



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 10:15 AM UTC

PDB ID : 8JF2 / pdb_00008jf2
EMDB ID : EMD-36207
Title : Cryo-EM structure of tetrameric DltB/DltC complex
Authors : Zhang, P.; Liu, Z.
Deposited on : 2023-05-17
Resolution : 3.50 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

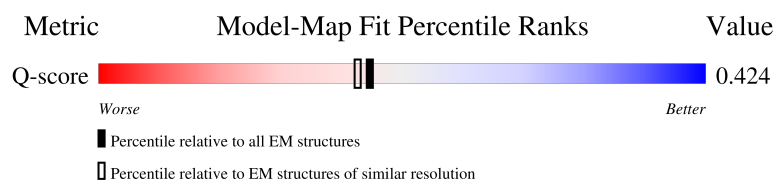
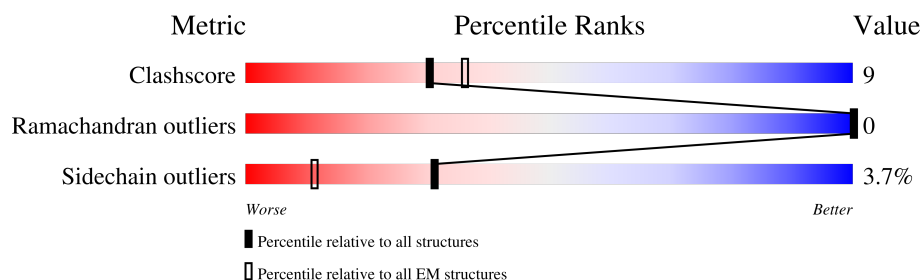
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 Å.

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



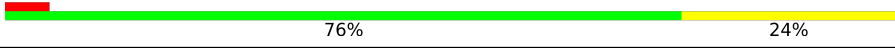
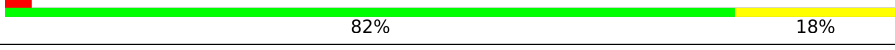
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13950 (3.00 - 4.00)

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	440	 70% 23% • 5%
1	B	440	 72% 22% • 5%
1	C	440	 70% 23% • 5%
1	D	440	 71% 24% 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	79	 89%11%
2	G	79	 75%25%
2	H	79	 5%76%24%
2	I	79	 82%18%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 17676 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 Teichoic acid D-alanyltransferase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	417	Total	C	N	O	S	0	0
			3461	2335	549	557	20		
1	B	419	Total	C	N	O	S	0	0
			3481	2349	552	560	20		
1	C	419	Total	C	N	O	S	0	0
			3484	2351	555	558	20		
1	D	419	Total	C	N	O	S	0	0
			3481	2349	552	560	20		

There are 100 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-24	MET	-	initiating methionine	UNP Q5M4V4
A	-23	GLY	-	expression tag	UNP Q5M4V4
A	-22	SER	-	expression tag	UNP Q5M4V4
A	-21	SER	-	expression tag	UNP Q5M4V4
A	-20	HIS	-	expression tag	UNP Q5M4V4
A	-19	HIS	-	expression tag	UNP Q5M4V4
A	-18	HIS	-	expression tag	UNP Q5M4V4
A	-17	HIS	-	expression tag	UNP Q5M4V4
A	-16	HIS	-	expression tag	UNP Q5M4V4
A	-15	HIS	-	expression tag	UNP Q5M4V4
A	-14	ASN	-	expression tag	UNP Q5M4V4
A	-13	TYR	-	expression tag	UNP Q5M4V4
A	-12	ASP	-	expression tag	UNP Q5M4V4
A	-11	ILE	-	expression tag	UNP Q5M4V4
A	-10	PRO	-	expression tag	UNP Q5M4V4
A	-9	THR	-	expression tag	UNP Q5M4V4
A	-8	THR	-	expression tag	UNP Q5M4V4
A	-7	GLU	-	expression tag	UNP Q5M4V4
A	-6	ASN	-	expression tag	UNP Q5M4V4
A	-5	LEU	-	expression tag	UNP Q5M4V4
A	-4	TYR	-	expression tag	UNP Q5M4V4
A	-3	PHE	-	expression tag	UNP Q5M4V4

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLN	-	expression tag	UNP Q5M4V4
A	-1	GLY	-	expression tag	UNP Q5M4V4
A	0	SER	-	expression tag	UNP Q5M4V4
B	-24	MET	-	initiating methionine	UNP Q5M4V4
B	-23	GLY	-	expression tag	UNP Q5M4V4
B	-22	SER	-	expression tag	UNP Q5M4V4
B	-21	SER	-	expression tag	UNP Q5M4V4
B	-20	HIS	-	expression tag	UNP Q5M4V4
B	-19	HIS	-	expression tag	UNP Q5M4V4
B	-18	HIS	-	expression tag	UNP Q5M4V4
B	-17	HIS	-	expression tag	UNP Q5M4V4
B	-16	HIS	-	expression tag	UNP Q5M4V4
B	-15	HIS	-	expression tag	UNP Q5M4V4
B	-14	ASN	-	expression tag	UNP Q5M4V4
B	-13	TYR	-	expression tag	UNP Q5M4V4
B	-12	ASP	-	expression tag	UNP Q5M4V4
B	-11	ILE	-	expression tag	UNP Q5M4V4
B	-10	PRO	-	expression tag	UNP Q5M4V4
B	-9	THR	-	expression tag	UNP Q5M4V4
B	-8	THR	-	expression tag	UNP Q5M4V4
B	-7	GLU	-	expression tag	UNP Q5M4V4
B	-6	ASN	-	expression tag	UNP Q5M4V4
B	-5	LEU	-	expression tag	UNP Q5M4V4
B	-4	TYR	-	expression tag	UNP Q5M4V4
B	-3	PHE	-	expression tag	UNP Q5M4V4
B	-2	GLN	-	expression tag	UNP Q5M4V4
B	-1	GLY	-	expression tag	UNP Q5M4V4
B	0	SER	-	expression tag	UNP Q5M4V4
C	-24	MET	-	initiating methionine	UNP Q5M4V4
C	-23	GLY	-	expression tag	UNP Q5M4V4
C	-22	SER	-	expression tag	UNP Q5M4V4
C	-21	SER	-	expression tag	UNP Q5M4V4
C	-20	HIS	-	expression tag	UNP Q5M4V4
C	-19	HIS	-	expression tag	UNP Q5M4V4
C	-18	HIS	-	expression tag	UNP Q5M4V4
C	-17	HIS	-	expression tag	UNP Q5M4V4
C	-16	HIS	-	expression tag	UNP Q5M4V4
C	-15	HIS	-	expression tag	UNP Q5M4V4
C	-14	ASN	-	expression tag	UNP Q5M4V4
C	-13	TYR	-	expression tag	UNP Q5M4V4
C	-12	ASP	-	expression tag	UNP Q5M4V4
C	-11	ILE	-	expression tag	UNP Q5M4V4

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	-10	PRO	-	expression tag	UNP Q5M4V4
C	-9	THR	-	expression tag	UNP Q5M4V4
C	-8	THR	-	expression tag	UNP Q5M4V4
C	-7	GLU	-	expression tag	UNP Q5M4V4
C	-6	ASN	-	expression tag	UNP Q5M4V4
C	-5	LEU	-	expression tag	UNP Q5M4V4
C	-4	TYR	-	expression tag	UNP Q5M4V4
C	-3	PHE	-	expression tag	UNP Q5M4V4
C	-2	GLN	-	expression tag	UNP Q5M4V4
C	-1	GLY	-	expression tag	UNP Q5M4V4
C	0	SER	-	expression tag	UNP Q5M4V4
D	-24	MET	-	initiating methionine	UNP Q5M4V4
D	-23	GLY	-	expression tag	UNP Q5M4V4
D	-22	SER	-	expression tag	UNP Q5M4V4
D	-21	SER	-	expression tag	UNP Q5M4V4
D	-20	HIS	-	expression tag	UNP Q5M4V4
D	-19	HIS	-	expression tag	UNP Q5M4V4
D	-18	HIS	-	expression tag	UNP Q5M4V4
D	-17	HIS	-	expression tag	UNP Q5M4V4
D	-16	HIS	-	expression tag	UNP Q5M4V4
D	-15	HIS	-	expression tag	UNP Q5M4V4
D	-14	ASN	-	expression tag	UNP Q5M4V4
D	-13	TYR	-	expression tag	UNP Q5M4V4
D	-12	ASP	-	expression tag	UNP Q5M4V4
D	-11	ILE	-	expression tag	UNP Q5M4V4
D	-10	PRO	-	expression tag	UNP Q5M4V4
D	-9	THR	-	expression tag	UNP Q5M4V4
D	-8	THR	-	expression tag	UNP Q5M4V4
D	-7	GLU	-	expression tag	UNP Q5M4V4
D	-6	ASN	-	expression tag	UNP Q5M4V4
D	-5	LEU	-	expression tag	UNP Q5M4V4
D	-4	TYR	-	expression tag	UNP Q5M4V4
D	-3	PHE	-	expression tag	UNP Q5M4V4
D	-2	GLN	-	expression tag	UNP Q5M4V4
D	-1	GLY	-	expression tag	UNP Q5M4V4
D	0	SER	-	expression tag	UNP Q5M4V4

- Molecule 2 is a protein called D-alanyl carrier protein.

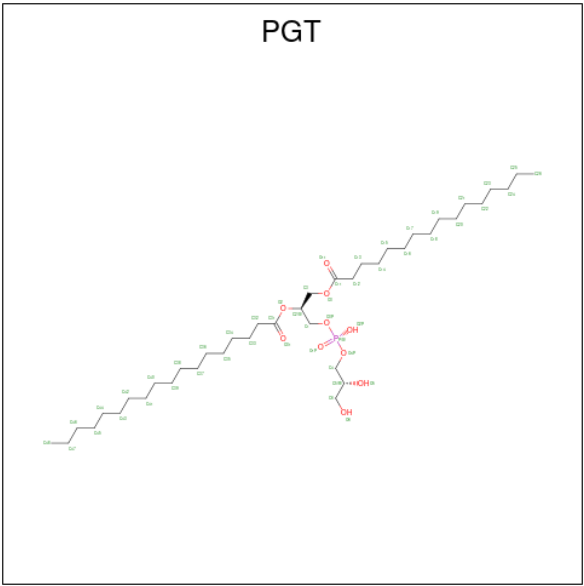
Mol	Chain	Residues	Atoms					AltConf	Trace
2	F	79	Total	C	N	O	S	0	0
			625	390	97	133	5		

Continued on next page...

Continued from previous page...

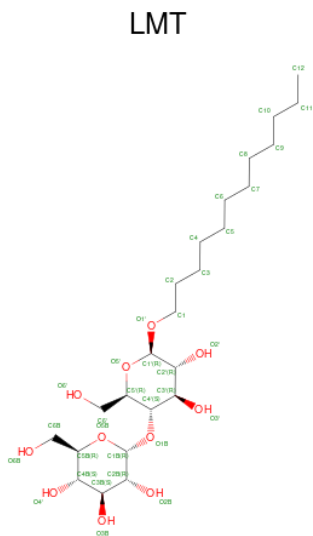
Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	79	Total	C	N	O	S	0	0
			625	390	97	133	5		
2	H	79	Total	C	N	O	S	0	0
			625	390	97	133	5		
2	I	79	Total	C	N	O	S	0	0
			625	390	97	133	5		

- Molecule 3 is (1S)-2-{{[(2R)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYL)OXY]METHYL]ETHYL STEARATE (CCD ID: PGT) (formula: C₄₀H₇₉O₁₀P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	O	P	0
			51	40	10	1	
3	B	1	Total	C	O	P	0
			51	40	10	1	
3	B	1	Total	C	O	P	0
			51	40	10	1	
3	C	1	Total	C	O	P	0
			51	40	10	1	
3	C	1	Total	C	O	P	0
			51	40	10	1	
3	D	1	Total	C	O	P	0
			51	40	10	1	

- Molecule 4 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).

