



Full wwPDB EM Validation Report ⓘ

Dec 6, 2023 – 12:17 PM JST

PDB ID : 8JZN
EMDB ID : EMD-36748
Title : Structure of a fungal 1,3-beta-glucan synthase
Authors : Zhao, C.; You, Z.; Chen, D.; Hang, J.; Wang, Z.; Meng, J.; Wang, L.; Zhao, P.; Qiao, J.; Yun, C.; Bai, L.
Deposited on : 2023-07-05
Resolution : 2.47 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:

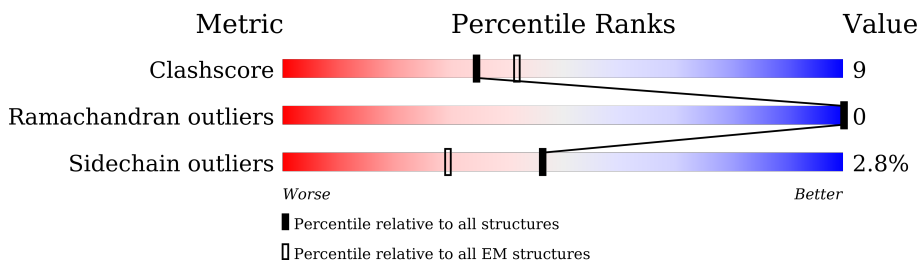
EMDB validation analysis : 0.0.1.dev70
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

1 Overall quality at a glance

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

The reported resolution of this entry is 2.47 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	1876	
2	B	2	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 12831 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 1,3-beta-glucan synthase component FKS1.

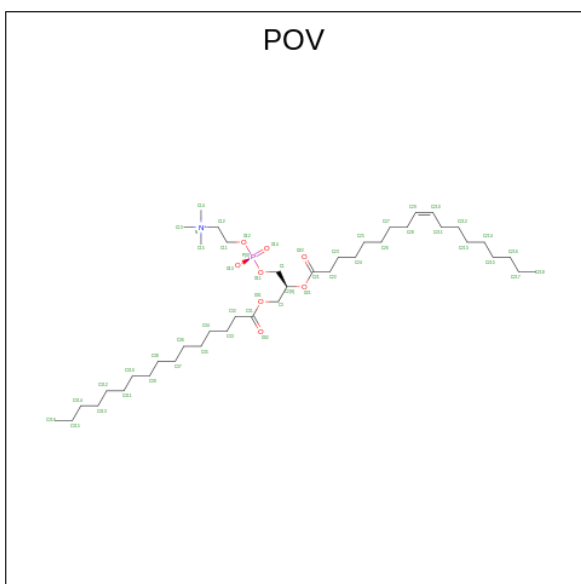
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1489	12155	7934	2038	2111	72	0	0

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



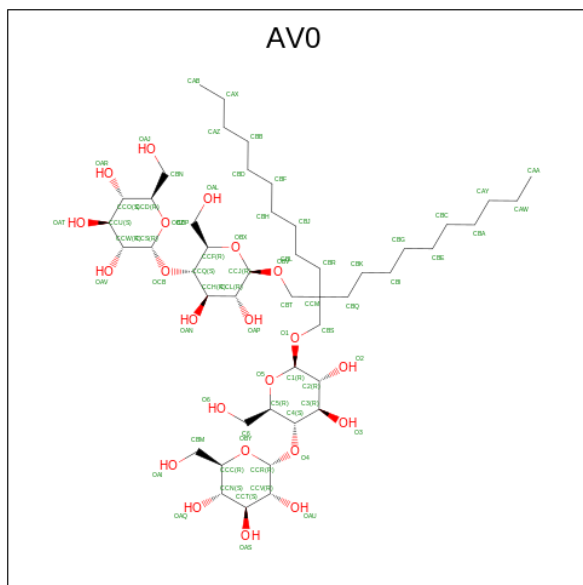
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	B	2	28	16	2	10	0	0

- Molecule 3 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylamm onio)ethyl phosphate (three-letter code: POV) (formula: C₄₂H₈₂NO₈P) (labeled as "Ligand of Interest" by depositor).



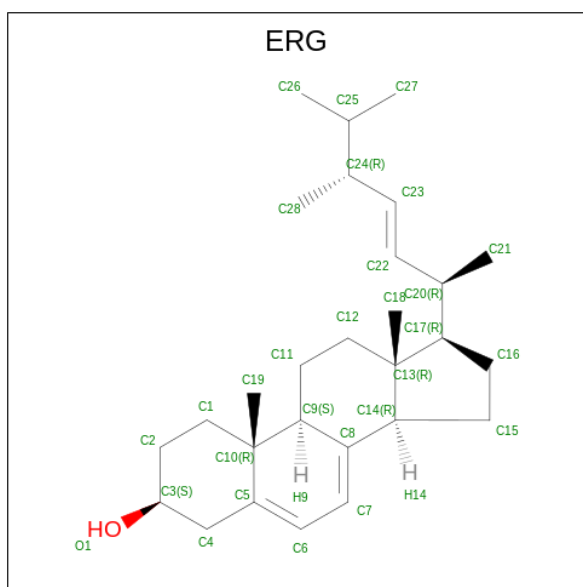
Mol	Chain	Residues	Atoms				AltConf	
3	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	A	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 4 is Lauryl Maltose Neopentyl Glycol (three-letter code: AV0) (formula: $C_{47}H_{88}O_{22}$).

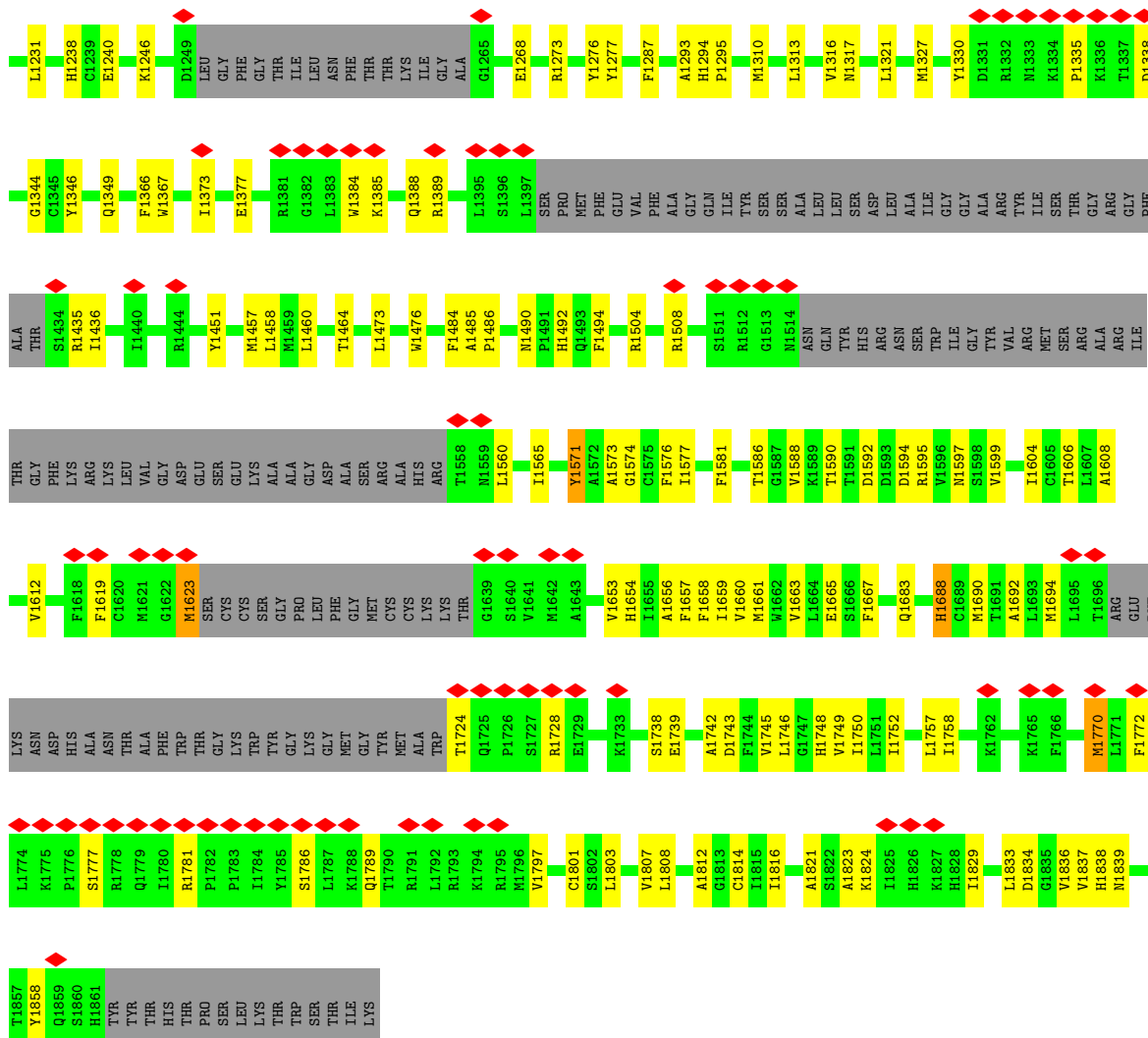


Mol	Chain	Residues	Atoms			AltConf
4	A	1	Total	C	O	0
			69	47	22	
4	A	1	Total	C	O	0
			69	47	22	

- Molecule 5 is ERGOSTEROL (three-letter code: ERG) (formula: $C_{28}H_{44}O$).



Mol	Chain	Residues	Atoms			AltConf
5	A	1	Total	C	O	0
			29	28	1	
5	A	1	Total	C	O	0
			29	28	1	
5	A	1	Total	C	O	0
			29	28	1	
5	A	1	Total	C	O	0
			29	28	1	
5	A	1	Total	C	O	0
			29	28	1	
5	A	1	Total	C	O	0
			29	28	1	
5	A	1	Total	C	O	0
			29	28	1	
5	A	1	Total	C	O	0
			29	28	1	
5	A	1	Total	C	O	0
			29	28	1	
5	A	1	Total	C	O	0
			29	28	1	
5	A	1	Total	C	O	0
			29	28	1	



● Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B: 100%

HAG1
HAG2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1077552	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.6	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	4.559	Depositor
Minimum map value	-2.647	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.094	Depositor
Recommended contour level	0.47	Depositor
Map size (\AA)	316.56, 316.56, 316.56	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.0552, 1.0552, 1.0552	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: ERG, AV0, POV, NAG

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	0.36	0/12481	0.45	0/16926

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	12155	0	12114	193	0
2	B	28	0	25	0	0
3	A	104	0	164	9	0
4	A	138	0	0	4	0
5	A	406	0	616	43	0
All	All	12831	0	12919	227	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (227) 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)
4:A:1902:AV0:OAI	4:A:1902:AV0:OAS	1.78	1.01
1:A:233:ASP:OD1	1:A:603:SER:HB2	1.79	0.81
1:A:1464:THR:HG21	1:A:1476:TRP:HE1	1.51	0.76
1:A:984:GLU:OE1	1:A:988:ARG:NH1	2.21	0.74
1:A:1786:SER:HB3	1:A:1789:GLN:HG3	1.69	0.73
1:A:1612:VAL:HG21	1:A:1653:VAL:HG21	1.71	0.70
1:A:779:GLN:HE21	1:A:788:ARG:HD2	1.56	0.70
1:A:1824:LYS:HE2	5:A:1915:ERG:H42	1.74	0.70
1:A:883:GLU:OE1	1:A:946:ARG:NH1	2.26	0.69
5:A:1906:ERG:H272	5:A:1907:ERG:H262	1.75	0.69
1:A:457:VAL:O	1:A:461:SER:HB3	1.93	0.69
1:A:877:LYS:HE2	1:A:884:TRP:CE2	2.28	0.69
1:A:1597:ASN:ND2	1:A:1836:VAL:O	2.26	0.68
1:A:891:THR:OG1	1:A:938:ARG:NH2	2.27	0.68
1:A:1654:HIS:HB3	3:A:1901:POV:H29	1.75	0.68
1:A:1175:THR:HG23	1:A:1373:ILE:HD12	1.75	0.67
1:A:456:TRP:HB3	1:A:460:ILE:HD12	1.76	0.66
1:A:303:ARG:NH2	1:A:337:ASP:OD1	2.29	0.66
1:A:852:ARG:HG3	1:A:852:ARG:HH11	1.60	0.66
1:A:601:VAL:HG11	1:A:1276:TYR:OH	1.97	0.65
5:A:1914:ERG:H282	5:A:1915:ERG:H211	1.79	0.65
1:A:839:MET:HG2	1:A:840:PRO:HD2	1.79	0.64
1:A:238:PHE:O	1:A:241:MET:HG2	1.96	0.64
5:A:1905:ERG:H263	5:A:1906:ERG:H283	1.80	0.64
1:A:399:TYR:CE1	1:A:603:SER:HB3	2.35	0.62
1:A:709:PHE:HA	1:A:714:SER:HB3	1.83	0.61
5:A:1911:ERG:H121	5:A:1917:ERG:H272	1.82	0.61
1:A:656:MET:HB2	1:A:670:LYS:HA	1.83	0.60
1:A:1458:LEU:HD21	3:A:1901:POV:H215	1.82	0.60
1:A:1104:ASN:OD1	1:A:1246:LYS:NZ	2.35	0.60
1:A:399:TYR:OH	1:A:603:SER:N	2.35	0.59
1:A:1855:MET:SD	1:A:1858:TYR:OH	2.52	0.59
1:A:839:MET:HG3	1:A:1116:ARG:HG2	1.85	0.59
4:A:1902:AV0:OAQ	4:A:1902:AV0:O4	2.20	0.59
1:A:646:ASP:OD2	1:A:649:ARG:NH2	2.28	0.59
1:A:1040:THR:OG1	1:A:1043:GLU:OE1	2.20	0.59
1:A:401:GLU:OE1	1:A:598:ARG:NH2	2.35	0.58
1:A:371:GLU:HB2	1:A:380:ARG:HG2	1.85	0.58
1:A:180:ASP:OD1	1:A:183:ARG:NH1	2.36	0.58
5:A:1905:ERG:H261	5:A:1916:ERG:H282	1.86	0.58
1:A:1436:ILE:O	1:A:1490:ASN:ND2	2.36	0.57
1:A:720:ARG:HA	1:A:799:GLN:HB3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1195:HIS:CD2	1:A:1196:PRO:HD3	2.39	0.57
1:A:237:GLY:HA3	1:A:604:GLN:HG3	1.84	0.57
1:A:1833:LEU:HB3	1:A:1837:VAL:HG13	1.85	0.57
1:A:399:TYR:CZ	1:A:603:SER:HB3	2.40	0.56
1:A:780:VAL:HG21	1:A:791:ARG:HE	1.69	0.56
1:A:243:LEU:HD21	1:A:1140:GLU:HG3	1.87	0.56
1:A:392:ASP:OD1	1:A:1273:ARG:NH2	2.27	0.55
1:A:514:GLU:OE1	1:A:531:ARG:NH2	2.40	0.55
1:A:1173:GLU:HA	1:A:1176:PHE:HB2	1.89	0.55
5:A:1914:ERG:H152	5:A:1915:ERG:H121	1.89	0.55
1:A:1812:ALA:O	1:A:1816:ILE:HD12	2.07	0.55
1:A:713:ILE:HG22	1:A:715:ILE:HG12	1.89	0.54
1:A:672:GLN:NE2	1:A:1317:ASN:OD1	2.36	0.54
1:A:453:ASN:O	1:A:457:VAL:HG23	2.08	0.54
1:A:459:HIS:CE1	1:A:692:THR:OG1	2.59	0.54
1:A:718:PRO:HB2	1:A:720:ARG:HD3	1.90	0.54
1:A:869:ARG:HD3	1:A:1781:ARG:HB2	1.88	0.54
1:A:999:LYS:HD2	1:A:1094:ARG:HB2	1.88	0.54
1:A:1590:THR:HB	1:A:1594:ASP:HB2	1.89	0.54
1:A:1604:ILE:HD13	5:A:1909:ERG:H7	1.89	0.54
1:A:450:THR:HG21	1:A:514:GLU:HB2	1.90	0.53
1:A:1385:LYS:HD2	1:A:1388:GLN:HE22	1.73	0.53
1:A:391:ASP:O	1:A:395:GLN:HG3	2.08	0.53
1:A:1494:PHE:HD1	1:A:1757:LEU:HD13	1.74	0.53
1:A:869:ARG:O	1:A:1781:ARG:NE	2.32	0.53
1:A:1451:TYR:OH	1:A:1743:ASP:OD1	2.26	0.52
1:A:717:THR:OG1	1:A:721:ASN:ND2	2.41	0.52
1:A:837:ASP:OD2	1:A:837:ASP:N	2.37	0.52
1:A:1460:LEU:O	1:A:1464:THR:HG23	2.10	0.52
1:A:1043:GLU:HG2	1:A:1044:GLU:H	1.75	0.52
1:A:1560:LEU:HD22	1:A:1692:ALA:HB2	1.91	0.51
1:A:1157:ILE:HA	1:A:1246:LYS:O	2.11	0.51
1:A:734:ILE:O	1:A:1116:ARG:NH2	2.43	0.51
1:A:459:HIS:HE1	1:A:692:THR:OG1	1.95	0.50
1:A:860:ILE:HA	1:A:872:LEU:HB3	1.91	0.50
1:A:1330:TYR:HB2	1:A:1349:GLN:HG2	1.94	0.50
1:A:1829:ILE:HD12	1:A:1829:ILE:H	1.76	0.50
1:A:1294:HIS:HB3	1:A:1295:PRO:HD3	1.94	0.50
1:A:1586:THR:O	1:A:1848:ASN:HB2	2.12	0.49
1:A:1377:GLU:HG3	1:A:1389:ARG:HG3	1.94	0.49
1:A:1573:ALA:O	1:A:1577:ILE:HG12	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:860:ILE:HG22	1:A:873:LEU:HB2	1.93	0.49
1:A:1222:ASP:HA	1:A:1225:ALA:HB2	1.95	0.49
1:A:671:VAL:HG21	5:A:1907:ERG:C7	2.42	0.49
1:A:454:ARG:O	1:A:458:MET:HG2	2.13	0.49
1:A:747:LYS:HD2	1:A:790:LEU:HB3	1.95	0.49
1:A:668:LEU:HD11	1:A:1577:ILE:HD12	1.95	0.48
1:A:195:SER:HB2	1:A:841:THR:H	1.79	0.48
1:A:675:ILE:HA	5:A:1906:ERG:H212	1.95	0.48
1:A:1772:PHE:HB3	1:A:1777:SER:HA	1.94	0.48
1:A:458:MET:O	1:A:462:ILE:HG12	2.13	0.48
1:A:1384:TRP:NE1	1:A:1388:GLN:OE1	2.47	0.48
1:A:245:LYS:HE2	4:A:1902:AV0:C6	2.43	0.48
1:A:315:ALA:HB1	1:A:318:VAL:HB	1.95	0.48
1:A:720:ARG:NE	1:A:802:ASN:OD1	2.43	0.48
1:A:942:TRP:O	1:A:946:ARG:HG2	2.14	0.47
1:A:171:LEU:HD22	1:A:336:LEU:HD21	1.96	0.47
1:A:467:PHE:HB3	5:A:1904:ERG:H271	1.95	0.47
1:A:1321:LEU:HA	1:A:1581:PHE:HE2	1.79	0.47
5:A:1906:ERG:H162	5:A:1906:ERG:H22	1.57	0.47
1:A:1335:PRO:HG2	1:A:1338:ASP:HB2	1.96	0.47
1:A:607:THR:HG23	1:A:1277:TYR:HB3	1.96	0.47
1:A:794:THR:O	1:A:798:SER:N	2.27	0.47
1:A:1742:ALA:HB2	3:A:1901:POV:H25	1.97	0.47
1:A:1770:MET:SD	1:A:1770:MET:N	2.88	0.47
5:A:1915:ERG:H111	5:A:1915:ERG:H193	1.70	0.47
1:A:317:GLN:HG3	1:A:362:TYR:HD1	1.79	0.46
1:A:383:ASP:OD1	1:A:383:ASP:N	2.42	0.46
1:A:1175:THR:CG2	1:A:1373:ILE:HD12	2.45	0.46
1:A:1592:ASP:OD2	1:A:1595:ARG:NH2	2.48	0.46
1:A:1656:ALA:HB2	5:A:1914:ERG:H273	1.97	0.46
1:A:408:LEU:HD13	1:A:425:ARG:HE	1.80	0.46
1:A:1310:MET:HG2	5:A:1916:ERG:H191	1.97	0.46
1:A:720:ARG:O	1:A:724:THR:OG1	2.23	0.46
1:A:1192:HIS:NE2	1:A:1194:GLY:HA3	2.31	0.46
1:A:514:GLU:HG2	1:A:528:LEU:HD21	1.98	0.46
1:A:736:ALA:HB2	1:A:833:PRO:HG2	1.97	0.46
1:A:671:VAL:HG21	5:A:1907:ERG:H7	1.96	0.45
1:A:1484:PHE:HE1	1:A:1750:ILE:HG23	1.81	0.45
1:A:934:GLU:O	1:A:938:ARG:HG3	2.16	0.45
1:A:382:ARG:NH2	1:A:386:LYS:O	2.50	0.45
1:A:486:GLN:N	1:A:487:PRO:HD2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:545:PRO:HB2	1:A:569:MET:HG3	1.99	0.45
1:A:1576:PHE:HZ	1:A:1599:VAL:HG13	1.82	0.45
1:A:1435:ARG:NE	1:A:1492:HIS:O	2.40	0.45
1:A:1494:PHE:CD1	1:A:1757:LEU:HD13	2.52	0.45
1:A:1565:ILE:CD1	1:A:1688:HIS:HB3	2.47	0.45
1:A:1101:ILE:HD13	1:A:1101:ILE:HA	1.85	0.45
3:A:1901:POV:H11A	3:A:1901:POV:H14A	1.66	0.45
5:A:1914:ERG:H281	5:A:1915:ERG:H272	1.98	0.45
1:A:462:ILE:HD12	5:A:1917:ERG:H271	1.99	0.45
1:A:636:SER:HB2	1:A:691:ASP:OD1	2.17	0.45
1:A:869:ARG:HB3	1:A:1781:ARG:NE	2.32	0.45
1:A:1752:ILE:HG12	1:A:1808:LEU:HD12	1.99	0.45
1:A:1797:VAL:O	1:A:1801:CYS:HB2	2.17	0.45
1:A:728:LYS:HD2	1:A:728:LYS:HA	1.74	0.44
5:A:1909:ERG:H121	5:A:1914:ERG:H12	1.99	0.44
1:A:642:LEU:HD23	1:A:642:LEU:HA	1.83	0.44
1:A:1829:ILE:HD12	1:A:1829:ILE:N	2.32	0.44
3:A:1918:POV:H39A	3:A:1918:POV:H28	1.97	0.44
1:A:587:GLY:HA3	4:A:1902:AV0:OAI	2.17	0.44
5:A:1908:ERG:H22	5:A:1908:ERG:H162	1.71	0.44
5:A:1909:ERG:H282	5:A:1909:ERG:H22	1.76	0.44
5:A:1913:ERG:H183	5:A:1913:ERG:H20	1.76	0.44
1:A:578:ILE:HG12	5:A:1911:ERG:H24	1.98	0.44
1:A:1757:LEU:HD12	1:A:1758:ILE:N	2.33	0.44
5:A:1915:ERG:H162	5:A:1915:ERG:H22	1.62	0.44
1:A:528:LEU:HD12	1:A:528:LEU:HA	1.89	0.44
1:A:1473:LEU:HD22	3:A:1918:POV:H21A	1.99	0.44
1:A:1608:ALA:HB3	1:A:1657:PHE:CE2	2.53	0.44
1:A:1175:THR:HA	1:A:1178:THR:HG23	2.00	0.43
1:A:1821:ALA:O	1:A:1824:LYS:HG2	2.18	0.43
1:A:1327:MET:HA	1:A:1346:TYR:O	2.17	0.43
1:A:1565:ILE:HD12	1:A:1688:HIS:HB3	2.00	0.43
5:A:1909:ERG:H183	5:A:1914:ERG:H12	1.98	0.43
3:A:1918:POV:H14A	3:A:1918:POV:H11	1.85	0.43
1:A:466:TYR:HD2	5:A:1917:ERG:H211	1.82	0.43
1:A:520:ARG:O	1:A:521:LYS:HD2	2.17	0.43
1:A:525:ALA:HA	1:A:528:LEU:HB2	1.99	0.43
1:A:1659:ILE:HD11	1:A:1814:CYS:HB3	2.01	0.43
1:A:1746:LEU:O	1:A:1750:ILE:HG13	2.17	0.43
5:A:1909:ERG:H152	5:A:1909:ERG:H181	1.82	0.43
1:A:735:LEU:HD23	1:A:735:LEU:HA	1.74	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1238:HIS:ND1	1:A:1240:GLU:OE1	2.41	0.43
1:A:1504:ARG:HD3	1:A:1508:ARG:NE	2.32	0.43
1:A:1745:VAL:O	1:A:1749:VAL:HG23	2.19	0.43
1:A:657:ARG:NH2	1:A:1344:GLY:O	2.31	0.43
1:A:780:VAL:HG11	1:A:791:ARG:HH21	1.84	0.43
1:A:839:MET:HG2	1:A:840:PRO:CD	2.47	0.43
1:A:888:VAL:HA	1:A:891:THR:HB	1.99	0.43
1:A:1147:PRO:HG2	1:A:1203:PHE:CD2	2.54	0.43
1:A:1571:TYR:CD1	5:A:1916:ERG:H41	2.53	0.43
1:A:456:TRP:HB3	1:A:460:ILE:CD1	2.48	0.43
1:A:843:THR:OG1	1:A:1094:ARG:O	2.32	0.43
5:A:1904:ERG:H183	5:A:1904:ERG:H20	1.78	0.43
1:A:1663:VAL:HG23	1:A:1667:PHE:CZ	2.54	0.43
5:A:1908:ERG:H20	5:A:1908:ERG:H183	1.54	0.43
1:A:1366:PHE:HD1	1:A:1367:TRP:CD1	2.37	0.42
1:A:445:TRP:O	1:A:449:VAL:HG23	2.19	0.42
1:A:1224:TYR:OH	1:A:1293:ALA:HB3	2.19	0.42
1:A:1837:VAL:HG21	5:A:1909:ERG:H42	2.00	0.42
5:A:1912:ERG:H111	5:A:1912:ERG:H193	1.66	0.42
5:A:1911:ERG:H21	5:A:1917:ERG:H121	2.01	0.42
1:A:1834:ASP:HA	1:A:1838:HIS:HB2	2.02	0.42
1:A:456:TRP:O	1:A:460:ILE:HB	2.19	0.42
1:A:1313:LEU:HD11	1:A:1574:GLY:HA3	2.00	0.42
5:A:1905:ERG:H183	5:A:1905:ERG:H20	1.78	0.42
1:A:607:THR:O	1:A:1231:LEU:HD22	2.19	0.42
1:A:1321:LEU:HA	1:A:1581:PHE:CE2	2.54	0.42
5:A:1908:ERG:H193	5:A:1908:ERG:H111	1.67	0.42
1:A:1661:MET:O	1:A:1665:GLU:HG2	2.20	0.42
3:A:1901:POV:H31D	3:A:1901:POV:H31G	1.77	0.42
1:A:726:LEU:HD22	1:A:823:ALA:HB2	2.01	0.41
5:A:1914:ERG:H183	5:A:1914:ERG:H20	1.84	0.41
1:A:877:LYS:HE2	1:A:884:TRP:CZ2	2.55	0.41
1:A:1485:ALA:HB3	1:A:1486:PRO:HD3	2.01	0.41
1:A:1657:PHE:HA	1:A:1660:VAL:HB	2.02	0.41
1:A:455:ILE:HG12	1:A:1287:PHE:CZ	2.55	0.41
1:A:635:GLU:HG2	1:A:695:TRP:HZ2	1.85	0.41
1:A:1619:PHE:O	1:A:1623:MET:N	2.53	0.41
1:A:856:SER:O	1:A:860:ILE:HG13	2.20	0.41
1:A:1152:GLY:HA2	1:A:1197:ASP:HB3	2.03	0.41
1:A:1588:VAL:O	1:A:1590:THR:HG23	2.20	0.41
3:A:1918:POV:O32	3:A:1918:POV:H23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:638:TYR:HH	5:A:1911:ERG:HO1	1.67	0.41
1:A:1823:ALA:O	1:A:1824:LYS:HD2	2.20	0.41
5:A:1911:ERG:H183	5:A:1911:ERG:H20	1.75	0.41
1:A:1803:LEU:O	1:A:1807:VAL:HG23	2.21	0.41
5:A:1906:ERG:H183	5:A:1906:ERG:H20	1.82	0.41
1:A:374:ASP:HB3	1:A:376:ARG:NH2	2.36	0.41
1:A:726:LEU:HD13	1:A:823:ALA:HA	2.03	0.41
1:A:685:PHE:CD2	5:A:1916:ERG:H211	2.56	0.40
1:A:755:ASN:O	1:A:759:ILE:HG12	2.20	0.40
5:A:1911:ERG:H21	5:A:1917:ERG:C11	2.51	0.40
1:A:882:VAL:HA	1:A:885:GLU:HG2	2.02	0.40
1:A:1571:TYR:HD1	5:A:1916:ERG:H41	1.86	0.40
1:A:1190:LYS:HD2	1:A:1238:HIS:HB2	2.04	0.40
1:A:1748:HIS:O	1:A:1752:ILE:HD12	2.21	0.40
1:A:238:PHE:O	1:A:241:MET:CG	2.67	0.40
1:A:1606:THR:HG23	1:A:1683:GLN:HG3	2.03	0.40
1:A:1724:THR:O	1:A:1728:ARG:N	2.53	0.40
5:A:1910:ERG:H23	5:A:1910:ERG:H213	1.81	0.40
1:A:467:PHE:HE1	1:A:648:ILE:HD11	1.87	0.40
1:A:895:ALA:HA	1:A:935:TYR:OH	2.22	0.40
1:A:1654:HIS:CE1	1:A:1738:SER:HG	2.40	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1461/1876 (78%)	1400 (96%)	61 (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	1309/1620 (81%)	1273 (97%)	36 (3%)	43 67

