



Full wwPDB EM Validation Report ⓘ

Mar 17, 2026 – 03:11 PM UTC

PDB ID : 9UTW / pdb_00009utw
EMDB ID : EMD-64502
Title : Structure of dimeric FKS1 in complex with tRNA
Authors : Li, J.L.; Zhu, A.Q.; Liu, J.X.; Dai, X.L.; Wang, X.; Yan, C.Y.; Deng, D.
Deposited on : 2025-05-05
Resolution : 2.96 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

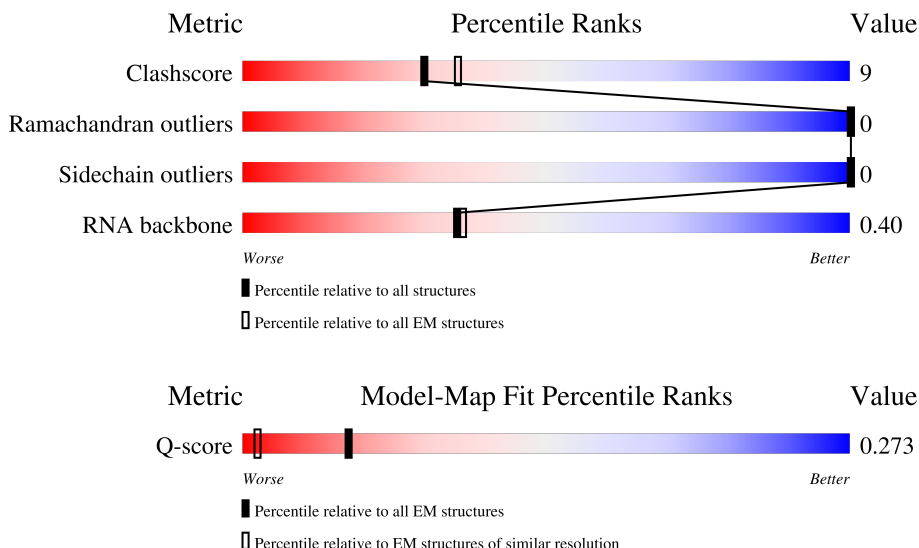
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.96 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	-
RNA backbone	8273	3508	-
Q-score	-	25397	13155 (2.46 - 3.46)

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	C	197	 10% 87%
1	G	197	 11% 87%
2	B	1876	 9% 65% 10% 25%

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Mol	Chain	Length	Quality of chain
2	H	1876	55% 20% 25%
3	A	76	61% 22% 39% 18% 18%
4	J	3	67% 67% 33%
5	D	2	100% 100%

2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 25408 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 Uncharacterized protein YMR295C.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	C	25	Total	C	N	O	0	0
			203	124	38	41		
1	G	25	Total	C	N	O	0	0
			203	124	38	41		

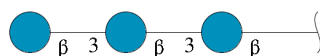
- Molecule 2 is a protein called 1,3-beta-glucan synthase component FKS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	1409	Total	C	N	O	S	0	0
			11499	7526	1918	1981	74		
2	B	1409	Total	C	N	O	S	0	0
			11499	7526	1918	1981	74		

- Molecule 3 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	62	Total	C	N	O	P	0	0
			1319	587	228	442	62		

- Molecule 4 is an oligosaccharide called beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms			AltConf	Trace
4	J	3	Total	C	O	0	0
			34	18	16		

- Molecule 5 is an oligosaccharide called beta-D-glucopyranose-(1-3)-beta-D-glucopyranose.

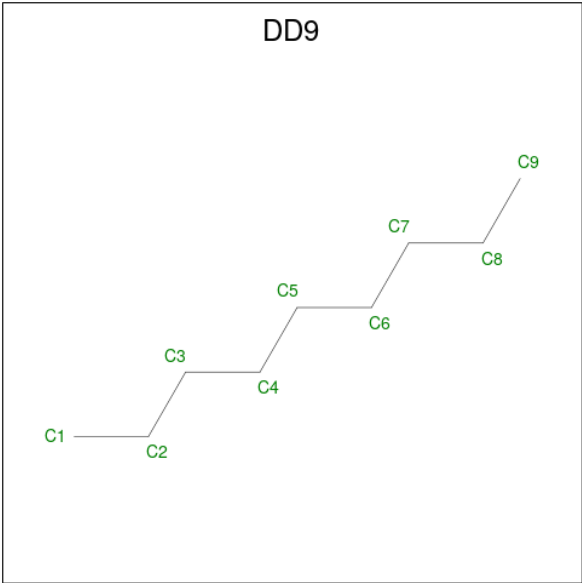


Mol	Chain	Residues	Atoms			AltConf	Trace
5	D	2	Total	C	O	0	0
			23	12	11		

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
6	H	1	Total	Mg	0
			1	1	
6	B	1	Total	Mg	0
			1	1	

- Molecule 7 is nonane (CCD ID: DD9) (formula: C₉H₂₀) (labeled as "Ligand of Interest" by depositor).



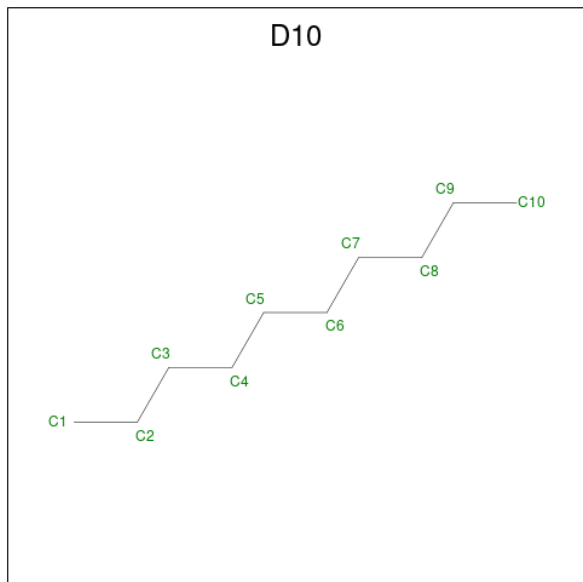
Mol	Chain	Residues	Atoms		AltConf
7	H	1	Total	C	0
			9	9	
7	H	1	Total	C	0
			9	9	
7	H	1	Total	C	0
			9	9	

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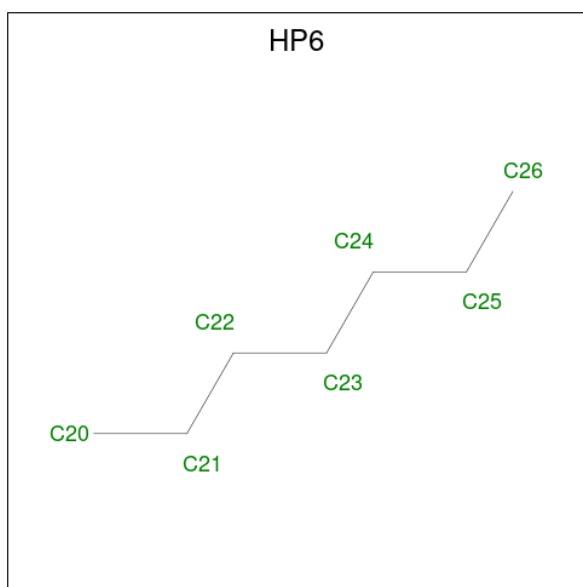
Mol	Chain	Residues	Atoms	AltConf
7	H	1	Total C 9 9	0
7	B	1	Total C 9 9	0
7	B	1	Total C 9 9	0
7	B	1	Total C 9 9	0
7	B	1	Total C 9 9	0

- Molecule 8 is DECANE (CCD ID: D10) (formula: $C_{10}H_{22}$) (labeled as "Ligand of Interest" by depositor).



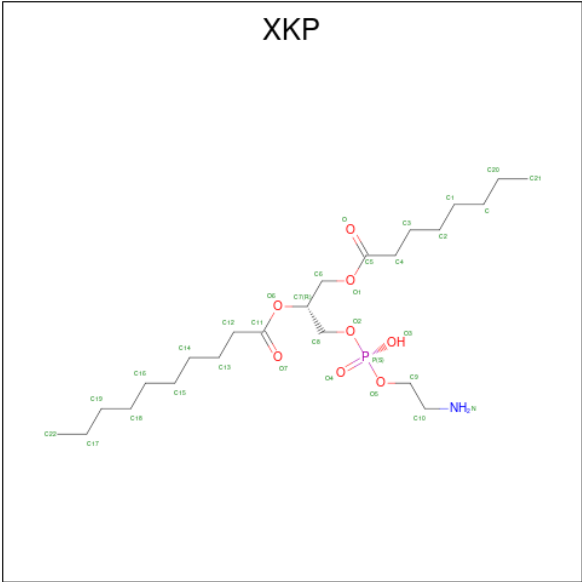
Mol	Chain	Residues	Atoms	AltConf
8	H	1	Total C 10 10	0
8	B	1	Total C 10 10	0

- Molecule 9 is HEPTANE (CCD ID: HP6) (formula: C_7H_{16}) (labeled as "Ligand of Interest" by depositor).



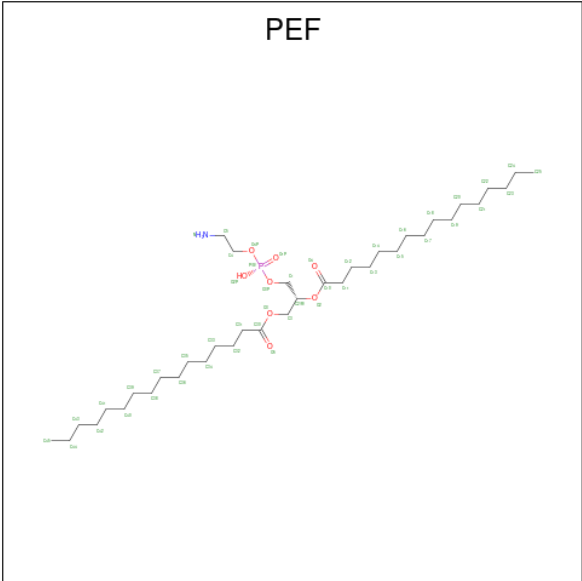
Mol	Chain	Residues	Atoms	AltConf
9	H	1	Total C 7 7	0
9	H	1	Total C 7 7	0
9	B	1	Total C 7 7	0
9	B	1	Total C 7 7	0
9	B	1	Total C 7 7	0
9	B	1	Total C 7 7	0

- Molecule 10 is (11R,14S)-17-amino-14-hydroxy-8,14-dioxo-9,13,15-trioxa-14lambda 5 -phosphahaheptadecan-11-yl decanoate (CCD ID: XKP) (formula: $C_{23}H_{46}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
10	H	1	Total	C	N	O	P	0
			33	23	1	8	1	
10	B	1	Total	C	N	O	P	0
			33	23	1	8	1	

- Molecule 11 is DI-PALMITOYL-3-SN-PHOSPHATIDYLETHANOLAMINE (CCD ID: PEF) (formula: C₃₇H₇₄NO₈P) (labeled as "Ligand of Interest" by depositor).



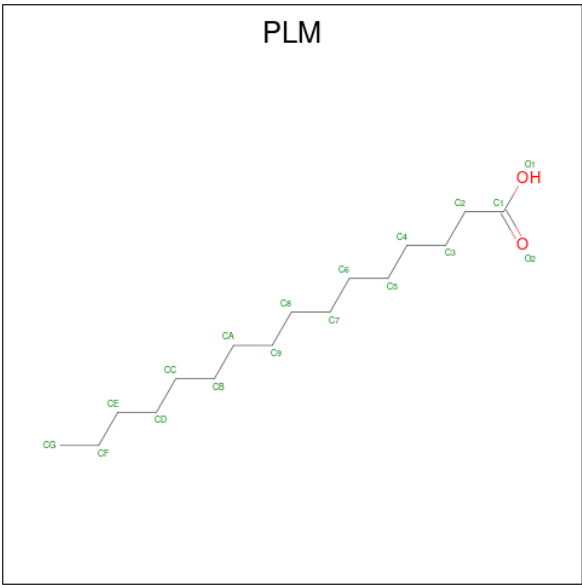
Mol	Chain	Residues	Atoms					AltConf
11	H	1	Total	C	N	O	P	0
			47	37	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
11	B	1	Total	C	N	O	P	0
			47	37	1	8	1	

- Molecule 12 is PALMITIC ACID (CCD ID: PLM) (formula: C₁₆H₃₂O₂) (labeled as "Ligand of Interest" by depositor).



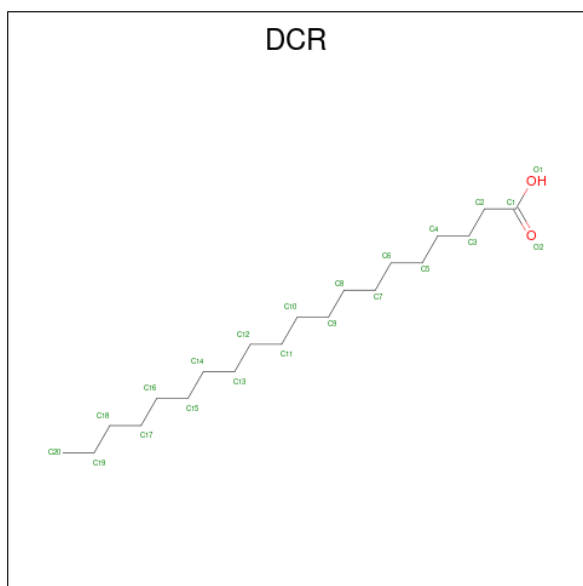
Mol	Chain	Residues	Atoms			AltConf
12	H	1	Total	C	O	0
			18	16	2	
12	H	1	Total	C	O	0
			18	16	2	
12	H	1	Total	C	O	0
			18	16	2	
12	H	1	Total	C	O	0
			18	16	2	
12	H	1	Total	C	O	0
			18	16	2	
12	H	1	Total	C	O	0
			18	16	2	
12	H	1	Total	C	O	0
			18	16	2	
12	B	1	Total	C	O	0
			18	16	2	
12	B	1	Total	C	O	0
			18	16	2	
12	B	1	Total	C	O	0
			18	16	2	

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Mol	Chain	Residues	Atoms			AltConf
12	B	1	Total	C	O	0
			18	16	2	
12	B	1	Total	C	O	0
			18	16	2	
12	B	1	Total	C	O	0
			18	16	2	
12	B	1	Total	C	O	0
			18	16	2	
12	B	1	Total	C	O	0
			18	16	2	
12	B	1	Total	C	O	0
			18	16	2	

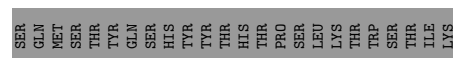
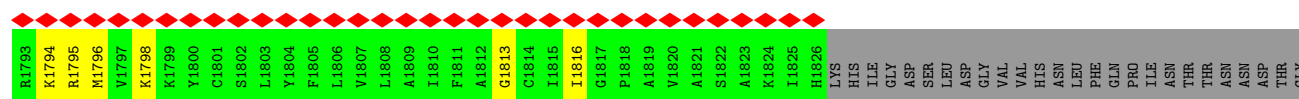
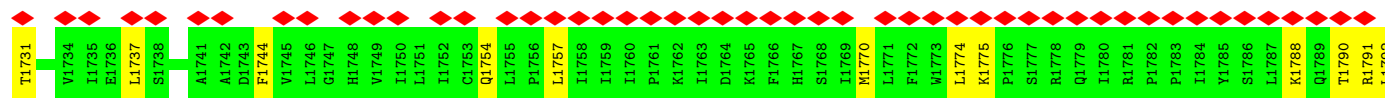
- Molecule 13 is icosanoic acid (CCD ID: DCR) (formula: $C_{20}H_{40}O_2$) (labeled as "Ligand of Interest" by depositor).



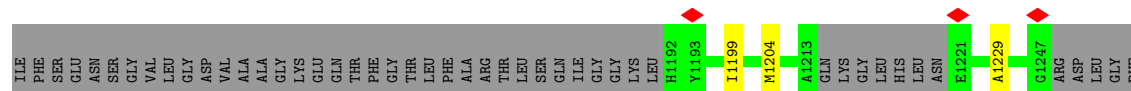
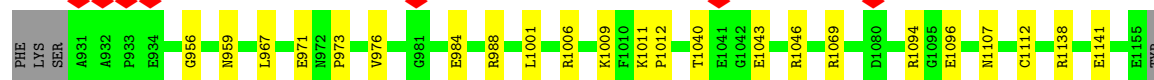
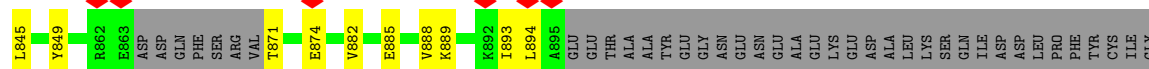
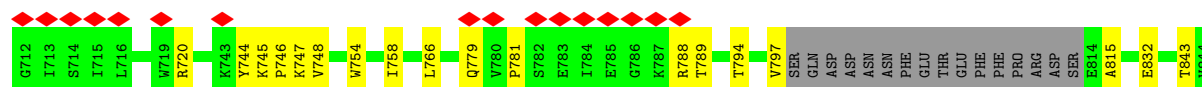
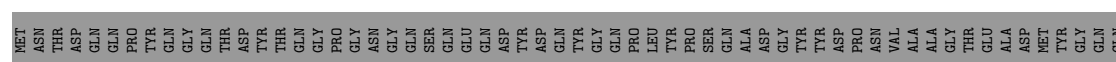
Mol	Chain	Residues	Atoms			AltConf
13	H	1	Total	C	O	0
			22	20	2	
13	B	1	Total	C	O	0
			22	20	2	

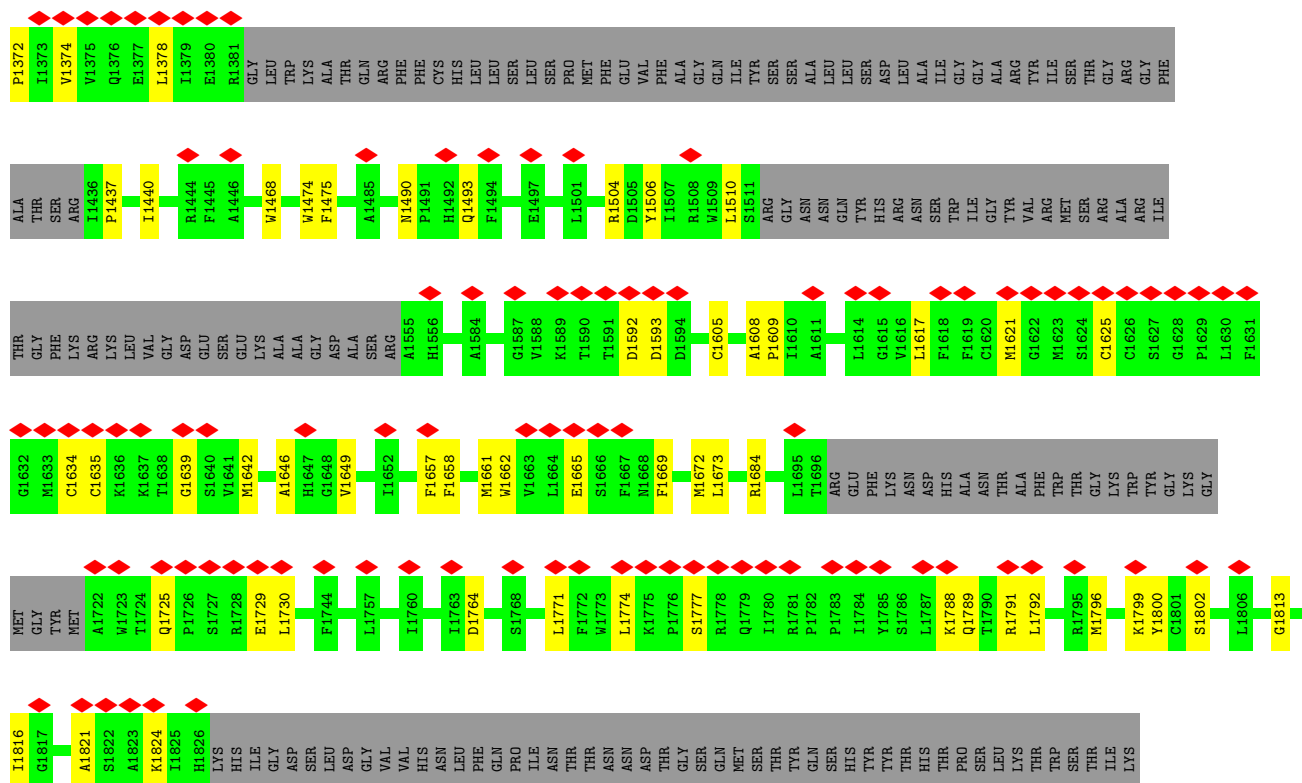




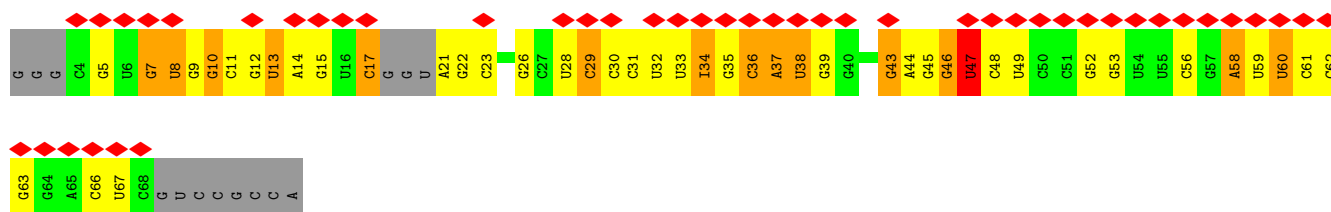
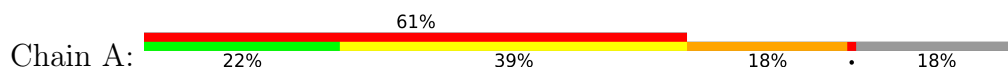


● Molecule 2: 1,3-beta-glucan synthase component FKS1





• Molecule 3: tRNA



• Molecule 4: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose



• Molecule 5: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	243849	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1100	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.750	Depositor
Minimum map value	-1.782	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.038	Depositor
Recommended contour level	0.2	Depositor
Map size ($\text{\AA}$)	440.0, 440.0, 440.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.1, 1.1, 1.1	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BGC, DCR, XKP, MG, PEF, HP6, D10, DD9, PLM

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	C	0.16	0/206	0.33	0/279
1	G	0.15	0/206	0.37	0/279
2	B	0.27	0/11813	0.48	1/16028 (0.0%)
2	H	0.18	0/11813	0.43	0/16028
3	A	0.40	2/1469 (0.1%)	0.37	1/2283 (0.0%)
All	All	0.24	2/25507 (0.0%)	0.45	2/34897 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	34	I	C5-C6	7.31	1.54	1.39
3	A	34	I	N3-C4	6.78	1.49	1.35

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1342	PRO	CA-N-CD	-14.28	92.01	112.00
3	A	47	U	P-O3'-C3'	-7.27	109.29	120.20

There are no chirality outliers.

There are no planarity outliers.

