



Full wwPDB EM Validation Report ⓘ

Mar 25, 2025 – 06:11 PM JST

PDB ID : 9KQI
EMDB ID : EMD-62505
Title : Cryo-EM structure of PSS1 with calcium
Authors : Ning, Y.; Yu, J.; Ge, J.
Deposited on : 2024-11-26
Resolution : 3.02 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.dev117
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41.4

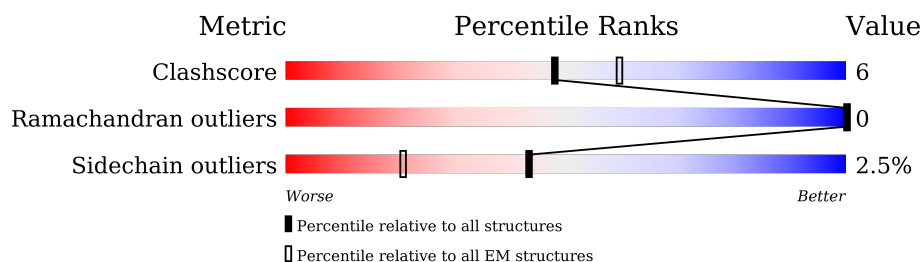
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.02 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	473	<div> <div>9%</div> <div>65%</div> <div>14%</div> <div>20%</div> </div>
1	B	473	<div> <div>10%</div> <div>67%</div> <div>13%</div> <div>20%</div> </div>

2 Entry composition [i](#)

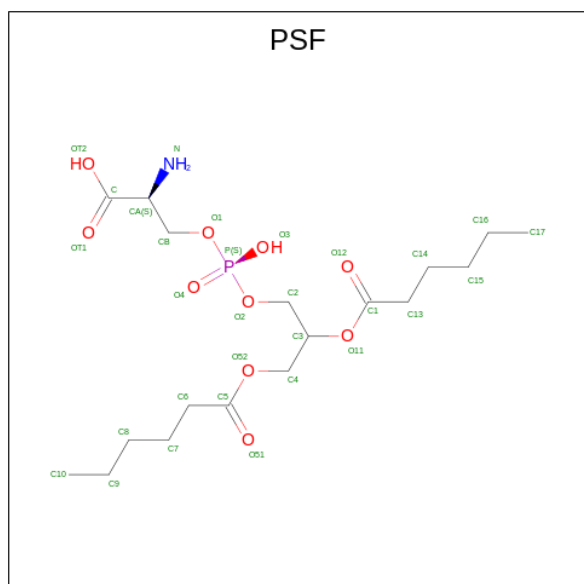
There are 8 unique types of molecules in this entry. The entry contains 7082 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Phosphatidylserine synthase 1.

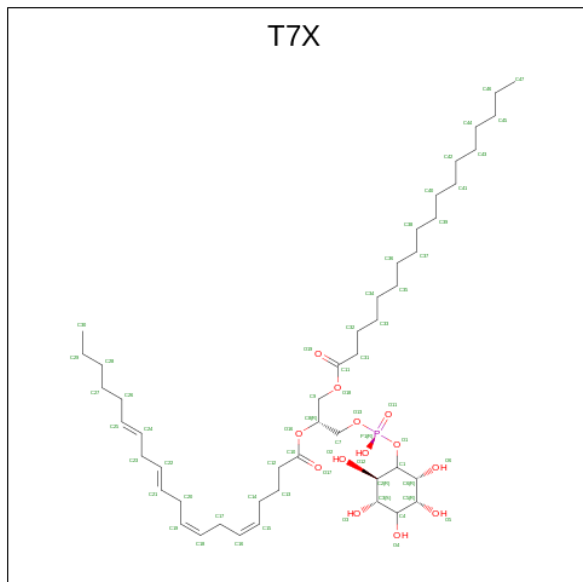
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	377	Total	C	N	O	S	0	0
			3171	2141	501	509	20		
1	B	377	Total	C	N	O	S	0	0
			3171	2141	501	509	20		

- Molecule 2 is 1,2-DICAPROYL-SN-PHOSPHATIDYL-L-SERINE (three-letter code: PSF) (formula: $C_{18}H_{34}NO_{10}P$) (labeled as "Ligand of Interest" by depositor).



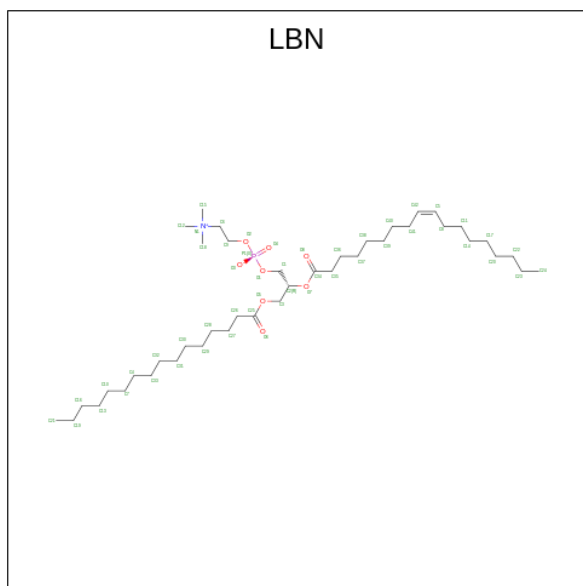
Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			30	18	1	10	1	
2	A	1	Total	C	N	O	P	0
			30	18	1	10	1	
2	B	1	Total	C	N	O	P	0
			30	18	1	10	1	
2	B	1	Total	C	N	O	P	0
			30	18	1	10	1	

- Molecule 3 is Phosphatidylinositol (three-letter code: T7X) (formula: $C_{47}H_{83}O_{13}P$) (labeled as "Ligand of Interest" by depositor).



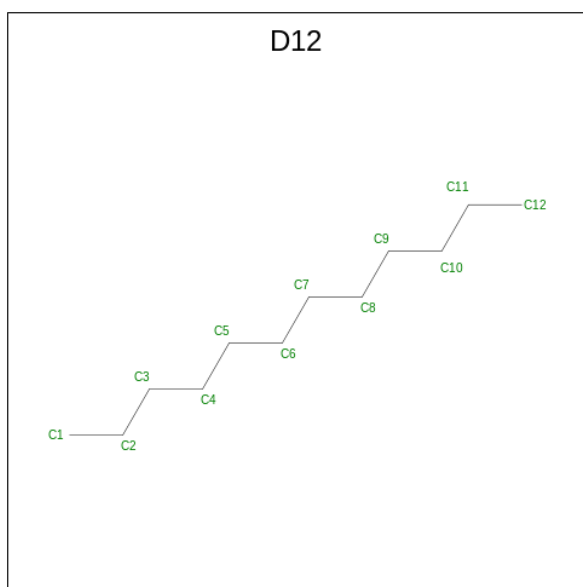
Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	O	P	0
			50	36	13	1	
3	B	1	Total	C	O	P	0
			50	36	13	1	

- Molecule 4 is 1-palmitoyl-2-oleoyl-sn-glycero-3-phosphocholine (three-letter code: LBN) (formula: $C_{42}H_{82}NO_8P$) (labeled as "Ligand of Interest" by depositor).



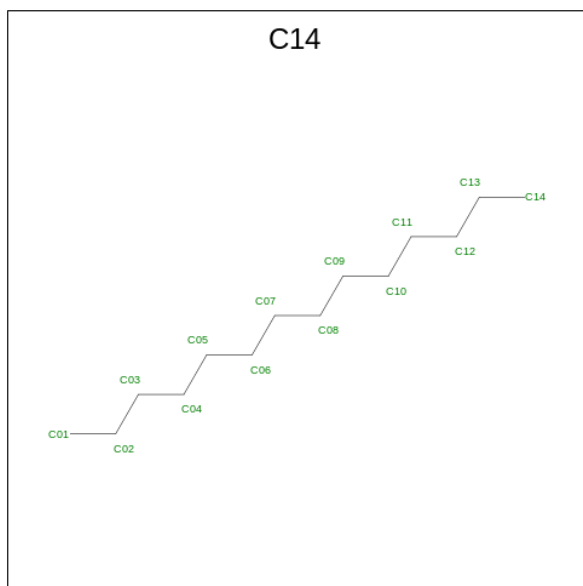
Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
4	A	1	Total	C	N	O	P	0
			32	22	1	8	1	
4	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
4	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
4	A	1	Total	C	N	O	P	0
			38	28	1	8	1	
4	B	1	Total	C	N	O	P	0
			38	28	1	8	1	
4	B	1	Total	C	N	O	P	0
			52	42	1	8	1	
4	B	1	Total	C	N	O	P	0
			32	22	1	8	1	
4	B	1	Total	C	N	O	P	0
			52	42	1	8	1	
4	B	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 5 is DODECANE (three-letter code: D12) (formula: $C_{12}H_{26}$).



Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	C	0
			12	12	
5	B	1	Total	C	0
			12	12	

- Molecule 6 is TETRADECANE (three-letter code: C14) (formula: $C_{14}H_{30}$).

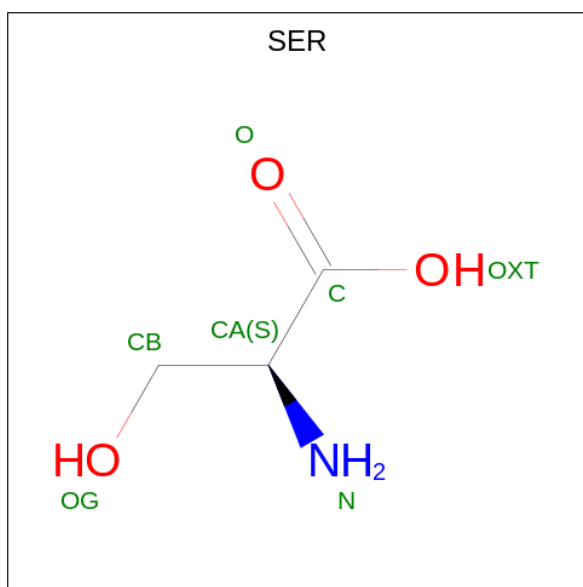


Mol	Chain	Residues	Atoms		AltConf
6	A	1	Total	C	0
			14	14	
6	B	1	Total	C	0
			14	14	

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
7	A	1	Total	Ca	0
			1	1	
7	B	1	Total	Ca	0
			1	1	

- Molecule 8 is SERINE (three-letter code: SER) (formula: $C_3H_7NO_3$).

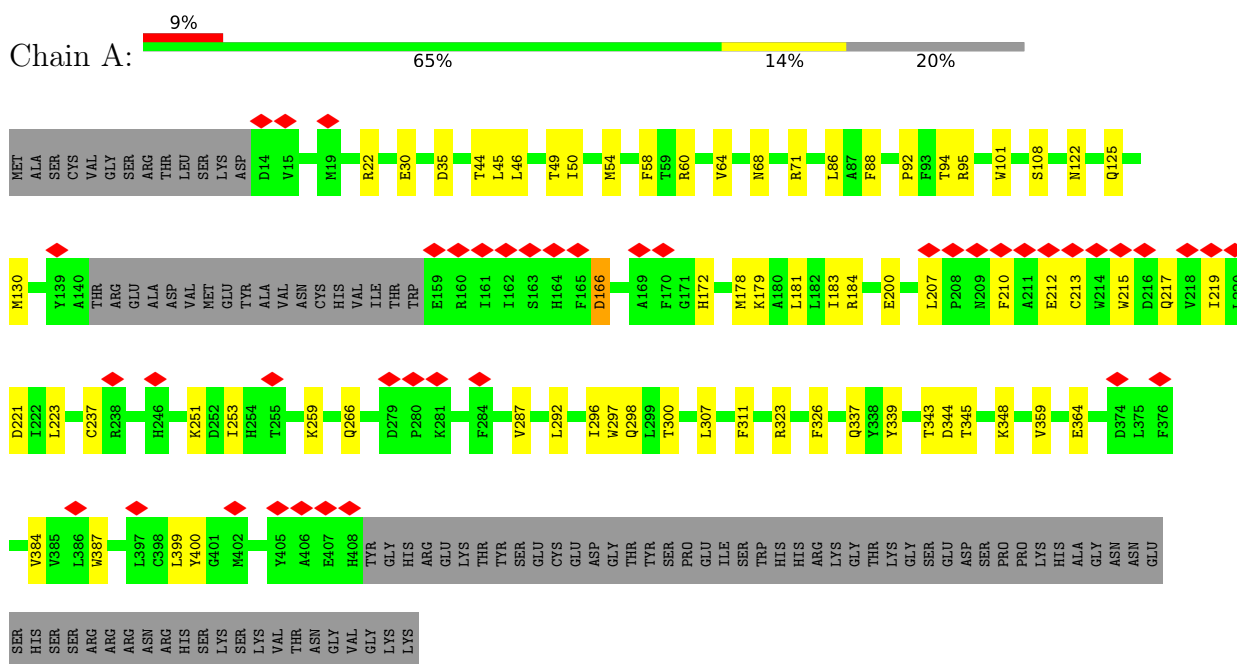


Mol	Chain	Residues	Atoms				AltConf
8	A	1	Total	C	N	O	0
			7	3	1	3	
8	B	1	Total	C	N	O	0
			7	3	1	3	

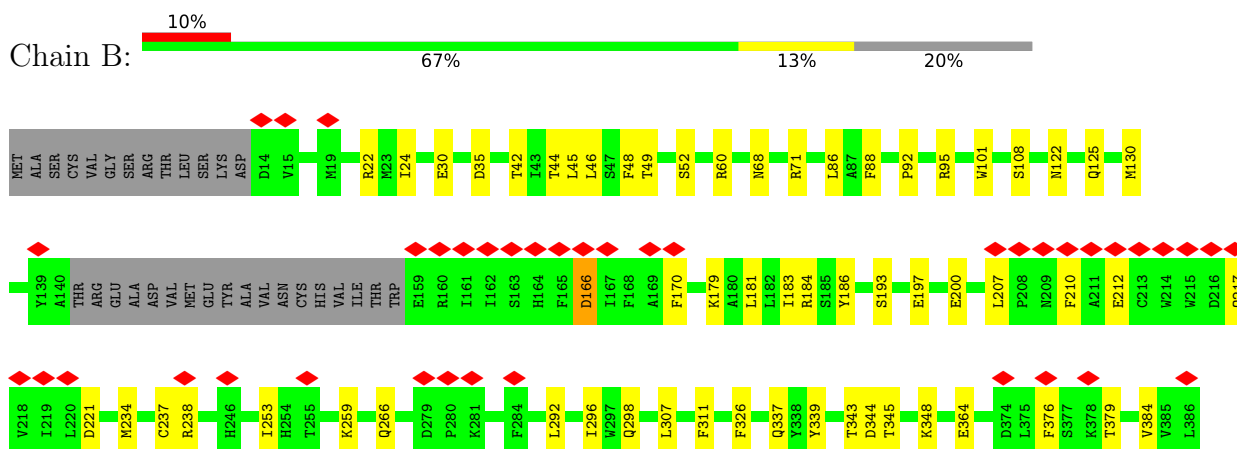
3 Residue-property plots

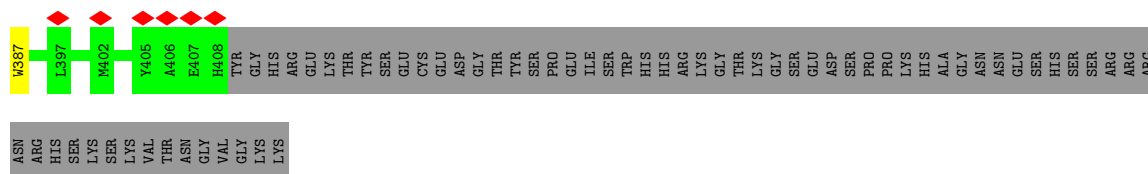
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Phosphatidylserine synthase 1



• Molecule 1: Phosphatidylserine synthase 1





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	446795	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 ($e^-/\text{\AA}^2$)	48	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.861	Depositor
Minimum map value	-3.064	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.105	Depositor
Recommended contour level	0.543	Depositor
Map size (\AA)	253.19998, 253.19998, 253.19998	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.055, 1.055, 1.055	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: C14, CA, T7X, D12, PSF, LBN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.31	0/3285	0.46	0/4474
1	B	0.31	0/3285	0.45	0/4474
All	All	0.31	0/6570	0.46	0/8948

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	3171	0	3137	40	0
1	B	3171	0	3137	37	0
2	A	60	0	64	4	0
2	B	60	0	64	4	0
3	A	50	0	0	0	0
3	B	50	0	0	0	0
4	A	226	0	0	2	0
4	B	226	0	0	2	0
5	A	12	0	26	0	0
5	B	12	0	26	0	0
6	A	14	0	30	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	14	0	30	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
8	A	7	0	4	2	0
8	B	7	0	4	2	0
All	All	7082	0	6522	77	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 6.