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	180	ASP
1	A	376	ARG
1	A	409	GLU
1	A	440	LYS
1	A	458	MET
1	A	473	THR
1	A	527	HIS
1	A	530	ARG
1	A	610	PHE
1	A	616	LEU
1	A	617	ASP
1	A	634	SER
1	A	740	MET
1	A	791	ARG
1	A	938	ARG
1	A	978	MET
1	A	991	GLU
1	A	1000	PHE
1	A	1006	ARG
1	A	1088	HIS
1	A	1093	TYR
1	A	1154	ARG
1	A	1193	TYR
1	A	1202	THR
1	A	1268	GLU
1	A	1316	VAL
1	A	1457	MET
1	A	1571	TYR
1	A	1623	MET
1	A	1658	PHE

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Mol	Chain	Res	Type
1	A	1688	HIS
1	A	1690	MET
1	A	1694	MET
1	A	1739	GLU
1	A	1770	MET
1	A	1839	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	459	HIS
1	A	779	GLN
1	A	1388	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	B	1	1,2	14,14,15	0.41	0	17,19,21	0.48	0
2	NAG	B	2	2	14,14,15	0.20	0	17,19,21	0.50	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	B	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	B	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.

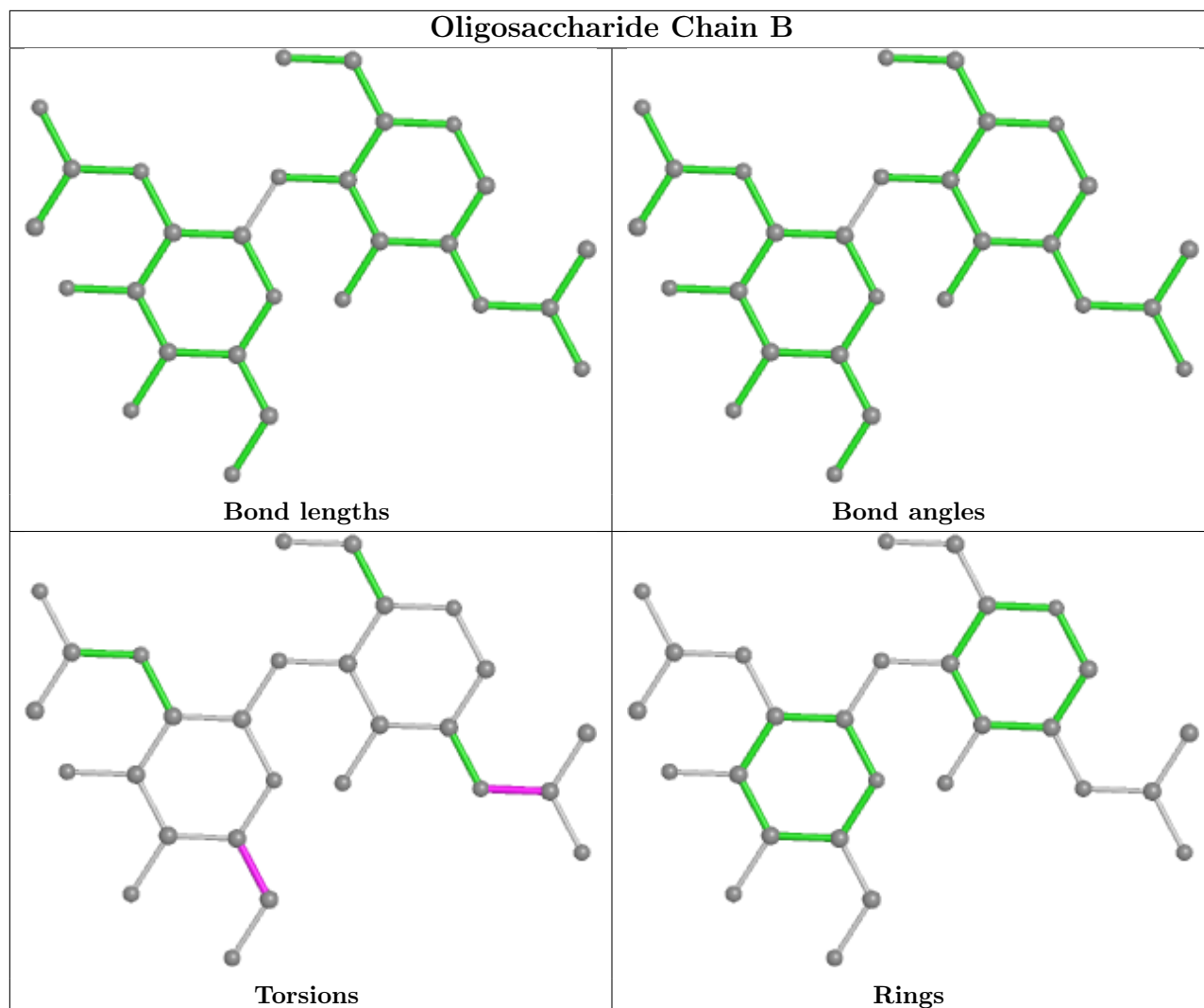
All (4) torsion outliers are listed below:

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

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](#)

18 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$
5	ERG	A	1912	-	31,32,32	4.26	17 (54%)	47,50,50	2.09	15 (31%)
5	ERG	A	1915	-	31,32,32	4.21	17 (54%)	47,50,50	2.13	15 (31%)
4	AV0	A	1902	-	72,72,72	1.41	7 (9%)	96,98,98	1.00	4 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	ERG	A	1913	-	31,32,32	4.20	17 (54%)	47,50,50	2.09	16 (34%)
5	ERG	A	1906	-	31,32,32	4.21	17 (54%)	47,50,50	2.08	18 (38%)
5	ERG	A	1904	-	31,32,32	4.14	17 (54%)	47,50,50	2.27	13 (27%)
5	ERG	A	1910	-	31,32,32	4.16	17 (54%)	47,50,50	2.14	15 (31%)
5	ERG	A	1905	-	31,32,32	4.16	17 (54%)	47,50,50	2.25	15 (31%)
5	ERG	A	1909	-	31,32,32	4.17	17 (54%)	47,50,50	2.27	18 (38%)
5	ERG	A	1914	-	31,32,32	4.12	17 (54%)	47,50,50	2.10	16 (34%)
5	ERG	A	1908	-	31,32,32	4.15	17 (54%)	47,50,50	2.42	15 (31%)
5	ERG	A	1916	-	31,32,32	4.12	17 (54%)	47,50,50	2.30	16 (34%)
5	ERG	A	1917	-	31,32,32	4.17	16 (51%)	47,50,50	2.57	16 (34%)
5	ERG	A	1907	-	31,32,32	4.16	16 (51%)	47,50,50	2.11	15 (31%)
4	AV0	A	1903	-	72,72,72	1.38	5 (6%)	96,98,98	1.07	4 (4%)
3	POV	A	1918	-	51,51,51	1.24	5 (9%)	57,59,59	1.04	2 (3%)
5	ERG	A	1911	-	31,32,32	4.19	17 (54%)	47,50,50	2.13	16 (34%)
3	POV	A	1901	-	51,51,51	1.20	4 (7%)	57,59,59	1.06	2 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ERG	A	1912	-	-	7/13/71/71	0/4/4/4
5	ERG	A	1915	-	-	7/13/71/71	0/4/4/4
4	AV0	A	1902	-	-	27/50/130/130	0/4/4/4
5	ERG	A	1913	-	-	11/13/71/71	0/4/4/4
5	ERG	A	1906	-	-	11/13/71/71	0/4/4/4
5	ERG	A	1904	-	-	11/13/71/71	0/4/4/4
5	ERG	A	1910	-	-	7/13/71/71	0/4/4/4
5	ERG	A	1905	-	-	6/13/71/71	0/4/4/4
5	ERG	A	1909	-	-	8/13/71/71	0/4/4/4
5	ERG	A	1914	-	-	11/13/71/71	0/4/4/4
5	ERG	A	1908	-	-	7/13/71/71	0/4/4/4
5	ERG	A	1916	-	-	12/13/71/71	0/4/4/4
5	ERG	A	1917	-	-	8/13/71/71	0/4/4/4
5	ERG	A	1907	-	-	3/13/71/71	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	AV0	A	1903	-	-	29/50/130/130	0/4/4/4
3	POV	A	1918	-	-	23/55/55/55	-
5	ERG	A	1911	-	-	8/13/71/71	0/4/4/4
3	POV	A	1901	-	-	25/55/55/55	-

