



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 01:20 PM UTC

PDB ID : 9KQJ / pdb_00009kqj
EMDB ID : EMD-62506
Title : Cryo-EM structure of PSS1 with calcium
Authors : Ning, Y.; Yu, J.; Ge, J.
Deposited on : 2024-11-26
Resolution : 2.95 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 EMD archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

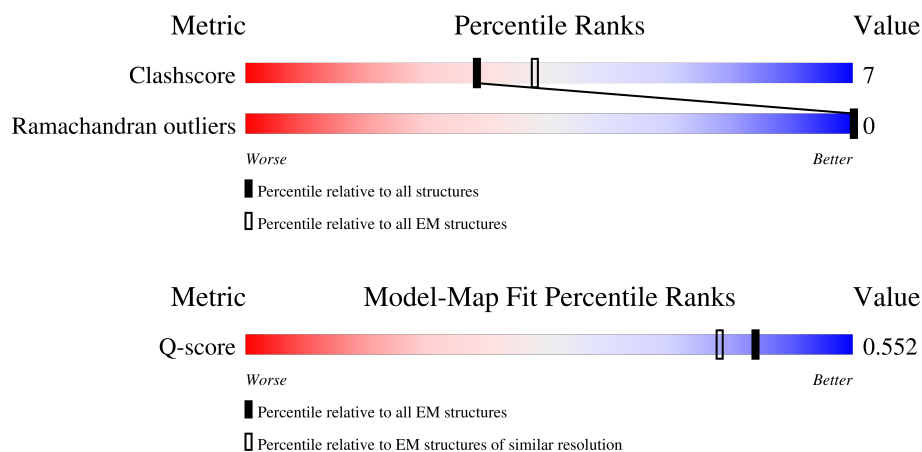
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.95 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	-
Q-score	-	25397	13114 (2.45 - 3.45)

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	9% 65% 15% 20%
1	B	473	9% 66% 14% 20%

2 Entry composition [i](#)

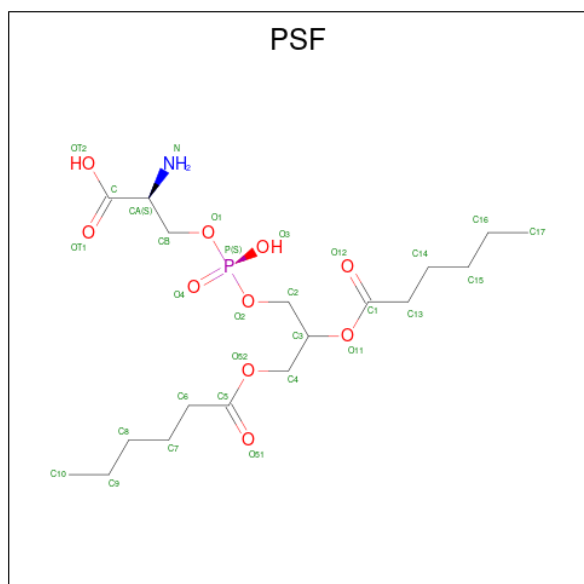
There are 7 unique types of molecules in this entry. The entry contains 7056 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

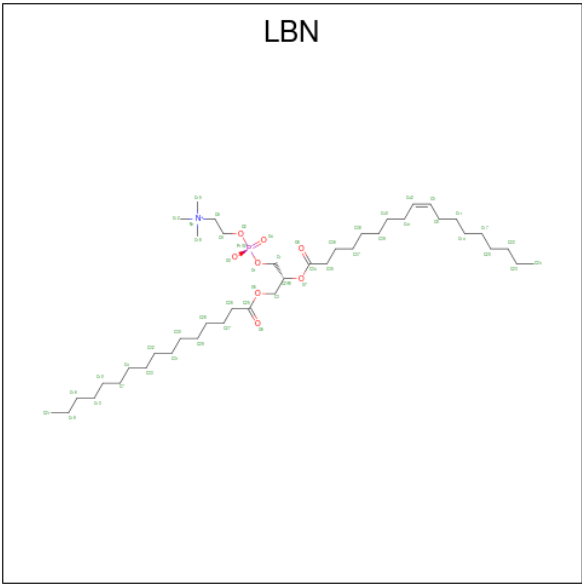
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	377	Total	C	N	O	S	0	0
			3171	2141	501	509	20		
1	B	377	Total	C	N	O	S	0	0
			3171	2141	501	509	20		

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



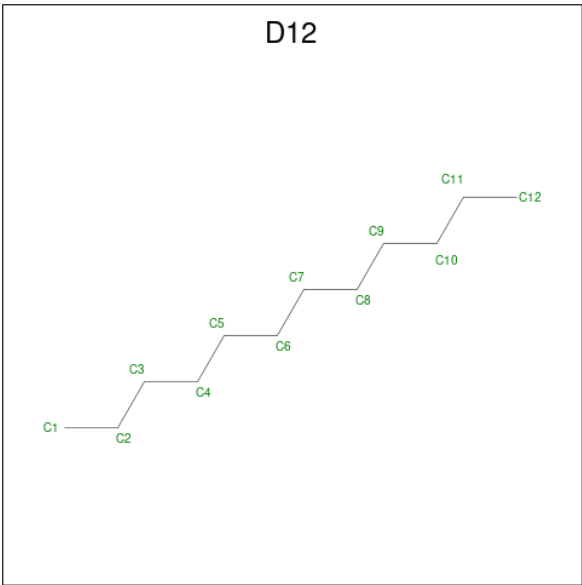
Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			30	18	1	10	1	
2	A	1	Total	C	N	O	P	0
			30	18	1	10	1	
2	B	1	Total	C	N	O	P	0
			30	18	1	10	1	
2	B	1	Total	C	N	O	P	0
			30	18	1	10	1	

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



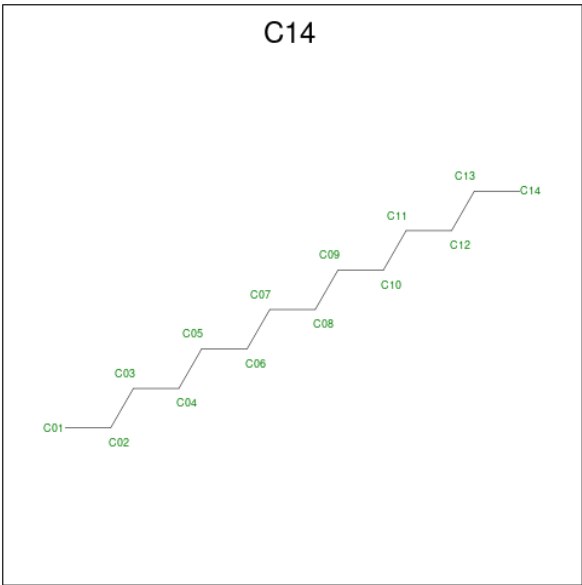
Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	A	1	Total	C	N	O	P	0
			32	22	1	8	1	
3	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	A	1	Total	C	N	O	P	0
			46	36	1	8	1	
3	A	1	Total	C	N	O	P	0
			38	28	1	8	1	
3	B	1	Total	C	N	O	P	0
			38	28	1	8	1	
3	B	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	B	1	Total	C	N	O	P	0
			32	22	1	8	1	
3	B	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	B	1	Total	C	N	O	P	0
			46	36	1	8	1	

- Molecule 4 is DODECANE (CCD ID: D12) (formula: $C_{12}H_{26}$).



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

- Molecule 5 is TETRADECANE (CCD ID: C14) (formula: C₁₄H₃₀).

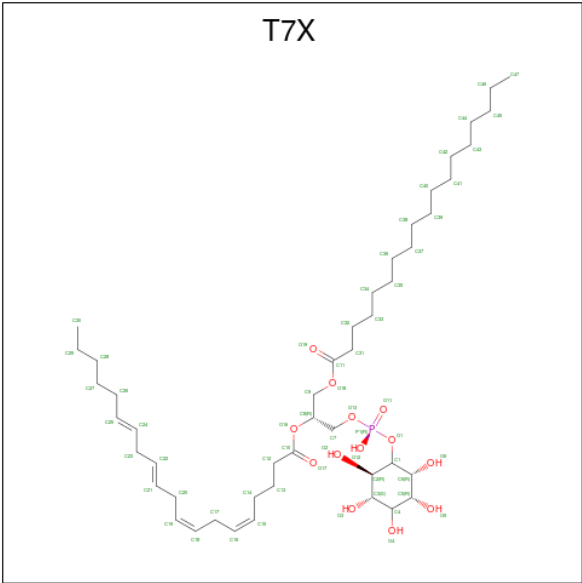


Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	C	0
			14	14	
5	B	1	Total	C	0
			14	14	

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 7 is Phosphatidylinositol (CCD ID: T7X) (formula: C₄₇H₈₃O₁₃P) (labeled as "Ligand of Interest" by depositor).

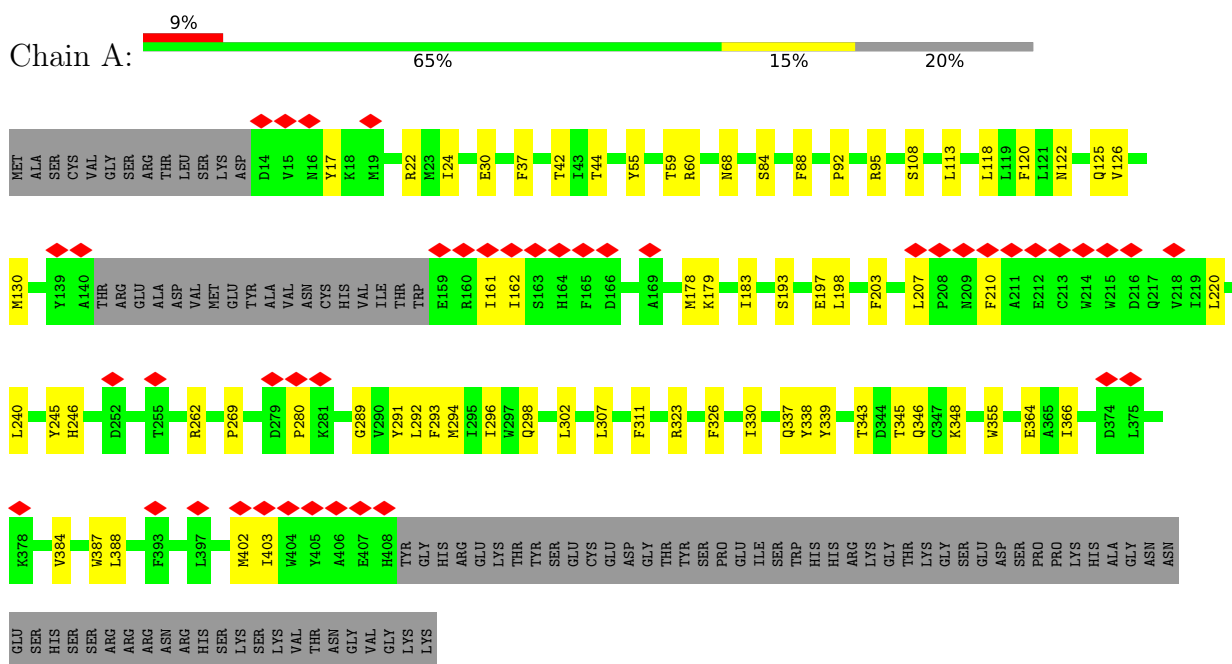


Mol	Chain	Residues	Atoms				AltConf
7	A	1	Total	C	O	P	0
			50	36	13	1	
7	B	1	Total	C	O	P	0
			50	36	13	1	

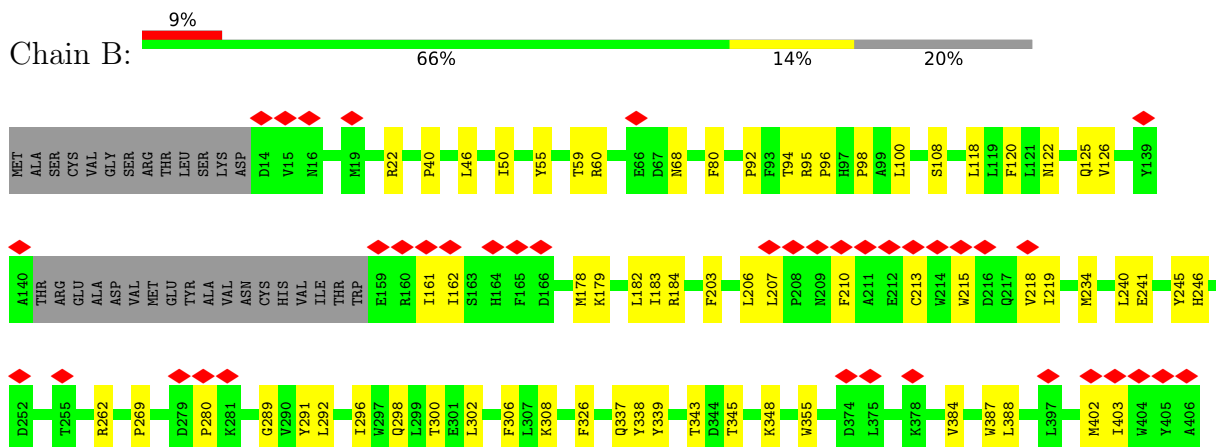
3 Residue-property plots

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



◆◆	
E407	
H408	
THR	
GLY	
HIS	
ARG	
GLU	
LYS	
THR	
TYR	
SER	
GLU	
CYS	
GLU	
ASP	
GLY	
THR	
TYR	
SER	
PRO	
GLU	
ILE	
SER	
TRP	
HIS	
HIS	
ARG	
LYS	
GLY	
THR	
LYS	
GLY	
SER	
GLU	
ASP	
SER	
PRO	
PRO	
LYS	
HIS	
ALA	
GLY	
ASN	
ASN	
GLU	
SER	
HIS	
SER	
SER	
ARG	
ARG	
ARG	
ASN	
ARG	
HIS	
SER	
LYS	
SER	
LYS	
VAL	

THR
ASN
GLY
VAL
GLY
LYS
LYS

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	455789	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	4.291	Depositor
Minimum map value	-3.079	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.093	Depositor
Recommended contour level	0.576	Depositor
Map size ($\text{\AA}$)	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 ($\text{\AA}$)	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: CA, C14, LBN, T7X, PSF, D12

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	0.20	0/3285	0.32	0/4474
1	B	0.20	0/3285	0.29	0/4474
All	All	0.20	0/6570	0.31	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	56	0
1	B	3171	0	3137	51	0
2	A	60	0	64	5	0
2	B	60	0	64	2	0
3	A	220	0	0	1	0
3	B	220	0	0	0	0
4	A	12	0	26	0	0
4	B	12	0	26	0	0
5	A	14	0	30	0	0
5	B	14	0	30	0	0
6	A	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	1	0	0	0	0
7	A	50	0	0	1	0
7	B	50	0	0	1	0
All	All	7056	0	6514	100	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 7.

