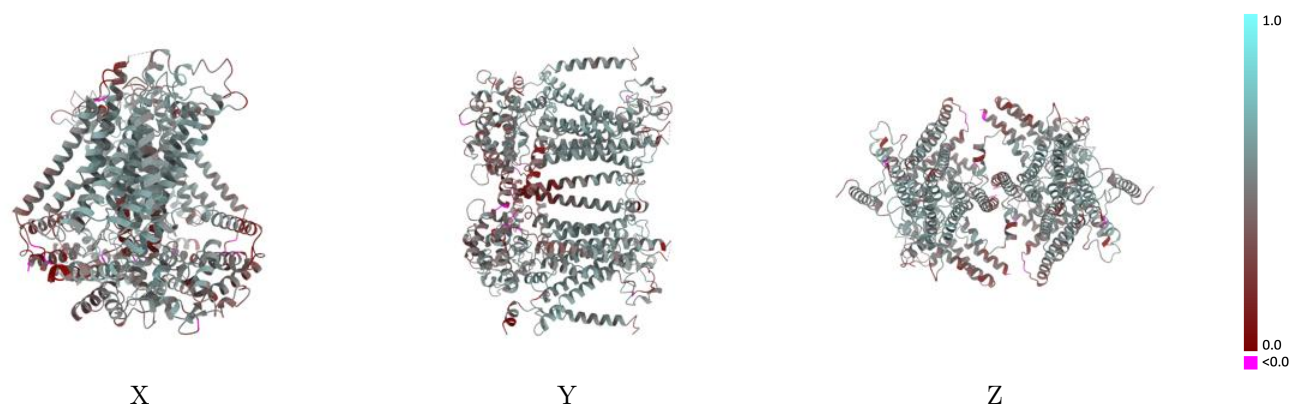
Y



Z

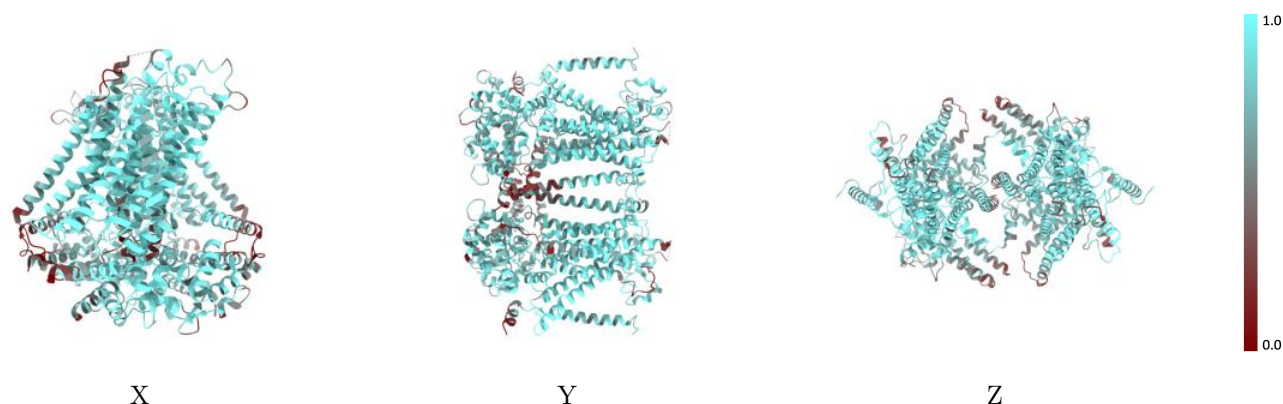
The images above show the 3D surface view of the map at the recommended contour level 5.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



