



## Full wwPDB EM Validation Report ⓘ

Apr 5, 2026 – 07:14 PM UTC

PDB ID : 9X04 / pdb\_00009x04  
EMDB ID : EMD-66419  
Title : Cryo-EM structure of Fks2 with intact active site  
Authors : Wang, L.X.; Bai, L.  
Deposited on : 2025-09-29  
Resolution : 3.41 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.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

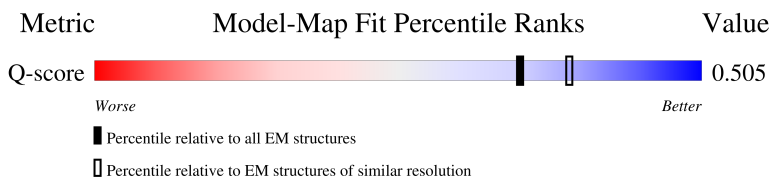
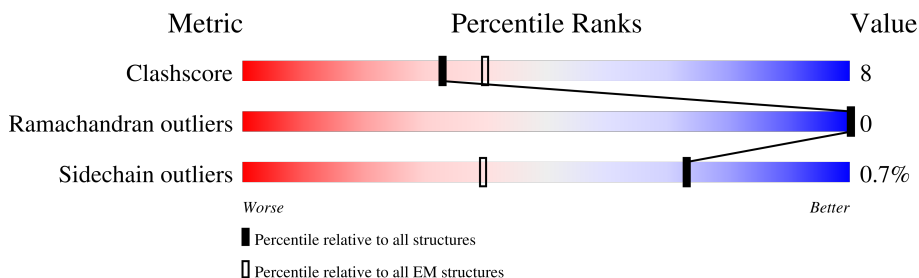
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.41 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	13997 ( 2.91 - 3.91 )

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

Mol	Chain	Length	Quality of chain
1	A	1895	
2	C	2	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ERG	A	1909	-	-	X	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 26639 atoms, of which 13392 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 1,3-beta-glucan synthase component GSC2.

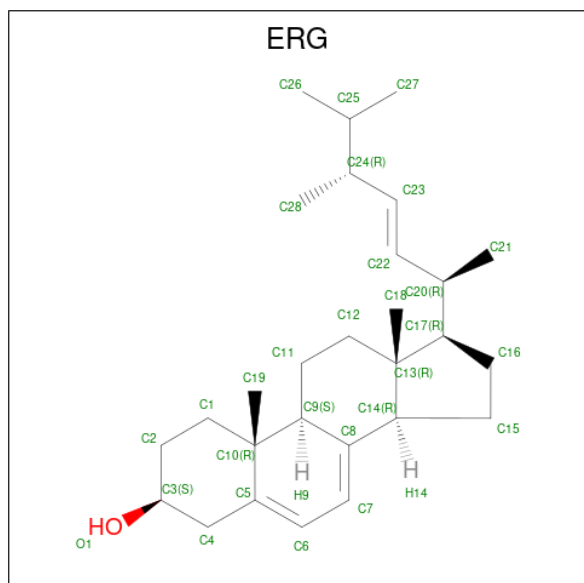
Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	1542	24883	8182	12346	2108	2170	77	0	0

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
2	C	2	53	16	25	2	10	0	0

- Molecule 3 is ERGOSTEROL (CCD ID: ERG) (formula: C<sub>28</sub>H<sub>44</sub>O).



[illegible]

- Molecule 4 is Enfumafungin (CCD ID: A1E06) (formula:  $C_{38}H_{60}O_{12}$ ) (labeled as "Ligand of Interest" by depositor).



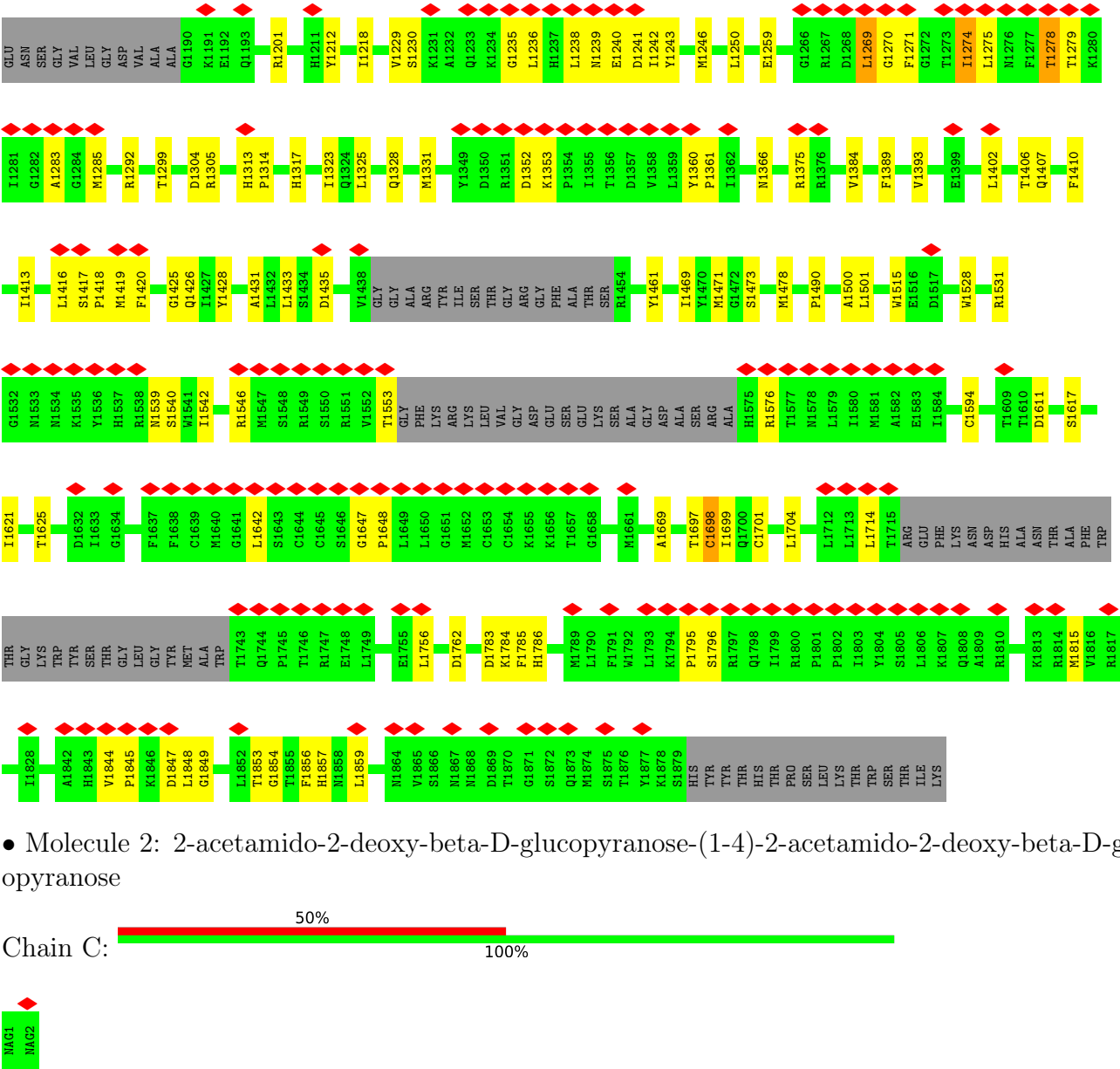
Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	H	O	0
			109	38	59	12	

- Molecule 5 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylammonio)ethyl phosphate (CCD ID: POV) (formula:  $C_{42}H_{82}NO_8P$ ).



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







## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	34524	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.625	Depositor
Minimum map value	-0.429	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	378.88, 378.88, 378.88	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.74, 0.74, 0.74	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, POV, ERG, A1E06

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	0.31	0/12879	0.46	8/17461 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1271	PHE	N-CA-C	7.99	120.77	111.02
1	A	1699	ILE	N-CA-C	-7.58	101.42	112.04
1	A	1701	CYS	CB-CA-C	-5.84	100.93	110.85
1	A	1854	GLY	N-CA-C	-5.58	99.97	113.18
1	A	1269	LEU	N-CA-C	5.50	115.81	108.38
1	A	1274	ILE	CB-CA-C	-5.39	105.07	111.81
1	A	1240	GLU	N-CA-C	5.27	117.71	111.33
1	A	1704	LEU	N-CA-C	-5.09	106.92	113.23

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1576	ARG	Sidechain

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	12537	12346	12537	177	0
2	C	28	25	25	0	0
3	A	580	880	880	92	0
4	A	50	59	0	0	0
5	A	52	82	82	0	0
All	All	13247	13392	13524	225	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 8.