All (100) 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:B:246:HIS:O	1:B:246:HIS:ND1	2.12	0.81
1:A:246:HIS:O	1:A:246:HIS:ND1	2.13	0.81
1:B:298:GLN:CD	1:B:387:TRP:HE1	1.99	0.70
1:B:55:TYR:O	1:B:59:THR:OG1	2.10	0.70
1:A:55:TYR:O	1:A:59:THR:OG1	2.10	0.69
1:B:95:ARG:HB2	2:B:503:PSF:H22	1.76	0.66
1:B:218:VAL:HG12	1:B:219:ILE:HD12	1.78	0.65
1:B:122:ASN:OD1	1:B:125:GLN:NE2	2.31	0.63
1:A:95:ARG:NH1	2:A:502:PSF:OT1	2.30	0.63
1:A:122:ASN:OD1	1:A:125:GLN:NE2	2.31	0.63
1:A:30:GLU:O	2:A:502:PSF:N	2.31	0.62
1:A:207:LEU:HD21	1:A:210:PHE:HB3	1.81	0.62
1:A:262:ARG:O	1:A:262:ARG:NH1	2.30	0.61
1:B:207:LEU:HD21	1:B:210:PHE:HB3	1.82	0.61
1:A:95:ARG:HB2	2:A:501:PSF:H22	1.82	0.60
1:A:161:ILE:HG23	1:A:220:LEU:HD21	1.83	0.60
1:A:84:SER:HB3	1:A:88:PHE:HD2	1.66	0.59
1:A:122:ASN:OD1	1:A:122:ASN:N	2.36	0.56
1:A:22:ARG:HH11	1:A:22:ARG:HG3	1.71	0.56
1:A:179:LYS:O	1:A:183:ILE:HG12	2.06	0.56
1:B:22:ARG:HG3	1:B:22:ARG:HH11	1.72	0.55
1:A:108:SER:HA	1:A:326:PHE:HZ	1.71	0.55
1:B:291:TYR:OH	1:B:388:LEU:HB2	2.06	0.55
1:B:161:ILE:HG12	1:B:215:TRP:HH2	1.72	0.54
1:A:291:TYR:OH	1:A:388:LEU:HB2	2.07	0.54
1:A:384:VAL:HG13	1:A:387:TRP:CE3	2.42	0.54
1:B:262:ARG:O	1:B:262:ARG:NH1	2.36	0.54
1:A:298:GLN:CD	1:A:387:TRP:HE1	2.16	0.53
1:B:269:PRO:HA	2:B:503:PSF:H21	1.91	0.53
1:A:292:LEU:O	1:A:296:ILE:HG12	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:384:VAL:HG13	1:B:387:TRP:CE3	2.45	0.52
1:A:345:THR:O	1:A:348:LYS:NZ	2.35	0.51
1:B:289:GLY:O	1:B:338:TYR:OH	2.18	0.50
1:B:92:PRO:HD3	1:B:337:GLN:HE21	1.77	0.50
1:A:384:VAL:O	1:A:388:LEU:HD23	2.11	0.50
1:B:384:VAL:O	1:B:388:LEU:HD23	2.12	0.50
1:A:307:LEU:HD11	1:A:364:GLU:HG2	1.93	0.50
1:A:269:PRO:HA	2:A:501:PSF:H21	1.94	0.50
1:B:203:PHE:HE2	1:B:302:LEU:HD11	1.78	0.49
1:B:179:LYS:O	1:B:183:ILE:HG12	2.12	0.49
1:B:108:SER:HA	1:B:326:PHE:HZ	1.78	0.49
1:A:298:GLN:HB2	1:A:387:TRP:HZ2	1.77	0.48
1:A:60:ARG:NH2	1:B:120:PHE:O	2.46	0.48
1:A:118:LEU:HD22	1:A:126:VAL:HG22	1.96	0.48
1:A:402:MET:SD	1:A:402:MET:N	2.87	0.47
1:A:203:PHE:HE2	1:A:302:LEU:HD11	1.79	0.47
1:A:92:PRO:HD3	1:A:337:GLN:HE21	1.78	0.47
1:A:193:SER:O	1:A:197:GLU:HG2	2.15	0.47
1:A:326:PHE:O	1:A:330:ILE:HG12	2.15	0.46
1:A:120:PHE:O	1:B:60:ARG:NH2	2.48	0.46
1:B:345:THR:O	1:B:348:LYS:NZ	2.39	0.46
1:B:384:VAL:HA	1:B:387:TRP:HB3	1.98	0.46
1:B:118:LEU:HD22	1:B:126:VAL:HG22	1.98	0.46
1:B:161:ILE:HG12	1:B:215:TRP:CH2	2.51	0.46
1:B:292:LEU:O	1:B:296:ILE:HG12	2.16	0.46
1:A:162:ILE:H	1:A:162:ILE:HG13	1.58	0.46
1:A:339:TYR:CE1	1:A:343:THR:HG21	2.51	0.45
1:B:184:ARG:NH2	1:B:241:GLU:OE2	2.47	0.45
1:B:402:MET:N	1:B:402:MET:SD	2.90	0.45
1:A:24:ILE:HA	1:A:24:ILE:HD13	1.69	0.45
1:A:125:GLN:NE2	1:B:68:ASN:HD22	2.14	0.45
1:B:178:MET:O	1:B:182:LEU:HD12	2.17	0.44
1:B:96:PRO:HD2	1:B:100:LEU:HD23	1.99	0.44
1:A:323:ARG:HH21	1:A:364:GLU:CD	2.25	0.43
1:A:113:LEU:HD11	1:B:80:PHE:HD1	1.83	0.43
1:B:308:LYS:HE3	1:B:308:LYS:HB2	1.75	0.43
7:A:510:T7X:O11	7:A:510:T7X:O6	2.36	0.43
1:A:68:ASN:HD22	1:B:125:GLN:NE2	2.16	0.43
7:B:501:T7X:O6	7:B:501:T7X:O11	2.37	0.43
1:B:240:LEU:O	1:B:245:TYR:OH	2.26	0.42
1:B:296:ILE:O	1:B:300:THR:HG23	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:PRO:HA	1:A:403:ILE:HG12	2.01	0.42
1:A:326:PHE:CE1	1:A:330:ILE:HD11	2.54	0.42
1:B:94:THR:HG22	1:B:98:PRO:HG3	2.01	0.42
1:A:289:GLY:O	1:A:338:TYR:OH	2.26	0.42
1:A:130:MET:HE1	1:A:311:PHE:HB3	2.02	0.42
1:A:294:MET:O	1:A:298:GLN:HG3	2.19	0.42
1:A:384:VAL:HG13	1:A:387:TRP:HE3	1.84	0.42
1:A:198:LEU:HD23	1:A:198:LEU:HA	1.90	0.42
1:A:42:THR:HG1	1:B:355:TRP:CD1	2.38	0.42
1:A:178:MET:HE3	1:A:178:MET:HB3	1.80	0.42
1:A:355:TRP:CD1	1:B:46:LEU:HD12	2.55	0.41
1:A:240:LEU:O	1:A:245:TYR:OH	2.30	0.41
1:A:384:VAL:HA	1:A:387:TRP:HB3	2.01	0.41
1:B:234:MET:HE3	1:B:234:MET:HB3	1.76	0.41
1:B:388:LEU:HD23	1:B:388:LEU:H	1.85	0.41
1:A:293:PHE:HB2	1:A:338:TYR:CE2	2.56	0.41
1:B:280:PRO:HA	1:B:403:ILE:HG12	2.03	0.41
1:B:122:ASN:OD1	1:B:122:ASN:N	2.37	0.41
1:B:162:ILE:H	1:B:162:ILE:HG13	1.59	0.41
1:A:17:TYR:OH	1:B:40:PRO:HG3	2.21	0.40
1:B:213:CYS:HB3	1:B:215:TRP:HD1	1.86	0.40
1:B:339:TYR:CE1	1:B:343:THR:HG21	2.56	0.40
1:A:44:THR:OG1	3:A:511:LBN:O3	2.31	0.40
1:A:37:PHE:CE2	2:A:502:PSF:H42	2.56	0.40
1:A:345:THR:HG23	1:A:346:GLN:HG2	2.03	0.40
1:A:366:ILE:HD11	1:B:50:ILE:HG23	2.04	0.40
1:B:206:LEU:HD23	1:B:206:LEU:HA	1.89	0.40
1:B:384:VAL:HG13	1:B:387:TRP:HE3	1.84	0.40
1:B:206:LEU:HD11	1:B:306:PHE:HE1	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	373/473 (79%)	364 (98%)	9 (2%)	0	100	100
1	B	373/473 (79%)	365 (98%)	8 (2%)	0	100	100
All	All	746/946 (79%)	729 (98%)	17 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 22 ligands modelled in this entry, 2 are monoatomic - leaving 20 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	$\# Z > 2$
3	LBN	A	507	-	51,51,51	0.48	0	57,59,59	0.57	1 (1%)
4	D12	A	505	-	11,11,11	0.22	0	10,10,10	0.29	0
2	PSF	A	501	-	28,29,29	0.74	0	30,36,36	1.05	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PSF	B	503	-	28,29,29	0.74	0	30,36,36	1.00	1 (3%)
5	C14	A	506	-	13,13,13	0.22	0	12,12,12	0.27	0
3	LBN	B	506	-	31,31,51	0.59	0	37,39,59	0.52	0
3	LBN	A	503	-	51,51,51	0.46	0	57,59,59	0.49	1 (1%)
3	LBN	B	505	-	51,51,51	0.46	0	57,59,59	0.49	1 (1%)
3	LBN	A	504	-	31,31,51	0.59	0	37,39,59	0.52	0
3	LBN	A	511	-	37,37,51	0.54	0	43,45,59	0.53	0
5	C14	B	508	-	13,13,13	0.22	0	12,12,12	0.28	0
2	PSF	A	502	-	28,29,29	0.73	0	30,36,36	0.95	1 (3%)
3	LBN	B	502	-	37,37,51	0.54	0	43,45,59	0.53	0
7	T7X	B	501	-	50,50,61	0.57	0	59,62,73	0.94	3 (5%)
7	T7X	A	510	-	50,50,61	0.57	0	59,62,73	0.93	4 (6%)
3	LBN	B	509	-	51,51,51	0.48	0	57,59,59	0.58	1 (1%)
3	LBN	A	508	-	45,45,51	0.49	0	51,53,59	0.51	0
2	PSF	B	504	-	28,29,29	0.73	0	30,36,36	0.84	1 (3%)
4	D12	B	507	-	11,11,11	0.22	0	10,10,10	0.29	0
3	LBN	B	510	-	45,45,51	0.49	0	51,53,59	0.50	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LBN	A	507	-	-	26/55/55/55	-
4	D12	A	505	-	-	0/9/9/9	-
2	PSF	A	501	-	-	7/35/35/35	-
2	PSF	B	503	-	-	11/35/35/35	-
5	C14	A	506	-	-	3/11/11/11	-
3	LBN	B	506	-	-	16/35/35/55	-
3	LBN	A	503	-	-	21/55/55/55	-
3	LBN	B	505	-	-	23/55/55/55	-
3	LBN	A	504	-	-	16/35/35/55	-
3	LBN	A	511	-	-	13/41/41/55	-
5	C14	B	508	-	-	3/11/11/11	-
2	PSF	A	502	-	-	15/35/35/35	-
3	LBN	B	502	-	-	16/41/41/55	-
7	T7X	B	501	-	-	9/45/69/80	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	T7X	A	510	-	-	8/45/69/80	0/1/1/1
3	LBN	B	509	-	-	21/55/55/55	-
3	LBN	A	508	-	-	18/49/49/55	-
2	PSF	B	504	-	-	9/35/35/35	-
4	D12	B	507	-	-	0/9/9/9	-
3	LBN	B	510	-	-	17/49/49/55	-

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	PSF	O1-CB-CA	4.82	112.26	108.06
2	B	503	PSF	O1-CB-CA	4.48	111.97	108.06
2	A	502	PSF	O1-CB-CA	4.02	111.56	108.06
2	B	504	PSF	O1-CB-CA	3.32	110.95	108.06
7	B	501	T7X	C6-C5-C4	2.86	115.84	110.83
7	A	510	T7X	C6-C5-C4	2.82	115.78	110.83
7	A	510	T7X	C4-C3-C2	2.79	115.74	110.83
7	B	501	T7X	C4-C3-C2	2.76	115.67	110.83
7	B	501	T7X	O1-C1-C6	2.56	114.14	108.73
7	A	510	T7X	O1-C1-C6	2.54	114.11	108.73
3	B	509	LBN	C2-O7-C34	2.52	123.83	117.80
3	A	507	LBN	C2-O7-C34	2.43	123.62	117.80
7	A	510	T7X	C5-C4-C3	2.07	114.46	110.83
3	A	503	LBN	C2-O7-C34	2.06	122.73	117.80
3	B	505	LBN	C2-O7-C34	2.05	122.70	117.80

There are no chirality outliers.