All (257) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1912	ERG	C6-C5	12.29	1.62	1.33
5	A	1908	ERG	C6-C5	12.05	1.61	1.33
5	A	1913	ERG	C6-C5	12.05	1.61	1.33
5	A	1915	ERG	C6-C5	12.00	1.61	1.33
5	A	1906	ERG	C6-C5	11.99	1.61	1.33
5	A	1910	ERG	C6-C5	11.99	1.61	1.33
5	A	1904	ERG	C6-C5	11.95	1.61	1.33
5	A	1909	ERG	C6-C5	11.93	1.61	1.33
5	A	1911	ERG	C6-C5	11.92	1.61	1.33
5	A	1917	ERG	C6-C5	11.92	1.61	1.33
5	A	1914	ERG	C6-C5	11.81	1.61	1.33
5	A	1907	ERG	C6-C5	11.76	1.61	1.33
5	A	1905	ERG	C6-C5	11.75	1.60	1.33
5	A	1916	ERG	C6-C5	11.73	1.60	1.33
5	A	1905	ERG	C20-C17	-10.59	1.36	1.54
5	A	1917	ERG	C20-C17	-10.57	1.36	1.54
5	A	1916	ERG	C20-C17	-10.48	1.36	1.54
5	A	1906	ERG	C20-C17	-10.47	1.36	1.54
5	A	1911	ERG	C20-C17	-10.47	1.36	1.54
5	A	1907	ERG	C20-C17	-10.40	1.36	1.54
5	A	1914	ERG	C20-C17	-10.37	1.37	1.54
5	A	1910	ERG	C20-C17	-10.30	1.37	1.54
5	A	1909	ERG	C20-C17	-10.24	1.37	1.54
5	A	1904	ERG	C20-C17	-10.23	1.37	1.54
5	A	1915	ERG	C20-C17	-10.17	1.37	1.54
5	A	1913	ERG	C20-C17	-9.99	1.37	1.54
5	A	1912	ERG	C20-C17	-9.99	1.37	1.54
5	A	1908	ERG	C20-C17	-9.96	1.37	1.54
5	A	1908	ERG	C9-C8	7.29	1.70	1.51
5	A	1905	ERG	C9-C8	7.01	1.69	1.51
5	A	1910	ERG	C9-C8	6.88	1.69	1.51
5	A	1916	ERG	C9-C8	6.84	1.69	1.51
5	A	1914	ERG	C9-C8	6.83	1.69	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1915	ERG	C9-C8	6.79	1.69	1.51
5	A	1912	ERG	C9-C8	6.77	1.69	1.51
5	A	1904	ERG	C9-C8	6.73	1.69	1.51
5	A	1911	ERG	C9-C8	6.61	1.68	1.51
5	A	1913	ERG	C9-C8	6.59	1.68	1.51
5	A	1909	ERG	C9-C8	6.59	1.68	1.51
5	A	1906	ERG	C9-C8	6.56	1.68	1.51
5	A	1912	ERG	C7-C6	6.42	1.60	1.41
5	A	1909	ERG	C13-C17	6.41	1.67	1.55
5	A	1907	ERG	C9-C8	6.38	1.68	1.51
5	A	1911	ERG	C10-C9	-6.26	1.47	1.55
5	A	1917	ERG	C9-C8	6.26	1.67	1.51
5	A	1912	ERG	C10-C9	-6.24	1.47	1.55
5	A	1911	ERG	C7-C6	6.24	1.59	1.41
5	A	1913	ERG	C7-C6	6.24	1.59	1.41
5	A	1909	ERG	C7-C6	6.21	1.59	1.41
5	A	1906	ERG	C7-C6	6.20	1.59	1.41
5	A	1913	ERG	C13-C17	6.16	1.66	1.55
5	A	1915	ERG	C7-C6	6.15	1.59	1.41
5	A	1909	ERG	C16-C17	6.15	1.67	1.54
5	A	1904	ERG	C7-C6	6.14	1.59	1.41
5	A	1907	ERG	C7-C6	6.12	1.59	1.41
5	A	1907	ERG	C13-C17	6.11	1.66	1.55
5	A	1913	ERG	C16-C17	6.06	1.67	1.54
5	A	1910	ERG	C7-C6	6.06	1.59	1.41
5	A	1917	ERG	C7-C6	6.06	1.59	1.41
5	A	1910	ERG	C13-C17	6.05	1.66	1.55
5	A	1905	ERG	C7-C6	6.05	1.59	1.41
5	A	1914	ERG	C7-C6	6.05	1.59	1.41
5	A	1906	ERG	C16-C17	6.04	1.66	1.54
5	A	1912	ERG	C13-C17	6.04	1.66	1.55
5	A	1908	ERG	C7-C6	6.03	1.58	1.41
5	A	1916	ERG	C13-C17	6.00	1.66	1.55
5	A	1910	ERG	C16-C17	5.98	1.66	1.54
5	A	1913	ERG	C10-C9	-5.98	1.47	1.55
5	A	1912	ERG	C16-C17	5.97	1.66	1.54
5	A	1904	ERG	C16-C17	5.96	1.66	1.54
5	A	1915	ERG	C13-C17	5.95	1.66	1.55
5	A	1916	ERG	C7-C6	5.92	1.58	1.41
5	A	1915	ERG	C16-C17	5.88	1.66	1.54
5	A	1917	ERG	C16-C17	5.87	1.66	1.54
5	A	1907	ERG	C16-C17	5.85	1.66	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1915	ERG	C10-C9	-5.85	1.48	1.55
5	A	1906	ERG	C13-C17	5.83	1.66	1.55
5	A	1909	ERG	C10-C9	-5.80	1.48	1.55
5	A	1911	ERG	C13-C17	5.79	1.66	1.55
5	A	1917	ERG	C13-C17	5.76	1.66	1.55
5	A	1907	ERG	C10-C9	-5.76	1.48	1.55
5	A	1912	ERG	C12-C13	-5.74	1.43	1.54
5	A	1911	ERG	C16-C17	5.74	1.66	1.54
5	A	1906	ERG	C10-C9	-5.74	1.48	1.55
5	A	1905	ERG	C12-C13	-5.74	1.43	1.54
5	A	1904	ERG	C13-C17	5.71	1.65	1.55
5	A	1914	ERG	C12-C13	-5.70	1.43	1.54
5	A	1915	ERG	C12-C13	-5.70	1.43	1.54
5	A	1916	ERG	C16-C17	5.67	1.66	1.54
5	A	1905	ERG	C16-C17	5.65	1.66	1.54
5	A	1908	ERG	C16-C17	5.64	1.66	1.54
5	A	1917	ERG	C12-C13	-5.61	1.44	1.54
5	A	1914	ERG	C13-C17	5.59	1.65	1.55
5	A	1914	ERG	C16-C17	5.57	1.65	1.54
5	A	1908	ERG	C12-C13	-5.54	1.44	1.54
5	A	1916	ERG	C12-C13	-5.53	1.44	1.54
5	A	1917	ERG	C10-C9	-5.50	1.48	1.55
5	A	1908	ERG	C13-C17	5.50	1.65	1.55
5	A	1911	ERG	C12-C13	-5.50	1.44	1.54
5	A	1905	ERG	C13-C17	5.50	1.65	1.55
5	A	1906	ERG	C12-C13	-5.48	1.44	1.54
5	A	1913	ERG	C12-C13	-5.45	1.44	1.54
5	A	1910	ERG	C12-C13	-5.43	1.44	1.54
5	A	1904	ERG	C12-C13	-5.42	1.44	1.54
5	A	1907	ERG	C12-C13	-5.40	1.44	1.54
5	A	1914	ERG	C10-C9	-5.35	1.48	1.55
5	A	1905	ERG	C10-C9	-5.07	1.49	1.55
5	A	1909	ERG	C12-C13	-5.02	1.45	1.54
5	A	1904	ERG	C10-C9	-4.75	1.49	1.55
5	A	1916	ERG	C10-C9	-4.72	1.49	1.55
4	A	1902	AV0	CBS-CCM	4.71	1.64	1.53
4	A	1903	AV0	CBS-CCM	4.69	1.64	1.53
5	A	1910	ERG	C10-C9	-4.66	1.49	1.55
4	A	1902	AV0	CBT-CCM	4.16	1.63	1.53
5	A	1908	ERG	C10-C9	-4.10	1.50	1.55
4	A	1903	AV0	CBT-CCM	3.87	1.62	1.53
5	A	1908	ERG	C15-C14	3.83	1.64	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1918	POV	O31-C31	3.81	1.44	1.33
5	A	1905	ERG	C15-C14	3.79	1.64	1.54
3	A	1901	POV	O31-C31	3.74	1.44	1.33
5	A	1910	ERG	C10-C5	3.69	1.60	1.52
5	A	1912	ERG	C15-C14	3.67	1.63	1.54
5	A	1911	ERG	C15-C14	3.67	1.63	1.54
5	A	1914	ERG	C15-C14	3.66	1.63	1.54
5	A	1904	ERG	C15-C14	3.63	1.63	1.54
5	A	1906	ERG	C15-C14	3.59	1.63	1.54
5	A	1908	ERG	C10-C5	3.59	1.60	1.52
5	A	1915	ERG	C15-C14	3.56	1.63	1.54
5	A	1913	ERG	C15-C14	3.54	1.63	1.54
5	A	1910	ERG	C15-C14	3.53	1.63	1.54
5	A	1916	ERG	C15-C14	3.53	1.63	1.54
5	A	1915	ERG	C10-C5	3.50	1.59	1.52
5	A	1906	ERG	C10-C5	3.50	1.59	1.52
4	A	1902	AV0	O5-C1	3.48	1.50	1.41
5	A	1907	ERG	C10-C5	3.47	1.59	1.52
5	A	1909	ERG	C15-C14	3.46	1.63	1.54
5	A	1917	ERG	C15-C14	3.45	1.63	1.54
4	A	1903	AV0	O5-C1	3.45	1.50	1.41
5	A	1909	ERG	C10-C5	3.43	1.59	1.52
5	A	1917	ERG	C10-C5	3.43	1.59	1.52
5	A	1904	ERG	C10-C5	3.41	1.59	1.52
5	A	1913	ERG	C10-C5	3.39	1.59	1.52
5	A	1907	ERG	C15-C14	3.36	1.63	1.54
5	A	1908	ERG	C13-C14	-3.36	1.50	1.56
5	A	1912	ERG	C10-C5	3.34	1.59	1.52
5	A	1913	ERG	C20-C22	3.34	1.59	1.51
5	A	1905	ERG	C10-C5	3.31	1.59	1.52
5	A	1916	ERG	C10-C5	3.27	1.59	1.52
5	A	1916	ERG	C20-C22	3.25	1.59	1.51
5	A	1908	ERG	C20-C22	3.25	1.59	1.51
5	A	1917	ERG	C13-C14	-3.24	1.50	1.56
5	A	1914	ERG	C20-C22	3.22	1.59	1.51
5	A	1907	ERG	C13-C14	-3.21	1.50	1.56
5	A	1911	ERG	C10-C5	3.21	1.59	1.52
5	A	1914	ERG	C10-C5	3.21	1.59	1.52
5	A	1908	ERG	C12-C11	3.19	1.60	1.53
5	A	1916	ERG	C13-C14	-3.19	1.50	1.56
5	A	1915	ERG	C20-C22	3.18	1.59	1.51
5	A	1912	ERG	C20-C22	3.14	1.59	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1906	ERG	C20-C22	3.13	1.59	1.51
5	A	1907	ERG	C20-C22	3.12	1.59	1.51
5	A	1904	ERG	C20-C22	3.10	1.59	1.51
5	A	1917	ERG	C20-C22	3.05	1.58	1.51
5	A	1905	ERG	C20-C22	3.03	1.58	1.51
5	A	1911	ERG	C13-C14	-3.03	1.51	1.56
5	A	1905	ERG	C13-C14	-3.02	1.51	1.56
5	A	1909	ERG	C20-C22	2.99	1.58	1.51
5	A	1915	ERG	C13-C14	-2.99	1.51	1.56
5	A	1911	ERG	C20-C22	2.98	1.58	1.51
5	A	1910	ERG	C13-C14	-2.94	1.51	1.56
5	A	1914	ERG	C13-C14	-2.93	1.51	1.56
5	A	1910	ERG	C20-C22	2.91	1.58	1.51
5	A	1912	ERG	C13-C14	-2.91	1.51	1.56
5	A	1913	ERG	C12-C11	2.90	1.59	1.53
5	A	1907	ERG	C12-C11	2.88	1.59	1.53
5	A	1917	ERG	C12-C11	2.87	1.59	1.53
5	A	1906	ERG	C13-C14	-2.85	1.51	1.56
5	A	1913	ERG	C13-C14	-2.85	1.51	1.56
5	A	1904	ERG	C4-C3	2.83	1.57	1.52
3	A	1918	POV	O21-C21	2.82	1.42	1.34
5	A	1915	ERG	C12-C11	2.80	1.59	1.53
5	A	1909	ERG	C12-C11	2.79	1.59	1.53
4	A	1903	AV0	OBY-CCR	2.78	1.48	1.41
5	A	1906	ERG	C4-C3	2.77	1.57	1.52
5	A	1904	ERG	C13-C14	-2.73	1.51	1.56
4	A	1903	AV0	CBQ-CCM	2.73	1.59	1.54
5	A	1914	ERG	C12-C11	2.71	1.59	1.53
4	A	1902	AV0	CBQ-CCM	2.68	1.59	1.54
5	A	1916	ERG	C12-C11	2.68	1.59	1.53
5	A	1906	ERG	C12-C11	2.67	1.59	1.53
5	A	1904	ERG	C4-C5	2.67	1.57	1.51
5	A	1912	ERG	C4-C3	2.67	1.56	1.52
5	A	1910	ERG	C12-C11	2.67	1.59	1.53
5	A	1908	ERG	C4-C3	2.67	1.56	1.52
5	A	1909	ERG	C13-C14	-2.66	1.51	1.56
5	A	1905	ERG	C4-C3	2.66	1.56	1.52
4	A	1902	AV0	OBY-CCR	2.66	1.48	1.41
3	A	1918	POV	P-O12	2.63	1.69	1.59
5	A	1905	ERG	C12-C11	2.63	1.59	1.53
3	A	1901	POV	O21-C21	2.63	1.41	1.34
5	A	1912	ERG	C12-C11	2.61	1.59	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1910	ERG	C4-C3	2.60	1.56	1.52
5	A	1913	ERG	C4-C3	2.60	1.56	1.52
5	A	1906	ERG	C4-C5	2.60	1.57	1.51
5	A	1917	ERG	C4-C3	2.58	1.56	1.52
5	A	1915	ERG	C4-C3	2.56	1.56	1.52
3	A	1901	POV	P-O12	2.56	1.69	1.59
5	A	1912	ERG	C4-C5	2.55	1.57	1.51
5	A	1904	ERG	C12-C11	2.55	1.58	1.53
5	A	1908	ERG	C4-C5	2.55	1.57	1.51
5	A	1910	ERG	C4-C5	2.52	1.57	1.51
5	A	1911	ERG	C12-C11	2.51	1.58	1.53
5	A	1913	ERG	C4-C5	2.51	1.57	1.51
5	A	1905	ERG	C4-C5	2.48	1.57	1.51
5	A	1915	ERG	C4-C5	2.48	1.57	1.51
5	A	1908	ERG	C21-C20	2.47	1.60	1.53
5	A	1907	ERG	C4-C3	2.43	1.56	1.52
5	A	1910	ERG	C21-C20	2.38	1.60	1.53
5	A	1907	ERG	C4-C5	2.36	1.56	1.51
5	A	1912	ERG	C21-C20	2.34	1.59	1.53
5	A	1917	ERG	C4-C5	2.32	1.56	1.51
5	A	1905	ERG	C21-C20	2.32	1.59	1.53
5	A	1912	ERG	C14-C8	2.32	1.57	1.51
5	A	1911	ERG	C4-C5	2.31	1.56	1.51
5	A	1915	ERG	C21-C20	2.30	1.59	1.53
3	A	1901	POV	C12-C11	2.30	1.58	1.51
5	A	1909	ERG	C4-C5	2.29	1.56	1.51
3	A	1918	POV	C12-C11	2.29	1.58	1.51
5	A	1909	ERG	C4-C3	2.27	1.56	1.52
5	A	1913	ERG	C21-C20	2.27	1.59	1.53
5	A	1904	ERG	C21-C20	2.27	1.59	1.53
5	A	1916	ERG	C4-C3	2.25	1.56	1.52
5	A	1916	ERG	C4-C5	2.25	1.56	1.51
5	A	1917	ERG	C14-C8	2.23	1.57	1.51
5	A	1908	ERG	C14-C8	2.23	1.57	1.51
5	A	1910	ERG	C14-C8	2.22	1.57	1.51
5	A	1909	ERG	C21-C20	2.22	1.59	1.53
5	A	1916	ERG	C21-C20	2.22	1.59	1.53
5	A	1907	ERG	C21-C20	2.22	1.59	1.53
5	A	1911	ERG	C21-C20	2.19	1.59	1.53
5	A	1904	ERG	C14-C8	2.19	1.57	1.51
5	A	1914	ERG	C4-C3	2.17	1.55	1.52
5	A	1905	ERG	C14-C8	2.16	1.57	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1902	AV0	OBZ-CCS	2.13	1.47	1.41
5	A	1914	ERG	C4-C5	2.12	1.56	1.51
5	A	1906	ERG	C14-C8	2.11	1.57	1.51
5	A	1911	ERG	C4-C3	2.11	1.55	1.52
5	A	1906	ERG	C21-C20	2.10	1.59	1.53
5	A	1915	ERG	C14-C8	2.10	1.57	1.51
5	A	1914	ERG	C14-C8	2.08	1.57	1.51
5	A	1914	ERG	C21-C20	2.07	1.59	1.53
5	A	1909	ERG	C14-C8	2.04	1.56	1.51
5	A	1913	ERG	C14-C8	2.03	1.56	1.51
4	A	1902	AV0	O5-C5	2.01	1.49	1.44
5	A	1911	ERG	C14-C8	2.01	1.56	1.51
5	A	1916	ERG	C14-C8	2.01	1.56	1.51
3	A	1918	POV	C22-C21	2.00	1.56	1.50