All (77) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:LEU:HD22	1:A:210:PHE:HB2	1.78	0.65
1:B:253:ILE:O	1:B:259:LYS:NZ	2.28	0.64
1:A:253:ILE:O	1:A:259:LYS:NZ	2.28	0.64
1:B:298:GLN:OE1	1:B:387:TRP:NE1	2.30	0.63
1:A:298:GLN:OE1	1:A:387:TRP:NE1	2.31	0.62
1:A:95:ARG:NH2	2:A:502:PSF:OT2	2.33	0.62
1:B:217:GLN:HA	1:B:221:ASP:HB2	1.81	0.62
1:B:95:ARG:NH2	2:B:503:PSF:OT2	2.32	0.62
1:A:92:PRO:HD3	1:A:337:GLN:HE21	1.66	0.61
1:A:166:ASP:OD1	1:A:166:ASP:N	2.34	0.60
1:B:266:GLN:HG2	2:B:503:PSF:H131	1.83	0.60
1:A:266:GLN:HG2	2:A:502:PSF:H131	1.84	0.59
1:B:30:GLU:O	2:B:503:PSF:N	2.37	0.58
1:B:207:LEU:HD22	1:B:210:PHE:HB2	1.86	0.58
1:A:30:GLU:O	2:A:502:PSF:N	2.37	0.56
1:A:345:THR:O	1:A:348:LYS:NZ	2.38	0.56
1:B:166:ASP:N	1:B:166:ASP:OD1	2.34	0.56
1:B:60:ARG:NH2	1:B:68:ASN:OD1	2.27	0.56
1:B:48:PHE:O	1:B:52:SER:OG	2.21	0.56
1:B:345:THR:O	1:B:348:LYS:NZ	2.39	0.56
1:A:101:TRP:HZ2	2:A:501:PSF:H41	1.73	0.54
1:A:108:SER:HA	1:A:326:PHE:HZ	1.71	0.54
1:A:60:ARG:NH2	1:A:68:ASN:OD1	2.29	0.53
1:B:200:GLU:OE2	8:B:512:SER:N	2.41	0.53
1:A:181:LEU:HA	1:A:237:CYS:SG	2.49	0.53
1:B:45:LEU:HD23	1:B:86:LEU:HD21	1.91	0.52
1:B:181:LEU:HA	1:B:237:CYS:SG	2.49	0.52
1:B:101:TRP:HZ2	2:B:502:PSF:H41	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:ASN:OD1	1:B:125:GLN:NE2	2.30	0.52
1:A:122:ASN:OD1	1:A:125:GLN:NE2	2.30	0.51
1:A:217:GLN:HA	1:A:221:ASP:HB2	1.93	0.51
1:B:45:LEU:O	1:B:49:THR:HG23	2.10	0.51
1:A:307:LEU:HD11	1:A:364:GLU:HG2	1.92	0.50
1:B:44:THR:OG1	4:B:501:LBN:O3	2.25	0.49
1:A:64:VAL:O	1:A:68:ASN:ND2	2.45	0.49
1:B:179:LYS:O	1:B:183:ILE:HG12	2.13	0.49
1:B:307:LEU:HD11	1:B:364:GLU:HG2	1.94	0.49
1:A:210:PHE:HD2	1:A:212:GLU:HG3	1.77	0.49
1:A:200:GLU:OE2	8:A:511:SER:N	2.46	0.49
1:A:46:LEU:O	1:A:50:ILE:HG12	2.14	0.48
1:A:339:TYR:CE1	1:A:343:THR:HG21	2.48	0.48
1:A:207:LEU:HD22	1:A:210:PHE:H	1.79	0.48
1:B:92:PRO:HD3	1:B:337:GLN:HE21	1.78	0.48
1:B:108:SER:HA	1:B:326:PHE:HZ	1.79	0.48
1:A:179:LYS:O	1:A:183:ILE:HG12	2.14	0.47
1:A:292:LEU:O	1:A:296:ILE:HG12	2.14	0.47
1:B:24:ILE:HG23	1:B:337:GLN:HG2	1.97	0.47
1:A:45:LEU:O	1:A:49:THR:HG23	2.14	0.47
1:B:193:SER:O	1:B:197:GLU:HG2	2.16	0.46
1:B:376:PHE:HD1	1:B:379:THR:HG1	1.63	0.46
1:A:94:THR:O	1:A:94:THR:OG1	2.30	0.46
4:B:506:LBN:O4	8:B:512:SER:OG	2.32	0.45
1:A:130:MET:SD	1:A:311:PHE:HB3	2.57	0.45
1:B:130:MET:SD	1:B:311:PHE:HB3	2.57	0.44
1:A:45:LEU:HD23	1:A:86:LEU:HD21	1.99	0.44
1:B:210:PHE:HD2	1:B:212:GLU:HG3	1.82	0.44
1:A:54:MET:HG2	1:A:58:PHE:HE2	1.83	0.44
1:B:42:THR:O	1:B:46:LEU:N	2.45	0.44
1:B:186:TYR:CE2	1:B:234:MET:HE2	2.53	0.44
1:A:122:ASN:OD1	1:A:122:ASN:N	2.51	0.43
1:A:384:VAL:HG13	1:A:387:TRP:CZ3	2.54	0.43
1:B:339:TYR:CE1	1:B:343:THR:HG21	2.54	0.43
4:A:505:LBN:O4	8:A:511:SER:OG	2.36	0.42
1:B:122:ASN:OD1	1:B:122:ASN:N	2.52	0.42
1:A:323:ARG:HH21	1:A:364:GLU:CD	2.23	0.42
1:A:359:VAL:HG13	1:B:46:LEU:HD13	2.01	0.42
1:B:92:PRO:HD3	1:B:337:GLN:NE2	2.35	0.42
1:B:292:LEU:O	1:B:296:ILE:HG12	2.19	0.42
1:A:44:THR:OG1	4:A:512:LBN:O3	2.26	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:TRP:O	1:A:300:THR:OG1	2.36	0.42
1:B:384:VAL:HG13	1:B:387:TRP:CZ3	2.55	0.42
1:A:22:ARG:HH21	1:B:22:ARG:NH1	2.17	0.42
1:A:213:CYS:HB3	1:A:215:TRP:CD1	2.55	0.42
1:B:207:LEU:HD22	1:B:210:PHE:H	1.85	0.41
1:A:287:VAL:HG22	1:A:399:LEU:HD11	2.03	0.41
1:A:251:LYS:HE3	1:A:251:LYS:HB2	1.85	0.41
1:A:219:ILE:HG23	1:A:223:LEU:HD22	2.03	0.41

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	373/473 (79%)	365 (98%)	8 (2%)	0	100	100
1	B	373/473 (79%)	368 (99%)	5 (1%)	0	100	100
All	All	746/946 (79%)	733 (98%)	13 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	339/423 (80%)	330 (97%)	9 (3%)	40	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	339/423 (80%)	331 (98%)	8 (2%)	44 73
All	All	678/846 (80%)	661 (98%)	17 (2%)	43 72

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	ASP
1	A	71	ARG
1	A	88	PHE
1	A	166	ASP
1	A	172	HIS
1	A	178	MET
1	A	184	ARG
1	A	344	ASP
1	A	400	TYR
1	B	35	ASP
1	B	71	ARG
1	B	88	PHE
1	B	166	ASP
1	B	170	PHE
1	B	184	ARG
1	B	238	ARG
1	B	344	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	337	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 2 are monoatomic - leaving 22 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
4	LBN	A	512	-	37,37,51	0.56	0	43,45,59	0.50	0
4	LBN	A	505	-	31,31,51	0.58	0	37,39,59	0.52	0
4	LBN	A	504	-	51,51,51	0.46	0	57,59,59	0.46	0
5	D12	A	506	-	11,11,11	0.22	0	10,10,10	0.23	0
4	LBN	B	506	-	31,31,51	0.57	0	37,39,59	0.52	0
8	SER	A	511	7	5,6,6	1.01	1 (20%)	5,7,7	1.61	2 (40%)
6	C14	A	507	-	13,13,13	0.21	0	12,12,12	0.24	0
2	PSF	A	501	-	28,29,29	0.71	0	32,36,36	1.01	1 (3%)
4	LBN	B	509	-	51,51,51	0.48	0	57,59,59	0.57	1 (1%)
4	LBN	A	508	-	51,51,51	0.48	0	57,59,59	0.56	1 (1%)
3	T7X	A	503	-	50,50,61	0.56	0	60,62,73	0.75	1 (1%)
6	C14	B	508	-	13,13,13	0.21	0	12,12,12	0.24	0
3	T7X	B	504	-	50,50,61	0.55	0	60,62,73	0.75	1 (1%)
8	SER	B	512	7	5,6,6	1.01	1 (20%)	5,7,7	1.60	2 (40%)
5	D12	B	507	-	11,11,11	0.22	0	10,10,10	0.23	0
2	PSF	B	503	-	28,29,29	0.72	0	32,36,36	1.00	1 (3%)
4	LBN	B	505	-	51,51,51	0.46	0	57,59,59	0.47	0
4	LBN	B	501	-	37,37,51	0.56	0	43,45,59	0.50	0
2	PSF	A	502	-	28,29,29	0.72	0	32,36,36	0.99	1 (3%)
2	PSF	B	502	-	28,29,29	0.71	0	32,36,36	1.01	1 (3%)
4	LBN	B	511	-	51,51,51	0.47	0	57,59,59	0.43	0
4	LBN	A	510	-	51,51,51	0.47	0	57,59,59	0.43	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
4	LBN	A	512	-	-	16/41/41/55	-
4	LBN	A	505	-	-	13/35/35/55	-
4	LBN	A	504	-	-	23/55/55/55	-
5	D12	A	506	-	-	0/9/9/9	-
4	LBN	B	506	-	-	13/35/35/55	-
8	SER	A	511	7	-	2/6/6/6	-
6	C14	A	507	-	-	4/11/11/11	-
2	PSF	A	501	-	-	16/35/35/35	-
4	LBN	B	509	-	-	15/55/55/55	-
4	LBN	A	508	-	-	15/55/55/55	-
3	T7X	A	503	-	-	9/45/69/80	0/1/1/1
6	C14	B	508	-	-	4/11/11/11	-
3	T7X	B	504	-	-	11/45/69/80	0/1/1/1
8	SER	B	512	7	-	3/6/6/6	-
5	D12	B	507	-	-	0/9/9/9	-
2	PSF	B	503	-	-	7/35/35/35	-
4	LBN	B	505	-	-	25/55/55/55	-
4	LBN	B	501	-	-	16/41/41/55	-
2	PSF	A	502	-	-	7/35/35/35	-
2	PSF	B	502	-	-	17/35/35/35	-
4	LBN	B	511	-	-	22/55/55/55	-
4	LBN	A	510	-	-	20/55/55/55	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	511	SER	OXT-C	-2.13	1.23	1.30
8	B	512	SER	OXT-C	-2.13	1.23	1.30

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	PSF	O1-CB-CA	4.33	111.83	108.06
2	B	502	PSF	O1-CB-CA	4.31	111.81	108.06
2	B	503	PSF	O1-CB-CA	4.18	111.70	108.06
2	A	502	PSF	O1-CB-CA	4.13	111.66	108.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	511	SER	OXT-C-O	-2.77	117.80	124.09
8	B	512	SER	OXT-C-O	-2.74	117.86	124.09
8	A	511	SER	OXT-C-CA	2.25	121.05	113.38
8	B	512	SER	OXT-C-CA	2.25	121.03	113.38
3	B	504	T7X	O3-C3-C2	-2.21	105.24	110.35
4	B	509	LBN	C2-O7-C34	2.20	123.21	117.79
3	A	503	T7X	O3-C3-C2	-2.19	105.28	110.35
4	A	508	LBN	C2-O7-C34	2.15	123.07	117.79

There are no chirality outliers.

All (258) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	PSF	C2-O2-P-O1
2	A	501	PSF	C2-O2-P-O4
2	A	501	PSF	N-CA-CB-O1
2	A	501	PSF	C-CA-CB-O1
2	A	501	PSF	OT1-C-CA-CB
2	A	501	PSF	OT2-C-CA-CB
2	A	502	PSF	OT1-C-CA-N
2	B	502	PSF	C2-O2-P-O1
2	B	502	PSF	C2-O2-P-O4
2	B	502	PSF	N-CA-CB-O1
2	B	502	PSF	C-CA-CB-O1
2	B	502	PSF	OT1-C-CA-CB
2	B	502	PSF	OT2-C-CA-CB
2	B	503	PSF	OT1-C-CA-N
3	A	503	T7X	C6-C1-O1-P1
3	B	504	T7X	C6-C1-O1-P1
4	A	504	LBN	C1-O1-P1-O2
4	A	504	LBN	N1-C6-C9-O2
4	A	504	LBN	C6-C9-O2-P1
4	A	505	LBN	N1-C6-C9-O2
4	A	505	LBN	C35-C34-O7-C2
4	A	508	LBN	C9-O2-P1-O1
4	A	508	LBN	C9-O2-P1-O3
4	A	508	LBN	C9-O2-P1-O4
4	A	510	LBN	C1-O1-P1-O4
4	A	510	LBN	O6-C25-O5-C3
4	A	512	LBN	C1-O1-P1-O3
4	A	512	LBN	C9-O2-P1-O3
4	A	512	LBN	C6-C9-O2-P1

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Mol	Chain	Res	Type	Atoms
4	B	501	LBN	C1-O1-P1-O3
4	B	501	LBN	C9-O2-P1-O3
4	B	501	LBN	C6-C9-O2-P1
4	B	505	LBN	C1-O1-P1-O2
4	B	505	LBN	C9-O2-P1-O1
4	B	505	LBN	N1-C6-C9-O2
4	B	505	LBN	C6-C9-O2-P1
4	B	506	LBN	N1-C6-C9-O2
4	B	506	LBN	C35-C34-O7-C2
4	B	509	LBN	C9-O2-P1-O1
4	B	509	LBN	C9-O2-P1-O3
4	B	509	LBN	C9-O2-P1-O4
4	B	511	LBN	C1-O1-P1-O4
4	B	511	LBN	O6-C25-O5-C3
4	A	510	LBN	C26-C25-O5-C3
4	B	511	LBN	C26-C25-O5-C3
4	A	505	LBN	C26-C25-O5-C3
4	B	506	LBN	C26-C25-O5-C3
4	A	505	LBN	O8-C34-O7-C2
4	B	506	LBN	O8-C34-O7-C2
2	A	501	PSF	O51-C5-O52-C4
2	B	502	PSF	O51-C5-O52-C4
4	A	508	LBN	O6-C25-O5-C3
2	A	501	PSF	C6-C5-O52-C4
2	B	502	PSF	C6-C5-O52-C4
4	B	509	LBN	C26-C25-O5-C3
4	B	506	LBN	O6-C25-O5-C3
4	B	509	LBN	O6-C25-O5-C3
2	A	502	PSF	C13-C1-O11-C3
2	B	503	PSF	C13-C1-O11-C3
4	B	505	LBN	C35-C34-O7-C2
4	A	508	LBN	C26-C25-O5-C3
4	A	505	LBN	O6-C25-O5-C3
4	A	508	LBN	C17-C20-C22-C23
4	A	504	LBN	C35-C34-O7-C2
2	A	502	PSF	OT2-C-CA-N
2	B	503	PSF	OT2-C-CA-N
4	A	504	LBN	C31-C32-C33-C4
4	B	511	LBN	C14-C17-C20-C22
4	A	510	LBN	C14-C17-C20-C22
4	B	509	LBN	C17-C20-C22-C23
2	A	502	PSF	O12-C1-O11-C3

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Mol	Chain	Res	Type	Atoms
2	B	503	PSF	O12-C1-O11-C3
4	A	504	LBN	O8-C34-O7-C2
4	B	505	LBN	O8-C34-O7-C2
4	A	512	LBN	C25-C26-C27-C28
4	B	501	LBN	C25-C26-C27-C28
4	A	512	LBN	C9-O2-P1-O1
4	B	501	LBN	C9-O2-P1-O1
4	A	504	LBN	C13-C10-C7-C4
2	A	501	PSF	C13-C1-O11-C3
2	B	502	PSF	C13-C1-O11-C3
4	A	505	LBN	C35-C36-C37-C38
4	B	505	LBN	C30-C31-C32-C33
4	B	506	LBN	C35-C36-C37-C38
4	B	511	LBN	C29-C30-C31-C32
4	A	510	LBN	C29-C30-C31-C32
4	A	510	LBN	C35-C36-C37-C38
4	A	512	LBN	C13-C10-C7-C4
2	A	501	PSF	O12-C1-O11-C3
2	B	502	PSF	O12-C1-O11-C3
4	A	512	LBN	C28-C29-C30-C31
4	B	501	LBN	C13-C10-C7-C4
4	B	511	LBN	C35-C36-C37-C38
4	B	501	LBN	C28-C29-C30-C31
4	B	505	LBN	C17-C20-C22-C23
8	B	512	SER	OXT-C-CA-N
4	B	505	LBN	C11-C14-C17-C20
3	A	503	T7X	C31-C32-C33-C34
3	B	504	T7X	C31-C32-C33-C34
4	B	505	LBN	C33-C4-C7-C10
3	A	503	T7X	C11-C31-C32-C33
8	A	511	SER	OXT-C-CA-N
4	A	512	LBN	C7-C10-C13-C16
4	B	501	LBN	C7-C10-C13-C16
4	A	504	LBN	C30-C31-C32-C33
3	A	503	T7X	C12-C13-C14-C15
3	B	504	T7X	C12-C13-C14-C15
4	B	509	LBN	C34-C35-C36-C37
4	A	510	LBN	C13-C16-C19-C21
2	A	502	PSF	C-CA-CB-O1
2	B	503	PSF	C-CA-CB-O1
4	A	504	LBN	C26-C25-O5-C3
3	A	503	T7X	O13-C7-C8-O16