All (252) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	PSF	C6-C5-O52-C4
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	C2-O2-P-O4
2	A	502	PSF	CB-O1-P-O4
2	A	502	PSF	CB-O1-P-O3
2	B	503	PSF	C2-O2-P-O1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	B	503	PSF	C2-O2-P-O3
2	B	503	PSF	C6-C5-O52-C4
2	B	503	PSF	N-CA-CB-O1
2	B	503	PSF	C-CA-CB-O1
2	B	503	PSF	OT1-C-CA-CB
2	B	503	PSF	OT2-C-CA-CB
2	B	504	PSF	C2-O2-P-O1
2	B	504	PSF	C2-O2-P-O4
2	B	504	PSF	C2-O2-P-O3
2	B	504	PSF	OT1-C-CA-CB
2	B	504	PSF	OT2-C-CA-CB
3	A	503	LBN	C9-O2-P1-O1
3	A	503	LBN	C9-O2-P1-O4
3	A	503	LBN	C3-C2-O7-C34
3	A	503	LBN	C35-C34-O7-C2
3	A	504	LBN	C1-O1-P1-O2
3	A	504	LBN	C1-O1-P1-O3
3	A	504	LBN	C1-O1-P1-O4
3	A	504	LBN	C9-O2-P1-O1
3	A	504	LBN	C9-O2-P1-O4
3	A	504	LBN	N1-C6-C9-O2
3	A	507	LBN	C1-O1-P1-O3
3	A	507	LBN	C1-O1-P1-O4
3	A	507	LBN	C9-O2-P1-O1
3	A	507	LBN	C9-O2-P1-O3
3	A	507	LBN	C9-O2-P1-O4
3	A	508	LBN	C1-O1-P1-O2
3	A	508	LBN	C1-O1-P1-O4
3	A	508	LBN	N1-C6-C9-O2
3	A	511	LBN	C9-O2-P1-O1
3	A	511	LBN	C9-O2-P1-O4
3	A	511	LBN	N1-C6-C9-O2
3	B	502	LBN	C1-O1-P1-O2
3	B	502	LBN	C1-O1-P1-O3
3	B	502	LBN	C9-O2-P1-O1
3	B	502	LBN	C9-O2-P1-O3
3	B	502	LBN	C9-O2-P1-O4
3	B	502	LBN	N1-C6-C9-O2
3	B	505	LBN	C9-O2-P1-O1
3	B	505	LBN	C9-O2-P1-O4
3	B	505	LBN	C3-C2-O7-C34
3	B	505	LBN	C35-C34-O7-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	B	506	LBN	C1-O1-P1-O2
3	B	506	LBN	C1-O1-P1-O3
3	B	506	LBN	C9-O2-P1-O4
3	B	506	LBN	N1-C6-C9-O2
3	B	509	LBN	C1-O1-P1-O3
3	B	509	LBN	C1-O1-P1-O4
3	B	509	LBN	C9-O2-P1-O1
3	B	509	LBN	C9-O2-P1-O3
3	B	509	LBN	C9-O2-P1-O4
3	B	510	LBN	C1-O1-P1-O2
3	B	510	LBN	C1-O1-P1-O4
3	B	510	LBN	N1-C6-C9-O2
7	A	510	T7X	C2-C1-O1-P1
7	A	510	T7X	C22-C23-C24-C25
7	B	501	T7X	C2-C1-O1-P1
2	A	501	PSF	O51-C5-O52-C4
2	B	503	PSF	O51-C5-O52-C4
3	A	507	LBN	C26-C25-O5-C3
3	B	509	LBN	C26-C25-O5-C3
3	A	507	LBN	O6-C25-O5-C3
3	B	509	LBN	O6-C25-O5-C3
3	A	503	LBN	O8-C34-O7-C2
3	B	505	LBN	O8-C34-O7-C2
3	B	505	LBN	C31-C32-C33-C4
2	A	502	PSF	C6-C5-O52-C4
2	A	502	PSF	C13-C1-O11-C3
2	B	504	PSF	C13-C1-O11-C3
2	A	502	PSF	O51-C5-O52-C4
3	A	503	LBN	C31-C32-C33-C4
2	B	504	PSF	O12-C1-O11-C3
3	A	508	LBN	C26-C25-O5-C3
3	B	510	LBN	C26-C25-O5-C3
3	A	508	LBN	C35-C36-C37-C38
2	A	502	PSF	O12-C1-O11-C3
3	B	510	LBN	C34-C35-C36-C37
3	A	508	LBN	C34-C35-C36-C37
3	B	506	LBN	C34-C35-C36-C37
3	B	510	LBN	C35-C36-C37-C38
3	B	510	LBN	O6-C25-O5-C3
7	A	510	T7X	C6-C1-O1-P1
3	A	508	LBN	O6-C25-O5-C3
3	A	504	LBN	C34-C35-C36-C37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	B	506	LBN	C35-C34-O7-C2
3	A	507	LBN	C34-C35-C36-C37
3	A	503	LBN	C7-C10-C13-C16
3	A	511	LBN	C7-C10-C13-C16
3	B	502	LBN	C7-C10-C13-C16
3	B	506	LBN	O8-C34-O7-C2
3	A	507	LBN	C28-C29-C30-C31
3	A	504	LBN	C35-C34-O7-C2
7	A	510	T7X	C12-C13-C14-C15
3	B	502	LBN	C26-C25-O5-C3
3	A	511	LBN	C26-C25-O5-C3
2	A	501	PSF	C13-C14-C15-C16
3	B	510	LBN	C42-C5-C8-C11
3	B	509	LBN	C17-C20-C22-C23
3	A	508	LBN	C35-C34-O7-C2
3	B	510	LBN	C35-C34-O7-C2
3	A	508	LBN	O8-C34-O7-C2
7	B	501	T7X	C12-C13-C14-C15
2	B	503	PSF	C13-C14-C15-C16
3	B	510	LBN	O8-C34-O7-C2
3	B	509	LBN	C8-C11-C14-C17
3	A	507	LBN	C17-C20-C22-C23
3	A	507	LBN	C30-C31-C32-C33
3	A	508	LBN	C42-C5-C8-C11
3	B	505	LBN	C13-C10-C7-C4
3	B	502	LBN	O6-C25-O5-C3
3	A	511	LBN	C13-C10-C7-C4
3	A	511	LBN	O6-C25-O5-C3
3	A	503	LBN	O1-C1-C2-C3
3	B	505	LBN	O1-C1-C2-C3
3	A	504	LBN	O8-C34-O7-C2
3	A	507	LBN	C8-C11-C14-C17
3	A	503	LBN	C33-C4-C7-C10
3	B	509	LBN	C38-C39-C40-C41
3	A	504	LBN	C1-C2-C3-O5
5	A	506	C14	C03-C04-C05-C06
5	A	506	C14	C04-C05-C06-C07
5	B	508	C14	C04-C05-C06-C07
3	A	503	LBN	C13-C10-C7-C4
3	B	506	LBN	C37-C38-C39-C40
5	B	508	C14	C03-C04-C05-C06
3	B	506	LBN	C26-C25-O5-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	B	502	LBN	C13-C10-C7-C4
7	A	510	T7X	C32-C33-C34-C35
3	B	510	LBN	C29-C30-C31-C32
3	A	508	LBN	C29-C30-C31-C32
7	B	501	T7X	C32-C33-C34-C35
7	B	501	T7X	C6-C1-O1-P1
2	A	502	PSF	O2-C2-C3-C4
3	B	509	LBN	C29-C30-C31-C32
3	B	505	LBN	C33-C4-C7-C10
3	A	503	LBN	C1-C2-C3-O5
3	B	505	LBN	C1-C2-C3-O5
3	B	506	LBN	C1-C2-C3-O5
3	A	504	LBN	C26-C27-C28-C29
2	A	502	PSF	OT1-C-CA-N
3	B	509	LBN	O1-C1-C2-O7
3	B	505	LBN	C7-C10-C13-C16
3	A	511	LBN	C31-C32-C33-C4
3	A	507	LBN	O7-C2-C3-O5
3	B	509	LBN	O7-C2-C3-O5
7	B	501	T7X	C22-C23-C24-C25
3	B	506	LBN	C36-C37-C38-C39
3	A	504	LBN	C26-C25-O5-C3
7	B	501	T7X	C31-C32-C33-C34
3	A	504	LBN	C37-C38-C39-C40
7	A	510	T7X	C31-C32-C33-C34
3	B	502	LBN	C33-C4-C7-C10
3	B	506	LBN	O6-C25-O5-C3
2	B	503	PSF	O2-C2-C3-O11
3	A	507	LBN	O1-C1-C2-O7
3	A	503	LBN	O7-C2-C3-O5
3	B	505	LBN	O7-C2-C3-O5
3	B	506	LBN	O7-C2-C3-O5
3	A	507	LBN	C11-C14-C17-C20
3	A	504	LBN	O6-C25-O5-C3
3	A	504	LBN	C36-C37-C38-C39
3	B	505	LBN	C32-C33-C4-C7
3	B	502	LBN	C31-C32-C33-C4
3	A	503	LBN	C42-C5-C8-C11
3	B	505	LBN	C42-C5-C8-C11
3	A	503	LBN	C32-C33-C4-C7
2	A	502	PSF	O2-C2-C3-O11
2	B	504	PSF	O2-C2-C3-O11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	A	503	LBN	O1-C1-C2-O7
3	A	504	LBN	O7-C2-C3-O5
2	A	502	PSF	C2-O2-P-O1
2	A	502	PSF	C2-O2-P-O3
2	A	502	PSF	CB-O1-P-O2
3	A	503	LBN	C9-O2-P1-O3
3	A	507	LBN	C1-O1-P1-O2
3	A	508	LBN	C1-O1-P1-O3
3	A	508	LBN	C9-O2-P1-O4
3	A	511	LBN	C9-O2-P1-O3
3	B	505	LBN	C9-O2-P1-O3
3	B	506	LBN	C1-O1-P1-O4
3	B	506	LBN	C9-O2-P1-O1
3	B	509	LBN	C1-O1-P1-O2
3	B	510	LBN	C1-O1-P1-O3
3	B	509	LBN	C2-C1-O1-P1
3	A	511	LBN	C33-C4-C7-C10
3	A	507	LBN	C13-C10-C7-C4
3	A	508	LBN	C1-C2-O7-C34
3	B	510	LBN	C1-C2-O7-C34
2	B	503	PSF	O2-C2-C3-C4
3	B	505	LBN	O1-C1-C2-O7
3	A	511	LBN	C26-C27-C28-C29
3	A	503	LBN	C26-C25-O5-C3
3	A	503	LBN	O6-C25-O5-C3
3	A	508	LBN	C30-C31-C32-C33
3	B	510	LBN	C30-C31-C32-C33
3	B	505	LBN	C10-C13-C16-C19
3	B	505	LBN	C26-C25-O5-C3
3	A	507	LBN	C2-C1-O1-P1
3	B	509	LBN	C28-C29-C30-C31
3	B	506	LBN	C26-C27-C28-C29
5	B	508	C14	C05-C06-C07-C08
3	A	507	LBN	C1-C2-O7-C34
3	B	509	LBN	C1-C2-O7-C34
3	B	509	LBN	C42-C5-C8-C11
3	A	507	LBN	C29-C30-C31-C32
3	B	509	LBN	C11-C14-C17-C20
5	A	506	C14	C05-C06-C07-C08
3	A	507	LBN	C42-C5-C8-C11
3	A	503	LBN	C17-C20-C22-C23
3	B	502	LBN	C10-C13-C16-C19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	B	505	LBN	O6-C25-O5-C3
2	A	502	PSF	OT2-C-CA-N
3	A	511	LBN	C10-C13-C16-C19
3	B	505	LBN	C26-C27-C28-C29
3	B	502	LBN	O5-C25-C26-C27
3	B	505	LBN	C17-C20-C22-C23
3	A	508	LBN	C17-C20-C22-C23
3	B	509	LBN	C13-C10-C7-C4
2	B	504	PSF	O2-C2-C3-C4
7	B	501	T7X	O13-C7-C8-C9
7	A	510	T7X	C1-O1-P1-O11
7	B	501	T7X	C1-O1-P1-O11
3	A	507	LBN	C2-C3-O5-C25
3	A	507	LBN	C32-C33-C4-C7
3	B	505	LBN	C36-C37-C38-C39
3	B	502	LBN	C34-C35-C36-C37
3	A	507	LBN	O7-C34-C35-C36
3	A	503	LBN	C36-C37-C38-C39
3	B	505	LBN	C29-C30-C31-C32
7	A	510	T7X	C33-C34-C35-C36
3	B	510	LBN	C17-C20-C22-C23
3	A	507	LBN	C38-C39-C40-C41
2	A	502	PSF	O11-C3-C4-O52
7	B	501	T7X	C33-C34-C35-C36
3	A	511	LBN	O5-C25-C26-C27
3	A	503	LBN	C29-C30-C31-C32
3	B	502	LBN	C26-C27-C28-C29
3	A	507	LBN	O8-C34-C35-C36
3	A	508	LBN	O7-C34-C35-C36
3	B	510	LBN	O7-C34-C35-C36
3	B	509	LBN	C2-C3-O5-C25
3	B	510	LBN	O5-C25-C26-C27
3	A	508	LBN	O5-C25-C26-C27

There are no ring outliers.

6 monomers are involved in 10 short contacts:

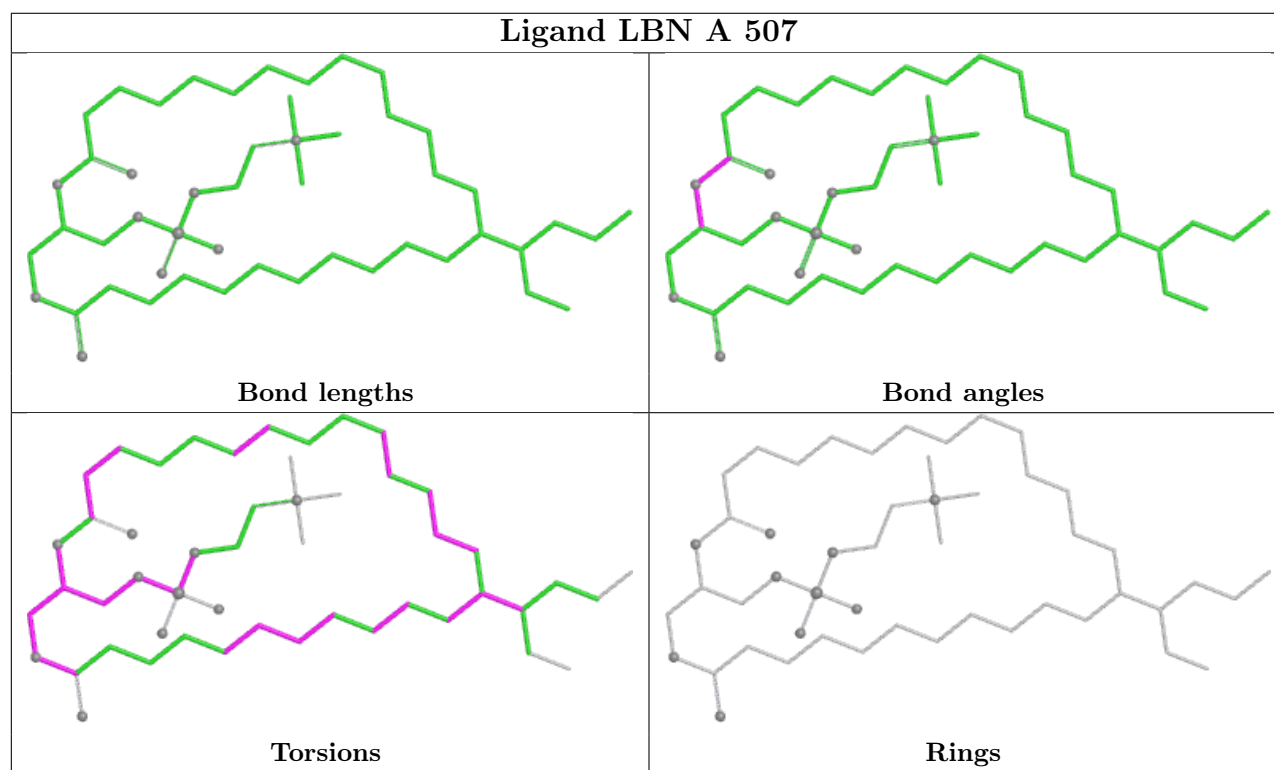
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	PSF	2	0
2	B	503	PSF	2	0
3	A	511	LBN	1	0
2	A	502	PSF	3	0

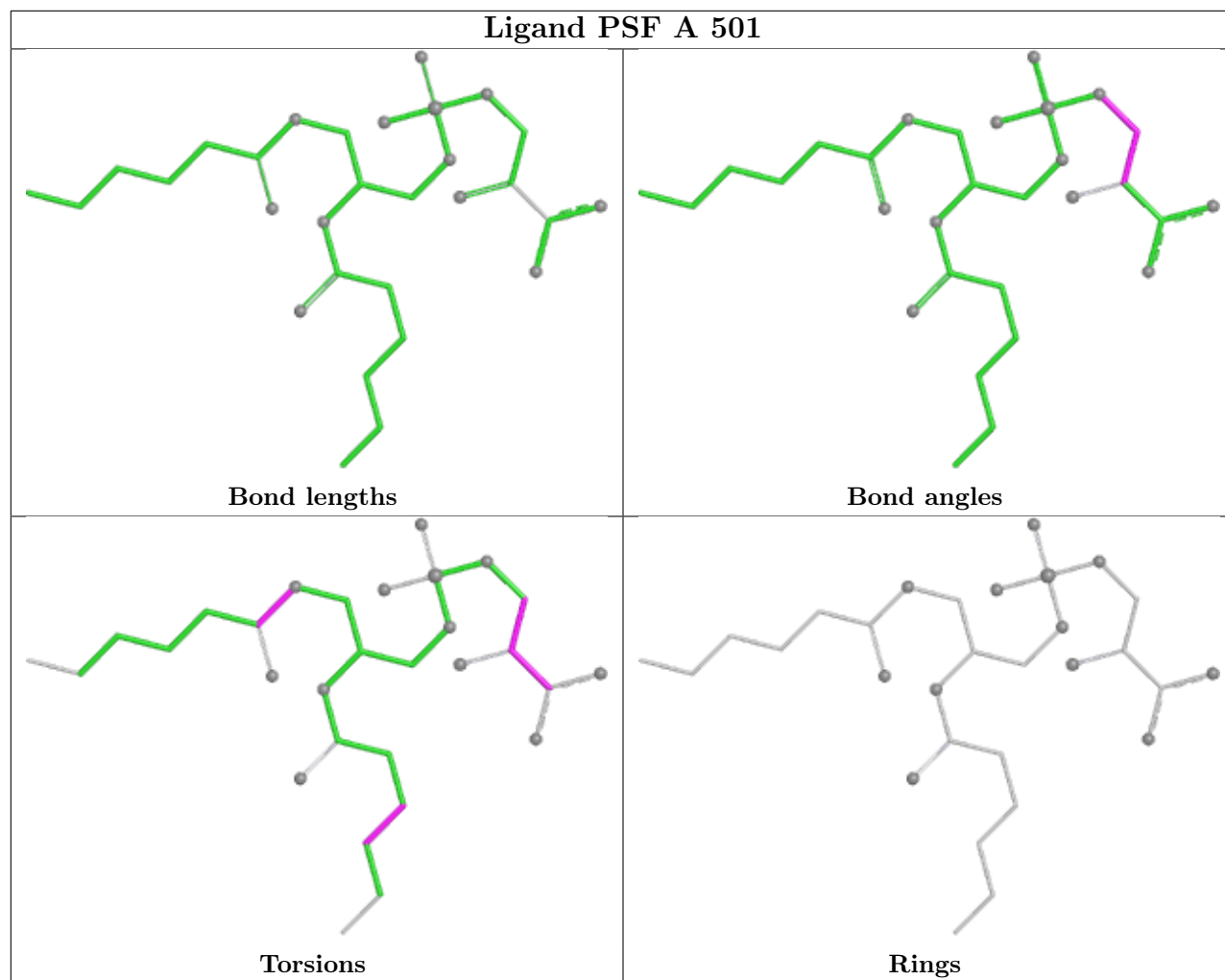
Continued on next page...