All (225) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1269:LEU:HD11	1:A:1274:ILE:HG12	1.20	1.15
3:A:1909:ERG:H181	3:A:1910:ERG:C18	1.81	1.10
3:A:1909:ERG:H152	3:A:1910:ERG:H182	1.11	1.06
1:A:717:VAL:HG21	3:A:1916:ERG:C26	1.93	0.99
3:A:1909:ERG:H152	3:A:1910:ERG:C18	1.93	0.98
3:A:1909:ERG:H181	3:A:1910:ERG:H183	1.47	0.97
1:A:1402:LEU:CD2	3:A:1909:ERG:H271	1.96	0.96
1:A:1402:LEU:HD21	3:A:1909:ERG:C27	1.97	0.94
3:A:1902:ERG:C12	3:A:1920:ERG:H152	1.99	0.92
1:A:1402:LEU:HD21	3:A:1909:ERG:H272	1.52	0.91
1:A:1515:TRP:CG	3:A:1903:ERG:H12	2.05	0.90
1:A:1269:LEU:CD1	1:A:1274:ILE:HG12	2.01	0.90
1:A:734:ILE:HG23	3:A:1913:ERG:H211	1.54	0.89
1:A:1126:ASN:ND2	1:A:1131:CYS:SG	2.46	0.88
1:A:1413:ILE:HG12	3:A:1919:ERG:C26	2.02	0.88
1:A:1402:LEU:HD22	3:A:1909:ERG:H271	1.58	0.84
1:A:1402:LEU:CD2	3:A:1909:ERG:C27	2.54	0.84
1:A:1413:ILE:CG1	3:A:1919:ERG:H261	2.09	0.83
1:A:680:GLU:OE2	1:A:1617:SER:OG	1.99	0.81
1:A:1278:THR:HG23	1:A:1428:TYR:CE1	2.21	0.75
1:A:717:VAL:HG21	3:A:1916:ERG:H263	1.69	0.75
1:A:1413:ILE:CG1	3:A:1919:ERG:C26	2.64	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1461:TYR:OH	1:A:1762:ASP:OD1	2.03	0.74
1:A:1201:ARG:NH1	1:A:1259:GLU:OE1	2.20	0.74
1:A:1413:ILE:HG12	3:A:1919:ERG:H263	1.66	0.74
1:A:837:ARG:NE	1:A:1129:GLU:OE2	2.20	0.74
1:A:1270:GLY:O	1:A:1274:ILE:HG13	1.87	0.74
3:A:1909:ERG:C15	3:A:1910:ERG:H111	2.18	0.73
1:A:1542:ILE:HD12	1:A:1542:ILE:H	1.52	0.73
1:A:338:ARG:NH1	1:A:1110:ILE:HD11	2.04	0.71
1:A:1407:GLN:NE2	3:A:1920:ERG:H193	2.06	0.71
3:A:1916:ERG:H283	3:A:1917:ERG:H183	1.72	0.71
1:A:1278:THR:HG23	1:A:1428:TYR:CZ	2.26	0.70
3:A:1902:ERG:H122	3:A:1920:ERG:H152	1.73	0.69
3:A:1906:ERG:H263	3:A:1909:ERG:H182	1.76	0.68
1:A:1325:LEU:CD1	3:A:1901:ERG:H7	2.23	0.68
1:A:1285:MET:HG3	1:A:1317:HIS:CE1	2.29	0.67
1:A:1325:LEU:HD13	3:A:1901:ERG:H7	1.76	0.67
1:A:1269:LEU:HD11	1:A:1274:ILE:CG1	2.13	0.66
3:A:1913:ERG:H151	3:A:1914:ERG:H211	1.78	0.65
1:A:428:GLU:N	1:A:428:GLU:OE1	2.30	0.65
1:A:1407:GLN:NE2	3:A:1920:ERG:C19	2.59	0.65
1:A:1030:LYS:HE3	1:A:1030:LYS:HA	1.77	0.64
3:A:1909:ERG:H152	3:A:1910:ERG:H111	1.79	0.63
1:A:1553:THR:HB	1:A:1714:LEU:HD21	1.80	0.63
1:A:1212:TYR:OH	1:A:1218:ILE:HD11	1.98	0.63
1:A:370:GLY:O	1:A:374:ASN:ND2	2.31	0.62
1:A:1279:THR:HG23	1:A:1431:ALA:HB2	1.81	0.62
3:A:1902:ERG:H121	3:A:1920:ERG:H152	1.81	0.62
1:A:1515:TRP:CD1	3:A:1903:ERG:C2	2.82	0.61
3:A:1910:ERG:H183	3:A:1910:ERG:H212	1.82	0.61
1:A:1175:TYR:O	1:A:1176:ILE:HB	2.01	0.59
1:A:739:ARG:HD2	1:A:819:ASP:HA	1.84	0.59
1:A:1515:TRP:CD2	3:A:1903:ERG:H12	2.38	0.58
3:A:1916:ERG:C28	3:A:1917:ERG:H183	2.33	0.58
1:A:1278:THR:HG23	1:A:1428:TYR:CD1	2.38	0.58
1:A:1328:GLN:HE21	1:A:1471:MET:HE3	1.68	0.57
1:A:1279:THR:HG23	1:A:1431:ALA:CB	2.36	0.56
1:A:1669:ALA:HB2	1:A:1756:LEU:HD22	1.87	0.56
1:A:1853:THR:HA	1:A:1856:PHE:HB2	1.88	0.56
3:A:1906:ERG:H25	3:A:1909:ERG:H191	1.88	0.56
1:A:405:LYS:O	1:A:406:VAL:HG23	2.04	0.56
1:A:1124:GLN:NE2	1:A:1174:GLU:OE2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:611:TYR:CE2	1:A:613:LYS:HB2	2.41	0.55
3:A:1902:ERG:H112	3:A:1920:ERG:C15	2.37	0.55
1:A:717:VAL:HG21	3:A:1916:ERG:H262	1.88	0.55
1:A:1515:TRP:CG	3:A:1903:ERG:C1	2.87	0.55
1:A:1786:HIS:CD2	3:A:1904:ERG:H261	2.42	0.54
1:A:1304:ASP:OD1	1:A:1305:ARG:N	2.40	0.54
1:A:1313:HIS:HB2	1:A:1314:PRO:HD3	1.88	0.54
3:A:1909:ERG:C15	3:A:1910:ERG:H182	2.07	0.54
1:A:334:ALA:O	1:A:338:ARG:NH1	2.41	0.53
3:A:1902:ERG:H121	3:A:1902:ERG:H212	1.91	0.53
3:A:1911:ERG:C7	3:A:1911:ERG:H191	2.39	0.53
1:A:1269:LEU:HG	1:A:1270:GLY:H	1.72	0.53
1:A:1848:LEU:N	1:A:1848:LEU:HD12	2.24	0.53
1:A:739:ARG:HH11	1:A:819:ASP:HA	1.73	0.53
3:A:1912:ERG:H183	3:A:1912:ERG:H212	1.91	0.53
1:A:783:GLU:O	1:A:783:GLU:OE2	2.27	0.52
3:A:1909:ERG:C18	3:A:1910:ERG:C18	2.72	0.52
3:A:1909:ERG:H181	3:A:1910:ERG:H181	1.86	0.52
1:A:550:ARG:NH1	1:A:604:LEU:O	2.43	0.52
1:A:1542:ILE:HD12	1:A:1542:ILE:N	2.24	0.52
1:A:1413:ILE:CD1	3:A:1919:ERG:H261	2.40	0.52
1:A:870:GLU:OE1	1:A:870:GLU:N	2.43	0.52
1:A:1531:ARG:C	1:A:1540:SER:HG	2.17	0.52
1:A:862:THR:OG1	1:A:1113:ARG:O	2.28	0.51
1:A:1542:ILE:O	1:A:1546:ARG:HG3	2.10	0.51
1:A:749:ILE:O	1:A:749:ILE:HG22	2.10	0.51
1:A:1323:ILE:HD11	1:A:1384:VAL:HG11	1.91	0.51
1:A:1413:ILE:HD11	3:A:1919:ERG:H261	1.92	0.51
1:A:1515:TRP:CH2	3:A:1903:ERG:H14	2.45	0.51
1:A:1853:THR:HA	1:A:1856:PHE:CB	2.40	0.51
1:A:1035:GLU:C	1:A:1035:GLU:OE1	2.53	0.51
1:A:1785:PHE:CZ	3:A:1904:ERG:H6	2.46	0.50
1:A:1269:LEU:HG	1:A:1270:GLY:N	2.27	0.50
3:A:1909:ERG:H151	3:A:1910:ERG:H111	1.91	0.50
1:A:1413:ILE:HD11	3:A:1919:ERG:C26	2.42	0.50
3:A:1902:ERG:C11	3:A:1920:ERG:H152	2.42	0.50
1:A:1419:MET:HG3	1:A:1420:PHE:N	2.27	0.50
1:A:1528:TRP:NE1	1:A:1539:ASN:O	2.45	0.49
1:A:1278:THR:HG23	1:A:1428:TYR:CE2	2.48	0.49
1:A:1331:MET:HB3	1:A:1478:MET:HE3	1.93	0.49
1:A:613:LYS:CD	1:A:613:LYS:N	2.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1325:LEU:CD2	3:A:1901:ERG:H6	2.42	0.49
3:A:1916:ERG:H121	3:A:1916:ERG:H212	1.94	0.49
1:A:1119:LEU:HD13	1:A:1212:TYR:OH	2.13	0.49
1:A:1783:ASP:OD1	1:A:1784:LYS:N	2.45	0.49
1:A:1501:LEU:O	1:A:1501:LEU:HD23	2.13	0.48
1:A:1413:ILE:CD1	3:A:1919:ERG:C26	2.91	0.48
1:A:476:ILE:HD11	1:A:526:GLN:HG2	1.96	0.48
1:A:1325:LEU:HD11	3:A:1901:ERG:H7	1.95	0.48
1:A:1175:TYR:CD2	1:A:1176:ILE:HG13	2.48	0.48
1:A:826:GLU:O	1:A:826:GLU:CG	2.63	0.47
1:A:411:ASP:OD1	1:A:1292:ARG:NH2	2.35	0.47
1:A:1621:ILE:HG23	1:A:1698:CYS:SG	2.55	0.47
1:A:783:GLU:OE2	1:A:783:GLU:C	2.57	0.47
1:A:1283:ALA:HB1	1:A:1435:ASP:OD2	2.15	0.47
1:A:1515:TRP:CD1	3:A:1903:ERG:H22A	2.49	0.47
1:A:1785:PHE:CE2	3:A:1904:ERG:C6	2.98	0.47
3:A:1909:ERG:C15	3:A:1910:ERG:C18	2.80	0.47
1:A:1847:ASP:O	1:A:1847:ASP:CG	2.57	0.47
1:A:1413:ILE:HG13	3:A:1919:ERG:H261	1.94	0.47
1:A:1417:SER:N	1:A:1418:PRO:CD	2.78	0.46
3:A:1906:ERG:H263	3:A:1909:ERG:C18	2.44	0.46
1:A:1242:ILE:HG22	1:A:1246:MET:HE3	1.98	0.46
1:A:1360:TYR:HB2	1:A:1361:PRO:HD3	1.98	0.46
1:A:665:ASP:OD2	1:A:1353:LYS:NZ	2.35	0.46
3:A:1914:ERG:H121	3:A:1914:ERG:H212	1.98	0.46
3:A:1912:ERG:H212	3:A:1912:ERG:H121	1.98	0.46
1:A:524:LEU:HD12	1:A:558:MET:HE1	1.99	0.45
3:A:1909:ERG:H212	3:A:1909:ERG:H183	1.97	0.45
1:A:1815:MET:SD	1:A:1815:MET:N	2.89	0.45
1:A:1433:LEU:HD13	3:A:1901:ERG:H42	1.99	0.45
1:A:622:SER:O	1:A:626:THR:HB	2.16	0.45
1:A:1410:PHE:CD2	3:A:1902:ERG:H272	2.52	0.45
1:A:611:TYR:CZ	1:A:613:LYS:HB2	2.51	0.45
1:A:1389:PHE:CE1	1:A:1393:VAL:HG23	2.52	0.45
1:A:1795:PRO:O	1:A:1796:SER:OG	2.32	0.45
3:A:1903:ERG:H121	3:A:1903:ERG:H212	1.99	0.44
3:A:1913:ERG:H121	3:A:1913:ERG:H212	1.99	0.44
1:A:1406:THR:OG1	3:A:1908:ERG:H261	2.18	0.44
3:A:1909:ERG:H212	3:A:1909:ERG:H121	1.99	0.44
1:A:1402:LEU:HD23	3:A:1912:ERG:H25	1.99	0.44
1:A:680:GLU:OE2	1:A:1617:SER:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1847:ASP:C	1:A:1848:LEU:HD12	2.43	0.44
1:A:1469:ILE:O	1:A:1473:SER:OG	2.30	0.44
1:A:1621:ILE:O	1:A:1625:THR:HG22	2.18	0.44
3:A:1906:ERG:H162	3:A:1906:ERG:H23	1.99	0.44
3:A:1911:ERG:H121	3:A:1911:ERG:H212	2.00	0.44
3:A:1917:ERG:H212	3:A:1917:ERG:H121	1.99	0.44
1:A:1325:LEU:HD22	3:A:1901:ERG:H6	2.00	0.44
1:A:192:ASN:O	1:A:366:PRO:HB3	2.18	0.44
1:A:1235:GLY:O	1:A:1236:LEU:C	2.59	0.44
1:A:1785:PHE:CE2	3:A:1904:ERG:C7	3.01	0.44
1:A:669:ILE:HD13	1:A:1366:ASN:O	2.18	0.44
1:A:672:THR:O	1:A:672:THR:OG1	2.33	0.44
1:A:1402:LEU:HD23	3:A:1912:ERG:H271	1.99	0.44
1:A:1542:ILE:H	1:A:1542:ILE:CD1	2.25	0.44
1:A:1402:LEU:HD23	3:A:1912:ERG:C25	2.48	0.43
1:A:969:LEU:O	1:A:973:ILE:HD12	2.18	0.43
1:A:1531:ARG:O	1:A:1540:SER:OG	2.35	0.43
3:A:1909:ERG:H151	3:A:1910:ERG:H191	2.00	0.43
1:A:1269:LEU:CG	1:A:1274:ILE:HG12	2.47	0.43
1:A:513:ALA:CB	1:A:568:VAL:HG22	2.48	0.43
1:A:1611:ASP:OD1	1:A:1611:ASP:N	2.52	0.43
1:A:1849:GLY:HA2	1:A:1859:LEU:HD12	2.01	0.43
3:A:1917:ERG:C22	3:A:1917:ERG:H263	2.48	0.43
1:A:826:GLU:O	1:A:826:GLU:HG2	2.19	0.43
1:A:1389:PHE:O	1:A:1389:PHE:CD1	2.72	0.43
1:A:521:VAL:O	1:A:525:ILE:HG12	2.19	0.43
1:A:1212:TYR:CD1	1:A:1212:TYR:C	2.97	0.43
1:A:1375:ARG:CG	1:A:1490:PRO:HG2	2.49	0.43
3:A:1901:ERG:C22	3:A:1901:ERG:H272	2.49	0.43
3:A:1904:ERG:H121	3:A:1904:ERG:H212	2.00	0.43
1:A:1236:LEU:HG	1:A:1238:LEU:HG	2.01	0.42
1:A:1236:LEU:HD11	1:A:1238:LEU:HD21	2.01	0.42
1:A:1239:ASN:HB2	1:A:1243:TYR:CE2	2.54	0.42
1:A:1269:LEU:CG	1:A:1270:GLY:H	2.31	0.42
1:A:565:VAL:CG1	1:A:566:ILE:HG23	2.50	0.42
1:A:1299:THR:HG22	1:A:1299:THR:O	2.17	0.42
1:A:1531:ARG:O	1:A:1542:ILE:HD13	2.19	0.42
1:A:1025:ARG:O	1:A:1025:ARG:HG2	2.18	0.42
1:A:824:GLU:OE1	1:A:824:GLU:HA	2.19	0.42
1:A:1275:LEU:O	1:A:1278:THR:HB	2.20	0.42
1:A:1844:VAL:HG12	1:A:1845:PRO:HD2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:872:ILE:HD12	1:A:872:ILE:N	2.34	0.42
1:A:406:VAL:O	1:A:456:LYS:NZ	2.52	0.42
1:A:629:PHE:CE1	1:A:1250:LEU:HD23	2.54	0.42
1:A:868:TYR:CD1	1:A:868:TYR:C	2.98	0.42
1:A:1285:MET:HG3	1:A:1317:HIS:CG	2.55	0.42
1:A:1402:LEU:HD22	3:A:1909:ERG:C27	2.33	0.42
1:A:801:SER:HB3	1:A:808:THR:HG23	2.02	0.42
3:A:1917:ERG:C22	3:A:1917:ERG:C26	2.98	0.42
1:A:1352:ASP:O	1:A:1352:ASP:CG	2.63	0.41
1:A:1375:ARG:HG3	1:A:1490:PRO:HG2	2.02	0.41
1:A:1389:PHE:HE1	1:A:1393:VAL:HG23	1.85	0.41
3:A:1901:ERG:C22	3:A:1901:ERG:C27	2.98	0.41
1:A:1119:LEU:HD11	1:A:1218:ILE:HD12	2.01	0.41
1:A:1425:GLY:O	1:A:1426:GLN:C	2.63	0.41
1:A:1278:THR:HG22	1:A:1279:THR:N	2.34	0.41
1:A:1515:TRP:CD1	3:A:1903:ERG:H21	2.55	0.41
1:A:452:ASP:C	1:A:452:ASP:OD1	2.62	0.41
1:A:1419:MET:HB2	1:A:1500:ALA:HB1	2.01	0.41
3:A:1905:ERG:C22	3:A:1905:ERG:H273	2.49	0.41
3:A:1908:ERG:H21	3:A:1909:ERG:H193	2.01	0.41
1:A:1212:TYR:O	1:A:1241:ASP:HB2	2.19	0.41
1:A:1229:VAL:HG23	1:A:1230:SER:N	2.35	0.41
3:A:1906:ERG:H23	3:A:1906:ERG:C16	2.51	0.41
1:A:1402:LEU:HD23	3:A:1912:ERG:C27	2.51	0.41
3:A:1906:ERG:C16	3:A:1906:ERG:C23	2.98	0.41
1:A:654:GLU:C	1:A:656:TYR:H	2.28	0.41
1:A:880:ILE:O	1:A:881:ARG:C	2.63	0.41
1:A:592:ALA:O	1:A:595:THR:HG22	2.20	0.41
1:A:338:ARG:NH2	1:A:1106:ASN:O	2.54	0.40
1:A:563:GLY:N	1:A:564:PRO:HD2	2.36	0.40
1:A:613:LYS:N	1:A:613:LYS:HD3	2.36	0.40
1:A:1594:CYS:HB3	1:A:1697:THR:HA	2.03	0.40
3:A:1917:ERG:H183	3:A:1917:ERG:H212	2.03	0.40
1:A:487:ALA:HB1	1:A:514:THR:HB	2.02	0.40
3:A:1906:ERG:H23	3:A:1906:ERG:H262	1.83	0.40
1:A:1170:VAL:HG23	1:A:1170:VAL:O	2.21	0.40
1:A:541:TRP:HA	1:A:541:TRP:CE3	2.57	0.40
1:A:1647:GLY:N	1:A:1648:PRO:CD	2.84	0.40
1:A:611:TYR:CE1	1:A:613:LYS:HE2	2.56	0.40

There are no symmetry-related clashes.



## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1522/1895 (80%)	1451 (95%)	71 (5%)	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	1352/1647 (82%)	1343 (99%)	9 (1%)	76	78

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	565	VAL
1	A	568	VAL
1	A	613	LYS
1	A	730	LEU
1	A	1278	THR
1	A	1416	LEU
1	A	1642	LEU
1	A	1698	CYS
1	A	1857	HIS

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

Mol	Chain	Res	Type
1	A	313	ASN
1	A	466	HIS
1	A	691	GLN
1	A	967	GLN
1	A	991	ASN
1	A	1032	HIS
1	A	1036	ASN
1	A	1106	ASN
1	A	1126	ASN
1	A	1148	GLN
1	A	1150	HIS
1	A	1237	HIS
1	A	1239	ASN
1	A	1319	ASN
1	A	1328	GLN
1	A	1602	ASN
1	A	1767	HIS
1	A	1786	HIS
1	A	1808	GLN
1	A	1857	HIS
1	A	1873	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](#)

2 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	C	1	1,2	14,14,15	0.31	0	17,19,21	0.50	0
2	NAG	C	2	2	14,14,15	0.17	0	17,19,21	0.41	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

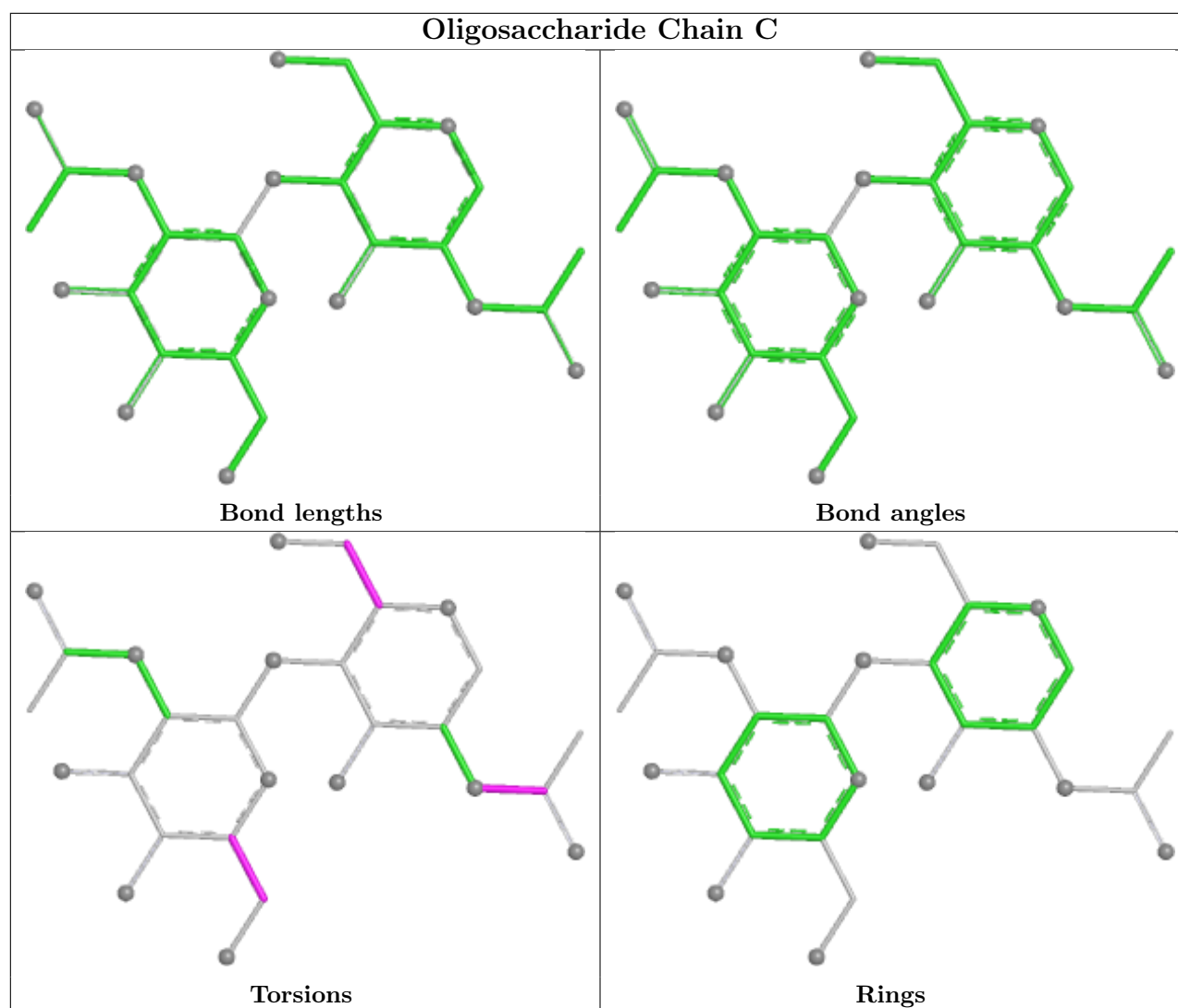
All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	2	NAG	C4-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
2	C	1	NAG	C8-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2
2	C	1	NAG	C4-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



## 5.6 Ligand geometry [i](#)

22 ligands are modelled in this entry.