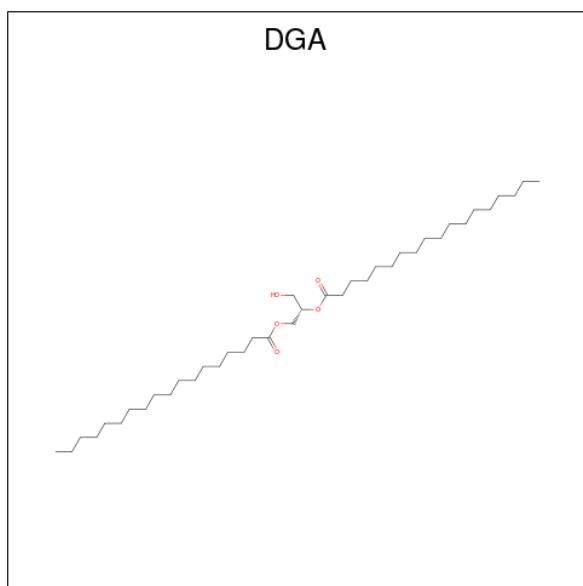


Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
4	C	1	Total	C	O	0
			35	24	11	
4	C	1	Total	C	O	0
			35	24	11	
4	C	1	Total	C	O	0
			35	24	11	
4	C	1	Total	C	O	0
			35	24	11	
4	D	1	Total	C	O	0
			35	24	11	
4	D	1	Total	C	O	0
			35	24	11	
4	D	1	Total	C	O	0
			35	24	11	
4	D	1	Total	C	O	0
			35	24	11	
4	D	1	Total	C	O	0
			35	24	11	
4	D	1	Total	C	O	0
			35	24	11	

- Molecule 5 is DIACYL GLYCEROL (CCD ID: DGA) (formula: $C_{39}H_{76}O_5$) (labeled as "Ligand of Interest" by depositor).



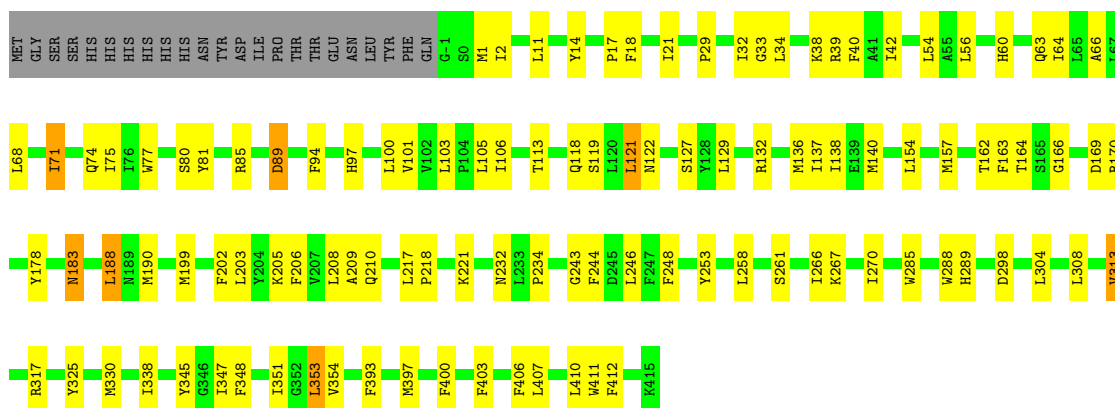
Mol	Chain	Residues	Atoms			AltConf
5	B	1	Total 44	C 39	O 5	0
5	C	1	Total 44	C 39	O 5	0

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.

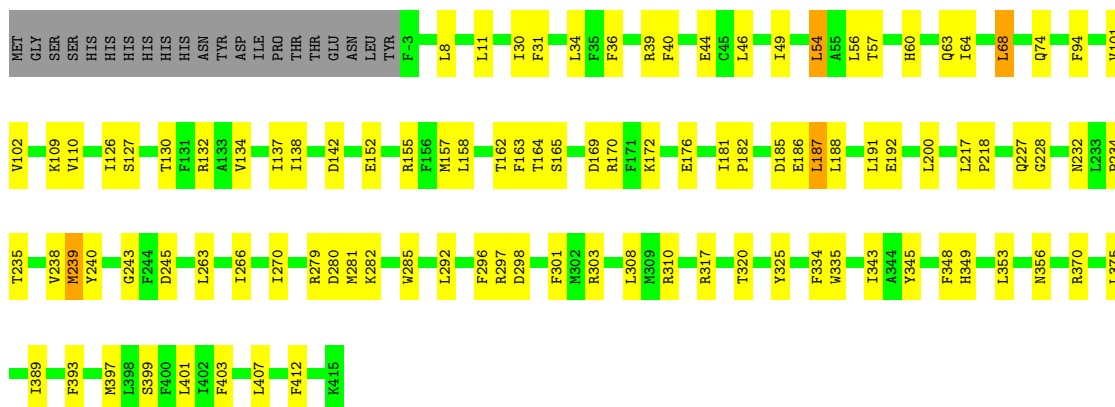
• Molecule 1: Teichoic acid D-alanyltransferase

Chain A: 



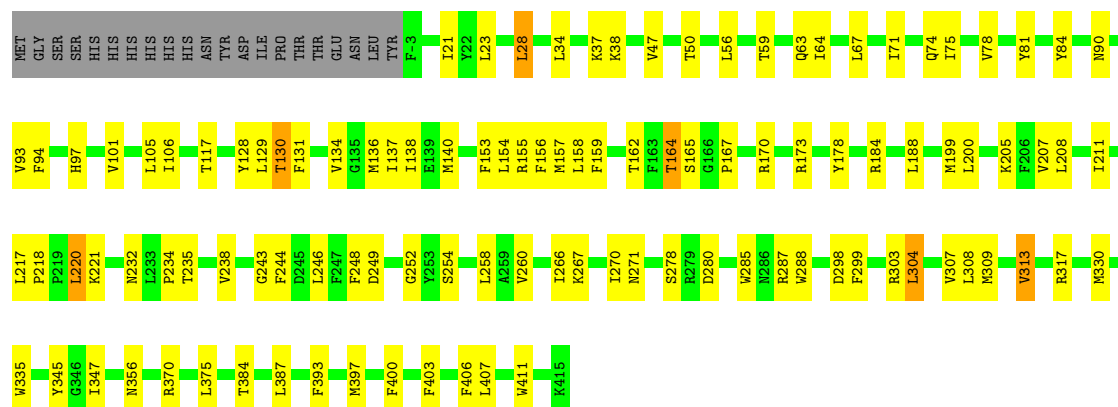
• Molecule 1: Teichoic acid D-alanyltransferase

Chain B: 



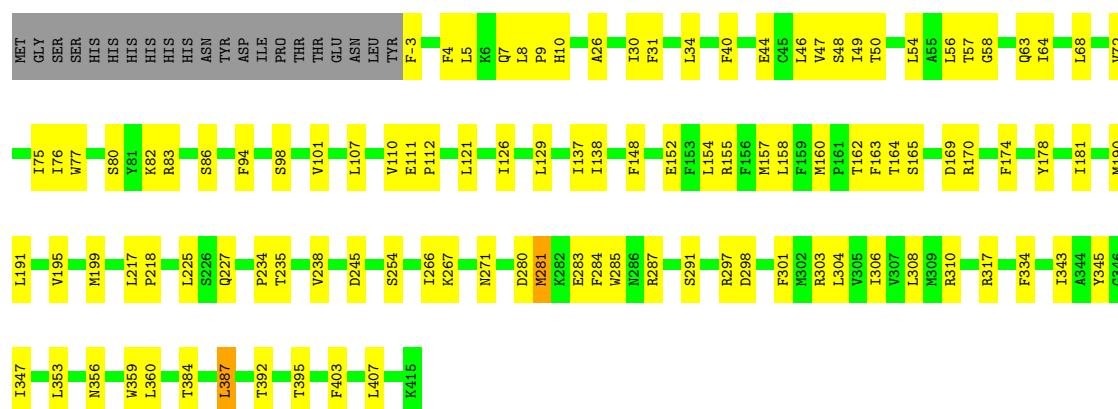
• Molecule 1: Teichoic acid D-alanyltransferase

Chain C: 



- Molecule 1: Teichoic acid D-alanyltransferase

Chain D: 71% 24% 5%



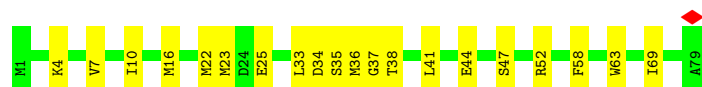
- Molecule 2: D-alanyl carrier protein

Chain F: 89% 11%



- Molecule 2: D-alanyl carrier protein

Chain G: 75% 25%

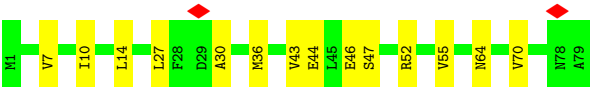
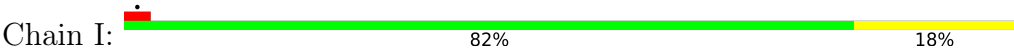


- Molecule 2: D-alanyl carrier protein

Chain H: 5% 76% 24%



• Molecule 2: D-alanyl carrier protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	377918	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	55	Depositor
Minimum defocus (nm)	1100	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.802	Depositor
Minimum map value	-0.596	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	265.6, 265.6, 265.6	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83000004, 0.83000004, 0.83000004	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: DGA, PGT, LMT

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	0.22	0/3569	0.33	0/4828
1	B	0.24	0/3590	0.32	0/4856
1	C	0.22	0/3593	0.33	0/4859
1	D	0.24	0/3590	0.32	0/4856
2	F	0.07	0/631	0.22	0/852
2	G	0.07	0/631	0.22	0/852
2	H	0.08	0/631	0.24	0/852
2	I	0.07	0/631	0.23	0/852
All	All	0.21	0/16866	0.31	0/22807