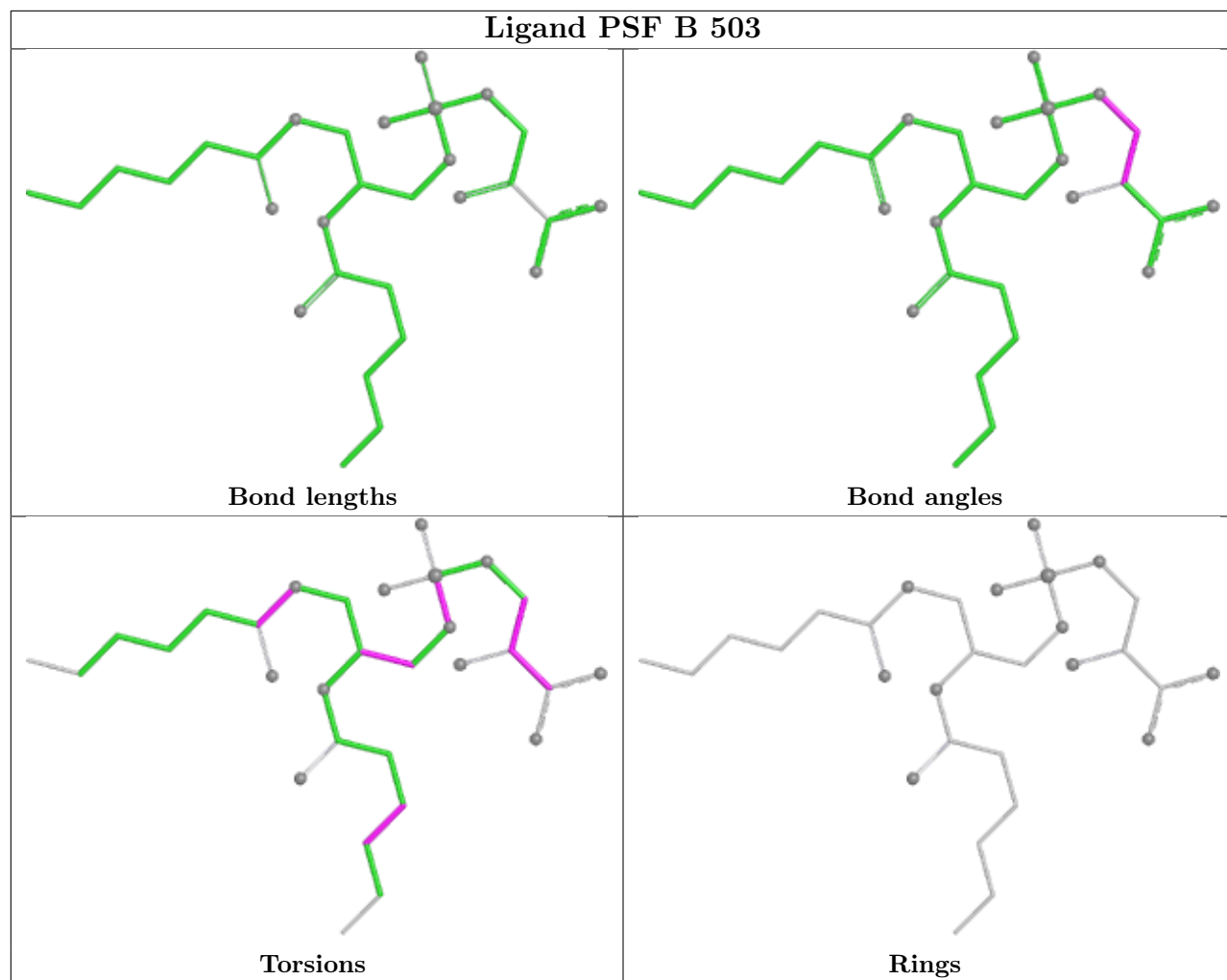
Continued from previous page...

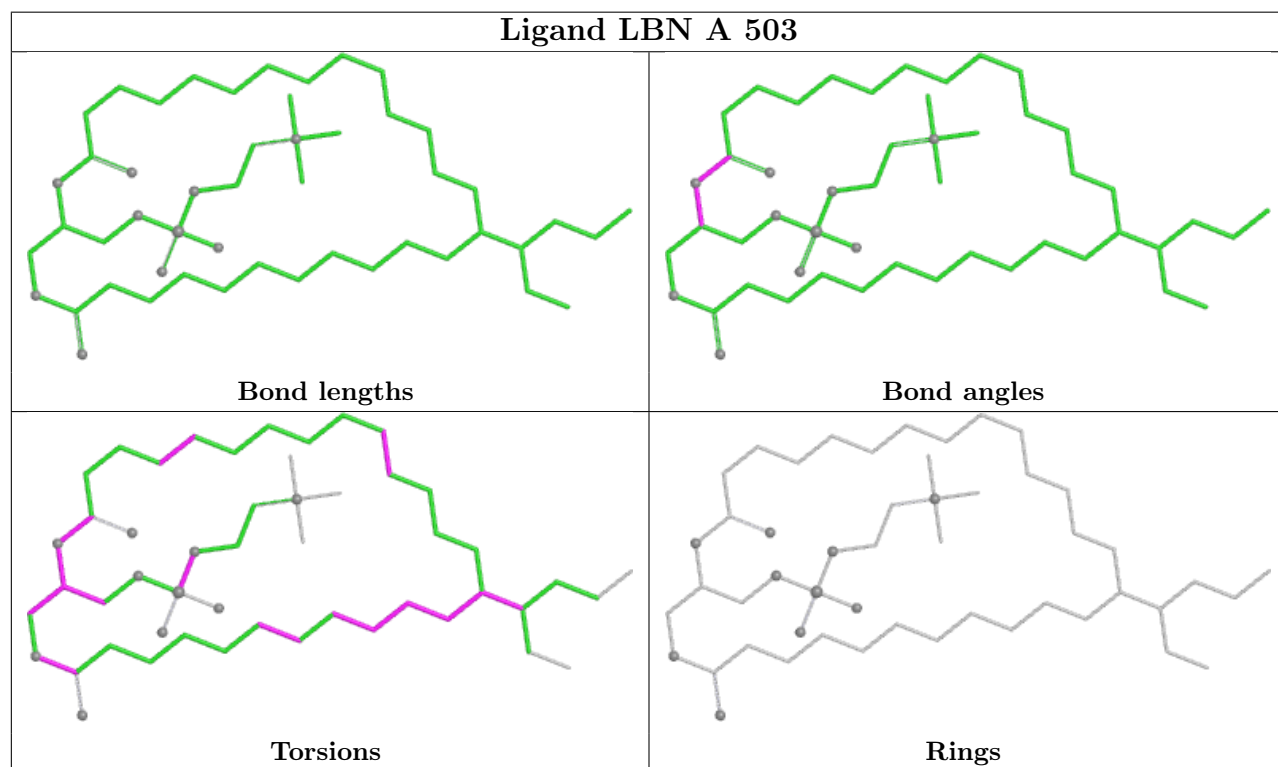
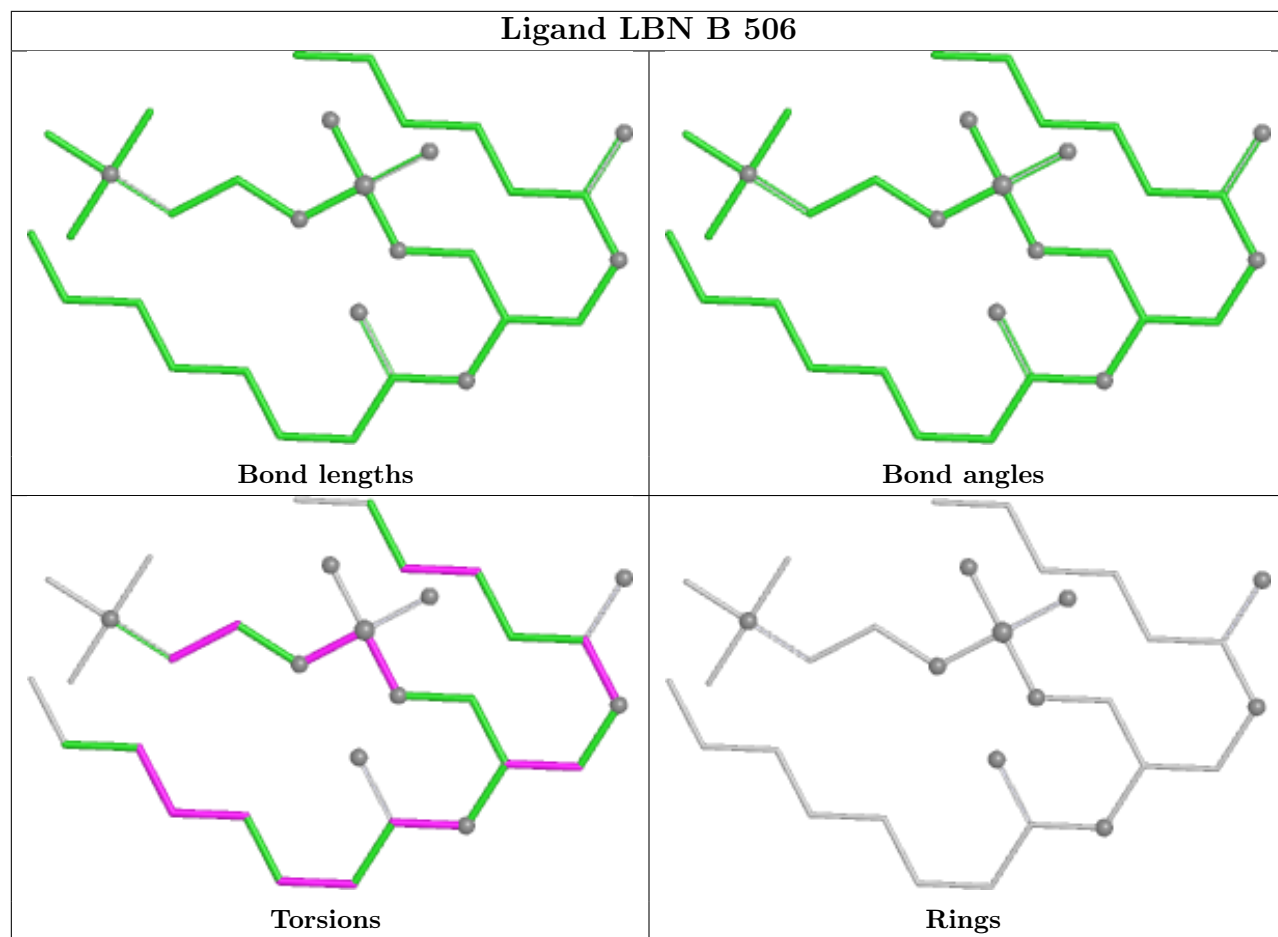
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	501	T7X	1	0
7	A	510	T7X	1	0

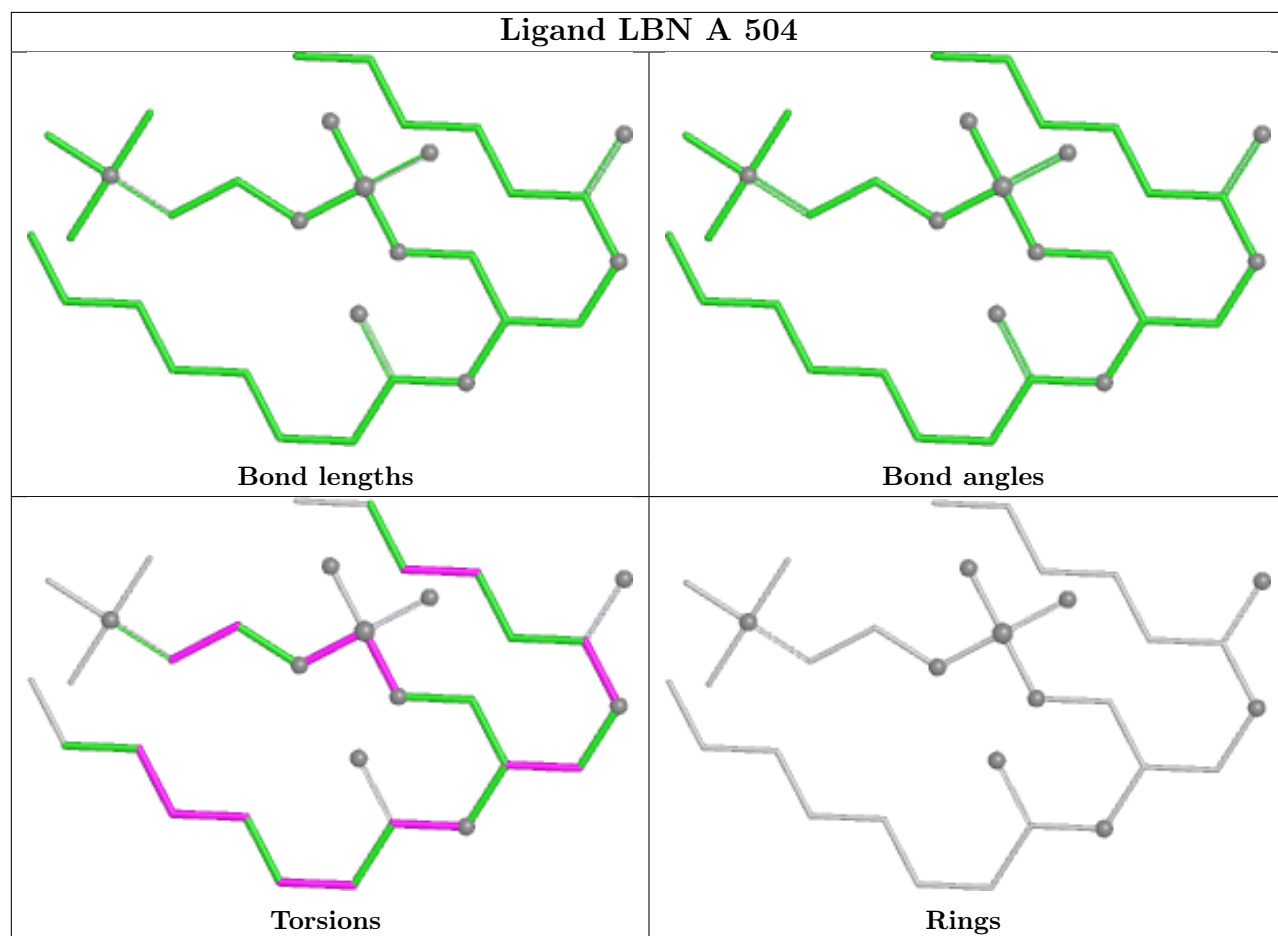
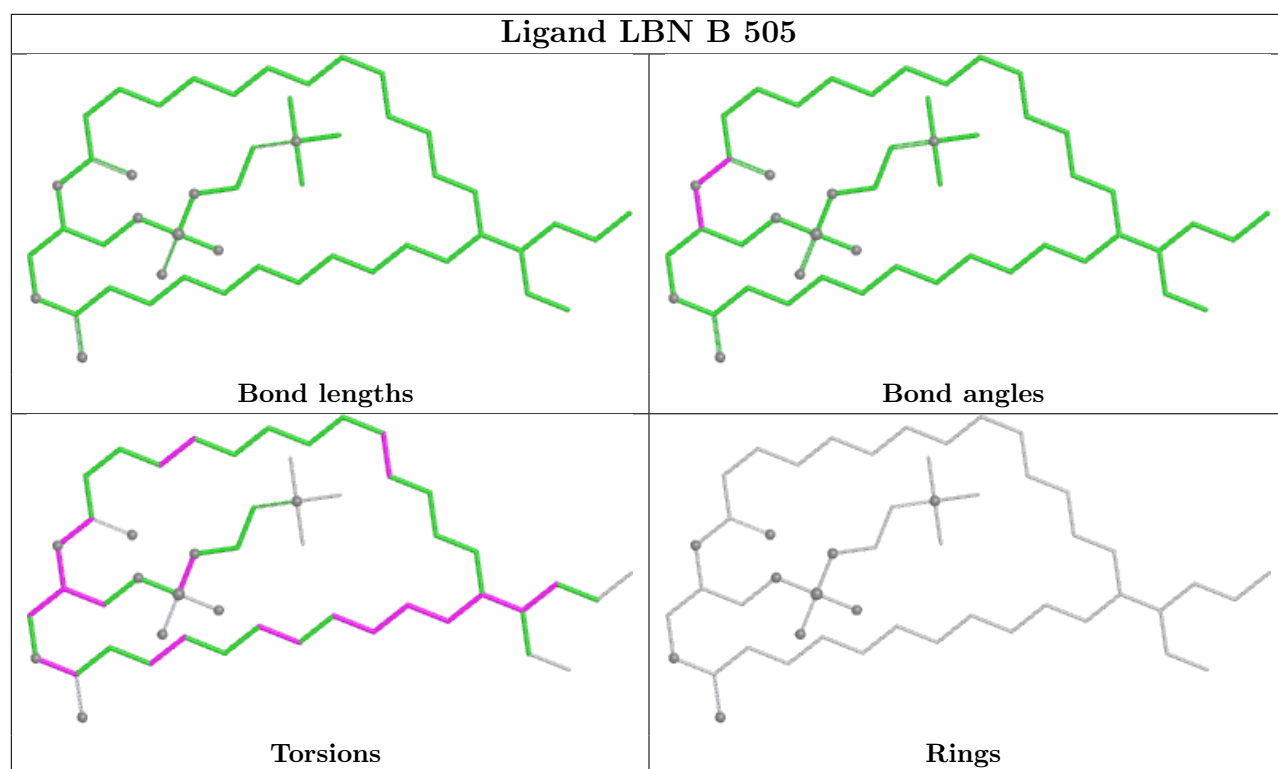
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