All (231) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1908	ERG	C13-C17-C20	-7.98	109.14	119.43
5	A	1917	ERG	C14-C8-C9	-7.79	102.93	114.66
5	A	1904	ERG	C14-C8-C9	-7.55	103.29	114.66
5	A	1909	ERG	C14-C8-C9	-7.09	103.98	114.66
5	A	1912	ERG	C4-C5-C10	-6.98	107.14	116.42
5	A	1905	ERG	C13-C17-C20	-6.91	110.52	119.43
5	A	1913	ERG	C4-C5-C10	-6.66	107.56	116.42
5	A	1917	ERG	C7-C6-C5	-6.62	111.59	123.20
5	A	1916	ERG	C4-C5-C10	-6.60	107.64	116.42
5	A	1916	ERG	C13-C17-C20	-6.01	111.67	119.43
5	A	1912	ERG	C14-C13-C17	5.91	106.03	99.72
5	A	1908	ERG	C14-C13-C17	5.80	105.91	99.72
5	A	1911	ERG	C13-C17-C20	-5.79	111.96	119.43
5	A	1908	ERG	C4-C5-C10	-5.70	108.85	116.42
5	A	1904	ERG	C12-C13-C14	5.67	116.27	107.27
5	A	1907	ERG	C14-C8-C9	-5.61	106.21	114.66
5	A	1909	ERG	C12-C13-C14	5.52	116.03	107.27
5	A	1914	ERG	C13-C17-C20	-5.45	112.40	119.43
5	A	1917	ERG	C12-C13-C14	5.40	115.83	107.27
5	A	1905	ERG	C7-C6-C5	-5.34	113.83	123.20
5	A	1915	ERG	C14-C13-C17	5.30	105.38	99.72
5	A	1915	ERG	C4-C5-C10	-5.29	109.39	116.42
5	A	1907	ERG	C4-C5-C10	-5.29	109.39	116.42
5	A	1906	ERG	C14-C8-C9	-5.27	106.72	114.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1916	ERG	C7-C6-C5	-5.27	113.96	123.20
5	A	1915	ERG	C13-C17-C20	-5.25	112.66	119.43
5	A	1917	ERG	C4-C5-C10	-5.22	109.49	116.42
5	A	1910	ERG	C4-C5-C10	-5.21	109.50	116.42
5	A	1905	ERG	C12-C13-C14	5.07	115.31	107.27
5	A	1904	ERG	C13-C17-C20	-5.02	112.96	119.43
5	A	1910	ERG	C14-C8-C9	-4.99	107.14	114.66
5	A	1909	ERG	C4-C5-C10	-4.90	109.90	116.42
5	A	1911	ERG	C4-C5-C10	-4.87	109.94	116.42
5	A	1914	ERG	C14-C8-C9	-4.74	107.52	114.66
5	A	1906	ERG	C12-C13-C14	4.74	114.79	107.27
5	A	1917	ERG	C6-C7-C8	-4.65	112.91	122.07
5	A	1917	ERG	C13-C17-C20	-4.58	113.53	119.43
5	A	1913	ERG	C13-C17-C20	-4.55	113.56	119.43
5	A	1904	ERG	C4-C5-C10	-4.54	110.39	116.42
5	A	1913	ERG	C14-C8-C9	-4.47	107.93	114.66
5	A	1910	ERG	C13-C17-C20	-4.45	113.69	119.43
5	A	1912	ERG	C13-C17-C20	-4.40	113.75	119.43
5	A	1916	ERG	C14-C13-C17	4.36	104.37	99.72
5	A	1910	ERG	C12-C13-C14	4.32	114.11	107.27
5	A	1908	ERG	C18-C13-C17	-4.31	103.67	111.71
5	A	1907	ERG	C12-C13-C14	4.31	114.10	107.27
5	A	1910	ERG	C7-C6-C5	-4.30	115.65	123.20
5	A	1908	ERG	C7-C6-C5	-4.28	115.68	123.20
5	A	1906	ERG	C13-C17-C20	-4.27	113.92	119.43
5	A	1911	ERG	C12-C13-C14	4.26	114.02	107.27
5	A	1914	ERG	C7-C6-C5	-4.18	115.86	123.20
5	A	1914	ERG	C12-C13-C14	4.18	113.91	107.27
5	A	1906	ERG	C4-C5-C10	-4.12	110.95	116.42
5	A	1917	ERG	C11-C9-C8	-4.11	102.11	111.33
5	A	1913	ERG	C12-C13-C14	4.09	113.75	107.27
4	A	1903	AV0	CCR-O4-C4	-3.99	108.10	117.96
3	A	1918	POV	O21-C21-C22	3.97	120.06	111.50
5	A	1915	ERG	C14-C8-C9	-3.87	108.83	114.66
5	A	1909	ERG	C12-C13-C17	3.86	122.35	116.57
3	A	1901	POV	O21-C21-C22	3.85	119.81	111.50
5	A	1907	ERG	C13-C17-C20	-3.85	114.46	119.43
5	A	1911	ERG	C12-C13-C17	3.83	122.31	116.57
5	A	1914	ERG	C4-C5-C10	-3.80	111.38	116.42
5	A	1911	ERG	C14-C8-C9	-3.78	108.97	114.66
5	A	1904	ERG	C7-C6-C5	-3.78	116.57	123.20
5	A	1916	ERG	C6-C7-C8	-3.71	114.77	122.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1908	ERG	C12-C13-C14	3.66	113.08	107.27
5	A	1905	ERG	C4-C5-C10	-3.64	111.58	116.42
5	A	1908	ERG	C6-C7-C8	-3.60	114.99	122.07
5	A	1916	ERG	C14-C8-C9	-3.58	109.26	114.66
5	A	1911	ERG	C18-C13-C17	-3.58	105.03	111.71
5	A	1905	ERG	C6-C7-C8	-3.57	115.05	122.07
5	A	1915	ERG	C7-C6-C5	-3.56	116.95	123.20
5	A	1913	ERG	C18-C13-C12	-3.55	104.98	110.59
5	A	1910	ERG	C14-C13-C17	3.52	103.48	99.72
5	A	1907	ERG	C7-C6-C5	-3.52	117.02	123.20
4	A	1902	AV0	CCR-O4-C4	-3.50	109.29	117.96
5	A	1916	ERG	C12-C13-C14	3.49	112.81	107.27
5	A	1912	ERG	C14-C8-C9	-3.48	109.42	114.66
4	A	1902	AV0	CCS-OCB-CCQ	-3.42	109.50	117.96
5	A	1909	ERG	C14-C8-C7	-3.42	117.65	124.38
5	A	1909	ERG	C17-C20-C22	-3.38	103.84	110.27
5	A	1905	ERG	C14-C8-C7	-3.37	117.74	124.38
5	A	1914	ERG	C12-C13-C17	3.35	121.58	116.57
5	A	1916	ERG	C18-C13-C12	-3.34	105.32	110.59
5	A	1916	ERG	C12-C13-C17	3.33	121.56	116.57
5	A	1905	ERG	C18-C13-C17	-3.29	105.58	111.71
5	A	1905	ERG	C12-C13-C17	3.28	121.48	116.57
5	A	1905	ERG	C18-C13-C12	-3.28	105.41	110.59
5	A	1909	ERG	C18-C13-C12	-3.27	105.43	110.59
5	A	1914	ERG	C18-C13-C17	-3.25	105.65	111.71
5	A	1911	ERG	C18-C13-C12	-3.22	105.51	110.59
5	A	1910	ERG	C18-C13-C17	-3.21	105.73	111.71
5	A	1913	ERG	C14-C13-C17	3.19	103.13	99.72
5	A	1906	ERG	C7-C6-C5	-3.19	117.60	123.20
5	A	1910	ERG	C6-C7-C8	-3.16	115.84	122.07
5	A	1904	ERG	C11-C9-C8	-3.16	104.26	111.33
5	A	1913	ERG	C7-C6-C5	-3.15	117.67	123.20
5	A	1914	ERG	C14-C8-C7	-3.15	118.19	124.38
5	A	1917	ERG	C18-C13-C17	-3.13	105.87	111.71
5	A	1907	ERG	C18-C13-C12	-3.13	105.65	110.59
5	A	1906	ERG	C18-C13-C17	-3.12	105.89	111.71
5	A	1907	ERG	C12-C13-C17	3.12	121.24	116.57
5	A	1910	ERG	C18-C13-C14	-3.11	105.21	110.24
5	A	1912	ERG	C18-C13-C14	-3.09	105.24	110.24
5	A	1904	ERG	C18-C13-C12	-3.06	105.75	110.59
5	A	1909	ERG	C7-C6-C5	-3.04	117.87	123.20
5	A	1906	ERG	C12-C13-C17	3.03	121.11	116.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1904	ERG	C18-C13-C17	-3.02	106.08	111.71
5	A	1907	ERG	C18-C13-C14	-3.02	105.35	110.24
5	A	1916	ERG	C18-C13-C17	-2.98	106.15	111.71
5	A	1905	ERG	C20-C22-C23	-2.97	116.44	125.67
5	A	1913	ERG	C12-C13-C17	2.97	121.02	116.57
5	A	1911	ERG	C14-C8-C7	-2.96	118.54	124.38
5	A	1911	ERG	C7-C6-C5	-2.96	118.00	123.20
5	A	1916	ERG	C18-C13-C14	-2.96	105.45	110.24
5	A	1914	ERG	C18-C13-C12	-2.96	105.92	110.59
5	A	1915	ERG	C6-C7-C8	-2.95	116.26	122.07
5	A	1915	ERG	C18-C13-C12	-2.94	105.94	110.59
5	A	1915	ERG	C18-C13-C17	-2.94	106.24	111.71
5	A	1906	ERG	C18-C13-C12	-2.93	105.97	110.59
5	A	1910	ERG	C12-C13-C17	2.92	120.94	116.57
5	A	1909	ERG	C24-C23-C22	-2.92	116.62	125.67
5	A	1911	ERG	C20-C22-C23	-2.88	116.72	125.67
5	A	1907	ERG	C14-C8-C7	-2.84	118.78	124.38
5	A	1910	ERG	C18-C13-C12	-2.83	106.11	110.59
5	A	1915	ERG	C12-C13-C17	2.83	120.80	116.57
5	A	1907	ERG	C14-C13-C17	2.82	102.72	99.72
5	A	1913	ERG	C18-C13-C17	-2.81	106.47	111.71
3	A	1918	POV	O31-C31-C32	2.80	120.71	111.91
5	A	1917	ERG	C12-C13-C17	2.79	120.75	116.57
5	A	1908	ERG	C20-C22-C23	-2.78	117.03	125.67
5	A	1912	ERG	C7-C6-C5	-2.78	118.32	123.20
5	A	1916	ERG	C20-C22-C23	-2.77	117.07	125.67
5	A	1912	ERG	C18-C13-C17	-2.74	106.60	111.71
5	A	1904	ERG	C18-C13-C14	-2.74	105.81	110.24
5	A	1907	ERG	C18-C13-C17	-2.73	106.61	111.71
5	A	1917	ERG	C18-C13-C12	-2.73	106.27	110.59
5	A	1915	ERG	C12-C13-C14	2.73	111.60	107.27
5	A	1910	ERG	C20-C22-C23	-2.72	117.22	125.67
5	A	1908	ERG	C19-C10-C1	-2.72	105.13	109.43
5	A	1917	ERG	C10-C5-C6	-2.72	117.80	122.58
5	A	1909	ERG	C11-C9-C8	-2.70	105.27	111.33
5	A	1915	ERG	C18-C13-C14	-2.69	105.89	110.24
5	A	1910	ERG	C11-C9-C8	-2.68	105.32	111.33
5	A	1911	ERG	C10-C5-C6	-2.67	117.88	122.58
5	A	1908	ERG	C18-C13-C14	-2.67	105.92	110.24
5	A	1915	ERG	C15-C14-C13	2.66	106.58	104.21
5	A	1914	ERG	C21-C20-C17	-2.66	107.69	113.06
5	A	1917	ERG	C18-C13-C14	-2.64	105.96	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1907	ERG	C10-C5-C6	-2.63	117.94	122.58
5	A	1917	ERG	C21-C20-C17	-2.63	107.75	113.06
5	A	1912	ERG	C10-C5-C6	-2.63	117.96	122.58
5	A	1911	ERG	C1-C10-C5	2.60	113.52	108.75
5	A	1904	ERG	C24-C23-C22	-2.60	117.61	125.67
5	A	1906	ERG	C24-C23-C22	-2.58	117.67	125.67
5	A	1908	ERG	C11-C12-C13	2.58	117.20	112.78
5	A	1914	ERG	C6-C7-C8	-2.58	117.00	122.07
5	A	1906	ERG	C18-C13-C14	-2.58	106.07	110.24
5	A	1909	ERG	C18-C13-C17	-2.57	106.92	111.71
5	A	1909	ERG	C16-C17-C20	-2.56	107.73	111.77
5	A	1906	ERG	C10-C5-C6	-2.54	118.11	122.58
5	A	1908	ERG	C12-C11-C9	2.53	118.96	112.60
5	A	1907	ERG	C11-C9-C8	-2.53	105.67	111.33
3	A	1901	POV	O31-C31-C32	2.52	119.81	111.91
5	A	1905	ERG	C16-C17-C13	-2.51	100.82	103.84
5	A	1905	ERG	C14-C8-C9	-2.51	110.88	114.66
5	A	1909	ERG	C13-C14-C8	2.51	118.34	113.48
5	A	1917	ERG	C11-C12-C13	2.50	117.07	112.78
5	A	1906	ERG	C6-C7-C8	-2.50	117.15	122.07
5	A	1906	ERG	C14-C8-C7	-2.50	119.47	124.38
5	A	1912	ERG	C12-C13-C14	2.47	111.19	107.27
4	A	1903	AV0	CCS-OCB-CCQ	-2.46	111.87	117.96
5	A	1908	ERG	C15-C14-C13	2.46	106.39	104.21
5	A	1913	ERG	C21-C20-C17	-2.45	108.10	113.06
5	A	1904	ERG	C6-C7-C8	-2.45	117.25	122.07
5	A	1917	ERG	C24-C23-C22	-2.41	118.20	125.67
5	A	1912	ERG	C6-C7-C8	-2.37	117.40	122.07
4	A	1902	AV0	CBL-CBR-CCM	-2.37	109.54	117.16
5	A	1914	ERG	C14-C13-C17	2.36	102.23	99.72
5	A	1906	ERG	C21-C20-C17	-2.35	108.31	113.06
5	A	1904	ERG	C12-C13-C17	2.35	120.09	116.57
4	A	1902	AV0	CBK-CBQ-CCM	-2.34	109.62	117.16
5	A	1910	ERG	C14-C8-C7	-2.34	119.77	124.38
5	A	1912	ERG	C18-C13-C12	-2.33	106.92	110.59
5	A	1904	ERG	C14-C8-C7	-2.32	119.81	124.38
5	A	1917	ERG	C1-C10-C5	2.32	113.00	108.75
5	A	1911	ERG	C6-C7-C8	-2.32	117.50	122.07
5	A	1911	ERG	C21-C20-C17	-2.32	108.37	113.06
5	A	1916	ERG	C10-C5-C6	-2.32	118.50	122.58
5	A	1914	ERG	C18-C13-C14	-2.32	106.49	110.24
5	A	1914	ERG	C1-C2-C3	2.31	113.44	110.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1914	ERG	C20-C22-C23	-2.31	118.52	125.67
5	A	1905	ERG	C18-C13-C14	-2.30	106.51	110.24
5	A	1913	ERG	C1-C2-C3	2.28	113.39	110.47
5	A	1913	ERG	C18-C13-C14	-2.26	106.58	110.24
5	A	1911	ERG	C14-C13-C17	2.26	102.13	99.72
5	A	1912	ERG	C11-C9-C10	-2.25	108.02	113.58
5	A	1916	ERG	C11-C9-C8	-2.23	106.34	111.33
5	A	1912	ERG	C12-C13-C17	2.22	119.89	116.57
5	A	1916	ERG	C1-C2-C3	2.21	113.31	110.47
5	A	1909	ERG	C18-C13-C14	-2.19	106.69	110.24
5	A	1906	ERG	C2-C3-C4	2.19	113.31	110.31
5	A	1910	ERG	C19-C10-C1	-2.19	105.97	109.43
5	A	1911	ERG	C18-C13-C14	-2.18	106.70	110.24
5	A	1913	ERG	C19-C10-C9	-2.18	107.37	111.03
4	A	1903	AV0	CCL-CCH-CCQ	2.16	114.62	109.68
5	A	1916	ERG	C14-C8-C7	-2.16	120.12	124.38
5	A	1909	ERG	C1-C10-C5	2.15	112.68	108.75
5	A	1912	ERG	C1-C10-C5	2.13	112.66	108.75
5	A	1905	ERG	C1-C2-C3	2.13	113.20	110.47
5	A	1913	ERG	C14-C8-C7	-2.13	120.18	124.38
5	A	1913	ERG	C6-C7-C8	-2.13	117.88	122.07
5	A	1913	ERG	C10-C5-C6	-2.12	118.86	122.58
5	A	1915	ERG	C19-C10-C9	-2.11	107.48	111.03
5	A	1912	ERG	C19-C10-C9	-2.11	107.48	111.03
5	A	1909	ERG	C10-C5-C6	-2.11	118.87	122.58
5	A	1909	ERG	C11-C12-C13	2.10	116.38	112.78
5	A	1906	ERG	C11-C9-C8	-2.09	106.64	111.33
5	A	1909	ERG	C1-C2-C3	2.09	113.15	110.47
5	A	1915	ERG	C1-C2-C3	2.08	113.13	110.47
5	A	1907	ERG	C1-C2-C3	2.07	113.13	110.47
5	A	1907	ERG	C20-C22-C23	-2.07	119.24	125.67
4	A	1903	AV0	C2-C3-C4	2.07	114.41	109.68
5	A	1906	ERG	C1-C10-C5	2.05	112.51	108.75
5	A	1906	ERG	C14-C13-C17	2.05	101.90	99.72
5	A	1908	ERG	C16-C15-C14	2.04	108.66	105.30
5	A	1915	ERG	C1-C10-C5	2.03	112.47	108.75
5	A	1905	ERG	C2-C3-C4	2.03	113.08	110.31
5	A	1908	ERG	C1-C2-C3	2.01	113.04	110.47
5	A	1914	ERG	C16-C17-C13	-2.00	101.43	103.84

There are no chirality outliers.

All (221) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1918	POV	O12-C11-C12-N
3	A	1918	POV	C22-C21-O21-C2
4	A	1902	AV0	CBL-CBR-CCM-CBQ
4	A	1902	AV0	CBL-CBR-CCM-CBS
4	A	1902	AV0	CBL-CBR-CCM-CBT
4	A	1902	AV0	O1-CBS-CCM-CBR
4	A	1902	AV0	OBV-CBT-CCM-CBQ
4	A	1902	AV0	OBV-CBT-CCM-CBR
4	A	1902	AV0	OBV-CBT-CCM-CBS
4	A	1903	AV0	O5-C1-O1-CBS
4	A	1903	AV0	CCM-CBS-O1-C1
4	A	1903	AV0	CBK-CBQ-CCM-CBR
4	A	1903	AV0	CBK-CBQ-CCM-CBS
4	A	1903	AV0	CBK-CBQ-CCM-CBT
4	A	1903	AV0	CBL-CBR-CCM-CBQ
4	A	1903	AV0	CBL-CBR-CCM-CBS
4	A	1903	AV0	CBL-CBR-CCM-CBT
4	A	1903	AV0	O1-CBS-CCM-CBQ
4	A	1903	AV0	O1-CBS-CCM-CBR
4	A	1903	AV0	OBV-CBT-CCM-CBQ
4	A	1903	AV0	OBV-CBT-CCM-CBR
5	A	1904	ERG	C13-C17-C20-C21
5	A	1904	ERG	C16-C17-C20-C21
5	A	1904	ERG	C16-C17-C20-C22
5	A	1904	ERG	C23-C24-C25-C27
5	A	1905	ERG	C13-C17-C20-C21
5	A	1905	ERG	C13-C17-C20-C22
5	A	1905	ERG	C16-C17-C20-C21
5	A	1905	ERG	C16-C17-C20-C22
5	A	1906	ERG	C13-C17-C20-C21
5	A	1906	ERG	C16-C17-C20-C21
5	A	1906	ERG	C16-C17-C20-C22
5	A	1906	ERG	C23-C24-C25-C27
5	A	1906	ERG	C28-C24-C25-C26
5	A	1906	ERG	C28-C24-C25-C27
5	A	1908	ERG	C13-C17-C20-C21
5	A	1908	ERG	C13-C17-C20-C22
5	A	1908	ERG	C16-C17-C20-C21
5	A	1908	ERG	C16-C17-C20-C22
5	A	1909	ERG	C17-C20-C22-C23
5	A	1911	ERG	C13-C17-C20-C21
5	A	1911	ERG	C16-C17-C20-C21
5	A	1913	ERG	C13-C17-C20-C21

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Mol	Chain	Res	Type	Atoms
5	A	1913	ERG	C13-C17-C20-C22
5	A	1913	ERG	C16-C17-C20-C21
5	A	1913	ERG	C16-C17-C20-C22
5	A	1914	ERG	C13-C17-C20-C21
5	A	1914	ERG	C13-C17-C20-C22
5	A	1914	ERG	C16-C17-C20-C21
5	A	1914	ERG	C16-C17-C20-C22
5	A	1914	ERG	C23-C24-C25-C27
5	A	1914	ERG	C28-C24-C25-C27
5	A	1915	ERG	C13-C17-C20-C21
5	A	1915	ERG	C16-C17-C20-C21
5	A	1916	ERG	C13-C17-C20-C21
5	A	1917	ERG	C13-C17-C20-C21
5	A	1917	ERG	C13-C17-C20-C22
5	A	1917	ERG	C16-C17-C20-C21
5	A	1917	ERG	C16-C17-C20-C22
5	A	1917	ERG	C17-C20-C22-C23
5	A	1917	ERG	C22-C23-C24-C25
3	A	1918	POV	O22-C21-O21-C2
4	A	1903	AV0	OAJ-CBN-CCD-CCO
4	A	1903	AV0	OAI-CBM-CCC-OBY
4	A	1903	AV0	OAL-CBP-CCF-OBX
4	A	1902	AV0	C3-C4-O4-CCR
4	A	1903	AV0	OAJ-CBN-CCD-OBZ
4	A	1903	AV0	OAL-CBP-CCF-CCQ
4	A	1903	AV0	O1-CBS-CCM-CBT
4	A	1903	AV0	OAI-CBM-CCC-CCN
5	A	1905	ERG	C17-C20-C22-C23
5	A	1908	ERG	C22-C23-C24-C25
5	A	1916	ERG	C17-C20-C22-C23
3	A	1901	POV	C21-C22-C23-C24
4	A	1903	AV0	OBV-CBT-CCM-CBS
3	A	1901	POV	C35-C36-C37-C38
5	A	1904	ERG	C28-C24-C25-C26
5	A	1904	ERG	C28-C24-C25-C27
5	A	1906	ERG	C23-C24-C25-C26
5	A	1912	ERG	C23-C24-C25-C27
5	A	1913	ERG	C28-C24-C25-C26
5	A	1914	ERG	C23-C24-C25-C26
5	A	1914	ERG	C28-C24-C25-C26
5	A	1916	ERG	C28-C24-C25-C26
3	A	1901	POV	C310-C311-C312-C313