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	3461	0	3537	64	0
1	B	3481	0	3554	68	0
1	C	3484	0	3563	71	0
1	D	3481	0	3554	66	0
2	F	625	0	601	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	625	0	601	15	0
2	H	625	0	601	11	0
2	I	625	0	601	11	0
3	A	51	0	78	0	0
3	B	102	0	156	7	0
3	C	102	0	156	5	0
3	D	51	0	78	5	0
4	A	140	0	181	10	0
4	B	280	0	360	13	0
4	C	210	0	271	3	0
4	D	245	0	315	16	0
5	B	44	0	76	5	0
5	C	44	0	76	4	0
All	All	17676	0	18359	324	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 (324) 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:243:GLY:HA3	1:B:397:MET:HE1	1.59	0.83
1:A:94:PHE:HZ	1:A:138:ILE:HD13	1.52	0.74
1:B:132:ARG:NH2	1:B:162:THR:OG1	2.22	0.73
1:B:280:ASP:OD1	1:B:356:ASN:ND2	2.22	0.72
1:D:359:TRP:NE1	4:D:605:LMT:O6'	2.23	0.72
1:D:334:PHE:HB3	3:D:601:PGT:H42	1.70	0.71
1:B:370:ARG:HG2	1:B:375:LEU:HB2	1.74	0.69
1:B:109:LYS:NZ	1:B:127:SER:OG	2.26	0.67
1:D:283:GLU:OE2	1:D:287:ARG:NH1	2.25	0.67
1:C:317:ARG:NH2	2:H:36:MET:SD	2.64	0.66
1:A:190:MET:SD	1:A:267:LYS:NZ	2.69	0.65
1:A:317:ARG:HH22	2:F:39:VAL:HB	1.61	0.65
1:A:243:GLY:HA3	1:A:397:MET:HE1	1.79	0.65
1:C:170:ARG:NH2	1:C:298:ASP:OD2	2.30	0.65
1:D:317:ARG:NH2	2:I:36:MET:O	2.31	0.64
1:C:205:LYS:NZ	1:C:249:ASP:OD1	2.29	0.64
1:C:28:LEU:HG	5:C:502:DGA:HAG3	1.81	0.62
1:A:34:LEU:HD12	1:A:39:ARG:HE	1.63	0.62
1:B:282:LYS:NZ	1:B:325:TYR:OH	2.32	0.62
3:C:501:PGT:H421	3:C:501:PGT:H201	1.82	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:192:GLU:HB3	4:B:506:LMT:H42	1.82	0.61
1:B:239:MET:HB2	1:B:401:LEU:HB2	1.80	0.61
1:D:121:LEU:HD23	1:D:121:LEU:H	1.64	0.61
1:D:56:LEU:O	1:D:63:GLN:NE2	2.34	0.61
1:A:317:ARG:NH2	2:F:36:MET:O	2.33	0.61
3:D:601:PGT:H352	3:D:601:PGT:H2	1.81	0.61
1:C:105:LEU:HB2	1:C:130:THR:HG21	1.82	0.61
1:C:243:GLY:HA3	1:C:397:MET:HE1	1.83	0.61
1:B:39:ARG:NH1	1:B:44:GLU:OE2	2.34	0.61
1:B:30:ILE:HD13	1:B:44:GLU:HG2	1.83	0.60
1:C:106:ILE:HG23	3:C:501:PGT:H41	1.82	0.60
1:B:56:LEU:O	1:B:63:GLN:NE2	2.35	0.60
5:C:502:DGA:HB62	1:D:49:ILE:HG21	1.84	0.60
1:C:138:ILE:HD11	1:C:303:ARG:CZ	2.32	0.60
1:B:40:PHE:HZ	4:B:507:LMT:H82	1.67	0.59
2:G:33:LEU:HD21	2:G:38:THR:HB	1.83	0.59
1:B:317:ARG:NH2	2:G:36:MET:SD	2.76	0.59
1:B:138:ILE:HD11	3:B:502:PGT:H182	1.85	0.59
1:D:310:ARG:HD3	2:I:52:ARG:HH22	1.68	0.58
1:C:56:LEU:HD12	1:C:63:GLN:HG3	1.86	0.58
1:C:164:THR:OG1	1:C:165:SER:N	2.37	0.58
2:I:7:VAL:HG21	2:I:70:VAL:HG22	1.86	0.57
1:D:297:ARG:HA	1:D:301:PHE:HB3	1.86	0.57
1:C:56:LEU:O	1:C:63:GLN:NE2	2.35	0.56
1:B:285:TRP:HD1	1:B:353:LEU:HD11	1.69	0.56
1:D:94:PHE:HZ	1:D:138:ILE:HD13	1.69	0.56
1:C:205:LYS:HB2	1:C:252:GLY:HA3	1.86	0.56
1:D:170:ARG:NH2	1:D:298:ASP:OD2	2.39	0.55
1:A:244:PHE:HD1	1:A:248:PHE:HE1	1.53	0.55
1:D:83:ARG:O	1:D:86:SER:OG	2.24	0.55
1:D:303:ARG:HE	3:D:601:PGT:H241	1.71	0.55
1:D:152:GLU:HG2	1:D:155:ARG:HH21	1.72	0.55
1:B:227:GLN:HG3	1:B:234:PRO:HG3	1.88	0.55
3:B:511:PGT:H372	4:D:602:LMT:H101	1.89	0.55
1:B:152:GLU:HG2	1:B:155:ARG:HH21	1.71	0.54
1:D:271:ASN:OD1	1:D:291:SER:OG	2.20	0.54
1:D:190:MET:SD	1:D:267:LYS:NZ	2.69	0.54
1:B:102:VAL:HG11	3:B:502:PGT:H342	1.89	0.54
1:D:227:GLN:HG3	1:D:234:PRO:HG3	1.89	0.54
1:B:188:LEU:HB3	4:B:506:LMT:H11	1.90	0.54
1:A:232:ASN:HB2	1:A:234:PRO:HD2	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:138:ILE:HD11	3:D:601:PGT:H182	1.90	0.53
1:B:310:ARG:HH11	2:G:52:ARG:HH22	1.55	0.53
1:A:66:ALA:HB1	1:A:121:LEU:HA	1.90	0.53
1:A:85:ARG:NH1	1:A:89:ASP:OD2	2.40	0.53
5:C:502:DGA:HB22	1:D:50:THR:HG22	1.91	0.53
1:B:34:LEU:HD23	1:B:187:LEU:HD11	1.90	0.53
1:D:395:THR:HG21	4:D:605:LMT:H92	1.90	0.53
1:A:29:PRO:HB3	4:A:604:LMT:H112	1.91	0.53
1:B:94:PHE:HZ	1:B:138:ILE:HD13	1.73	0.53
1:B:164:THR:OG1	1:B:165:SER:N	2.42	0.53
1:A:199:MET:HG3	1:B:46:LEU:HD13	1.91	0.53
1:D:254:SER:OG	1:D:271:ASN:ND2	2.35	0.53
2:F:15:PHE:HB3	2:F:17:GLU:HG3	1.90	0.53
1:A:33:GLY:HA3	1:A:40:PHE:HE2	1.73	0.52
1:B:170:ARG:NH2	1:B:298:ASP:OD2	2.42	0.52
1:D:384:THR:HA	1:D:387:LEU:HD23	1.91	0.52
1:C:244:PHE:O	1:C:248:PHE:HD1	1.93	0.52
2:G:44:GLU:O	2:G:47:SER:OG	2.21	0.52
1:C:136:MET:HE3	1:C:153:PHE:CD1	2.45	0.51
1:D:195:VAL:HG11	4:D:604:LMT:H112	1.92	0.51
1:A:217:LEU:HD11	1:A:221:LYS:HE3	1.92	0.51
1:A:351:ILE:HA	1:A:354:VAL:HG12	1.92	0.51
1:D:157:MET:HG2	1:D:158:LEU:HD23	1.92	0.51
1:C:299:PHE:CE1	2:H:56:SER:HB2	2.45	0.51
1:C:303:ARG:HH21	3:C:501:PGT:H461	1.75	0.51
1:B:74:GLN:OE1	1:B:101:VAL:HG13	2.10	0.51
1:A:75:ILE:HD11	1:A:154:LEU:HD11	1.93	0.51
1:C:21:ILE:HD11	5:C:502:DGA:HA31	1.92	0.51
1:A:113:THR:HG21	1:A:338:ILE:HB	1.92	0.51
4:C:505:LMT:H91	1:D:40:PHE:HZ	1.76	0.51
1:A:103:LEU:HA	1:A:106:ILE:HG22	1.93	0.50
1:A:308:LEU:HD22	1:A:313:VAL:HG11	1.92	0.50
3:B:511:PGT:H351	4:D:602:LMT:H92	1.92	0.50
1:C:199:MET:HG3	1:D:46:LEU:HD13	1.93	0.50
2:I:27:LEU:HA	2:I:30:ALA:HB3	1.93	0.50
1:A:11:LEU:HD12	1:A:54:LEU:HD23	1.92	0.50
1:B:297:ARG:HA	1:B:301:PHE:HB3	1.93	0.50
1:C:71:ILE:HD11	1:C:158:LEU:HD21	1.92	0.50
1:D:54:LEU:HD21	4:D:608:LMT:H32	1.94	0.50
1:D:34:LEU:HD13	1:D:181:ILE:HG23	1.92	0.50
4:B:503:LMT:O2'	3:B:511:PGT:O2P	2.30	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:244:PHE:HD1	1:C:248:PHE:HE1	1.59	0.50
1:D:44:GLU:HA	1:D:47:VAL:HG12	1.93	0.50
1:B:142:ASP:OD2	1:B:303:ARG:NH2	2.44	0.49
1:C:184:ARG:HD3	4:C:503:LMT:H11	1.93	0.49
1:C:345:TYR:CD1	1:C:403:PHE:HB2	2.47	0.49
1:C:254:SER:OG	1:C:271:ASN:HB2	2.11	0.49
1:D:280:ASP:OD1	1:D:281:MET:N	2.45	0.49
4:D:603:LMT:H102	4:D:606:LMT:H92	1.94	0.49
1:C:136:MET:O	1:C:140:MET:HG2	2.11	0.49
1:A:17:PRO:HB3	1:A:202:PHE:CE1	2.48	0.49
1:A:330:MET:HE1	1:A:347:ILE:HD12	1.95	0.49
1:B:132:ARG:NH1	1:B:169:ASP:OD2	2.44	0.49
1:C:370:ARG:HB3	1:C:375:LEU:HB2	1.95	0.49
1:B:109:LYS:HE2	1:B:335:TRP:O	2.13	0.49
1:B:235:THR:O	1:B:238:VAL:HG12	2.13	0.49
1:A:121:LEU:HD23	1:A:121:LEU:H	1.78	0.49
1:D:31:PHE:HE2	1:D:191:LEU:HD22	1.77	0.49
1:C:393:PHE:O	1:C:397:MET:HG2	2.13	0.49
1:A:345:TYR:CD1	1:A:403:PHE:HB2	2.47	0.49
3:B:511:PGT:H262	3:B:511:PGT:H471	1.94	0.49
1:C:330:MET:HE1	1:C:347:ILE:HD12	1.95	0.48
1:B:217:LEU:HB3	1:B:218:PRO:HD3	1.94	0.48
1:B:228:GLY:O	1:B:232:ASN:ND2	2.46	0.48
3:C:509:PGT:H341	4:D:603:LMT:H61	1.95	0.48
1:A:393:PHE:O	1:A:397:MET:HG2	2.14	0.48
2:H:9:GLU:HG3	2:H:13:GLU:HG3	1.95	0.48
1:C:23:LEU:HD21	1:C:260:VAL:HG13	1.96	0.48
2:G:63:TRP:HE3	2:G:69:ILE:HD13	1.77	0.48
1:C:159:PHE:CZ	1:C:266:ILE:HD12	2.48	0.48
1:D:235:THR:O	1:D:238:VAL:HG12	2.14	0.48
1:D:306:ILE:HD11	2:I:55:VAL:HG11	1.96	0.48
1:B:31:PHE:HE2	1:B:191:LEU:HD22	1.79	0.48
1:A:105:LEU:HD11	1:A:127:SER:HA	1.96	0.48
1:A:258:LEU:HD11	1:A:270:ILE:HA	1.94	0.48
1:D:195:VAL:HG12	1:D:199:MET:HE3	1.96	0.48
1:C:81:TYR:HB2	1:C:97:HIS:CD2	2.49	0.47
1:A:203:LEU:HD13	5:B:501:DGA:HA91	1.97	0.47
1:B:334:PHE:CD1	1:B:343:ILE:HD11	2.49	0.47
1:A:244:PHE:O	1:A:248:PHE:HD1	1.98	0.47
4:A:604:LMT:H61	4:D:604:LMT:H52	1.95	0.47
2:I:10:ILE:HG12	2:I:44:GLU:HG3	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:ARG:NH1	1:A:178:TYR:O	2.47	0.47
1:C:157:MET:HE3	1:C:157:MET:HB2	1.78	0.47
1:C:317:ARG:HH22	2:H:39:VAL:HB	1.79	0.47
1:B:157:MET:HG2	1:B:158:LEU:HD23	1.97	0.47
1:C:162:THR:HG23	1:C:167:PRO:HD2	1.96	0.47
1:D:217:LEU:HB3	1:D:218:PRO:HD3	1.96	0.47
1:D:280:ASP:O	1:D:284:PHE:N	2.47	0.47
1:D:334:PHE:CD1	1:D:343:ILE:HD11	2.50	0.47
4:D:602:LMT:H1B	4:D:603:LMT:H6'1	1.97	0.47
2:G:4:LYS:HD2	2:G:23:MET:HE2	1.97	0.47
1:D:8:LEU:HB2	1:D:9:PRO:HD2	1.96	0.47
1:D:310:ARG:HD3	2:I:52:ARG:NH2	2.30	0.47
1:B:279:ARG:HA	1:B:389:ILE:HA	1.97	0.47
2:G:35:SER:OG	2:G:36:MET:N	2.48	0.46
1:A:1:MET:HG3	1:A:2:ILE:H	1.79	0.46
1:D:44:GLU:OE2	1:D:178:TYR:OH	2.21	0.46
1:D:164:THR:OG1	1:D:165:SER:N	2.44	0.46
1:A:407:LEU:HG	1:A:411:TRP:CD1	2.51	0.46
4:A:603:LMT:H5B	4:A:603:LMT:H6D	1.96	0.46
1:A:118:GLN:OE1	1:A:122:ASN:ND2	2.49	0.46
1:B:172:LYS:NZ	1:B:176:GLU:OE2	2.49	0.46
1:D:56:LEU:HD11	1:D:163:PHE:HE2	1.81	0.46