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Mol	Chain	Res	Type	Atoms
3	B	504	T7X	O13-C7-C8-O16
4	B	506	LBN	O1-C1-C2-O7
3	B	504	T7X	C11-C31-C32-C33
4	A	508	LBN	C30-C31-C32-C33
4	A	508	LBN	C28-C29-C30-C31
3	A	503	T7X	C7-O13-P1-O1
4	A	504	LBN	C9-O2-P1-O1
4	A	508	LBN	C1-O1-P1-O2
4	B	509	LBN	C1-O1-P1-O2
4	B	511	LBN	C9-O2-P1-O1
2	A	501	PSF	C5-C6-C7-C8
2	B	502	PSF	C5-C6-C7-C8
2	A	501	PSF	C13-C14-C15-C16
6	A	507	C14	C05-C06-C07-C08
2	B	502	PSF	C13-C14-C15-C16
6	A	507	C14	C03-C04-C05-C06
6	B	508	C14	C03-C04-C05-C06
4	A	504	LBN	C1-C2-C3-O5
4	B	511	LBN	C37-C38-C39-C40
4	A	504	LBN	C10-C13-C16-C19
4	A	510	LBN	C37-C38-C39-C40
4	A	505	LBN	O1-C1-C2-O7
4	A	510	LBN	O1-C1-C2-O7
4	B	511	LBN	O1-C1-C2-O7
4	A	505	LBN	C25-C26-C27-C28
4	B	506	LBN	C25-C26-C27-C28
4	A	504	LBN	O6-C25-O5-C3
4	B	511	LBN	C13-C16-C19-C21
6	B	508	C14	C05-C06-C07-C08
4	B	505	LBN	C26-C25-O5-C3
4	B	506	LBN	C36-C37-C38-C39
4	A	505	LBN	O1-C1-C2-C3
4	A	505	LBN	C36-C37-C38-C39
4	A	508	LBN	C2-C1-O1-P1
4	B	509	LBN	C2-C1-O1-P1
4	B	505	LBN	C1-C2-C3-O5
4	B	506	LBN	C1-C2-C3-O5
3	B	504	T7X	C7-O13-P1-O1
4	A	510	LBN	C9-O2-P1-O1
4	A	510	LBN	C14-C11-C8-C5
4	B	511	LBN	C28-C29-C30-C31
4	A	510	LBN	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
8	A	511	SER	O-C-CA-N
8	B	512	SER	O-C-CA-N
4	A	512	LBN	C2-C1-O1-P1
4	B	501	LBN	C2-C1-O1-P1
4	B	505	LBN	C31-C32-C33-C4
4	B	505	LBN	O5-C25-C26-C27
4	A	510	LBN	C28-C29-C30-C31
3	A	503	T7X	O13-C7-C8-C9
3	B	504	T7X	O13-C7-C8-C9
4	A	510	LBN	O1-C1-C2-C3
4	B	506	LBN	O1-C1-C2-C3
4	B	511	LBN	O1-C1-C2-C3
4	B	511	LBN	C27-C28-C29-C30
4	B	505	LBN	C8-C11-C14-C17
2	A	501	PSF	C2-C3-C4-O52
2	B	502	PSF	C2-C3-C4-O52
4	A	505	LBN	C1-C2-C3-O5
4	B	505	LBN	O6-C25-O5-C3
6	B	508	C14	C04-C05-C06-C07
4	B	505	LBN	C28-C29-C30-C31
4	B	501	LBN	C10-C13-C16-C19
4	A	504	LBN	C36-C37-C38-C39
4	A	504	LBN	C1-O1-P1-O3
4	A	504	LBN	C9-O2-P1-O3
4	B	505	LBN	C1-O1-P1-O3
4	B	505	LBN	C9-O2-P1-O3
2	A	502	PSF	O2-C2-C3-C4
2	B	503	PSF	O2-C2-C3-C4
6	A	507	C14	C04-C05-C06-C07
4	B	505	LBN	C27-C28-C29-C30
4	B	511	LBN	C14-C11-C8-C5
4	A	510	LBN	C17-C20-C22-C23
2	A	502	PSF	O2-C2-C3-O11
2	B	503	PSF	O2-C2-C3-O11
4	A	510	LBN	C9-C6-N1-C15
4	B	511	LBN	C9-C6-N1-C15
4	A	512	LBN	N1-C6-C9-O2
4	B	501	LBN	N1-C6-C9-O2
2	A	501	PSF	O11-C3-C4-O52
2	B	502	PSF	O11-C3-C4-O52
4	A	504	LBN	O7-C2-C3-O5
4	B	505	LBN	O7-C2-C3-O5

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Mol	Chain	Res	Type	Atoms
4	A	508	LBN	C13-C10-C7-C4
4	A	512	LBN	C10-C13-C16-C19
2	B	502	PSF	C1-C13-C14-C15
2	A	501	PSF	C1-C13-C14-C15
4	B	509	LBN	C30-C31-C32-C33
4	A	504	LBN	C3-C2-O7-C34
4	B	505	LBN	C3-C2-O7-C34
4	A	504	LBN	O5-C25-C26-C27
4	A	505	LBN	O7-C2-C3-O5
4	B	506	LBN	O7-C2-C3-O5
4	A	505	LBN	C9-O2-P1-O1
4	A	510	LBN	C1-O1-P1-O2
4	A	512	LBN	C1-O1-P1-O2
4	B	506	LBN	C9-O2-P1-O1
4	B	511	LBN	C1-O1-P1-O2
4	A	504	LBN	C38-C39-C40-C41
4	B	509	LBN	C13-C10-C7-C4
4	B	511	LBN	C17-C20-C22-C23
4	A	508	LBN	O7-C2-C3-O5
4	B	501	LBN	C26-C27-C28-C29
3	A	503	T7X	C1-O1-P1-O11
3	B	504	T7X	C1-O1-P1-O11
4	A	512	LBN	C26-C27-C28-C29
2	A	501	PSF	C4-C3-O11-C1
2	B	502	PSF	C4-C3-O11-C1
4	A	508	LBN	C1-C2-O7-C34
4	B	509	LBN	C1-C2-O7-C34
3	B	504	T7X	C22-C23-C24-C25
4	B	501	LBN	C1-O1-P1-O2
4	A	512	LBN	C29-C30-C31-C32
4	B	505	LBN	C10-C13-C16-C19
4	B	509	LBN	C28-C29-C30-C31
6	A	507	C14	C02-C03-C04-C05
6	B	508	C14	C02-C03-C04-C05
4	B	511	LBN	C20-C22-C23-C24
4	A	508	LBN	C14-C11-C8-C5
4	B	501	LBN	C31-C32-C33-C4
4	A	510	LBN	C9-C6-N1-C18
4	B	511	LBN	C30-C31-C32-C33
4	A	504	LBN	C17-C20-C22-C23
4	A	504	LBN	C37-C38-C39-C40
4	B	509	LBN	O7-C2-C3-O5

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Mol	Chain	Res	Type	Atoms
4	B	511	LBN	C9-C6-N1-C18
8	B	512	SER	OXT-C-CA-CB
4	B	501	LBN	C29-C30-C31-C32
3	B	504	T7X	C32-C33-C34-C35
3	A	503	T7X	C7-O13-P1-O11
3	B	504	T7X	C7-O13-P1-O11
4	A	508	LBN	C1-O1-P1-O4
4	A	510	LBN	C9-C6-N1-C12
4	A	510	LBN	C9-O2-P1-O4
4	A	512	LBN	C1-O1-P1-O4
4	B	501	LBN	C1-O1-P1-O4
4	B	509	LBN	C1-O1-P1-O4
4	B	511	LBN	C9-O2-P1-O4
4	A	512	LBN	C31-C32-C33-C4
4	B	505	LBN	O6-C25-C26-C27
4	B	505	LBN	C35-C36-C37-C38
2	B	502	PSF	OT2-C-CA-N
4	A	504	LBN	C28-C29-C30-C31
4	B	511	LBN	C9-C6-N1-C12

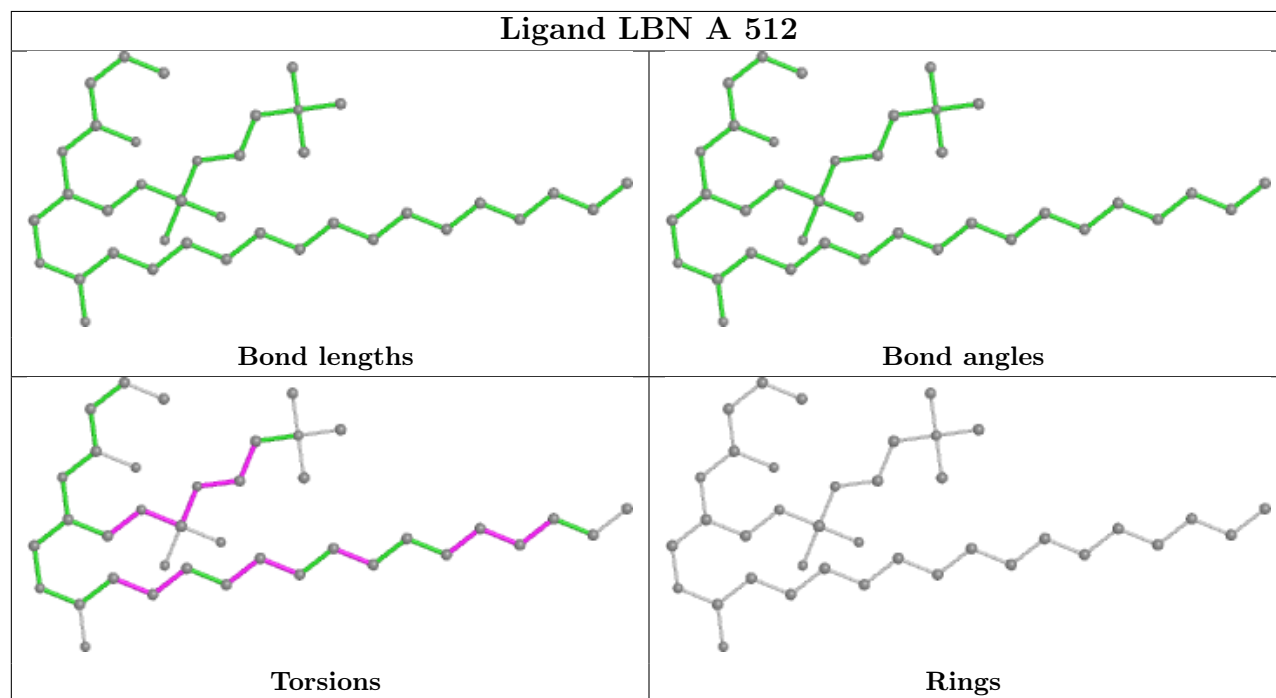
There are no ring outliers.

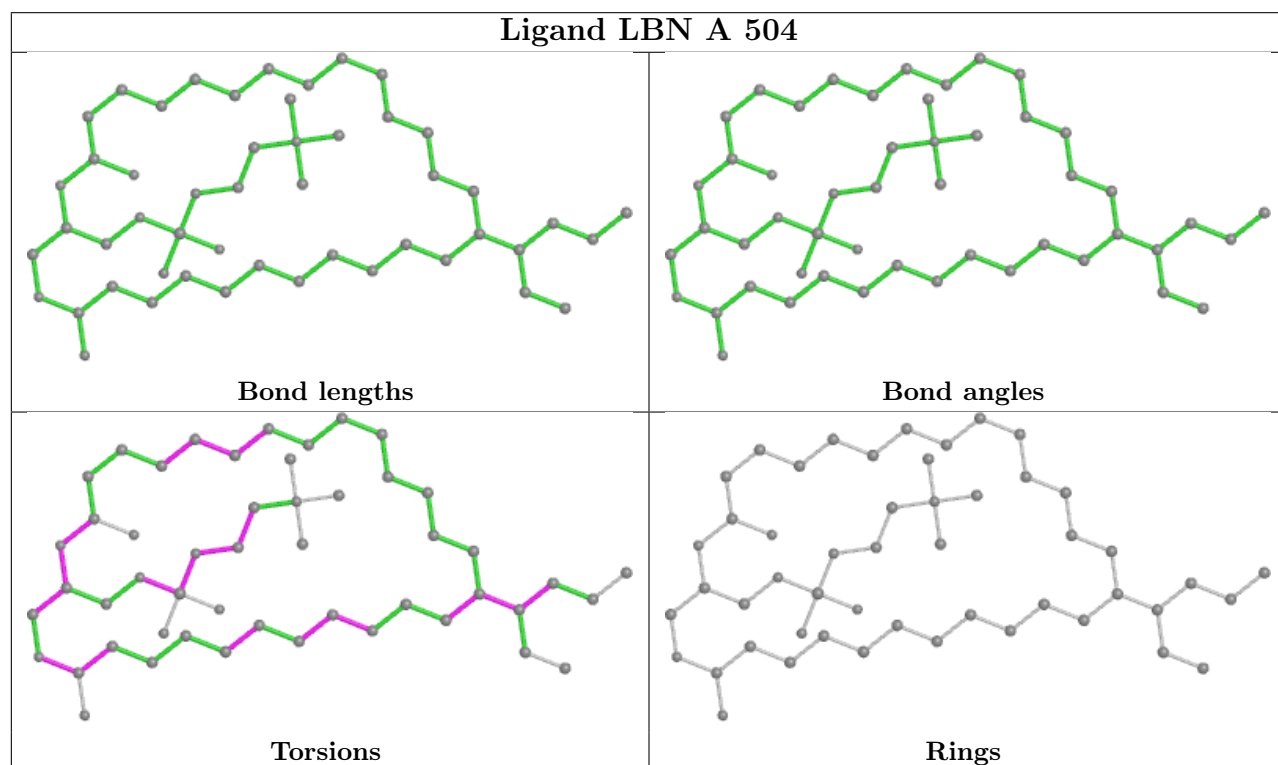
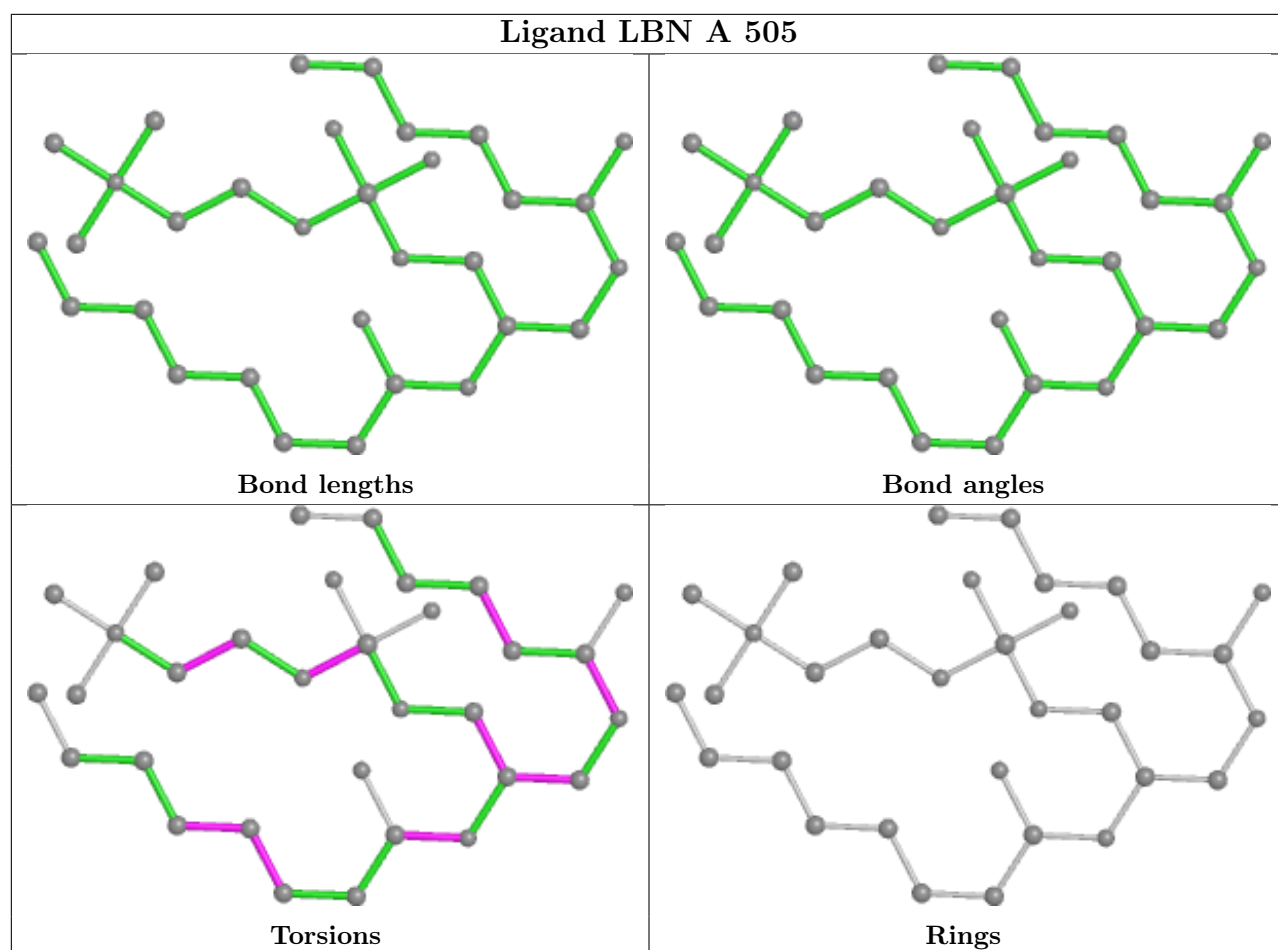
10 monomers are involved in 14 short contacts:

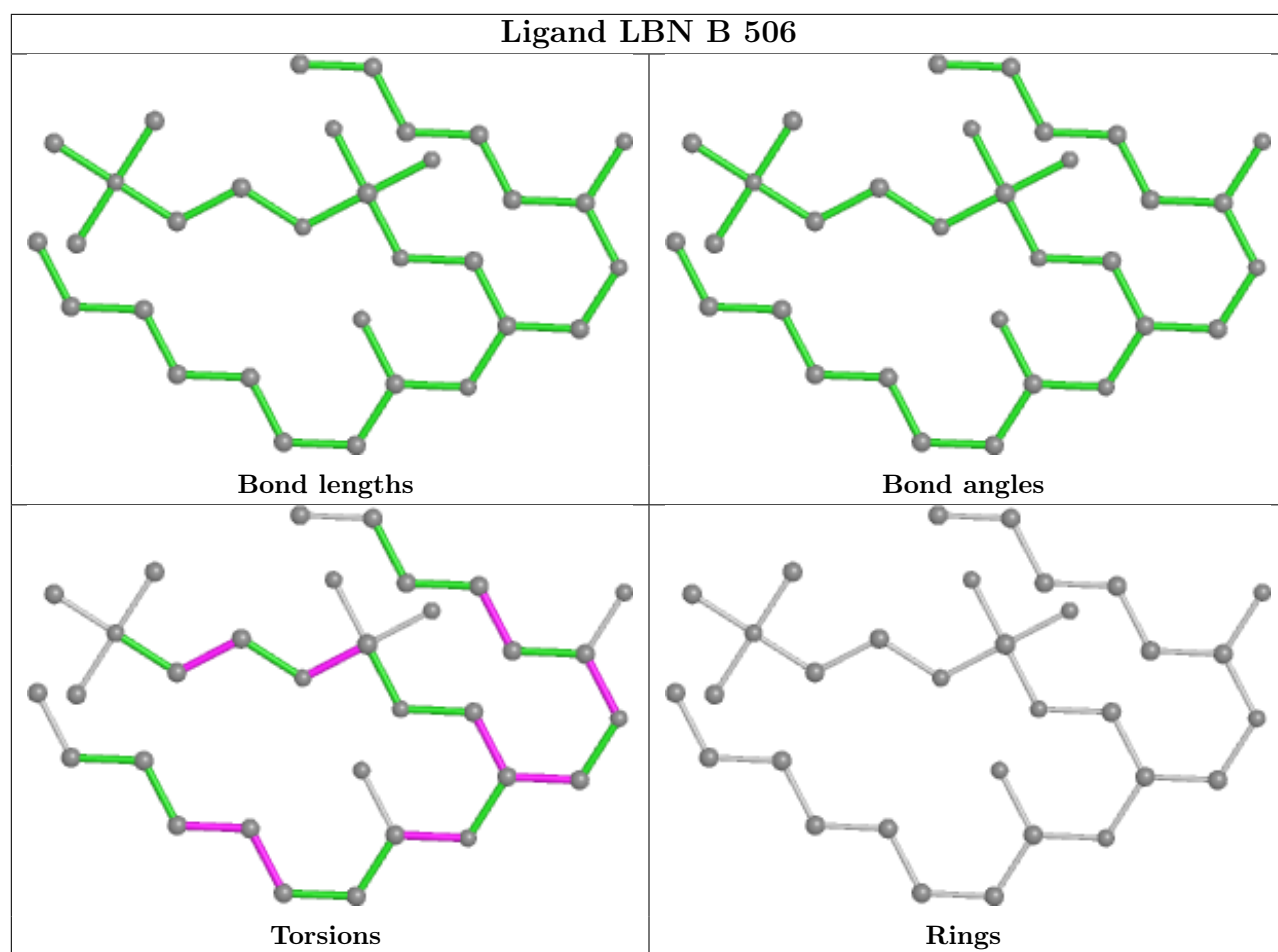
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	512	LBN	1	0
4	A	505	LBN	1	0
4	B	506	LBN	1	0
8	A	511	SER	2	0
2	A	501	PSF	1	0
8	B	512	SER	2	0
2	B	503	PSF	3	0
4	B	501	LBN	1	0
2	A	502	PSF	3	0
2	B	502	PSF	1	0

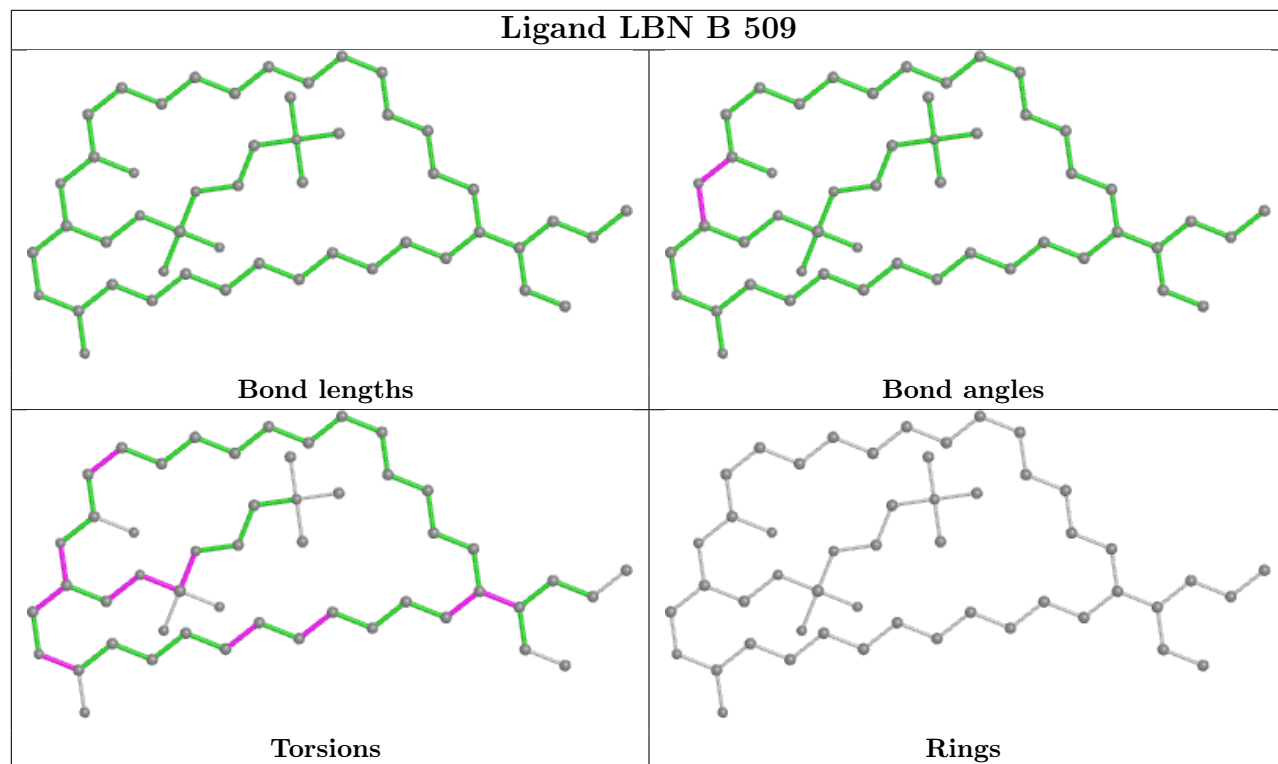
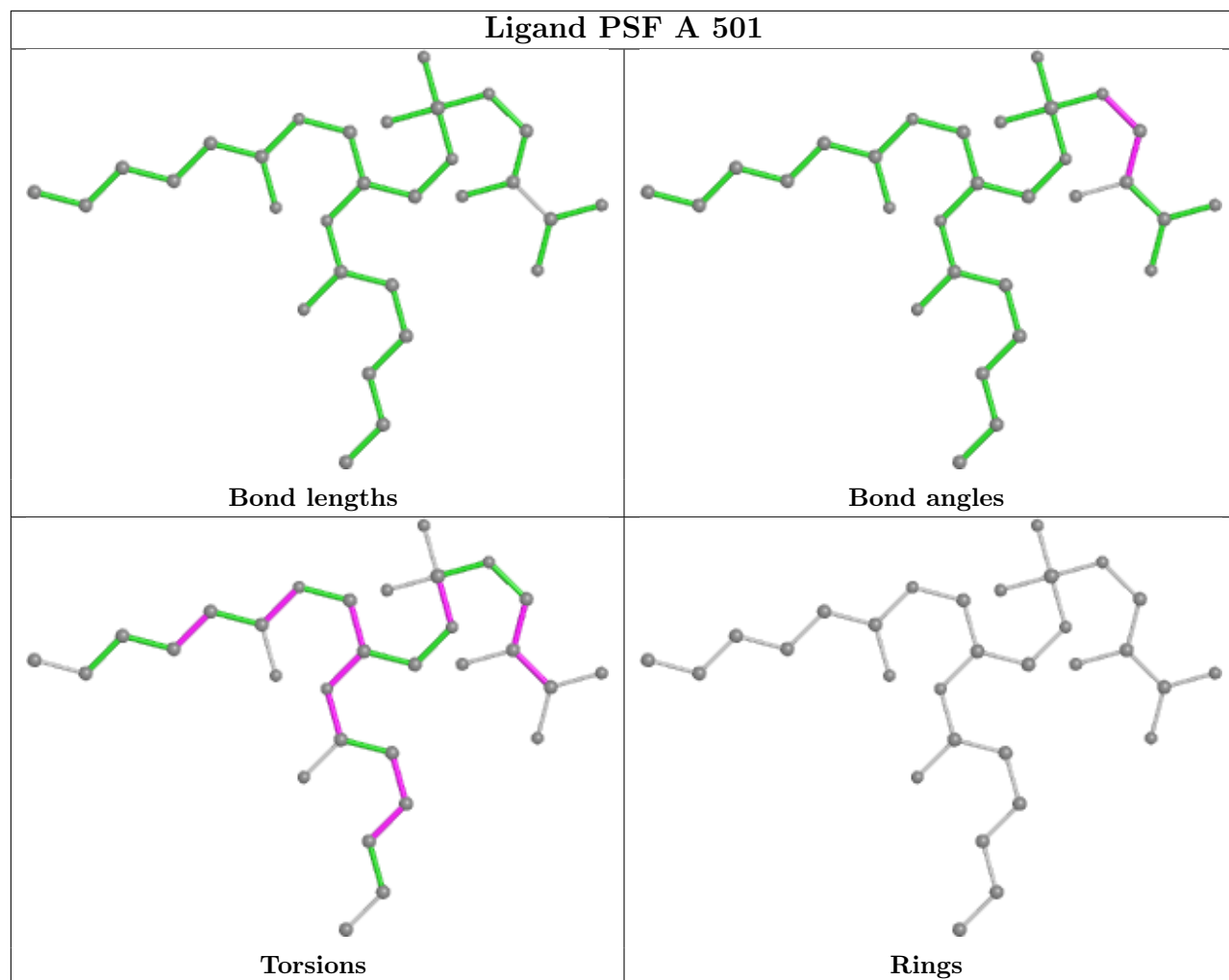
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