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	ERG	A	1913	-	32,32,32	0.83	1 (3%)	45,50,50	1.32	6 (13%)
3	ERG	A	1920	-	32,32,32	0.76	1 (3%)	45,50,50	0.64	1 (2%)
5	POV	A	1922	-	51,51,51	0.53	0	57,59,59	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	ERG	A	1906	-	32,32,32	0.76	1 (3%)	45,50,50	0.70	1 (2%)
4	A1E06	A	1921	-	52,55,55	0.45	0	75,91,91	1.47	6 (8%)
3	ERG	A	1908	-	32,32,32	0.76	1 (3%)	45,50,50	0.74	1 (2%)
3	ERG	A	1905	-	32,32,32	1.10	3 (9%)	45,50,50	1.53	9 (20%)
3	ERG	A	1901	-	32,32,32	0.94	1 (3%)	45,50,50	1.44	6 (13%)
3	ERG	A	1909	-	32,32,32	0.88	1 (3%)	45,50,50	1.44	9 (20%)
3	ERG	A	1902	-	32,32,32	0.93	1 (3%)	45,50,50	1.28	7 (15%)
3	ERG	A	1907	-	32,32,32	0.65	1 (3%)	45,50,50	0.62	1 (2%)
3	ERG	A	1910	-	32,32,32	0.85	1 (3%)	45,50,50	1.36	7 (15%)
3	ERG	A	1912	-	32,32,32	1.12	3 (9%)	45,50,50	1.67	12 (26%)
3	ERG	A	1903	-	32,32,32	0.82	1 (3%)	45,50,50	1.32	6 (13%)
3	ERG	A	1911	-	32,32,32	1.05	2 (6%)	45,50,50	5.16	14 (31%)
3	ERG	A	1904	-	32,32,32	0.82	1 (3%)	45,50,50	1.31	8 (17%)
3	ERG	A	1918	-	32,32,32	0.71	1 (3%)	45,50,50	0.61	1 (2%)
3	ERG	A	1917	-	32,32,32	0.85	1 (3%)	45,50,50	1.27	5 (11%)
3	ERG	A	1914	-	32,32,32	0.85	1 (3%)	45,50,50	1.32	5 (11%)
3	ERG	A	1916	-	32,32,32	0.89	1 (3%)	45,50,50	1.29	6 (13%)
3	ERG	A	1919	-	32,32,32	0.68	1 (3%)	45,50,50	0.61	1 (2%)
3	ERG	A	1915	-	32,32,32	0.83	1 (3%)	45,50,50	1.41	6 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ERG	A	1913	-	-	2/13/71/71	0/4/4/4
3	ERG	A	1920	-	-	3/13/71/71	0/4/4/4
5	POV	A	1922	-	-	14/55/55/55	-
3	ERG	A	1906	-	-	4/13/71/71	0/4/4/4
4	A1E06	A	1921	-	-	3/24/138/138	0/7/6/6
3	ERG	A	1908	-	-	4/13/71/71	0/4/4/4
3	ERG	A	1905	-	-	2/13/71/71	0/4/4/4
3	ERG	A	1901	-	-	2/13/71/71	0/4/4/4
3	ERG	A	1909	-	-	7/13/71/71	0/4/4/4
3	ERG	A	1902	-	-	1/13/71/71	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ERG	A	1907	-	-	0/13/71/71	0/4/4/4
3	ERG	A	1910	-	-	10/13/71/71	0/4/4/4
3	ERG	A	1912	-	-	2/13/71/71	0/4/4/4
3	ERG	A	1903	-	-	1/13/71/71	0/4/4/4
3	ERG	A	1911	-	-	2/13/71/71	0/4/4/4
3	ERG	A	1904	-	-	0/13/71/71	0/4/4/4
3	ERG	A	1918	-	-	4/13/71/71	0/4/4/4
3	ERG	A	1917	-	-	4/13/71/71	0/4/4/4
3	ERG	A	1914	-	-	0/13/71/71	0/4/4/4
3	ERG	A	1916	-	-	3/13/71/71	0/4/4/4
3	ERG	A	1919	-	-	3/13/71/71	0/4/4/4
3	ERG	A	1915	-	-	2/13/71/71	0/4/4/4

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1908	ERG	C10-C9	3.89	1.60	1.55
3	A	1906	ERG	C10-C9	3.85	1.60	1.55
3	A	1920	ERG	C10-C9	3.84	1.60	1.55
3	A	1918	ERG	C10-C9	3.55	1.60	1.55
3	A	1919	ERG	C10-C9	3.42	1.60	1.55
3	A	1907	ERG	C10-C9	3.25	1.59	1.55
3	A	1901	ERG	C13-C14	-3.11	1.51	1.56
3	A	1912	ERG	C13-C14	-3.06	1.51	1.56
3	A	1915	ERG	C13-C14	-3.06	1.51	1.56
3	A	1905	ERG	C13-C14	-3.03	1.51	1.56
3	A	1914	ERG	C13-C14	-3.02	1.51	1.56
3	A	1902	ERG	C13-C14	-3.01	1.51	1.56
3	A	1917	ERG	C13-C14	-2.98	1.51	1.56
3	A	1903	ERG	C13-C14	-2.97	1.51	1.56
3	A	1911	ERG	C13-C14	-2.96	1.51	1.56
3	A	1913	ERG	C13-C14	-2.93	1.51	1.56
3	A	1904	ERG	C13-C14	-2.91	1.51	1.56
3	A	1909	ERG	C13-C14	-2.89	1.51	1.56
3	A	1910	ERG	C13-C14	-2.88	1.51	1.56
3	A	1916	ERG	C13-C14	-2.87	1.51	1.56
3	A	1905	ERG	C4-C3	2.81	1.57	1.52
3	A	1912	ERG	C4-C3	2.62	1.56	1.52
3	A	1911	ERG	C1-C10	2.46	1.58	1.54
3	A	1912	ERG	C2-C3	2.46	1.57	1.51
3	A	1905	ERG	C2-C3	2.36	1.57	1.51

All (118) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1911	ERG	C19-C10-C5	-19.18	79.09	108.38
3	A	1911	ERG	C19-C10-C1	-19.10	80.37	109.43
3	A	1911	ERG	C19-C10-C9	-17.80	81.41	110.98
4	A	1921	A1E06	C7-C5-C2	-7.79	106.07	115.16
3	A	1911	ERG	C1-C10-C9	6.54	121.10	108.39
4	A	1921	A1E06	C29-O2-C16	6.32	127.01	116.26
3	A	1905	ERG	C9-C10-C5	3.97	115.99	109.66
3	A	1911	ERG	C9-C10-C5	3.89	115.86	109.66
3	A	1912	ERG	C9-C10-C5	3.86	115.81	109.66
3	A	1912	ERG	C2-C3-C4	3.82	115.66	110.29
3	A	1905	ERG	C2-C3-C4	3.76	115.58	110.29
3	A	1901	ERG	C9-C10-C5	3.74	115.63	109.66
3	A	1917	ERG	C9-C10-C5	3.66	115.49	109.66
3	A	1916	ERG	C9-C10-C5	3.65	115.48	109.66
3	A	1915	ERG	C13-C14-C8	-3.64	107.16	113.59
3	A	1909	ERG	C9-C10-C5	3.63	115.45	109.66
3	A	1913	ERG	C9-C10-C5	3.63	115.44	109.66
3	A	1904	ERG	C9-C10-C5	3.57	115.35	109.66
4	A	1921	A1E06	C22-C3-C8	3.52	113.77	110.36
3	A	1902	ERG	C9-C10-C5	3.50	115.24	109.66
3	A	1912	ERG	C13-C17-C20	-3.50	115.19	119.38
3	A	1901	ERG	C3-C4-C5	-3.49	106.50	112.05
3	A	1911	ERG	C2-C1-C10	-3.47	105.39	112.78
3	A	1911	ERG	C1-C10-C5	3.46	114.71	108.74
3	A	1914	ERG	C9-C10-C5	3.35	115.00	109.66
3	A	1915	ERG	C9-C10-C5	3.35	115.00	109.66
3	A	1903	ERG	C9-C10-C5	3.31	114.94	109.66
3	A	1911	ERG	C13-C14-C8	-3.26	107.84	113.59
3	A	1901	ERG	C17-C20-C22	-3.25	104.10	110.49
3	A	1912	ERG	C13-C14-C8	-3.21	107.92	113.59
3	A	1910	ERG	C9-C10-C5	3.21	114.77	109.66
3	A	1915	ERG	C13-C17-C20	-3.20	115.55	119.38
3	A	1903	ERG	C13-C14-C8	-3.20	107.95	113.59
3	A	1915	ERG	C14-C13-C17	3.18	103.05	99.72
3	A	1901	ERG	C13-C14-C8	-3.16	108.02	113.59
3	A	1910	ERG	C3-C4-C5	-3.12	107.08	112.05
3	A	1914	ERG	C13-C14-C8	-3.03	108.24	113.59
3	A	1910	ERG	C17-C20-C22	-3.01	104.59	110.49
3	A	1913	ERG	C13-C14-C8	-2.94	108.39	113.59
3	A	1909	ERG	C3-C4-C5	-2.88	107.47	112.05
3	A	1913	ERG	C13-C17-C20	-2.83	115.99	119.38
3	A	1905	ERG	C13-C14-C8	-2.83	108.60	113.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1903	ERG	C13-C17-C20	-2.82	116.00	119.38
3	A	1904	ERG	C13-C14-C8	-2.80	108.65	113.59
3	A	1911	ERG	C13-C17-C20	-2.79	116.04	119.38
3	A	1912	ERG	C21-C20-C22	-2.79	103.60	109.91
3	A	1914	ERG	C13-C17-C20	-2.78	116.05	119.38
3	A	1911	ERG	C4-C5-C10	2.74	119.93	116.42
3	A	1916	ERG	C13-C17-C20	-2.72	116.12	119.38
3	A	1902	ERG	C17-C20-C22	-2.71	105.16	110.49
3	A	1905	ERG	O1-C3-C4	2.71	115.81	109.71
3	A	1917	ERG	C13-C14-C8	-2.70	108.83	113.59
3	A	1911	ERG	C11-C9-C10	-2.67	107.23	113.65
3	A	1904	ERG	C13-C17-C20	-2.67	116.18	119.38
3	A	1912	ERG	C14-C13-C17	2.66	102.50	99.72
4	A	1921	A1E06	C12-C5-C2	2.65	114.78	111.14
3	A	1917	ERG	C13-C17-C20	-2.65	116.20	119.38
3	A	1902	ERG	C3-C4-C5	-2.64	107.85	112.05
3	A	1909	ERG	C1-C10-C5	-2.60	104.26	108.74
3	A	1901	ERG	C24-C23-C22	-2.58	117.99	125.81
3	A	1913	ERG	C3-C4-C5	-2.58	107.94	112.05
3	A	1902	ERG	C24-C23-C22	-2.58	118.01	125.81
3	A	1917	ERG	C3-C4-C5	-2.56	107.97	112.05
3	A	1913	ERG	C14-C13-C17	2.56	102.39	99.72
3	A	1909	ERG	C27-C25-C26	2.56	117.61	110.58
3	A	1916	ERG	C13-C14-C8	-2.54	109.10	113.59
3	A	1907	ERG	C9-C10-C5	2.54	113.71	109.66
3	A	1905	ERG	C13-C17-C20	-2.53	116.35	119.38
3	A	1909	ERG	C13-C14-C8	-2.51	109.16	113.59
3	A	1912	ERG	O1-C3-C4	2.51	115.36	109.71
3	A	1904	ERG	C14-C13-C17	2.50	102.34	99.72
3	A	1904	ERG	C3-C4-C5	-2.48	108.11	112.05
3	A	1910	ERG	C11-C9-C8	-2.46	105.88	111.28
3	A	1903	ERG	C14-C13-C17	2.44	102.27	99.72
3	A	1908	ERG	C9-C10-C5	2.38	113.45	109.66
3	A	1906	ERG	C9-C10-C5	2.37	113.44	109.66
3	A	1915	ERG	C20-C22-C23	-2.37	118.64	125.81
3	A	1905	ERG	C17-C20-C22	-2.35	105.87	110.49
3	A	1916	ERG	C3-C4-C5	-2.34	108.32	112.05
3	A	1912	ERG	O1-C3-C2	2.34	116.28	110.17
3	A	1902	ERG	C11-C9-C8	-2.34	106.14	111.28
3	A	1911	ERG	C14-C13-C17	2.31	102.13	99.72
3	A	1918	ERG	C9-C10-C5	2.31	113.33	109.66
3	A	1919	ERG	C9-C10-C5	2.30	113.33	109.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1912	ERG	C3-C4-C5	-2.29	108.40	112.05
3	A	1909	ERG	C11-C9-C8	-2.28	106.27	111.28
3	A	1910	ERG	C15-C14-C13	-2.25	102.19	104.21
3	A	1909	ERG	C24-C23-C22	-2.24	119.02	125.81
3	A	1910	ERG	C16-C15-C14	-2.24	101.60	105.25
3	A	1910	ERG	C24-C23-C22	-2.24	119.04	125.81
3	A	1916	ERG	C20-C22-C23	-2.22	119.10	125.81
3	A	1920	ERG	C9-C10-C5	2.22	113.19	109.66
3	A	1912	ERG	C25-C24-C23	-2.21	105.35	112.02
3	A	1901	ERG	C11-C9-C8	-2.17	106.51	111.28
3	A	1913	ERG	C20-C22-C23	-2.17	119.26	125.81
3	A	1904	ERG	C20-C22-C23	-2.17	119.26	125.81
3	A	1905	ERG	O1-C3-C2	2.16	115.82	110.17
3	A	1914	ERG	C14-C13-C17	2.16	101.98	99.72
3	A	1914	ERG	C20-C22-C23	-2.16	119.28	125.81
3	A	1911	ERG	C24-C23-C22	-2.15	119.31	125.81
3	A	1909	ERG	C19-C10-C1	-2.13	106.19	109.43
3	A	1902	ERG	C16-C15-C14	-2.13	101.77	105.25
3	A	1909	ERG	C15-C14-C13	-2.13	102.31	104.21
3	A	1905	ERG	C4-C5-C10	2.12	119.13	116.42
3	A	1903	ERG	C24-C23-C22	-2.11	119.43	125.81
3	A	1916	ERG	C24-C23-C22	-2.10	119.46	125.81
3	A	1905	ERG	C20-C22-C23	-2.10	119.46	125.81
3	A	1912	ERG	C24-C23-C22	-2.09	119.50	125.81
3	A	1902	ERG	C13-C14-C8	-2.08	109.92	113.59
3	A	1904	ERG	C11-C12-C13	-2.06	109.26	112.74
4	A	1921	A1E06	C22-C3-C14	-2.06	103.76	107.10
3	A	1911	ERG	C20-C22-C23	-2.05	119.62	125.81
3	A	1903	ERG	C20-C22-C23	-2.03	119.66	125.81
4	A	1921	A1E06	C3-C8-C9	-2.03	116.62	118.01
3	A	1904	ERG	C24-C23-C22	-2.03	119.68	125.81
3	A	1917	ERG	C14-C13-C17	2.03	101.84	99.72
3	A	1912	ERG	C4-C5-C10	2.02	119.01	116.42
3	A	1915	ERG	C24-C23-C22	-2.01	119.74	125.81

There are no chirality outliers.

All (73) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1906	ERG	C22-C23-C24-C25
3	A	1908	ERG	C22-C23-C24-C25
3	A	1909	ERG	C23-C24-C25-C27

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Mol	Chain	Res	Type	Atoms
3	A	1909	ERG	C28-C24-C25-C27
3	A	1910	ERG	C13-C17-C20-C21
3	A	1910	ERG	C16-C17-C20-C21
3	A	1910	ERG	C16-C17-C20-C22
3	A	1913	ERG	C22-C23-C24-C25
3	A	1918	ERG	C20-C22-C23-C24
3	A	1919	ERG	C20-C22-C23-C24
5	A	1922	POV	C1-O11-P-O14
5	A	1922	POV	O21-C2-C3-O31
4	A	1921	A1E06	O7-C29-O2-C16
3	A	1919	ERG	C22-C23-C24-C28
3	A	1920	ERG	C22-C23-C24-C28
4	A	1921	A1E06	C33-C29-O2-C16
3	A	1908	ERG	C17-C20-C22-C23
3	A	1910	ERG	C17-C20-C22-C23
3	A	1915	ERG	C22-C23-C24-C25
3	A	1919	ERG	C22-C23-C24-C25
3	A	1920	ERG	C22-C23-C24-C25
3	A	1915	ERG	C22-C23-C24-C28
3	A	1906	ERG	C21-C20-C22-C23
3	A	1909	ERG	C21-C20-C22-C23
3	A	1910	ERG	C21-C20-C22-C23
3	A	1920	ERG	C20-C22-C23-C24
3	A	1909	ERG	C16-C17-C20-C22
3	A	1910	ERG	C13-C17-C20-C22
3	A	1906	ERG	C17-C20-C22-C23
3	A	1905	ERG	C22-C23-C24-C28
3	A	1917	ERG	C22-C23-C24-C28
3	A	1918	ERG	C22-C23-C24-C28
5	A	1922	POV	C22-C21-O21-C2
5	A	1922	POV	O22-C21-O21-C2
3	A	1902	ERG	C17-C20-C22-C23
3	A	1909	ERG	C17-C20-C22-C23
3	A	1916	ERG	C22-C23-C24-C25
3	A	1918	ERG	C22-C23-C24-C25
4	A	1921	A1E06	O7-C35-C38-O12
5	A	1922	POV	C1-C2-C3-O31
3	A	1906	ERG	C22-C23-C24-C28
3	A	1901	ERG	C22-C23-C24-C28
5	A	1922	POV	C24-C25-C26-C27
3	A	1910	ERG	C22-C23-C24-C28
3	A	1912	ERG	C21-C20-C22-C23

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Mol	Chain	Res	Type	Atoms
3	A	1917	ERG	C21-C20-C22-C23
3	A	1908	ERG	C21-C20-C22-C23
3	A	1917	ERG	C22-C23-C24-C25
5	A	1922	POV	C34-C35-C36-C37
3	A	1901	ERG	C22-C23-C24-C25
3	A	1905	ERG	C22-C23-C24-C25
5	A	1922	POV	C1-O11-P-O12
3	A	1909	ERG	C23-C24-C25-C26
5	A	1922	POV	C213-C214-C215-C216
5	A	1922	POV	O32-C31-O31-C3
5	A	1922	POV	C32-C31-O31-C3
3	A	1910	ERG	C22-C23-C24-C25
3	A	1917	ERG	C17-C20-C22-C23
3	A	1910	ERG	C23-C24-C25-C26
3	A	1918	ERG	C23-C24-C25-C27
3	A	1913	ERG	C22-C23-C24-C28
3	A	1912	ERG	C17-C20-C22-C23
5	A	1922	POV	C37-C38-C39-C310
3	A	1911	ERG	C22-C23-C24-C28
3	A	1916	ERG	C21-C20-C22-C23
5	A	1922	POV	C26-C27-C28-C29
5	A	1922	POV	C211-C212-C213-C214
3	A	1911	ERG	C22-C23-C24-C25
3	A	1916	ERG	C17-C20-C22-C23
3	A	1908	ERG	C23-C24-C25-C27
3	A	1903	ERG	C22-C23-C24-C28
3	A	1909	ERG	C28-C24-C25-C26
3	A	1910	ERG	C23-C24-C25-C27

There are no ring outliers.