1:A:18:PHE:HA	1:A:21:ILE:HG12	1.97	0.46
1:A:136:MET:O	1:A:140:MET:HG2	2.16	0.46
4:B:503:LMT:H1'	4:B:503:LMT:H21	1.66	0.46
1:C:84:TYR:CZ	1:C:93:VAL:HG21	2.51	0.46
1:C:173:ARG:NH2	1:C:267:LYS:O	2.49	0.46
1:D:57:THR:HG22	1:D:64:ILE:HG13	1.98	0.46
1:A:183:ASN:OD1	1:A:183:ASN:N	2.47	0.45
5:B:501:DGA:OXT	5:B:501:DGA:OG1	2.33	0.45
1:C:136:MET:HE3	1:C:153:PHE:HD1	1.81	0.45
1:C:217:LEU:HB3	1:C:218:PRO:HD3	1.97	0.45
1:D:235:THR:HA	1:D:238:VAL:HG12	1.98	0.45
1:A:68:LEU:O	1:A:71:ILE:HG23	2.16	0.45
1:A:261:SER:OG	1:A:266:ILE:O	2.22	0.45
1:C:308:LEU:HD22	1:C:313:VAL:HG11	1.98	0.45
1:A:14:TYR:O	1:A:205:LYS:NZ	2.39	0.45
1:A:32:ILE:HB	4:A:604:LMT:H91	1.98	0.45
1:B:239:MET:HE2	1:B:240:TYR:CE1	2.51	0.45
1:B:345:TYR:CD1	1:B:403:PHE:HB2	2.51	0.45
1:D:101:VAL:HG11	1:D:137:ILE:HD12	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:TYR:CD1	1:A:353:LEU:HD23	2.52	0.45
2:G:34:ASP:O	2:G:36:MET:N	2.50	0.45
1:B:317:ARG:NH1	2:G:37:GLY:HA2	2.32	0.45
1:D:98:SER:O	1:D:101:VAL:HG12	2.17	0.45
1:A:206:PHE:HB3	4:A:603:LMT:H21	1.99	0.45
3:B:502:PGT:H321	3:B:502:PGT:H2	1.69	0.45
1:C:220:LEU:HD13	1:C:220:LEU:HA	1.87	0.44
1:A:38:LYS:HE3	4:D:604:LMT:H11	2.00	0.44
1:A:40:PHE:O	1:A:42:ILE:N	2.49	0.44
1:B:54:LEU:HD21	4:B:509:LMT:H81	1.99	0.44
1:C:155:ARG:HD2	1:C:178:TYR:CZ	2.52	0.44
4:B:508:LMT:H51	4:B:508:LMT:H22	1.68	0.44
1:B:130:THR:O	1:B:134:VAL:HG23	2.17	0.44
1:D:280:ASP:OD2	1:D:356:ASN:ND2	2.51	0.44
2:H:6:GLU:O	2:H:10:ILE:HG12	2.18	0.44
1:B:36:PHE:HD2	4:B:507:LMT:H52	1.83	0.44
1:B:49:ILE:HG21	5:B:501:DGA:HA42	1.99	0.44
1:C:221:LYS:HE3	1:C:406:PHE:HD1	1.83	0.44
1:C:407:LEU:HG	1:C:411:TRP:CD1	2.53	0.44
3:D:601:PGT:H351	3:D:601:PGT:H382	1.68	0.44
1:D:345:TYR:CD1	1:D:403:PHE:HB2	2.53	0.44
1:B:232:ASN:HB2	1:B:234:PRO:HD2	2.00	0.44
1:C:94:PHE:HE1	1:C:137:ILE:HG22	1.83	0.44
1:A:217:LEU:HB3	1:A:218:PRO:HD3	2.00	0.43
1:B:182:PRO:HB2	1:B:187:LEU:HD22	2.00	0.43
1:D:26:ALA:HB2	4:D:608:LMT:H91	1.98	0.43
1:D:30:ILE:O	1:D:34:LEU:HD23	2.18	0.43
1:C:74:GLN:OE1	1:C:101:VAL:HG13	2.18	0.43
4:A:605:LMT:H1'	4:A:605:LMT:H21	1.54	0.43
1:B:200:LEU:HD12	1:B:200:LEU:HA	1.83	0.43
1:C:254:SER:HB2	1:C:271:ASN:HD22	1.83	0.43
1:D:285:TRP:CD1	1:D:353:LEU:HD11	2.54	0.43
1:A:94:PHE:HE1	1:A:137:ILE:HG22	1.84	0.43
4:D:607:LMT:H1B	4:D:607:LMT:H5'	1.50	0.43
1:A:210:GLN:OE1	4:A:603:LMT:O2'	2.36	0.43
4:C:506:LMT:H3'	4:C:506:LMT:H1B	1.59	0.43
2:H:22:MET:HE1	2:H:27:LEU:HG	2.01	0.43
1:C:47:VAL:HA	1:C:50:THR:HG22	1.98	0.43
2:G:22:MET:SD	2:G:25:GLU:HB3	2.59	0.43
2:H:73:VAL:HA	2:H:76:LEU:HG	2.00	0.43
1:B:31:PHE:CE1	1:B:187:LEU:HD12	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:317:ARG:NH2	2:G:36:MET:O	2.52	0.43
1:D:77:TRP:O	1:D:80:SER:HB3	2.18	0.43
1:C:232:ASN:HB2	1:C:234:PRO:HD2	2.00	0.43
1:B:348:PHE:HE2	1:B:399:SER:HB2	1.83	0.43
2:I:43:VAL:O	2:I:46:GLU:HB3	2.18	0.43
1:A:170:ARG:NH2	1:A:298:ASP:OD2	2.52	0.42
1:C:64:ILE:O	1:C:67:LEU:HB3	2.19	0.42
1:C:235:THR:O	1:C:238:VAL:HG12	2.19	0.42
1:C:280:ASP:HB3	1:C:356:ASN:OD1	2.19	0.42
1:D:82:LYS:HD3	1:D:148:PHE:HE1	1.84	0.42
1:B:68:LEU:HD13	1:B:68:LEU:HA	1.83	0.42
1:B:393:PHE:O	1:B:397:MET:HG2	2.18	0.42
2:G:58:PHE:HE1	2:G:63:TRP:HB2	1.83	0.42
1:C:78:VAL:HG22	1:C:137:ILE:HD11	2.01	0.42
1:D:48:SER:HA	1:D:160:MET:HG3	2.01	0.42
2:G:41:LEU:O	2:G:44:GLU:HB2	2.19	0.42
1:A:166:GLY:N	1:A:253:TYR:OH	2.53	0.42
1:B:11:LEU:HD12	1:B:11:LEU:HA	1.84	0.42
4:D:605:LMT:H71	4:D:605:LMT:H41	1.87	0.42
4:A:603:LMT:H51	4:A:603:LMT:H22	1.84	0.42
1:B:281:MET:HA	1:B:281:MET:HE3	2.01	0.42
4:B:510:LMT:H1B	4:B:510:LMT:H3'	1.84	0.42
1:C:94:PHE:CE1	1:C:137:ILE:HG22	2.55	0.42
1:C:136:MET:HE2	1:C:156:PHE:CD2	2.54	0.42
2:H:61:ASP:O	2:H:64:ASN:ND2	2.52	0.42
1:A:205:LYS:O	1:A:209:ALA:HB3	2.20	0.42
1:B:36:PHE:CD2	4:B:507:LMT:H52	2.54	0.42
1:B:325:TYR:CD1	1:B:353:LEU:HD23	2.55	0.42
1:C:78:VAL:HG11	1:C:153:PHE:CE1	2.54	0.42
1:D:72:VAL:O	1:D:76:ILE:HG13	2.19	0.42
1:D:75:ILE:HD11	1:D:154:LEU:HD21	2.02	0.42
1:D:107:LEU:HD12	1:D:121:LEU:HD11	2.02	0.42
1:A:56:LEU:HD12	1:A:63:GLN:HG3	2.02	0.42
1:A:157:MET:HE3	1:A:157:MET:HB2	1.75	0.42
1:B:235:THR:HA	1:B:238:VAL:HG12	2.01	0.42
1:C:207:VAL:O	1:C:211:ILE:HG12	2.19	0.42
1:D:68:LEU:HD13	1:D:68:LEU:HA	1.81	0.42
1:B:8:LEU:HD22	1:B:57:THR:HG21	2.02	0.41
1:B:270:ILE:H	1:B:270:ILE:HG12	1.69	0.41
3:C:501:PGT:H141	3:C:501:PGT:H171	1.76	0.41
1:D:174:PHE:CE1	1:D:266:ILE:HG21	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:7:VAL:HA	2:G:10:ILE:HG22	2.02	0.41
2:I:44:GLU:O	2:I:47:SER:OG	2.33	0.41
1:A:285:TRP:CZ3	1:A:288:TRP:HD1	2.38	0.41
1:B:280:ASP:OD1	1:B:281:MET:N	2.51	0.41
1:C:304:LEU:HA	1:C:307:VAL:HG12	2.02	0.41
1:D:111:GLU:HB3	1:D:112:PRO:HD3	2.02	0.41
2:F:11:ILE:HD12	2:F:19:VAL:HG23	2.02	0.41
1:A:188:LEU:HD13	1:A:188:LEU:HA	1.85	0.41
4:B:505:LMT:H1B	4:B:505:LMT:H6'2	1.87	0.41
1:C:131:PHE:HD1	1:C:131:PHE:HA	1.77	0.41
1:C:278:SER:OG	1:C:287:ARG:HD2	2.19	0.41
1:C:309:MET:HE3	2:H:43:VAL:HG21	2.02	0.41
4:A:604:LMT:H6D	4:D:606:LMT:H5'	2.02	0.41
1:B:185:ASP:OD1	1:B:186:GLU:N	2.53	0.41
1:D:75:ILE:HD11	1:D:154:LEU:HD11	2.02	0.41
2:G:63:TRP:CE3	2:G:69:ILE:HD13	2.55	0.41
1:A:136:MET:HG3	1:A:140:MET:HE2	2.01	0.41
1:A:246:LEU:HD23	1:A:400:PHE:CE2	2.56	0.41
1:A:258:LEU:HD23	1:A:258:LEU:HA	1.90	0.41
1:C:384:THR:O	1:C:387:LEU:HG	2.21	0.41
1:D:4:PHE:O	1:D:7:GLN:NE2	2.53	0.41
2:H:66:ALA:O	2:H:69:ILE:HG12	2.20	0.41
1:C:75:ILE:HD11	1:C:154:LEU:HD11	2.03	0.41
1:C:90:ASN:HB3	1:C:93:VAL:HG23	2.02	0.41
1:C:101:VAL:HG21	1:C:137:ILE:HG13	2.03	0.41
1:D:310:ARG:HH11	2:I:52:ARG:HH12	1.68	0.41
1:A:132:ARG:NH2	1:A:162:THR:OG1	2.51	0.41
1:B:292:LEU:HD11	1:B:296:PHE:HE1	1.85	0.41
1:D:10:HIS:CG	1:D:58:GLY:HA2	2.55	0.41
1:A:81:TYR:HB2	1:A:97:HIS:CD2	2.56	0.41
1:A:348:PHE:HA	1:A:351:ILE:HG12	2.02	0.41
1:B:263:LEU:HD23	1:B:263:LEU:HA	1.87	0.41
4:B:505:LMT:H123	4:B:506:LMT:H122	2.02	0.41
1:D:285:TRP:HD1	1:D:353:LEU:HD11	1.86	0.41
1:A:74:GLN:OE1	1:A:101:VAL:HG13	2.21	0.41
1:A:77:TRP:HA	1:A:80:SER:HB3	2.03	0.41
1:B:240:TYR:HA	1:B:397:MET:HE2	2.02	0.41
1:C:37:LYS:HA	1:C:37:LYS:HD3	1.89	0.41
1:C:285:TRP:CZ3	1:C:288:TRP:HD1	2.39	0.41
4:D:603:LMT:H41	4:D:606:LMT:H32	2.03	0.41
1:A:56:LEU:HD21	1:A:163:PHE:HE2	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:LEU:HD11	1:B:163:PHE:HE2	1.86	0.41
1:B:181:ILE:HA	1:B:182:PRO:HD3	1.97	0.41
1:C:38:LYS:HE2	1:C:38:LYS:HB2	1.90	0.41
1:C:200:LEU:HA	1:C:200:LEU:HD23	1.87	0.41
2:I:64:ASN:OD1	2:I:64:ASN:N	2.54	0.40
1:A:406:PHE:HE2	1:A:410:LEU:HD12	1.85	0.40
5:B:501:DGA:HBH2	5:B:501:DGA:HBT1	1.97	0.40
1:C:134:VAL:O	1:C:138:ILE:HG22	2.21	0.40
1:C:246:LEU:HD23	1:C:400:PHE:CE2	2.57	0.40
4:A:604:LMT:H62	4:A:604:LMT:H31	1.76	0.40
1:B:317:ARG:O	1:B:320:THR:OG1	2.27	0.40
5:B:501:DGA:HB31	4:B:509:LMT:H101	2.03	0.40
2:F:3:VAL:HG12	2:F:49:PHE:HE1	1.87	0.40
1:C:128:TYR:CZ	1:C:335:TRP:HH2	2.39	0.40
1:C:258:LEU:HD11	1:C:270:ILE:HA	2.02	0.40
1:D:308:LEU:HD13	1:D:308:LEU:HA	1.96	0.40
2:H:67:ASN:OD1	2:H:68:LYS:N	2.55	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	415/440 (94%)	398 (96%)	17 (4%)	0	100	100
1	B	417/440 (95%)	397 (95%)	20 (5%)	0	100	100
1	C	417/440 (95%)	402 (96%)	15 (4%)	0	100	100
1	D	417/440 (95%)	395 (95%)	22 (5%)	0	100	100
2	F	77/79 (98%)	76 (99%)	1 (1%)	0	100	100
2	G	77/79 (98%)	72 (94%)	5 (6%)	0	100	100
2	H	77/79 (98%)	69 (90%)	8 (10%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	I	77/79 (98%)	73 (95%)	4 (5%)	0	100	100
All	All	1974/2076 (95%)	1882 (95%)	92 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	371/394 (94%)	353 (95%)	18 (5%)	22	48
1	B	373/394 (95%)	358 (96%)	15 (4%)	28	54
1	C	373/394 (95%)	361 (97%)	12 (3%)	34	59
1	D	373/394 (95%)	357 (96%)	16 (4%)	26	51
2	F	71/71 (100%)	70 (99%)	1 (1%)	59	71
2	G	71/71 (100%)	70 (99%)	1 (1%)	59	71
2	H	71/71 (100%)	70 (99%)	1 (1%)	59	71
2	I	71/71 (100%)	70 (99%)	1 (1%)	59	71
All	All	1774/1860 (95%)	1709 (96%)	65 (4%)	31	56