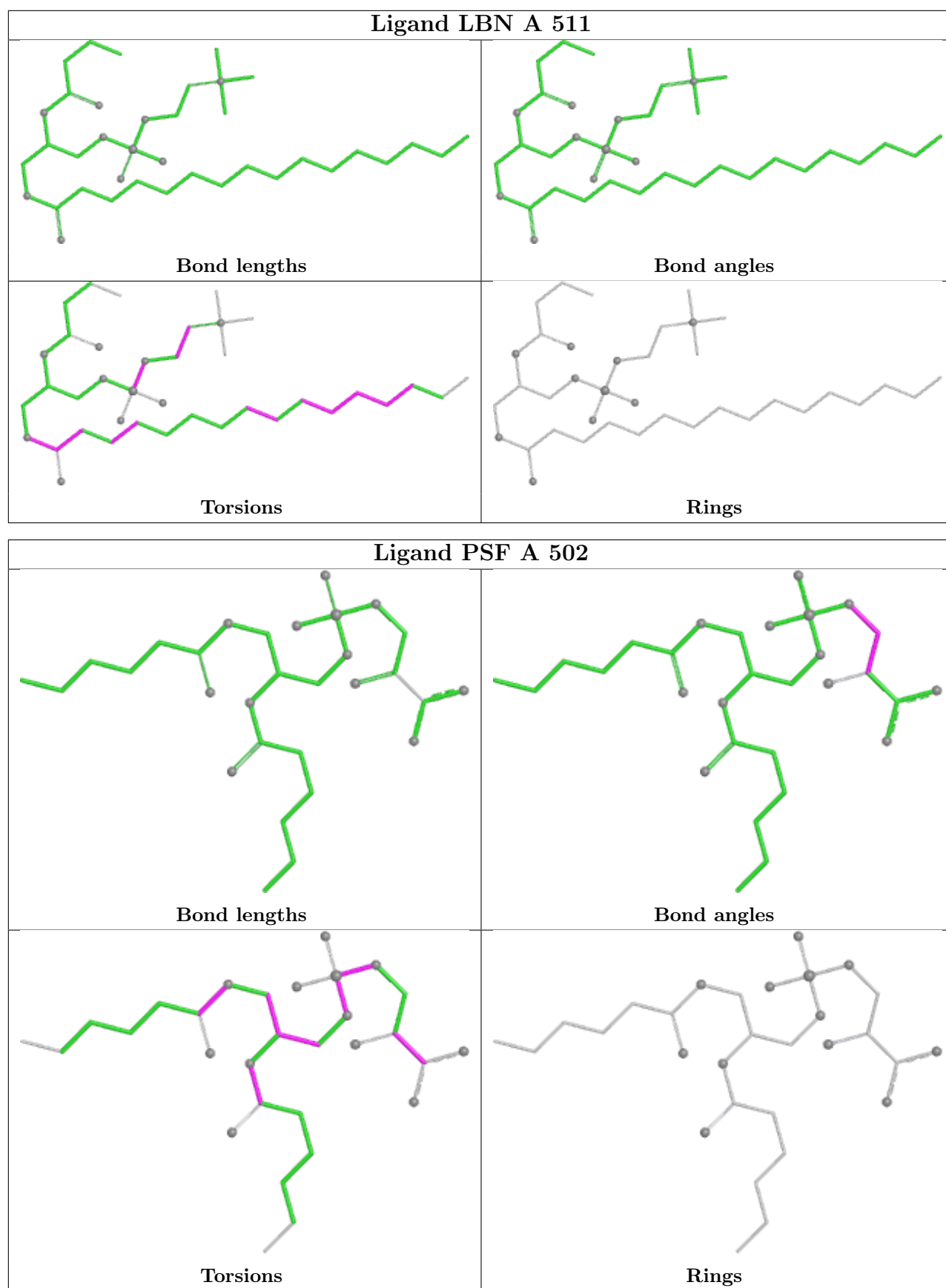


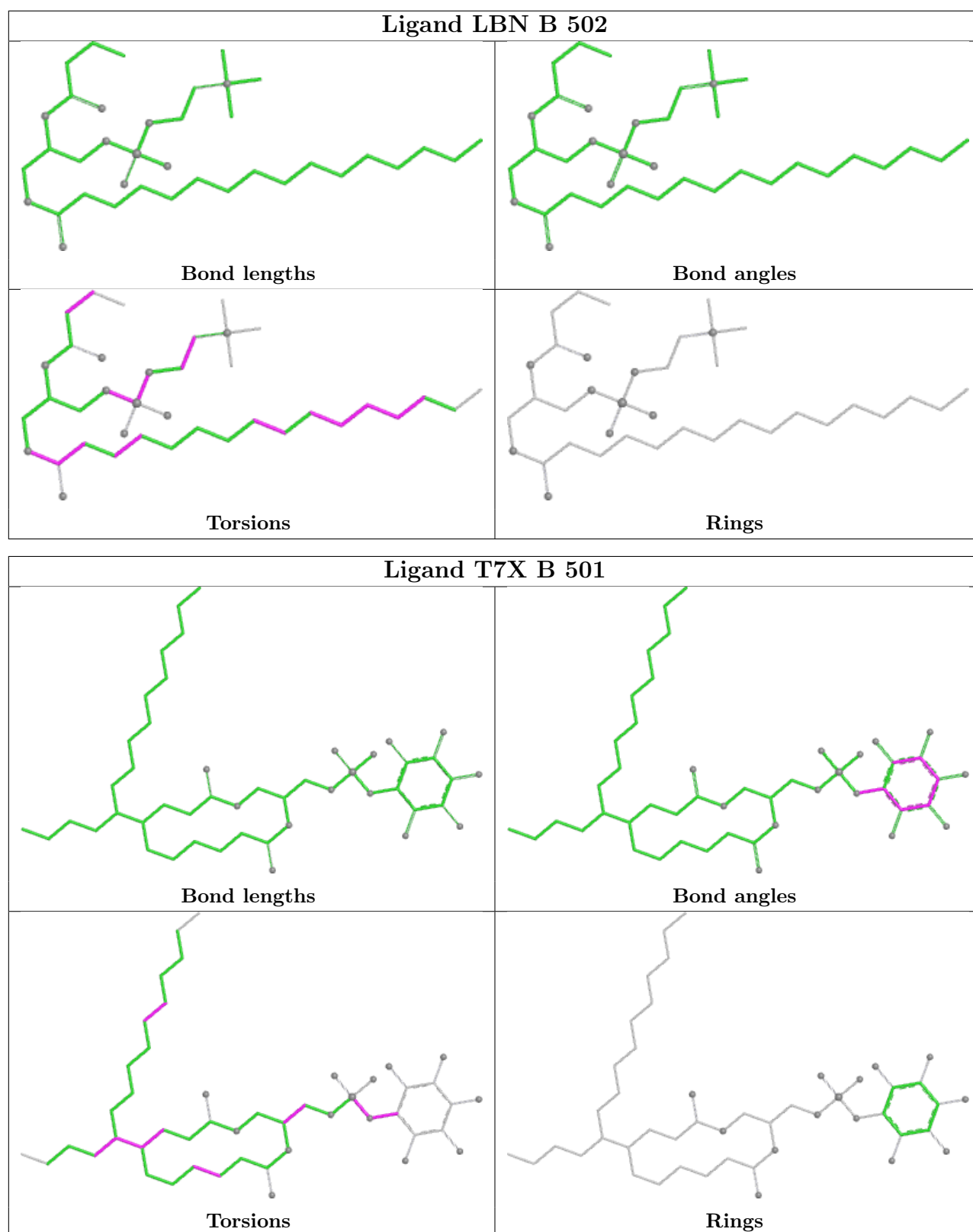




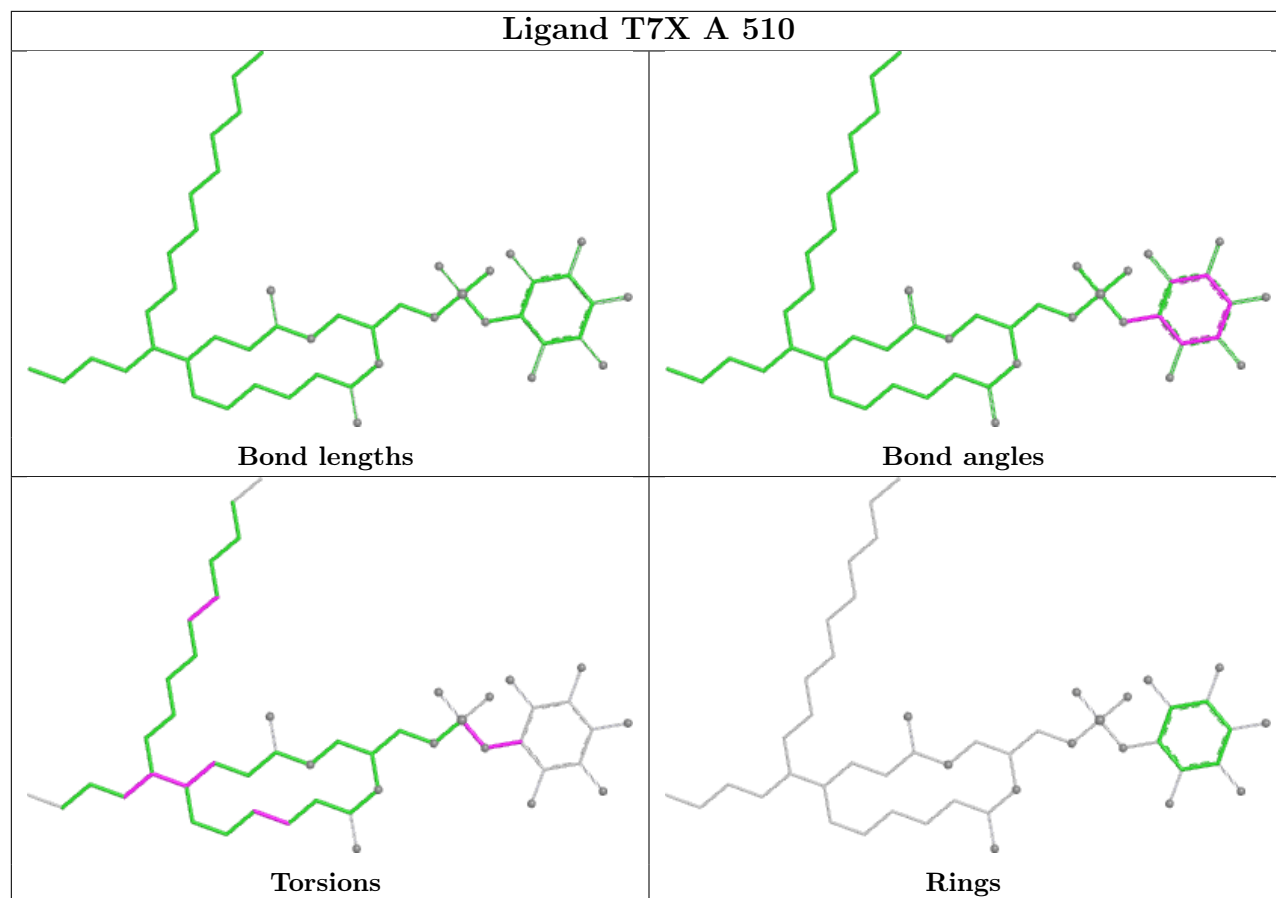




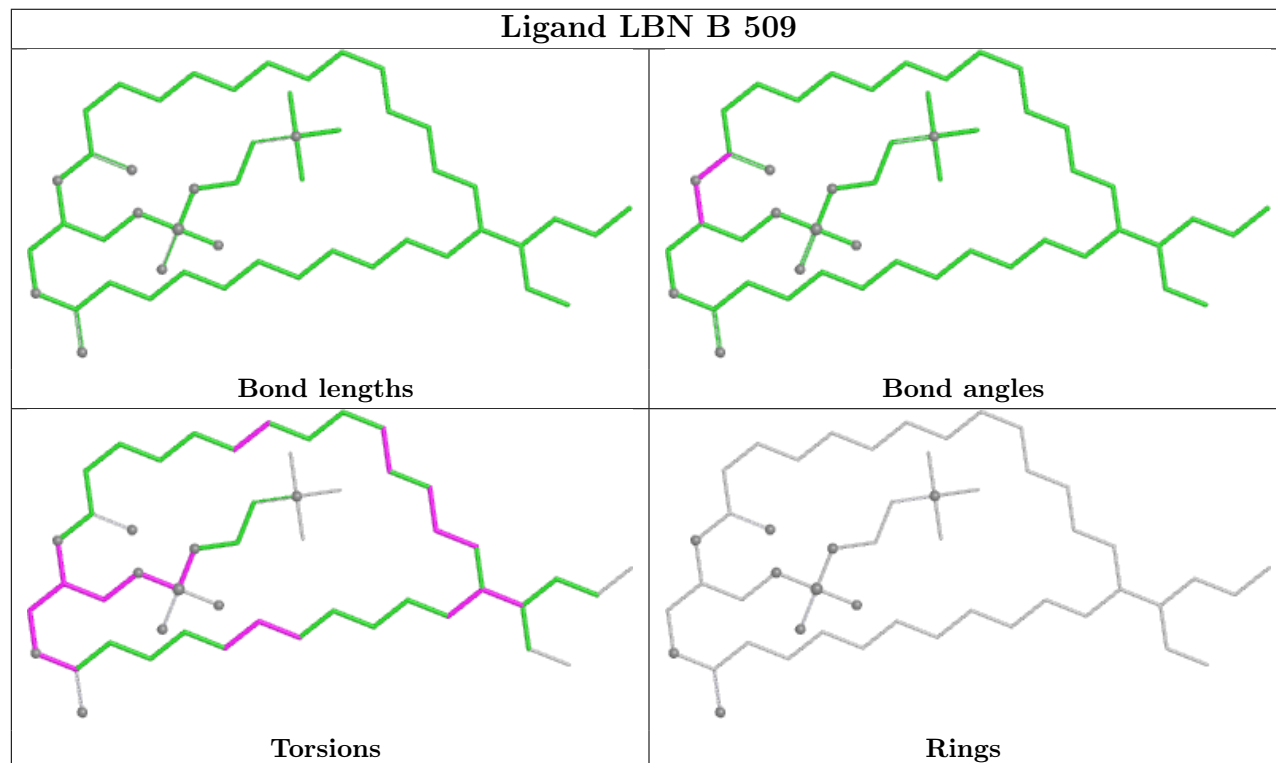


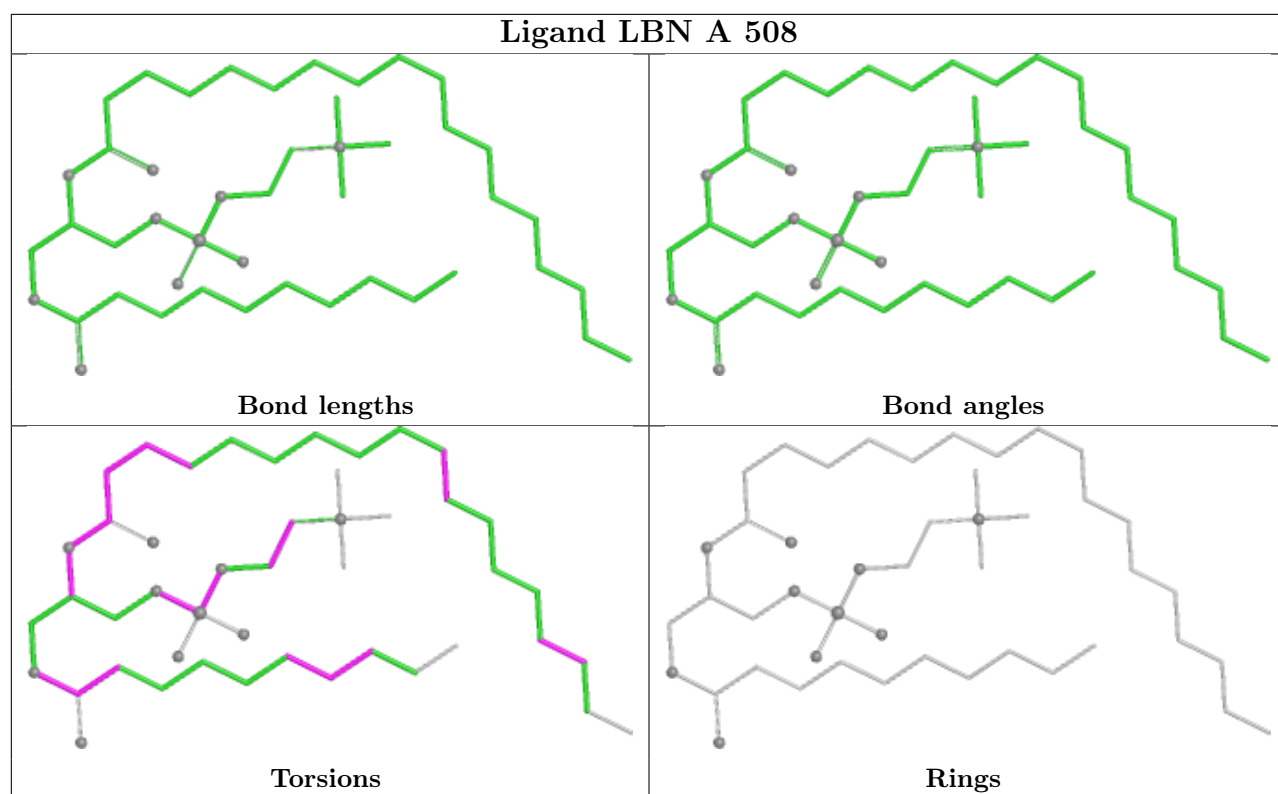


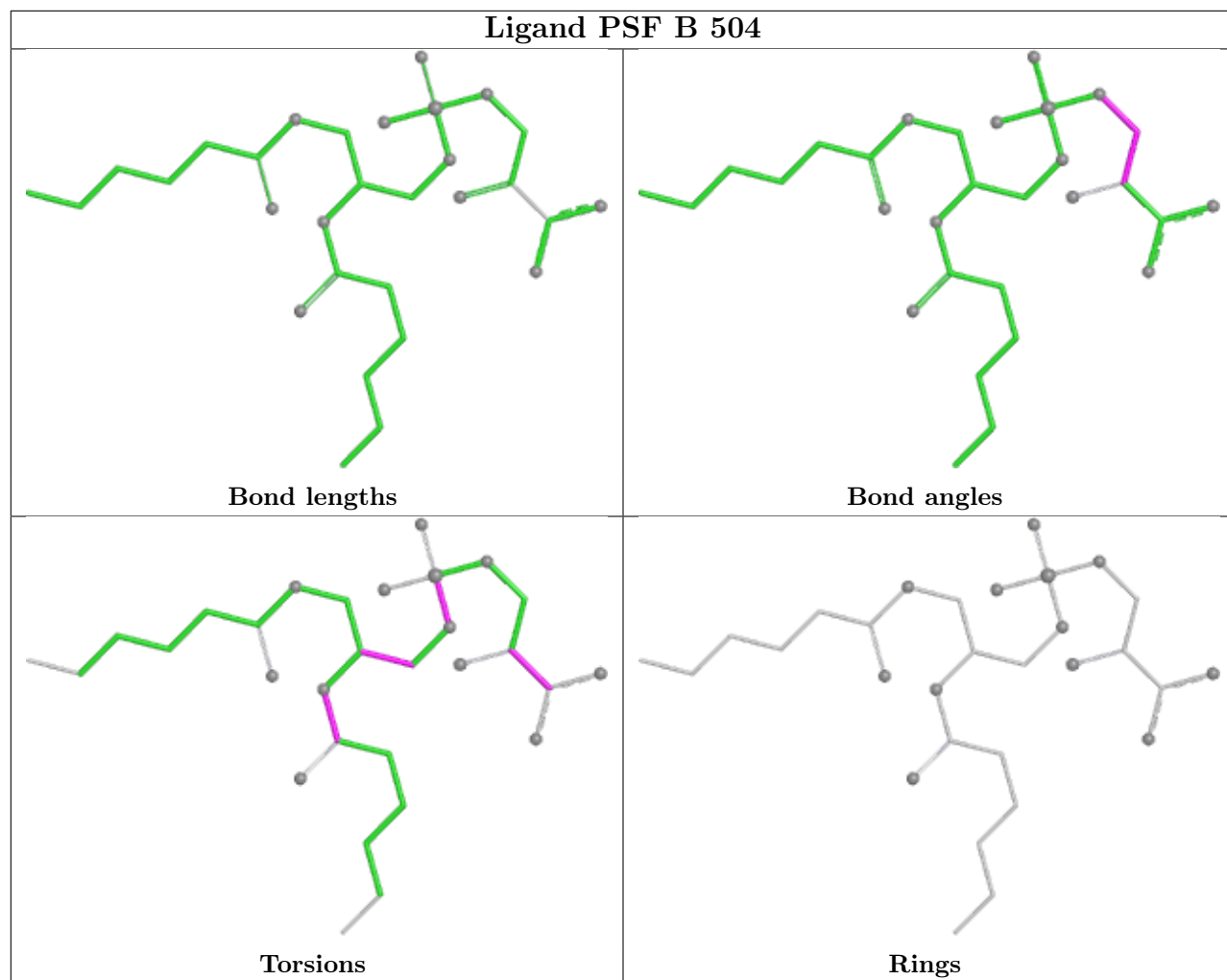
Ligand T7X A 510

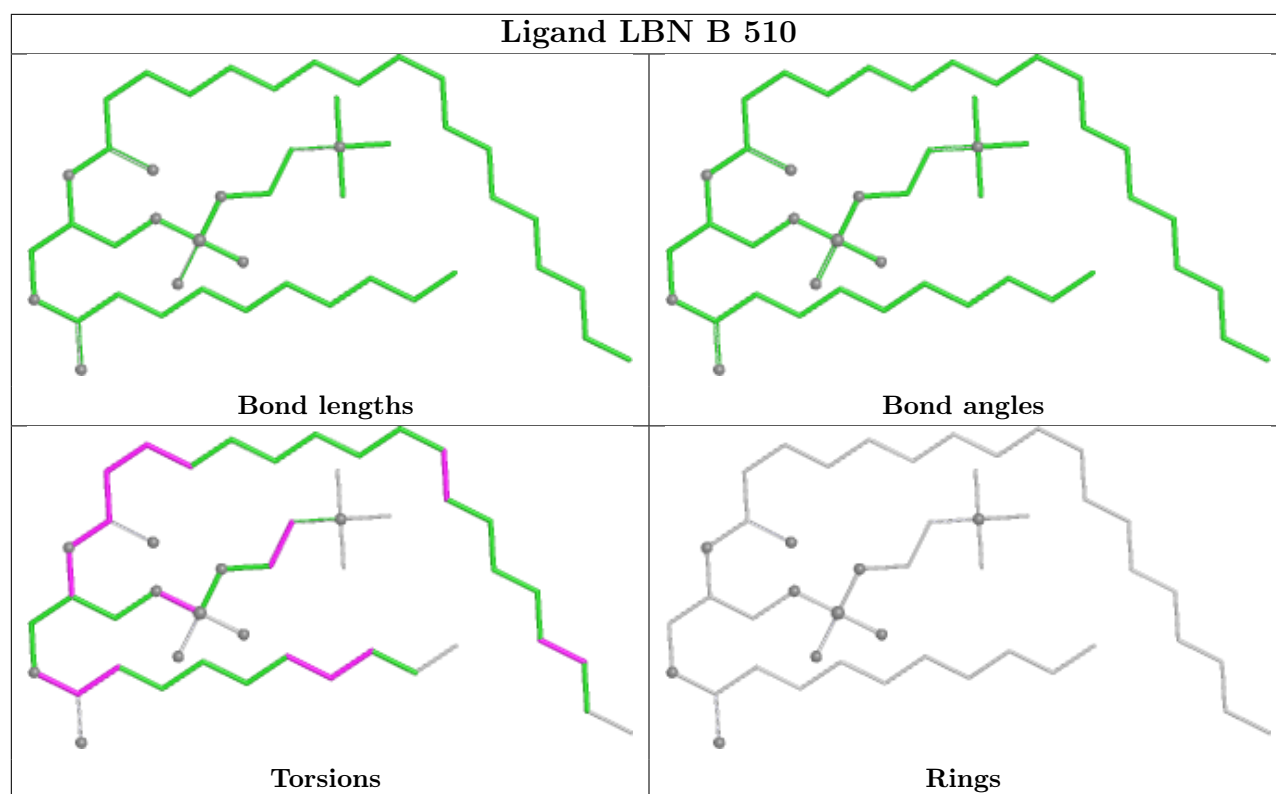


Ligand LBN B 509









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.

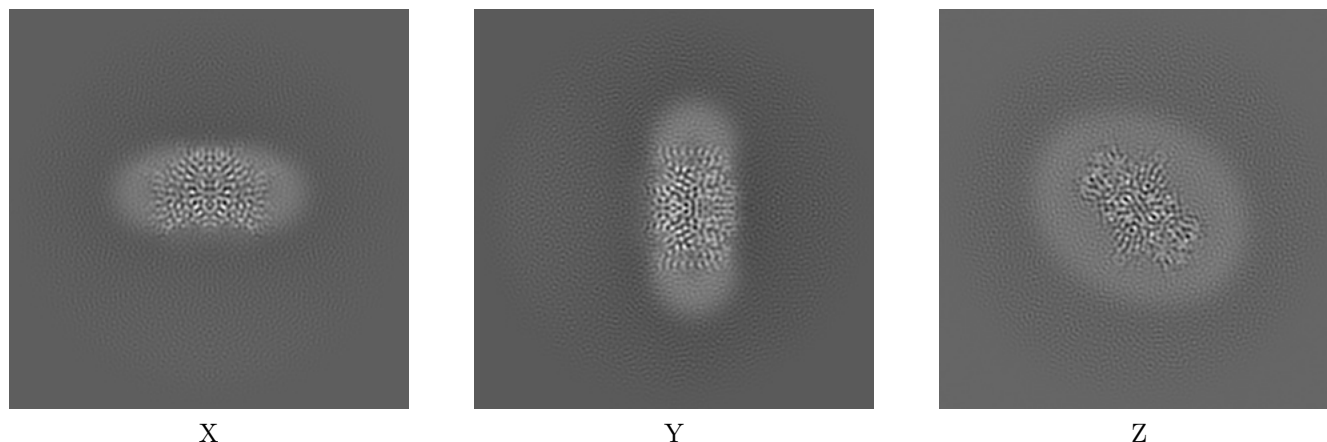
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62506. These allow visual inspection of the internal detail of the map and identification of artifacts.

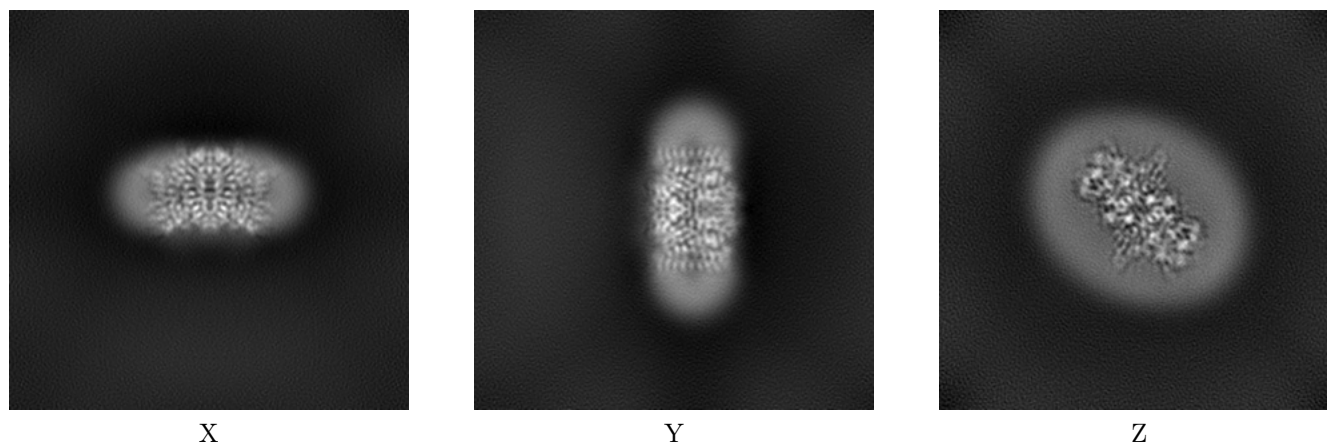