17 monomers are involved in 92 short contacts:

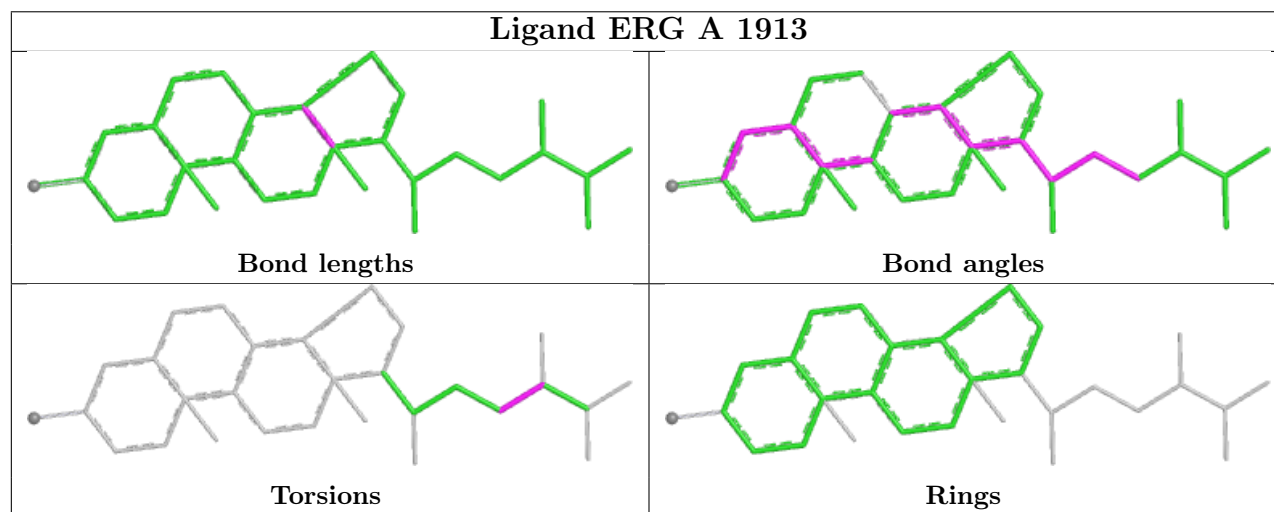
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1913	ERG	3	0
3	A	1920	ERG	7	0
3	A	1906	ERG	7	0
3	A	1908	ERG	2	0
3	A	1905	ERG	1	0
3	A	1901	ERG	8	0
3	A	1909	ERG	24	0
3	A	1902	ERG	7	0
3	A	1910	ERG	13	0

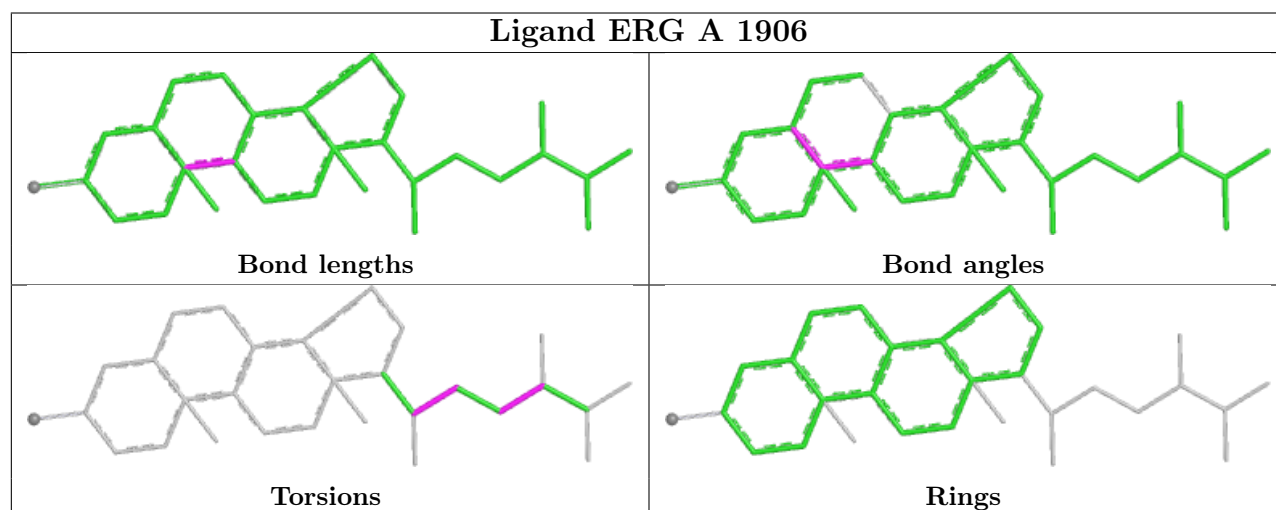
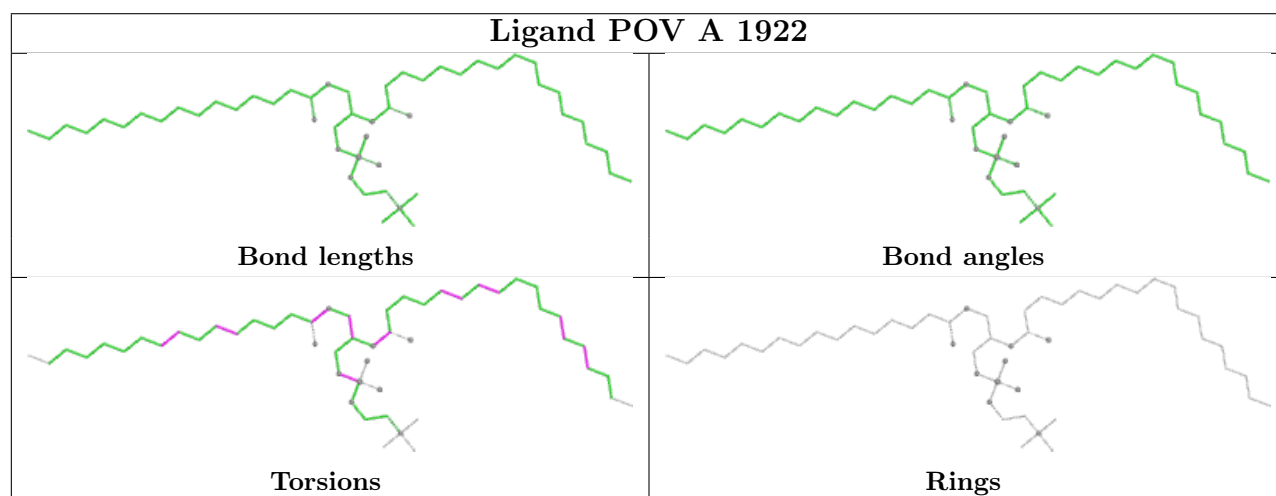
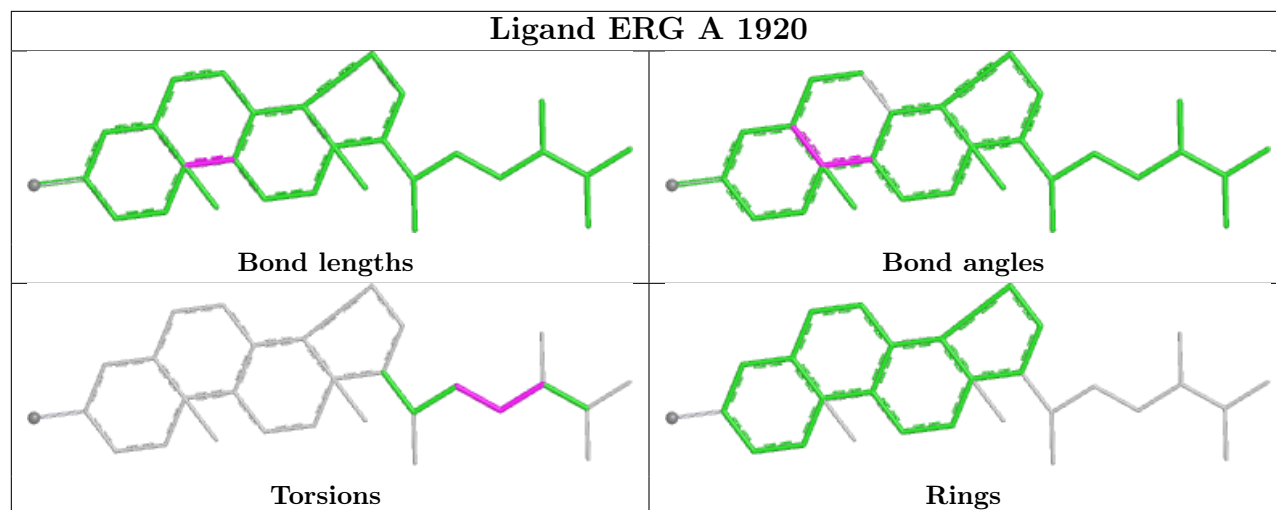
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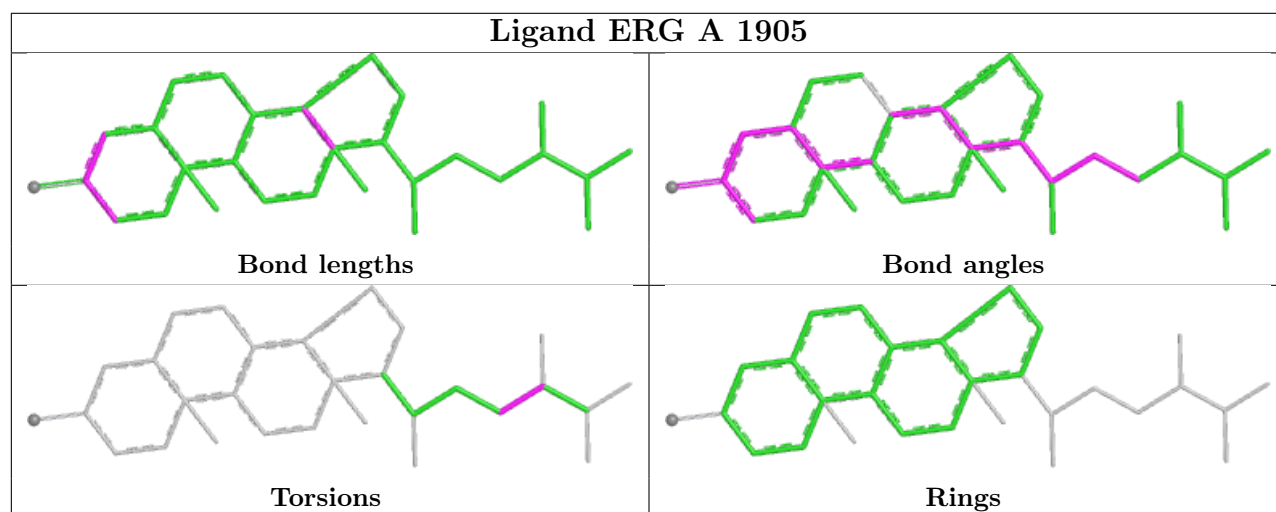
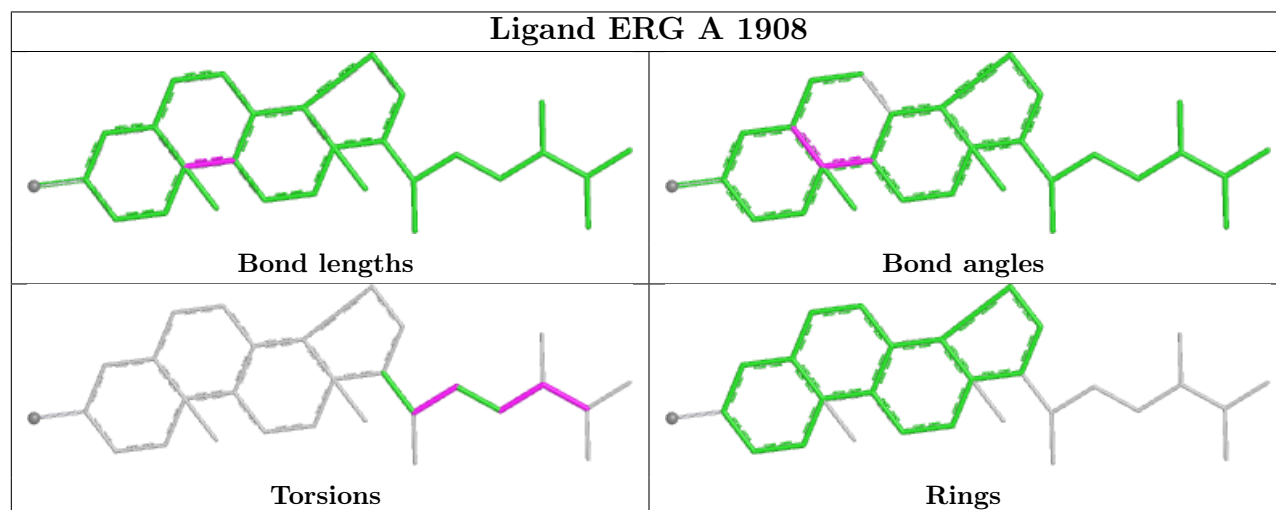
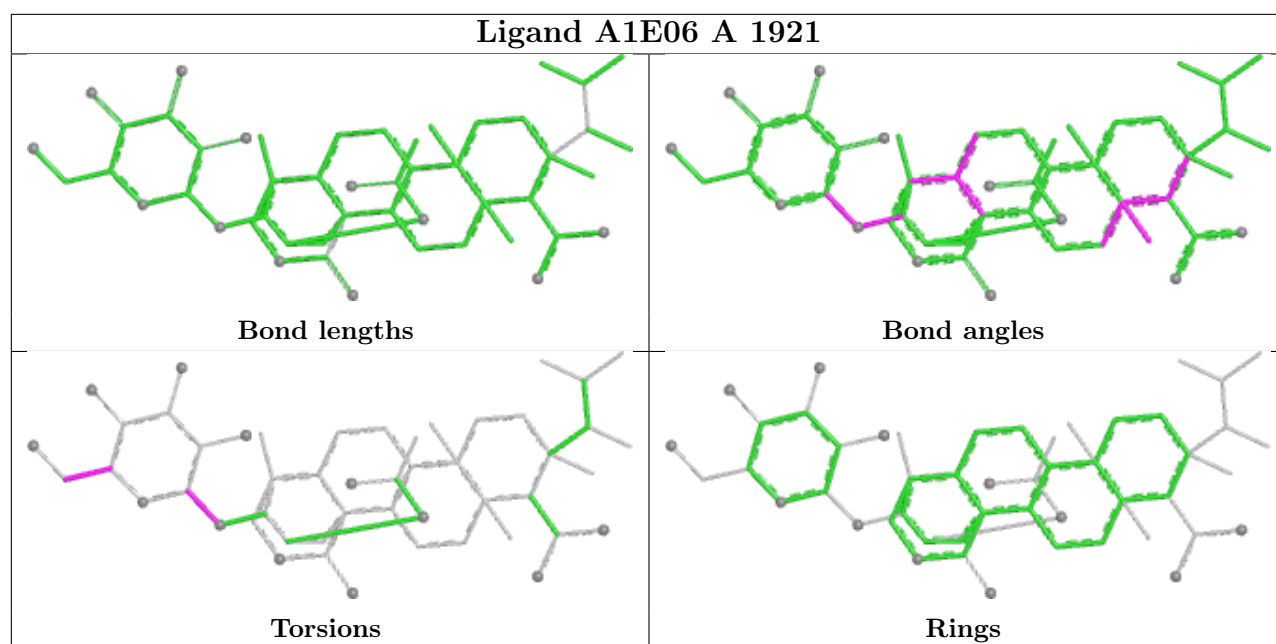
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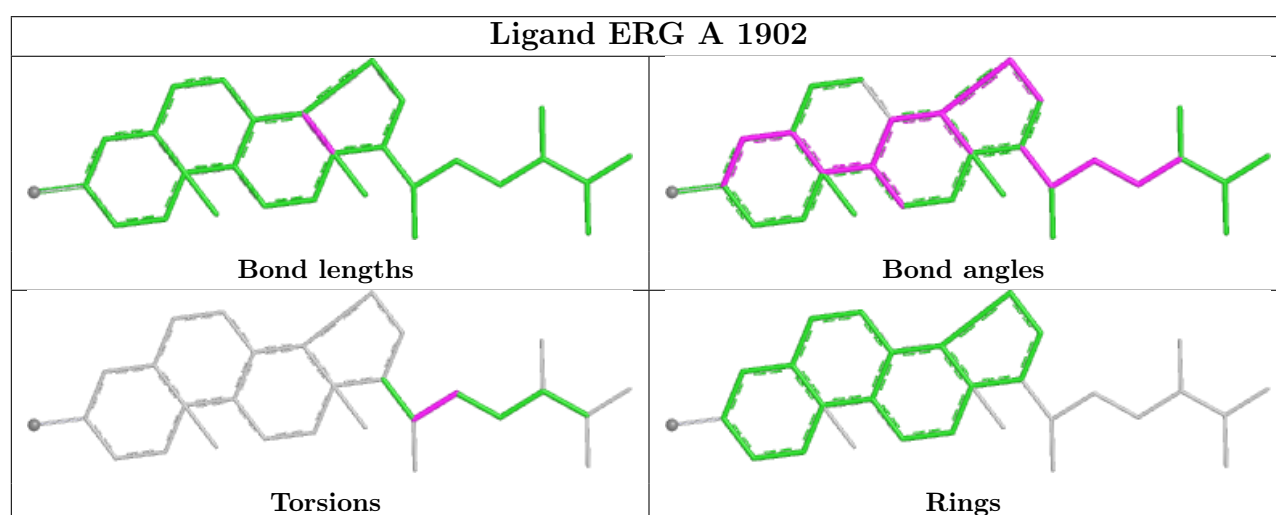
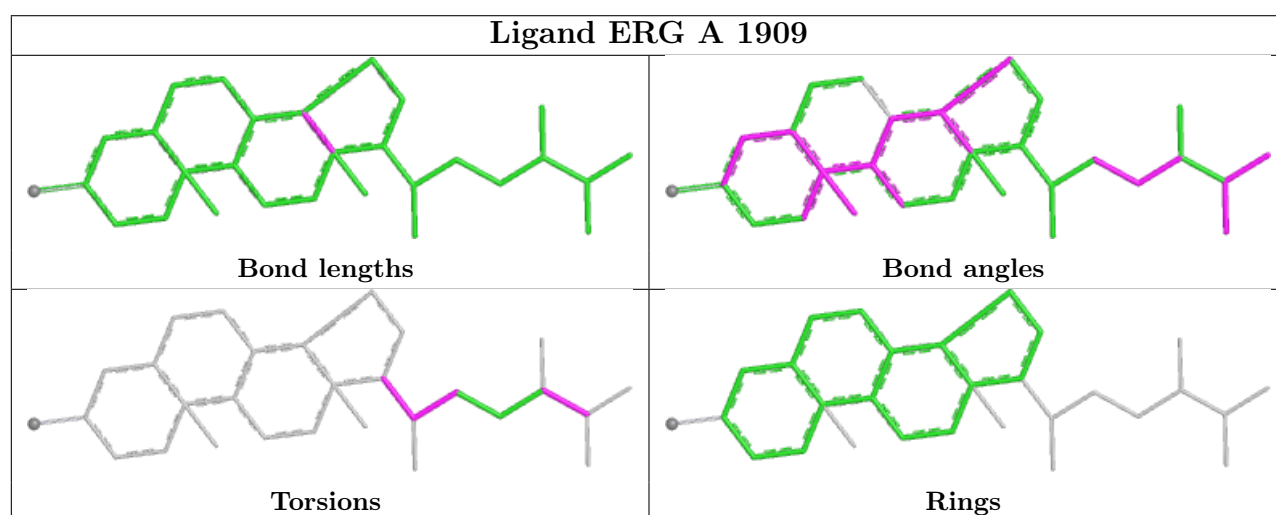
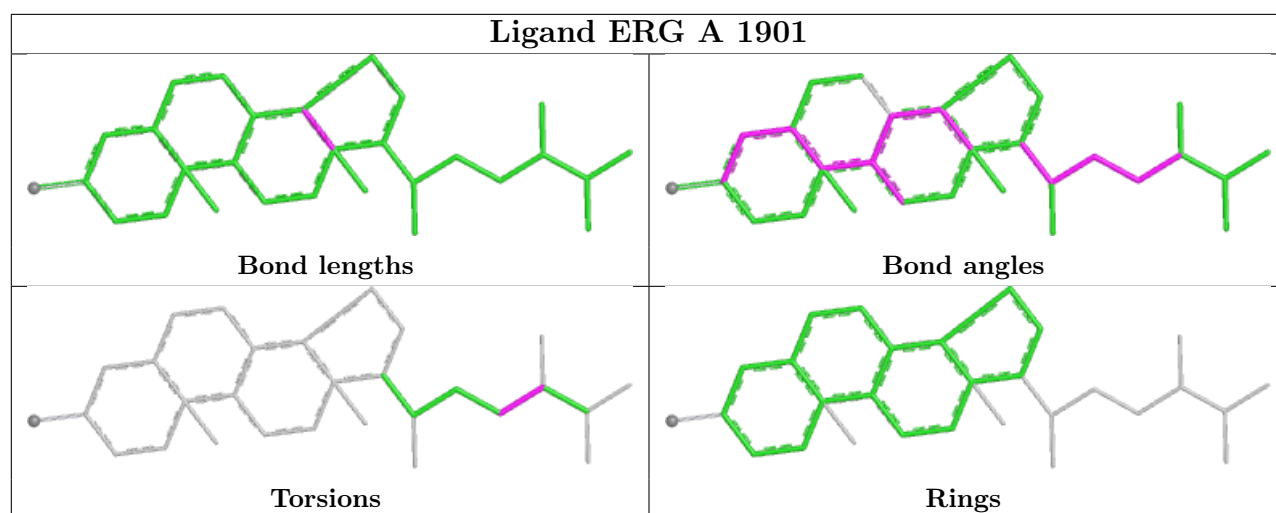
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1912	ERG	6	0
3	A	1903	ERG	8	0
3	A	1911	ERG	2	0
3	A	1904	ERG	5	0
3	A	1917	ERG	6	0
3	A	1914	ERG	2	0
3	A	1916	ERG	6	0
3	A	1919	ERG	9	0