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	C	203	0	194	4	0
1	G	203	0	194	3	0
2	B	11499	0	11514	132	0
2	H	11499	0	11513	274	0
3	A	1319	0	668	35	0
4	J	34	0	28	1	0
5	D	23	0	21	0	0
6	B	1	0	0	0	0
6	H	1	0	0	0	0
7	B	36	0	80	0	0
7	H	36	0	80	1	0
8	B	10	0	22	0	0
8	H	10	0	22	0	0
9	B	28	0	64	1	0
9	H	14	0	32	0	0
10	B	33	0	0	0	0
10	H	33	0	0	0	0
11	B	47	0	73	6	0
11	H	47	0	73	7	0
12	B	162	0	279	9	0
12	H	126	0	217	18	0
13	B	22	0	39	0	0
13	H	22	0	39	0	0
All	All	25408	0	25152	461	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 (461) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:660:GLY:HA3	2:B:666:ALA:HA	1.44	0.97
2:H:514:GLU:OE1	2:H:531:ARG:NH2	2.02	0.93
2:H:1579:PHE:HA	2:H:1674:ILE:HD12	1.53	0.90
2:H:671:VAL:HG13	2:H:674:LYS:HE2	1.55	0.86
2:B:1107:ASN:ND2	2:B:1112:CYS:SG	2.53	0.82
2:H:408:LEU:HD21	2:H:414:LEU:HD13	1.63	0.79
1:G:100:ALA:HB3	1:G:103:GLU:HG3	1.65	0.79
2:H:658:CYS:HG	2:H:1586:THR:HG1	1.23	0.79
2:H:172:THR:HG23	2:H:177:PHE:HB2	1.66	0.78
2:B:442:THR:HG22	2:B:443:ARG:H	1.48	0.76
2:H:618:ARG:NH2	2:H:1285:ASP:OD2	2.20	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:387:ILE:O	2:B:437:LYS:NZ	2.20	0.74
2:H:1207:ARG:HE	2:H:1232:ARG:HB3	1.51	0.73
2:B:1342:PRO:HD2	2:B:1342:PRO:O	1.88	0.73
3:A:30:C:C4	3:A:31:C:N4	2.57	0.73
2:H:421:GLU:HB2	2:H:425:ARG:HH21	1.53	0.72
2:H:1321:LEU:HA	2:H:1581:PHE:HE2	1.55	0.72
3:A:5:G:H22	3:A:67:U:H3	1.36	0.71
2:B:283:GLU:OE1	2:B:283:GLU:N	2.22	0.70
2:H:1690:MET:HE1	2:H:1731:THR:HB	1.74	0.70
2:H:1792:LEU:HA	2:H:1795:ARG:HG2	1.72	0.70
2:H:441:GLU:HB3	2:H:1271:LEU:HD22	1.74	0.69
2:H:1207:ARG:HE	2:H:1232:ARG:CB	2.06	0.69
2:H:418:PRO:O	2:H:425:ARG:NH2	2.26	0.69
2:B:1662:TRP:HA	2:B:1665:GLU:HB2	1.73	0.69
2:H:822:PHE:CE2	2:H:1110:GLU:HB2	2.28	0.69
2:B:1605:CYS:HA	2:B:1657:PHE:CZ	2.28	0.69
2:B:845:LEU:HD13	2:B:1001:LEU:HD23	1.75	0.68
3:A:30:C:N4	3:A:31:C:N4	2.41	0.68
2:H:1123:GLU:OE2	2:H:1237:LYS:NZ	2.24	0.68
2:B:1662:TRP:HE1	2:B:1672:MET:HE1	1.59	0.68
2:H:962:ARG:HG3	2:H:1109:LEU:HD21	1.75	0.68
2:B:1788:LYS:NZ	3:A:9:G:OP1	2.27	0.67
2:B:1788:LYS:HG3	2:B:1791:ARG:HH21	1.59	0.67
2:H:167:ILE:HG12	2:H:303:ARG:HE	1.58	0.67
2:H:233:ASP:OD1	2:H:605:THR:OG1	2.12	0.67
2:B:368:GLN:HA	2:B:380:ARG:HH21	1.60	0.67
2:H:323:GLU:HG3	2:H:398:TRP:CD1	2.30	0.66
2:H:593:MET:HB3	2:H:595:LYS:HG2	1.78	0.66
2:H:196:ARG:HD3	2:H:209:LEU:HG	1.78	0.66
2:H:1795:ARG:HE	2:H:1796:MET:HE3	1.62	0.65
2:B:1437:PRO:HG2	2:B:1440:ILE:HG12	1.79	0.65
2:B:1789:GLN:NE2	3:A:10:G:O2'	2.30	0.65
11:B:1912:PEF:H422	11:B:1912:PEF:H211	1.79	0.65
2:B:593:MET:HB3	2:B:595:LYS:HG3	1.77	0.64
3:A:15:G:H22	3:A:21:A:H1'	1.62	0.64
2:B:335:TYR:HE1	2:B:340:LEU:HD22	1.62	0.64
2:B:493:TRP:HB2	2:B:566:ALA:HB1	1.79	0.64
2:B:779:GLN:HA	2:B:789:THR:O	1.98	0.63
2:H:1490:ASN:ND2	2:H:1493:GLN:OE1	2.32	0.63
2:H:1294:HIS:HB2	2:H:1295:PRO:HD3	1.79	0.63
2:H:1650:ALA:O	2:H:1654:HIS:ND1	2.25	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:565:VAL:O	2:H:569:MET:HG2	1.99	0.62
3:A:34:I:H5'	3:A:35:G:C4	2.34	0.62
2:H:1114:LYS:HZ1	2:H:1242:TYR:HB2	1.65	0.62
2:B:1006:ARG:HH11	2:B:1009:LYS:HZ2	1.46	0.62
2:B:849:TYR:CE2	2:B:1006:ARG:HD3	2.35	0.61
2:H:1479:LEU:O	2:H:1482:LEU:HB3	2.00	0.61
2:H:843:THR:HG22	2:H:1098:ILE:HG12	1.81	0.61
2:B:1359:THR:HG22	2:B:1475:PHE:HE2	1.65	0.61
2:H:633:TYR:HB2	12:H:1918:PLM:HA2	1.83	0.61
2:H:844:VAL:HG22	2:H:1099:GLN:HB3	1.83	0.60
2:H:179:ARG:O	2:H:182:MET:HG3	2.00	0.60
2:B:367:ASN:O	2:B:380:ARG:NH2	2.33	0.60
2:B:1684:ARG:HH22	12:B:1915:PLM:H42	1.66	0.60
2:H:199:ARG:HG3	2:H:200:MET:SD	2.42	0.60
2:H:750:ILE:HG22	2:H:754:TRP:CD1	2.37	0.60
2:H:952:ARG:NH1	2:H:1106:ASP:OD1	2.34	0.60
2:H:453:ASN:HA	2:H:456:TRP:CE3	2.37	0.60
2:B:1634:CYS:SG	2:B:1635:CYS:N	2.75	0.60
2:H:771:HIS:HA	2:H:774:LYS:HD3	1.84	0.59
2:H:1665:GLU:HB3	2:H:1668:ASN:HB3	1.84	0.59
2:B:482:LEU:HD13	2:B:1337:THR:HG21	1.83	0.59
2:H:858:ARG:NH2	3:A:17:C:OP2	2.27	0.59
2:H:453:ASN:HA	2:H:456:TRP:HE3	1.67	0.59
2:B:442:THR:HG22	2:B:443:ARG:N	2.17	0.59
2:H:167:ILE:HG23	2:H:303:ARG:HD3	1.84	0.59
2:H:538:ILE:HD13	2:H:580:PHE:HZ	1.68	0.59
2:B:656:MET:HE3	2:B:1346:TYR:CE2	2.39	0.58
2:H:1634:CYS:SG	2:H:1635:CYS:N	2.76	0.58
2:B:745:LYS:O	2:B:748:VAL:HG12	2.03	0.58
2:B:1821:ALA:HA	2:B:1824:LYS:HG2	1.85	0.58
2:H:1579:PHE:HD1	2:H:1674:ILE:HG13	1.68	0.58
2:H:750:ILE:HG22	2:H:754:TRP:HD1	1.68	0.58
2:H:1114:LYS:NZ	2:H:1242:TYR:HB2	2.19	0.58
1:C:100:ALA:HB3	1:C:103:GLU:HG3	1.86	0.58
2:B:1199:ILE:HG23	2:B:1204:MET:HG3	1.86	0.58
2:H:534:PHE:HA	2:H:537:ILE:HB	1.85	0.58
2:H:1658:PHE:HD2	2:H:1672:MET:HE1	1.69	0.57
2:H:185:MET:HE2	2:H:309:LEU:O	2.04	0.57
2:H:472:PRO:O	2:H:476:THR:HG23	2.04	0.57
3:A:7:G:C5	3:A:49:U:H1'	2.39	0.57
2:H:1109:LEU:O	2:H:1113:LEU:HG	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:984:GLU:O	2:B:988:ARG:HG2	2.04	0.57
2:H:759:ILE:HB	2:H:763:ARG:HH12	1.70	0.57
2:H:1557:ARG:O	2:H:1561:ILE:HG13	2.05	0.56
2:H:296:LEU:HD23	2:H:301:ARG:HG2	1.87	0.56
2:B:1138:ARG:HB2	2:B:1141:GLU:OE1	2.06	0.56
2:H:843:THR:CG2	2:H:1098:ILE:HG12	2.35	0.56
2:H:186:PHE:O	2:H:190:MET:HG2	2.05	0.56
2:H:392:ASP:OD1	2:H:438:THR:OG1	2.20	0.55
2:B:832:GLU:N	2:B:832:GLU:OE1	2.37	0.55
3:A:62:C:H2'	3:A:63:G:H8	1.70	0.55
2:H:480:GLN:HB3	2:H:483:VAL:HG22	1.89	0.55
2:H:444:THR:HA	2:H:1270:MET:HE1	1.87	0.55
2:H:686:ILE:HD13	2:H:1310:MET:HG3	1.88	0.55
2:H:672:GLN:HG2	2:H:1321:LEU:HD13	1.87	0.55
2:H:1562:MET:O	2:H:1565:ILE:HG22	2.06	0.55
2:B:1011:LYS:HD3	3:A:36:C:H41	1.71	0.55
2:H:965:LYS:HB3	2:H:990:LEU:HD23	1.88	0.55
2:H:583:MET:SD	2:H:588:LEU:HD23	2.47	0.55
2:H:1090:LEU:HD11	2:H:1210:VAL:HG11	1.89	0.54
2:H:1788:LYS:HA	2:H:1791:ARG:HE	1.72	0.54
2:H:315:ALA:HB3	2:H:319:ARG:HG3	1.89	0.54
2:H:687:LEU:HD12	2:H:690:LEU:HD12	1.90	0.54
2:H:531:ARG:O	2:H:535:LEU:HG	2.07	0.54
2:H:759:ILE:HG13	2:H:763:ARG:HH22	1.73	0.54
2:B:514:GLU:OE1	2:B:531:ARG:NH2	2.36	0.54
2:H:1790:THR:HG22	2:H:1794:LYS:NZ	2.23	0.54
2:B:1285:ASP:OD1	2:B:1286:ARG:N	2.41	0.54
2:H:1498:ASP:OD1	2:H:1499:PHE:N	2.41	0.54
2:B:1294:HIS:HB2	2:B:1295:PRO:HD3	1.89	0.54
2:H:1051:LEU:HD23	2:H:1067:LYS:HE2	1.90	0.53
2:H:1437:PRO:HG2	2:H:1440:ILE:HG12	1.91	0.53
2:B:1669:PHE:HA	2:B:1672:MET:HE1	1.90	0.53
2:H:332:ALA:O	2:H:336:LEU:HG	2.08	0.53
2:H:367:ASN:O	2:H:380:ARG:NH2	2.41	0.53
2:B:1592:ASP:OD1	2:B:1593:ASP:N	2.41	0.53
2:H:213:TYR:CZ	2:H:1202:THR:HG23	2.44	0.53
2:H:1592:ASP:OD1	2:H:1593:ASP:N	2.42	0.53
2:H:1568:CYS:HB2	12:H:1913:PLM:H51	1.91	0.53
2:H:1153:ALA:HB1	2:H:1242:TYR:O	2.09	0.53
2:H:1813:GLY:HA2	2:H:1816:ILE:HG12	1.90	0.52
2:H:1147:PRO:HG2	2:H:1203:PHE:CE2	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:239:ARG:O	2:B:243:LEU:HG	2.09	0.52
2:H:757:ILE:O	2:H:760:SER:OG	2.22	0.52
2:H:957:PHE:HE2	2:H:1105:GLN:HB3	1.74	0.52
2:B:745:LYS:HG2	2:B:747:LYS:NZ	2.25	0.52
2:H:1060:ASP:N	2:H:1060:ASP:OD1	2.42	0.52
2:H:1472:LEU:HA	2:H:1475:PHE:HD2	1.75	0.52
2:H:1662:TRP:HA	2:H:1665:GLU:HB2	1.92	0.52
2:H:1019:GLU:O	2:H:1023:ARG:HG2	2.09	0.52
2:H:1504:ARG:NH2	2:H:1508:ARG:HE	2.08	0.52
2:H:509:VAL:HG11	11:H:1910:PEF:H32	1.91	0.52
2:H:468:ALA:HB2	12:H:1916:PLM:HG1	1.92	0.51
2:H:408:LEU:HD22	2:H:428:ASP:HB2	1.93	0.51
2:B:480:GLN:HB3	2:B:483:VAL:HG22	1.92	0.51
2:H:1657:PHE:HA	2:H:1660:VAL:HG12	1.92	0.51
2:H:1658:PHE:CD2	2:H:1672:MET:HE1	2.45	0.51
2:B:1788:LYS:NZ	3:A:11:C:OP2	2.43	0.51
2:H:1790:THR:O	2:H:1794:LYS:HG2	2.10	0.51
2:B:1349:GLN:HA	2:B:1352:VAL:HG22	1.93	0.51
2:H:297:SER:HB2	2:H:300:GLU:OE1	2.10	0.51
2:H:963:ALA:HB1	2:H:1113:LEU:HD23	1.93	0.51
2:H:1306:LEU:O	2:H:1310:MET:HG2	2.10	0.51
2:B:195:SER:OG	2:B:1096:GLU:OE2	2.26	0.51
2:B:745:LYS:HG2	2:B:747:LYS:HZ3	1.76	0.51
2:H:873:LEU:O	2:H:877:LYS:HE3	2.11	0.51
2:H:493:TRP:HB2	2:H:566:ALA:HB1	1.91	0.51
2:B:1617:LEU:HD13	2:B:1730:LEU:HD22	1.93	0.51
2:H:664:TRP:HE3	2:H:668:LEU:HD11	1.76	0.51
2:B:505:LEU:HD23	11:B:1912:PEF:H42	1.92	0.51
2:H:323:GLU:HG3	2:H:398:TRP:HD1	1.72	0.50
2:B:1359:THR:HG22	2:B:1475:PHE:CE2	2.45	0.50
2:H:422:ARG:HG2	2:H:425:ARG:HH12	1.77	0.50
2:H:454:ARG:NH2	2:H:583:MET:O	2.44	0.50
2:B:491:TYR:OH	2:B:555:ASP:OD1	2.28	0.50
2:B:1306:LEU:HD11	9:B:1908:HP6:H222	1.93	0.50
2:H:472:PRO:HA	2:H:475:TYR:CZ	2.46	0.50
2:B:667:VAL:HG23	2:B:668:LEU:HD12	1.93	0.50
2:H:501:THR:HG22	2:H:542:ASN:HB3	1.92	0.50
2:B:392:ASP:OD1	2:B:1273:ARG:NH2	2.40	0.50
2:H:818:ARG:HD3	2:H:1110:GLU:HG3	1.93	0.50
2:H:1683:GLN:NE2	2:H:1684:ARG:HG3	2.26	0.50
2:H:1597:ASN:OD1	2:H:1598:SER:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:32:U:H2'	3:A:33:U:C6	2.47	0.50
2:H:348:MET:HG3	2:H:349:PRO:HD2	1.94	0.49
2:H:617:ASP:OD1	2:H:618:ARG:N	2.45	0.49
3:A:34:I:H5'	3:A:35:G:N3	2.27	0.49
2:H:344:ARG:NH2	2:H:346:GLU:O	2.33	0.49
2:H:733:LYS:NZ	2:H:828:THR:O	2.41	0.49
2:H:1469:GLN:HB2	2:H:1472:LEU:HG	1.94	0.49
2:B:661:GLU:N	2:B:665:GLY:O	2.44	0.49
2:H:1201:ALA:O	2:H:1205:THR:OG1	2.11	0.49
2:B:698:ILE:O	2:B:701:THR:HG22	2.12	0.49
2:B:973:PRO:HA	2:B:976:VAL:HG22	1.95	0.49
2:H:1067:LYS:HG3	2:H:1068:PHE:N	2.27	0.49
2:H:237:GLY:O	2:H:241:MET:HG2	2.12	0.49
3:A:28:U:H1'	3:A:43:G:H22	1.76	0.49
2:H:595:LYS:O	2:H:599:ARG:NH1	2.46	0.49
2:H:1646:ALA:HA	2:H:1649:VAL:HG22	1.95	0.49
2:H:941:ILE:HG23	2:H:951:TYR:HE1	1.78	0.49
2:H:1114:LYS:HD2	2:H:1118:VAL:HG23	1.93	0.49
1:G:104:ARG:NH2	2:H:165:GLU:OE1	2.46	0.49
2:H:225:TYR:CZ	2:H:229:GLN:HG2	2.48	0.49
2:H:694:LEU:HD13	2:H:1368:ILE:HG21	1.94	0.49
2:B:707:LYS:HG3	2:B:711:LEU:HD23	1.95	0.49
3:A:46:G:O2'	3:A:47:U:H5'	2.12	0.49
2:B:1774:LEU:O	2:B:1777:SER:OG	2.31	0.49
2:H:696:TYR:O	2:H:700:ASN:ND2	2.45	0.49
2:B:1490:ASN:ND2	2:B:1493:GLN:OE1	2.45	0.49
2:H:507:GLN:NE2	2:H:535:LEU:HD22	2.28	0.48
2:B:885:GLU:HA	2:B:888:VAL:HG22	1.94	0.48
2:B:893:ILE:HG22	2:B:894:LEU:HD12	1.95	0.48
2:H:504:SER:O	2:H:507:GLN:HG2	2.14	0.48
2:H:1076:PRO:HG2	2:H:1077:ILE:HD12	1.94	0.48
2:H:1114:LYS:HD2	2:H:1114:LYS:O	2.13	0.48
2:B:1011:LYS:HZ2	3:A:36:C:H5	1.61	0.48
3:A:58:A:O2'	3:A:60:U:OP2	2.21	0.48
2:H:177:PHE:O	2:H:350:GLU:HG3	2.13	0.48
2:H:308:TYR:OH	2:H:1206:THR:HG22	2.13	0.48
2:H:451:ASN:ND2	2:H:1275:TYR:HB3	2.28	0.48
2:H:975:ILE:HA	2:H:978:MET:HE2	1.95	0.48
2:B:766:LEU:HD21	2:B:815:ALA:HB2	1.95	0.48
2:H:1200:ASN:ND2	2:H:1203:PHE:HB2	2.29	0.48
2:H:1310:MET:N	2:H:1310:MET:HE2	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:960:TYR:HE1	2:H:1107:ASN:ND2	2.11	0.48
2:B:401:GLU:OE1	2:B:523:ALA:HB2	2.13	0.48
2:H:508:ILE:HG23	2:H:532:PHE:HE1	1.78	0.48
2:H:757:ILE:O	2:H:761:MET:HG2	2.14	0.48
2:H:952:ARG:NH1	2:H:1105:GLN:O	2.47	0.48
11:B:1912:PEF:H232	11:B:1912:PEF:H431	1.95	0.48
2:B:781:PRO:HB2	2:B:788:ARG:O	2.13	0.48
2:B:1011:LYS:CD	3:A:36:C:H41	2.26	0.48
2:H:613:LEU:HD22	2:H:617:ASP:OD2	2.14	0.48
2:B:678:GLY:HA3	12:B:1914:PLM:HB2	1.96	0.48
2:B:889:LYS:O	2:B:893:ILE:HG12	2.14	0.48
2:H:365:ILE:HD13	2:H:390:TYR:CE1	2.49	0.48
2:H:499:GLY:HA3	2:H:577:ILE:HD11	1.95	0.48
2:H:731:TYR:CD1	2:H:746:PRO:HB3	2.49	0.48
2:B:1011:LYS:HD2	3:A:36:C:C5	2.49	0.48
2:H:625:TRP:HB2	12:H:1914:PLM:H72	1.96	0.47
2:H:1051:LEU:HD22	2:H:1092:PHE:CD1	2.49	0.47
2:B:1204:MET:HE1	2:B:1229:ALA:HB2	1.96	0.47
2:H:975:ILE:HG22	2:H:979:PHE:CE1	2.50	0.47
12:H:1912:PLM:HG1	12:H:1913:PLM:HF1	1.97	0.47
2:B:1764:ASP:OD1	2:B:1764:ASP:N	2.45	0.47
2:H:382:ARG:HH21	2:H:386:LYS:HE2	1.78	0.47
2:B:1330:TYR:OH	2:B:1347:ASN:HB3	2.15	0.47
2:B:476:THR:HB	2:B:479:TYR:HB2	1.95	0.47
2:B:473:THR:HG22	2:B:479:TYR:CZ	2.50	0.47
2:H:166:ASP:OD1	2:H:167:ILE:N	2.48	0.47
2:H:764:GLU:HG3	2:H:766:LEU:HG	1.97	0.47
2:H:526:GLN:NE2	2:H:598:ARG:O	2.48	0.47
2:H:179:ARG:HA	2:H:182:MET:HG3	1.97	0.46
2:H:640:LEU:HG	2:H:644:LEU:HD12	1.96	0.46
12:H:1912:PLM:H52	12:H:1912:PLM:H82	1.74	0.46
2:H:151:TRP:CZ3	2:H:202:PRO:HB3	2.51	0.46
2:H:356:ARG:NH2	2:H:424:LEU:O	2.49	0.46
2:H:451:ASN:HD21	2:H:1275:TYR:C	2.24	0.46
2:H:1005:GLN:NE2	2:H:1085:ASN:OD1	2.48	0.46
1:C:95:SER:O	2:B:1069:ARG:NH1	2.49	0.46
1:G:104:ARG:O	1:G:108:THR:HG23	2.16	0.46
2:H:452:PHE:HD1	2:H:1287:PHE:CE1	2.32	0.46
2:H:958:MET:HE1	2:H:1025:TYR:CD2	2.51	0.46
2:H:451:ASN:OD1	2:H:1279:GLY:HA3	2.16	0.46
2:H:515:TRP:CH2	2:H:520:ARG:HG3	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1310:MET:HE1	12:H:1913:PLM:HA1	1.98	0.46
2:B:661:GLU:O	2:B:665:GLY:N	2.22	0.46
2:H:1624:SER:HB3	2:H:1630:LEU:HD22	1.97	0.46
2:B:500:GLY:HA3	2:B:542:ASN:HD21	1.81	0.46
12:B:1915:PLM:H92	12:B:1915:PLM:H61	1.59	0.46
2:H:1639:GLY:HA2	2:H:1642:MET:HE3	1.98	0.46
2:B:843:THR:OG1	2:B:1094:ARG:O	2.33	0.46
2:H:184:ASN:HA	2:H:1068:PHE:CE2	2.51	0.46
2:H:1684:ARG:HH21	12:H:1913:PLM:H41	1.81	0.46
11:B:1912:PEF:H142	11:B:1912:PEF:H172	1.64	0.46
2:H:960:TYR:HE1	2:H:1107:ASN:HD21	1.64	0.46
2:B:1330:TYR:H	2:B:1349:GLN:HG3	1.82	0.46
2:H:417:LEU:HB3	2:H:418:PRO:HD2	1.98	0.45
2:H:530:ARG:HB3	2:H:593:MET:HE3	1.97	0.45
2:H:846:THR:OG1	2:H:1002:VAL:HG22	2.16	0.45
2:H:445:TRP:CD1	2:H:445:TRP:H	2.34	0.45
2:H:1583:ASN:OD1	2:H:1671:ARG:HD3	2.17	0.45
2:H:825:SER:O	2:H:828:THR:HG22	2.16	0.45
2:H:148:TYR:CZ	2:H:190:MET:HB2	2.52	0.45
2:H:451:ASN:HD21	2:H:1275:TYR:HB3	1.80	0.45
2:H:488:LEU:HD21	2:H:558:TYR:HE1	1.82	0.45
2:H:1086:GLN:O	2:H:1090:LEU:HB2	2.16	0.45
2:H:1600:LEU:HA	2:H:1603:ILE:HG12	1.98	0.45
2:H:1790:THR:HG22	2:H:1794:LYS:HZ3	1.81	0.45
2:B:569:MET:HB3	2:B:569:MET:HE3	1.83	0.45
2:H:656:MET:HE1	2:H:1581:PHE:CE1	2.52	0.45
2:H:737:THR:HA	2:H:740:MET:HE3	1.97	0.45
2:H:758:ILE:HG21	2:H:775:LEU:HD11	1.99	0.45
2:H:1367:TRP:O	2:H:1371:VAL:HG23	2.16	0.45
3:A:36:C:C2	3:A:37:A:H1'	2.52	0.45
3:A:62:C:H2'	3:A:63:G:C8	2.51	0.45
2:H:323:GLU:HB2	2:H:397:PHE:HB2	1.98	0.45
11:H:1910:PEF:H453	11:H:1910:PEF:H421	1.77	0.45
3:A:38:U:H2'	3:A:39:G:C8	2.52	0.45
2:H:1617:LEU:O	2:H:1621:MET:HG2	2.17	0.45
2:B:745:LYS:HD2	2:B:746:PRO:HD2	1.98	0.45
2:B:1367:TRP:O	2:B:1371:VAL:HG23	2.18	0.45
12:H:1911:PLM:H52	12:H:1911:PLM:H81	1.77	0.44
3:A:15:G:N2	3:A:21:A:H1'	2.30	0.44
2:H:746:PRO:O	2:H:750:ILE:HG12	2.16	0.44
2:B:720:ARG:NH1	2:B:797:VAL:O	2.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1510:LEU:HD13	2:H:1744:PHE:CE1	2.52	0.44
2:H:588:LEU:HB3	2:H:589:PHE:CD2	2.53	0.44
2:H:843:THR:HA	2:H:999:LYS:O	2.18	0.44
12:H:1911:PLM:H91	12:H:1911:PLM:HC1	1.47	0.44
12:B:1920:PLM:H62	12:B:1920:PLM:H91	1.49	0.44
2:H:565:VAL:HG13	2:H:569:MET:HE3	1.99	0.44
2:H:843:THR:O	2:H:1098:ILE:HA	2.18	0.44
2:H:213:TYR:CE1	2:H:1202:THR:HG23	2.52	0.44
2:H:875:TYR:HA	2:H:878:GLN:HG2	1.99	0.44
2:H:285:ALA:O	2:H:289:TRP:HD1	1.99	0.44
2:H:396:LEU:HD23	2:H:397:PHE:CZ	2.52	0.44
2:B:659:THR:HB	2:B:662:TYR:OH	2.18	0.44
2:B:1799:LYS:O	2:B:1802:SER:OG	2.34	0.44
2:H:407:VAL:HG22	2:H:408:LEU:O	2.18	0.44
2:H:745:LYS:O	2:H:748:VAL:HG12	2.18	0.44
2:H:1227:MET:SD	2:H:1274:GLU:HB3	2.58	0.44
2:H:1305:GLN:HG2	2:H:1309:GLN:NE2	2.32	0.43
3:A:11:C:H2'	3:A:12:G:H8	1.84	0.43
2:H:979:PHE:CZ	2:H:989:GLU:HG3	2.53	0.43
2:B:1725:GLN:O	2:B:1729:GLU:HG3	2.18	0.43
2:H:480:GLN:HG3	2:H:482:LEU:H	1.83	0.43
2:H:1770:MET:O	2:H:1774:LEU:HG	2.19	0.43
11:H:1910:PEF:H401	11:H:1910:PEF:H432	1.77	0.43
2:B:650:ILE:HD13	2:B:650:ILE:HA	1.87	0.43
2:B:1506:TYR:CZ	2:B:1510:LEU:HD11	2.53	0.43
12:B:1919:PLM:HC2	12:B:1919:PLM:H91	1.54	0.43
2:H:1118:VAL:HG11	2:H:1198:PHE:CZ	2.53	0.43
2:H:1147:PRO:HG2	2:H:1203:PHE:HE2	1.84	0.43
2:B:707:LYS:HD3	2:B:707:LYS:HA	1.82	0.43
2:H:1506:TYR:CE2	2:H:1510:LEU:HD21	2.54	0.43
2:B:1608:ALA:HB3	2:B:1609:PRO:HD3	2.00	0.43
2:H:553:ASP:OD1	2:H:554:LYS:N	2.51	0.43
2:H:1495:ALA:O	2:H:1499:PHE:HD2	2.01	0.43
12:H:1917:PLM:H62	12:H:1917:PLM:H91	1.82	0.43
2:B:1363:PHE:HE1	2:B:1474:TRP:HB3	1.84	0.43
3:A:13:U:H3	3:A:22:G:H1	1.67	0.43
2:H:210:HIS:HD2	2:H:214:ILE:HD13	1.83	0.43
2:H:415:ILE:O	2:H:422:ARG:NH2	2.52	0.43
2:H:469:TYR:CE2	7:H:1902:DD9:H2	2.53	0.43
11:B:1912:PEF:H342	11:B:1912:PEF:H312	1.86	0.43
2:H:445:TRP:CE3	11:H:1910:PEF:H342	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1209:GLY:O	2:H:1212:LYS:HE3	2.19	0.43
2:H:1378:LEU:O	2:H:1378:LEU:HD23	2.18	0.43
2:B:373:VAL:HG12	2:B:374:ASP:OD2	2.19	0.43
2:B:1672:MET:HG2	2:B:1673:LEU:N	2.33	0.43
2:H:979:PHE:HZ	2:H:989:GLU:HG3	1.83	0.43
2:H:1680:ILE:O	2:H:1683:GLN:HG3	2.19	0.43
2:H:1692:ALA:HA	2:H:1695:LEU:HD12	2.00	0.43
2:B:1006:ARG:HH11	2:B:1009:LYS:NZ	2.15	0.43
2:B:1646:ALA:HA	2:B:1649:VAL:HG22	2.00	0.43
2:H:1563:ALA:O	2:H:1566:ILE:HG22	2.19	0.43
1:C:105:PRO:HG3	2:B:182:MET:HE3	2.00	0.42
2:H:957:PHE:CE2	2:H:1105:GLN:HB3	2.52	0.42
11:B:1912:PEF:H402	11:B:1912:PEF:H371	1.59	0.42
2:H:322:ALA:O	2:H:325:LEU:HG	2.18	0.42
2:B:645:ARG:HE	2:B:645:ARG:HB2	1.69	0.42
2:B:956:GLY:O	2:B:959:ASN:ND2	2.48	0.42
3:A:52:G:H2'	3:A:53:G:H8	1.83	0.42
2:H:658:CYS:SG	2:H:1586:THR:OG1	2.39	0.42
2:B:1328:CYS:HB3	2:B:1340:LEU:HD13	2.01	0.42
2:H:486:GLN:OE1	2:H:487:PRO:HD2	2.19	0.42
2:H:1754:GLN:OE1	2:H:1757:LEU:HB3	2.19	0.42
11:H:1910:PEF:H201	11:H:1910:PEF:H231	1.78	0.42
2:B:882:VAL:O	2:B:885:GLU:HG3	2.20	0.42
2:B:1468:TRP:CD1	12:B:1921:PLM:H21	2.55	0.42
2:B:1771:LEU:HA	2:B:1774:LEU:HD12	2.00	0.42
3:A:7:G:H4'	3:A:8:U:OP2	2.19	0.42
2:H:644:LEU:HD21	2:H:684:ASP:OD2	2.20	0.42
2:H:776:LEU:O	2:H:793:PRO:HG3	2.20	0.42
2:B:553:ASP:OD1	2:B:554:LYS:N	2.52	0.42
2:B:1669:PHE:HA	2:B:1672:MET:CE	2.50	0.42
3:A:13:U:H2'	3:A:14:A:H8	1.83	0.42
3:A:66:C:H2'	3:A:67:U:C6	2.54	0.42
2:H:553:ASP:O	2:H:557:VAL:HG12	2.20	0.42
2:H:1794:LYS:O	2:H:1798:LYS:HG2	2.19	0.42
2:B:1366:PHE:CE1	4:J:1:BGC:H3	2.54	0.42
2:H:179:ARG:HA	2:H:182:MET:CG	2.50	0.42
2:H:201:SER:HB3	2:H:204:GLN:HG3	2.01	0.42
2:H:839:MET:HE1	2:H:1119:LEU:HD12	2.01	0.42
2:H:894:LEU:HD22	2:H:938:ARG:HH12	1.84	0.42
2:B:794:THR:HA	2:B:797:VAL:HG22	2.02	0.42
2:B:871:THR:HB	2:B:874:GLU:OE1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1813:GLY:HA2	2:B:1816:ILE:HG12	2.00	0.42
3:A:11:C:C2	3:A:12:G:C8	3.07	0.42
3:A:29:C:H2'	3:A:30:C:C6	2.55	0.42
2:H:958:MET:HE1	2:H:1025:TYR:CG	2.55	0.42
2:H:1002:VAL:HG23	2:H:1028:LEU:HD11	2.02	0.42
12:H:1916:PLM:HA1	12:H:1916:PLM:HD2	1.71	0.42
2:B:515:TRP:HE1	2:B:520:ARG:NH2	2.17	0.42
2:B:1199:ILE:HD13	2:B:1199:ILE:HA	1.92	0.42
12:B:1915:PLM:HC1	12:B:1915:PLM:H91	1.73	0.42
2:H:873:LEU:O	2:H:877:LYS:HG2	2.20	0.42
2:H:889:LYS:O	2:H:893:ILE:HG12	2.20	0.42
11:H:1910:PEF:H361	11:H:1910:PEF:H392	1.84	0.42
2:B:1639:GLY:O	2:B:1642:MET:HG2	2.20	0.42
12:B:1921:PLM:HC1	12:B:1921:PLM:HF2	1.45	0.42
2:H:465:MET:HG3	2:H:496:CYS:HB3	2.02	0.41
2:B:425:ARG:O	2:B:427:GLY:N	2.53	0.41
2:B:1011:LYS:HB2	2:B:1012:PRO:HD2	2.01	0.41
2:B:1040:THR:OG1	2:B:1043:GLU:OE1	2.38	0.41
2:B:1046:ARG:HE	2:B:1046:ARG:HB2	1.73	0.41
2:H:476:THR:HG22	2:H:487:PRO:HG3	2.02	0.41
2:H:731:TYR:CZ	2:H:746:PRO:HG3	2.55	0.41
2:H:1506:TYR:HE2	2:H:1510:LEU:HD21	1.85	0.41
12:H:1918:PLM:H31	12:H:1918:PLM:H62	1.72	0.41
2:B:1621:MET:O	2:B:1625:CYS:HB2	2.21	0.41
3:A:30:C:C4	3:A:31:C:C4	3.08	0.41
2:H:844:VAL:HG23	2:H:998:PHE:HE1	1.85	0.41
2:H:1134:ALA:HB3	2:H:1137:LEU:HB2	2.02	0.41
2:H:1310:MET:SD	12:H:1913:PLM:HD2	2.60	0.41
2:B:583:MET:HE3	2:B:583:MET:HB3	1.94	0.41
2:B:481:GLN:HB2	2:B:649:ARG:HD2	2.02	0.41
2:H:174:ARG:HD3	2:H:341:CYS:SG	2.61	0.41
2:H:1223:ILE:O	2:H:1227:MET:HG3	2.20	0.41
2:H:1283:PRO:HG2	2:H:1286:ARG:HG3	2.02	0.41
2:B:744:TYR:HB3	2:B:748:VAL:CG1	2.50	0.41
2:H:328:ILE:HA	2:H:331:CYS:SG	2.61	0.41
2:H:1453:GLY:O	2:H:1457:MET:HG2	2.20	0.41
2:B:1672:MET:HB3	2:B:1672:MET:HE2	1.75	0.41
2:H:481:GLN:HB2	2:H:649:ARG:HD2	2.01	0.41
2:H:822:PHE:CE1	2:H:826:LEU:HD11	2.55	0.41
2:H:1380:GLU:O	2:H:1775:LYS:HE3	2.20	0.41
2:B:1371:VAL:N	2:B:1372:PRO:HD2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:106:LEU:O	1:C:109:ILE:HG22	2.21	0.41
2:H:409:GLU:HG2	2:H:428:ASP:O	2.21	0.41
2:H:1452:MET:HA	2:H:1455:ARG:HG2	2.02	0.41
2:H:1506:TYR:O	2:H:1510:LEU:HG	2.20	0.41
2:H:1646:ALA:HB3	2:H:1737:LEU:HD21	2.03	0.41
2:B:1792:LEU:O	2:B:1796:MET:HG3	2.21	0.41
2:H:359:THR:HB	2:H:360:PRO:HD3	2.03	0.41
2:H:959:ASN:HB3	2:H:1109:LEU:HD23	2.03	0.41
2:H:1146:HIS:HB3	2:H:1233:GLY:O	2.21	0.41
2:H:1452:MET:O	2:H:1455:ARG:HG2	2.21	0.41
2:H:1461:LEU:HA	2:H:1464:THR:HG22	2.03	0.41
2:H:1571:TYR:HB2	12:H:1913:PLM:H92	2.02	0.41
12:H:1914:PLM:H52	12:H:1914:PLM:H81	1.79	0.41
2:B:425:ARG:C	2:B:427:GLY:H	2.28	0.41
2:B:967:LEU:O	2:B:971:GLU:HG2	2.21	0.41
2:H:308:TYR:HB2	2:H:329:TYR:HE1	1.85	0.41
2:H:1455:ARG:HH12	2:H:1684:ARG:CZ	2.33	0.41
2:H:1504:ARG:HA	2:H:1507:ILE:HG12	2.03	0.41
2:B:1657:PHE:HB3	2:B:1661:MET:HE3	2.02	0.41
3:A:30:C:H2'	3:A:31:C:C6	2.56	0.41
3:A:31:C:H2'	3:A:32:U:C6	2.56	0.41
2:H:164:ILE:HB	2:H:190:MET:HE1	2.02	0.40
2:H:314:GLU:HB2	2:H:353:PHE:HE2	1.86	0.40
2:H:458:MET:SD	12:H:1914:PLM:HE1	2.61	0.40
11:H:1910:PEF:H211	11:H:1910:PEF:H422	2.02	0.40
12:B:1913:PLM:H22	12:B:1913:PLM:H52	1.61	0.40
2:H:472:PRO:HB3	2:H:492:LYS:NZ	2.36	0.40
2:H:1051:LEU:HD13	2:H:1092:PHE:CD2	2.56	0.40
2:H:1104:ASN:N	2:H:1104:ASN:HD22	2.18	0.40
2:H:1310:MET:HE1	12:H:1913:PLM:CA	2.52	0.40
2:B:671:VAL:O	2:B:671:VAL:HG12	2.22	0.40
2:B:1011:LYS:H	2:B:1011:LYS:HG2	1.56	0.40
2:B:1374:VAL:O	2:B:1378:LEU:HB2	2.22	0.40
2:B:1504:ARG:HG2	2:B:1800:TYR:CZ	2.56	0.40
2:B:1658:PHE:CE1	2:B:1672:MET:SD	3.15	0.40
2:B:754:TRP:O	2:B:758:ILE:HG12	2.21	0.40
2:H:792:ALA:HA	2:H:793:PRO:HD3	1.99	0.40
2:H:1455:ARG:HH12	2:H:1684:ARG:NH2	2.20	0.40
2:H:1602:ILE:O	2:H:1606:THR:HG23	2.21	0.40
2:H:1621:MET:HE1	2:H:1730:LEU:HD11	2.02	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	C	23/197 (12%)	23 (100%)	0	0	100	100
1	G	23/197 (12%)	23 (100%)	0	0	100	100
2	B	1387/1876 (74%)	1339 (96%)	48 (4%)	0	100	100
2	H	1387/1876 (74%)	1342 (97%)	45 (3%)	0	100	100
All	All	2820/4146 (68%)	2727 (97%)	93 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	22/167 (13%)	22 (100%)	0	100	100
1	G	22/167 (13%)	22 (100%)	0	100	100
2	B	1238/1620 (76%)	1238 (100%)	0	100	100
2	H	1238/1620 (76%)	1238 (100%)	0	100	100
All	All	2520/3574 (70%)	2520 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	220	ASN
2	H	368	GLN
2	H	385	ASN
2	H	451	ASN
2	H	459	HIS
2	H	604	GLN
2	H	614	HIS
2	H	948	GLN
2	H	1029	GLN
2	H	1086	GLN
2	H	1087	ASN
2	H	1104	ASN
2	H	1107	ASN
2	H	1347	ASN
2	H	1349	GLN
2	H	1376	GLN
2	H	1681	GLN
2	H	1683	GLN
2	H	1688	HIS
2	B	280	ASN
2	B	316	ASN
2	B	394	ASN
2	B	447	HIS
2	B	604	GLN
2	B	614	HIS
2	B	1107	ASN
2	B	1142	GLN
2	B	1281	GLN
2	B	1300	ASN
2	B	1469	GLN
2	B	1789	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	A	58/76 (76%)	21 (36%)	2 (3%)