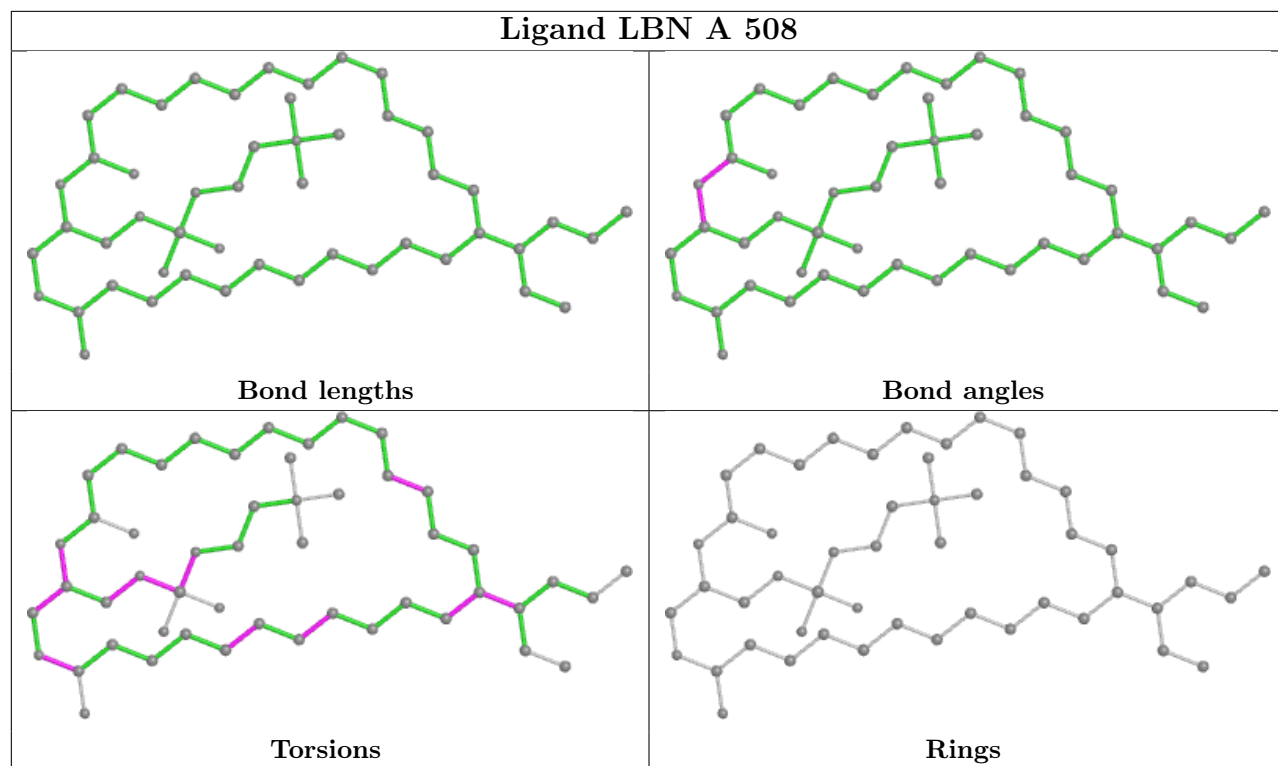




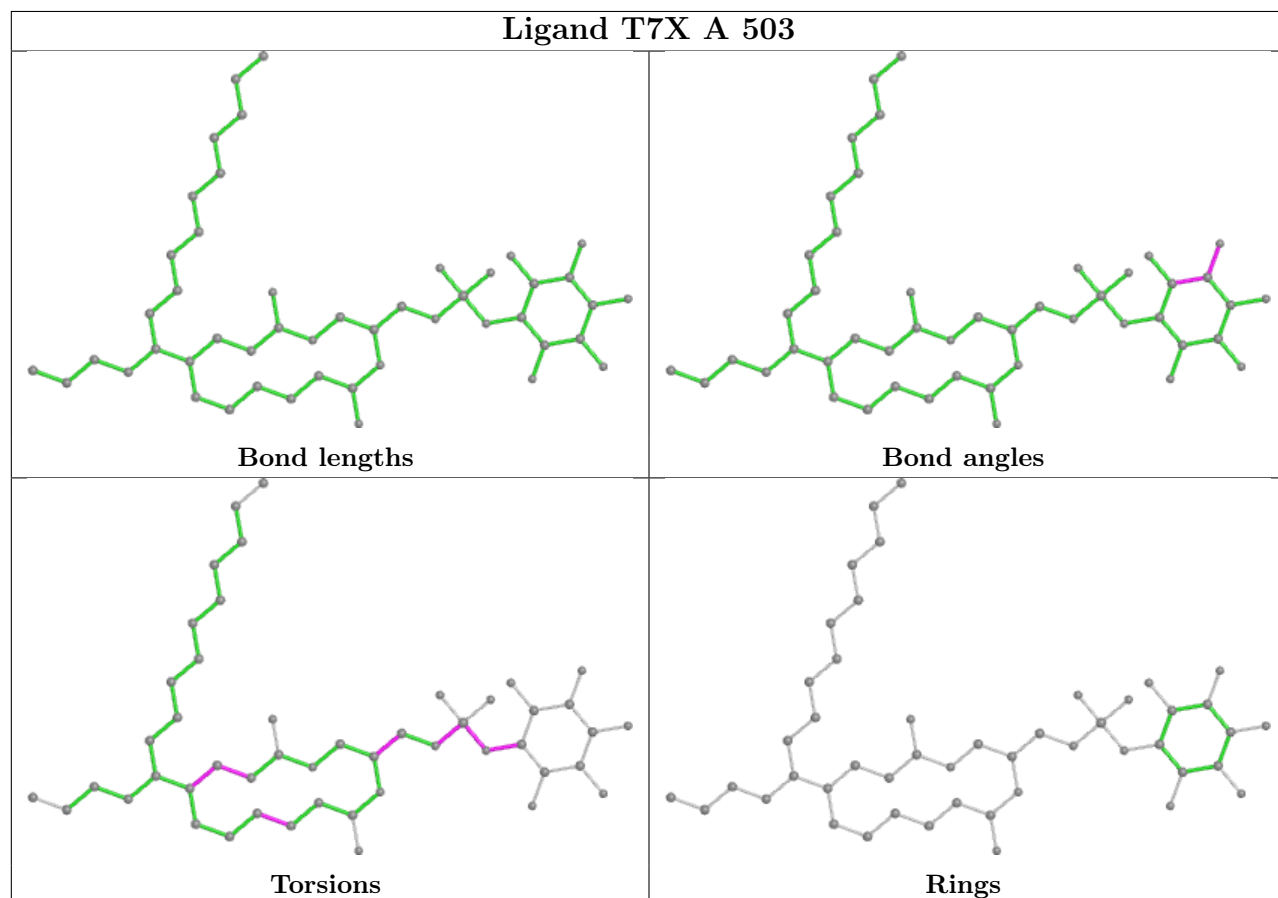


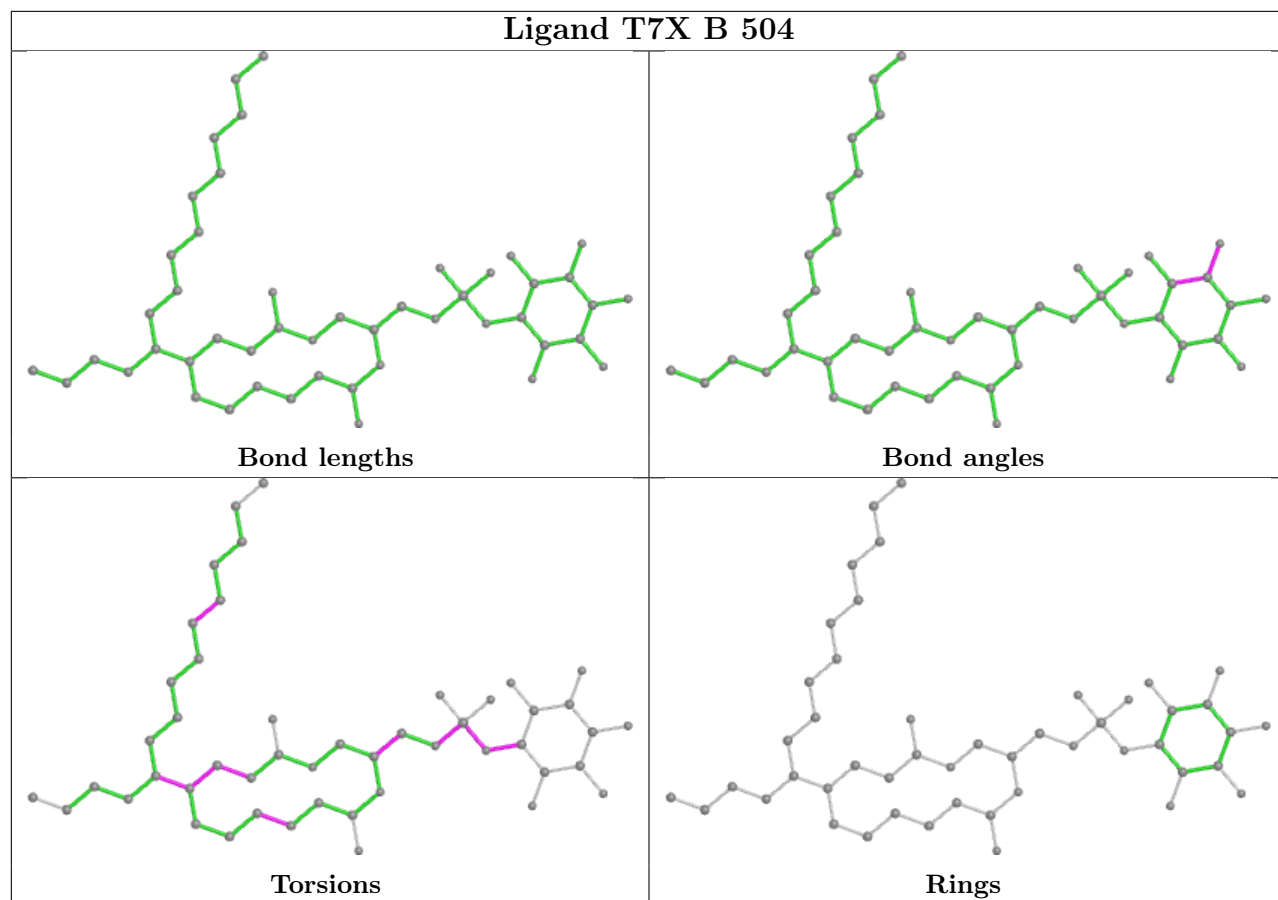


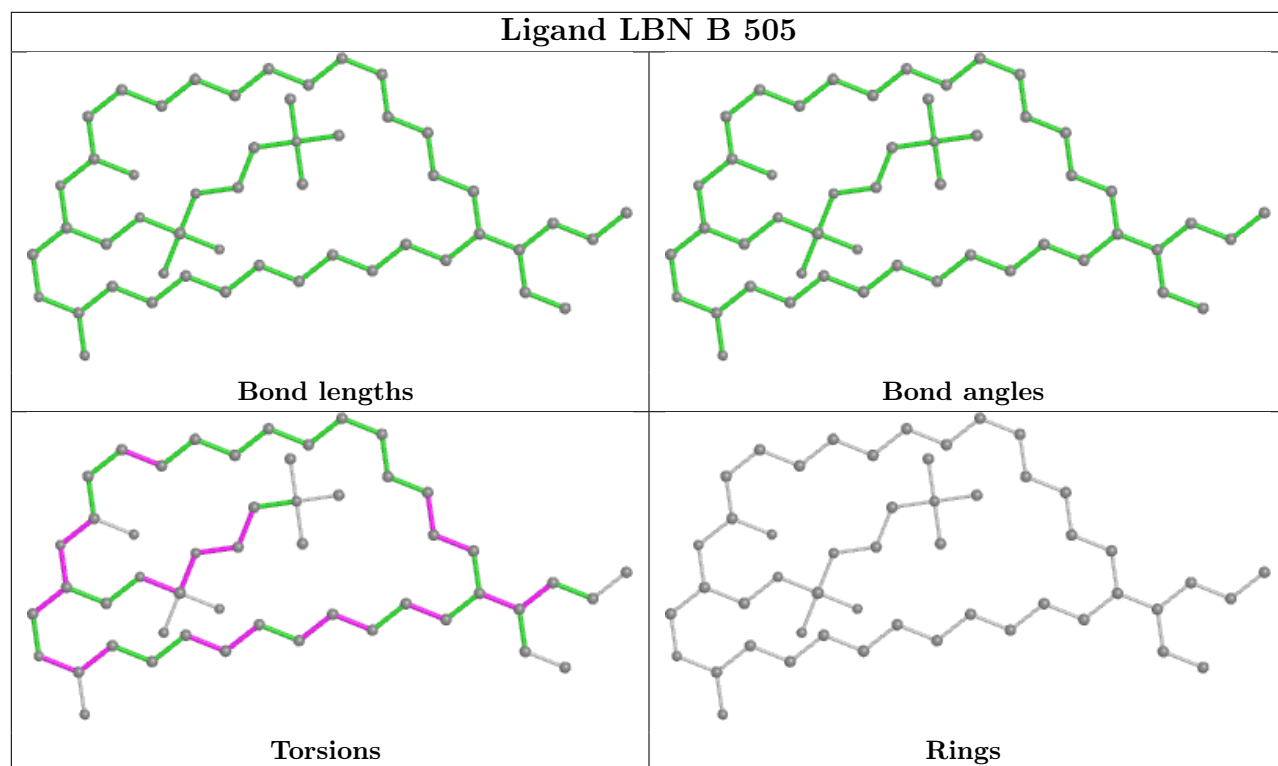
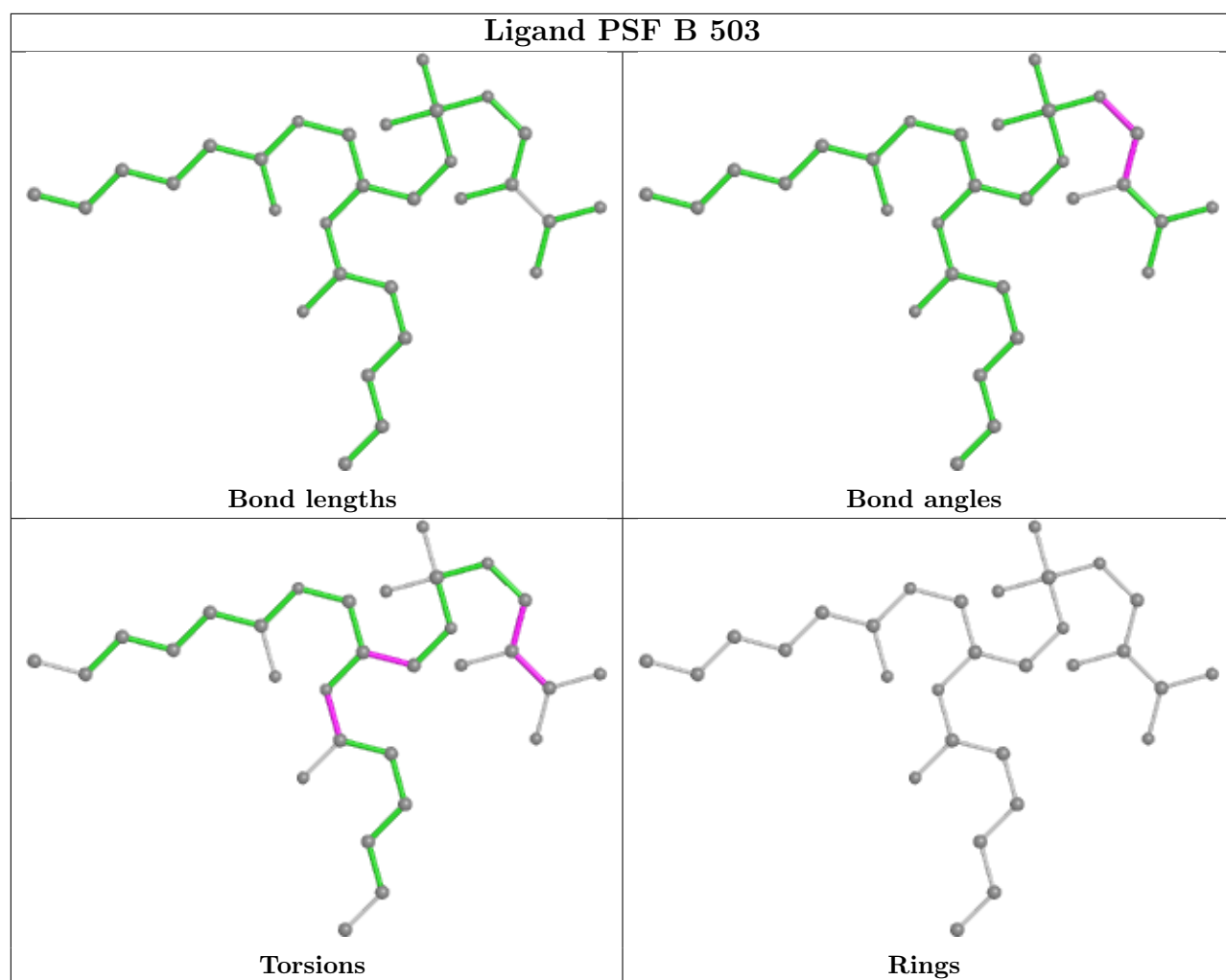
Ligand LBN A 508