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	HIS
1	A	64	ILE
1	A	71	ILE
1	A	89	ASP
1	A	100	LEU
1	A	119	SER
1	A	121	LEU
1	A	129	LEU
1	A	164	THR
1	A	169	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	183	ASN
1	A	188	LEU
1	A	208	LEU
1	A	289	HIS
1	A	304	LEU
1	A	313	VAL
1	A	353	LEU
1	A	412	PHE
1	B	54	LEU
1	B	60	HIS
1	B	64	ILE
1	B	68	LEU
1	B	110	VAL
1	B	126	ILE
1	B	137	ILE
1	B	187	LEU
1	B	239	MET
1	B	245	ASP
1	B	266	ILE
1	B	308	LEU
1	B	349	HIS
1	B	407	LEU
1	B	412	PHE
1	C	28	LEU
1	C	34	LEU
1	C	59	THR
1	C	117	THR
1	C	129	LEU
1	C	130	THR
1	C	164	THR
1	C	188	LEU
1	C	208	LEU
1	C	220	LEU
1	C	304	LEU
1	C	313	VAL
1	D	-3	PHE
1	D	5	LEU
1	D	110	VAL
1	D	126	ILE
1	D	129	LEU
1	D	162	THR
1	D	169	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	225	LEU
1	D	245	ASP
1	D	281	MET
1	D	304	LEU
1	D	347	ILE
1	D	360	LEU
1	D	387	LEU
1	D	392	THR
1	D	407	LEU
2	F	55	VAL
2	G	16	MET
2	H	51	ILE
2	I	14	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	311	ASN
1	D	356	ASN
2	G	78	ASN
2	I	78	ASN