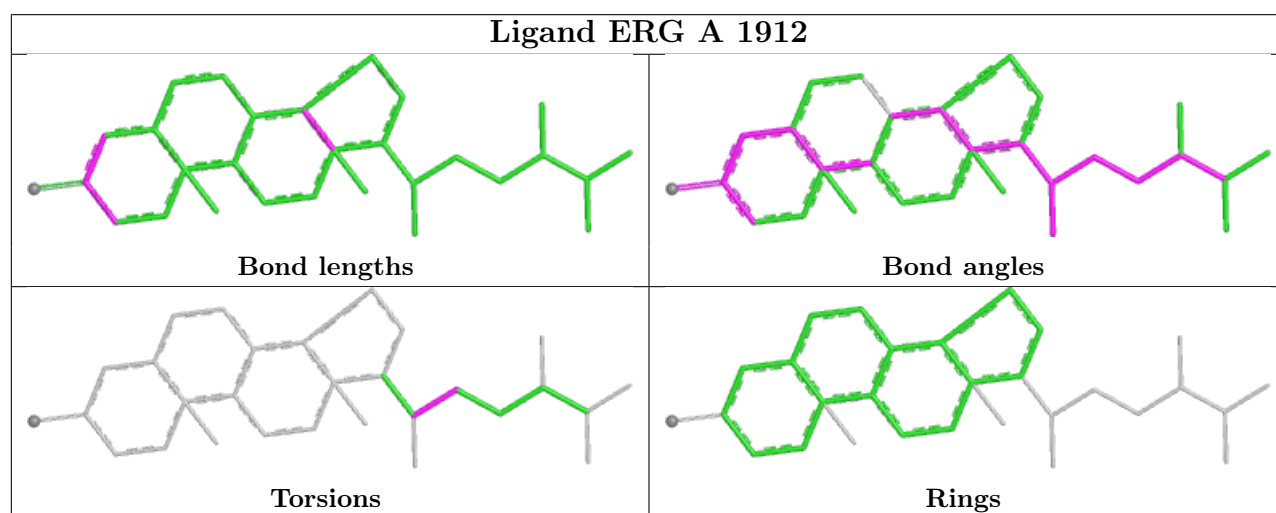
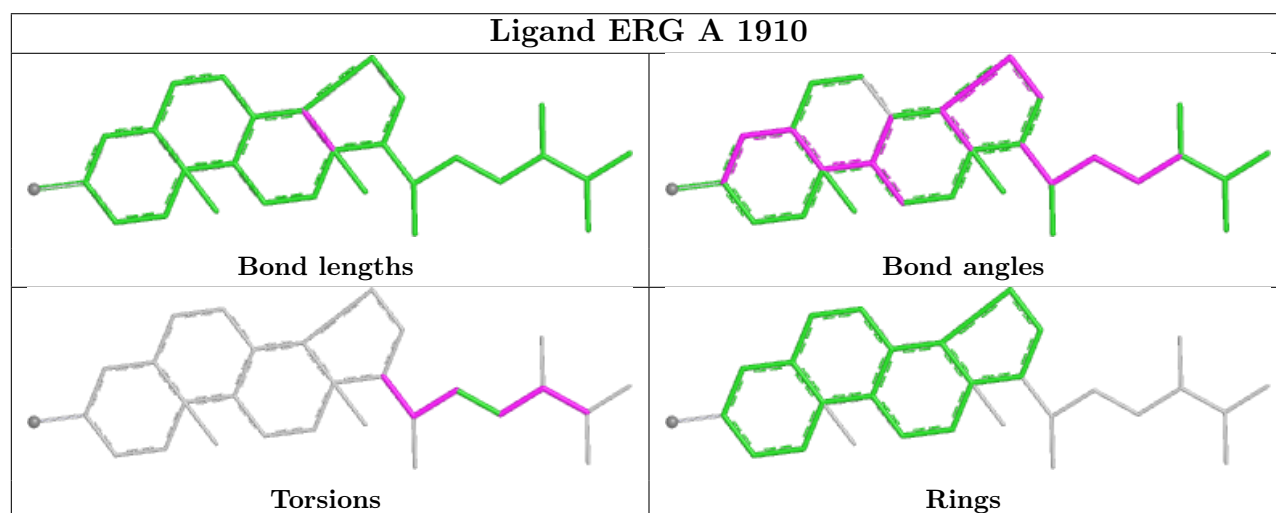
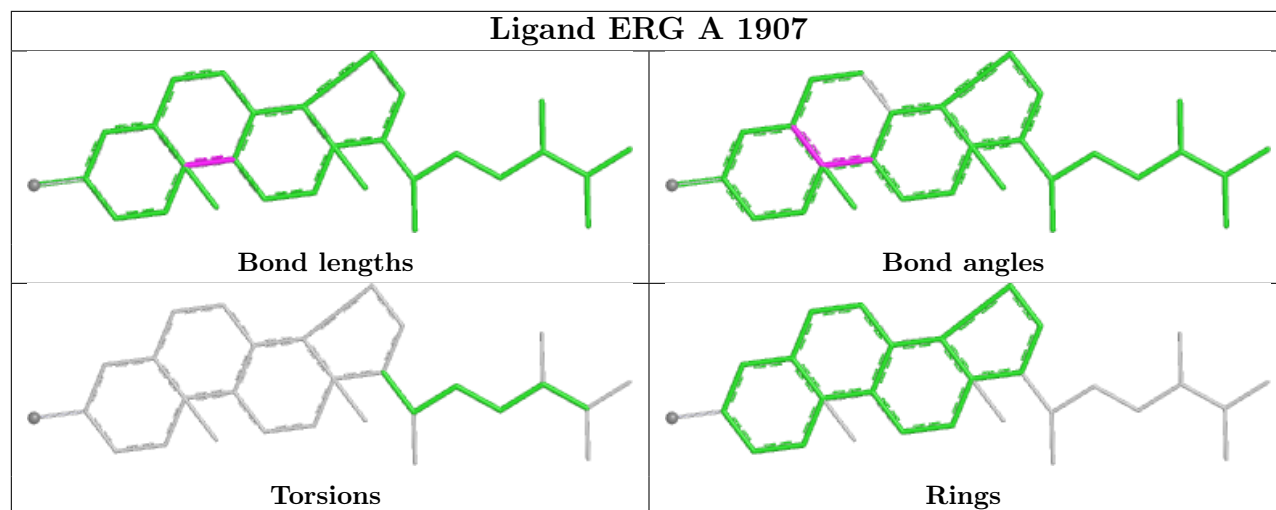
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



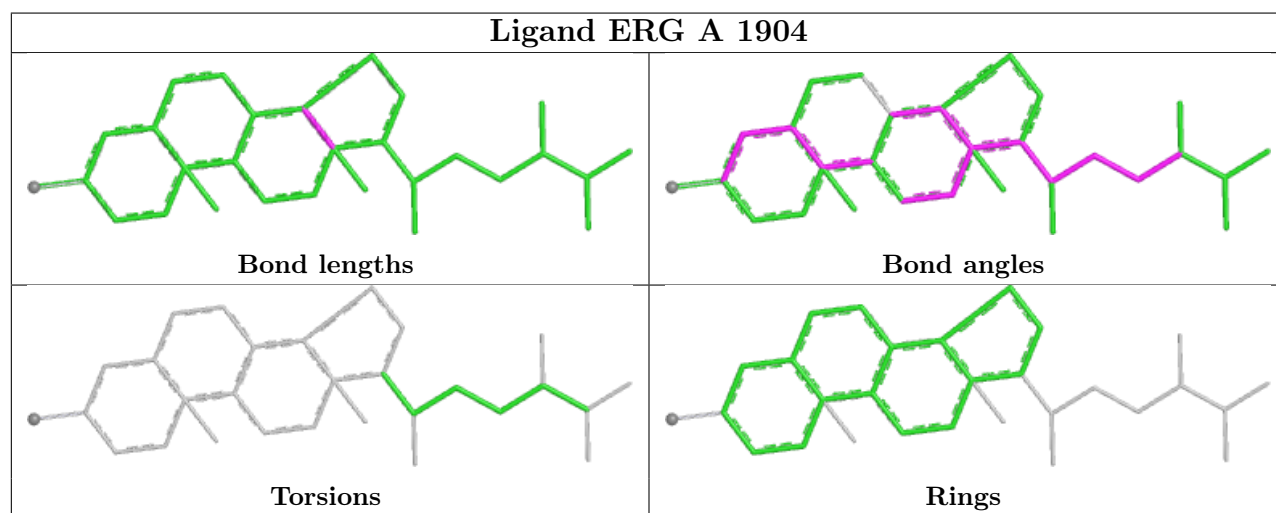
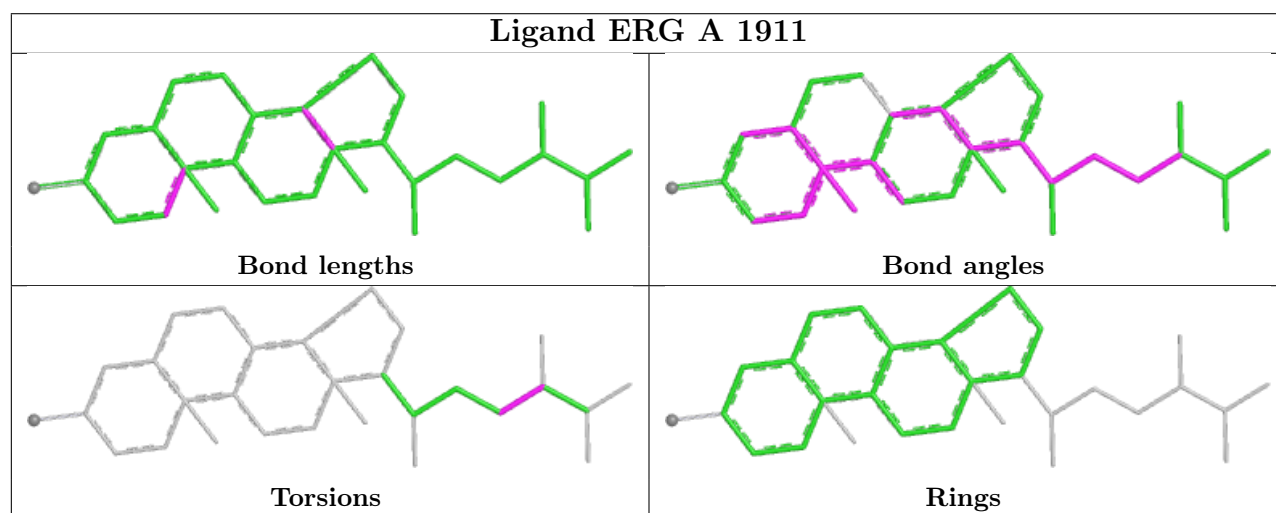
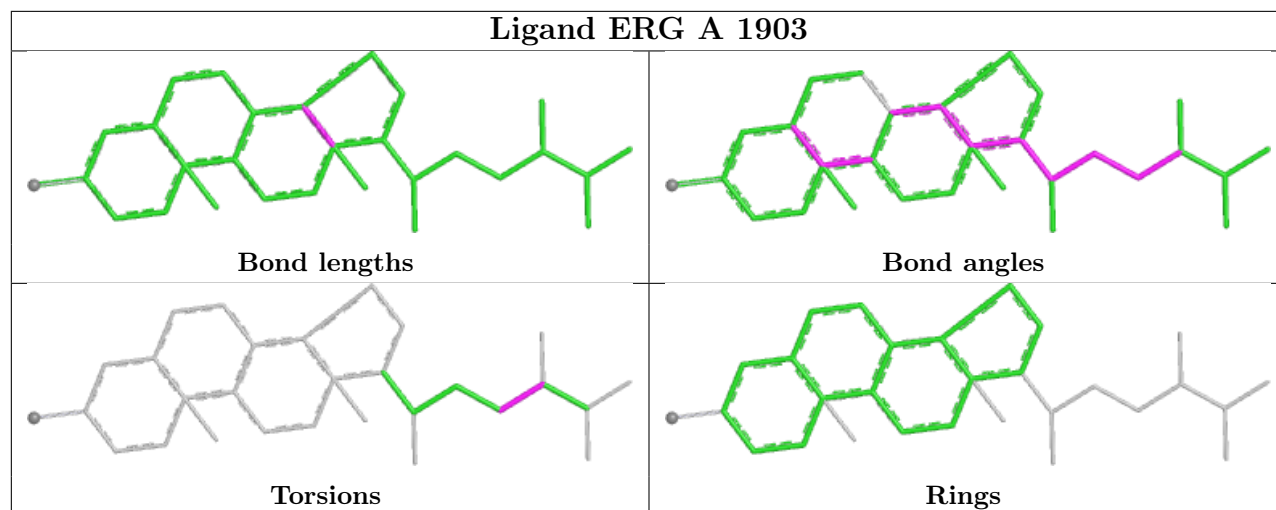