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Mol	Chain	Res	Type	Atoms
3	A	1901	POV	C37-C38-C39-C310
4	A	1902	AV0	CBD-CBF-CBH-CBJ
3	A	1918	POV	C37-C38-C39-C310
3	A	1918	POV	C33-C34-C35-C36
3	A	1901	POV	C214-C215-C216-C217
3	A	1901	POV	C312-C313-C314-C315
4	A	1902	AV0	CBG-CBI-CBK-CBQ
5	A	1904	ERG	C13-C17-C20-C22
5	A	1906	ERG	C13-C17-C20-C22
5	A	1907	ERG	C13-C17-C20-C21
5	A	1911	ERG	C13-C17-C20-C22
5	A	1916	ERG	C16-C17-C20-C21
3	A	1918	POV	C23-C24-C25-C26
3	A	1918	POV	C36-C37-C38-C39
4	A	1902	AV0	CAZ-CBB-CBD-CBF
5	A	1904	ERG	C22-C23-C24-C25
5	A	1913	ERG	C22-C23-C24-C25
5	A	1914	ERG	C22-C23-C24-C25
5	A	1915	ERG	C22-C23-C24-C25
5	A	1906	ERG	C22-C23-C24-C28
5	A	1908	ERG	C21-C20-C22-C23
5	A	1910	ERG	C21-C20-C22-C23
5	A	1911	ERG	C21-C20-C22-C23
5	A	1911	ERG	C22-C23-C24-C28
5	A	1915	ERG	C22-C23-C24-C28
3	A	1918	POV	C35-C36-C37-C38
3	A	1918	POV	C34-C35-C36-C37
3	A	1901	POV	C26-C27-C28-C29
3	A	1918	POV	C210-C211-C212-C213
3	A	1918	POV	C26-C27-C28-C29
3	A	1918	POV	C213-C214-C215-C216
3	A	1901	POV	C211-C212-C213-C214
5	A	1904	ERG	C22-C23-C24-C28
5	A	1905	ERG	C21-C20-C22-C23
5	A	1914	ERG	C22-C23-C24-C28
5	A	1916	ERG	C21-C20-C22-C23
4	A	1902	AV0	CAW-CAY-CBA-CBC
4	A	1903	AV0	CAZ-CBB-CBD-CBF
3	A	1901	POV	C33-C34-C35-C36
3	A	1918	POV	C212-C213-C214-C215
4	A	1903	AV0	CBE-CBG-CBI-CBK
5	A	1904	ERG	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
5	A	1912	ERG	C23-C24-C25-C26
5	A	1913	ERG	C23-C24-C25-C26
5	A	1913	ERG	C23-C24-C25-C27
5	A	1913	ERG	C28-C24-C25-C27
5	A	1916	ERG	C23-C24-C25-C26
5	A	1916	ERG	C23-C24-C25-C27
5	A	1916	ERG	C28-C24-C25-C27
4	A	1903	AV0	CBC-CBE-CBG-CBI
3	A	1901	POV	C34-C35-C36-C37
3	A	1918	POV	C1-C2-C3-O31
3	A	1918	POV	C211-C212-C213-C214
5	A	1906	ERG	C22-C23-C24-C25
5	A	1908	ERG	C17-C20-C22-C23
5	A	1911	ERG	C17-C20-C22-C23
5	A	1913	ERG	C22-C23-C24-C28
5	A	1916	ERG	C22-C23-C24-C28
4	A	1902	AV0	CBC-CBE-CBG-CBI
4	A	1902	AV0	CBE-CBG-CBI-CBK
4	A	1903	AV0	C2-C1-O1-CBS
3	A	1901	POV	C25-C26-C27-C28
4	A	1902	AV0	C5-C4-O4-CCR
5	A	1907	ERG	C13-C17-C20-C22
5	A	1907	ERG	C16-C17-C20-C21
5	A	1910	ERG	C13-C17-C20-C21
5	A	1915	ERG	C13-C17-C20-C22
5	A	1916	ERG	C13-C17-C20-C22
4	A	1902	AV0	CAA-CAW-CAY-CBA
4	A	1902	AV0	CBK-CBQ-CCM-CBR
5	A	1909	ERG	C22-C23-C24-C28
4	A	1903	AV0	CAW-CAY-CBA-CBC
5	A	1910	ERG	C23-C24-C25-C27
3	A	1918	POV	C311-C312-C313-C314
3	A	1901	POV	O21-C2-C3-O31
3	A	1918	POV	C215-C216-C217-C218
4	A	1902	AV0	C4-C5-C6-O6
4	A	1903	AV0	CBA-CBC-CBE-CBG
3	A	1901	POV	C1-C2-C3-O31
4	A	1902	AV0	O1-CBS-CCM-CBT
5	A	1915	ERG	C21-C20-C22-C23
4	A	1902	AV0	O1-CBS-CCM-CBQ
3	A	1901	POV	C11-O12-P-O11
5	A	1909	ERG	C28-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
5	A	1912	ERG	C28-C24-C25-C27
4	A	1902	AV0	CAX-CAZ-CBB-CBD
3	A	1901	POV	C32-C33-C34-C35
3	A	1901	POV	C313-C314-C315-C316
4	A	1902	AV0	CBK-CBQ-CCM-CBS
4	A	1902	AV0	CBK-CBQ-CCM-CBT
3	A	1918	POV	O21-C2-C3-O31
5	A	1910	ERG	C17-C20-C22-C23
5	A	1911	ERG	C22-C23-C24-C25
5	A	1916	ERG	C22-C23-C24-C25
4	A	1902	AV0	CBF-CBH-CBJ-CBL
3	A	1901	POV	C23-C24-C25-C26
4	A	1902	AV0	CAY-CBA-CBC-CBE
3	A	1918	POV	C31-C32-C33-C34
3	A	1901	POV	C1-O11-P-O12
5	A	1909	ERG	C23-C24-C25-C26
5	A	1909	ERG	C23-C24-C25-C27
5	A	1910	ERG	C23-C24-C25-C26
5	A	1912	ERG	C28-C24-C25-C26
5	A	1912	ERG	C22-C23-C24-C28
5	A	1912	ERG	C13-C17-C20-C21
5	A	1915	ERG	C16-C17-C20-C22
3	A	1901	POV	C210-C211-C212-C213
3	A	1918	POV	C24-C25-C26-C27
5	A	1906	ERG	C21-C20-C22-C23
4	A	1902	AV0	O5-C5-C6-O6
4	A	1903	AV0	CBB-CBD-CBF-CBH
4	A	1902	AV0	OBX-CCJ-OBV-CBT
5	A	1904	ERG	C21-C20-C22-C23
5	A	1914	ERG	C21-C20-C22-C23
3	A	1918	POV	O11-C1-C2-O21
3	A	1901	POV	C311-C312-C313-C314
4	A	1903	AV0	CBI-CBK-CBQ-CCM
5	A	1911	ERG	C16-C17-C20-C22
5	A	1916	ERG	C16-C17-C20-C22
5	A	1909	ERG	C21-C20-C22-C23
5	A	1917	ERG	C22-C23-C24-C28
3	A	1918	POV	C29-C210-C211-C212
5	A	1909	ERG	C22-C23-C24-C25
3	A	1901	POV	O11-C1-C2-C3
4	A	1903	AV0	CBD-CBF-CBH-CBJ
5	A	1910	ERG	C22-C23-C24-C28

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Mol	Chain	Res	Type	Atoms
5	A	1912	ERG	C21-C20-C22-C23
5	A	1913	ERG	C21-C20-C22-C23
5	A	1917	ERG	C21-C20-C22-C23
3	A	1901	POV	C29-C210-C211-C212
3	A	1901	POV	C1-O11-P-O14
3	A	1918	POV	C1-O11-P-O14
5	A	1909	ERG	C28-C24-C25-C27
5	A	1910	ERG	C16-C17-C20-C21
3	A	1901	POV	C311-C310-C39-C38
3	A	1901	POV	C212-C213-C214-C215

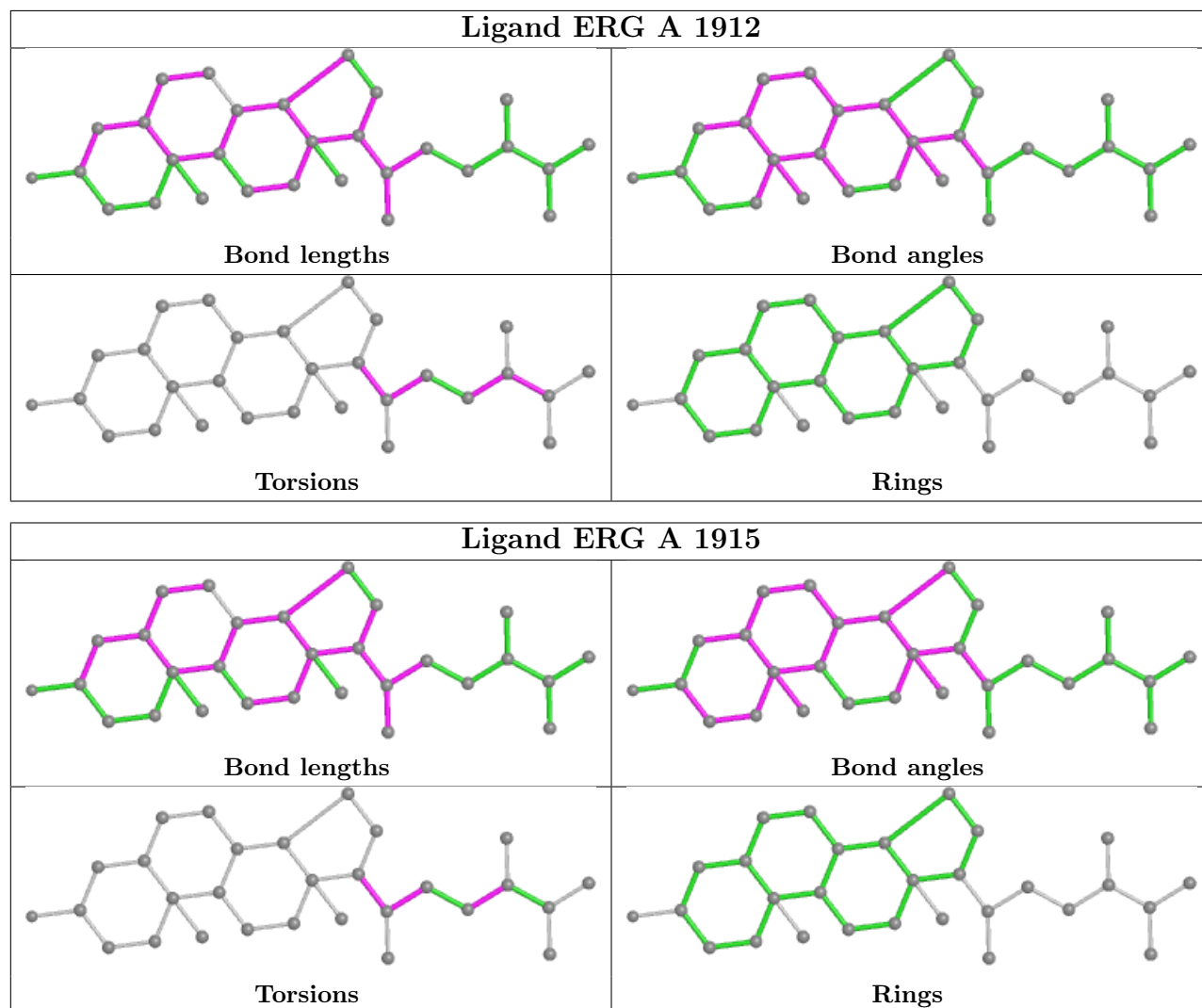
There are no ring outliers.

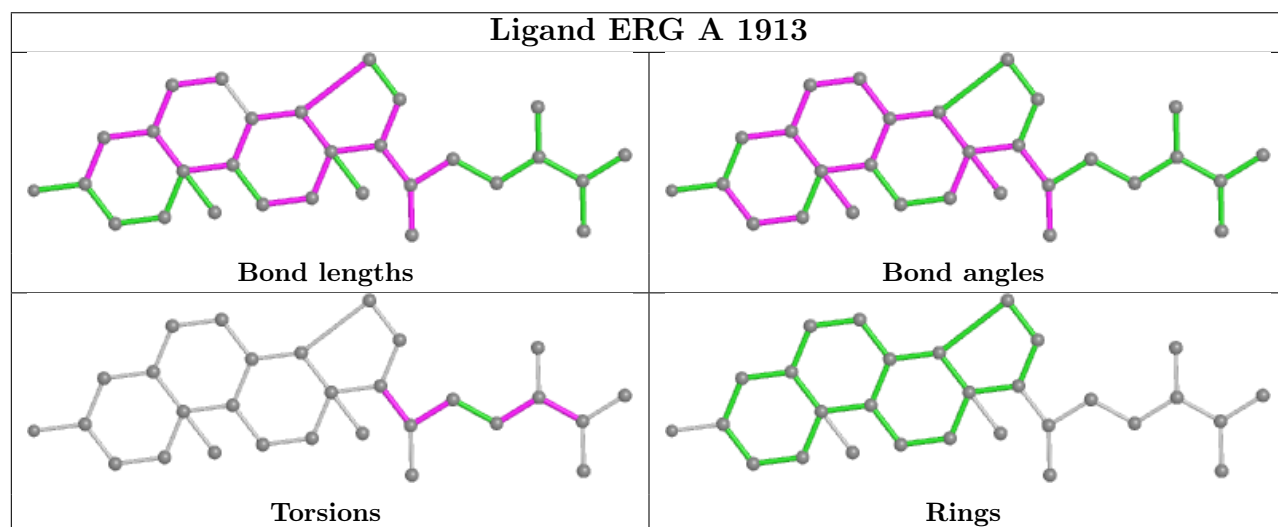
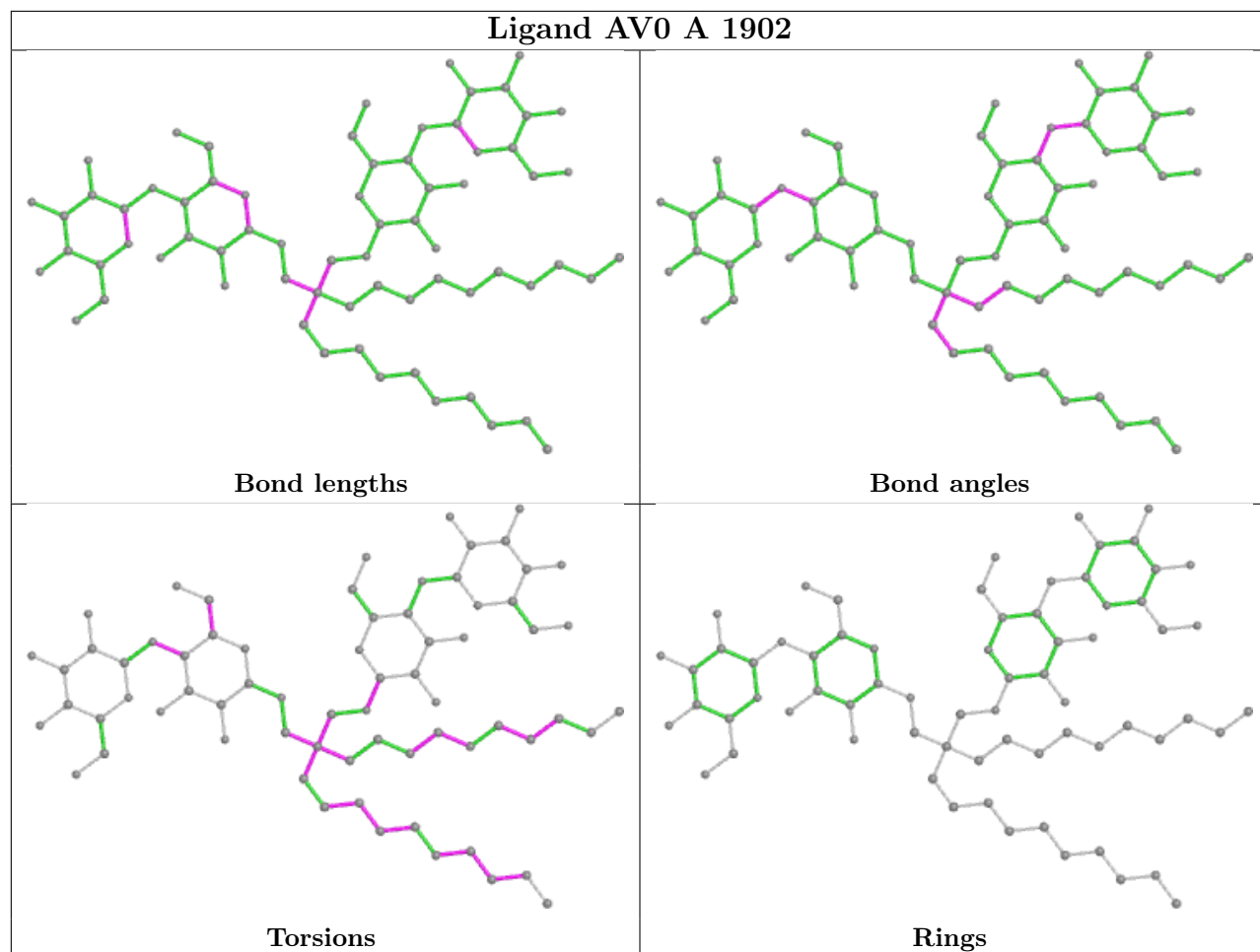
17 monomers are involved in 56 short contacts:

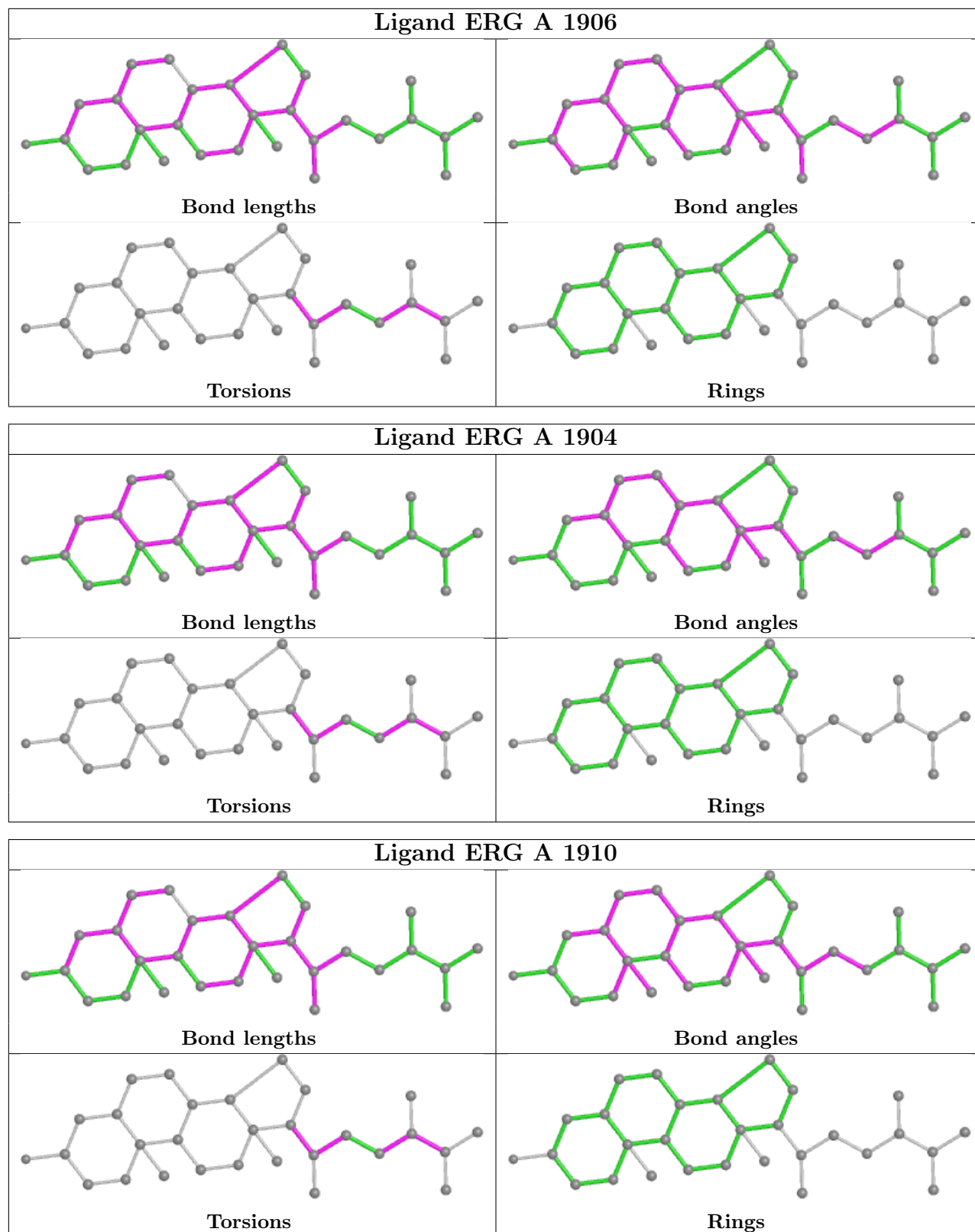
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1912	ERG	1	0
5	A	1915	ERG	6	0
4	A	1902	AV0	4	0
5	A	1913	ERG	1	0
5	A	1906	ERG	5	0
5	A	1904	ERG	2	0
5	A	1910	ERG	1	0
5	A	1905	ERG	3	0
5	A	1909	ERG	6	0
5	A	1914	ERG	7	0
5	A	1908	ERG	3	0
5	A	1916	ERG	5	0
5	A	1917	ERG	5	0
5	A	1907	ERG	3	0
3	A	1918	POV	4	0
5	A	1911	ERG	6	0
3	A	1901	POV	5	0