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](#)

33 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	PGT	A	601	-	50,50,50	0.47	0	53,56,56	0.49	0
3	PGT	C	501	-	50,50,50	0.49	0	53,56,56	0.43	0
4	LMT	C	504	-	36,36,36	1.13	4 (11%)	47,47,47	0.97	2 (4%)
4	LMT	D	602	-	36,36,36	1.13	4 (11%)	47,47,47	0.96	1 (2%)
3	PGT	B	502	-	50,50,50	0.49	0	53,56,56	0.49	0
4	LMT	B	505	-	36,36,36	1.09	4 (11%)	47,47,47	0.97	3 (6%)
4	LMT	C	503	-	36,36,36	1.18	6 (16%)	47,47,47	0.95	1 (2%)
4	LMT	B	504	-	36,36,36	1.09	4 (11%)	47,47,47	0.97	2 (4%)
4	LMT	A	604	-	36,36,36	1.14	5 (13%)	47,47,47	0.99	1 (2%)
4	LMT	C	508	-	36,36,36	1.13	5 (13%)	47,47,47	1.04	1 (2%)
5	DGA	C	502	-	43,43,43	0.18	0	45,45,45	0.17	0
4	LMT	D	607	-	36,36,36	1.15	5 (13%)	47,47,47	0.99	2 (4%)
4	LMT	D	608	-	36,36,36	1.15	6 (16%)	47,47,47	0.96	1 (2%)
4	LMT	C	506	-	36,36,36	1.14	5 (13%)	47,47,47	1.00	1 (2%)
3	PGT	B	511	-	50,50,50	0.49	0	53,56,56	0.45	0
4	LMT	B	507	-	36,36,36	1.14	5 (13%)	47,47,47	0.98	2 (4%)
4	LMT	A	602	-	36,36,36	1.11	4 (11%)	47,47,47	0.99	3 (6%)
4	LMT	C	505	-	36,36,36	1.10	4 (11%)	47,47,47	0.96	3 (6%)
5	DGA	B	501	-	43,43,43	0.19	0	45,45,45	0.21	0
4	LMT	A	603	-	36,36,36	1.14	5 (13%)	47,47,47	1.03	3 (6%)
4	LMT	D	603	-	36,36,36	1.14	5 (13%)	47,47,47	0.98	2 (4%)
3	PGT	D	601	-	50,50,50	0.48	0	53,56,56	0.52	0
4	LMT	B	509	-	36,36,36	1.12	4 (11%)	47,47,47	0.98	1 (2%)
4	LMT	B	506	-	36,36,36	1.15	5 (13%)	47,47,47	1.01	2 (4%)
4	LMT	B	510	-	36,36,36	1.14	6 (16%)	47,47,47	0.95	2 (4%)
4	LMT	D	606	-	36,36,36	1.08	4 (11%)	47,47,47	1.01	3 (6%)
4	LMT	A	605	-	36,36,36	1.09	4 (11%)	47,47,47	0.98	4 (8%)
4	LMT	B	508	-	36,36,36	1.15	6 (16%)	47,47,47	1.08	3 (6%)
3	PGT	C	509	-	50,50,50	0.49	0	53,56,56	0.45	0
4	LMT	B	503	-	36,36,36	1.12	5 (13%)	47,47,47	0.98	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	LMT	C	507	-	36,36,36	1.15	5 (13%)	47,47,47	1.00	2 (4%)
4	LMT	D	604	-	36,36,36	1.15	5 (13%)	47,47,47	1.00	2 (4%)
4	LMT	D	605	-	36,36,36	1.18	5 (13%)	47,47,47	1.14	4 (8%)

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	PGT	A	601	-	-	21/55/55/55	-
3	PGT	C	501	-	-	25/55/55/55	-
4	LMT	C	504	-	-	9/21/61/61	0/2/2/2
4	LMT	D	602	-	-	10/21/61/61	0/2/2/2
3	PGT	B	502	-	-	18/55/55/55	-
4	LMT	B	505	-	-	9/21/61/61	0/2/2/2
4	LMT	C	503	-	-	12/21/61/61	0/2/2/2
4	LMT	B	504	-	-	12/21/61/61	0/2/2/2
4	LMT	A	604	-	-	12/21/61/61	0/2/2/2
4	LMT	C	508	-	-	15/21/61/61	0/2/2/2
5	DGA	C	502	-	-	20/45/45/45	-
4	LMT	D	607	-	-	11/21/61/61	0/2/2/2
4	LMT	D	608	-	-	10/21/61/61	0/2/2/2
4	LMT	C	506	-	-	8/21/61/61	0/2/2/2
3	PGT	B	511	-	-	14/55/55/55	-
4	LMT	B	507	-	-	7/21/61/61	0/2/2/2
4	LMT	A	602	-	-	5/21/61/61	0/2/2/2
4	LMT	C	505	-	-	7/21/61/61	0/2/2/2
5	DGA	B	501	-	-	18/45/45/45	-
4	LMT	A	603	-	-	11/21/61/61	0/2/2/2
4	LMT	D	603	-	-	7/21/61/61	0/2/2/2
3	PGT	D	601	-	-	30/55/55/55	-
4	LMT	B	509	-	-	6/21/61/61	0/2/2/2
4	LMT	B	506	-	-	11/21/61/61	0/2/2/2
4	LMT	B	510	-	-	10/21/61/61	0/2/2/2
4	LMT	D	606	-	-	8/21/61/61	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	LMT	A	605	-	-	10/21/61/61	0/2/2/2
4	LMT	B	508	-	-	10/21/61/61	0/2/2/2
3	PGT	C	509	-	-	22/55/55/55	-
4	LMT	B	503	-	-	5/21/61/61	0/2/2/2
4	LMT	C	507	-	-	7/21/61/61	0/2/2/2
4	LMT	D	604	-	-	14/21/61/61	0/2/2/2
4	LMT	D	605	-	-	7/21/61/61	0/2/2/2