All (21) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	A	8	U
3	A	10	G

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Mol	Chain	Res	Type
3	A	13	U
3	A	17	C
3	A	23	C
3	A	26	G
3	A	29	C
3	A	36	C
3	A	37	A
3	A	38	U
3	A	43	G
3	A	44	A
3	A	45	G
3	A	46	G
3	A	47	U
3	A	48	C
3	A	56	C
3	A	58	A
3	A	59	U
3	A	60	U
3	A	61	C

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	A	7	G
3	A	37	A

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](#)

5 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
5	BGC	D	1	5	12,12,12	0.18	0	17,17,17	0.15	0
5	BGC	D	2	5	11,11,12	0.21	0	15,15,17	0.51	0
4	BGC	J	1	4	12,12,12	0.34	0	17,17,17	0.57	0
4	BGC	J	2	4	11,11,12	0.35	0	15,15,17	0.70	0
4	BGC	J	3	4	11,11,12	0.21	0	15,15,17	0.55	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
5	BGC	D	1	5	-	2/2/22/22	0/1/1/1
5	BGC	D	2	5	-	2/2/19/22	0/1/1/1
4	BGC	J	1	4	-	2/2/22/22	0/1/1/1
4	BGC	J	2	4	-	2/2/19/22	0/1/1/1
4	BGC	J	3	4	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

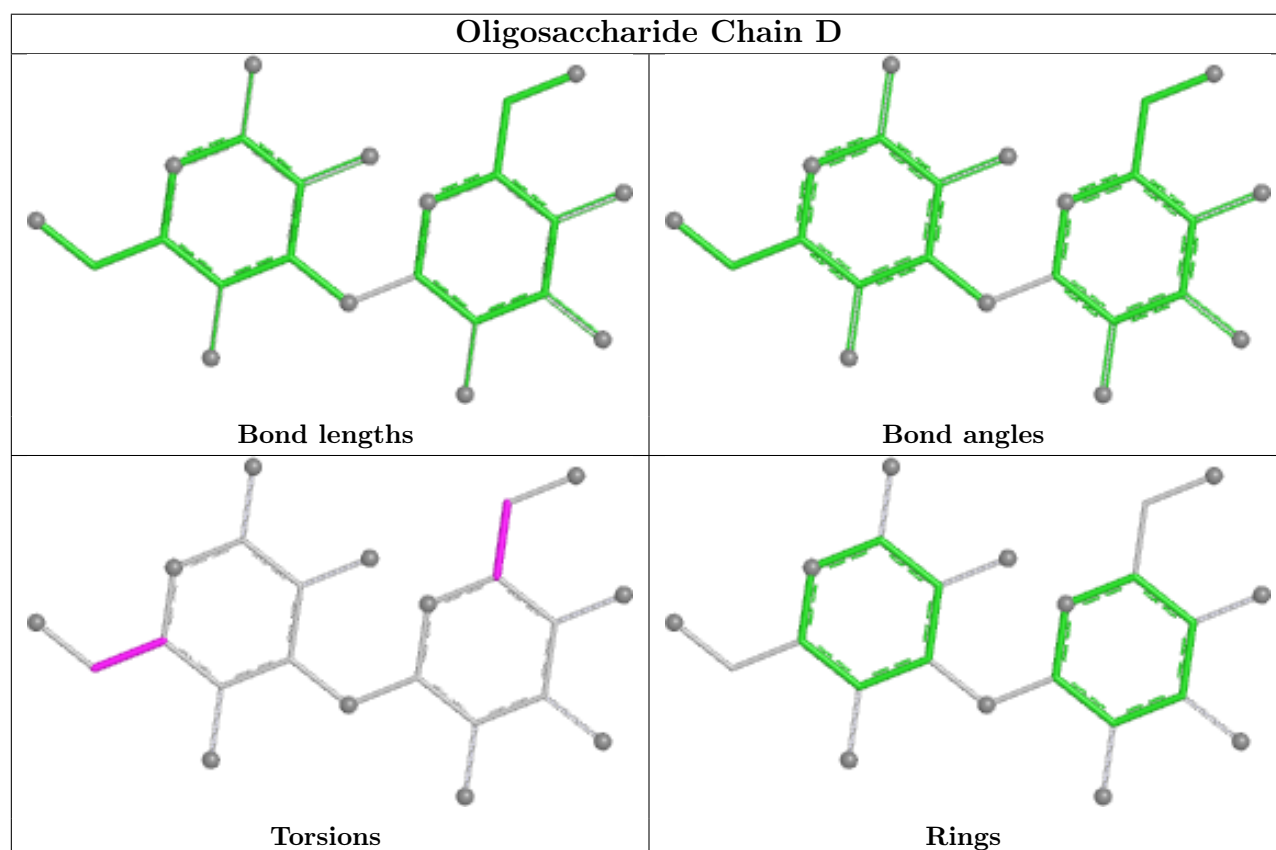
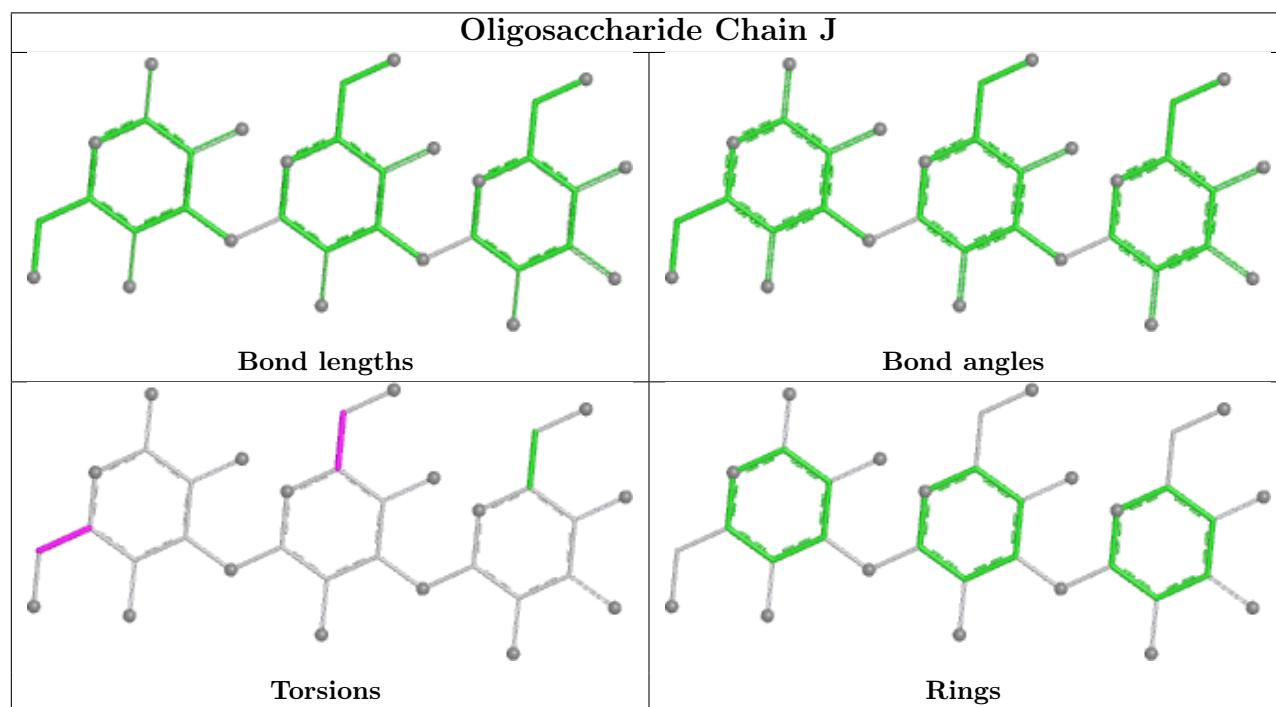
Mol	Chain	Res	Type	Atoms
5	D	2	BGC	O5-C5-C6-O6
5	D	2	BGC	C4-C5-C6-O6
4	J	2	BGC	C4-C5-C6-O6
4	J	1	BGC	C4-C5-C6-O6
4	J	1	BGC	O5-C5-C6-O6
4	J	2	BGC	O5-C5-C6-O6
5	D	1	BGC	C4-C5-C6-O6
5	D	1	BGC	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	J	1	BGC	1	0

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

Of 40 ligands modelled in this entry, 2 are monoatomic - leaving 38 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	HP6	H	1908	-	6,6,6	0.32	0	5,5,5	0.66	0
12	PLM	B	1913	-	17,17,17	0.57	0	17,17,17	1.10	0
13	DCR	B	1917	-	21,21,21	0.52	0	21,21,21	1.07	0
7	DD9	B	1902	-	8,8,8	0.26	0	7,7,7	0.86	0
12	PLM	H	1914	-	17,17,17	0.60	0	17,17,17	1.05	0
9	HP6	B	1908	-	6,6,6	0.29	0	5,5,5	0.72	0
12	PLM	H	1912	-	17,17,17	0.59	0	17,17,17	1.08	0
12	PLM	H	1916	-	17,17,17	0.61	0	17,17,17	1.06	0
7	DD9	H	1903	-	8,8,8	0.30	0	7,7,7	0.79	0
10	XKP	H	1909	-	32,32,32	1.07	4 (12%)	35,37,37	1.05	2 (5%)
9	HP6	B	1907	-	6,6,6	0.31	0	5,5,5	0.65	0
12	PLM	B	1920	-	17,17,17	0.57	0	17,17,17	1.11	1 (5%)
12	PLM	B	1922	-	17,17,17	0.59	0	17,17,17	1.10	0
12	PLM	H	1913	-	17,17,17	0.56	0	17,17,17	1.09	1 (5%)
13	DCR	H	1915	-	21,21,21	0.55	0	21,21,21	1.02	0
8	D10	H	1906	-	9,9,9	0.32	0	8,8,8	0.78	0
12	PLM	B	1915	-	17,17,17	0.57	0	17,17,17	1.14	0
9	HP6	H	1907	-	6,6,6	0.35	0	5,5,5	0.60	0
12	PLM	H	1917	-	17,17,17	0.59	0	17,17,17	1.11	0
12	PLM	B	1916	-	17,17,17	0.57	0	17,17,17	1.08	0
11	PEF	B	1912	-	46,46,46	1.32	6 (13%)	49,51,51	1.19	2 (4%)
10	XKP	B	1911	-	32,32,32	1.08	4 (12%)	35,37,37	1.01	2 (5%)
12	PLM	B	1918	-	17,17,17	0.58	0	17,17,17	1.11	1 (5%)
7	DD9	B	1905	-	8,8,8	0.30	0	7,7,7	0.80	0
8	D10	B	1906	-	9,9,9	0.27	0	8,8,8	0.84	0
7	DD9	H	1902	-	8,8,8	0.29	0	7,7,7	0.78	0
7	DD9	B	1904	-	8,8,8	0.31	0	7,7,7	0.73	0
12	PLM	B	1921	-	17,17,17	0.54	0	17,17,17	1.17	1 (5%)
9	HP6	B	1909	-	6,6,6	0.32	0	5,5,5	0.65	0
7	DD9	H	1905	-	8,8,8	0.31	0	7,7,7	0.85	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	PLM	B	1914	-	17,17,17	0.56	0	17,17,17	1.09	0
7	DD9	B	1903	-	8,8,8	0.29	0	7,7,7	0.81	0
12	PLM	H	1911	-	17,17,17	0.59	0	17,17,17	1.06	0
12	PLM	B	1919	-	17,17,17	0.57	0	17,17,17	1.09	0
12	PLM	H	1918	-	17,17,17	0.62	0	17,17,17	1.06	0
11	PEF	H	1910	-	46,46,46	1.37	6 (13%)	49,51,51	1.01	2 (4%)
7	DD9	H	1904	-	8,8,8	0.31	0	7,7,7	0.79	0
9	HP6	B	1910	-	6,6,6	0.31	0	5,5,5	0.69	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
9	HP6	H	1908	-	-	0/4/4/4	-
12	PLM	B	1913	-	-	6/15/15/15	-
13	DCR	B	1917	-	-	7/19/19/19	-
7	DD9	B	1902	-	-	2/6/6/6	-
12	PLM	H	1914	-	-	4/15/15/15	-
9	HP6	B	1908	-	-	0/4/4/4	-
12	PLM	H	1912	-	-	7/15/15/15	-
12	PLM	H	1916	-	-	6/15/15/15	-
7	DD9	H	1903	-	-	1/6/6/6	-
10	XKP	H	1909	-	-	21/36/36/36	-
9	HP6	B	1907	-	-	0/4/4/4	-
12	PLM	B	1920	-	-	9/15/15/15	-
12	PLM	B	1922	-	-	11/15/15/15	-
12	PLM	H	1913	-	-	10/15/15/15	-
13	DCR	H	1915	-	-	7/19/19/19	-
8	D10	H	1906	-	-	3/7/7/7	-
12	PLM	B	1915	-	-	10/15/15/15	-
9	HP6	H	1907	-	-	0/4/4/4	-
12	PLM	H	1917	-	-	5/15/15/15	-
12	PLM	B	1916	-	-	7/15/15/15	-
11	PEF	B	1912	-	-	18/50/50/50	-
10	XKP	B	1911	-	-	13/36/36/36	-
12	PLM	B	1918	-	-	6/15/15/15	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	DD9	B	1905	-	-	0/6/6/6	-
8	D10	B	1906	-	-	2/7/7/7	-
7	DD9	H	1902	-	-	2/6/6/6	-
7	DD9	B	1904	-	-	2/6/6/6	-
12	PLM	B	1921	-	-	10/15/15/15	-
9	HP6	B	1909	-	-	1/4/4/4	-
7	DD9	H	1905	-	-	0/6/6/6	-
12	PLM	B	1914	-	-	5/15/15/15	-
7	DD9	B	1903	-	-	1/6/6/6	-
12	PLM	H	1911	-	-	8/15/15/15	-
12	PLM	B	1919	-	-	4/15/15/15	-
12	PLM	H	1918	-	-	7/15/15/15	-
11	PEF	H	1910	-	-	20/50/50/50	-
7	DD9	H	1904	-	-	3/6/6/6	-
9	HP6	B	1910	-	-	0/4/4/4	-