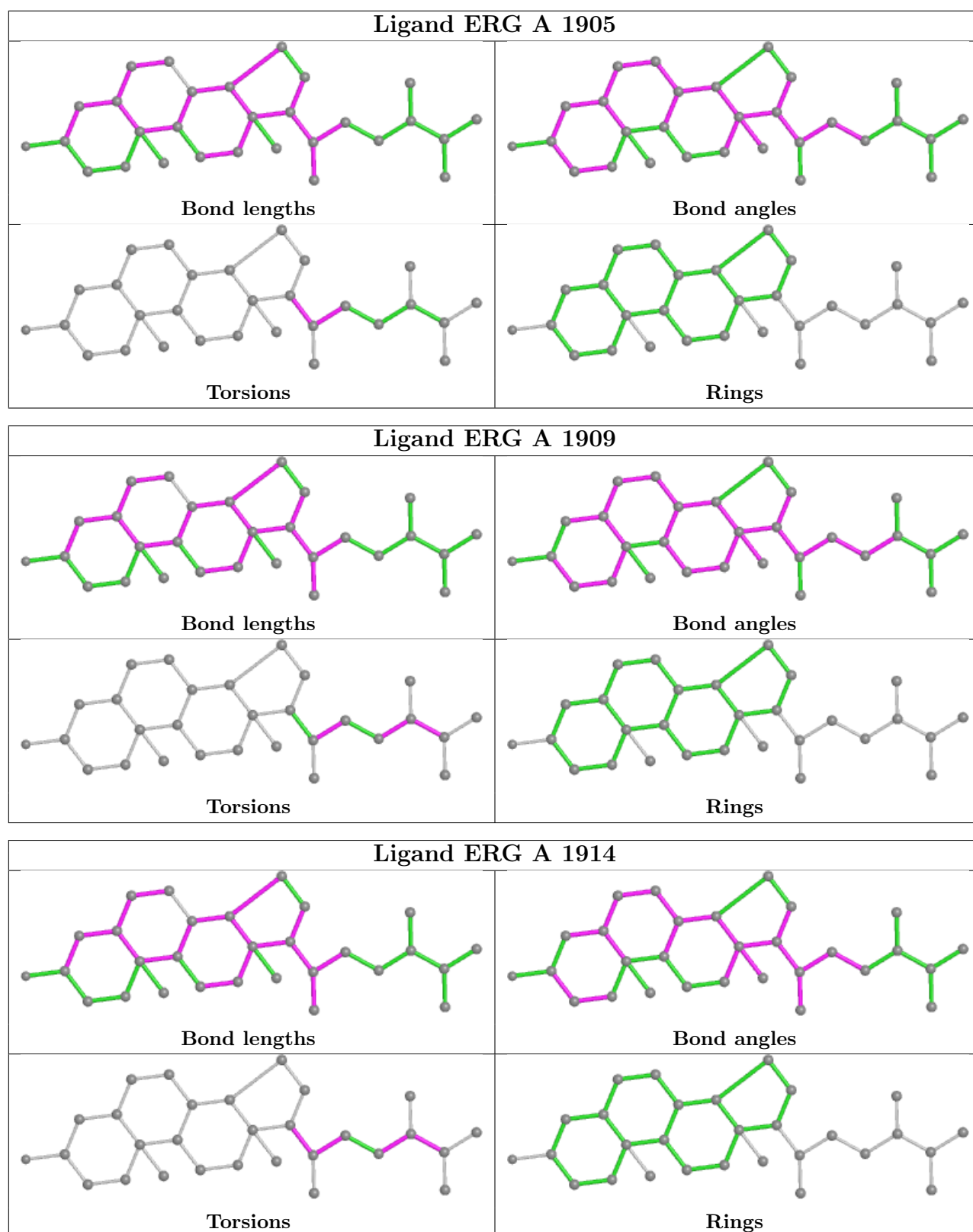
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

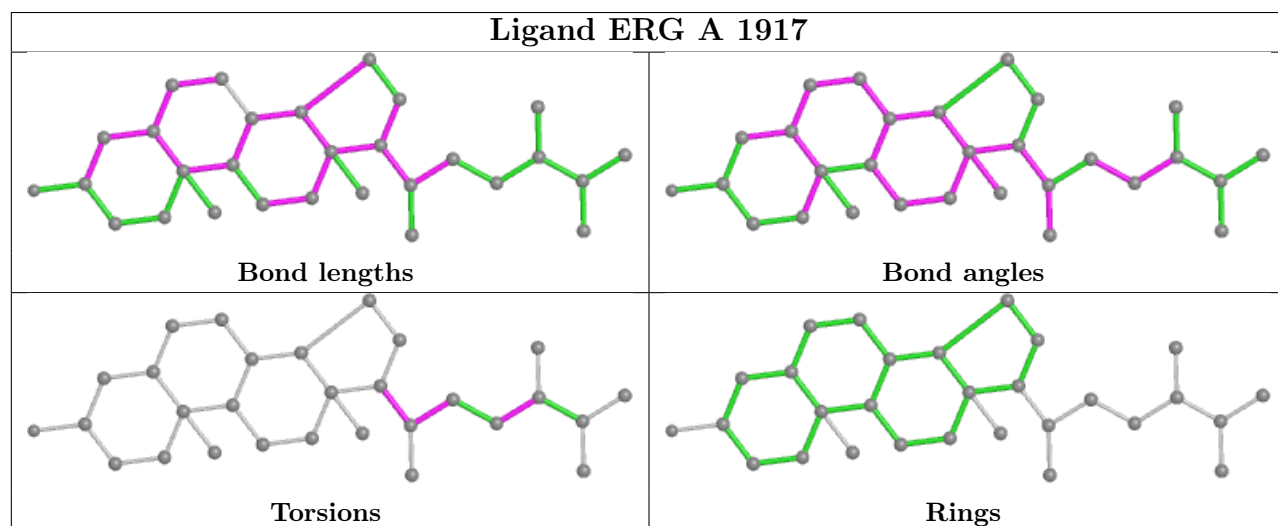
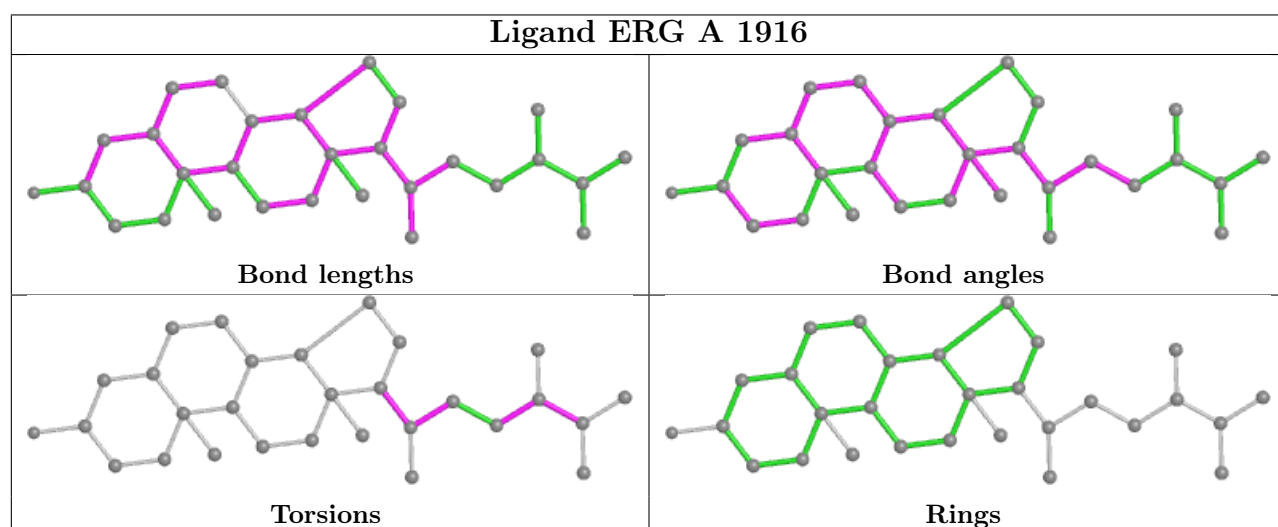
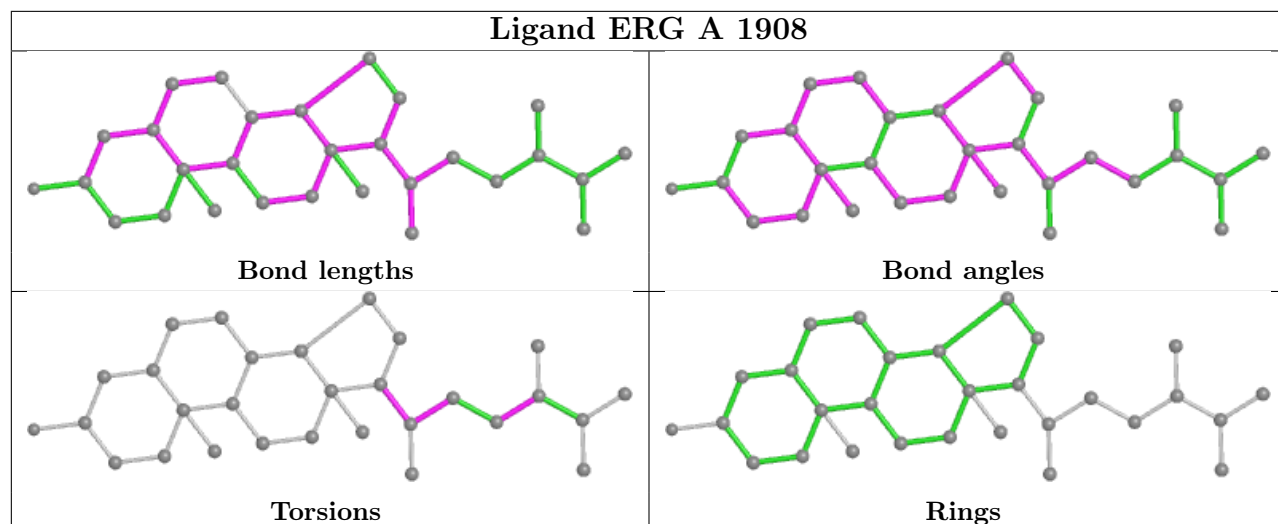
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

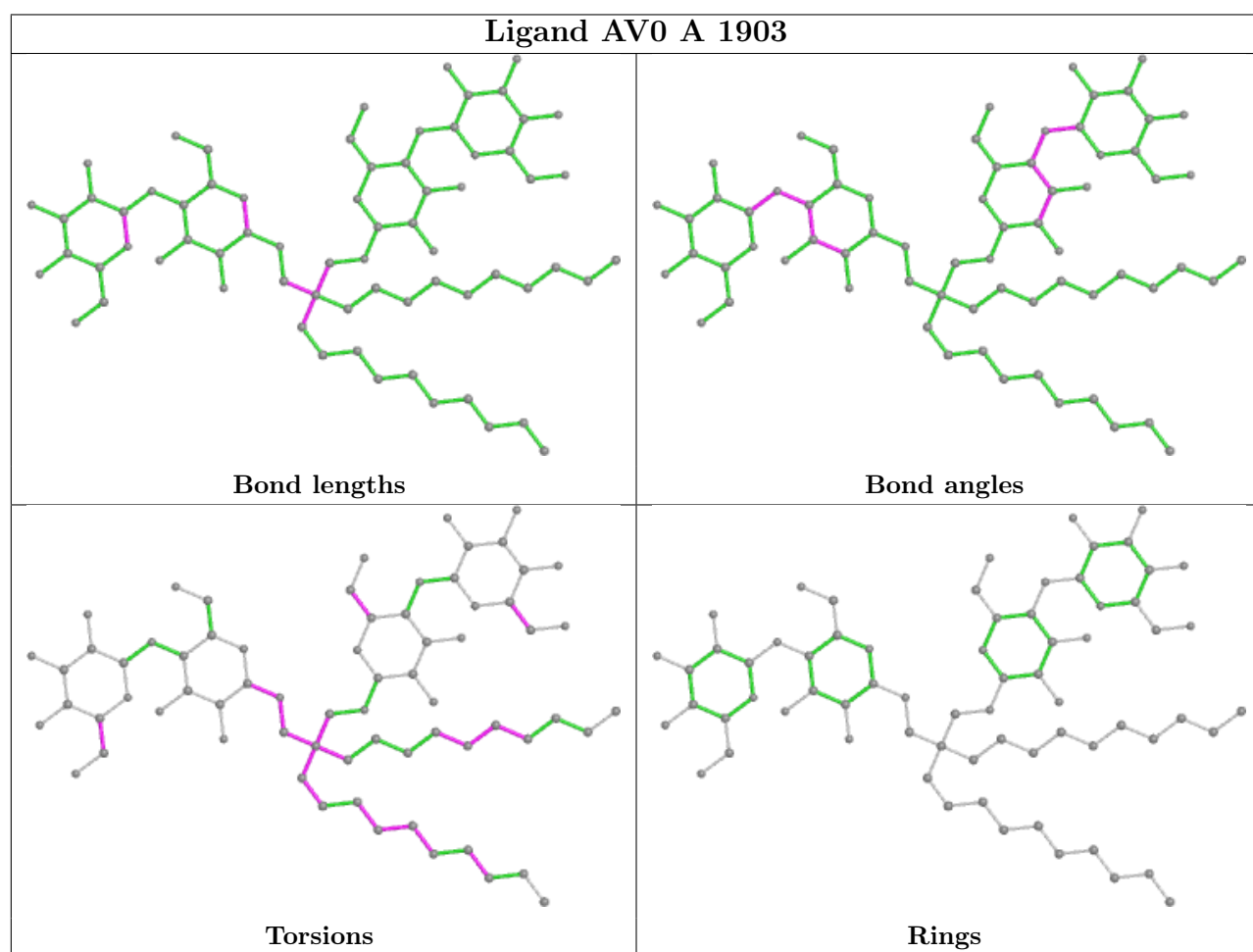
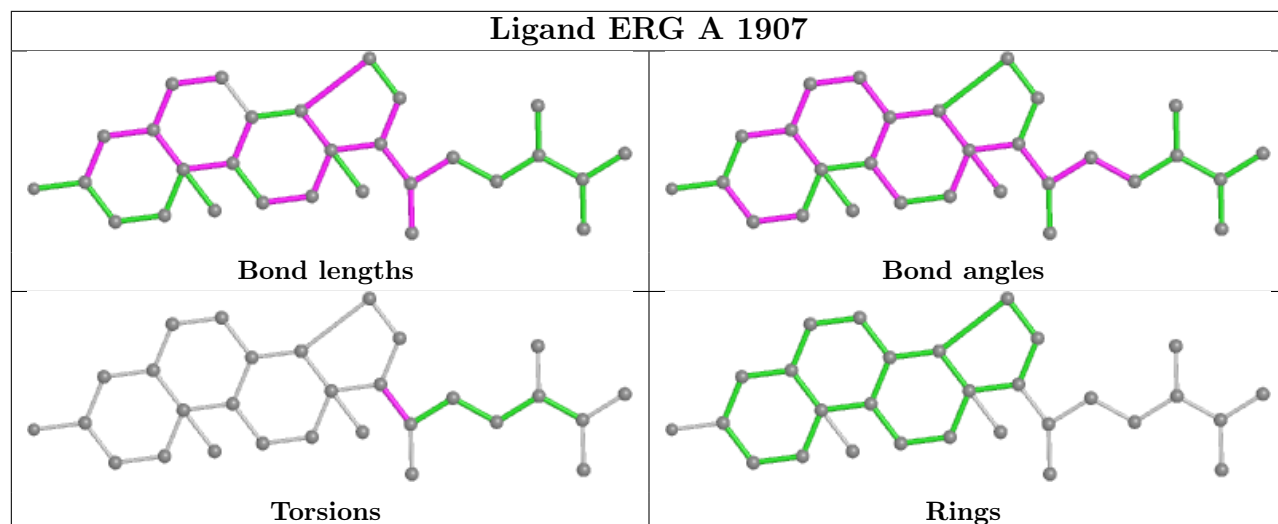


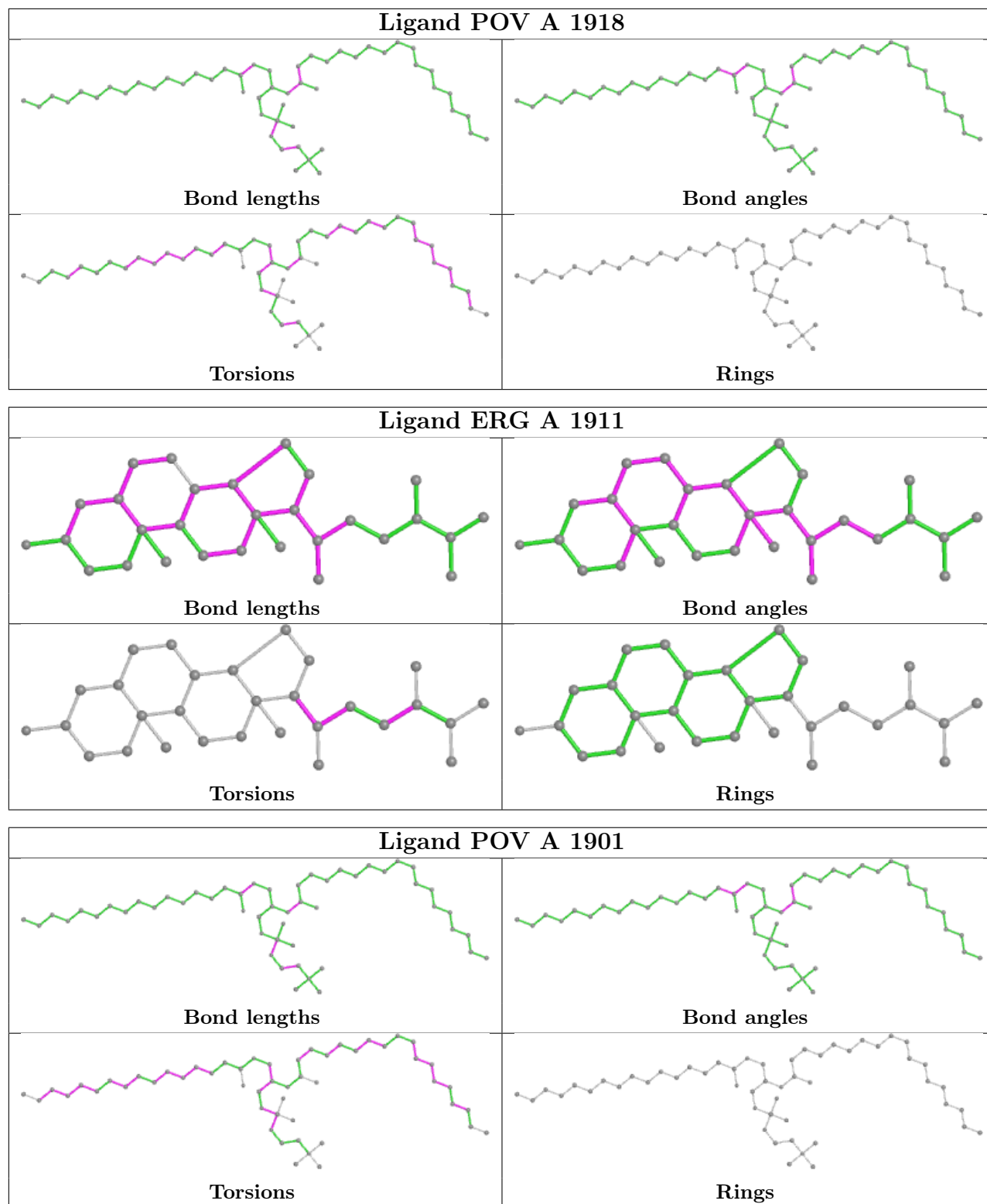












5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

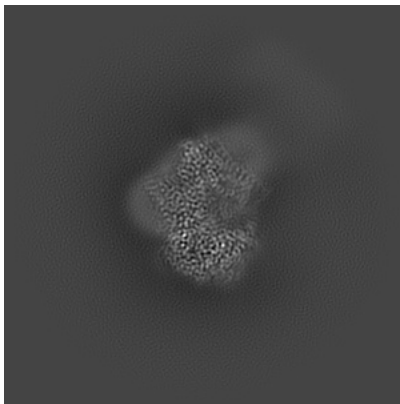
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36748. These allow visual inspection of the internal detail of the map and identification of artifacts.