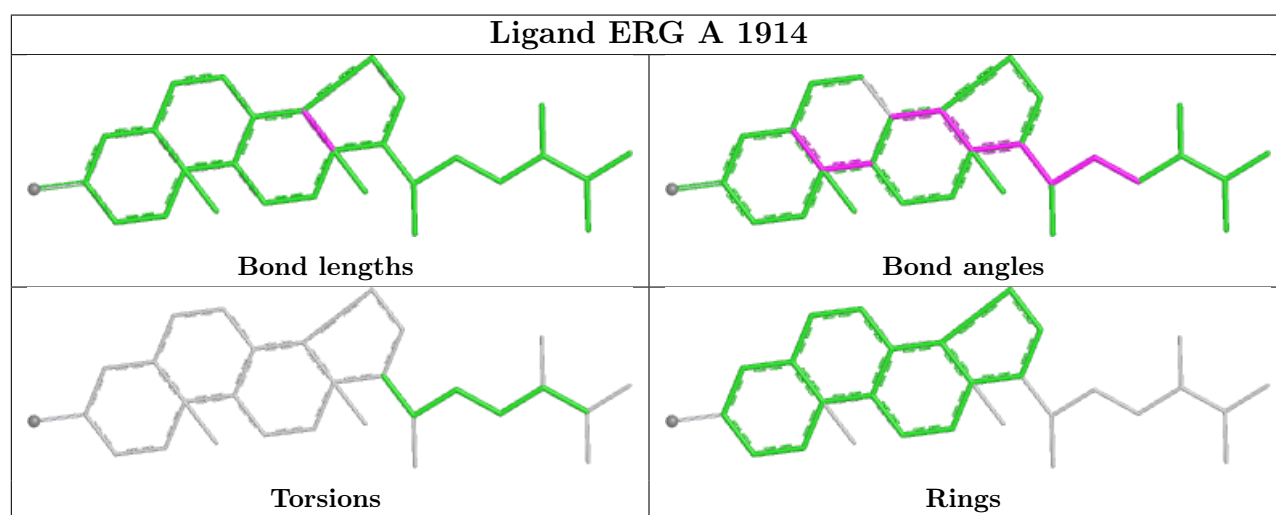
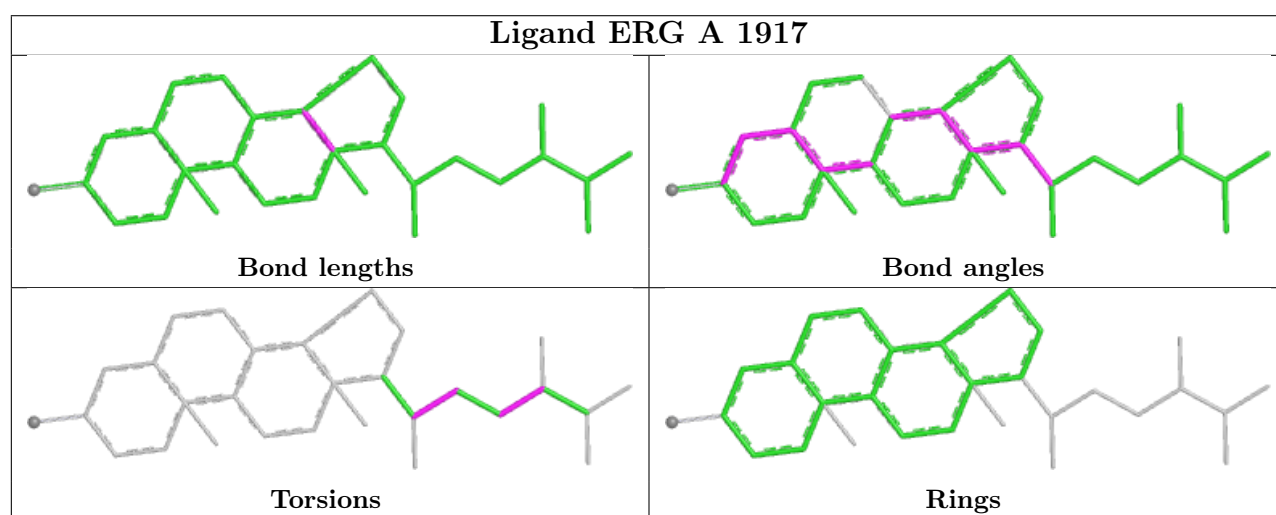
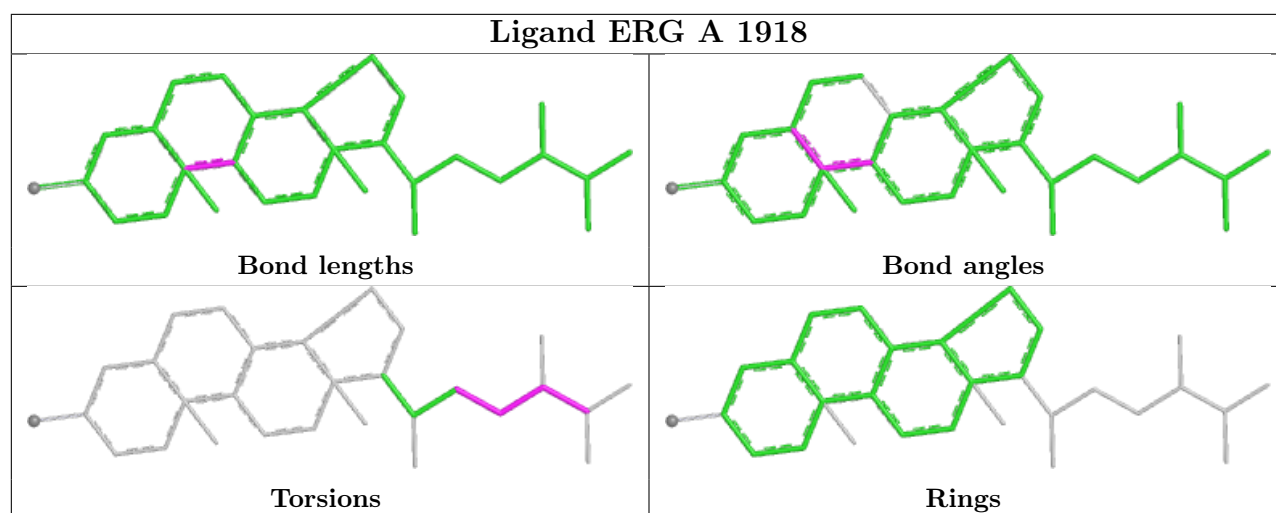


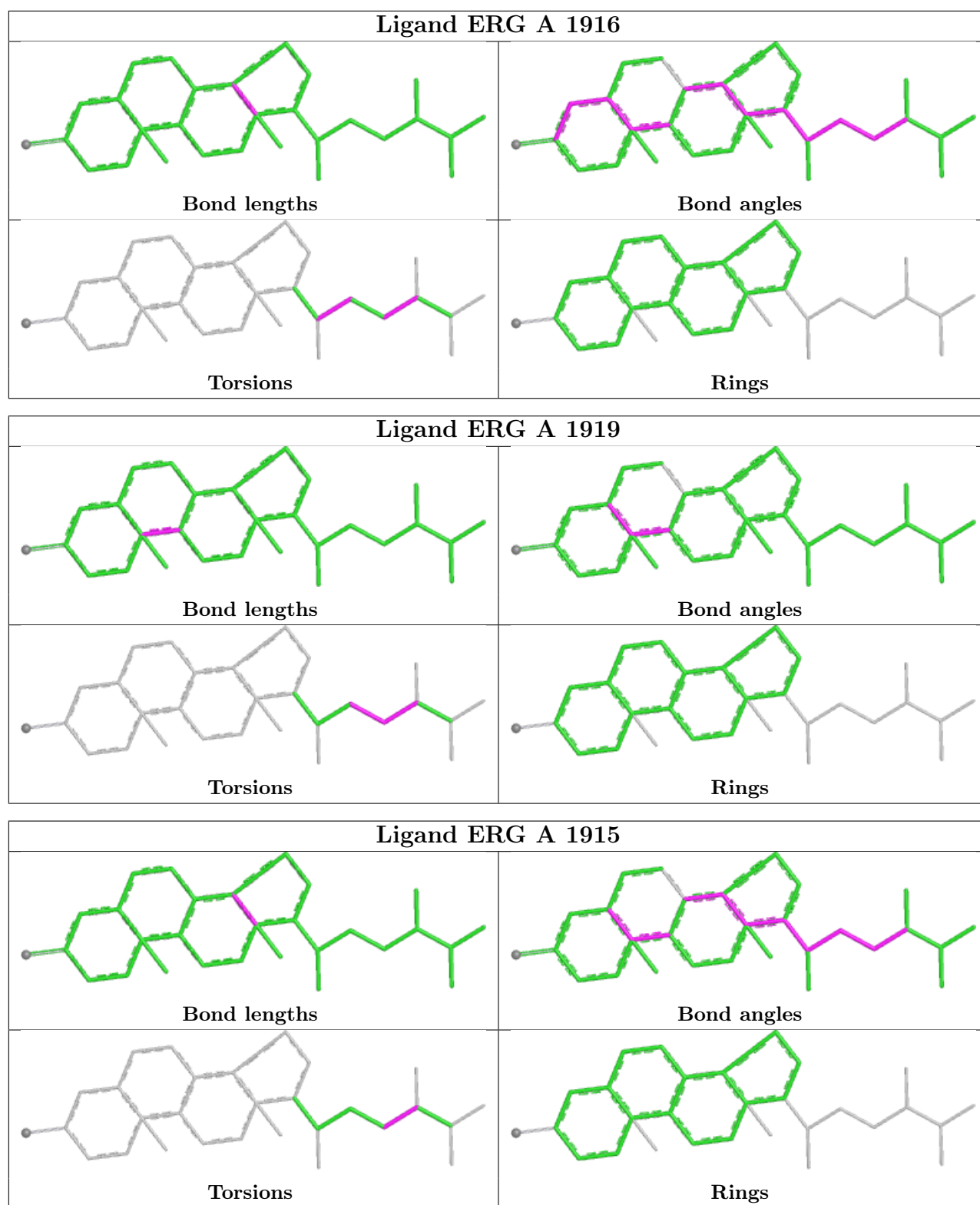












## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

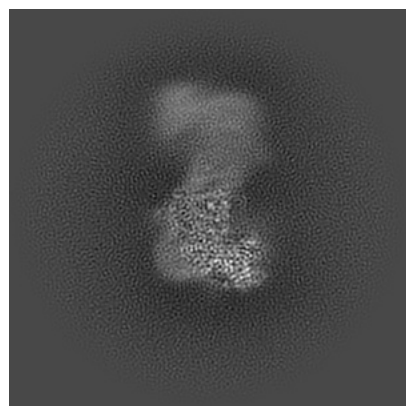
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-66419. These allow visual inspection of the internal detail of the map and identification of artifacts.

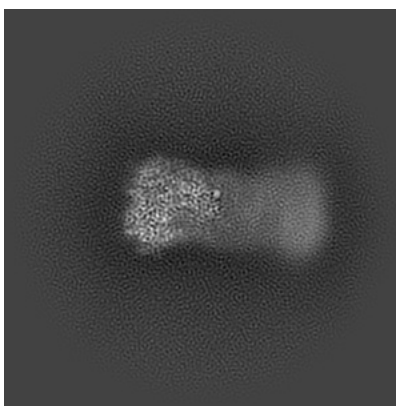
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

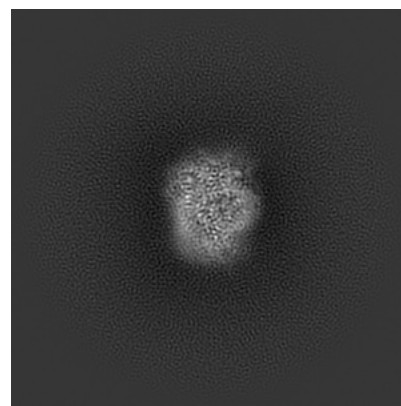
#### 6.1.1 Primary map



X

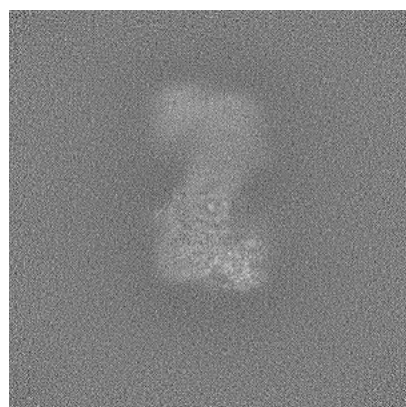


Y

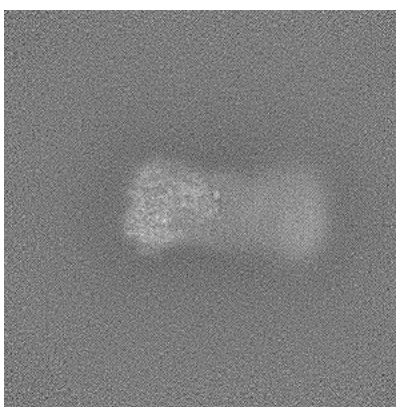


Z

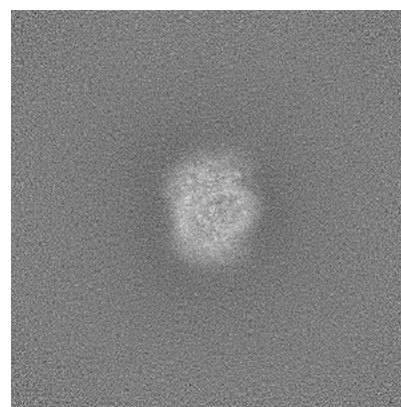
#### 6.1.2 Raw map



X



Y



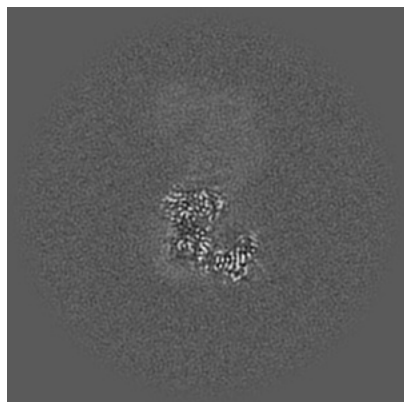
Z

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

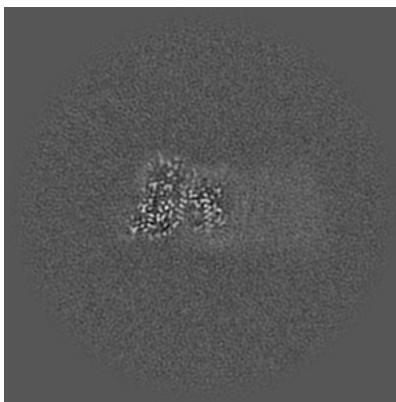


## 6.2 Central slices [i](#)

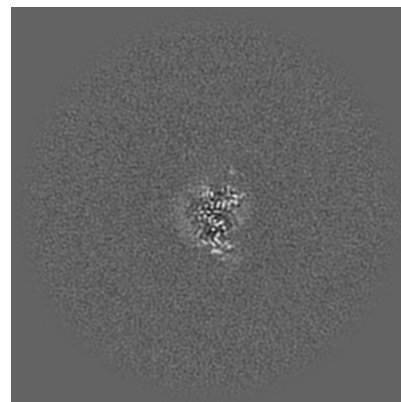
### 6.2.1 Primary map



X Index: 256

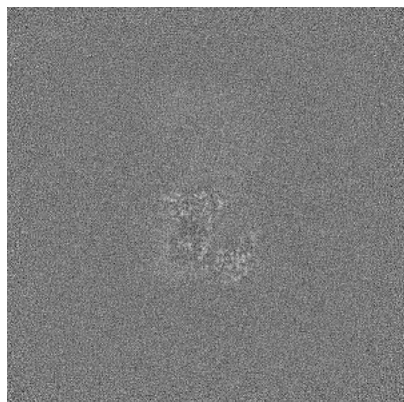


Y Index: 256

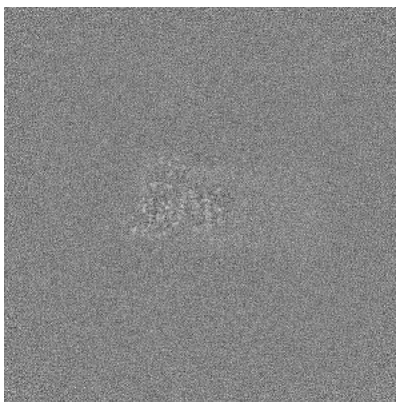


Z Index: 256

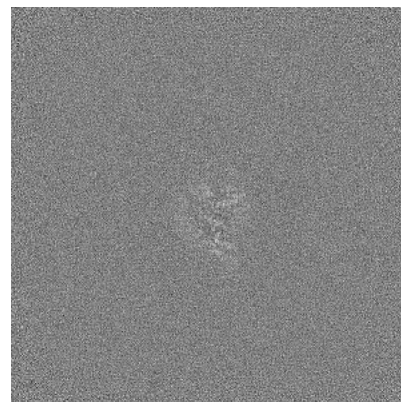
### 6.2.2 Raw map



X Index: 256



Y Index: 256

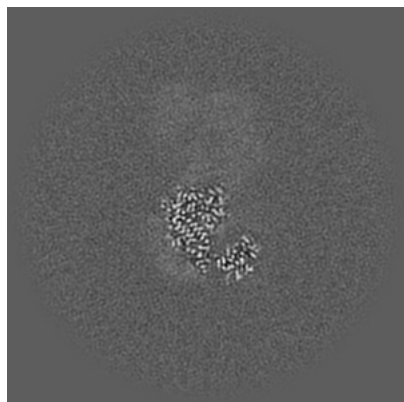


Z Index: 256

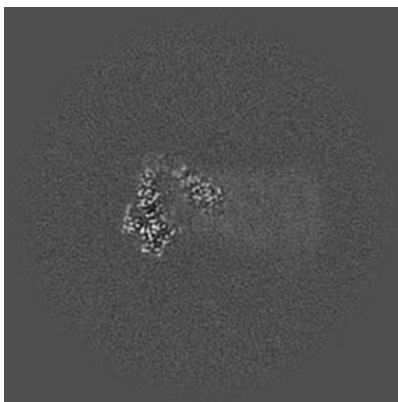
The images above show central slices of the map in three orthogonal directions.