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	H	1910	PEF	O2-C10	3.83	1.45	1.34
11	B	1912	PEF	O3-C30	3.81	1.44	1.33
11	H	1910	PEF	O3-C30	3.79	1.44	1.33
11	B	1912	PEF	O2-C10	3.63	1.44	1.34
11	B	1912	PEF	O2-C2	-2.74	1.40	1.46
10	B	1911	XKP	O6-C7	-2.66	1.40	1.46
11	H	1910	PEF	C31-C30	2.65	1.58	1.50
11	H	1910	PEF	O2-C2	-2.61	1.40	1.46
10	H	1909	XKP	O6-C7	-2.59	1.40	1.46
11	B	1912	PEF	C31-C30	2.59	1.58	1.50
11	H	1910	PEF	C11-C10	2.49	1.57	1.50
10	B	1911	XKP	O1-C5	2.44	1.40	1.33
10	H	1909	XKP	O1-C5	2.39	1.40	1.33
11	H	1910	PEF	P-O3P	2.31	1.68	1.59
11	B	1912	PEF	P-O3P	2.30	1.68	1.59
11	B	1912	PEF	C11-C10	2.22	1.57	1.50
10	B	1911	XKP	O6-C11	2.17	1.40	1.34
10	H	1909	XKP	O6-C11	2.15	1.40	1.34
10	H	1909	XKP	O1-C6	-2.14	1.40	1.45
10	B	1911	XKP	O1-C6	-2.06	1.40	1.45

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	1912	PEF	O2-C10-C11	4.18	120.52	111.48
10	H	1909	XKP	O6-C11-C12	4.05	120.24	111.48
10	B	1911	XKP	O6-C11-C12	4.00	120.14	111.48
11	H	1910	PEF	O2-C10-C11	3.66	119.39	111.48
10	B	1911	XKP	O1-C5-C4	2.90	120.69	111.83
10	H	1909	XKP	O1-C5-C4	2.75	120.22	111.83
11	H	1910	PEF	O3-C30-C31	2.71	120.09	111.83
11	B	1912	PEF	O3-C30-C31	2.69	120.03	111.83
12	H	1913	PLM	O1-C1-C2	2.64	122.35	114.00
12	B	1921	PLM	C3-C2-C1	-2.13	108.96	114.51
12	B	1918	PLM	C3-C2-C1	-2.04	109.20	114.51
12	B	1920	PLM	C3-C2-C1	-2.03	109.21	114.51

There are no chirality outliers.

All (218) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	H	1909	XKP	C12-C11-O6-C7
10	H	1909	XKP	C7-C8-O2-P
10	H	1909	XKP	C8-O2-P-O3
10	H	1909	XKP	C8-O2-P-O4
10	H	1909	XKP	C8-O2-P-O5
10	H	1909	XKP	C9-O5-P-O4
10	B	1911	XKP	C12-C11-O6-C7
10	B	1911	XKP	C7-C8-O2-P
10	B	1911	XKP	C8-O2-P-O3
10	B	1911	XKP	C8-O2-P-O5
11	H	1910	PEF	O3P-C1-C2-O2
10	H	1909	XKP	O7-C11-O6-C7
10	B	1911	XKP	O7-C11-O6-C7
10	H	1909	XKP	O-C5-O1-C6
10	H	1909	XKP	C4-C5-O1-C6
10	B	1911	XKP	C4-C5-O1-C6
10	B	1911	XKP	O-C5-O1-C6
11	B	1912	PEF	C35-C36-C37-C38
12	H	1917	PLM	C1-C2-C3-C4
11	B	1912	PEF	C10-C11-C12-C13
10	B	1911	XKP	C11-C12-C13-C14
12	H	1913	PLM	C1-C2-C3-C4
12	B	1921	PLM	C1-C2-C3-C4
12	B	1920	PLM	CA-CB-CC-CD

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Mol	Chain	Res	Type	Atoms
11	H	1910	PEF	C20-C21-C22-C23
10	H	1909	XKP	C11-C12-C13-C14
12	B	1914	PLM	C1-C2-C3-C4
12	B	1920	PLM	C6-C7-C8-C9
12	B	1920	PLM	C4-C5-C6-C7
12	H	1912	PLM	C7-C8-C9-CA
11	B	1912	PEF	C12-C13-C14-C15
12	H	1911	PLM	CB-CC-CD-CE
12	B	1913	PLM	CB-CC-CD-CE
12	B	1915	PLM	C4-C5-C6-C7
12	B	1918	PLM	C1-C2-C3-C4
12	H	1913	PLM	C3-C4-C5-C6
12	B	1913	PLM	C7-C8-C9-CA
11	H	1910	PEF	C34-C35-C36-C37
12	H	1912	PLM	C4-C5-C6-C7
12	B	1916	PLM	C6-C7-C8-C9
11	B	1912	PEF	C34-C35-C36-C37
11	H	1910	PEF	C15-C16-C17-C18
11	B	1912	PEF	C36-C37-C38-C39
11	H	1910	PEF	C10-C11-C12-C13
11	B	1912	PEF	C15-C16-C17-C18
11	B	1912	PEF	C18-C19-C20-C21
12	H	1916	PLM	C6-C7-C8-C9
12	B	1918	PLM	C8-C9-CA-CB
12	B	1920	PLM	C9-CA-CB-CC
12	B	1921	PLM	C4-C5-C6-C7
12	H	1917	PLM	C3-C4-C5-C6
12	B	1915	PLM	C2-C3-C4-C5
12	H	1914	PLM	C4-C5-C6-C7
11	B	1912	PEF	C30-C31-C32-C33
11	H	1910	PEF	C35-C36-C37-C38
12	H	1916	PLM	CB-CC-CD-CE
12	B	1915	PLM	C7-C8-C9-CA
12	B	1920	PLM	C2-C3-C4-C5
12	B	1921	PLM	C8-C9-CA-CB
12	B	1920	PLM	CB-CC-CD-CE
12	B	1921	PLM	CB-CC-CD-CE
7	B	1902	DD9	C3-C4-C5-C6
12	H	1917	PLM	C8-C9-CA-CB
12	B	1913	PLM	C4-C5-C6-C7
13	H	1915	DCR	C13-C14-C15-C16
12	B	1921	PLM	CC-CD-CE-CF

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Mol	Chain	Res	Type	Atoms
13	H	1915	DCR	C15-C16-C17-C18
12	B	1920	PLM	C1-C2-C3-C4
12	H	1913	PLM	C8-C9-CA-CB
11	H	1910	PEF	C18-C19-C20-C21
12	H	1918	PLM	C8-C9-CA-CB
12	B	1922	PLM	C1-C2-C3-C4
12	B	1921	PLM	C6-C7-C8-C9
12	H	1913	PLM	CC-CD-CE-CF
12	B	1914	PLM	CB-CC-CD-CE
13	B	1917	DCR	C13-C14-C15-C16
8	H	1906	D10	C3-C4-C5-C6
12	B	1918	PLM	C6-C7-C8-C9
12	H	1912	PLM	CC-CD-CE-CF
12	H	1911	PLM	CC-CD-CE-CF
12	B	1914	PLM	CA-CB-CC-CD
11	B	1912	PEF	C37-C38-C39-C40
12	B	1915	PLM	C9-CA-CB-CC
12	H	1914	PLM	C8-C9-CA-CB
12	H	1918	PLM	C4-C5-C6-C7
12	B	1916	PLM	CA-CB-CC-CD
12	B	1921	PLM	CA-CB-CC-CD
12	B	1922	PLM	C9-CA-CB-CC
12	H	1918	PLM	C1-C2-C3-C4
12	B	1919	PLM	C9-CA-CB-CC
12	H	1911	PLM	C9-CA-CB-CC
12	H	1913	PLM	C6-C7-C8-C9
12	H	1911	PLM	CD-CE-CF-CG
12	H	1916	PLM	C8-C9-CA-CB
7	H	1902	DD9	C3-C4-C5-C6
12	H	1912	PLM	CB-CC-CD-CE
12	H	1916	PLM	C1-C2-C3-C4
11	B	1912	PEF	C11-C10-O2-C2
9	B	1909	HP6	C23-C24-C25-C26
10	H	1909	XKP	C13-C14-C15-C16
11	H	1910	PEF	C33-C34-C35-C36
12	H	1914	PLM	CD-CE-CF-CG
10	H	1909	XKP	C6-C7-C8-O2
11	B	1912	PEF	C19-C20-C21-C22
11	B	1912	PEF	C38-C39-C40-C41
12	B	1914	PLM	CC-CD-CE-CF
10	H	1909	XKP	C1-C2-C3-C4
13	H	1915	DCR	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
12	H	1911	PLM	C7-C8-C9-CA
12	B	1921	PLM	CD-CE-CF-CG
12	B	1922	PLM	C8-C9-CA-CB
10	H	1909	XKP	O6-C7-C8-O2
12	H	1916	PLM	CA-CB-CC-CD
10	B	1911	XKP	C1-C2-C3-C4
12	H	1911	PLM	C8-C9-CA-CB
12	H	1912	PLM	C9-CA-CB-CC
11	H	1910	PEF	C30-C31-C32-C33
12	H	1917	PLM	C7-C8-C9-CA
12	H	1918	PLM	CB-CC-CD-CE
12	B	1922	PLM	CB-CC-CD-CE
11	H	1910	PEF	O3P-C1-C2-C3
12	B	1920	PLM	C3-C4-C5-C6
7	B	1902	DD9	C2-C3-C4-C5
10	H	1909	XKP	C6-C7-O6-C11
10	B	1911	XKP	C6-C7-O6-C11
10	H	1909	XKP	C15-C16-C18-C19
11	B	1912	PEF	C11-C12-C13-C14
12	H	1914	PLM	C9-CA-CB-CC
12	B	1915	PLM	C8-C9-CA-CB
11	B	1912	PEF	O4-C10-O2-C2
12	B	1914	PLM	C6-C7-C8-C9
12	B	1916	PLM	C5-C6-C7-C8
10	B	1911	XKP	C6-C7-C8-O2
11	H	1910	PEF	C42-C43-C44-C45
12	B	1913	PLM	C2-C3-C4-C5
8	B	1906	D10	C7-C8-C9-C10
11	H	1910	PEF	C36-C37-C38-C39
12	B	1922	PLM	CD-CE-CF-CG
10	B	1911	XKP	O6-C7-C8-O2
12	B	1922	PLM	C2-C3-C4-C5
12	H	1911	PLM	CA-CB-CC-CD
12	B	1918	PLM	C4-C5-C6-C7
12	B	1922	PLM	C3-C4-C5-C6
8	B	1906	D10	C5-C6-C7-C8
10	H	1909	XKP	C2-C3-C4-C5
10	H	1909	XKP	N-C10-C9-O5
10	B	1911	XKP	N-C10-C9-O5
11	H	1910	PEF	C1-O3P-P-O1P
12	B	1921	PLM	C3-C4-C5-C6
11	B	1912	PEF	C2-C1-O3P-P

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Mol	Chain	Res	Type	Atoms
7	B	1903	DD9	C6-C7-C8-C9
11	B	1912	PEF	C13-C14-C15-C16
13	B	1917	DCR	C2-C3-C4-C5
7	B	1904	DD9	C4-C5-C6-C7
13	H	1915	DCR	C7-C8-C9-C10
11	H	1910	PEF	C41-C42-C43-C44
7	H	1904	DD9	C3-C4-C5-C6
12	H	1917	PLM	C9-CA-CB-CC
12	B	1918	PLM	CD-CE-CF-CG
11	H	1910	PEF	C13-C14-C15-C16
12	B	1921	PLM	C5-C6-C7-C8
13	B	1917	DCR	O2-C1-C2-C3
13	B	1917	DCR	C9-C10-C11-C12
12	B	1920	PLM	CC-CD-CE-CF
13	B	1917	DCR	C14-C15-C16-C17
12	H	1913	PLM	CB-CC-CD-CE
12	H	1913	PLM	O2-C1-C2-C3
12	B	1913	PLM	C1-C2-C3-C4
12	B	1919	PLM	O2-C1-C2-C3
13	B	1917	DCR	O1-C1-C2-C3
12	H	1912	PLM	CD-CE-CF-CG
12	B	1916	PLM	C9-CA-CB-CC
12	B	1922	PLM	O2-C1-C2-C3
12	B	1916	PLM	CD-CE-CF-CG
12	H	1911	PLM	C2-C3-C4-C5
12	H	1913	PLM	O1-C1-C2-C3
12	B	1919	PLM	O1-C1-C2-C3
13	H	1915	DCR	C16-C17-C18-C19
12	B	1922	PLM	O1-C1-C2-C3
11	B	1912	PEF	C14-C15-C16-C17
12	H	1913	PLM	CA-CB-CC-CD
10	H	1909	XKP	O1-C6-C7-C8
11	H	1910	PEF	C16-C17-C18-C19
13	B	1917	DCR	C15-C16-C17-C18
12	B	1922	PLM	C4-C5-C6-C7
13	H	1915	DCR	O2-C1-C2-C3
13	H	1915	DCR	O1-C1-C2-C3
12	H	1912	PLM	C5-C6-C7-C8
12	H	1918	PLM	C6-C7-C8-C9
12	B	1915	PLM	C5-C6-C7-C8
7	B	1904	DD9	C6-C7-C8-C9
12	H	1913	PLM	CD-CE-CF-CG

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Mol	Chain	Res	Type	Atoms
12	B	1915	PLM	O2-C1-C2-C3
7	H	1902	DD9	C6-C7-C8-C9
12	B	1915	PLM	O1-C1-C2-C3
12	B	1919	PLM	C3-C4-C5-C6
7	H	1903	DD9	C6-C7-C8-C9
10	H	1909	XKP	C-C1-C2-C3
7	H	1904	DD9	C5-C6-C7-C8
8	H	1906	D10	C5-C6-C7-C8
12	B	1922	PLM	CC-CD-CE-CF
8	H	1906	D10	C6-C7-C8-C9
11	B	1912	PEF	C22-C23-C24-C25
12	H	1918	PLM	O2-C1-C2-C3
11	H	1910	PEF	O5-C30-O3-C3
12	H	1918	PLM	O1-C1-C2-C3
11	H	1910	PEF	C31-C30-O3-C3
12	B	1918	PLM	C3-C4-C5-C6
12	B	1913	PLM	CC-CD-CE-CF
11	H	1910	PEF	O2-C10-C11-C12
12	H	1916	PLM	C9-CA-CB-CC
12	B	1915	PLM	C6-C7-C8-C9
7	H	1904	DD9	C2-C3-C4-C5
10	H	1909	XKP	C14-C15-C16-C18
12	B	1915	PLM	CB-CC-CD-CE
12	B	1916	PLM	O1-C1-C2-C3
12	B	1916	PLM	O2-C1-C2-C3
11	H	1910	PEF	O4-C10-C11-C12

There are no ring outliers.

17 monomers are involved in 42 short contacts:

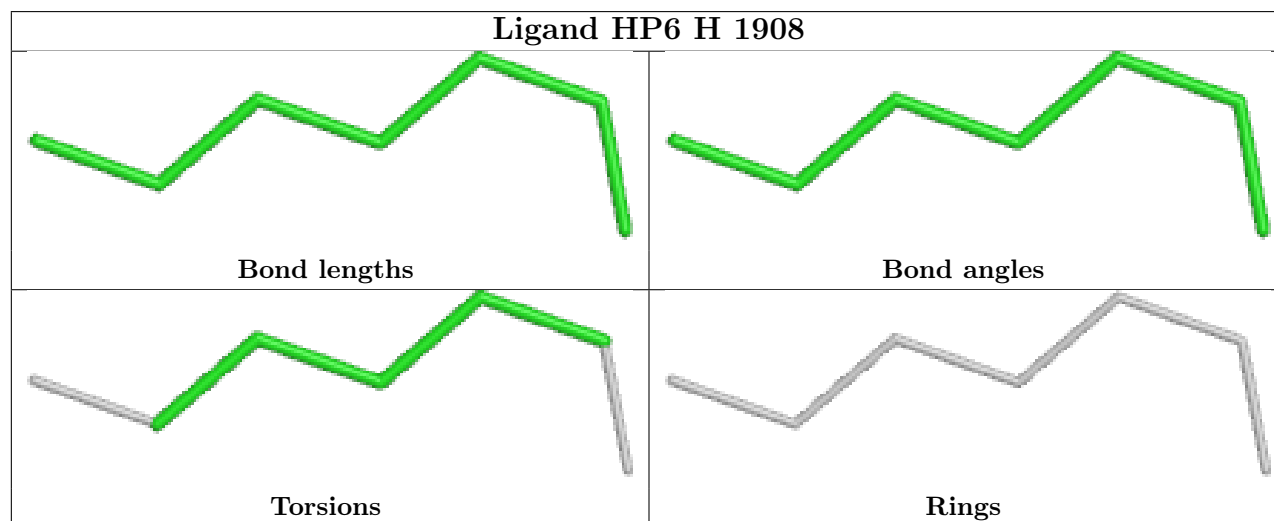
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	B	1913	PLM	1	0
12	H	1914	PLM	3	0
9	B	1908	HP6	1	0
12	H	1912	PLM	2	0
12	H	1916	PLM	2	0
12	B	1920	PLM	1	0
12	H	1913	PLM	7	0
12	B	1915	PLM	3	0
12	H	1917	PLM	1	0
11	B	1912	PEF	6	0
7	H	1902	DD9	1	0

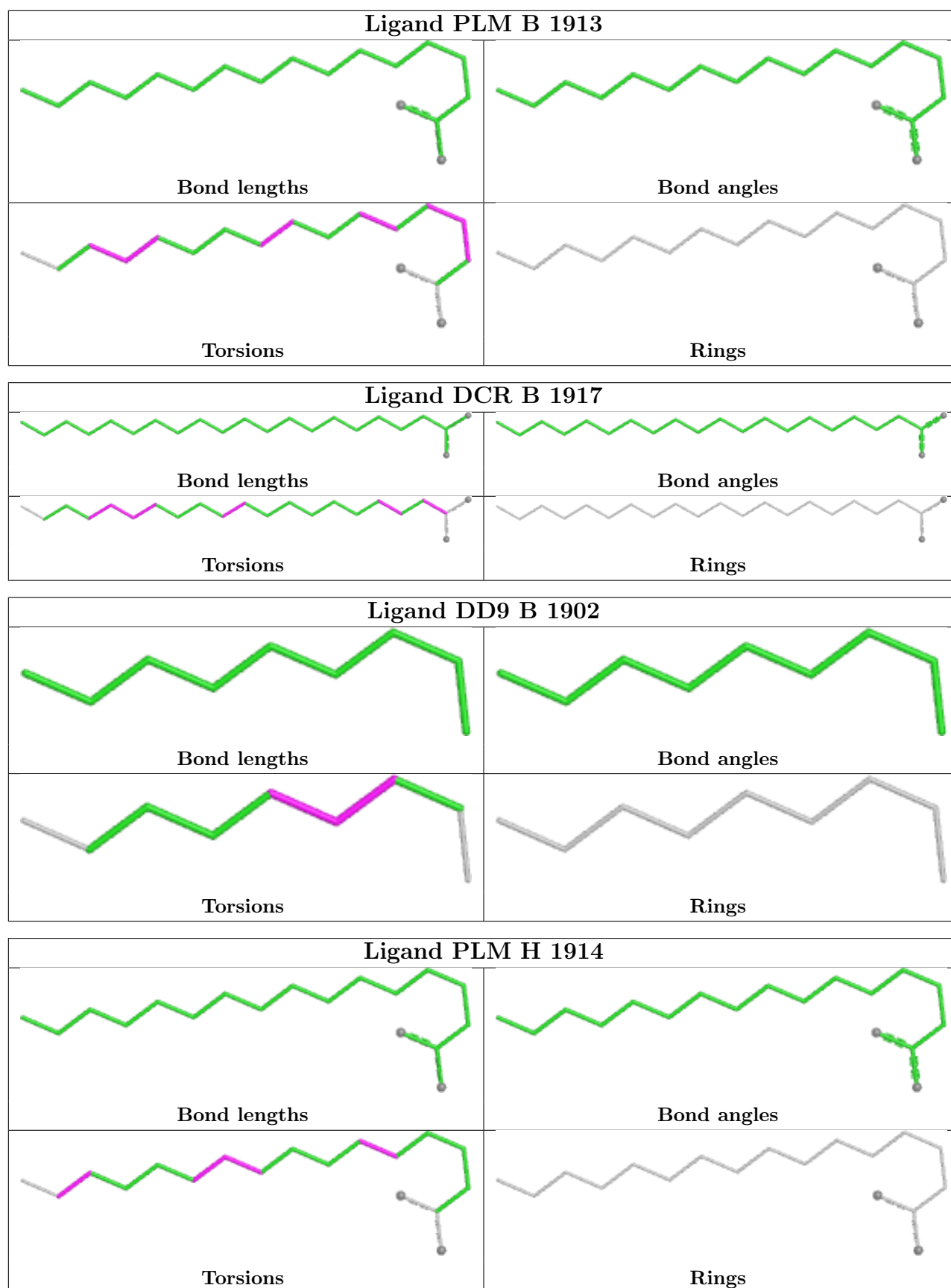
Continued on next page...