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



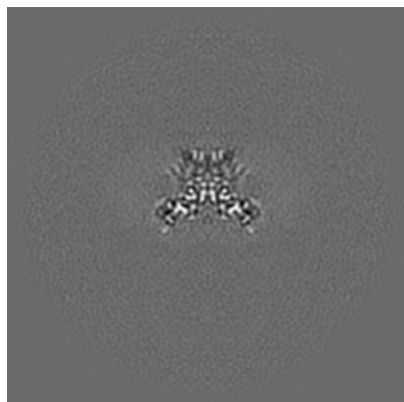
6.1.2 Raw map



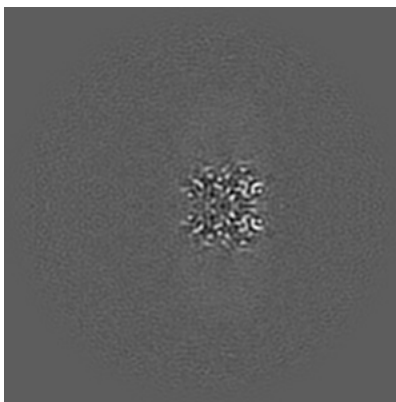
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

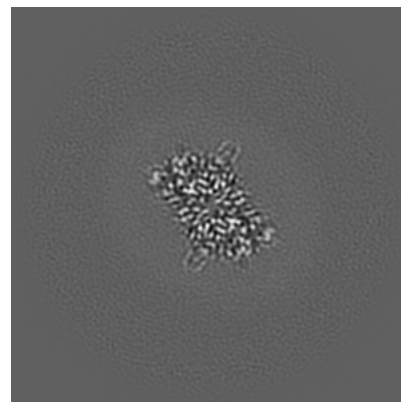
6.2.1 Primary map



X Index: 120

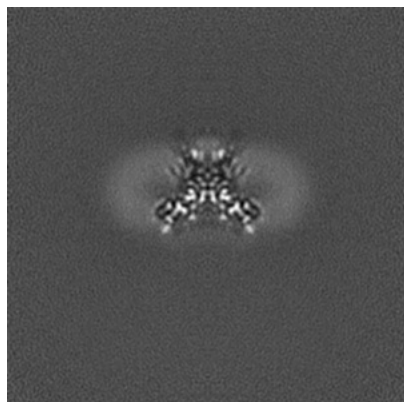


Y Index: 120

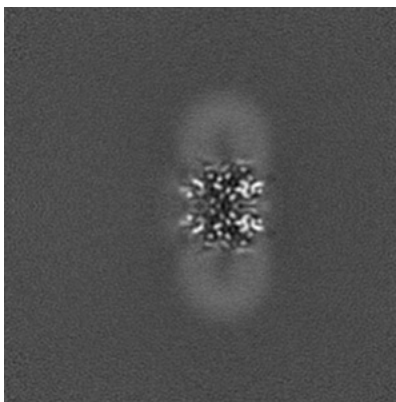


Z Index: 120

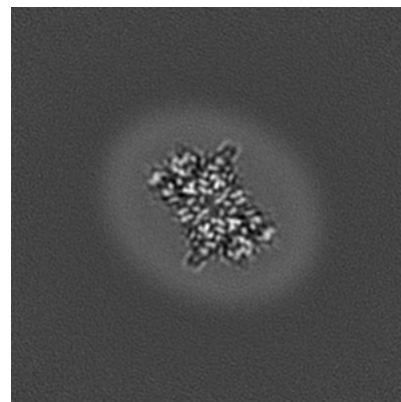
6.2.2 Raw map



X Index: 120



Y Index: 120

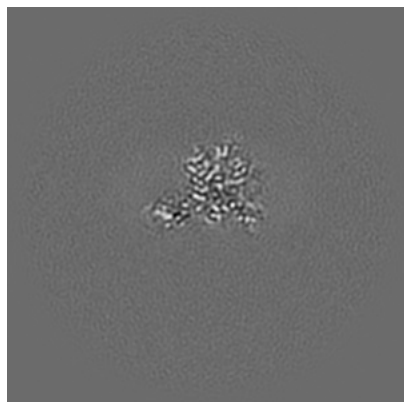


Z Index: 120

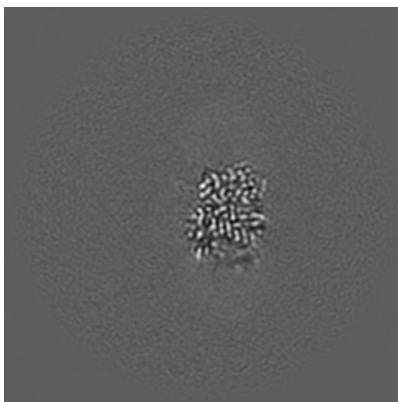
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