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

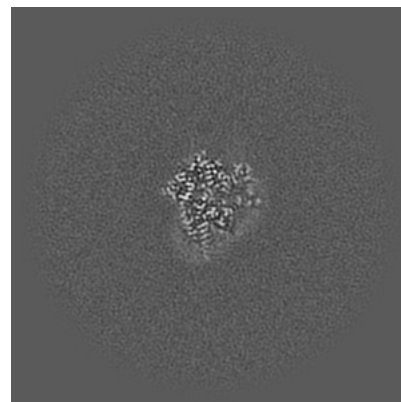
### 6.3.1 Primary map



X Index: 262

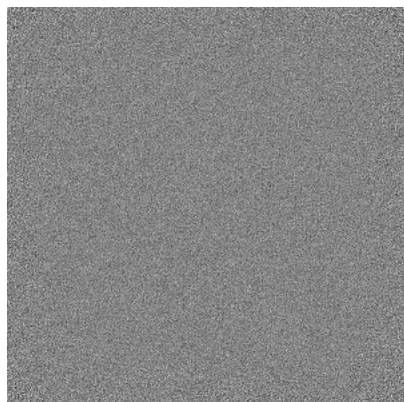


Y Index: 278

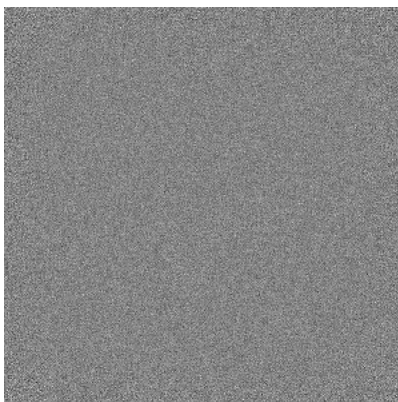


Z Index: 196

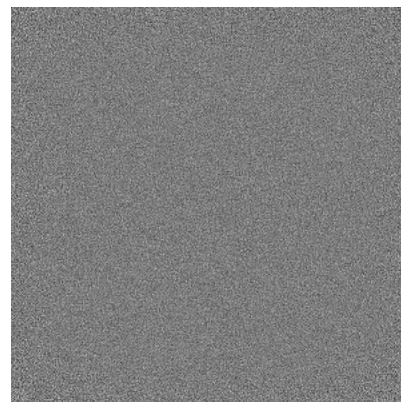
### 6.3.2 Raw map



X Index: 0



Y Index: 0

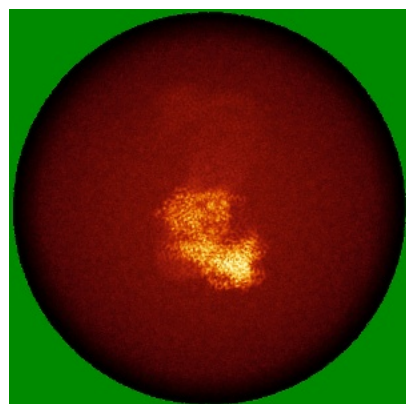


Z Index: 0

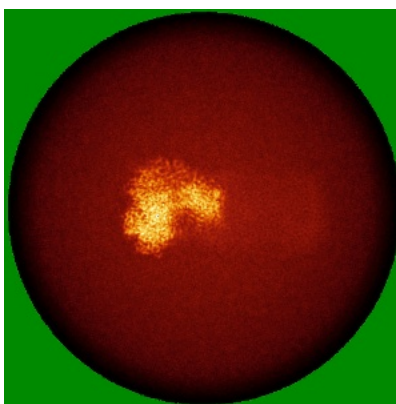
The images above show the largest variance slices of the map in three orthogonal directions.

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

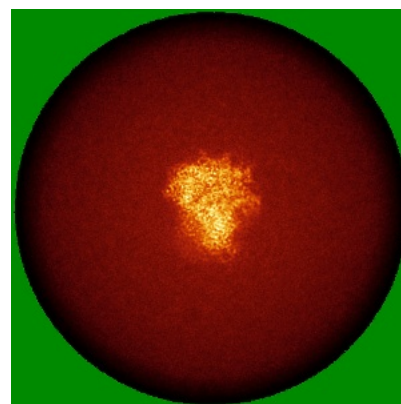
### 6.4.1 Primary map



X

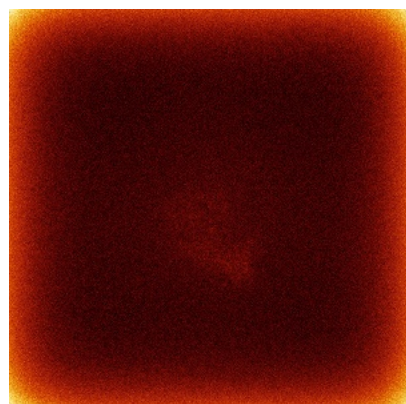


Y

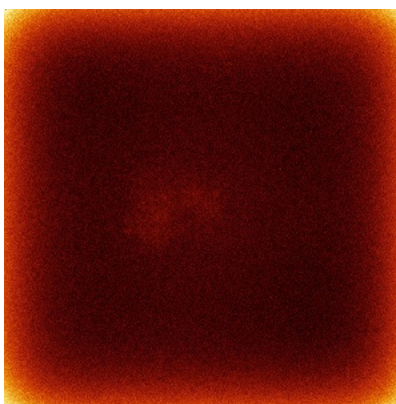


Z

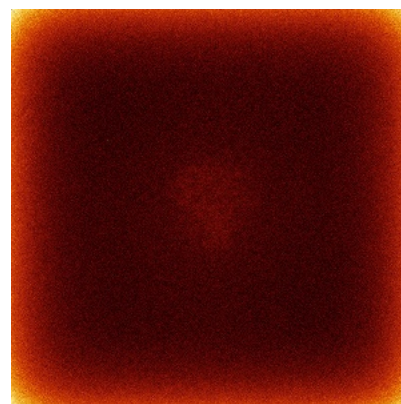
### 6.4.2 Raw map



X



Y



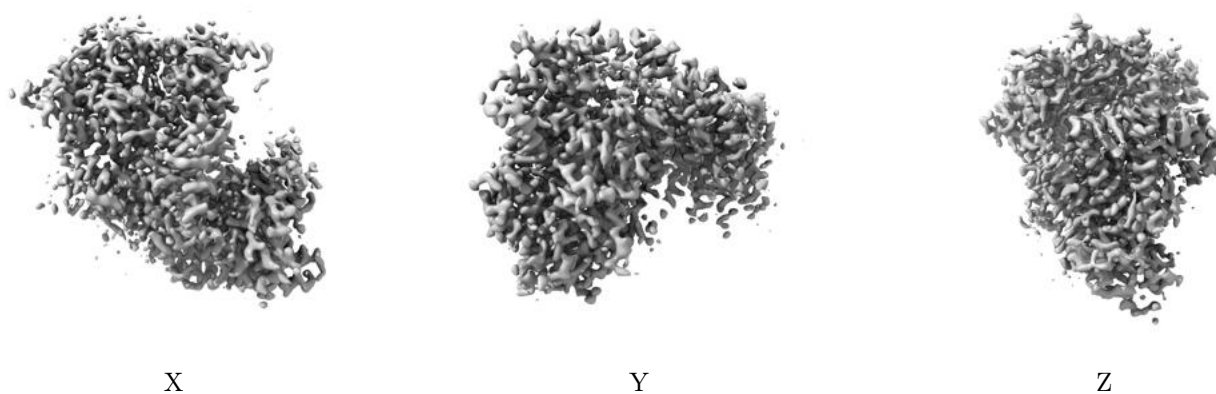
Z

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.



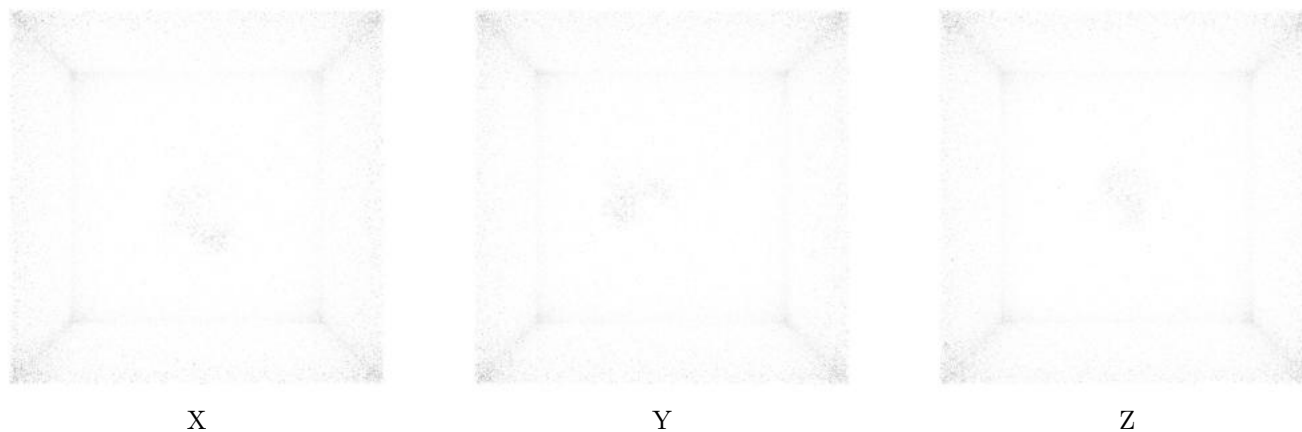
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.15. 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.

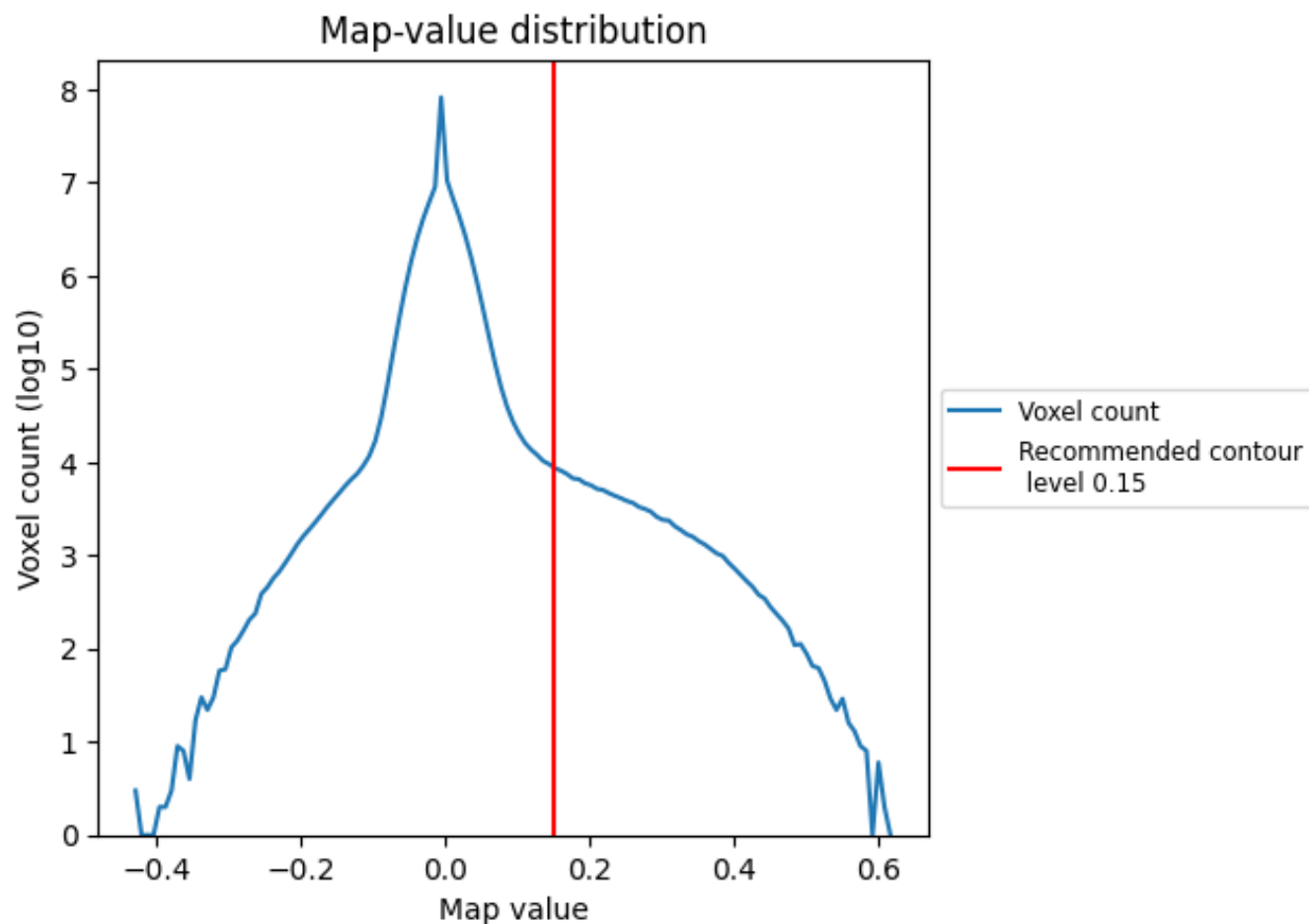
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

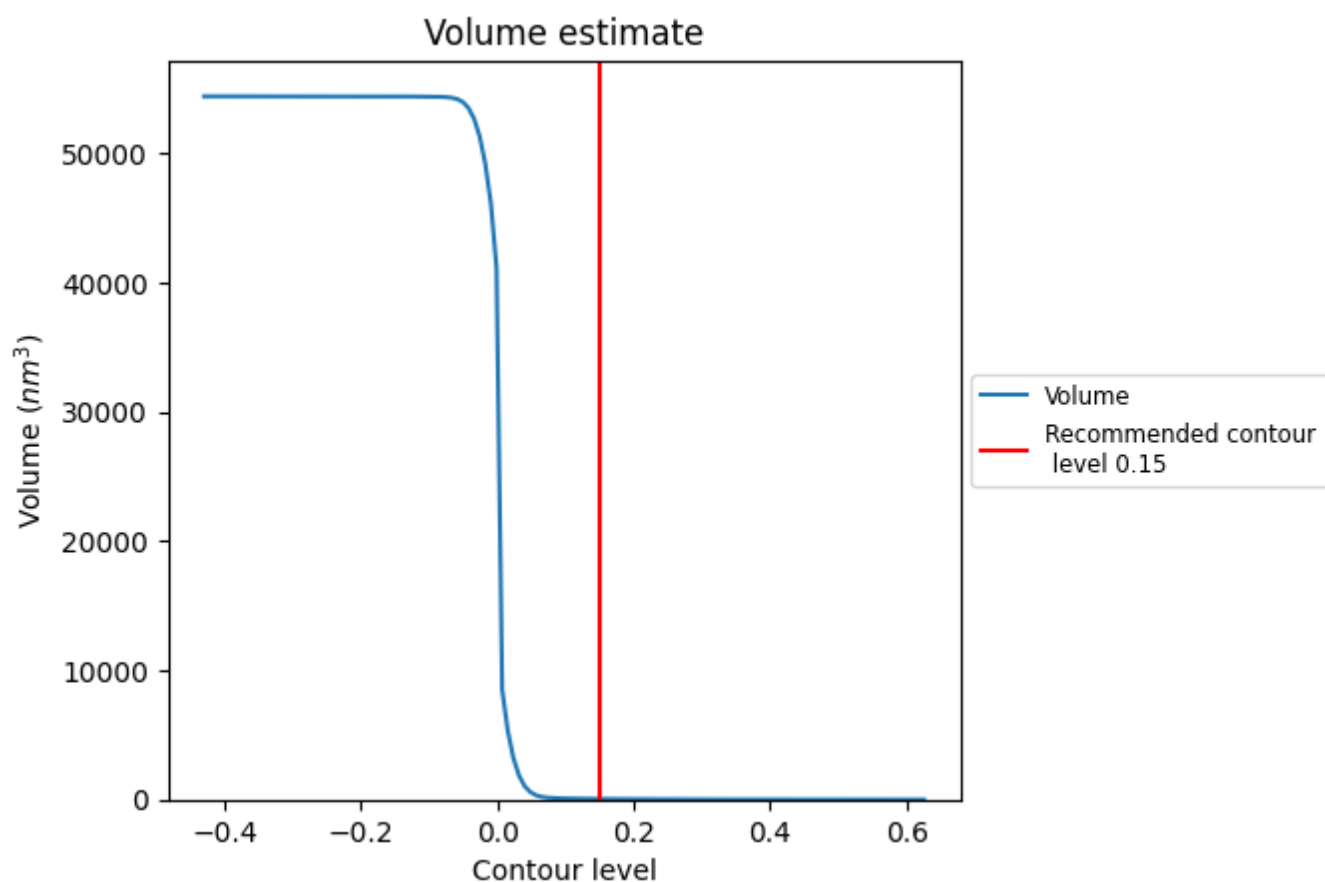
This section contains the results of statistical analysis of the map.