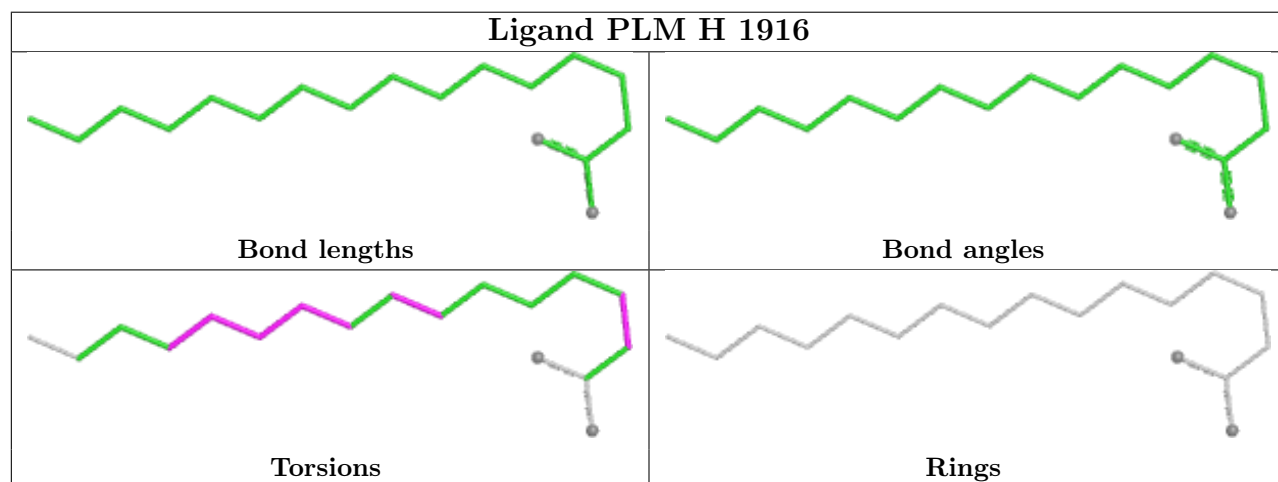
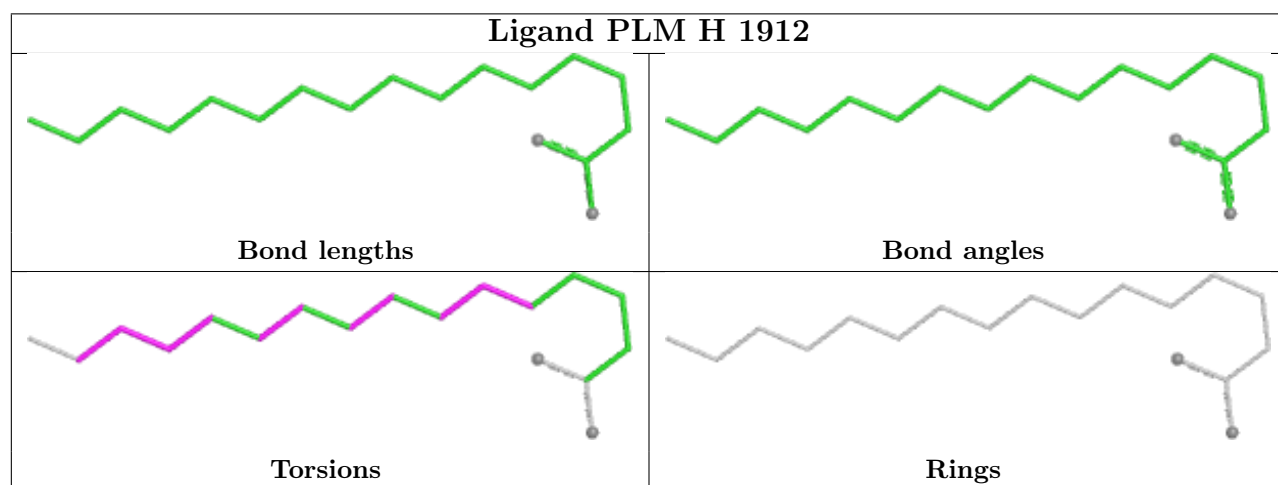
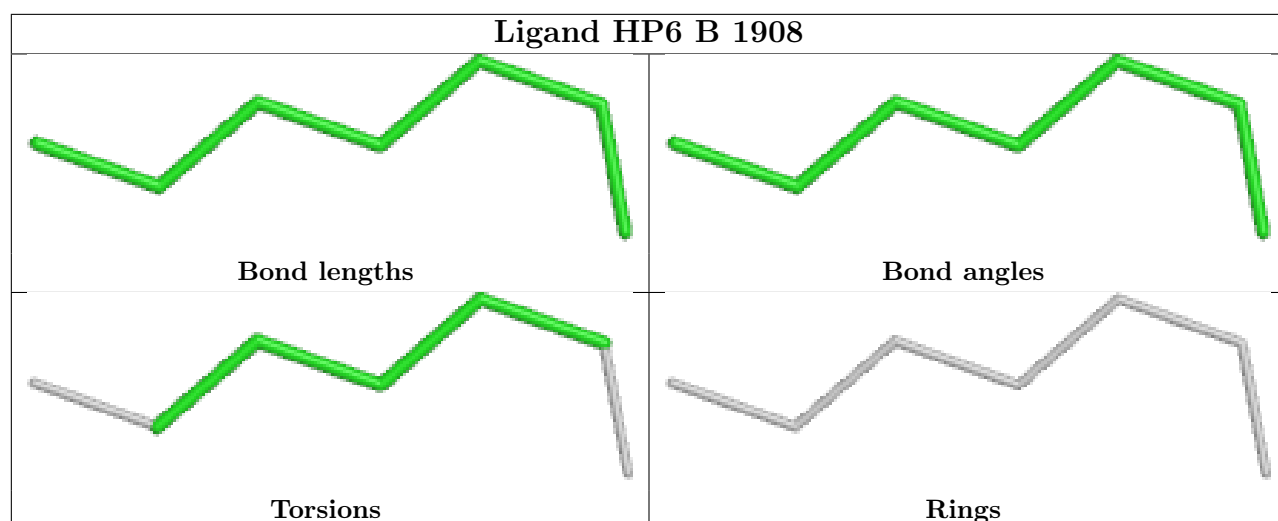
Continued from previous page...

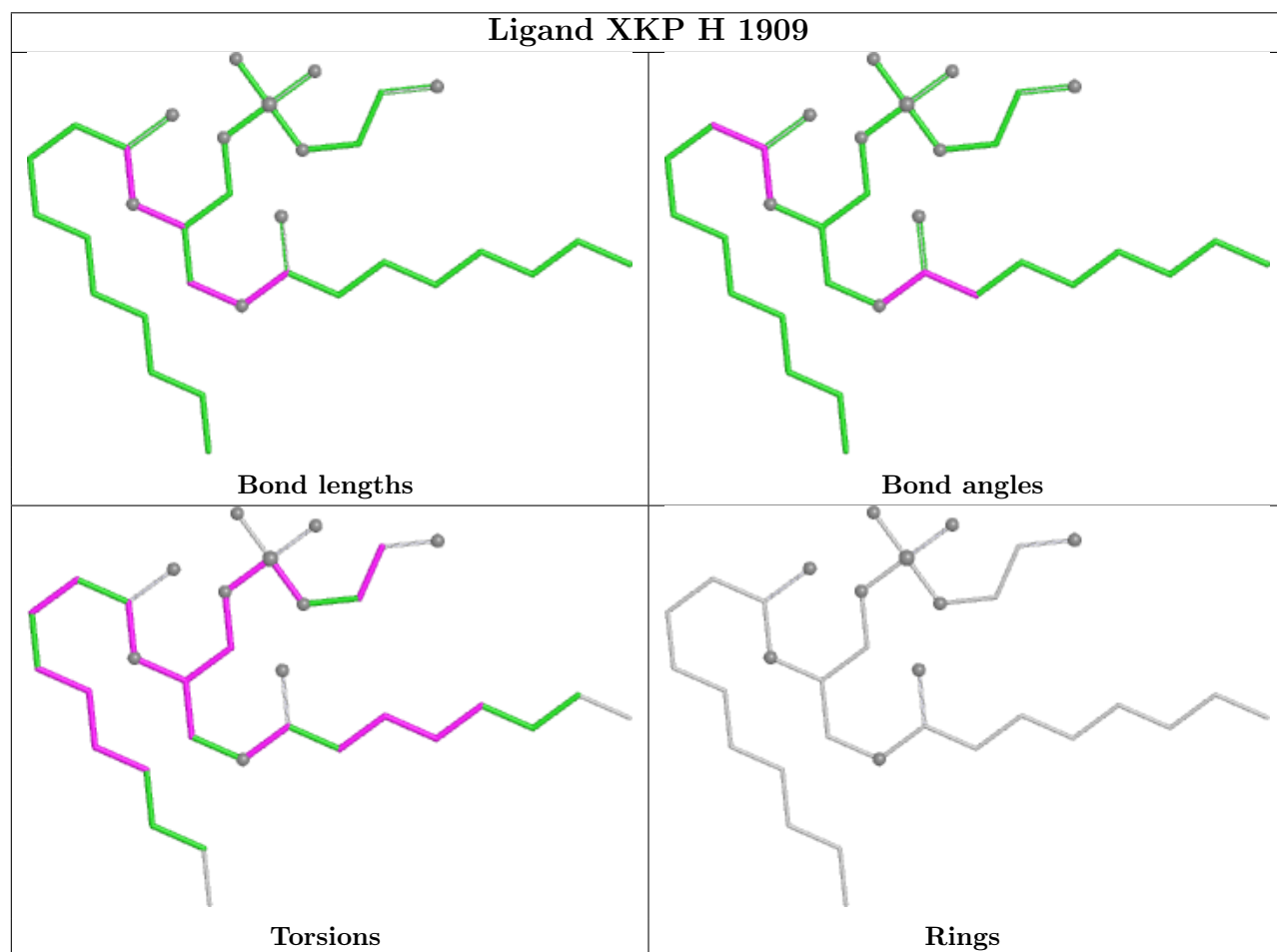
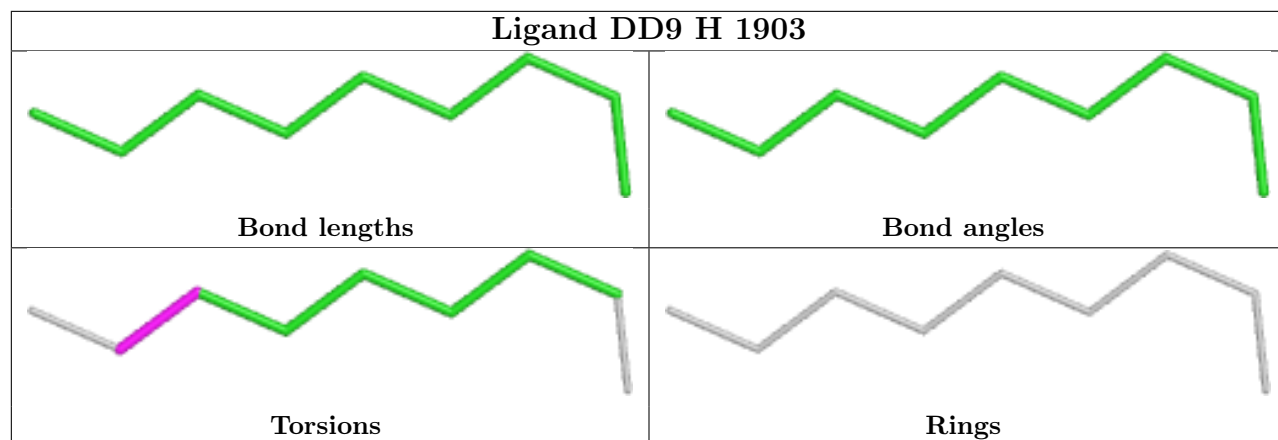
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	B	1921	PLM	2	0
12	B	1914	PLM	1	0
12	H	1911	PLM	2	0
12	B	1919	PLM	1	0
12	H	1918	PLM	2	0
11	H	1910	PEF	7	0

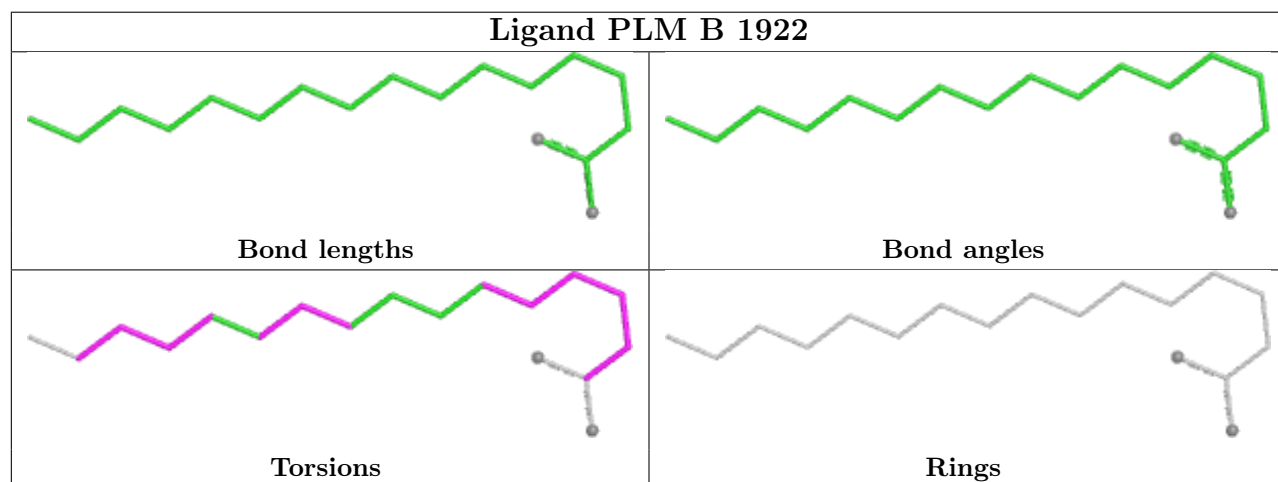
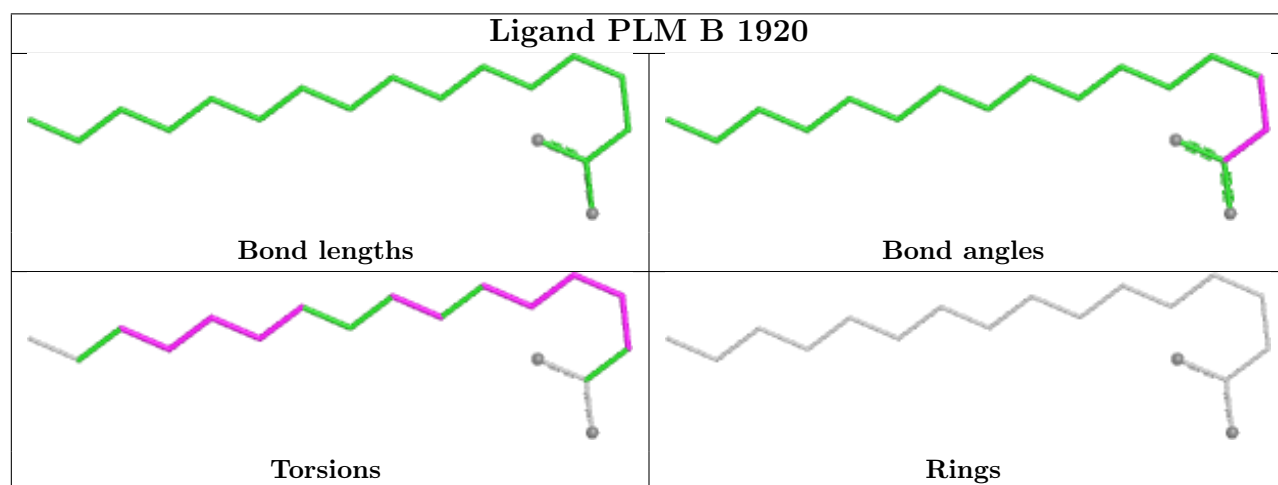
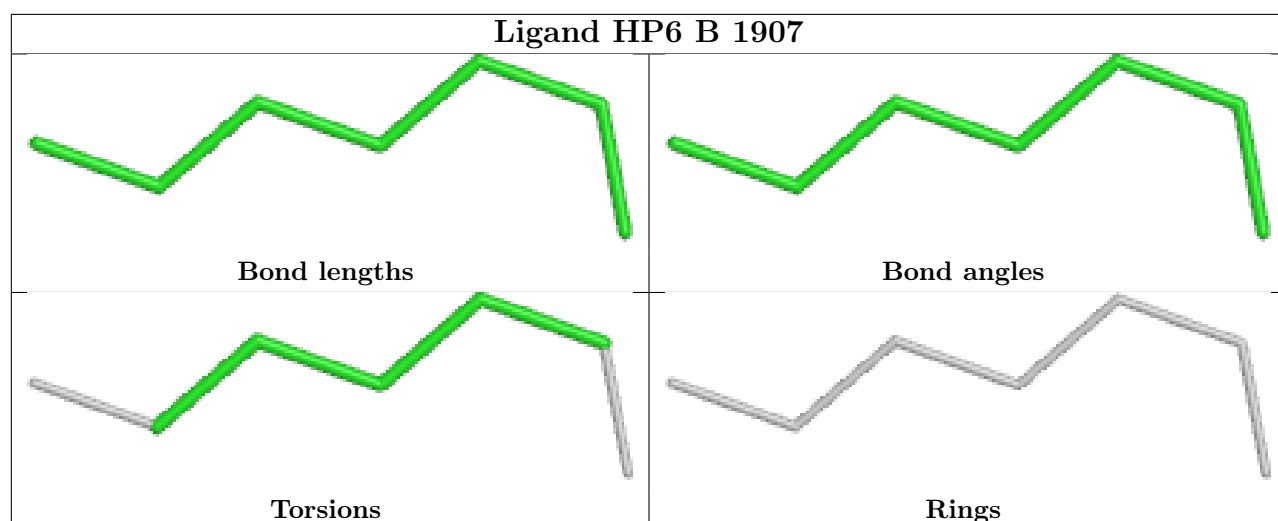
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

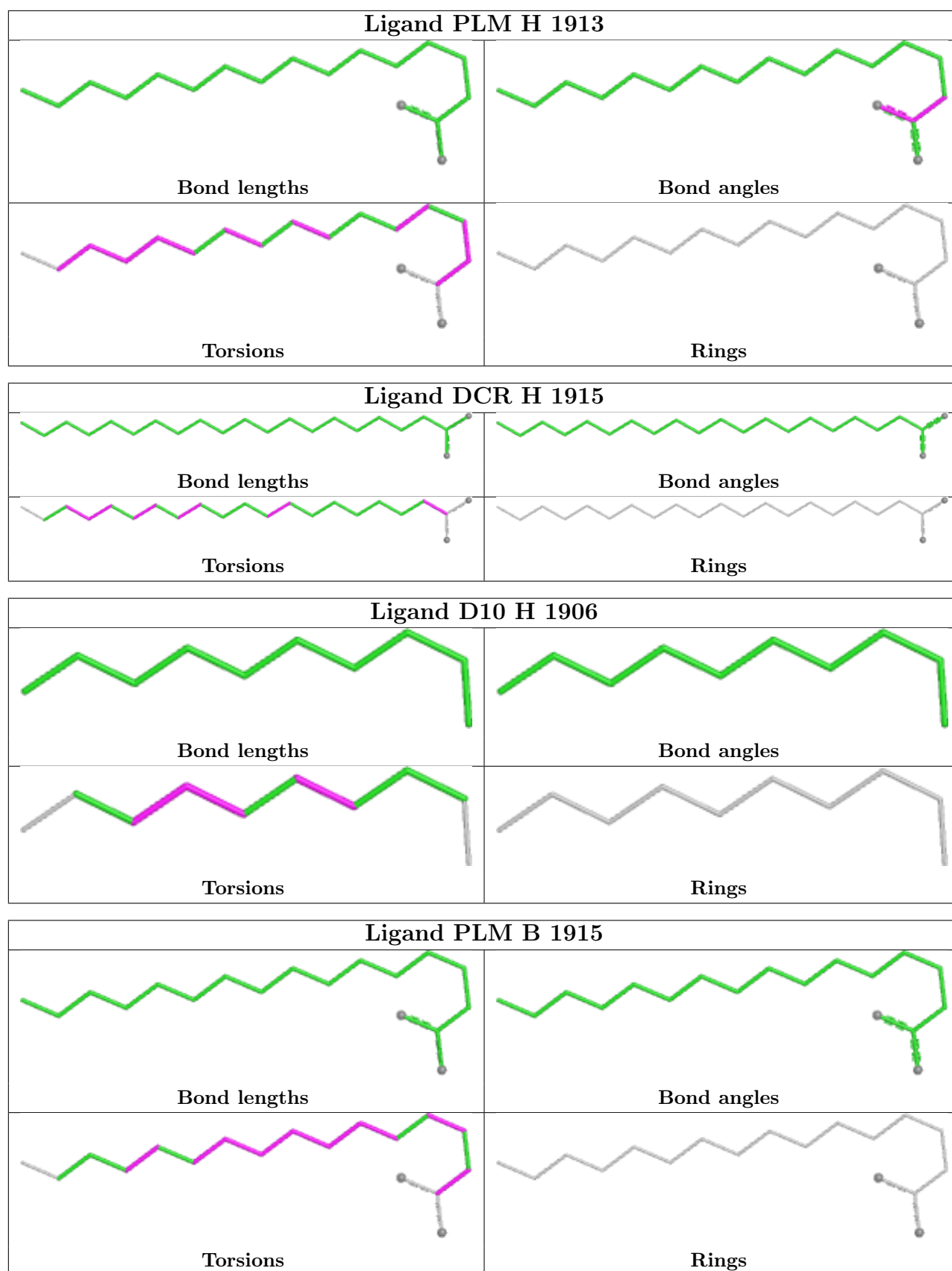


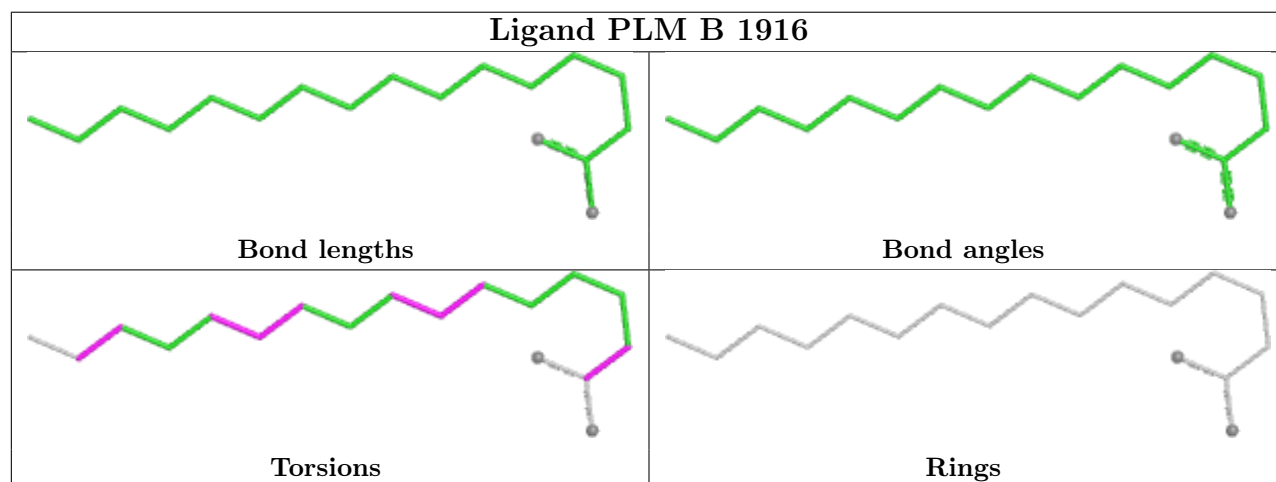
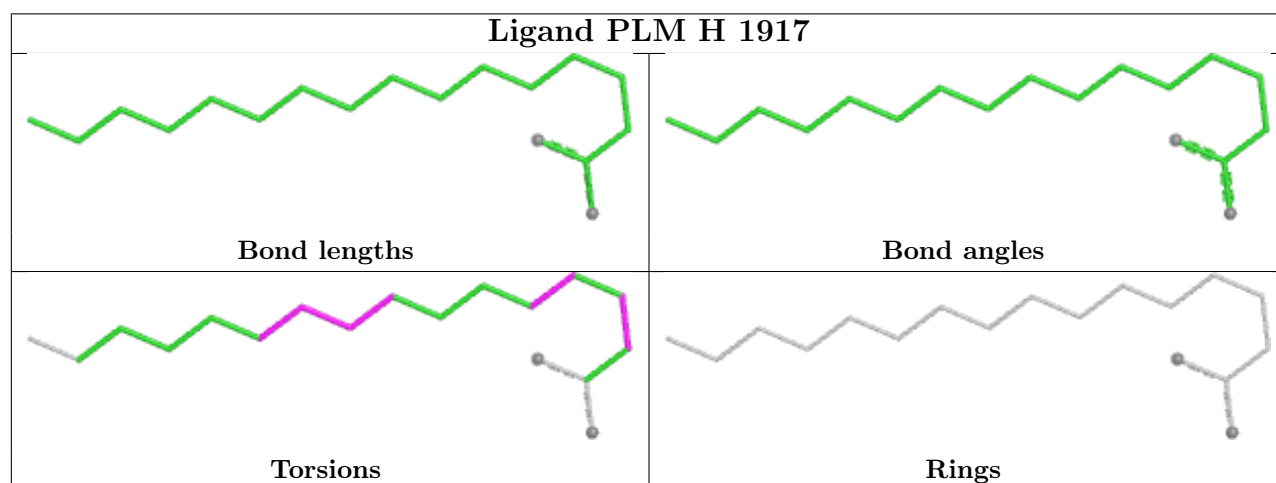
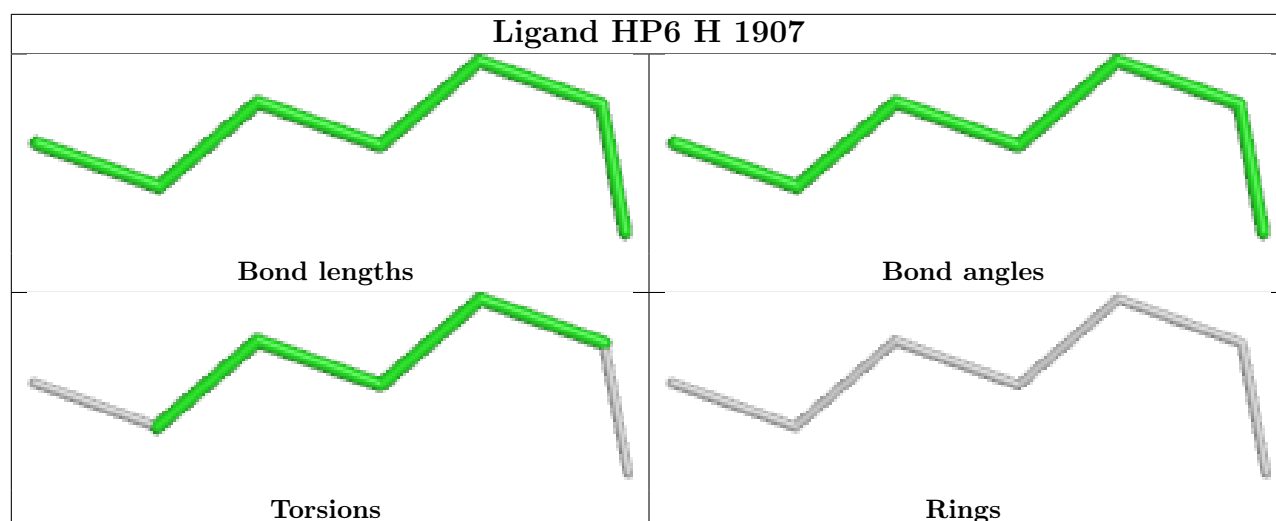