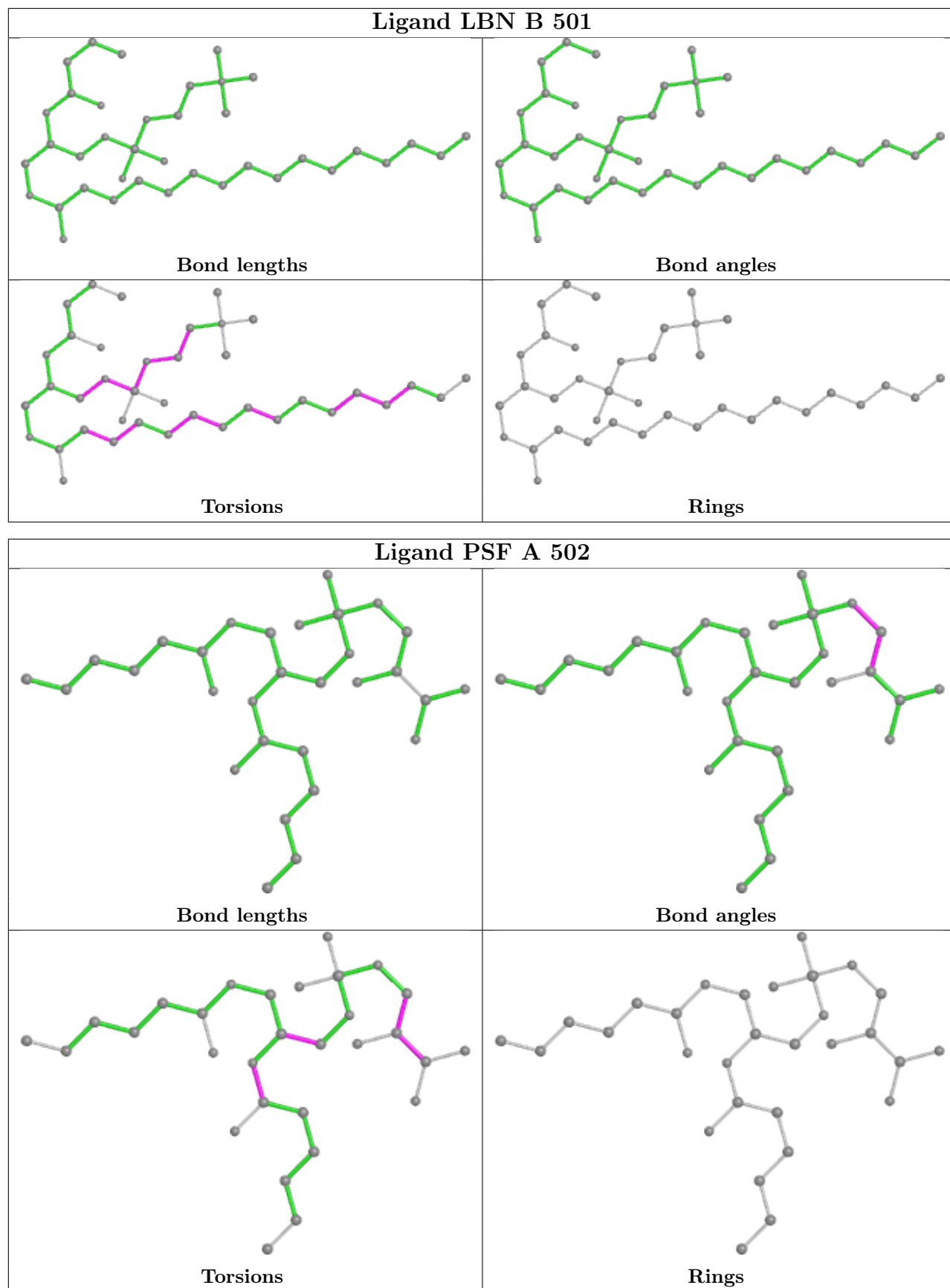


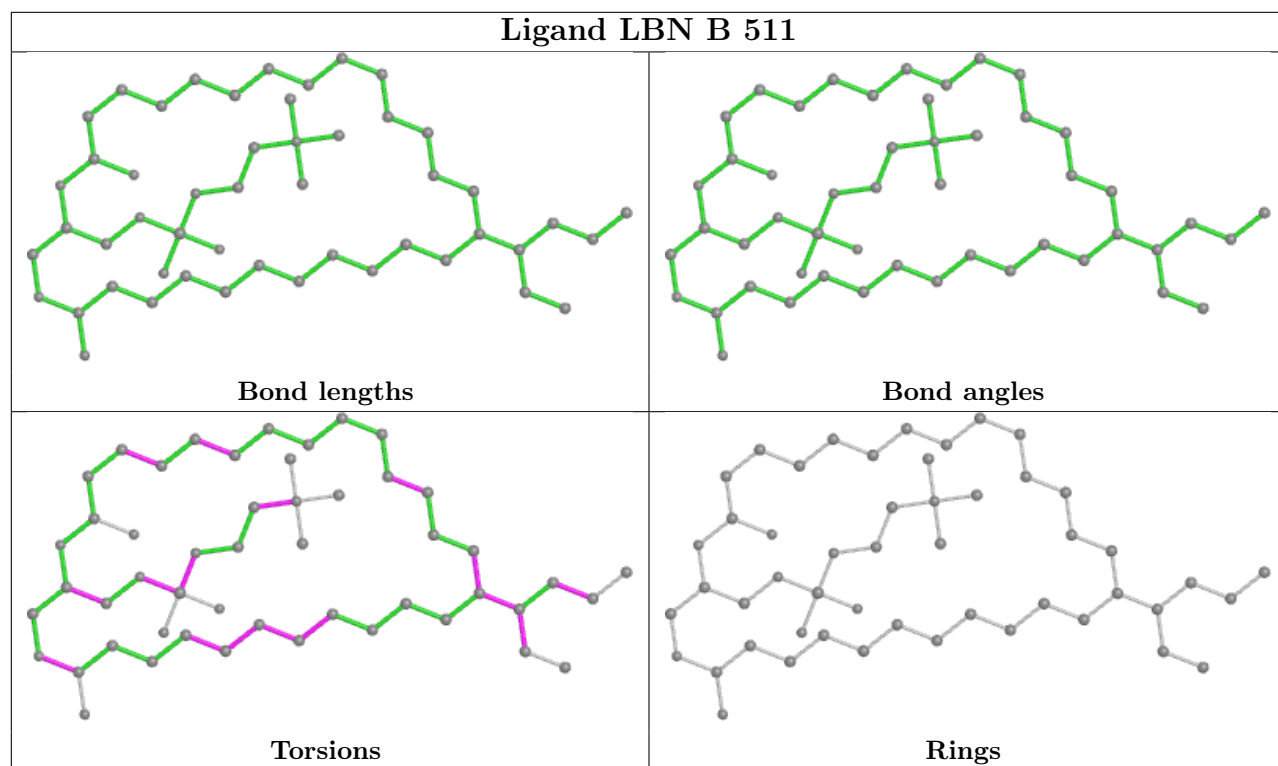
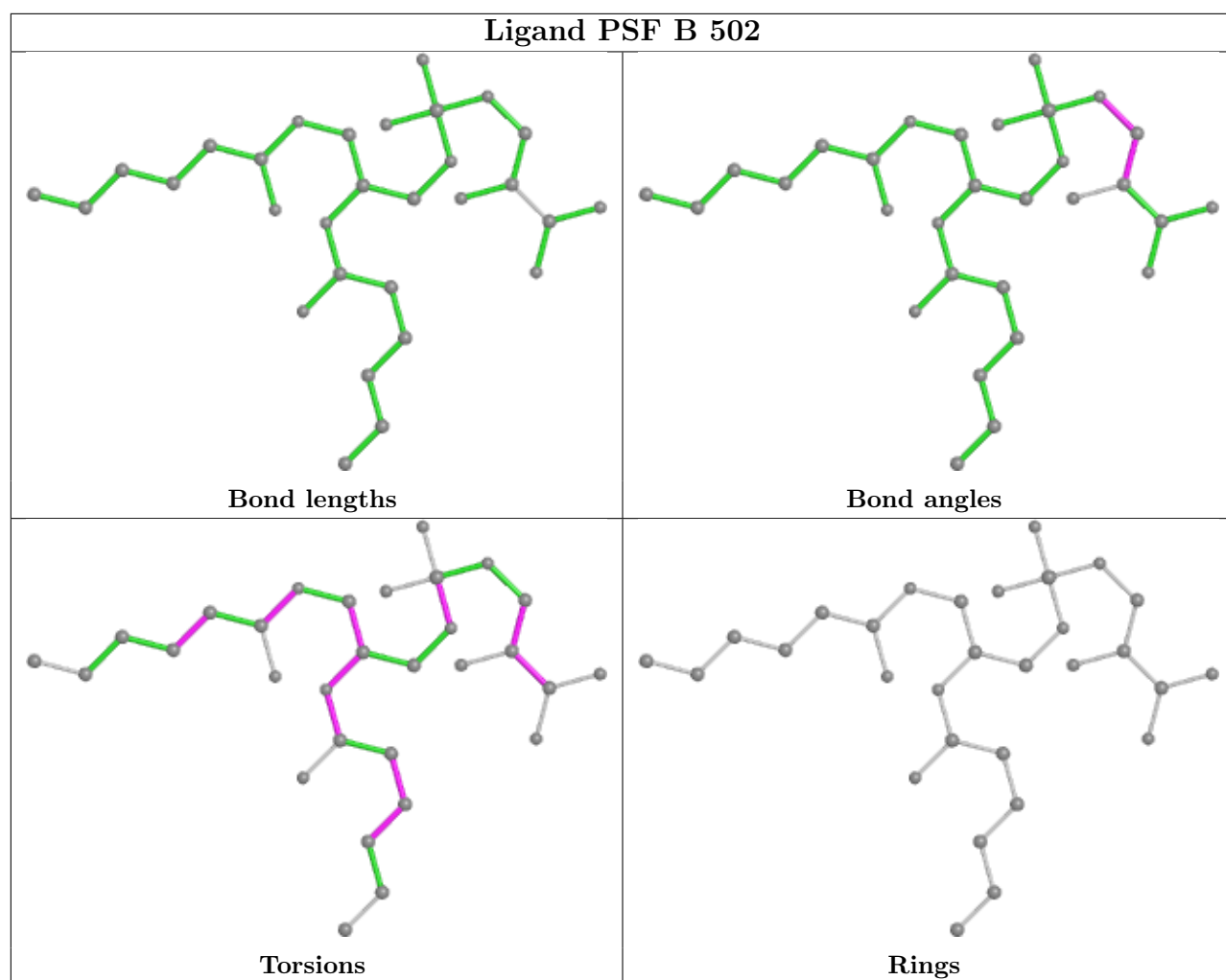
Ligand T7X A 503

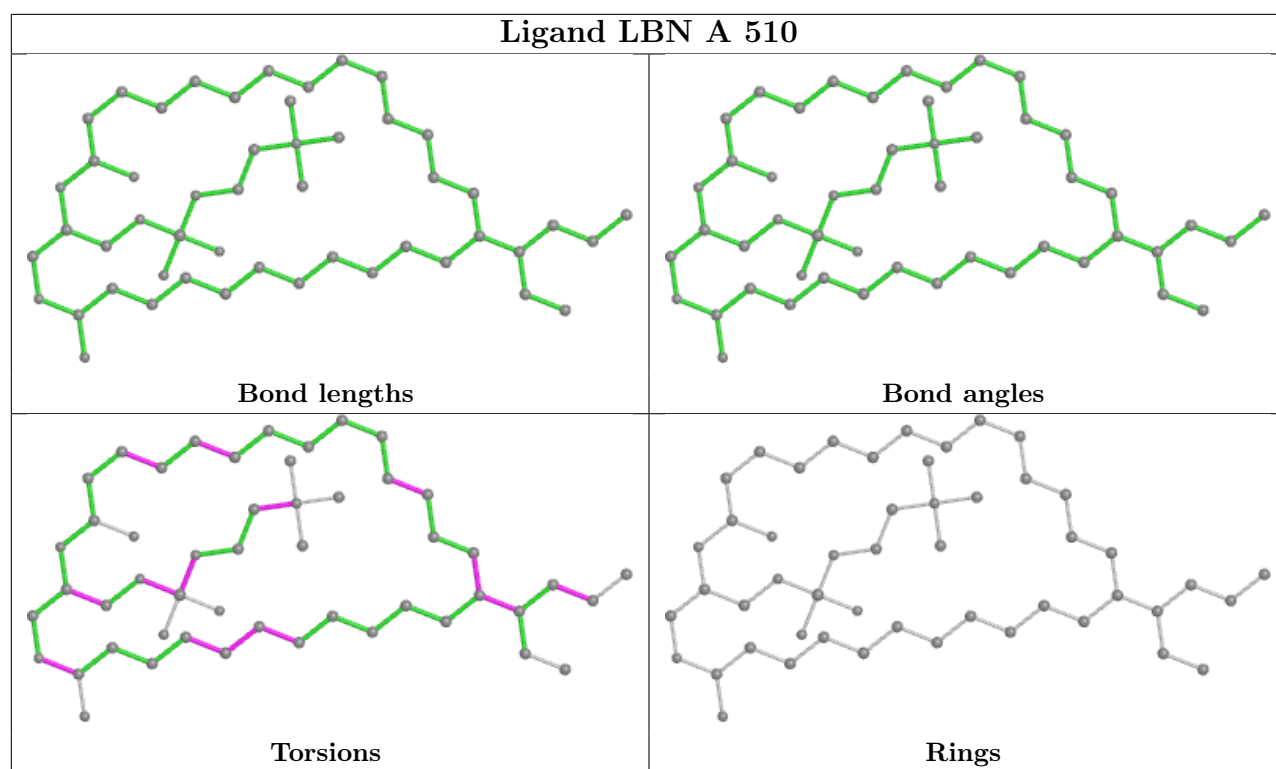












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

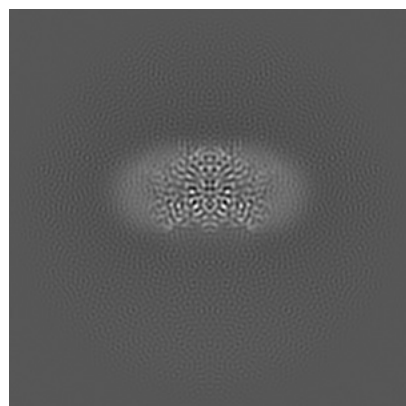
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62505. These allow visual inspection of the internal detail of the map and identification of artifacts.

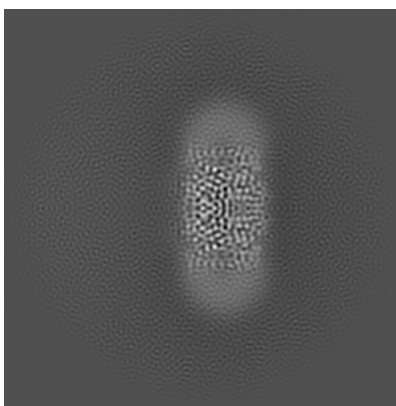
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

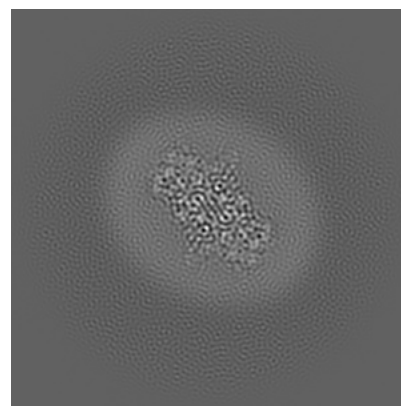
6.1.1 Primary map



X

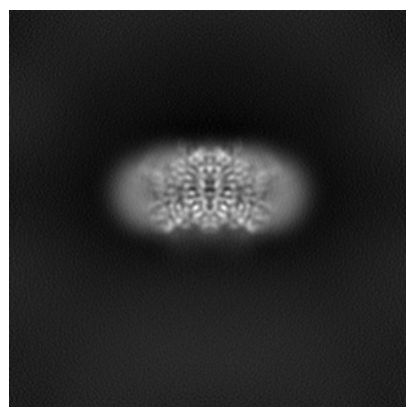


Y

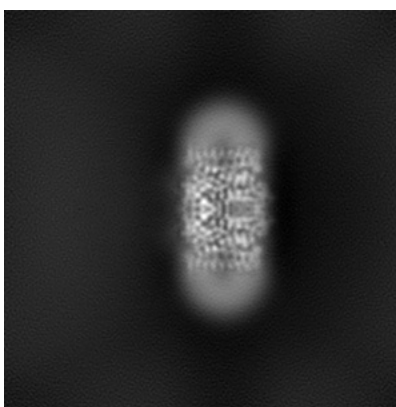


Z

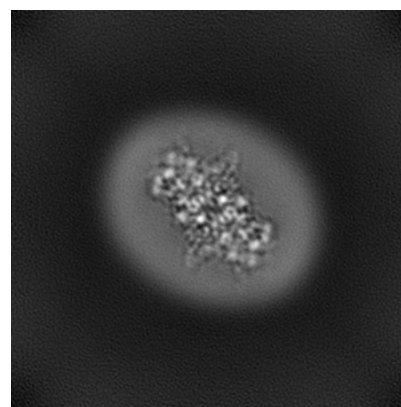
6.1.2 Raw map



X



Y

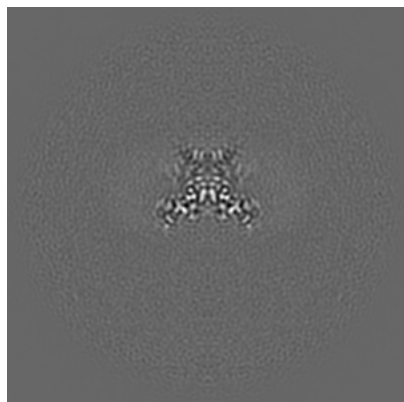


Z

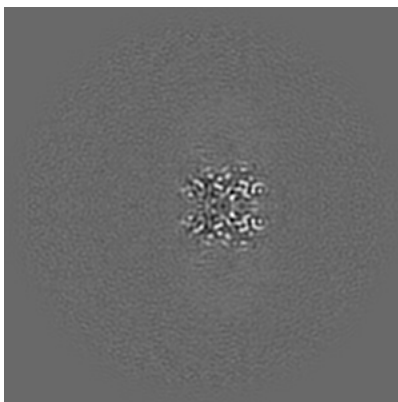
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

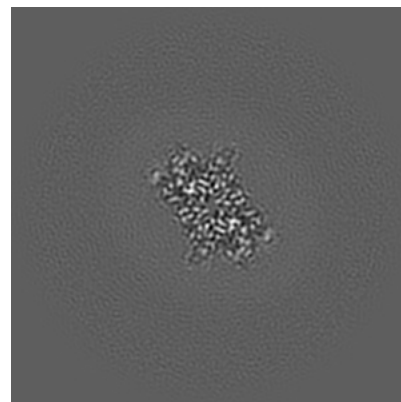
6.2.1 Primary map



X Index: 120

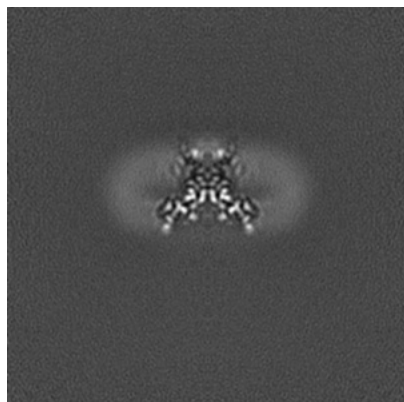


Y Index: 120

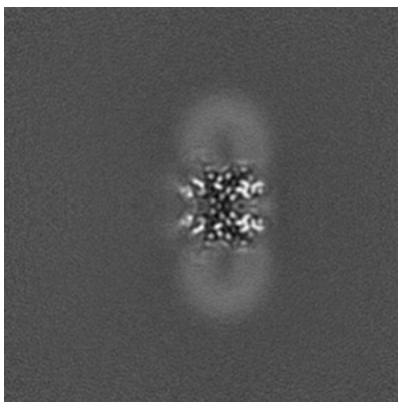


Z Index: 120

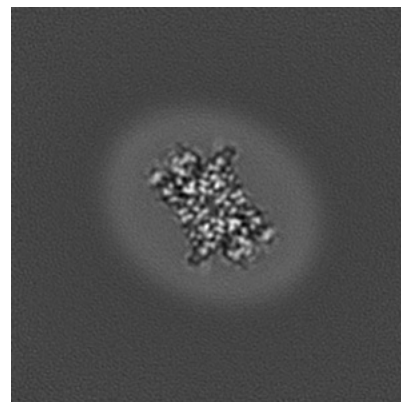
6.2.2 Raw map



X Index: 120



Y Index: 120

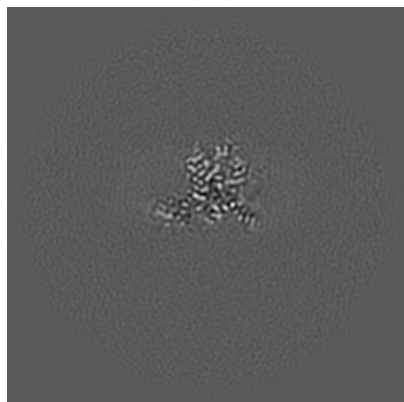


Z Index: 120

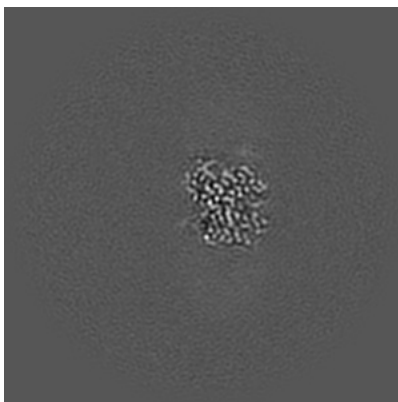
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