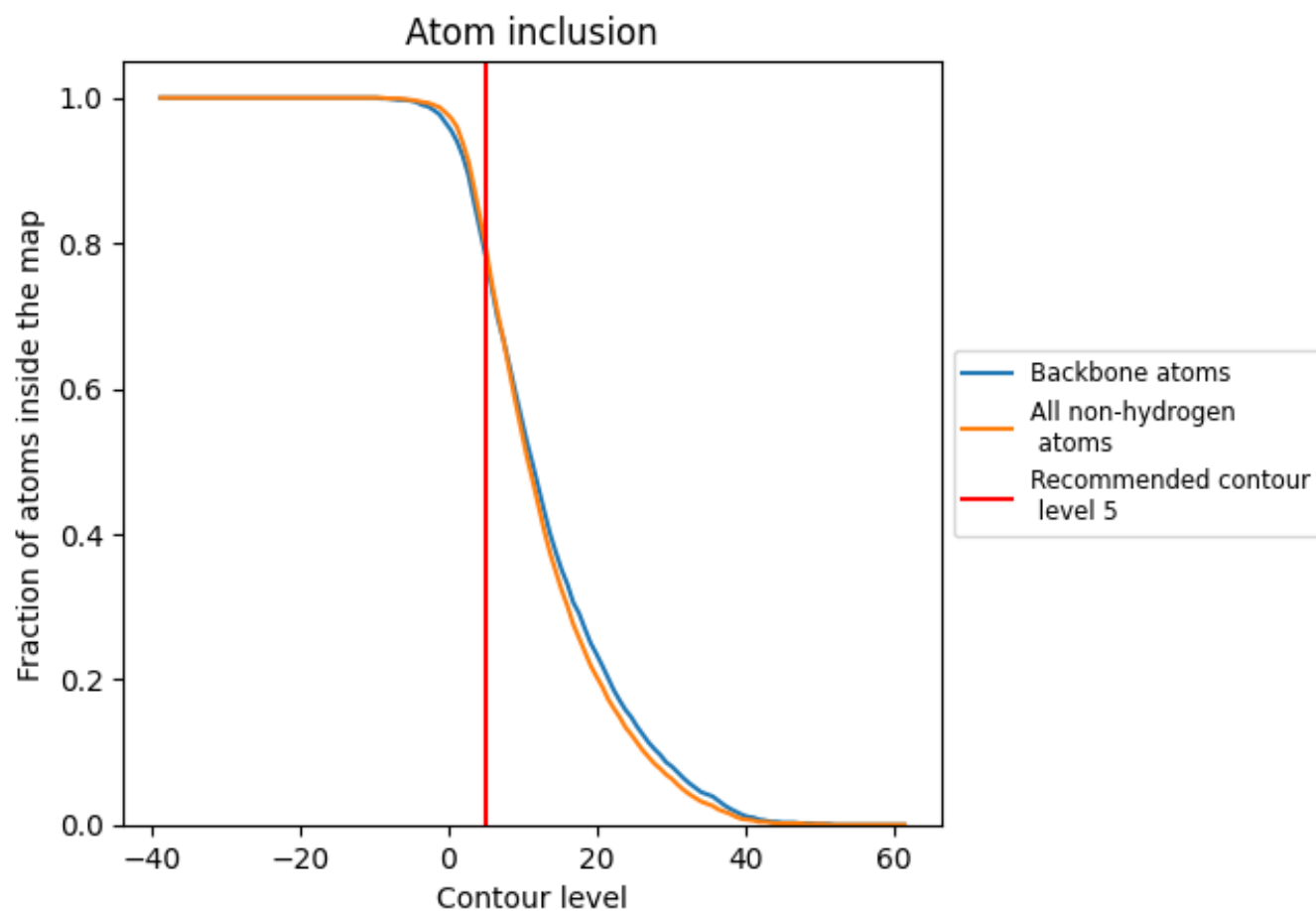
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 80% 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 (5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.7950	<div><div></div></div> 0.4800
A	<div><div></div></div> 0.7980	<div><div></div></div> 0.4840
B	<div><div></div></div> 0.7990	<div><div></div></div> 0.4850
C	<div><div></div></div> 0.7940	<div><div></div></div> 0.4670
D	<div><div></div></div> 0.7480	<div><div></div></div> 0.4740
E	<div><div></div></div> 0.7960	<div><div></div></div> 0.4640
F	<div><div></div></div> 0.7480	<div><div></div></div> 0.4770

1.0

0.0

<0.0