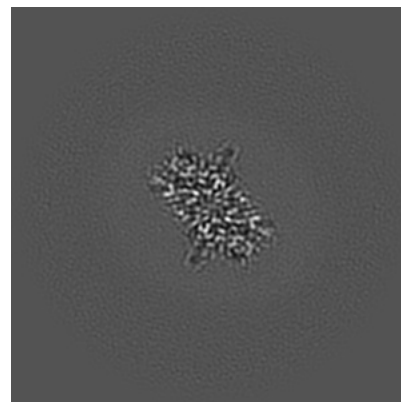
6.3.1 Primary map



X Index: 114

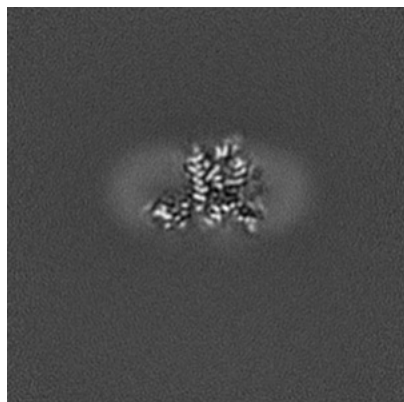


Y Index: 126

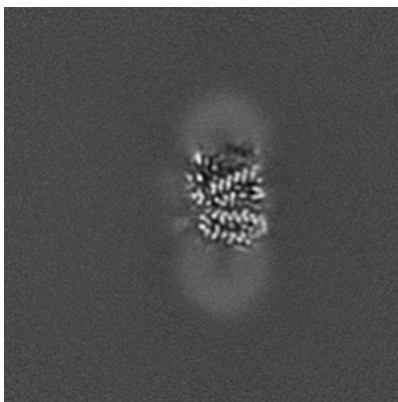


Z Index: 121

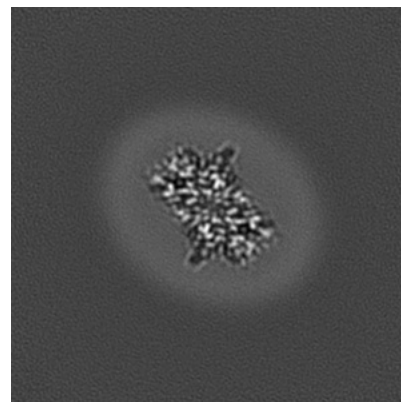
6.3.2 Raw map



X Index: 114



Y Index: 114

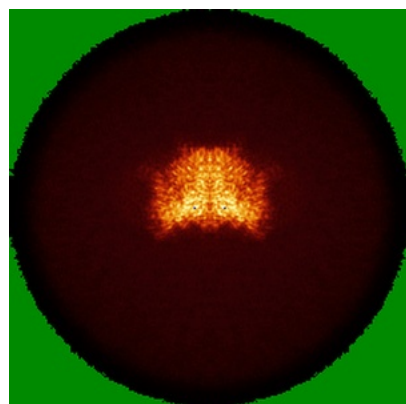


Z Index: 121

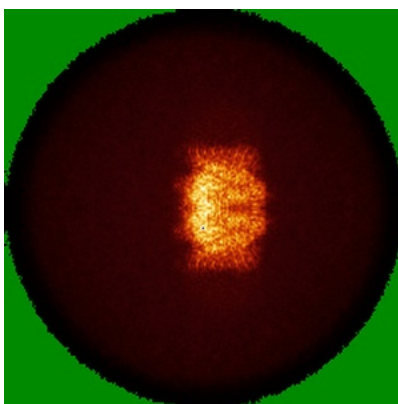
The images above show the largest variance slices of the map in three orthogonal directions.

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

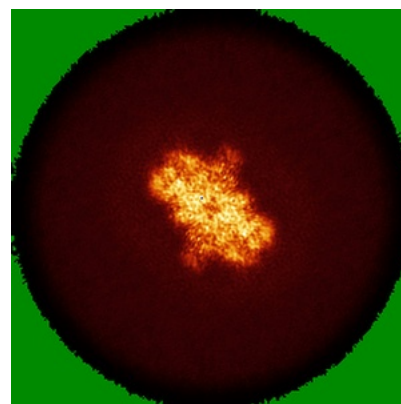
6.4.1 Primary map



X



Y

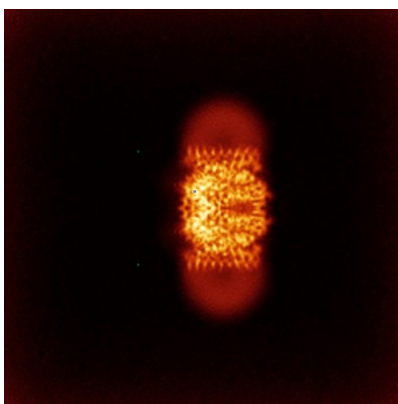


Z

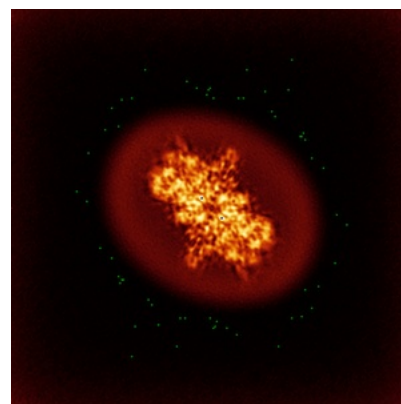
6.4.2 Raw map



X



Y

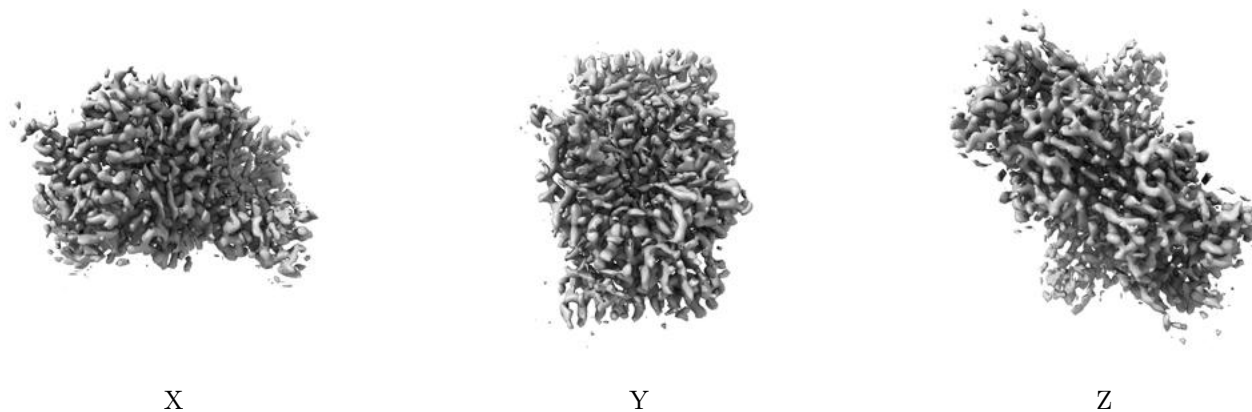


Z

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.

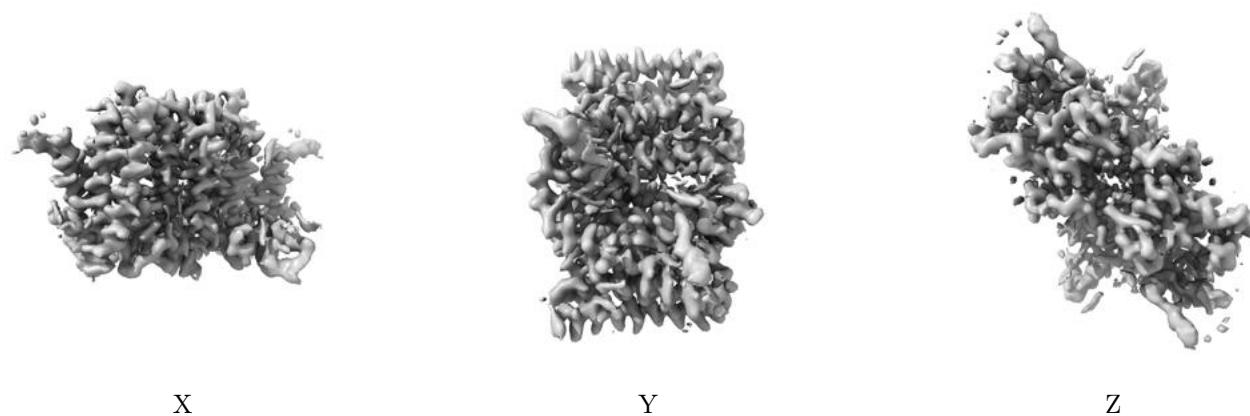
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.576. 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.

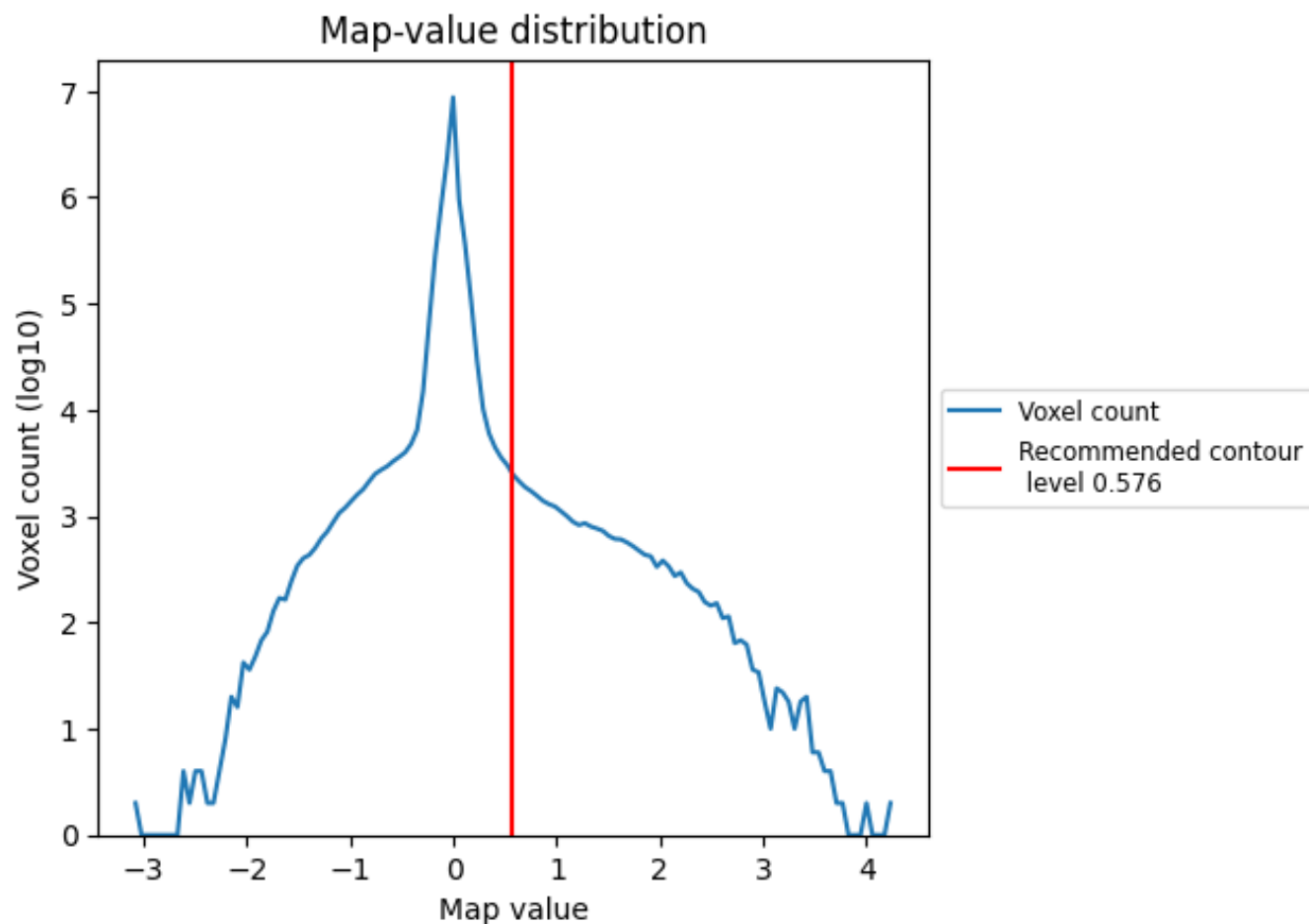
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

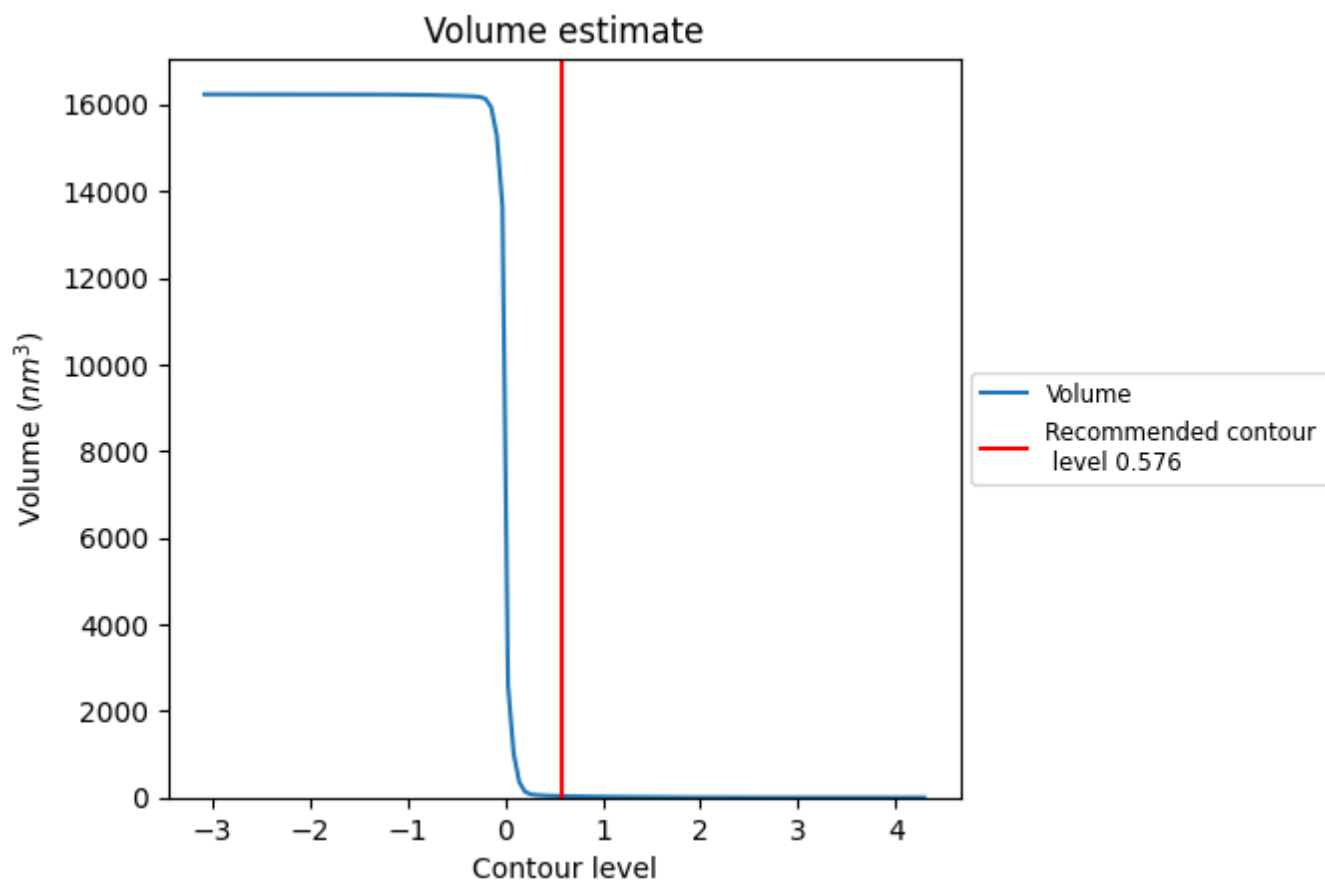
This section contains the results of statistical analysis of the map.