All (120) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	603	LMT	O3'-C3'	-2.65	1.36	1.43
4	B	508	LMT	O4'-C4B	-2.61	1.36	1.43
4	B	507	LMT	O3'-C3'	-2.58	1.36	1.43
4	A	602	LMT	O3'-C3'	-2.57	1.36	1.43
4	D	607	LMT	O3'-C3'	-2.55	1.36	1.43
4	D	604	LMT	O3'-C3'	-2.54	1.36	1.43
4	D	608	LMT	O3'-C3'	-2.53	1.36	1.43
4	C	505	LMT	O3'-C3'	-2.53	1.36	1.43
4	D	605	LMT	O3'-C3'	-2.52	1.36	1.43
4	B	504	LMT	O3'-C3'	-2.52	1.36	1.43
4	C	503	LMT	O3'-C3'	-2.52	1.36	1.43
4	A	605	LMT	O3'-C3'	-2.51	1.36	1.43
4	C	508	LMT	O3'-C3'	-2.50	1.36	1.43
4	A	603	LMT	O3'-C3'	-2.50	1.36	1.43
4	C	507	LMT	O3'-C3'	-2.50	1.36	1.43
4	B	509	LMT	O3'-C3'	-2.50	1.36	1.43
4	B	505	LMT	O3'-C3'	-2.50	1.36	1.43
4	B	508	LMT	O3'-C3'	-2.49	1.36	1.43
4	B	510	LMT	O3'-C3'	-2.49	1.36	1.43
4	B	503	LMT	O3'-C3'	-2.49	1.36	1.43
4	D	607	LMT	O4'-C4B	-2.48	1.36	1.43
4	C	504	LMT	O3'-C3'	-2.48	1.36	1.43
4	B	506	LMT	O3'-C3'	-2.47	1.36	1.43
4	C	506	LMT	O3'-C3'	-2.46	1.36	1.43
4	A	604	LMT	O3'-C3'	-2.44	1.36	1.43
4	D	602	LMT	O3'-C3'	-2.44	1.36	1.43
4	D	604	LMT	O2'-C2'	-2.42	1.37	1.43
4	D	606	LMT	O3'-C3'	-2.42	1.37	1.43
4	D	607	LMT	O3B-C3B	-2.37	1.37	1.43
4	A	602	LMT	O2'-C2'	-2.37	1.37	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	508	LMT	O3B-C3B	-2.36	1.37	1.43
4	D	605	LMT	O2'-C2'	-2.33	1.37	1.43
4	D	608	LMT	O2B-C2B	-2.32	1.37	1.43
4	D	604	LMT	O2B-C2B	-2.31	1.37	1.43
4	B	507	LMT	O2'-C2'	-2.30	1.37	1.43
4	B	508	LMT	O2B-C2B	-2.28	1.37	1.43
4	C	503	LMT	O2'-C2'	-2.27	1.37	1.43
4	C	504	LMT	O2B-C2B	-2.26	1.37	1.43
4	B	509	LMT	O2B-C2B	-2.25	1.37	1.43
4	C	504	LMT	O3B-C3B	-2.25	1.37	1.43
4	D	608	LMT	O2'-C2'	-2.24	1.37	1.43
4	D	607	LMT	O2B-C2B	-2.23	1.37	1.43
4	A	603	LMT	O2B-C2B	-2.23	1.37	1.43
4	D	603	LMT	O2B-C2B	-2.23	1.37	1.43
4	B	510	LMT	O1'-C1'	-2.23	1.36	1.40
4	C	507	LMT	O2B-C2B	-2.23	1.37	1.43
4	B	504	LMT	O2B-C2B	-2.22	1.37	1.43
4	A	602	LMT	O2B-C2B	-2.22	1.37	1.43
4	D	606	LMT	O3B-C3B	-2.22	1.37	1.43
4	D	607	LMT	O2'-C2'	-2.22	1.37	1.43
4	A	605	LMT	O2B-C2B	-2.22	1.37	1.43
4	B	506	LMT	O3B-C3B	-2.21	1.37	1.43
4	B	507	LMT	O3B-C3B	-2.21	1.37	1.43
4	A	602	LMT	O3B-C3B	-2.21	1.37	1.43
4	D	603	LMT	O3B-C3B	-2.21	1.37	1.43
4	A	603	LMT	O2'-C2'	-2.21	1.37	1.43
4	A	604	LMT	O3B-C3B	-2.21	1.37	1.43
4	A	604	LMT	O2'-C2'	-2.21	1.37	1.43
4	C	503	LMT	O1'-C1'	-2.21	1.36	1.40
4	B	506	LMT	O2B-C2B	-2.20	1.37	1.43
4	B	506	LMT	O2'-C2'	-2.20	1.37	1.43
4	D	603	LMT	O2'-C2'	-2.20	1.37	1.43
4	D	606	LMT	O2B-C2B	-2.20	1.37	1.43
4	D	608	LMT	O3B-C3B	-2.20	1.37	1.43
4	D	605	LMT	O2B-C2B	-2.19	1.37	1.43
4	C	507	LMT	O3B-C3B	-2.19	1.37	1.43
4	B	505	LMT	O2B-C2B	-2.19	1.37	1.43
4	B	510	LMT	O3B-C3B	-2.19	1.37	1.43
4	D	604	LMT	O3B-C3B	-2.19	1.37	1.43
4	B	503	LMT	O2B-C2B	-2.19	1.37	1.43
4	D	602	LMT	O3B-C3B	-2.19	1.37	1.43
4	B	510	LMT	O2B-C2B	-2.19	1.37	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	506	LMT	O2B-C2B	-2.19	1.37	1.43
4	A	604	LMT	O2B-C2B	-2.19	1.37	1.43
4	C	506	LMT	O3B-C3B	-2.19	1.37	1.43
4	C	505	LMT	O2B-C2B	-2.18	1.37	1.43
4	A	603	LMT	O3B-C3B	-2.18	1.37	1.43
4	B	504	LMT	O3B-C3B	-2.18	1.37	1.43
4	B	509	LMT	O3B-C3B	-2.18	1.37	1.43
4	D	602	LMT	O2B-C2B	-2.18	1.37	1.43
4	D	602	LMT	O2'-C2'	-2.17	1.37	1.43
4	B	505	LMT	O3B-C3B	-2.17	1.37	1.43
4	C	505	LMT	O3B-C3B	-2.17	1.37	1.43
4	B	503	LMT	O3B-C3B	-2.17	1.37	1.43
4	B	504	LMT	O2'-C2'	-2.17	1.37	1.43
4	B	508	LMT	O2'-C2'	-2.17	1.37	1.43
4	B	503	LMT	O2'-C2'	-2.16	1.37	1.43
4	C	503	LMT	O3B-C3B	-2.16	1.37	1.43
4	C	508	LMT	O2'-C2'	-2.16	1.37	1.43
4	A	604	LMT	O1'-C1'	-2.15	1.36	1.40
4	C	503	LMT	O2B-C2B	-2.15	1.37	1.43
4	C	508	LMT	O3B-C3B	-2.15	1.37	1.43
4	B	506	LMT	O1'-C1'	-2.15	1.36	1.40
4	B	509	LMT	O2'-C2'	-2.14	1.37	1.43
4	B	507	LMT	O2B-C2B	-2.14	1.37	1.43
4	C	507	LMT	O2'-C2'	-2.14	1.37	1.43
4	B	505	LMT	O2'-C2'	-2.13	1.37	1.43
4	C	505	LMT	O2'-C2'	-2.13	1.37	1.43
4	C	504	LMT	O2'-C2'	-2.12	1.37	1.43
4	A	605	LMT	O2'-C2'	-2.12	1.37	1.43
4	B	507	LMT	O1'-C1'	-2.12	1.36	1.40
4	C	508	LMT	O2B-C2B	-2.10	1.37	1.43
4	D	606	LMT	O2'-C2'	-2.10	1.37	1.43
4	C	506	LMT	O2'-C2'	-2.09	1.37	1.43
4	D	604	LMT	O1'-C1'	-2.09	1.36	1.40
4	D	603	LMT	O1'-C1'	-2.09	1.36	1.40
4	D	605	LMT	O3B-C3B	-2.09	1.37	1.43
4	C	507	LMT	O1'-C1'	-2.08	1.36	1.40
4	A	605	LMT	O3B-C3B	-2.08	1.37	1.43
4	A	603	LMT	O1'-C1'	-2.07	1.36	1.40
4	B	510	LMT	O2'-C2'	-2.07	1.37	1.43
4	C	503	LMT	O4'-C4B	-2.07	1.37	1.43
4	C	506	LMT	O1'-C1'	-2.06	1.36	1.40
4	D	605	LMT	O1'-C1'	-2.03	1.36	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	608	LMT	O4'-C4B	-2.02	1.38	1.43
4	B	508	LMT	O1'-C1'	-2.01	1.36	1.40
4	C	508	LMT	O1'-C1'	-2.01	1.36	1.40
4	B	503	LMT	O4'-C4B	-2.01	1.38	1.43
4	D	608	LMT	O1'-C1'	-2.00	1.36	1.40
4	B	510	LMT	O4'-C4B	-2.00	1.38	1.43

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	605	LMT	C3'-C4'-C5'	-3.40	103.40	110.93
4	B	508	LMT	C1'-O5'-C5'	-3.16	107.54	113.72
4	C	508	LMT	C1'-O5'-C5'	-3.08	107.70	113.72
4	B	506	LMT	C1'-O5'-C5'	-3.08	107.70	113.72
4	D	605	LMT	C1'-O5'-C5'	-3.01	107.84	113.72
4	A	603	LMT	C1'-O5'-C5'	-3.00	107.87	113.72
4	C	506	LMT	C1'-O5'-C5'	-2.90	108.05	113.72
4	D	602	LMT	C1'-O5'-C5'	-2.83	108.20	113.72
4	D	604	LMT	C1'-O5'-C5'	-2.78	108.29	113.72
4	C	507	LMT	C1'-O5'-C5'	-2.76	108.33	113.72
4	C	503	LMT	C1'-O5'-C5'	-2.72	108.41	113.72
4	B	503	LMT	C1'-O5'-C5'	-2.72	108.41	113.72
4	B	509	LMT	C1'-O5'-C5'	-2.63	108.58	113.72
4	C	504	LMT	C1'-O5'-C5'	-2.57	108.70	113.72
4	B	507	LMT	C1'-O5'-C5'	-2.54	108.75	113.72
4	C	507	LMT	C3'-C4'-C5'	-2.54	105.30	110.93
4	A	602	LMT	O5'-C5'-C6'	2.53	112.70	106.44
4	D	607	LMT	C1'-O5'-C5'	-2.52	108.81	113.72
4	D	606	LMT	O5'-C5'-C6'	2.49	112.60	106.44
4	A	603	LMT	C3'-C4'-C5'	-2.47	105.45	110.93
4	D	608	LMT	C1'-O5'-C5'	-2.40	109.03	113.72
4	B	504	LMT	C3'-C4'-C5'	-2.39	105.64	110.93
4	B	503	LMT	C3'-C4'-C5'	-2.37	105.67	110.93
4	C	504	LMT	C3'-C4'-C5'	-2.36	105.71	110.93
4	D	603	LMT	C3'-C4'-C5'	-2.34	105.75	110.93
4	D	606	LMT	O5'-C5'-C4'	2.31	114.49	109.72
4	B	510	LMT	C1'-O5'-C5'	-2.30	109.22	113.72
4	A	605	LMT	O5'-C5'-C4'	2.28	114.43	109.72
4	D	603	LMT	C1'-O5'-C5'	-2.25	109.33	113.72
4	C	505	LMT	O5'-C5'-C4'	2.24	114.36	109.72
4	D	604	LMT	C3'-C4'-C5'	-2.24	105.96	110.93
4	B	505	LMT	O1'-C1'-C2'	2.23	111.66	108.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	505	LMT	O5'-C5'-C4'	2.23	114.33	109.72
4	B	505	LMT	C3'-C4'-C5'	-2.20	106.04	110.93
4	C	505	LMT	C3'-C4'-C5'	-2.19	106.08	110.93
4	A	602	LMT	O1'-C1'-C2'	2.18	111.58	108.27
4	B	504	LMT	O5'-C5'-C4'	2.17	114.21	109.72
4	C	505	LMT	O1'-C1'-C2'	2.14	111.53	108.27
4	D	605	LMT	O5B-C5B-C4B	2.13	113.54	109.70
4	B	506	LMT	C3'-C4'-C5'	-2.13	106.22	110.93
4	B	508	LMT	O5B-C5B-C6B	2.11	111.67	106.44
4	A	605	LMT	C3'-C4'-C5'	-2.09	106.30	110.93
4	A	605	LMT	O5B-C5B-C6B	2.08	111.58	106.44
4	B	508	LMT	O5B-C5B-C4B	2.06	113.42	109.70
4	D	607	LMT	O5B-C5B-C6B	2.05	111.52	106.44
4	A	604	LMT	C1'-O5'-C5'	-2.04	109.73	113.72
4	A	602	LMT	O5'-C5'-C4'	2.03	113.93	109.72
4	D	605	LMT	O5B-C5B-C6B	2.02	111.46	106.44
4	B	507	LMT	C3'-C4'-C5'	-2.02	106.44	110.93
4	A	605	LMT	O1'-C1'-C2'	2.01	111.33	108.27
4	D	606	LMT	O1'-C1'-C2'	2.01	111.33	108.27
4	A	603	LMT	O5B-C5B-C4B	2.01	113.32	109.70
4	B	510	LMT	C3'-C4'-C5'	-2.00	106.49	110.93

There are no chirality outliers.