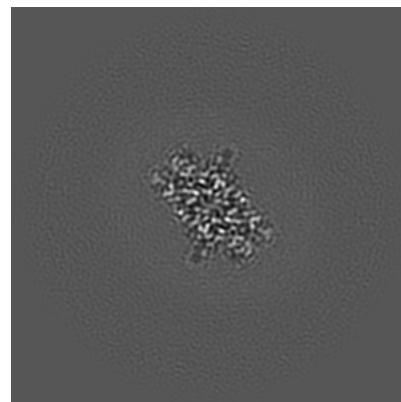
6.3.1 Primary map



X Index: 114

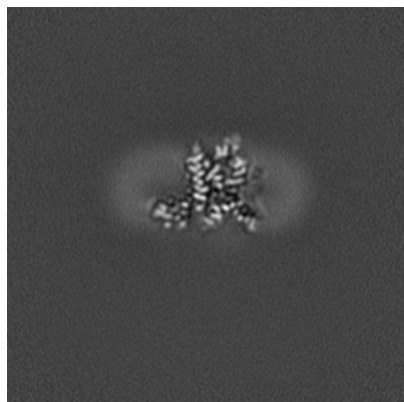


Y Index: 116

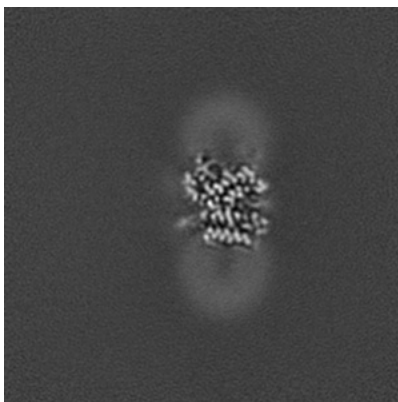


Z Index: 121

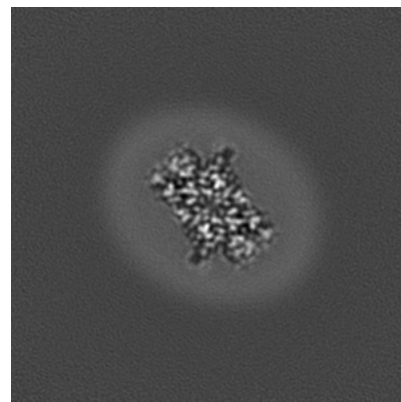
6.3.2 Raw map



X Index: 114



Y Index: 116

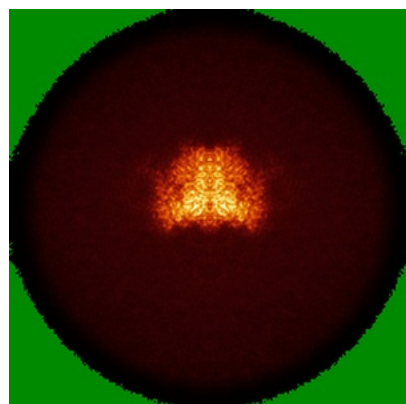


Z Index: 121

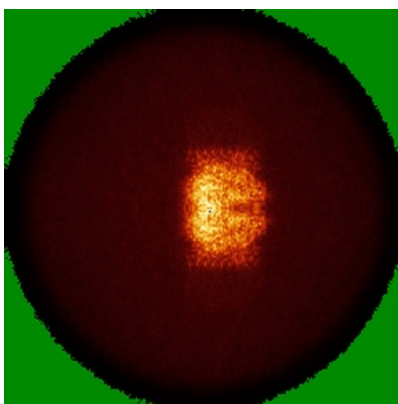
The images above show the largest variance slices of the map in three orthogonal directions.

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

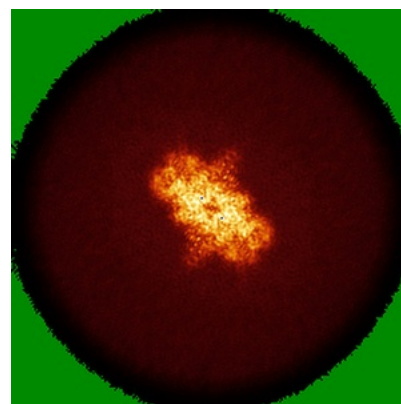
6.4.1 Primary map



X

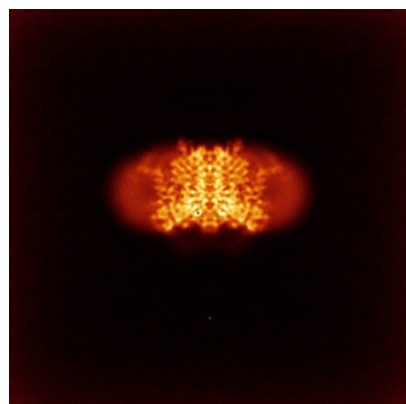


Y

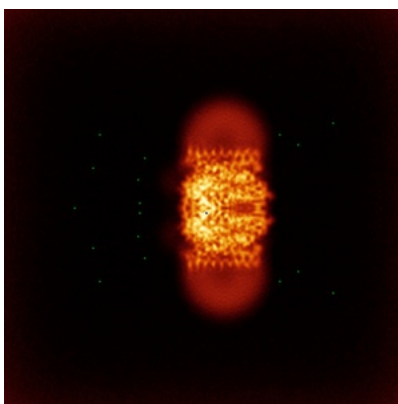


Z

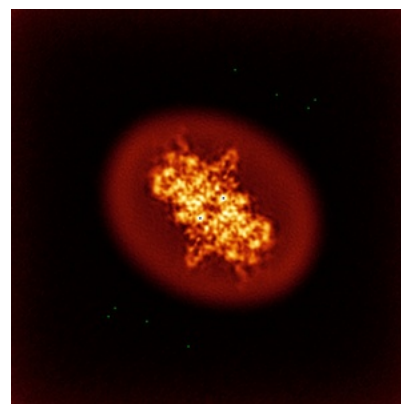
6.4.2 Raw map



X



Y

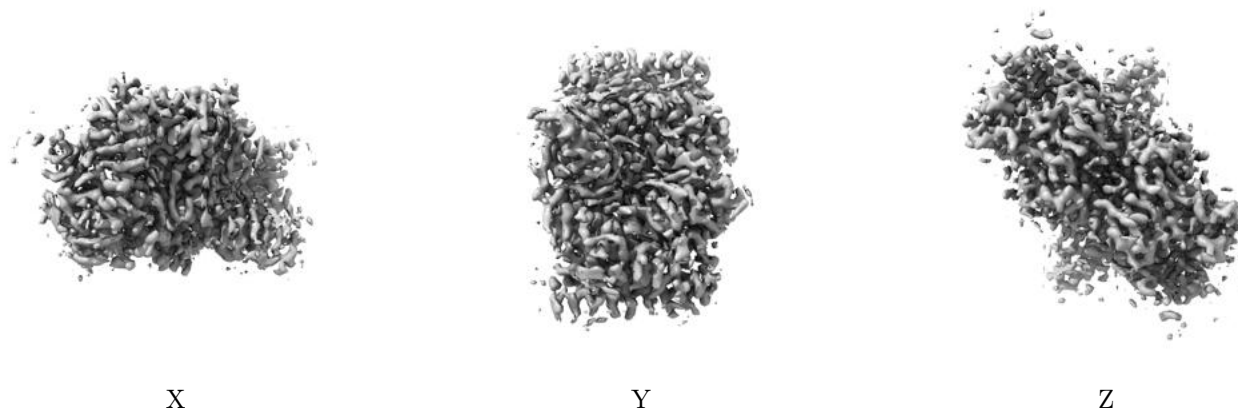


Z

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.

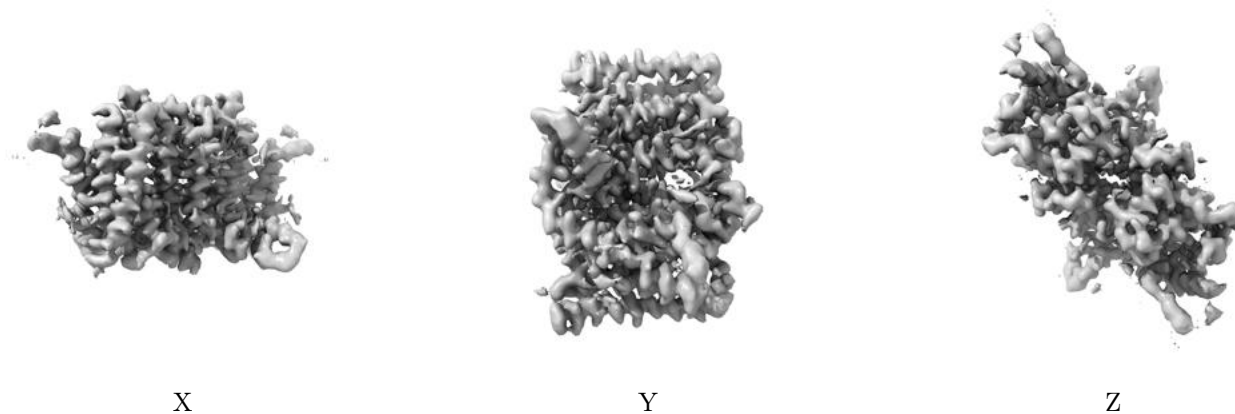
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.543. 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.

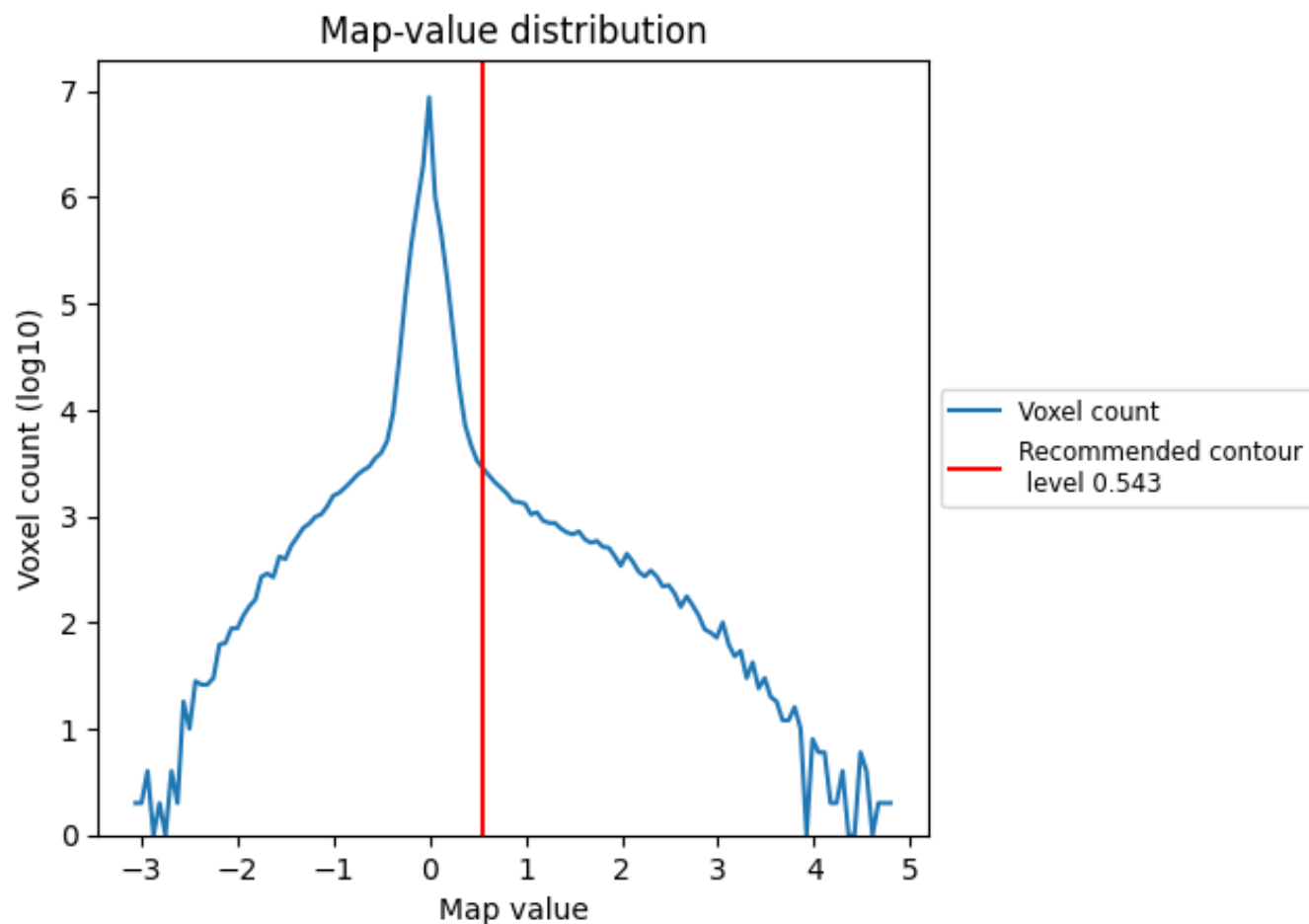
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

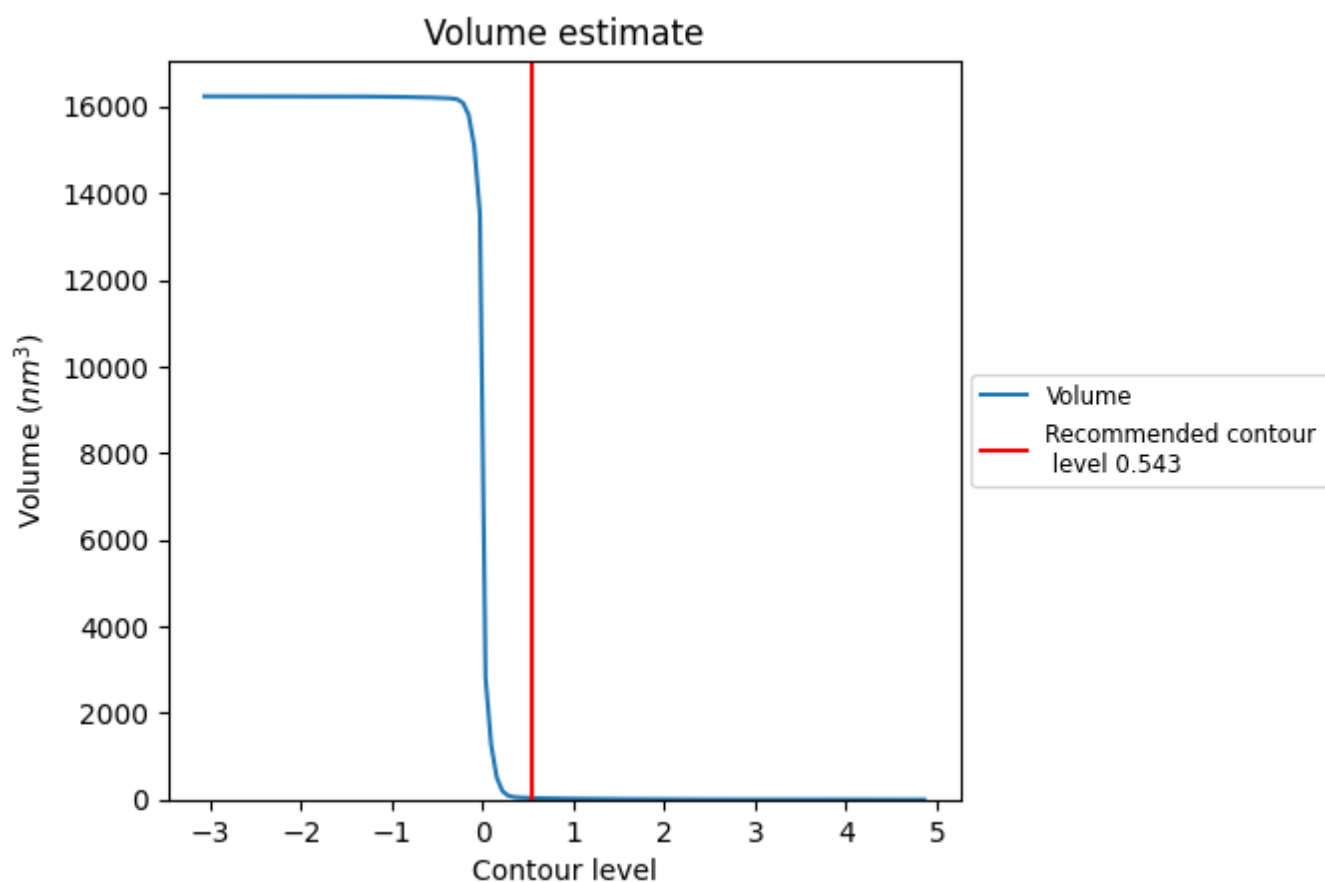
This section contains the results of statistical analysis of the map.

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.