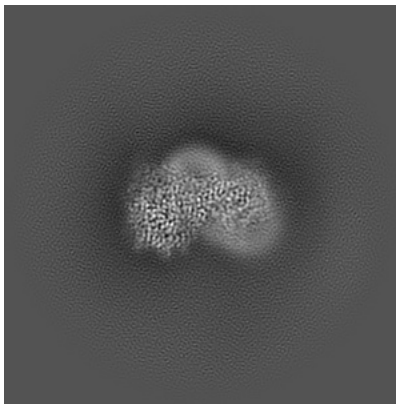
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

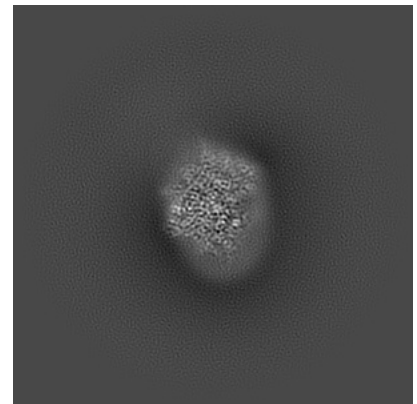
6.1.1 Primary map



X

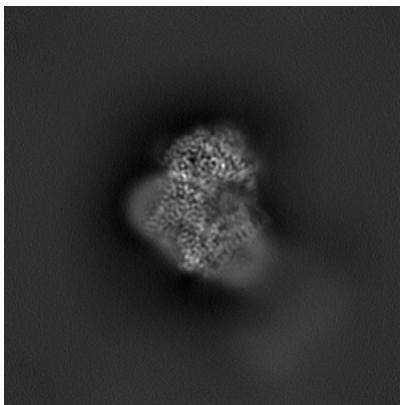


Y

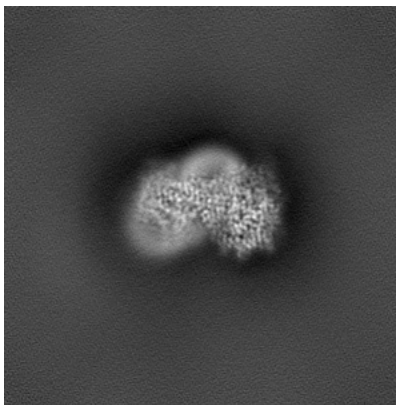


Z

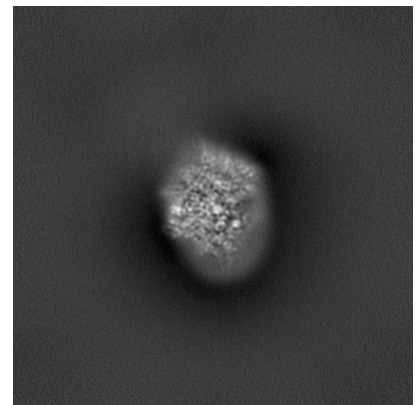
6.1.2 Raw map



X



Y

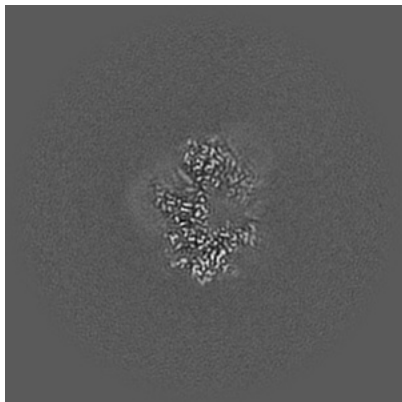


Z

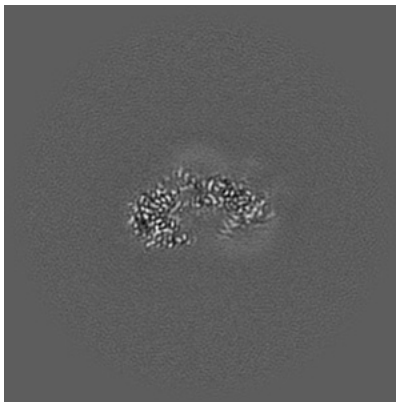
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

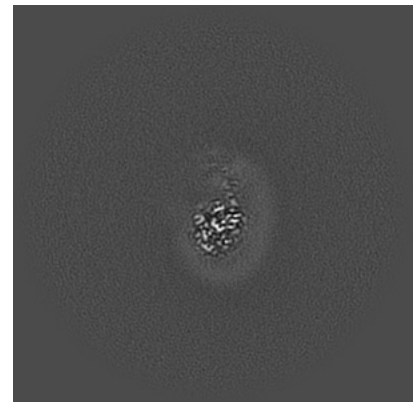
6.2.1 Primary map



X Index: 150

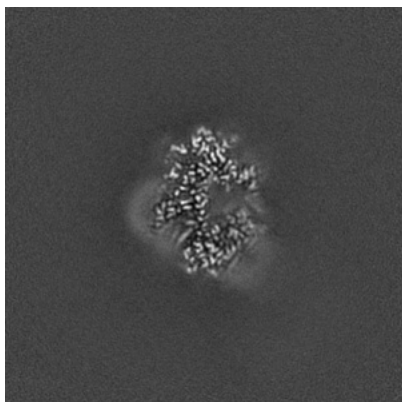


Y Index: 150

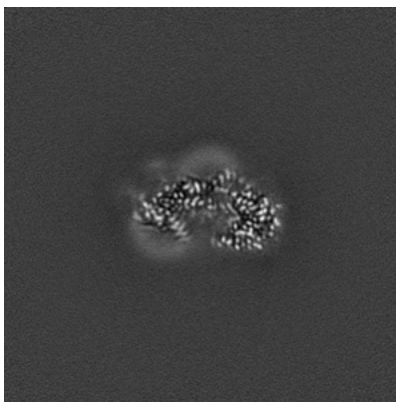


Z Index: 150

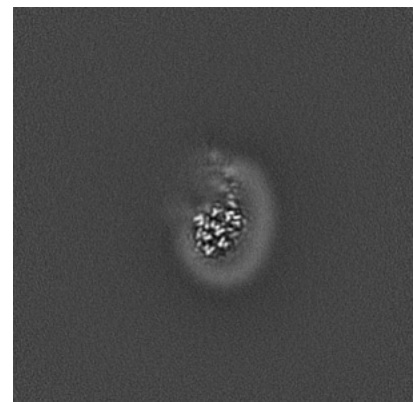
6.2.2 Raw map



X Index: 150



Y Index: 150

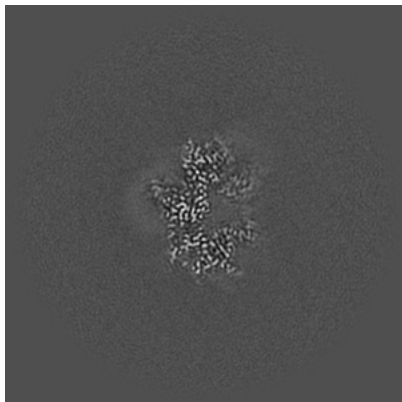


Z Index: 150

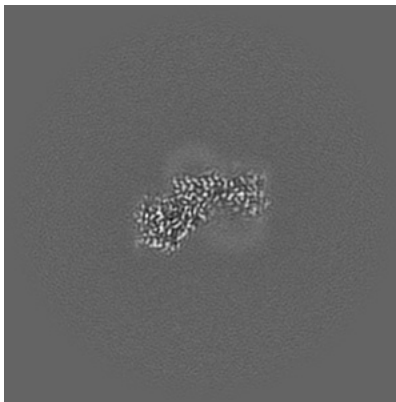
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

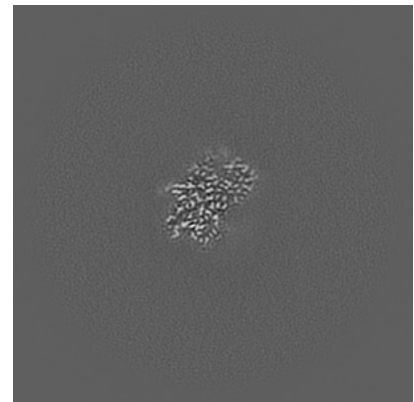
6.3.1 Primary map



X Index: 153

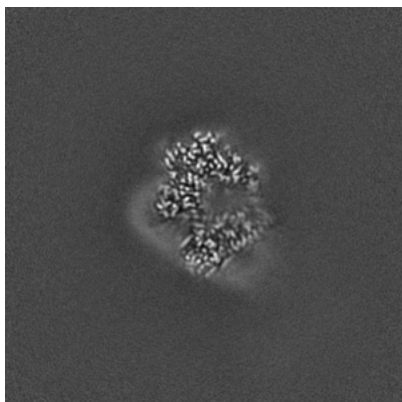


Y Index: 137

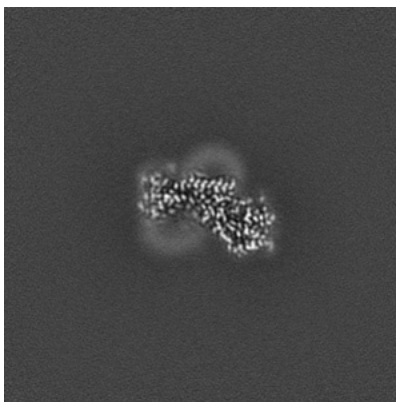


Z Index: 119

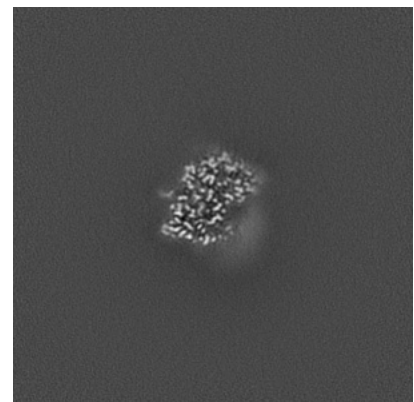
6.3.2 Raw map



X Index: 146



Y Index: 137

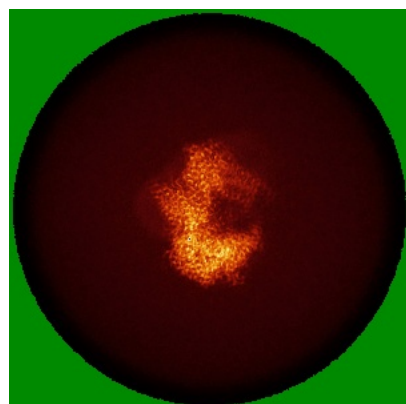


Z Index: 175

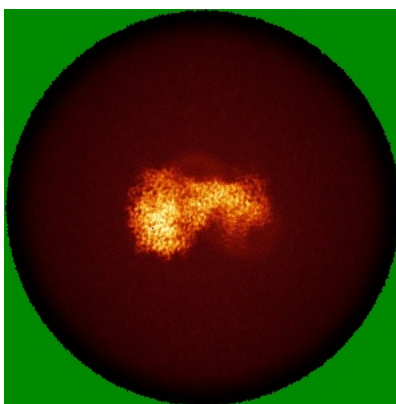
The images above show the largest variance slices of the map in three orthogonal directions.

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

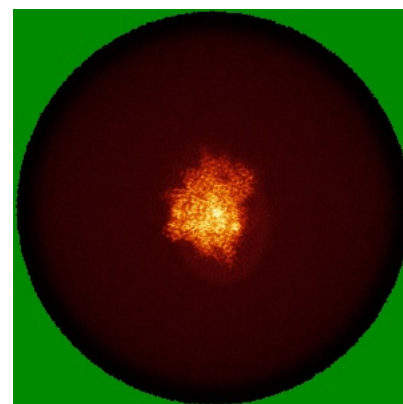
6.4.1 Primary map



X

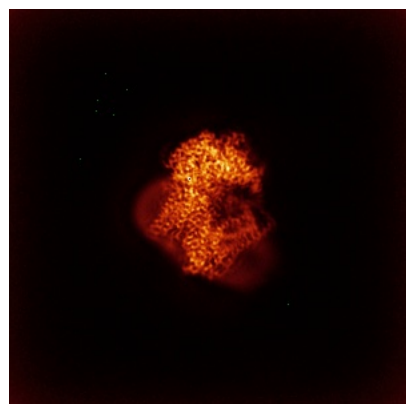


Y

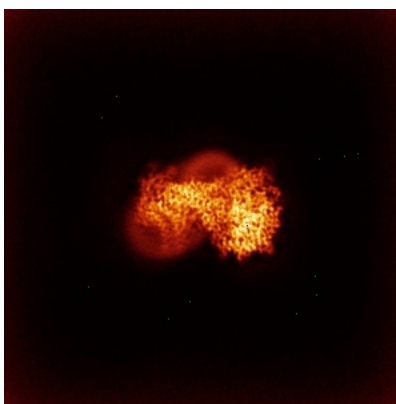


Z

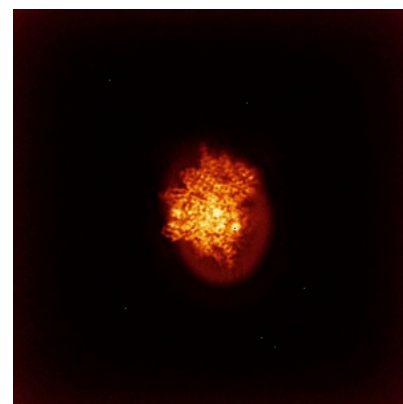
6.4.2 Raw map



X



Y

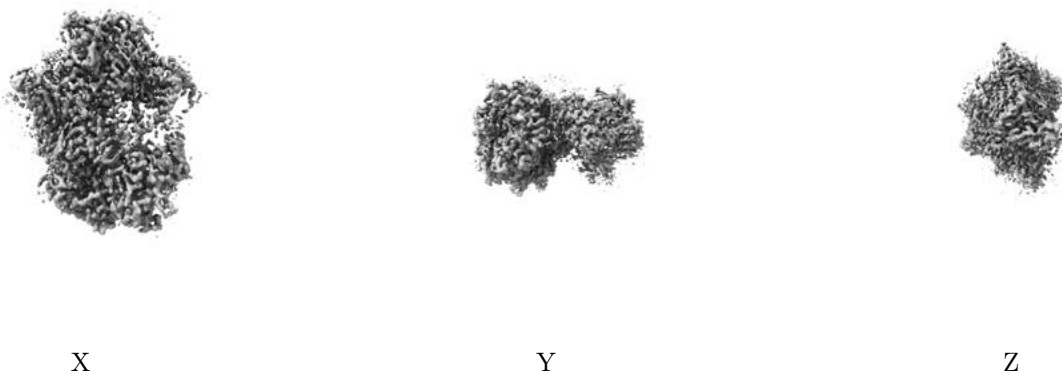


Z

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.

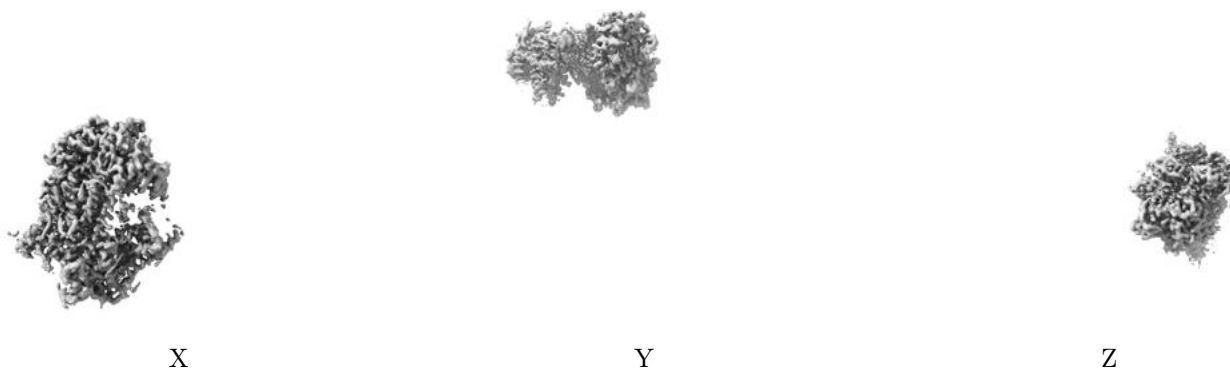
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.47. 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.

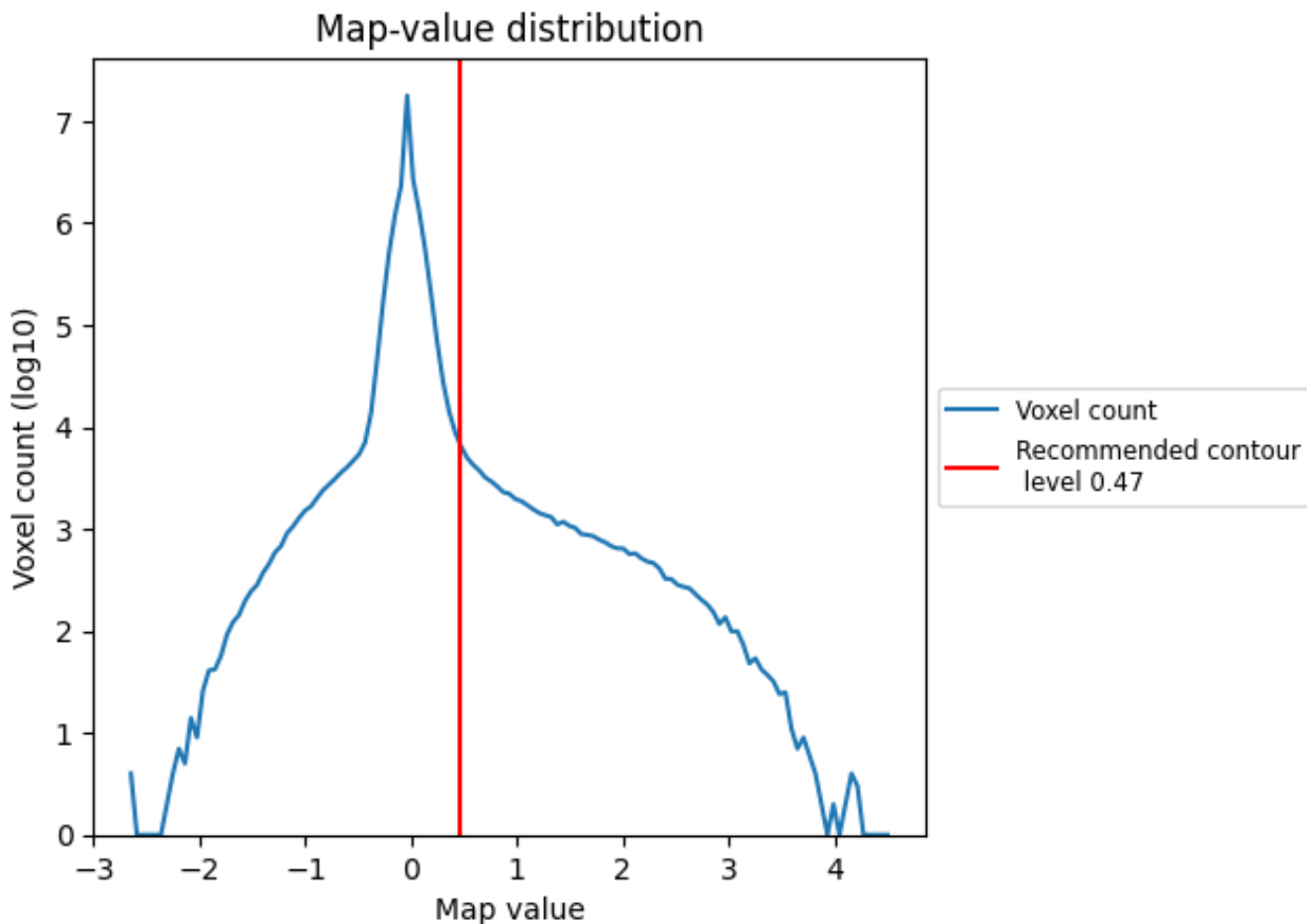
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