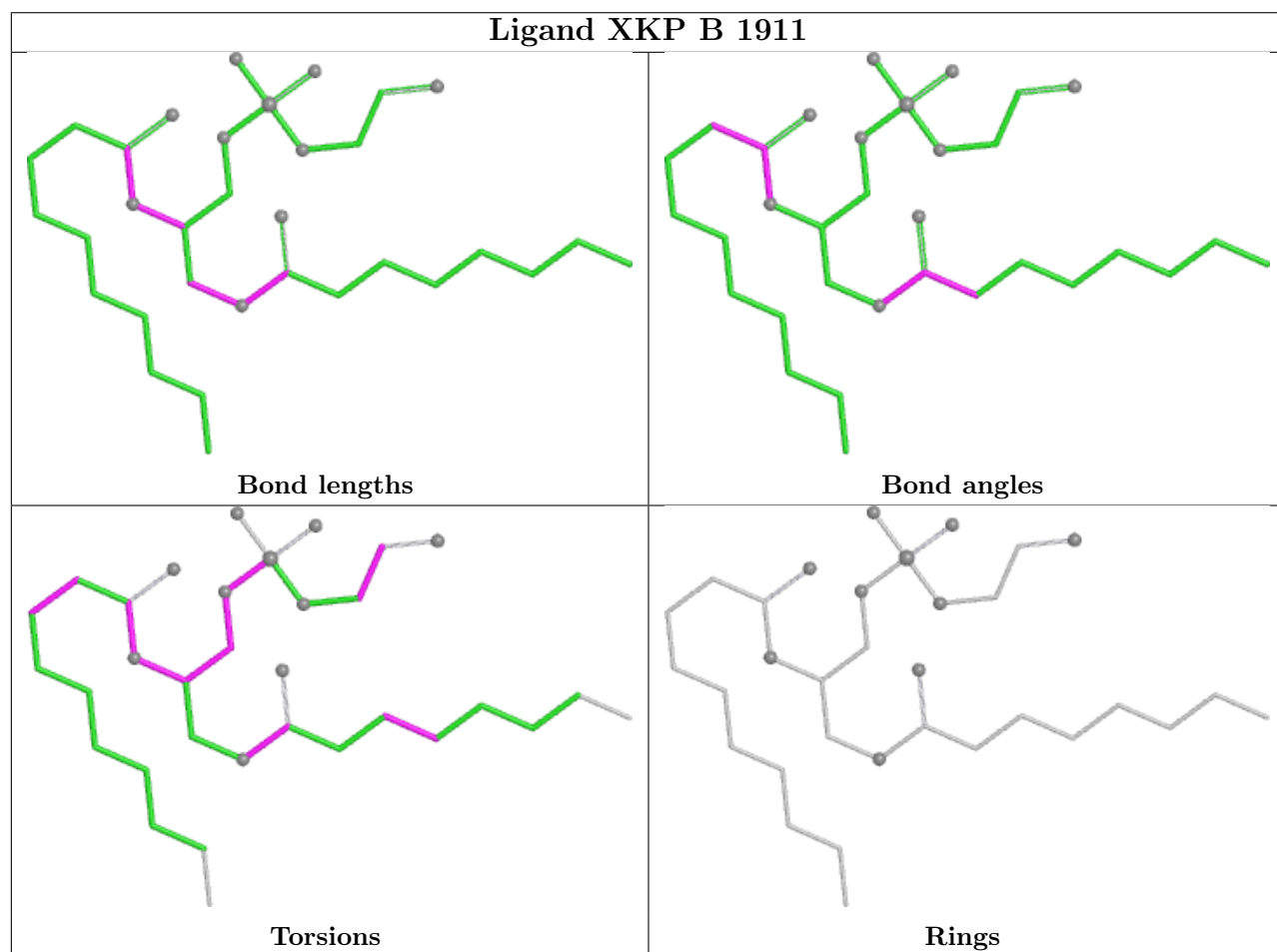
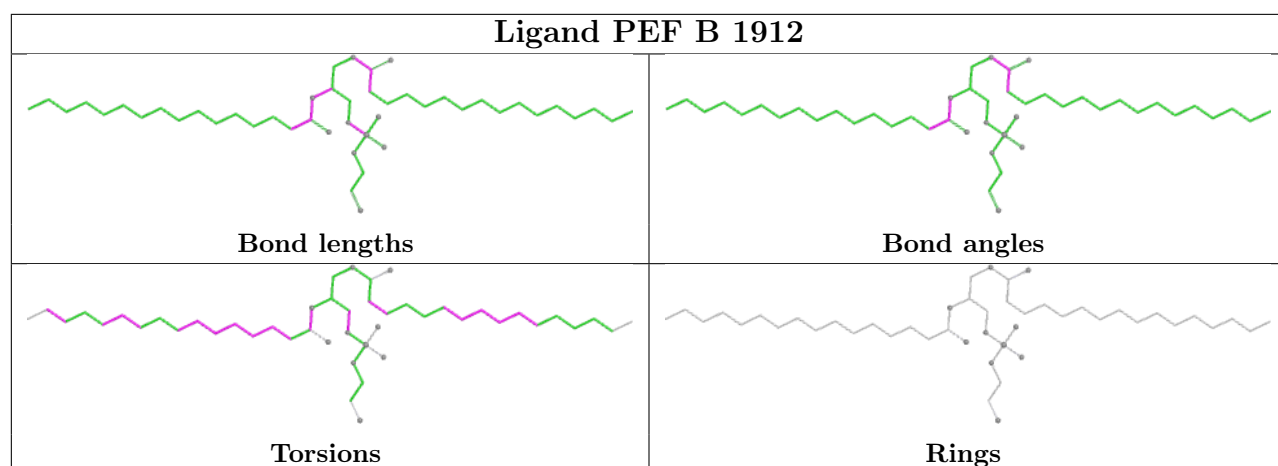


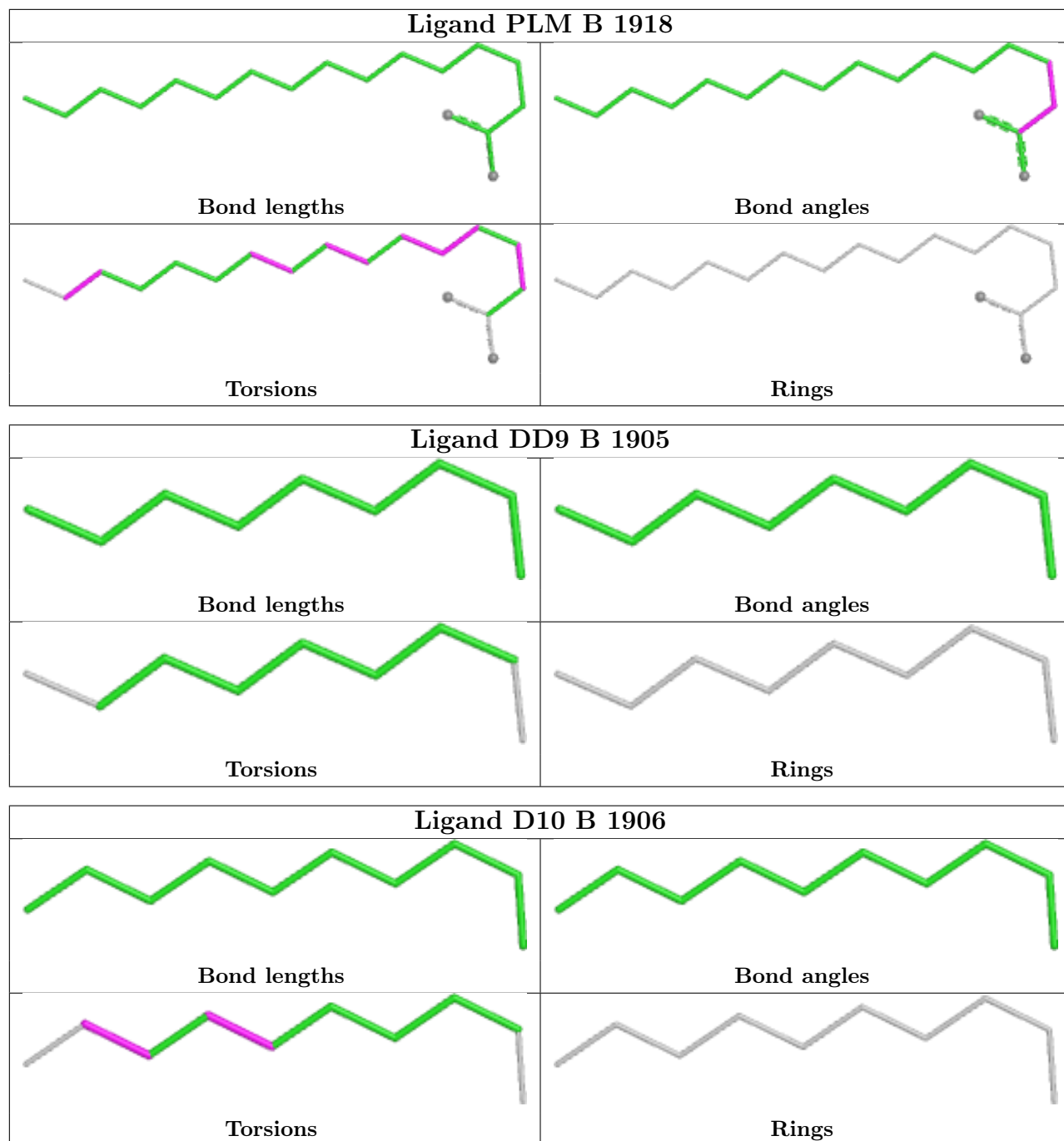


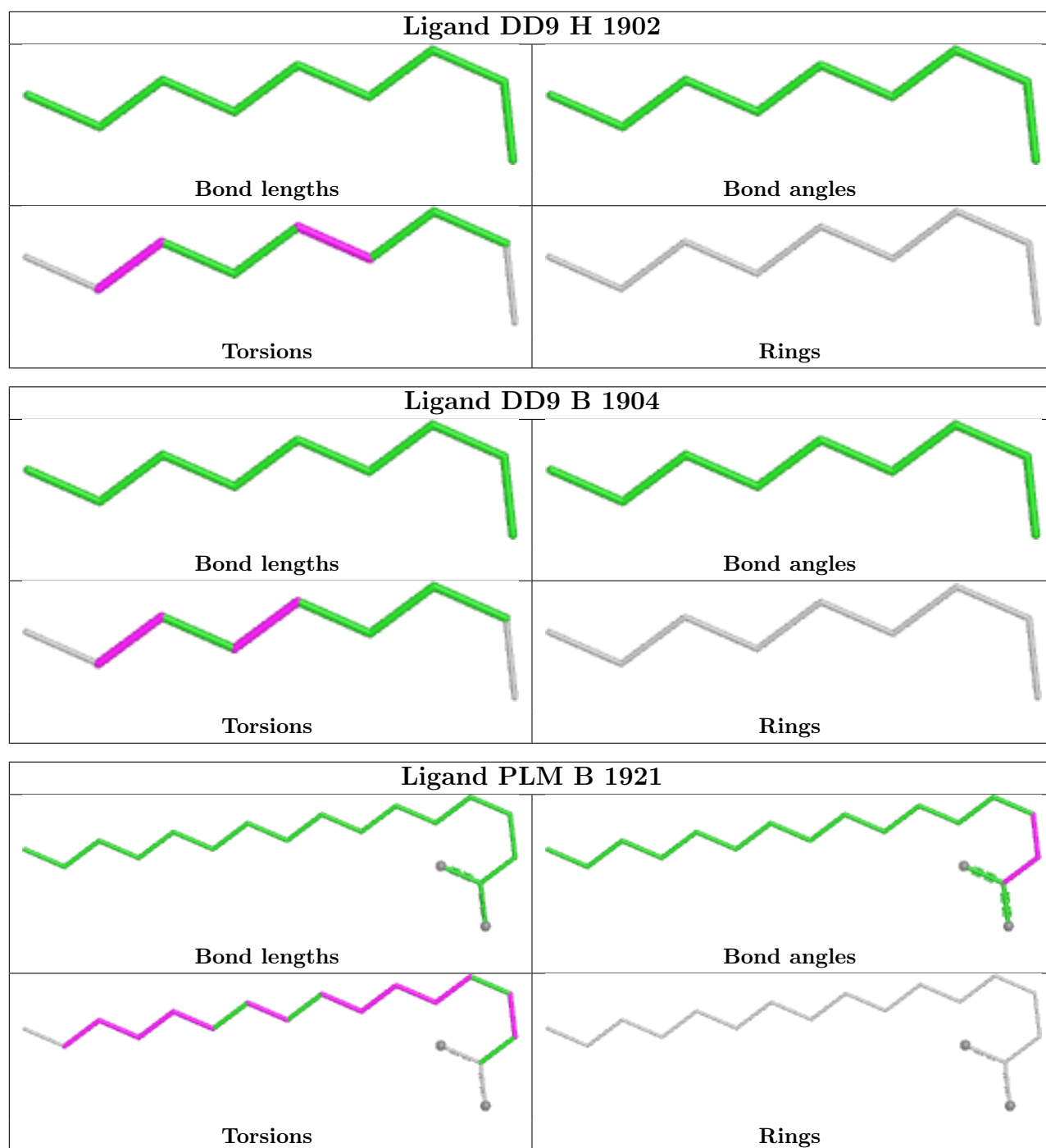


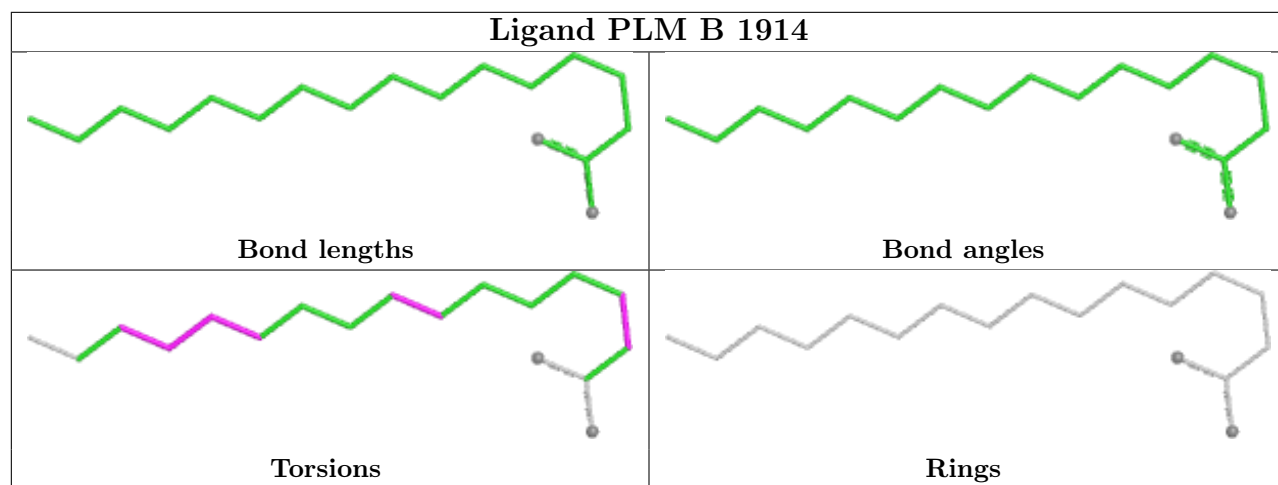
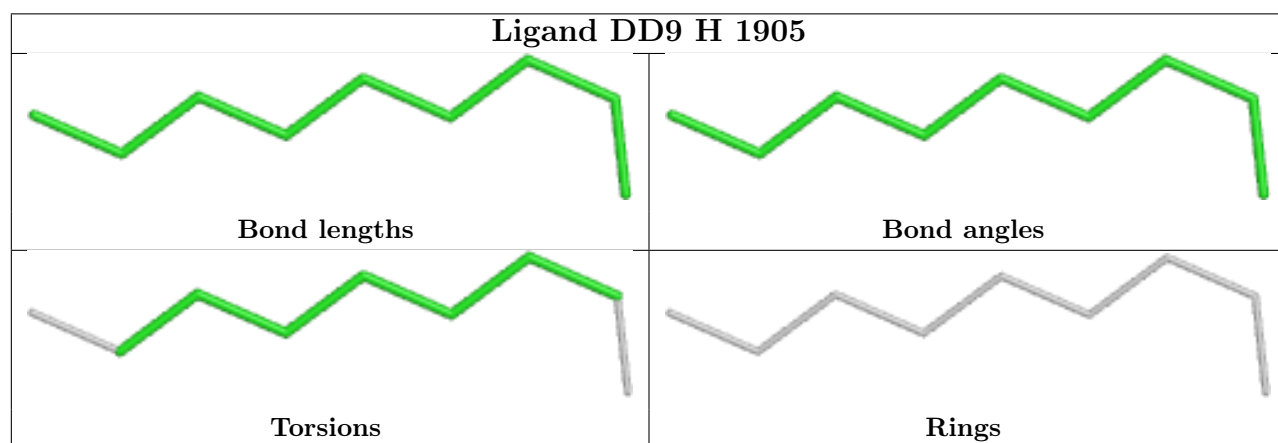
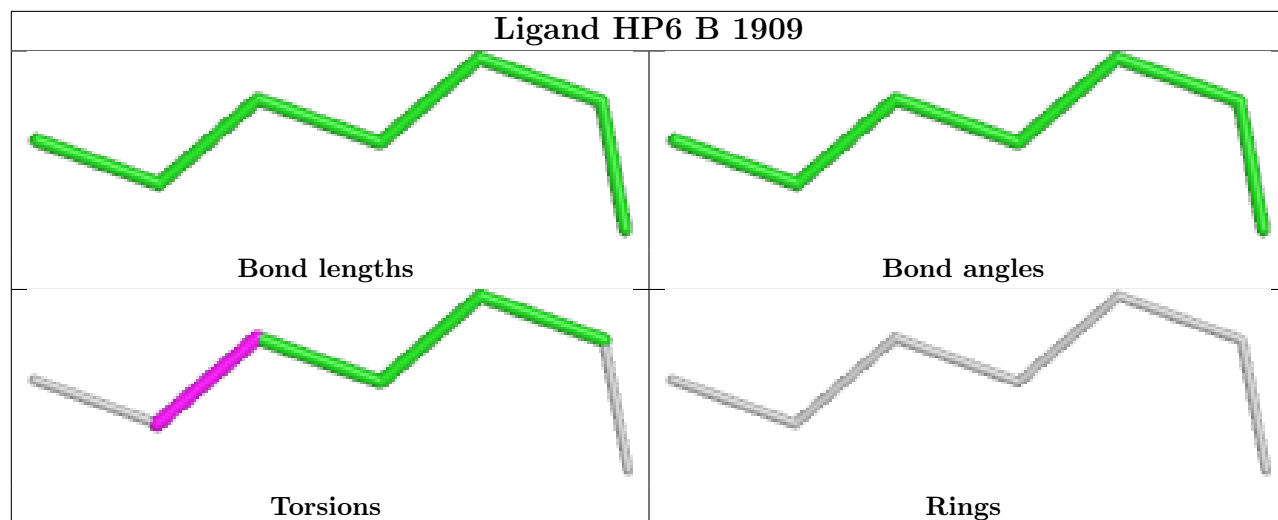


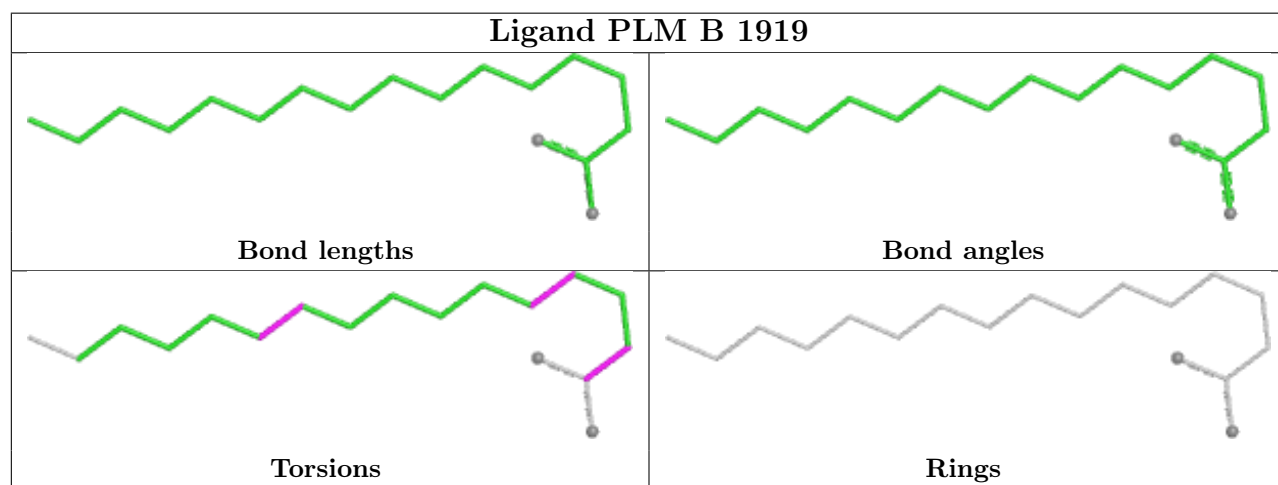
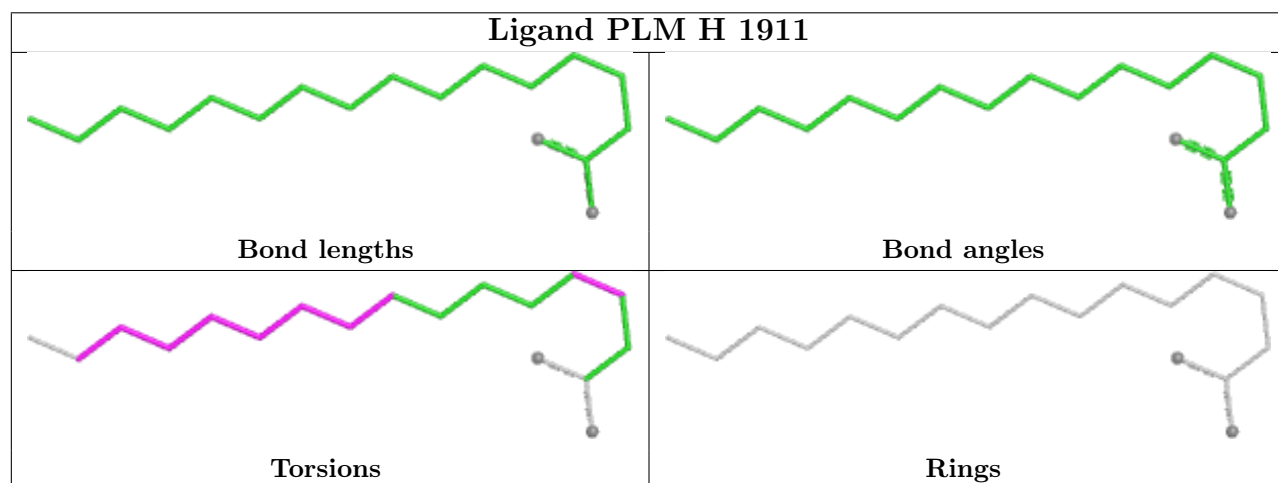
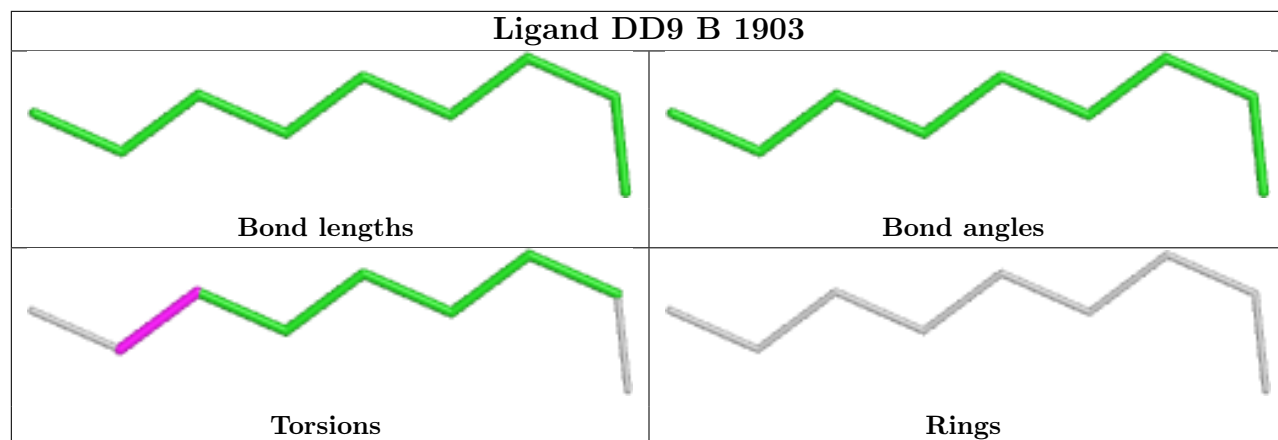