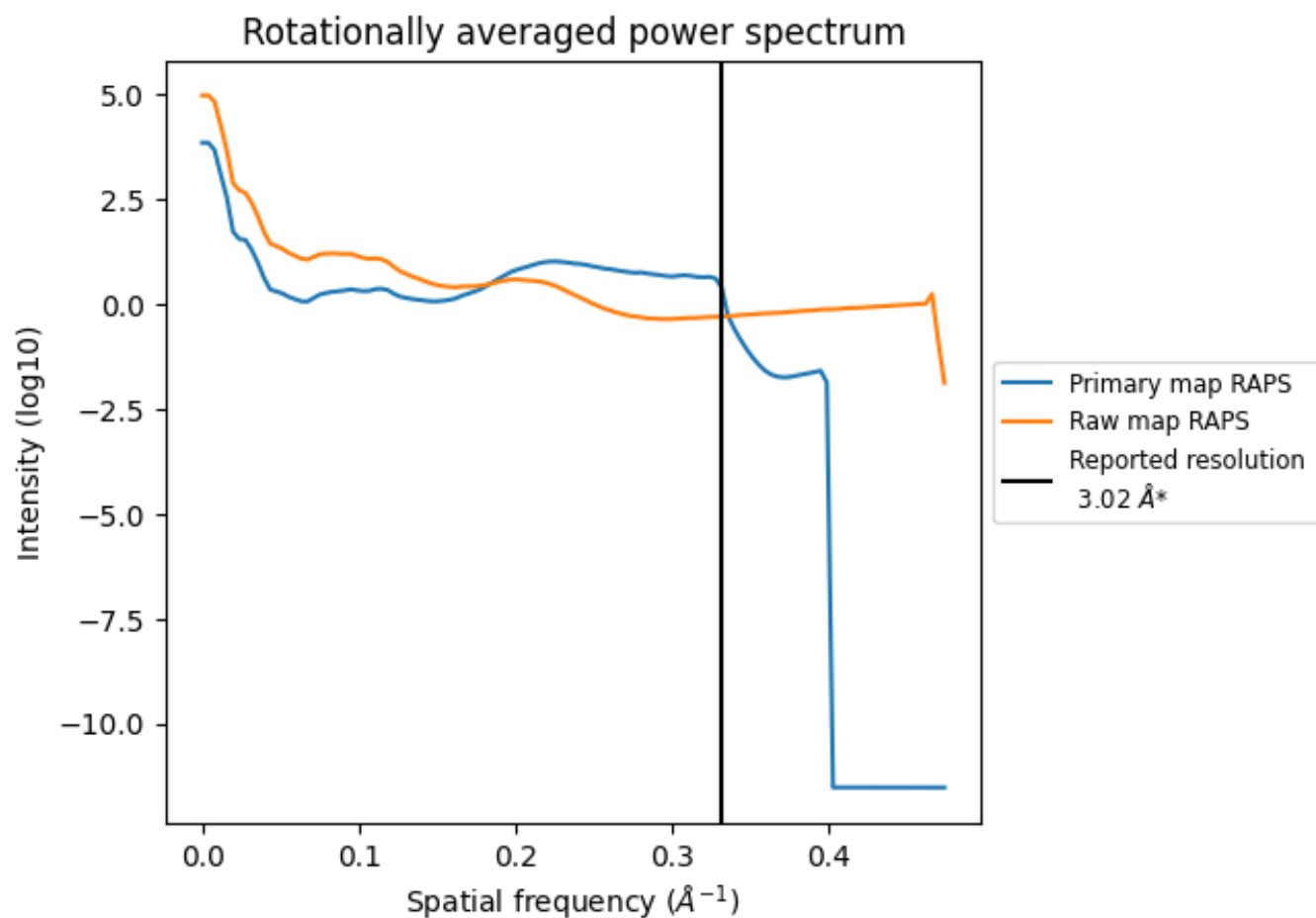
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 36 nm^3 ; this corresponds to an approximate mass of 32 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 ⓘ

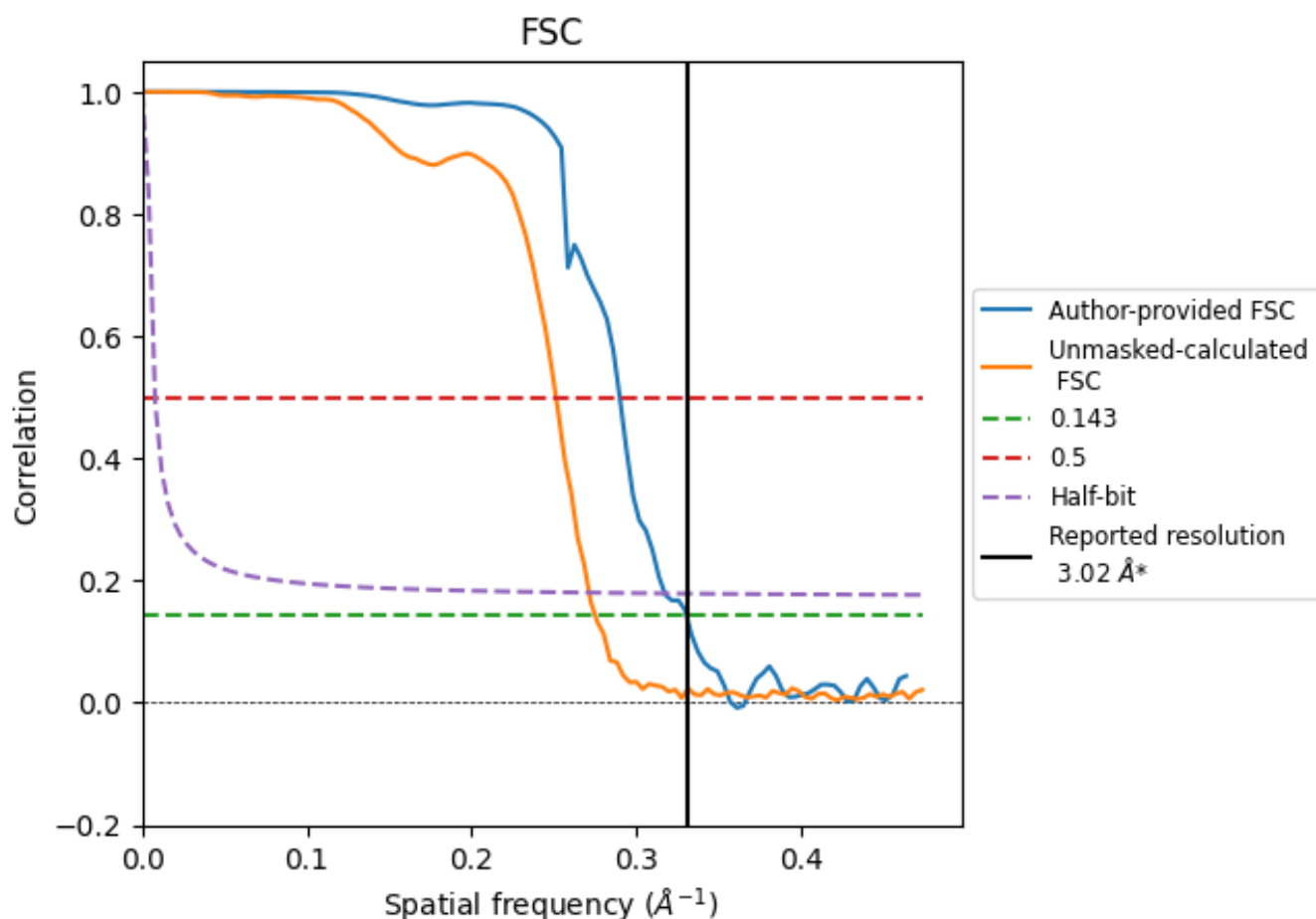


*Reported resolution corresponds to spatial frequency of 0.331 Å⁻¹

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 0.331 \AA^{-1}

8.2 Resolution estimates [i](#)

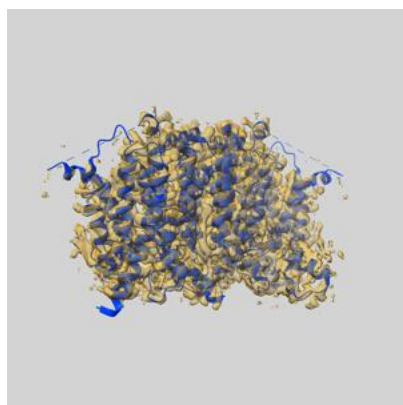
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.02	-	-
Author-provided FSC curve	3.02	3.45	3.15
Unmasked-calculated*	3.63	3.98	3.68

*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 3.63 differs from the reported value 3.02 by more than 10 %

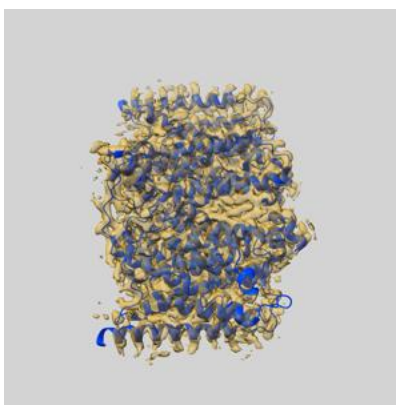
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-62505 and PDB model 9KQI. Per-residue inclusion information can be found in section [3](#) on page [8](#).

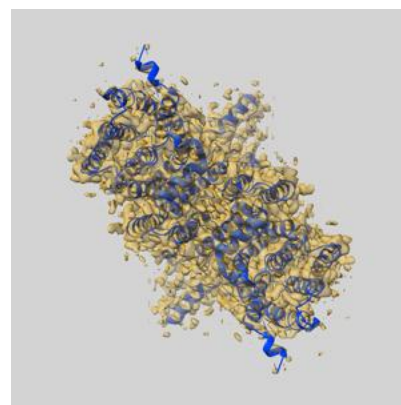
9.1 Map-model overlay [i](#)



X



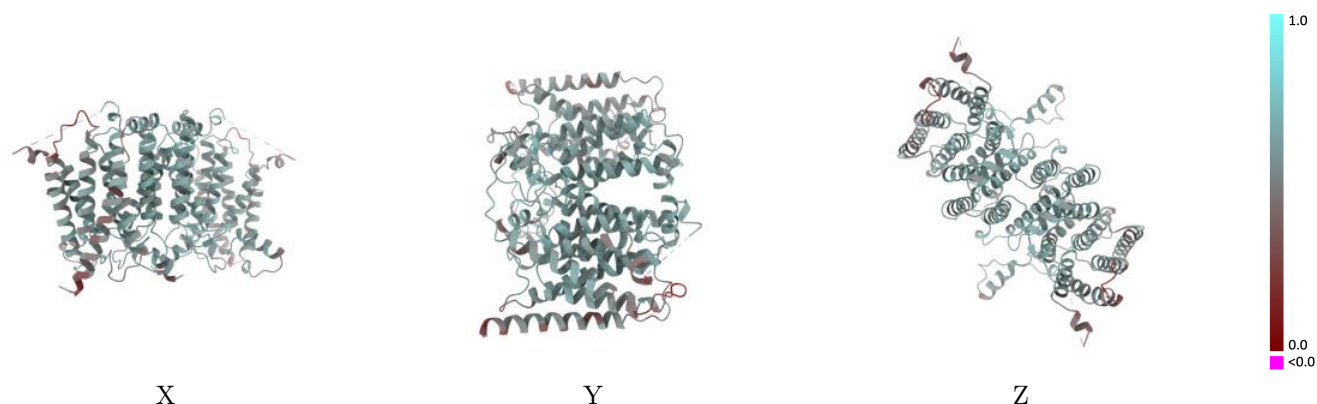
Y



Z

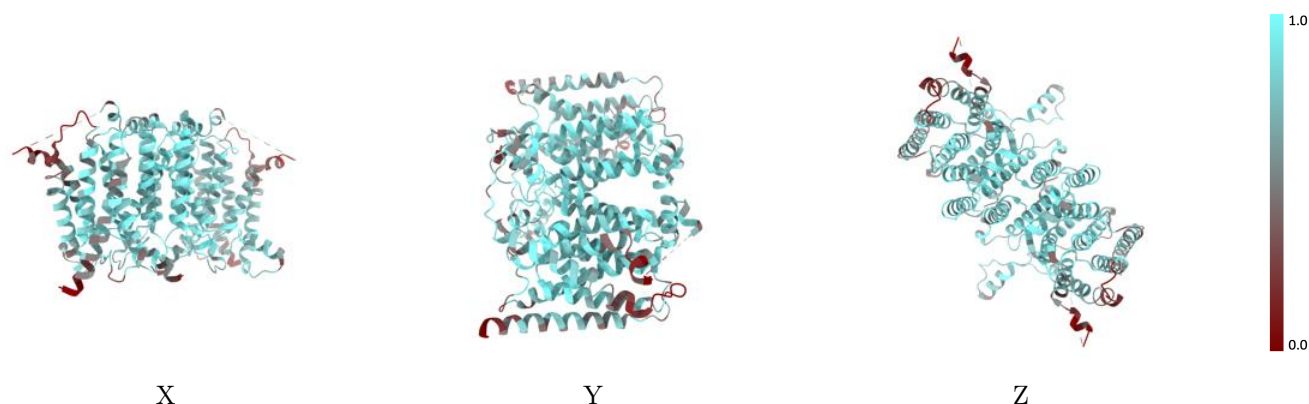
The images above show the 3D surface view of the map at the recommended contour level 0.543 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



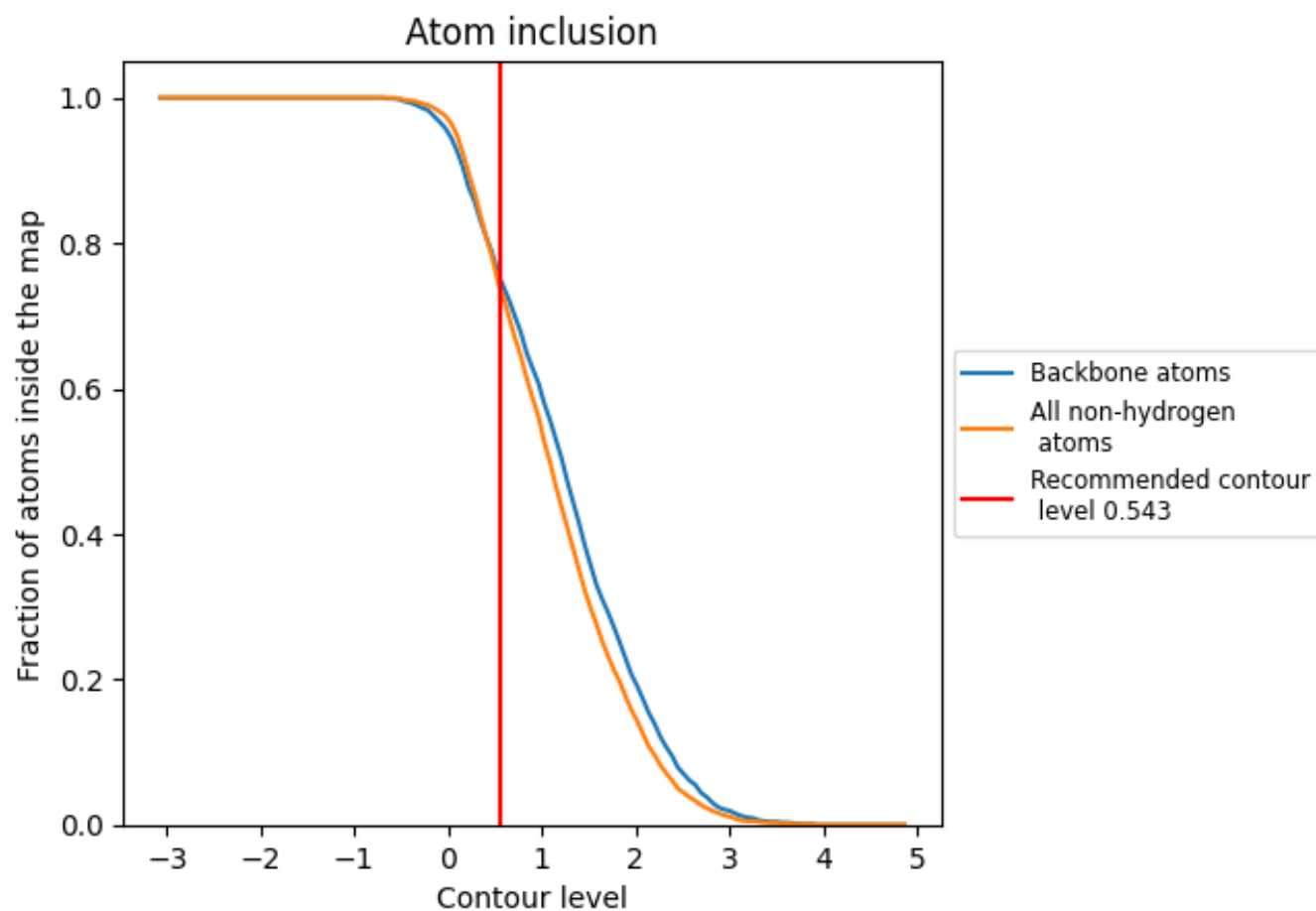
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.543).

9.4 Atom inclusion ⓘ



At the recommended contour level, 75% of all backbone atoms, 74% 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 (0.543) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7400	<div></div> 0.5530
A	<div></div> 0.7410	<div></div> 0.5510
B	<div></div> 0.7390	<div></div> 0.5540