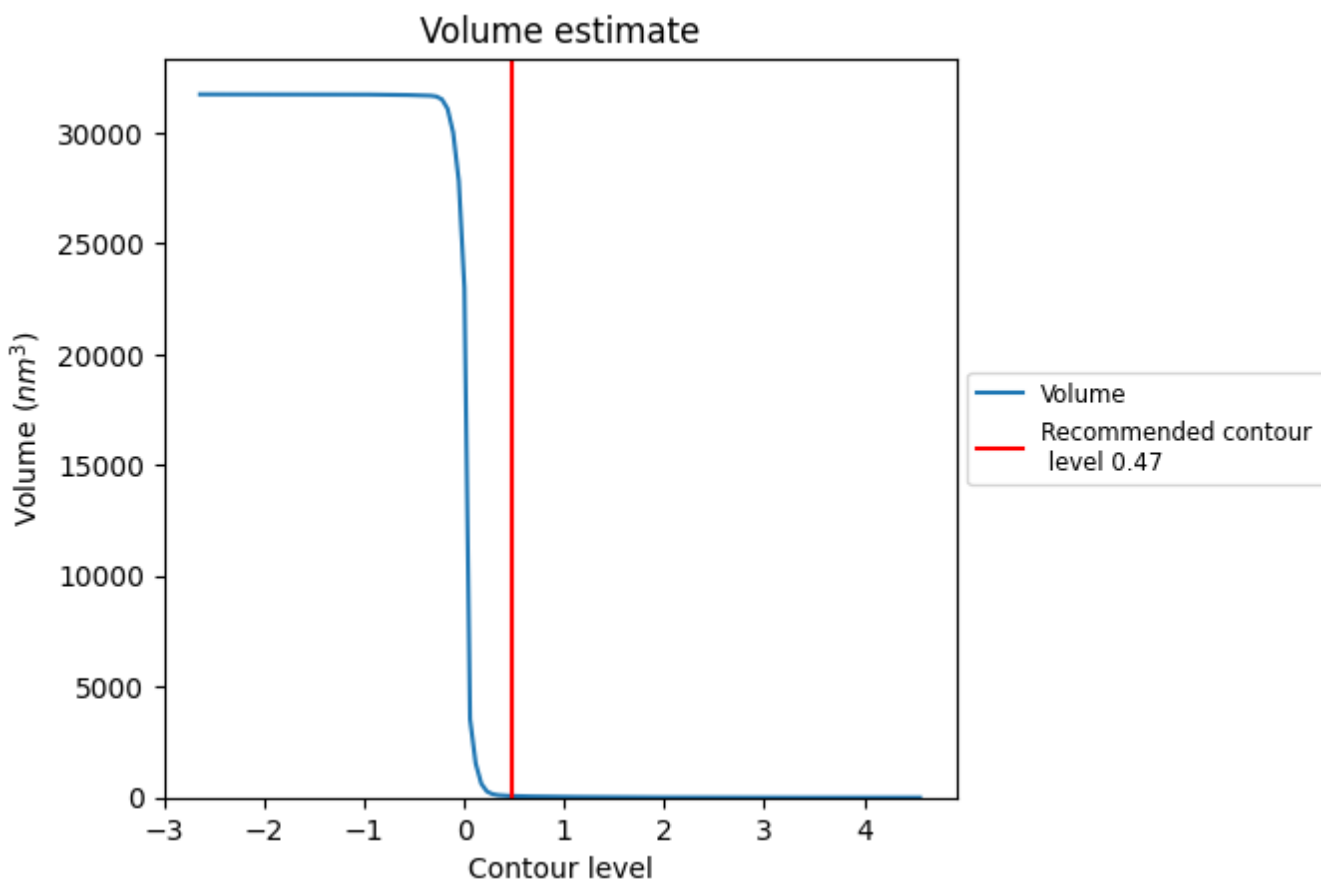
This section contains the results of statistical analysis of the map.

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.

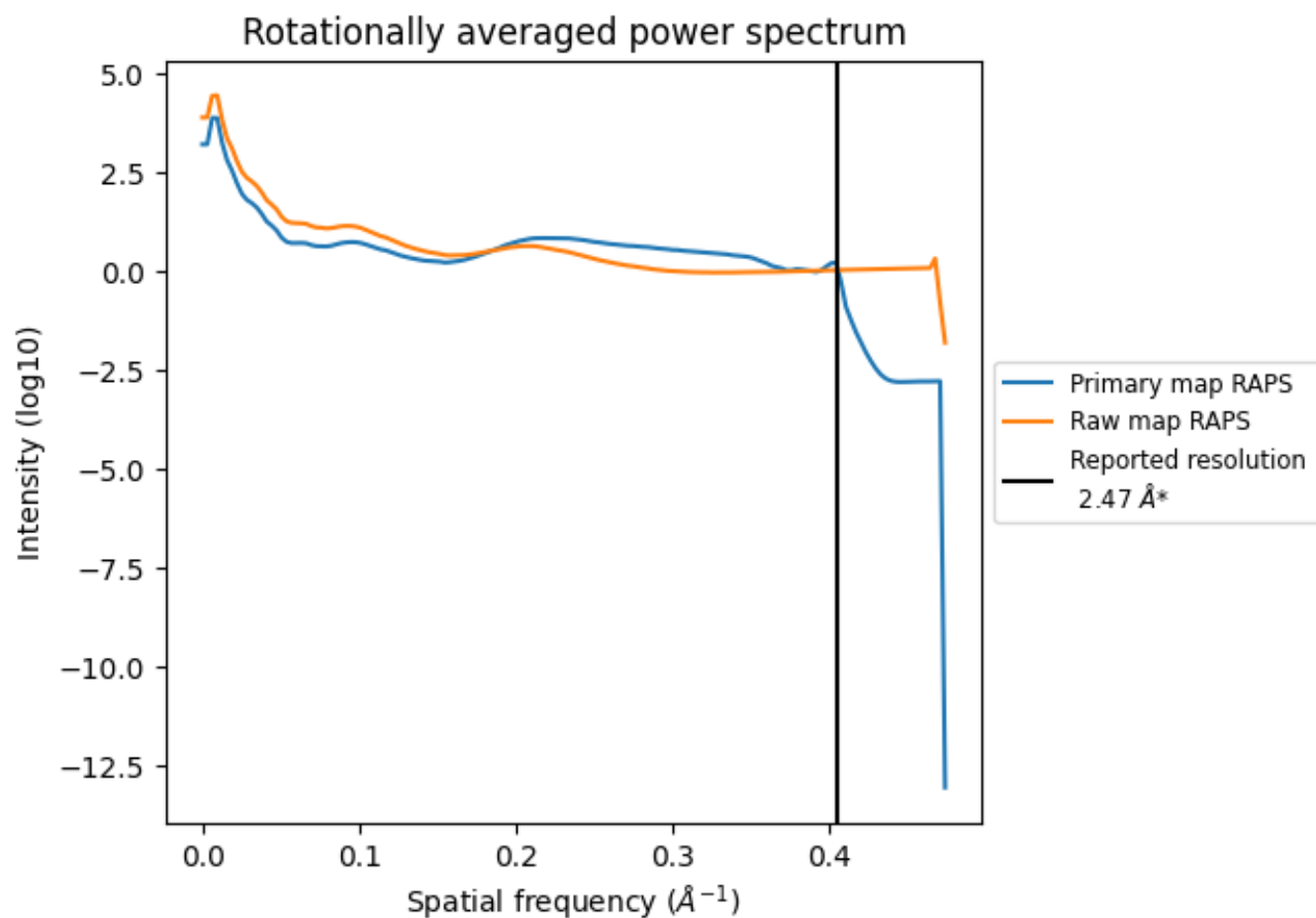
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 72 nm^3 ; this corresponds to an approximate mass of 65 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum i

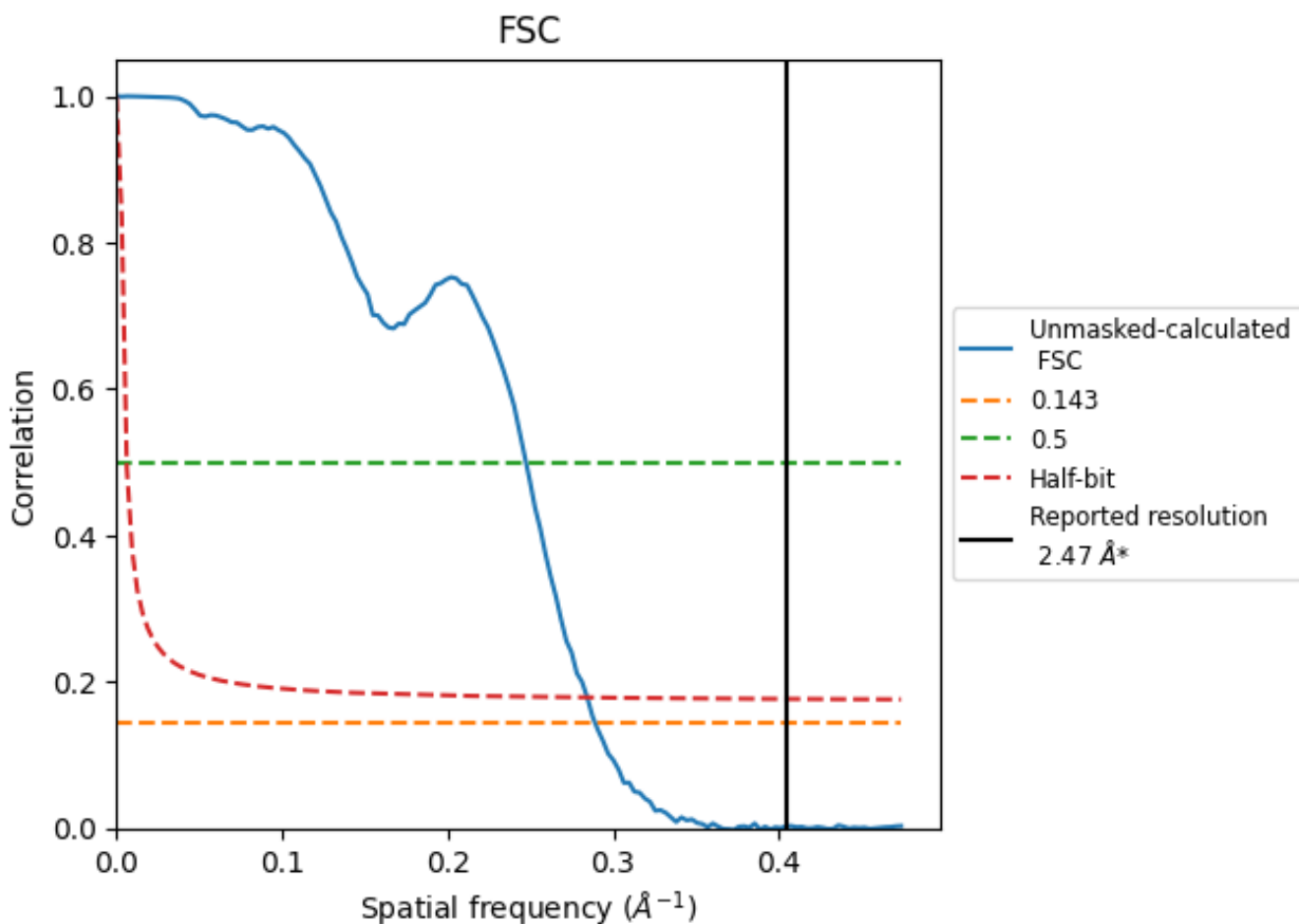


*Reported resolution corresponds to spatial frequency of 0.405 Å⁻¹

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 0.405 Å⁻¹

8.2 Resolution estimates [i](#)

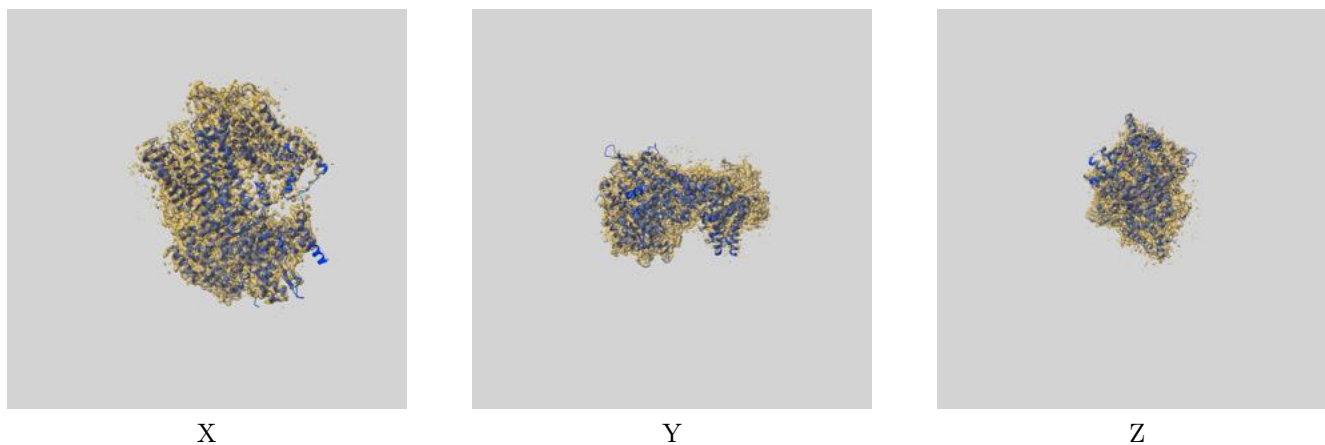
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.47	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.46	4.05	3.52

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.46 differs from the reported value 2.47 by more than 10 %

9 Map-model fit [i](#)

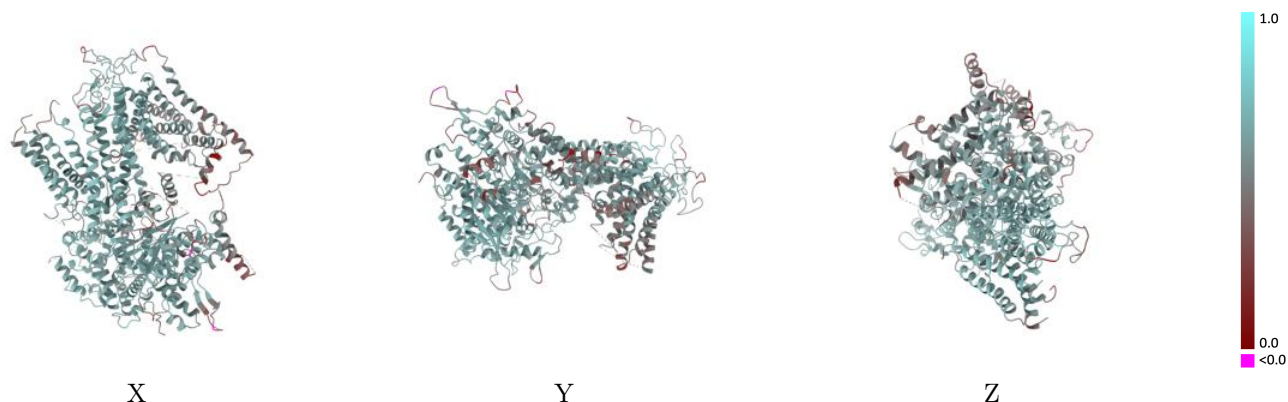
This section contains information regarding the fit between EMDB map EMD-36748 and PDB model 8JZN. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



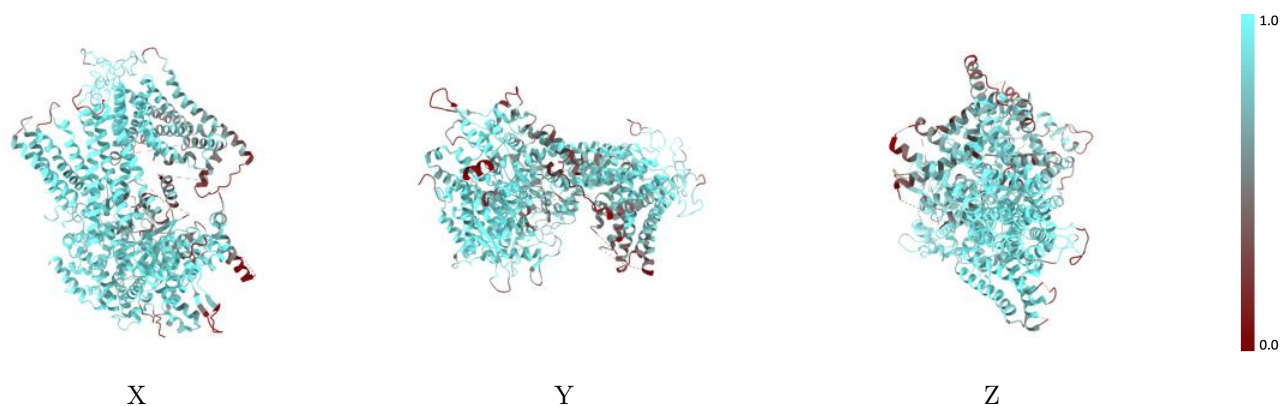
The images above show the 3D surface view of the map at the recommended contour level 0.47 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



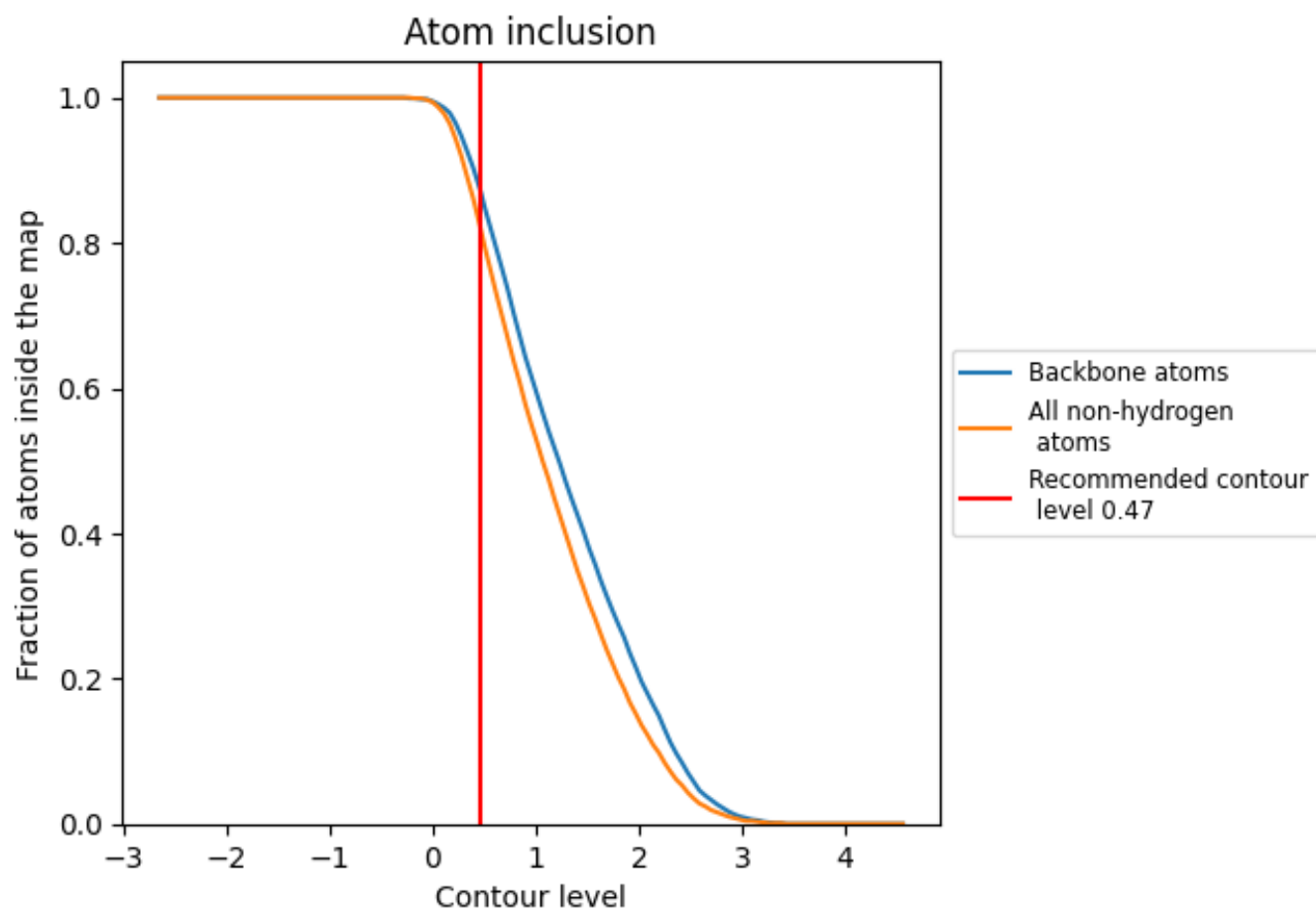
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.47).







9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 82% 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 (0.47) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8170	 0.5770
A	 0.8170	 0.5770
B	 0.7860	 0.5610