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.

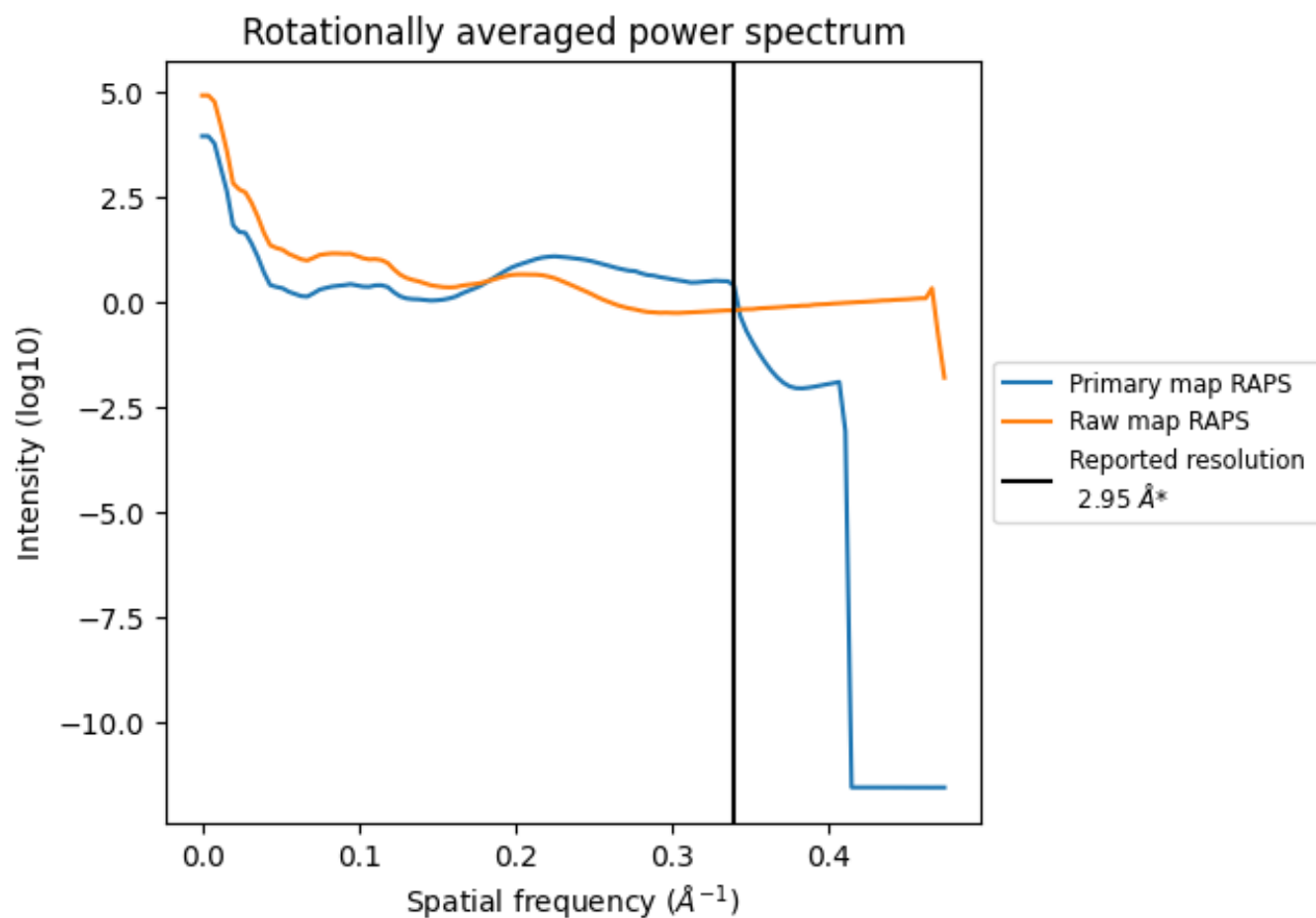
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 33 nm³; this corresponds to an approximate mass of 30 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 ⓘ

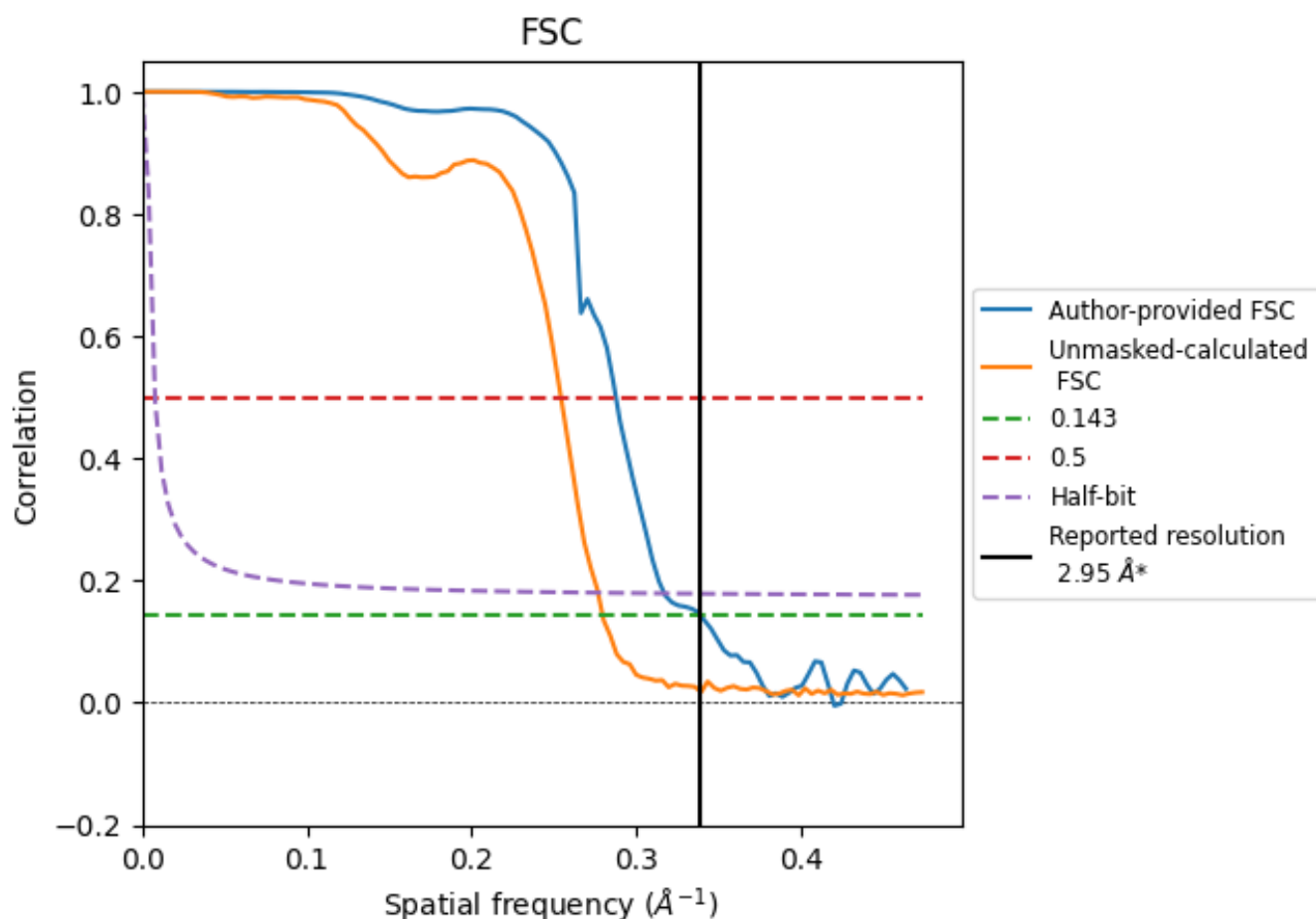


*Reported resolution corresponds to spatial frequency of 0.339 Å⁻¹

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 $0.339 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.95	-	-
Author-provided FSC curve	2.95	3.47	3.15
Unmasked-calculated*	3.57	3.93	3.61

*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 3.57 differs from the reported value 2.95 by more than 10 %

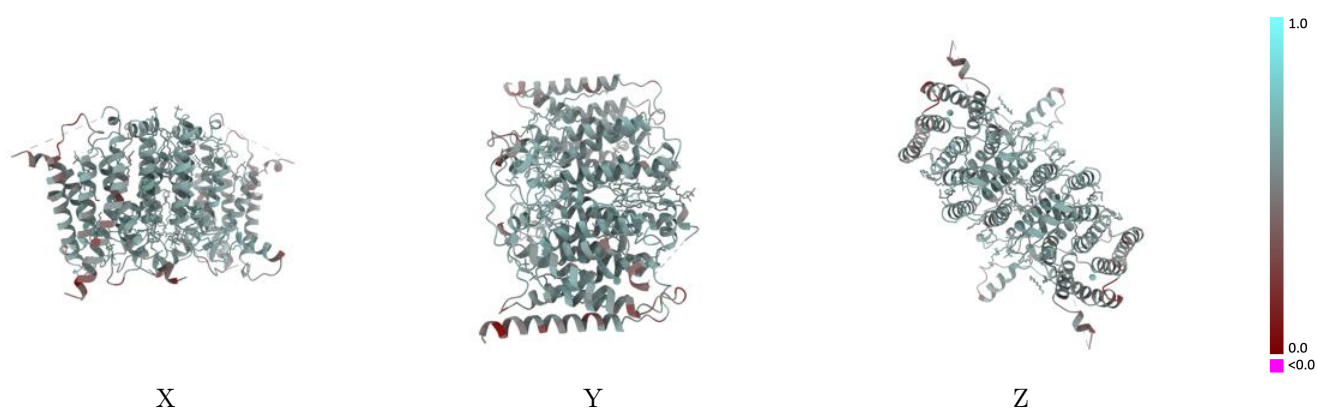
9 Map-model fit [i](#)

This section contains information regarding the fit between EMD map EMD-62506 and PDB model 9KQJ. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)

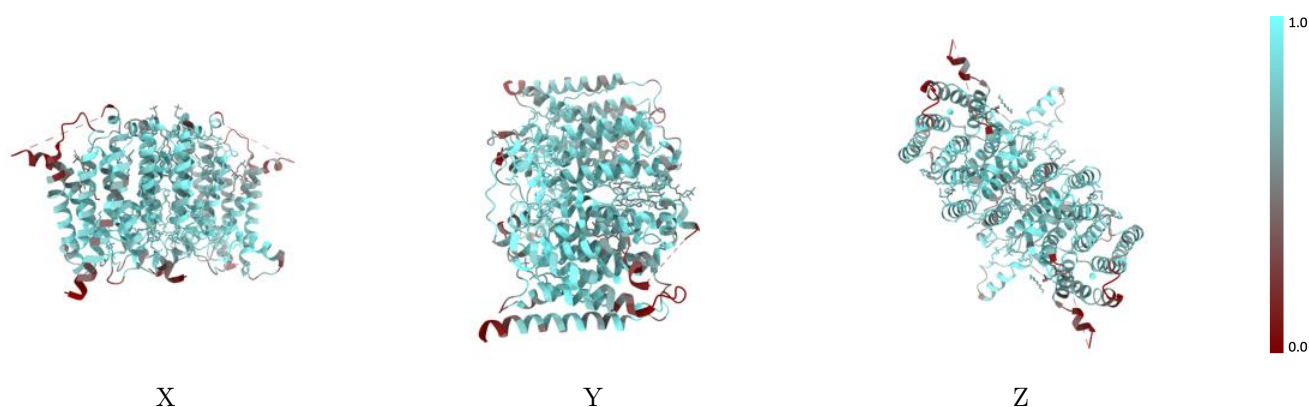
This section was not generated.

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



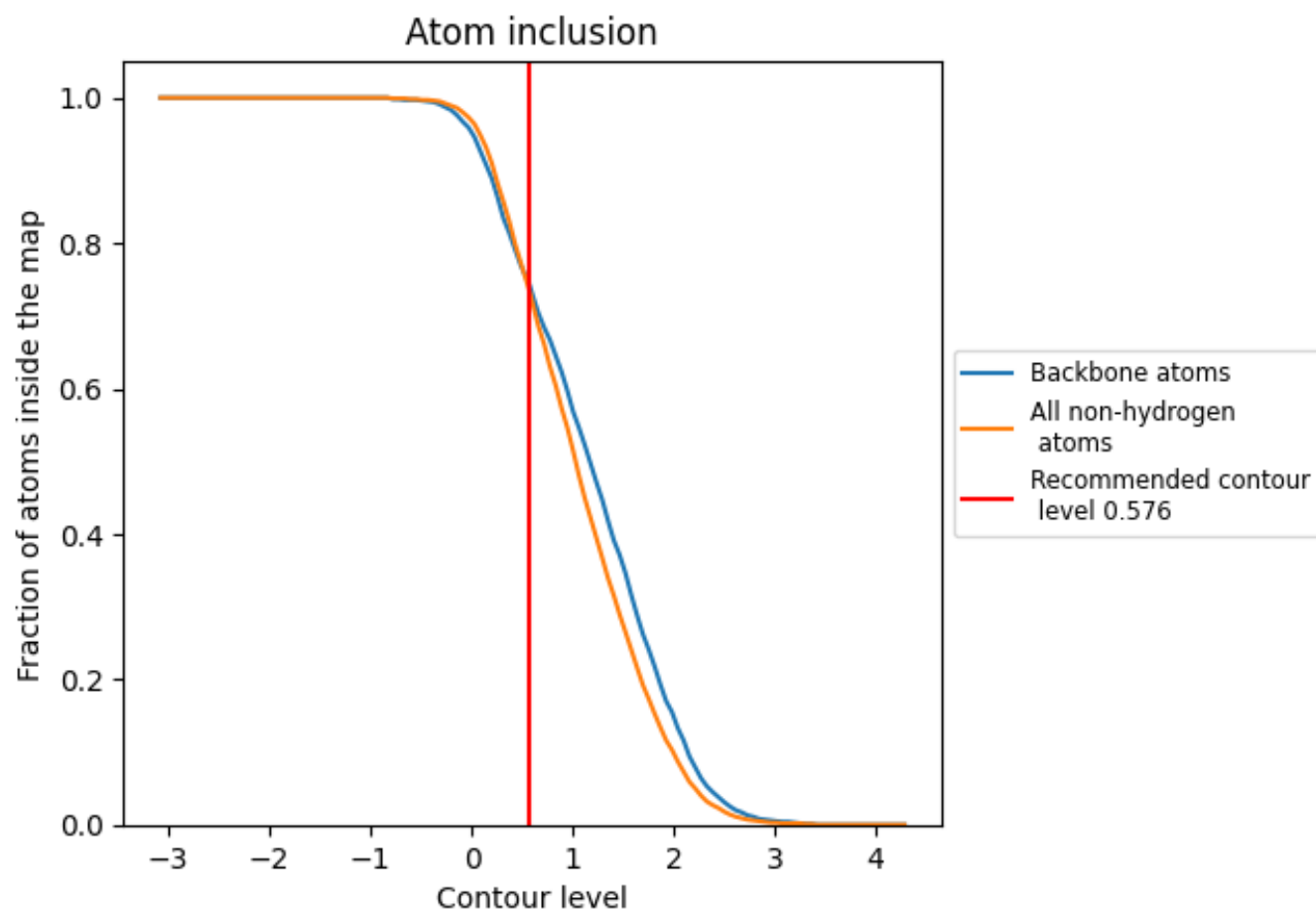
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.576).

9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 73% 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 (0.576) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7340	0.5520
A	0.7300	0.5500
B	0.7380	0.5540