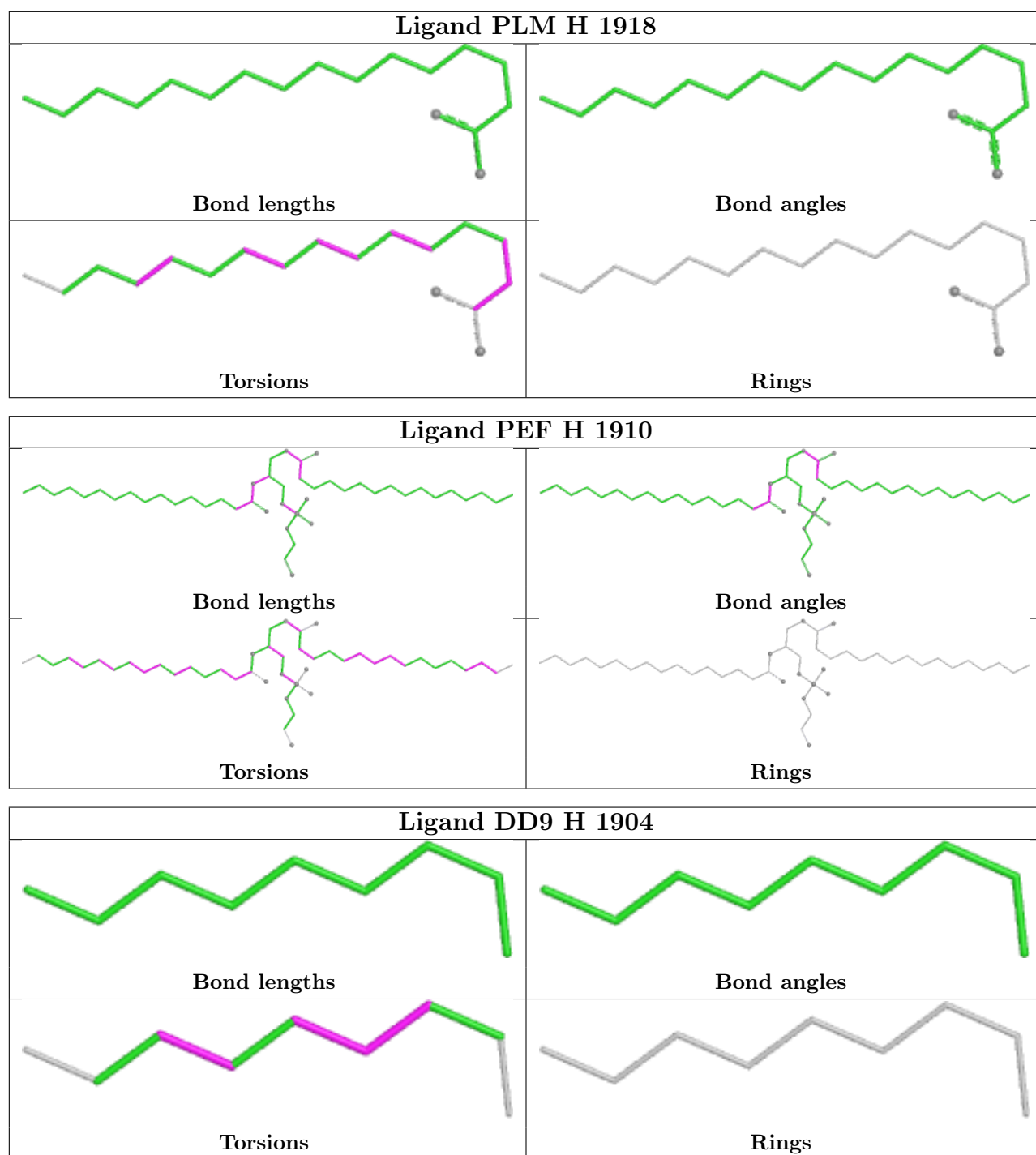


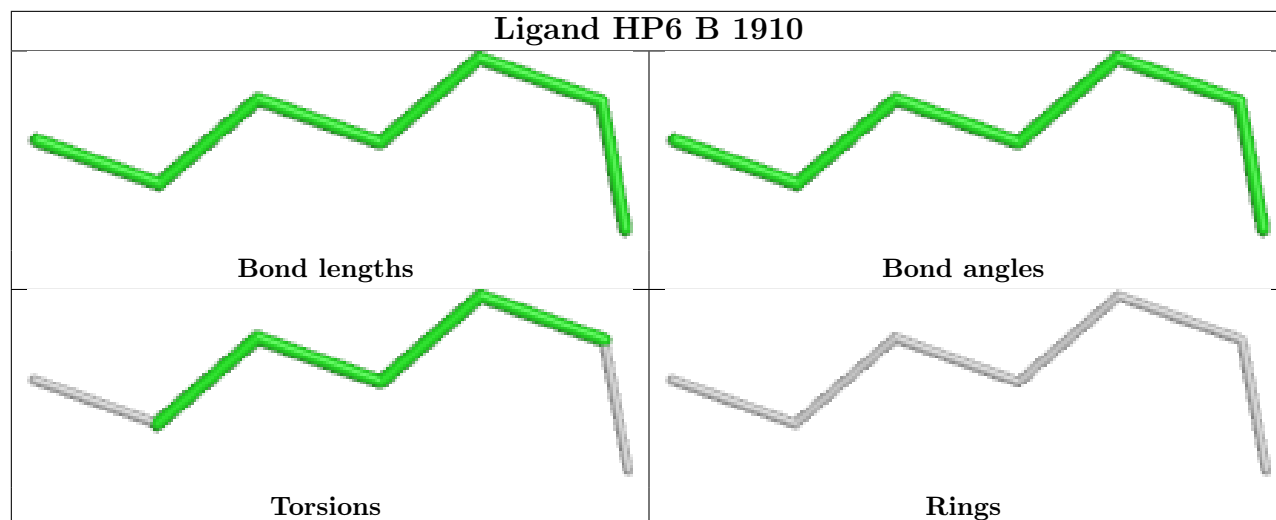












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

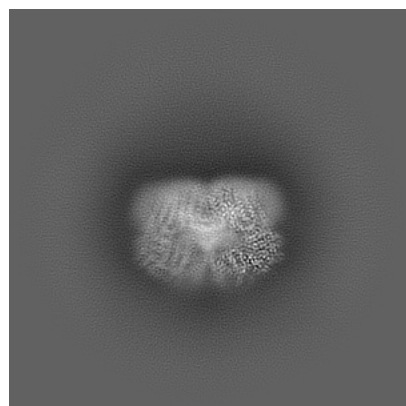
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-64502. These allow visual inspection of the internal detail of the map and identification of artifacts.

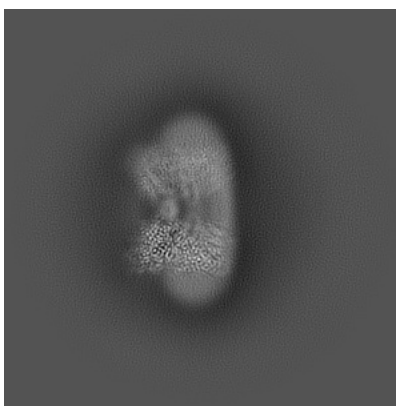
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

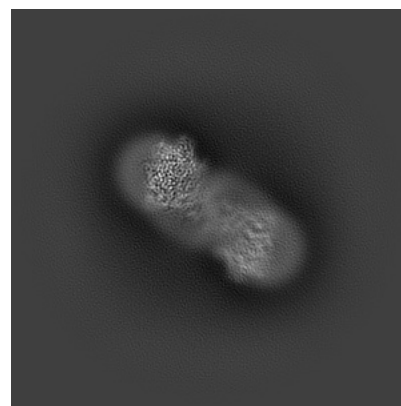
6.1.1 Primary map



X

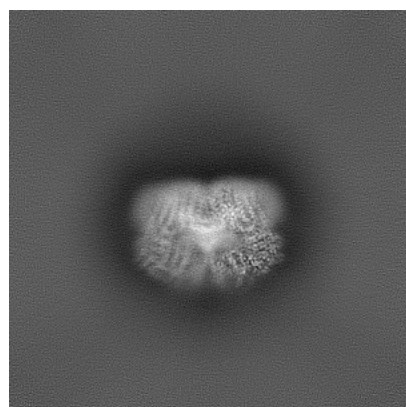


Y

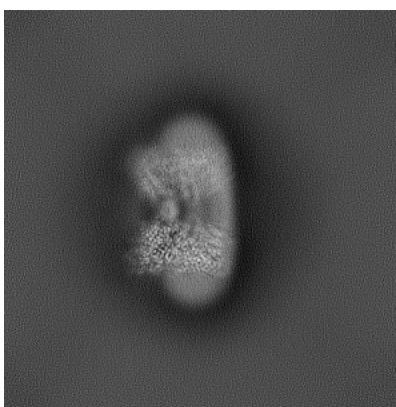


Z

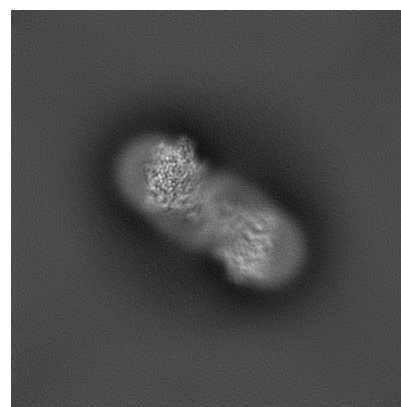
6.1.2 Raw map



X



Y

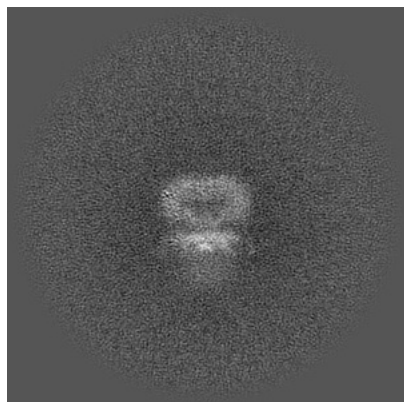


Z

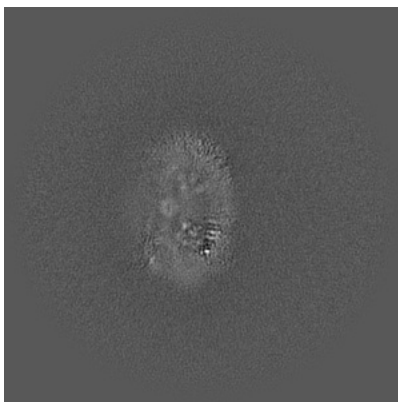
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

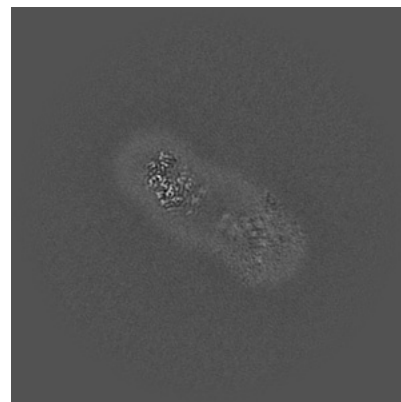
6.2.1 Primary map



X Index: 200

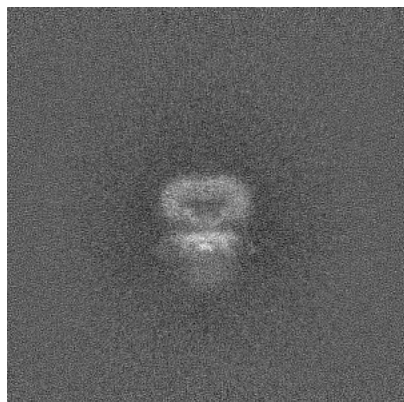


Y Index: 200

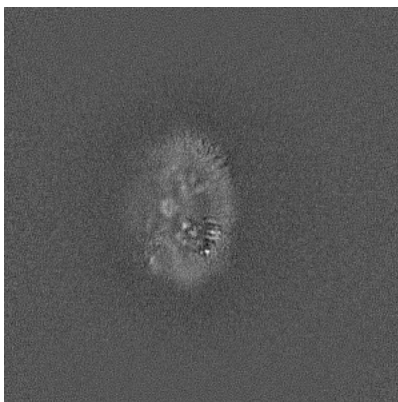


Z Index: 200

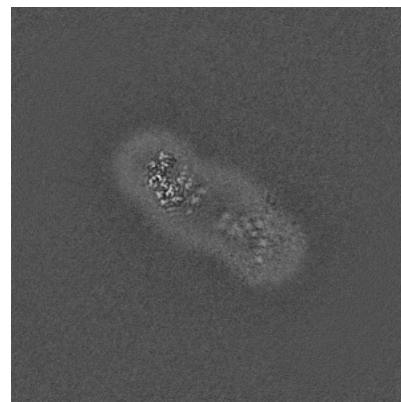
6.2.2 Raw map



X Index: 200



Y Index: 200

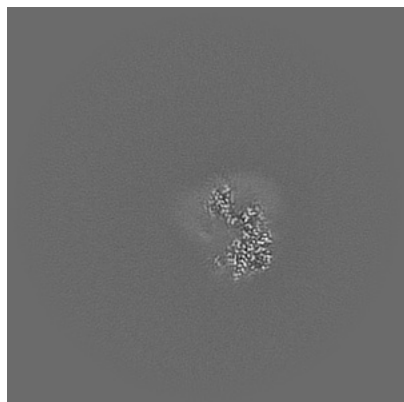


Z Index: 200

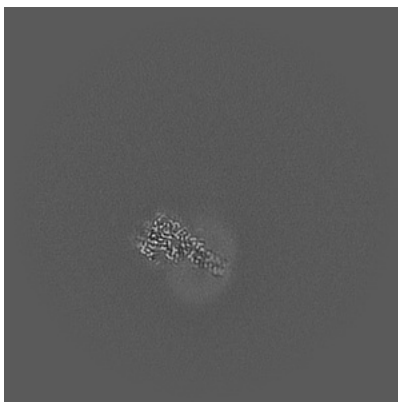
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

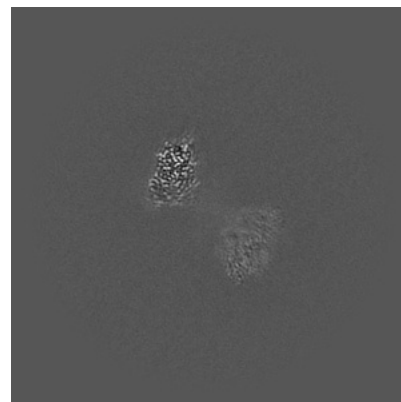
6.3.1 Primary map



X Index: 159

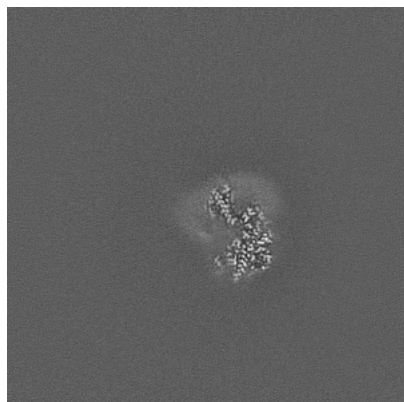


Y Index: 245

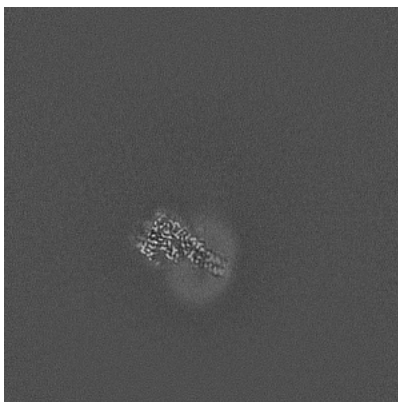


Z Index: 148

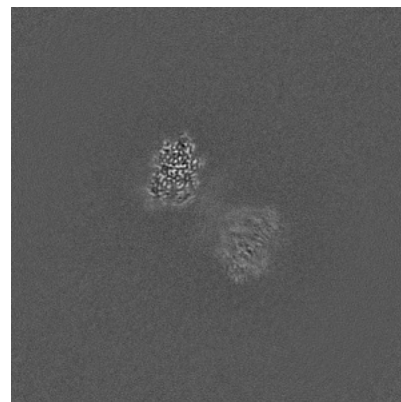
6.3.2 Raw map



X Index: 159



Y Index: 245

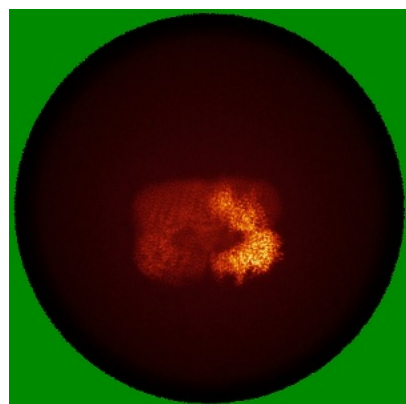


Z Index: 151

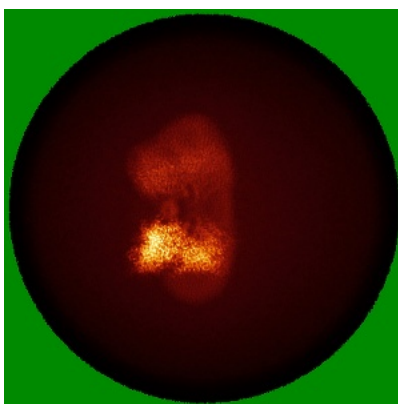
The images above show the largest variance slices of the map in three orthogonal directions.

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

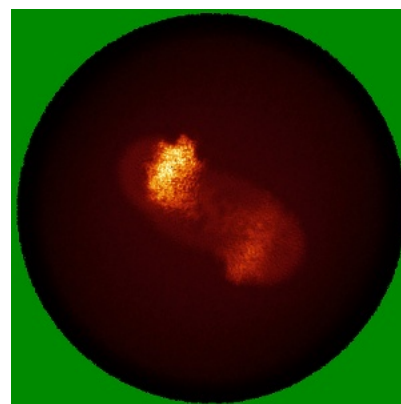
6.4.1 Primary map



X

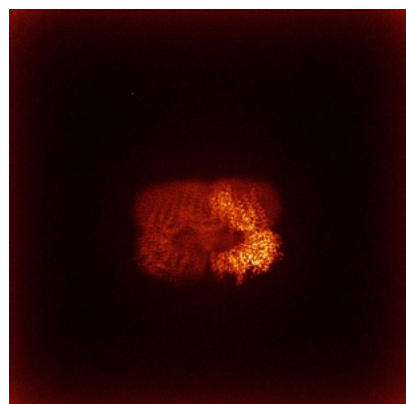


Y

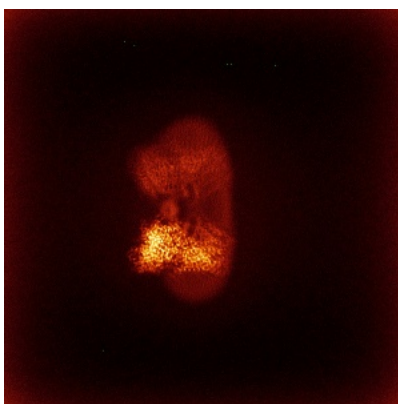


Z

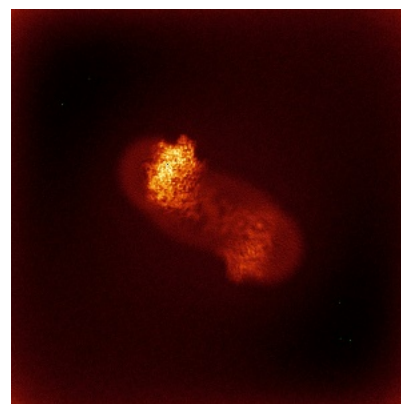
6.4.2 Raw map



X



Y

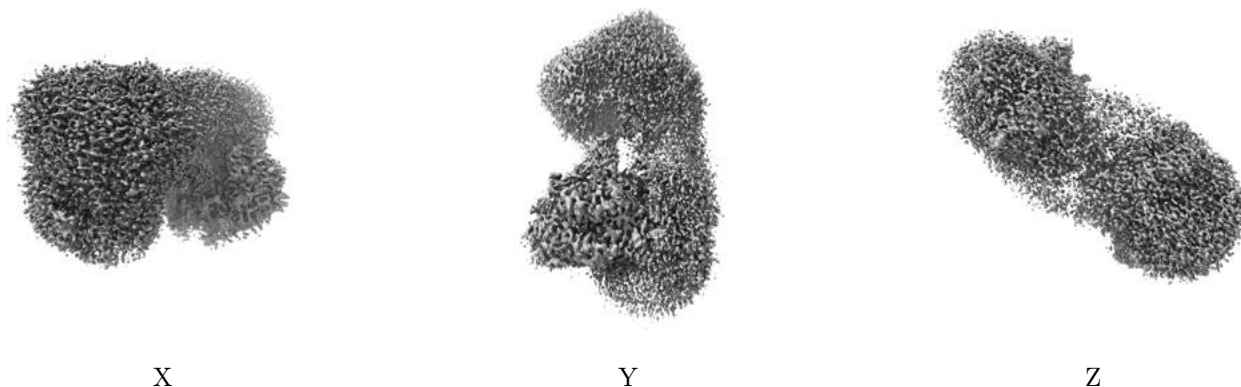


Z

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.