### 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.

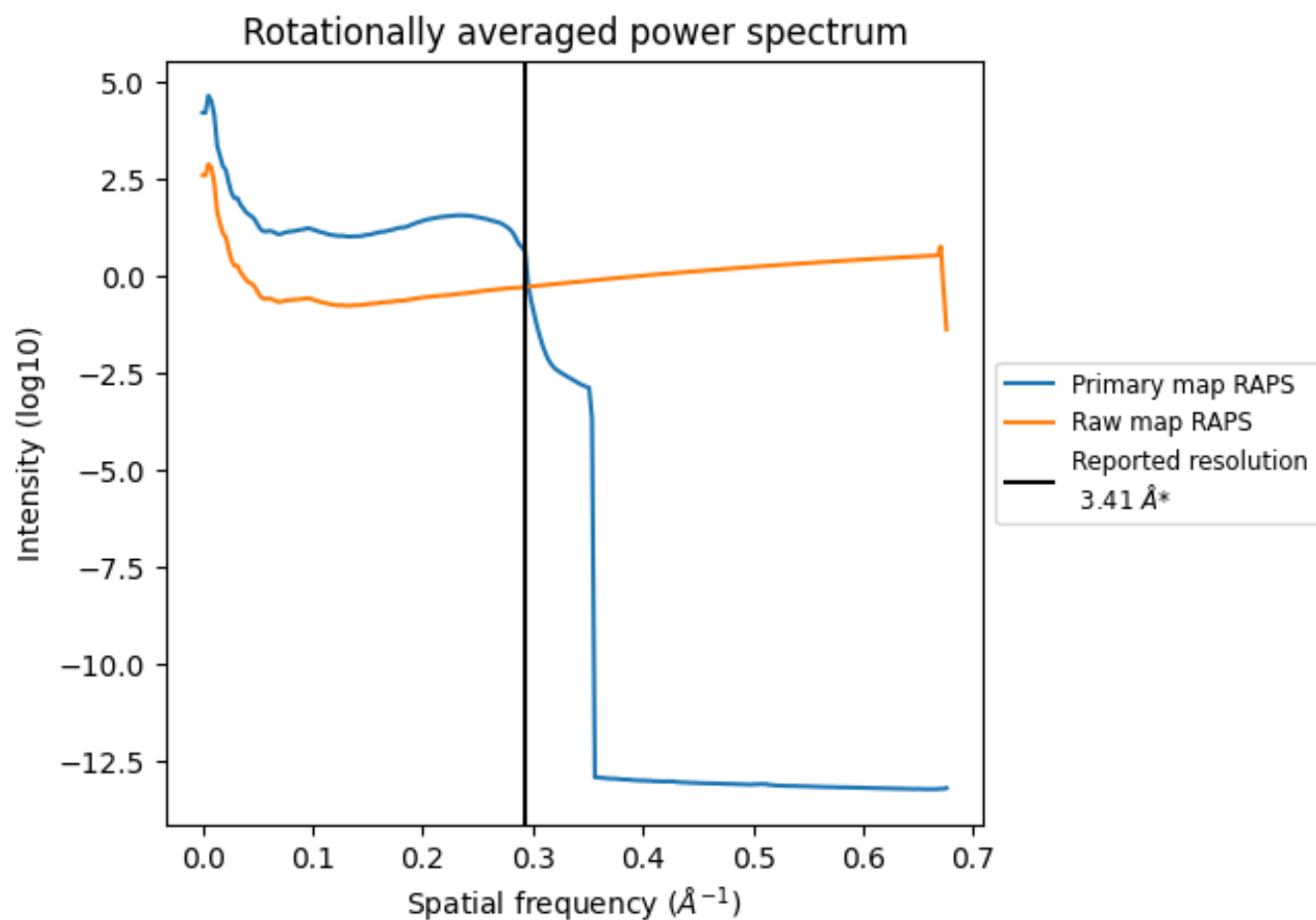
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 48 nm<sup>3</sup>; this corresponds to an approximate mass of 43 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 ⓘ

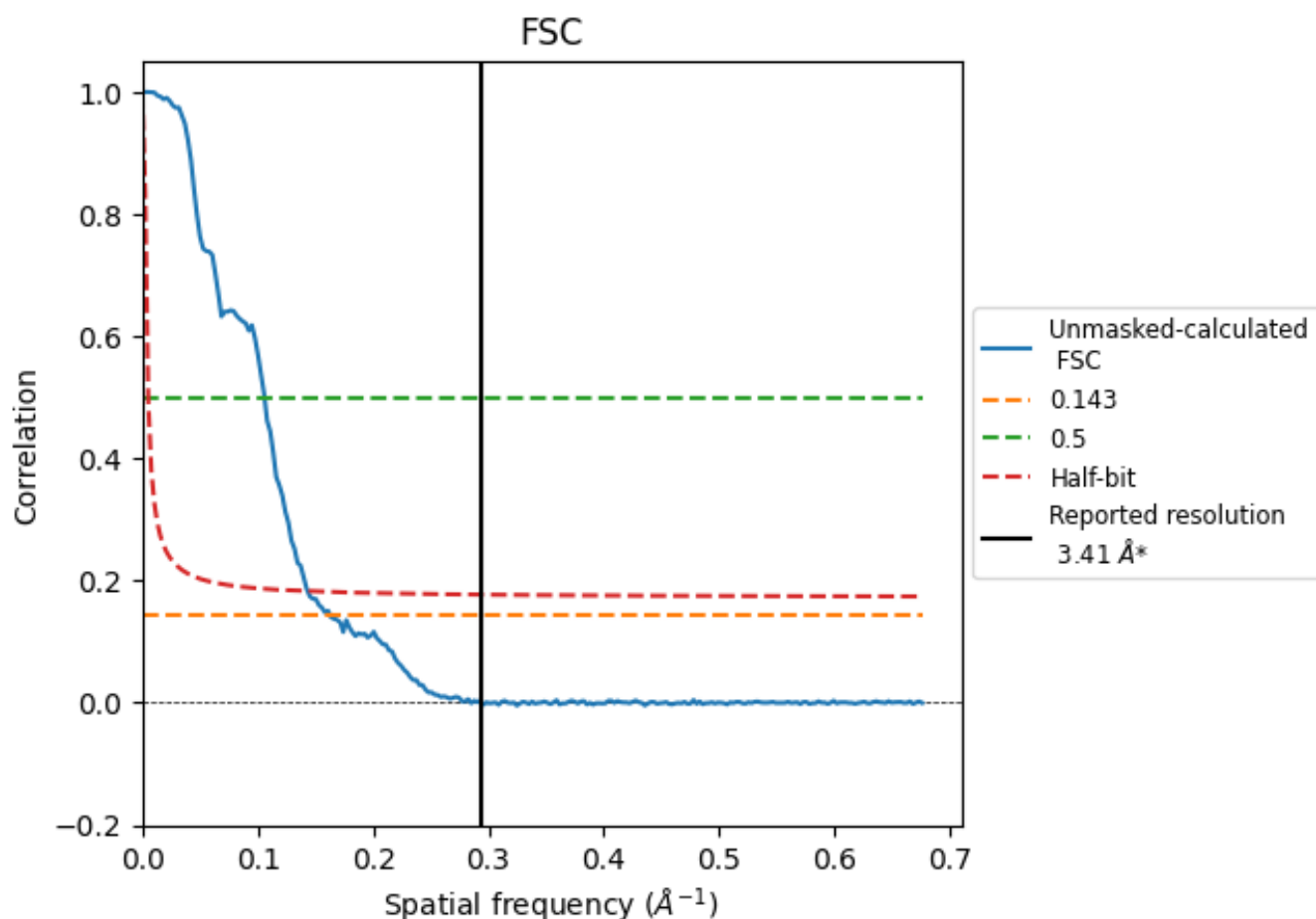


\*Reported resolution corresponds to spatial frequency of 0.293 Å<sup>-1</sup>

## 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  $0.293 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

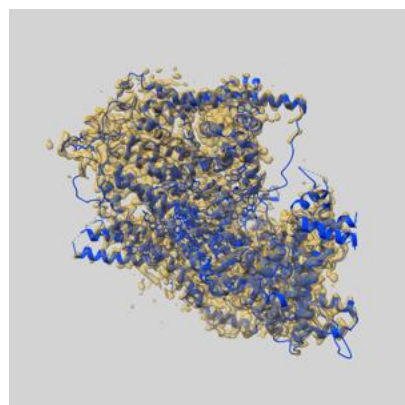
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.41	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.14	9.44	6.97

\*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 6.14 differs from the reported value 3.41 by more than 10 %

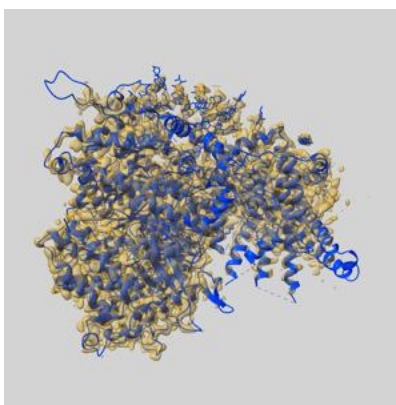
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-66419 and PDB model 9X04. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

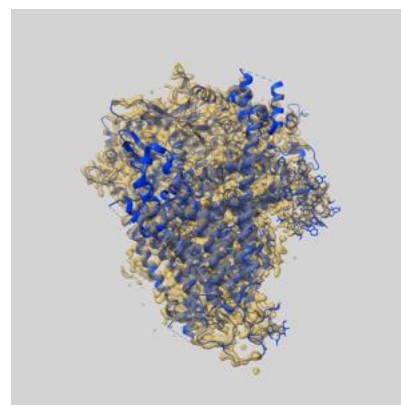
### 9.1 Map-model overlay [i](#)



X



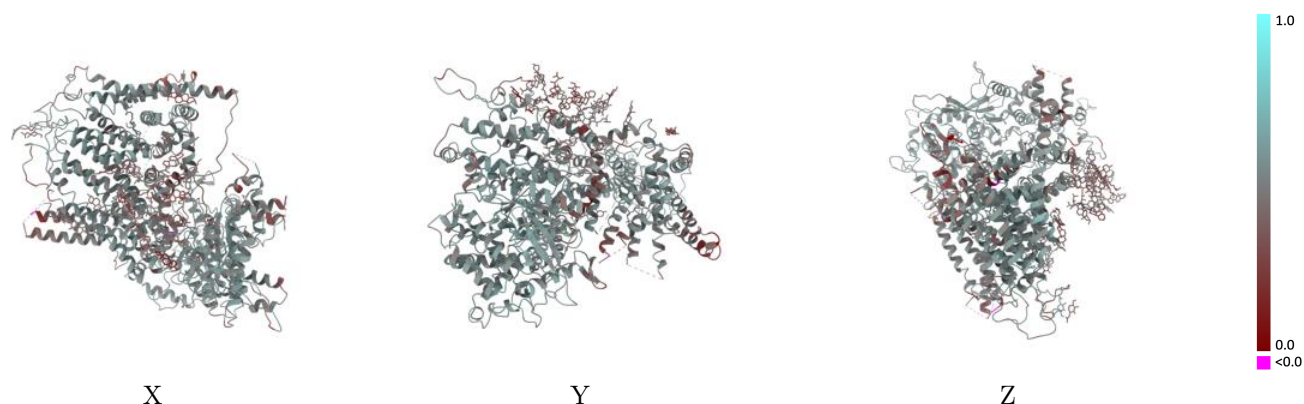
Y



Z

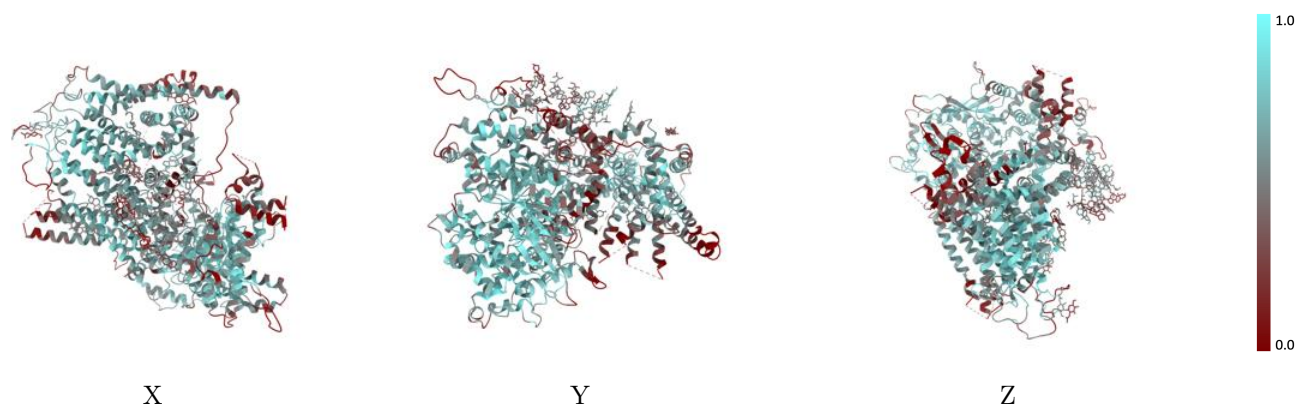
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

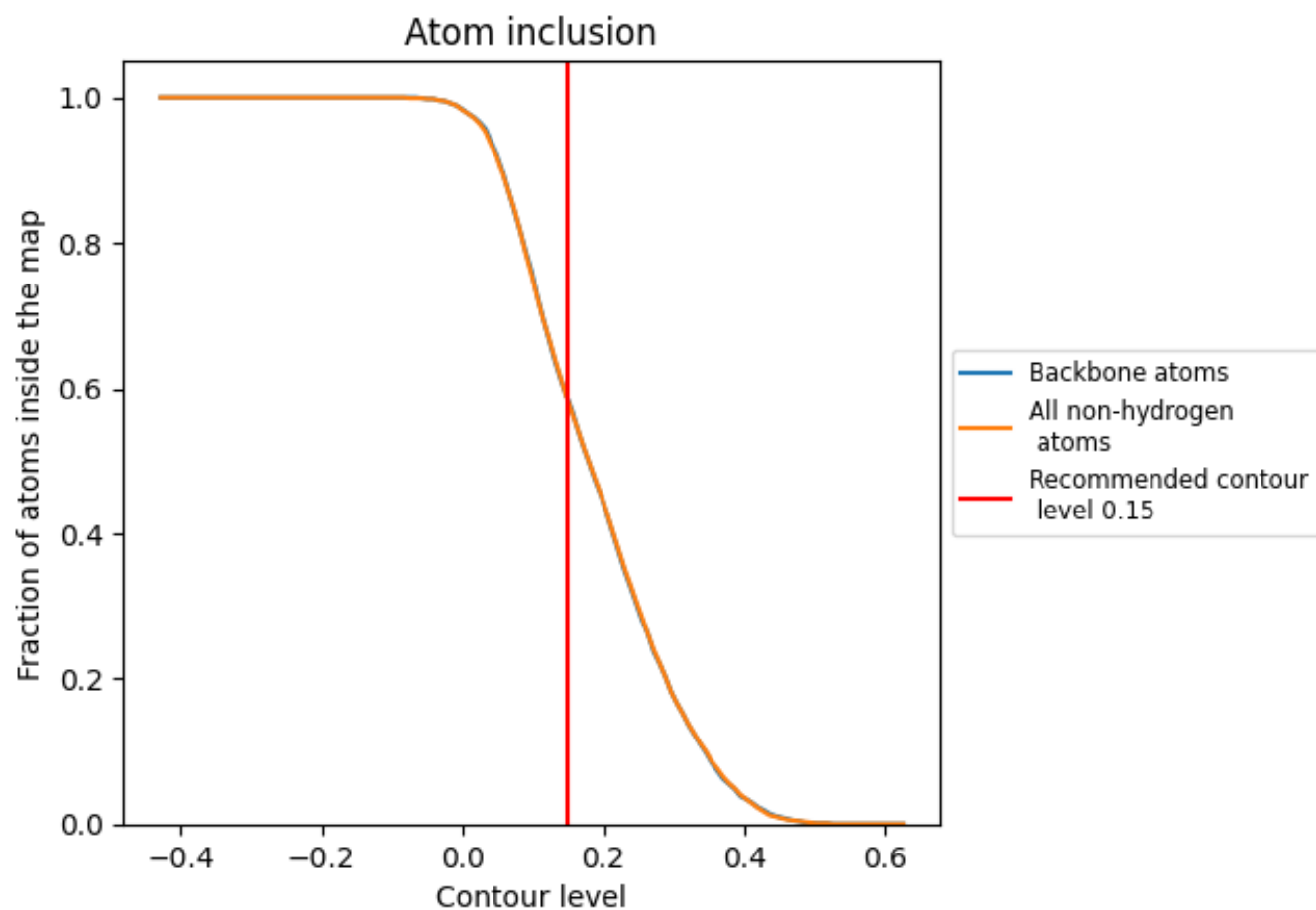
## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.15).



## 9.4 Atom inclusion [i](#)



At the recommended contour level, 58% of all backbone atoms, 58% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.5800	<div></div> 0.5050
A	<div></div> 0.5910	<div></div> 0.5050
C	<div></div> 0.3570	<div></div> 0.4570