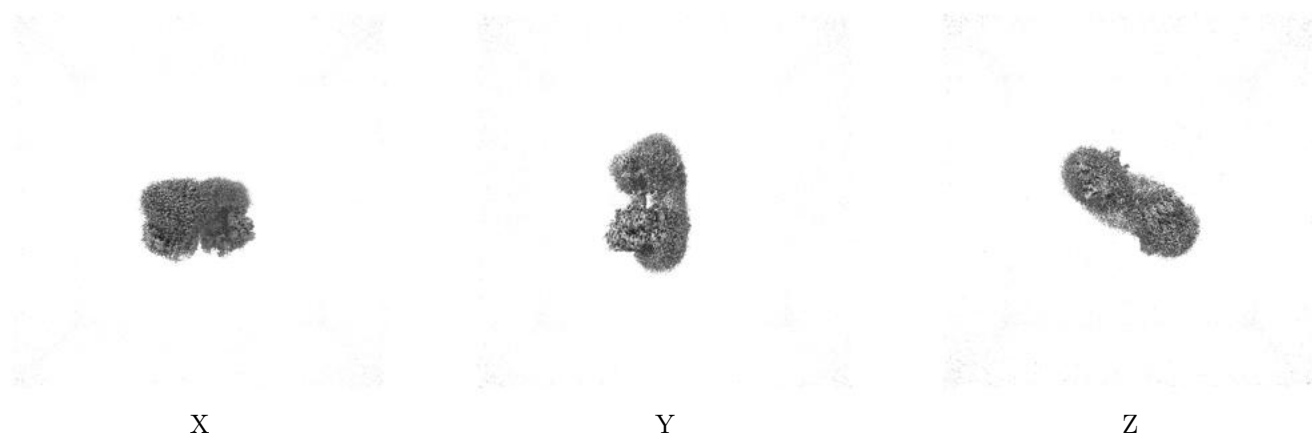
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

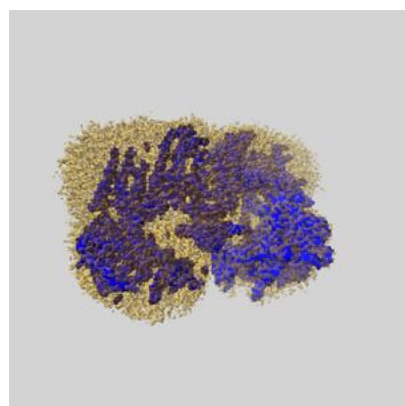
6.6 Mask visualisation [i](#)

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

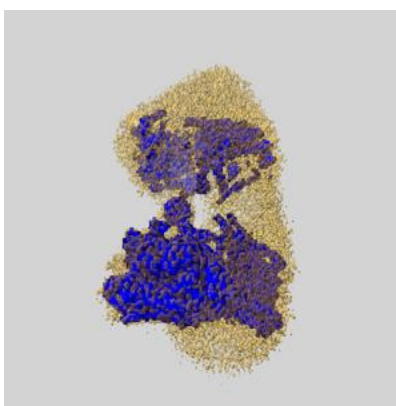
A mask typically either:

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

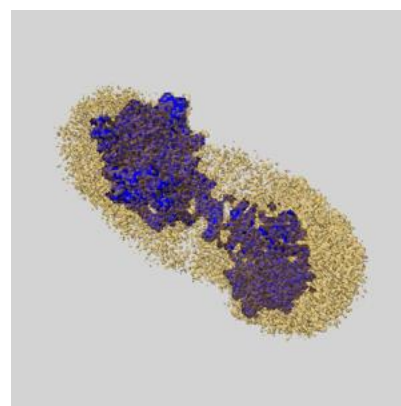
6.6.1 emd_64502_msk_1.map [i](#)



X



Y

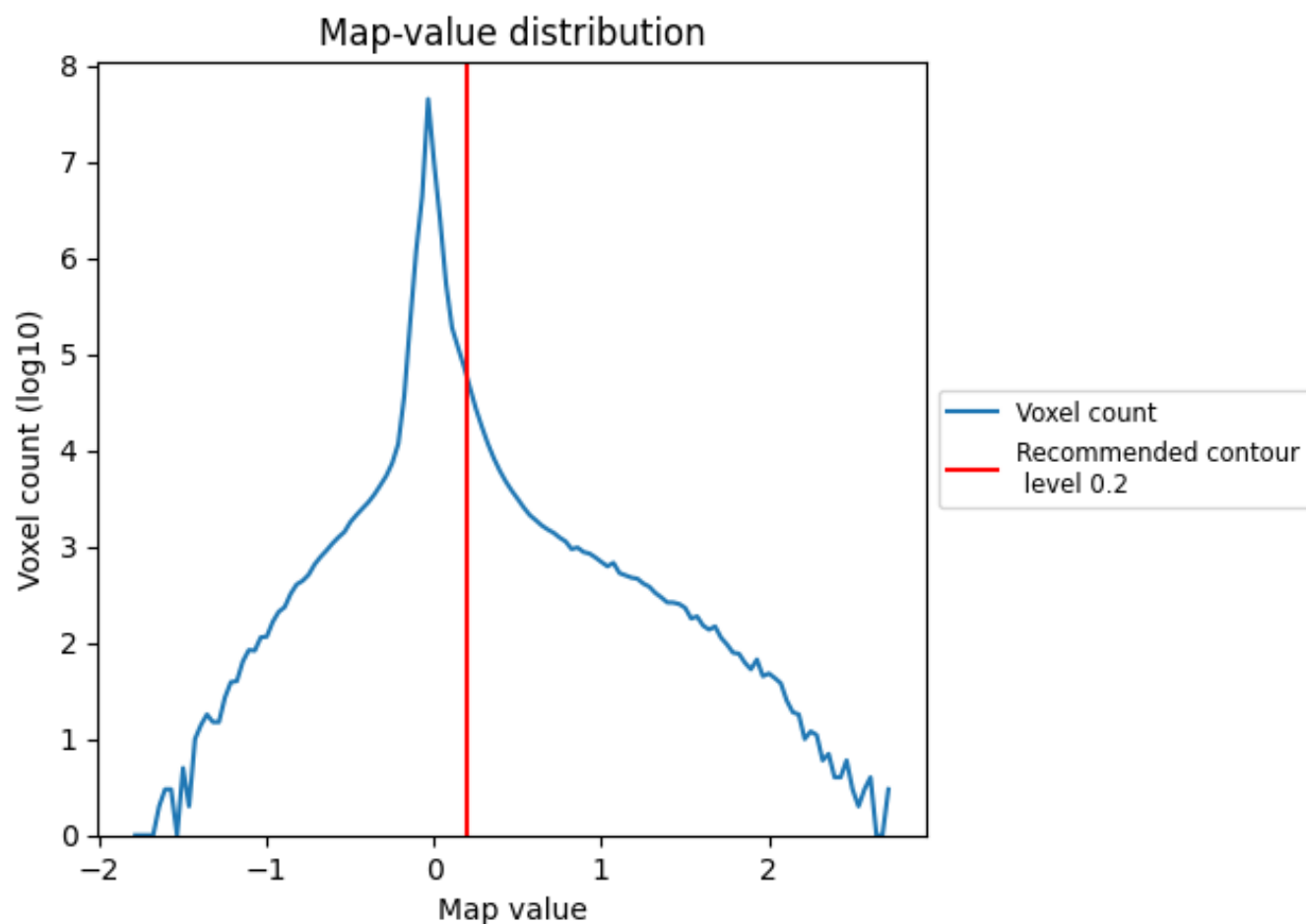


Z

7 Map analysis [i](#)

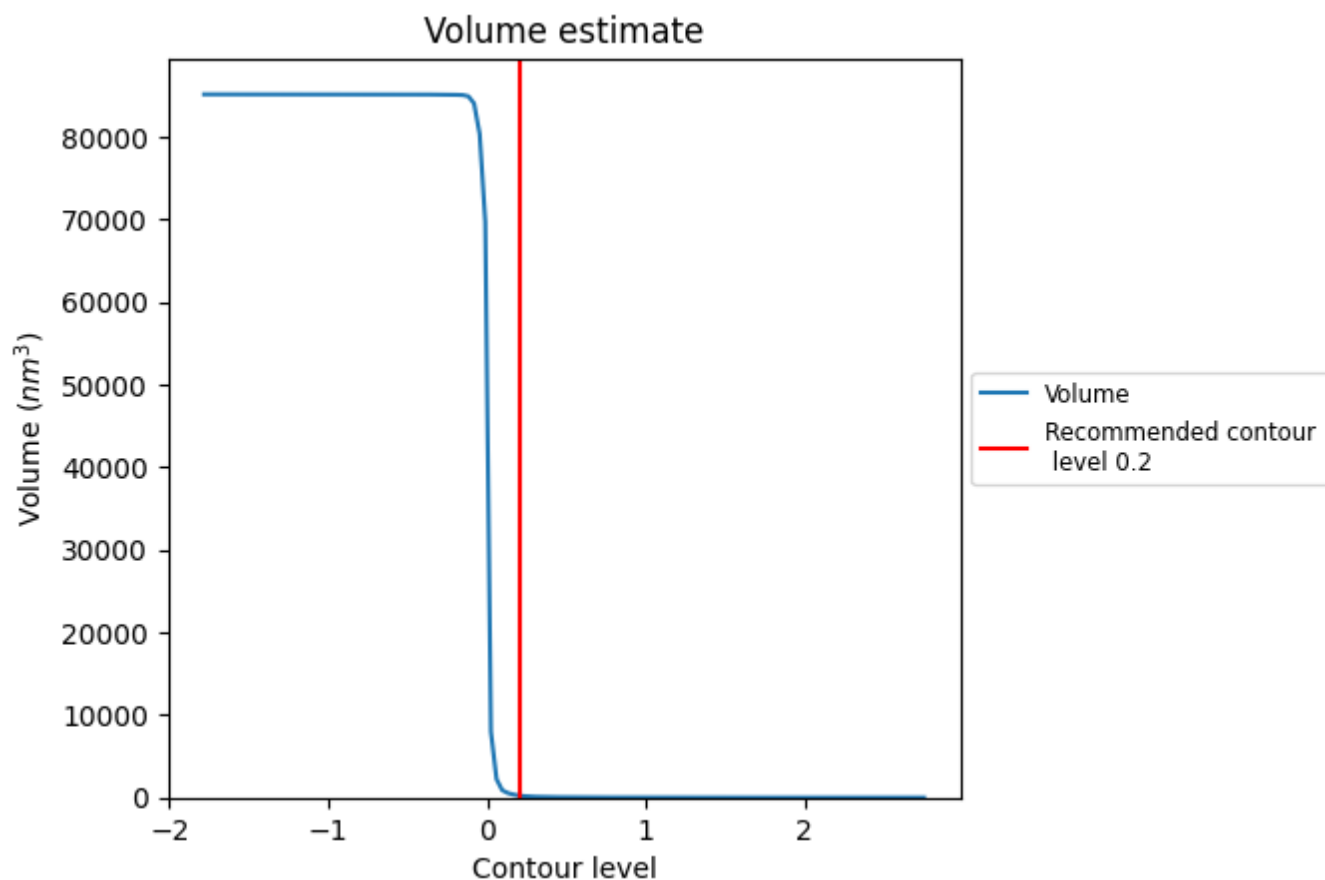
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

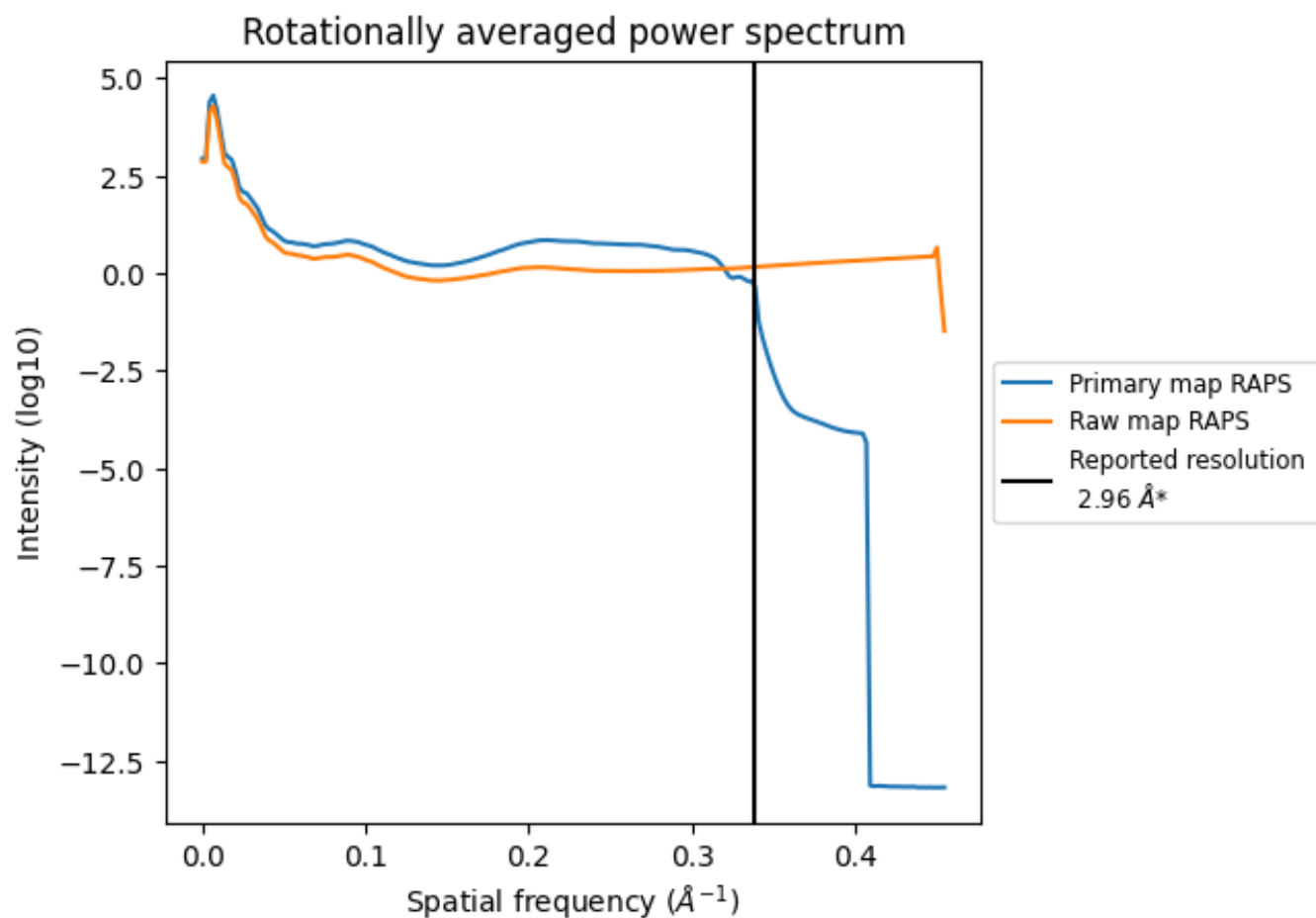
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 244 nm³; this corresponds to an approximate mass of 220 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 ⓘ

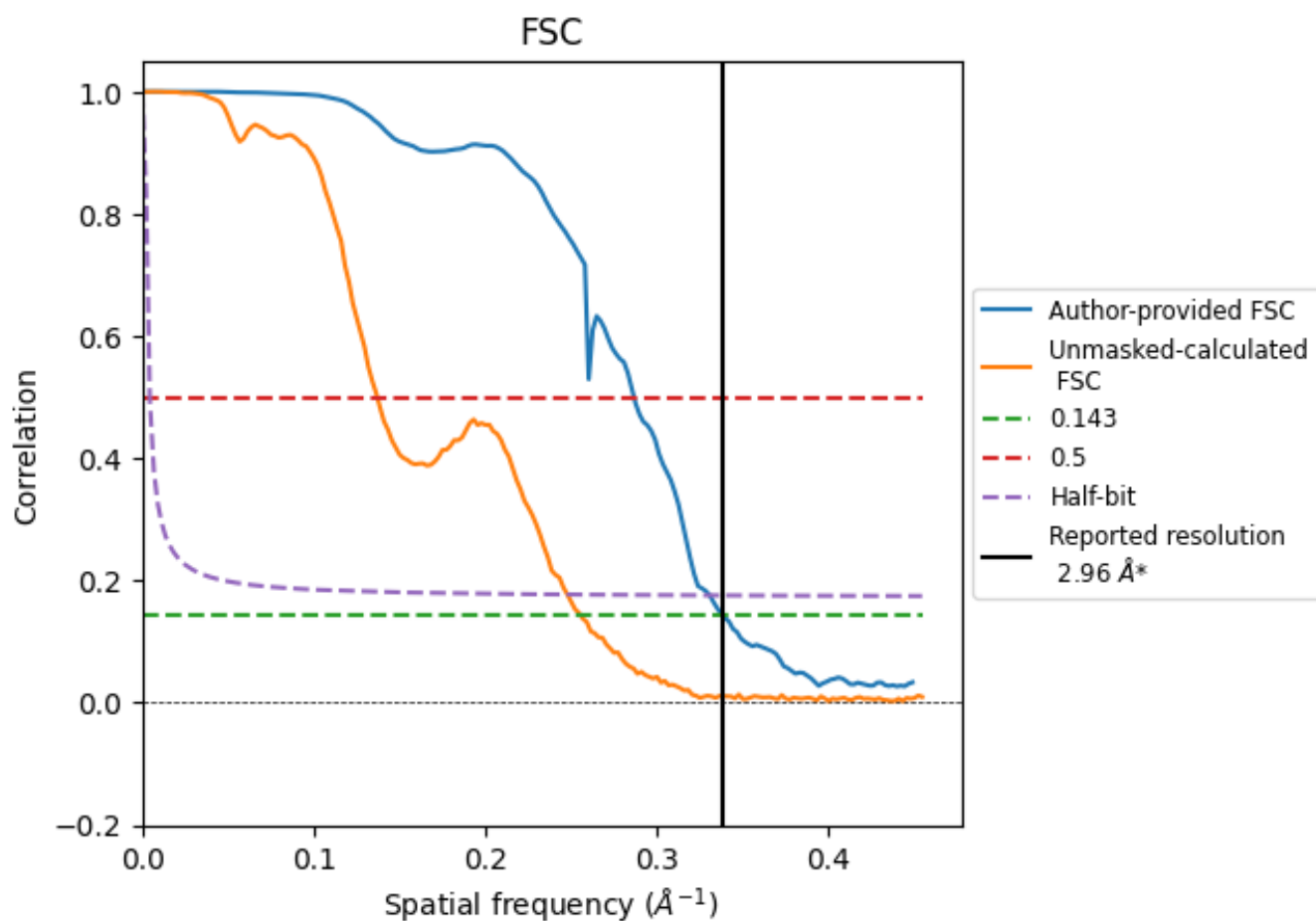


*Reported resolution corresponds to spatial frequency of 0.338 Å⁻¹

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 0.338 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

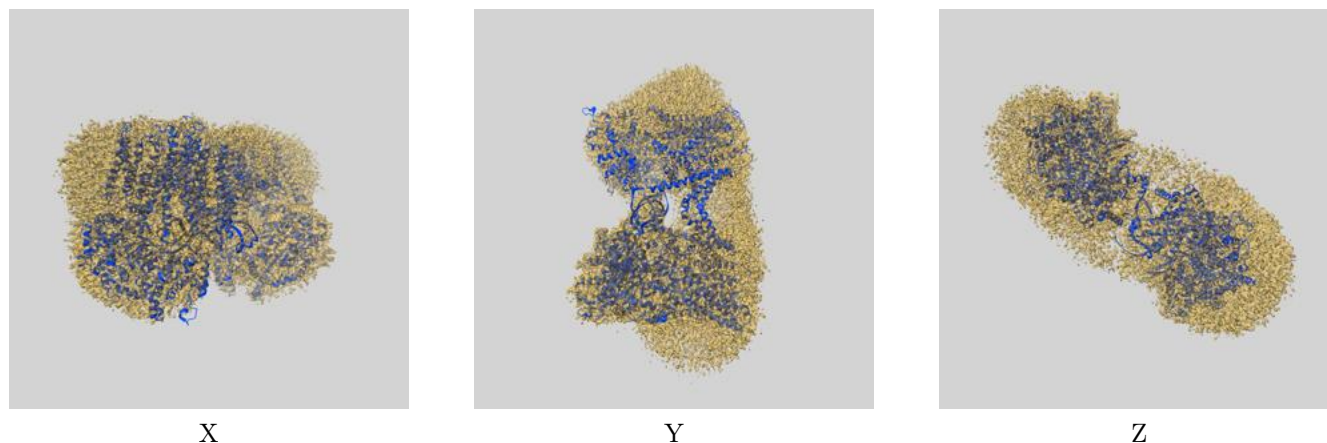
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.96	-	-
Author-provided FSC curve	2.96	3.49	3.02
Unmasked-calculated*	3.91	7.30	4.04

*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 3.91 differs from the reported value 2.96 by more than 10 %

9 Map-model fit [i](#)

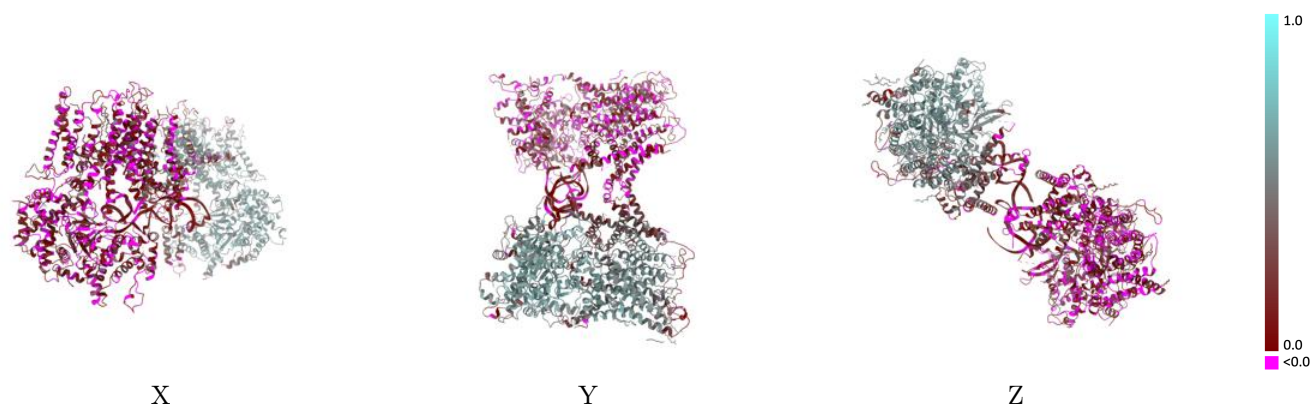
This section contains information regarding the fit between EMDB map EMD-64502 and PDB model 9UTW. Per-residue inclusion information can be found in section [3](#) on page [11](#).

9.1 Map-model overlay [i](#)



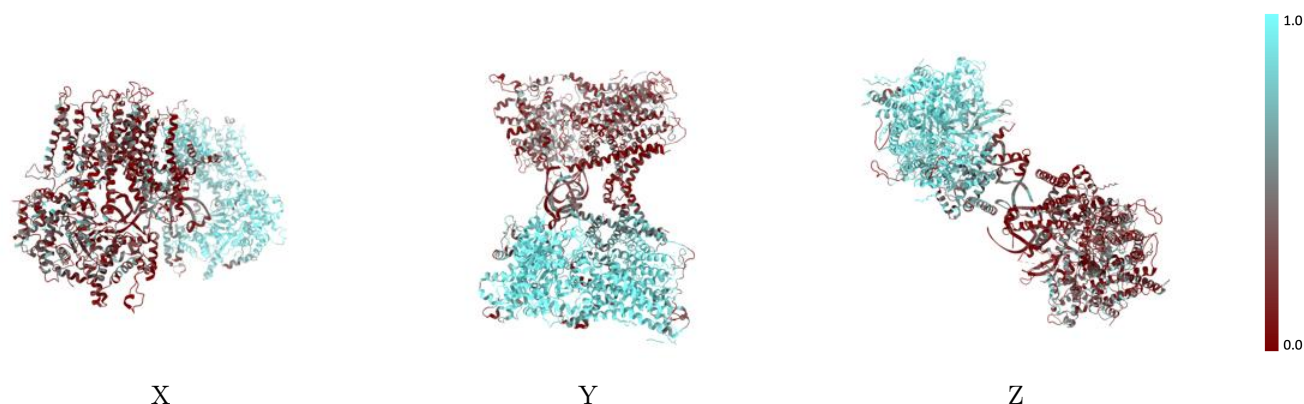
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



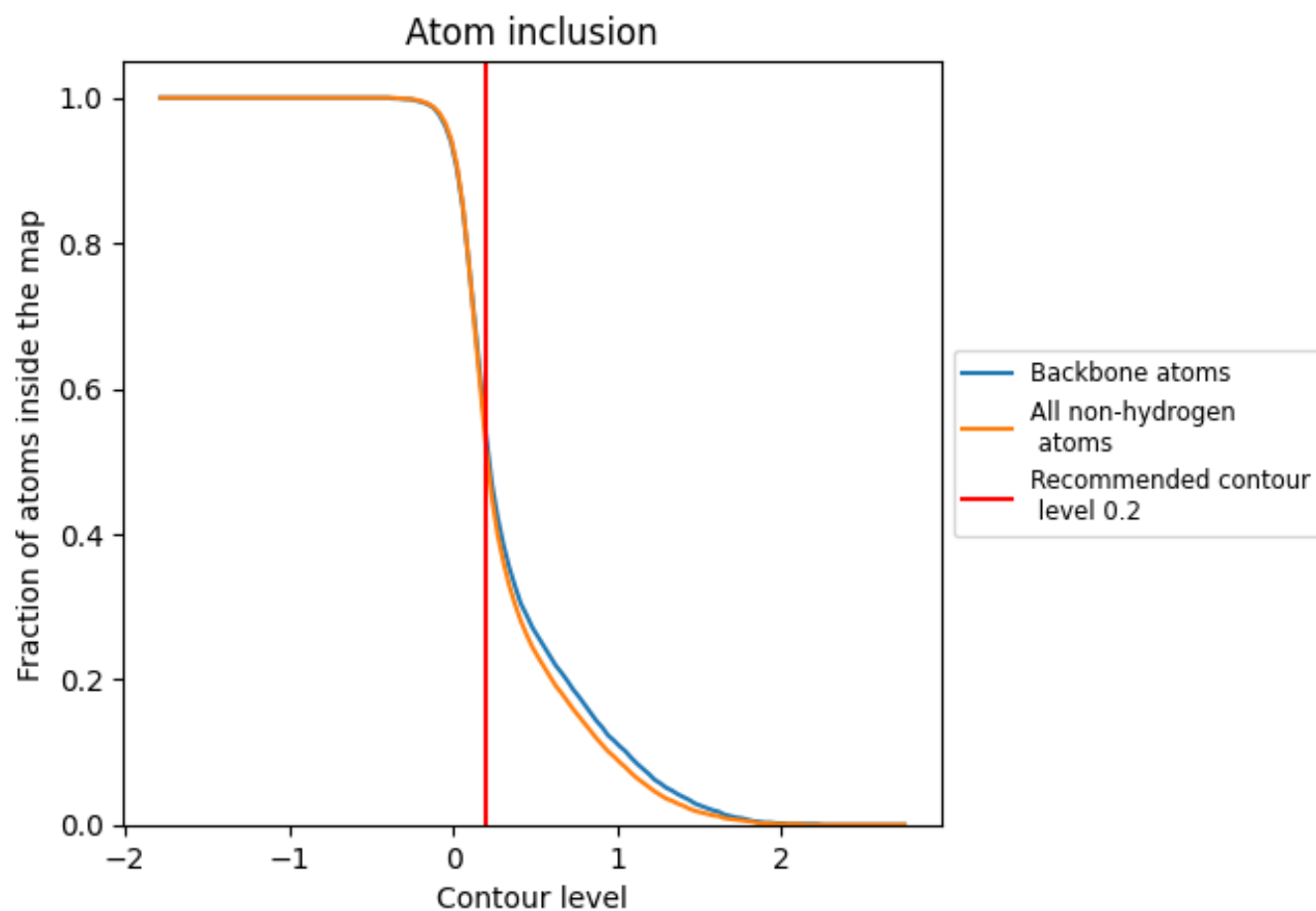
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 54% of all backbone atoms, 52% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5210	0.2730
A	0.2460	0.0720
B	0.8090	0.4790
C	0.5510	0.4170
D	0.1300	0.0170
G	0.2470	0.1020
H	0.2700	0.0900
J	0.2650	0.1750

1.0

0.0

<0.0