All (401) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	601	PGT	C1-O3P-P-O2P
3	A	601	PGT	C4-O4P-P-O3P
3	A	601	PGT	C4-O4P-P-O1P
3	A	601	PGT	C4-O4P-P-O2P
3	A	601	PGT	C4-C5-C6-O6
3	B	502	PGT	C32-C31-O2-C2
3	B	502	PGT	O31-C31-O2-C2
3	B	502	PGT	C4-C5-C6-O6
3	B	511	PGT	C1-O3P-P-O4P
3	B	511	PGT	C4-C5-C6-O6
3	C	501	PGT	C32-C31-O2-C2
3	C	501	PGT	O31-C31-O2-C2
3	C	501	PGT	C1-O3P-P-O1P
3	C	501	PGT	C4-O4P-P-O2P
3	C	501	PGT	C4-C5-C6-O6
3	D	601	PGT	O31-C31-O2-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	D	601	PGT	C1-O3P-P-O1P
3	D	601	PGT	C4-C5-C6-O6
3	D	601	PGT	O11-C11-O3-C3
3	D	601	PGT	C12-C11-O3-C3
4	A	603	LMT	O5'-C1'-O1'-C1
4	A	604	LMT	O5'-C1'-O1'-C1
4	A	605	LMT	C2-C1-O1'-C1'
4	B	505	LMT	O5'-C1'-O1'-C1
4	B	507	LMT	O5'-C1'-O1'-C1
4	B	509	LMT	O5'-C1'-O1'-C1
4	C	503	LMT	C2'-C1'-O1'-C1
4	C	503	LMT	O5'-C1'-O1'-C1
4	C	504	LMT	O5'-C1'-O1'-C1
4	D	603	LMT	O5'-C1'-O1'-C1
4	D	605	LMT	C2-C1-O1'-C1'
4	D	607	LMT	O5'-C1'-O1'-C1
4	D	607	LMT	C2-C1-O1'-C1'
4	D	608	LMT	O5'-C1'-O1'-C1
4	D	608	LMT	C2-C1-O1'-C1'
5	C	502	DGA	CB2-CB1-OG2-CG2
5	C	502	DGA	CG1-CG2-CG3-OXT
5	C	502	DGA	OG2-CG2-CG3-OXT
4	A	604	LMT	C5'-C4'-O1B-C1B
5	C	502	DGA	OA1-CA1-OG1-CG1
4	A	602	LMT	O5B-C1B-O1B-C4'
4	D	604	LMT	O5B-C1B-O1B-C4'
4	D	608	LMT	O5B-C1B-O1B-C4'
5	C	502	DGA	CA2-CA1-OG1-CG1
3	C	509	PGT	O11-C11-O3-C3
4	A	605	LMT	O5B-C1B-O1B-C4'
5	B	501	DGA	OB1-CB1-OG2-CG2
5	C	502	DGA	OB1-CB1-OG2-CG2
4	B	508	LMT	C4'-C5'-C6'-O6'
4	D	607	LMT	C5'-C4'-O1B-C1B
3	C	509	PGT	C12-C11-O3-C3
4	A	603	LMT	O5'-C5'-C6'-O6'
3	D	601	PGT	C32-C31-O2-C2
5	B	501	DGA	CB2-CB1-OG2-CG2
4	C	508	LMT	O5'-C5'-C6'-O6'
4	B	504	LMT	O5B-C5B-C6B-O6B
4	C	503	LMT	O5B-C5B-C6B-O6B
4	C	504	LMT	O5B-C5B-C6B-O6B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	B	508	LMT	C3'-C4'-O1B-C1B
4	D	604	LMT	O5B-C5B-C6B-O6B
4	D	608	LMT	O5'-C5'-C6'-O6'
4	B	506	LMT	C4B-C5B-C6B-O6B
4	C	506	LMT	C3'-C4'-O1B-C1B
4	B	504	LMT	C2B-C1B-O1B-C4'
3	C	501	PGT	O4P-C4-C5-O5
3	C	509	PGT	O4P-C4-C5-O5
4	C	503	LMT	O5'-C5'-C6'-O6'
4	D	605	LMT	O5B-C5B-C6B-O6B
4	D	603	LMT	O5B-C5B-C6B-O6B
4	B	503	LMT	C4B-C5B-C6B-O6B
4	D	603	LMT	C4B-C5B-C6B-O6B
4	A	602	LMT	O5'-C5'-C6'-O6'
4	C	508	LMT	O5B-C5B-C6B-O6B
4	D	604	LMT	O5'-C5'-C6'-O6'
4	A	603	LMT	C4'-C5'-C6'-O6'
4	B	506	LMT	O5B-C5B-C6B-O6B
4	C	507	LMT	O5'-C5'-C6'-O6'
4	D	606	LMT	C4B-C5B-C6B-O6B
4	B	504	LMT	O5B-C1B-O1B-C4'
4	B	508	LMT	O5B-C5B-C6B-O6B
4	D	608	LMT	O5B-C5B-C6B-O6B
4	A	602	LMT	C4'-C5'-C6'-O6'
4	C	508	LMT	C4'-C5'-C6'-O6'
4	D	604	LMT	C4B-C5B-C6B-O6B
4	B	503	LMT	O5B-C5B-C6B-O6B
4	B	504	LMT	C4B-C5B-C6B-O6B
4	C	503	LMT	C4B-C5B-C6B-O6B
4	B	510	LMT	O5'-C1'-O1'-C1
4	D	604	LMT	O5'-C1'-O1'-C1
4	D	606	LMT	C4'-C5'-C6'-O6'
5	B	501	DGA	CDA-CEA-CFA-CGA
4	A	603	LMT	O5B-C5B-C6B-O6B
4	B	504	LMT	O5'-C5'-C6'-O6'
4	B	508	LMT	O5'-C5'-C6'-O6'
4	B	510	LMT	O5B-C5B-C6B-O6B
4	A	604	LMT	C4B-C5B-C6B-O6B
4	D	602	LMT	C4B-C5B-C6B-O6B
4	C	503	LMT	C4'-C5'-C6'-O6'
4	C	504	LMT	C4B-C5B-C6B-O6B
4	B	510	LMT	C5'-C4'-O1B-C1B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	C	501	PGT	O4P-C4-C5-C6
4	D	606	LMT	O5'-C5'-C6'-O6'
4	D	605	LMT	C4B-C5B-C6B-O6B
4	B	505	LMT	C3'-C4'-O1B-C1B
4	B	510	LMT	C4B-C5B-C6B-O6B
4	A	604	LMT	C2'-C1'-O1'-C1
4	B	510	LMT	C2'-C1'-O1'-C1
4	C	504	LMT	C2'-C1'-O1'-C1
4	D	604	LMT	C2'-C1'-O1'-C1
4	D	607	LMT	C2'-C1'-O1'-C1
4	D	608	LMT	C2'-C1'-O1'-C1
3	A	601	PGT	O4P-C4-C5-O5
4	D	604	LMT	C4'-C5'-C6'-O6'
4	C	505	LMT	O5'-C5'-C6'-O6'
4	A	603	LMT	C4B-C5B-C6B-O6B
4	D	606	LMT	O5B-C5B-C6B-O6B
4	D	608	LMT	C4'-C5'-C6'-O6'
3	A	601	PGT	O2-C2-C3-O3
3	D	601	PGT	C14-C15-C16-C17
3	A	601	PGT	O5-C5-C6-O6
3	B	511	PGT	O5-C5-C6-O6
3	C	501	PGT	O5-C5-C6-O6
3	D	601	PGT	O5-C5-C6-O6
4	B	505	LMT	C4B-C5B-C6B-O6B
4	A	604	LMT	O5B-C5B-C6B-O6B
4	A	605	LMT	O5'-C5'-C6'-O6'
4	A	604	LMT	O1'-C1-C2-C3
4	C	508	LMT	C4B-C5B-C6B-O6B
4	B	504	LMT	C4'-C5'-C6'-O6'
4	C	507	LMT	C4'-C5'-C6'-O6'
4	D	608	LMT	C4B-C5B-C6B-O6B
4	C	506	LMT	O5'-C1'-O1'-C1
4	D	602	LMT	O5B-C5B-C6B-O6B
4	B	508	LMT	C4B-C5B-C6B-O6B
4	C	506	LMT	O5B-C5B-C6B-O6B
4	D	605	LMT	O1'-C1-C2-C3
4	B	507	LMT	O1'-C1-C2-C3
4	D	602	LMT	C5'-C4'-O1B-C1B
3	C	509	PGT	O4P-C4-C5-C6
5	C	502	DGA	CA9-CAA-CBA-CCA
4	C	504	LMT	O1'-C1-C2-C3
4	B	505	LMT	C5'-C4'-O1B-C1B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	D	607	LMT	C2B-C1B-O1B-C4'
4	B	505	LMT	C2'-C1'-O1'-C1
4	C	506	LMT	C2'-C1'-O1'-C1
5	B	501	DGA	CG1-CG2-OG2-CB1
4	D	602	LMT	C1-C2-C3-C4
4	C	507	LMT	O5B-C5B-C6B-O6B
3	D	601	PGT	C16-C17-C18-C19
3	B	502	PGT	C22-C23-C24-C25
5	B	501	DGA	CB7-CB8-CB9-CAB
4	B	506	LMT	C4-C5-C6-C7
4	D	603	LMT	C1-C2-C3-C4
4	A	605	LMT	C3-C4-C5-C6
5	B	501	DGA	CA2-CA3-CA4-CA5
3	B	502	PGT	O5-C5-C6-O6
4	B	504	LMT	C2-C1-O1'-C1'
4	B	505	LMT	C2-C1-O1'-C1'
4	B	510	LMT	C2-C1-O1'-C1'
4	C	505	LMT	C2-C1-O1'-C1'
4	C	506	LMT	C2-C1-O1'-C1'
4	B	510	LMT	C3'-C4'-O1B-C1B
3	A	601	PGT	C32-C31-O2-C2
3	B	502	PGT	C31-C32-C33-C34
4	D	606	LMT	C1-C2-C3-C4
4	A	603	LMT	C4-C5-C6-C7
4	C	503	LMT	O1'-C1-C2-C3
3	A	601	PGT	C36-C37-C38-C39
4	D	602	LMT	C6-C7-C8-C9
4	D	602	LMT	C11-C10-C9-C8
3	A	601	PGT	O31-C31-O2-C2
4	B	504	LMT	C3-C4-C5-C6
4	D	608	LMT	C7-C8-C9-C10
4	D	607	LMT	O5B-C1B-O1B-C4'
3	B	502	PGT	C21-C22-C23-C24
3	C	509	PGT	C13-C14-C15-C16
4	C	507	LMT	C5-C6-C7-C8
4	C	508	LMT	O5'-C1'-O1'-C1
4	B	507	LMT	C2'-C1'-O1'-C1
4	B	507	LMT	C3-C4-C5-C6
5	C	502	DGA	CBB-CAB-CB9-CB8
4	B	503	LMT	O1'-C1-C2-C3
3	C	509	PGT	C32-C31-O2-C2
5	B	501	DGA	CB9-CAB-CBB-CCB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	B	508	LMT	C5'-C4'-O1B-C1B
4	B	509	LMT	C11-C10-C9-C8
4	C	503	LMT	C3-C4-C5-C6
4	D	604	LMT	C2-C3-C4-C5
5	C	502	DGA	CDA-CEA-CFA-CGA
4	C	503	LMT	C5'-C4'-O1B-C1B
3	D	601	PGT	O3P-C1-C2-O2
3	C	501	PGT	C34-C35-C36-C37
4	A	605	LMT	C7-C8-C9-C10
3	A	601	PGT	C16-C17-C18-C19
4	B	505	LMT	C2-C3-C4-C5
4	B	505	LMT	O5B-C5B-C6B-O6B
3	D	601	PGT	C42-C43-C44-C45
3	A	601	PGT	C14-C15-C16-C17
4	A	603	LMT	C6-C7-C8-C9
3	C	501	PGT	C12-C13-C14-C15
4	B	504	LMT	C11-C10-C9-C8
4	D	602	LMT	C3'-C4'-O1B-C1B
4	D	602	LMT	O5'-C5'-C6'-O6'
3	C	509	PGT	O31-C31-O2-C2
3	B	511	PGT	C31-C32-C33-C34
3	D	601	PGT	C31-C32-C33-C34
4	C	505	LMT	C6-C7-C8-C9
4	C	505	LMT	O5B-C5B-C6B-O6B
4	D	607	LMT	O5B-C5B-C6B-O6B
4	A	603	LMT	O1'-C1-C2-C3
5	B	501	DGA	CFA-CGA-CHA-CIA
4	B	509	LMT	C2'-C1'-O1'-C1
3	A	601	PGT	C1-C2-C3-O3
4	D	604	LMT	C11-C10-C9-C8
4	B	509	LMT	O5B-C5B-C6B-O6B
3	B	511	PGT	C37-C38-C39-C40
4	B	506	LMT	C5-C6-C7-C8
4	C	508	LMT	C11-C10-C9-C8
3	D	601	PGT	C2-C1-O3P-P
4	D	603	LMT	C4-C5-C6-C7
4	A	605	LMT	O5B-C5B-C6B-O6B
4	C	506	LMT	C5'-C4'-O1B-C1B
4	B	505	LMT	C1-C2-C3-C4
3	C	509	PGT	C42-C43-C44-C45
4	A	605	LMT	C6-C7-C8-C9
3	C	509	PGT	C40-C41-C42-C43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	D	601	PGT	C17-C18-C19-C20
3	B	511	PGT	O2-C2-C3-O3
5	C	502	DGA	CB7-CB8-CB9-CAB
4	A	605	LMT	C5-C6-C7-C8
4	B	507	LMT	O5B-C5B-C6B-O6B
3	D	601	PGT	C35-C36-C37-C38
3	B	502	PGT	C45-C46-C47-C48
4	B	503	LMT	C2-C1-O1'-C1'
4	B	507	LMT	C2-C1-O1'-C1'
4	B	508	LMT	C2-C1-O1'-C1'
4	D	602	LMT	C2-C1-O1'-C1'
4	C	507	LMT	C2'-C1'-O1'-C1
4	D	603	LMT	C2'-C1'-O1'-C1
3	D	601	PGT	O3P-C1-C2-C3
3	C	501	PGT	C33-C34-C35-C36
4	C	507	LMT	C4-C5-C6-C7
4	C	503	LMT	C3'-C4'-O1B-C1B
5	B	501	DGA	CAA-CBA-CCA-CDA
3	B	502	PGT	C1-C2-C3-O3
3	B	511	PGT	C1-C2-C3-O3
3	C	501	PGT	C1-C2-C3-O3
3	C	509	PGT	C1-C2-C3-O3
3	C	509	PGT	C34-C35-C36-C37
4	C	508	LMT	O5B-C1B-O1B-C4'
4	A	603	LMT	C11-C10-C9-C8
3	B	511	PGT	O3P-C1-C2-O2
3	D	601	PGT	C12-C13-C14-C15
3	B	502	PGT	C5-C4-O4P-P
5	C	502	DGA	CB3-CB4-CB5-CB6
4	D	605	LMT	C3-C4-C5-C6
3	C	501	PGT	O2-C2-C3-O3
3	D	601	PGT	C32-C33-C34-C35
4	C	508	LMT	C4-C5-C6-C7
4	A	603	LMT	C5-C6-C7-C8
3	D	601	PGT	O4P-C4-C5-O5
5	B	501	DGA	CBB-CAB-CB9-CB8
3	A	601	PGT	C17-C18-C19-C20
4	B	504	LMT	C2-C3-C4-C5
5	C	502	DGA	CB4-CB5-CB6-CB7
4	C	504	LMT	C5-C6-C7-C8
5	B	501	DGA	CA4-CA5-CA6-CA7
3	C	501	PGT	C12-C11-O3-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	D	601	PGT	C1-C2-C3-O3
5	C	502	DGA	OG1-CG1-CG2-CG3
3	D	601	PGT	C41-C42-C43-C44
3	B	502	PGT	O2-C2-C3-O3
3	C	509	PGT	O2-C2-C3-O3
5	C	502	DGA	OG1-CG1-CG2-OG2
4	D	604	LMT	C3-C4-C5-C6
3	C	509	PGT	C37-C38-C39-C40
4	B	510	LMT	C7-C8-C9-C10
4	C	508	LMT	C2'-C1'-O1'-C1
3	B	511	PGT	C12-C11-O3-C3
4	A	602	LMT	C2-C1-O1'-C1'
4	C	504	LMT	C2-C1-O1'-C1'
4	C	508	LMT	C2-C1-O1'-C1'
3	C	509	PGT	C39-C40-C41-C42
3	C	509	PGT	C20-C21-C22-C23
3	B	511	PGT	O3P-C1-C2-C3
4	B	508	LMT	C11-C10-C9-C8
3	D	601	PGT	C34-C35-C36-C37
4	B	506	LMT	C3-C4-C5-C6
5	B	501	DGA	CB4-CB5-CB6-CB7
3	C	501	PGT	O11-C11-O3-C3
3	D	601	PGT	C23-C24-C25-C26
3	A	601	PGT	C23-C24-C25-C26
3	B	511	PGT	O11-C11-O3-C3
3	D	601	PGT	O2-C2-C3-O3
3	B	502	PGT	C38-C39-C40-C41
3	C	501	PGT	C38-C39-C40-C41
3	B	511	PGT	C1-O3P-P-O1P
3	C	501	PGT	C4-O4P-P-O3P
3	C	501	PGT	C4-O4P-P-O1P
3	C	509	PGT	C4-O4P-P-O1P
3	D	601	PGT	C4-O4P-P-O1P
4	C	508	LMT	C5'-C4'-O1B-C1B
3	C	509	PGT	C5-C4-O4P-P
4	D	604	LMT	C7-C8-C9-C10
3	C	501	PGT	C15-C16-C17-C18
3	A	601	PGT	C1-C2-O2-C31
4	B	509	LMT	C1-C2-C3-C4
4	D	607	LMT	C9-C10-C11-C12
3	C	501	PGT	O3P-C1-C2-O2
4	C	504	LMT	C6-C7-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	C	501	PGT	C23-C24-C25-C26
5	B	501	DGA	CCB-CDB-CEB-CFB
4	D	607	LMT	C3'-C4'-O1B-C1B
4	C	503	LMT	C5-C6-C7-C8
4	B	508	LMT	C4-C5-C6-C7
5	B	501	DGA	CFB-CGB-CHB-CIB
4	D	606	LMT	C9-C10-C11-C12
5	B	501	DGA	CDB-CEB-CFB-CGB
3	C	509	PGT	C31-C32-C33-C34
4	C	508	LMT	C2B-C1B-O1B-C4'
3	C	501	PGT	C45-C46-C47-C48
4	B	506	LMT	C2-C1-O1'-C1'
4	D	604	LMT	C2-C1-O1'-C1'
5	C	502	DGA	CEA-CFA-CGA-CHA
4	B	507	LMT	C5'-C4'-O1B-C1B
3	B	502	PGT	C17-C18-C19-C20
3	A	601	PGT	C20-C21-C22-C23
4	B	504	LMT	C5-C6-C7-C8
5	B	501	DGA	CA6-CA7-CA8-CA9
3	A	601	PGT	C19-C20-C21-C22
3	B	502	PGT	C19-C20-C21-C22
4	B	510	LMT	C11-C10-C9-C8
4	D	608	LMT	C11-C10-C9-C8
4	A	604	LMT	O5B-C1B-O1B-C4'
4	B	509	LMT	O5'-C5'-C6'-O6'
4	C	506	LMT	C4B-C5B-C6B-O6B
5	B	501	DGA	CEA-CFA-CGA-CHA
4	D	606	LMT	C11-C10-C9-C8
4	C	506	LMT	C3-C4-C5-C6
4	A	604	LMT	C2-C3-C4-C5
3	C	501	PGT	C17-C18-C19-C20
4	D	602	LMT	C3-C4-C5-C6
3	C	509	PGT	C41-C42-C43-C44
4	C	508	LMT	C7-C8-C9-C10
3	B	511	PGT	C40-C41-C42-C43
4	C	504	LMT	C3-C4-C5-C6
3	D	601	PGT	C22-C23-C24-C25
3	B	502	PGT	O3-C11-C12-C13
3	C	509	PGT	C32-C33-C34-C35
3	B	511	PGT	C18-C19-C20-C21
3	C	501	PGT	C14-C15-C16-C17
4	A	604	LMT	C7-C8-C9-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	A	605	LMT	C4-C5-C6-C7
4	A	605	LMT	C11-C10-C9-C8
4	D	603	LMT	C3-C4-C5-C6
3	D	601	PGT	C19-C20-C21-C22
4	C	507	LMT	C9-C10-C11-C12
4	B	510	LMT	C3-C4-C5-C6
4	C	508	LMT	C3-C4-C5-C6
4	B	506	LMT	O5'-C1'-O1'-C1
4	B	504	LMT	C4-C5-C6-C7
4	C	505	LMT	C4-C5-C6-C7
3	C	509	PGT	C14-C15-C16-C17
3	A	601	PGT	O3P-C1-C2-C3
3	C	501	PGT	O3P-C1-C2-C3
3	B	502	PGT	C23-C24-C25-C26
4	C	503	LMT	C11-C10-C9-C8
4	B	506	LMT	O5B-C1B-O1B-C4'
3	B	502	PGT	C44-C45-C46-C47
4	C	505	LMT	C9-C10-C11-C12
5	C	502	DGA	OG1-CA1-CA2-CA3
4	A	604	LMT	C2-C1-O1'-C1'
4	D	606	LMT	C2-C1-O1'-C1'
3	D	601	PGT	O3-C11-C12-C13
4	B	506	LMT	C5'-C4'-O1B-C1B
4	A	603	LMT	C5'-C4'-O1B-C1B
4	B	506	LMT	C6-C7-C8-C9
3	A	601	PGT	C12-C13-C14-C15
5	C	502	DGA	CDB-CEB-CFB-CGB
3	C	509	PGT	C21-C22-C23-C24
4	D	607	LMT	O1'-C1-C2-C3
4	D	605	LMT	C2-C3-C4-C5
4	A	604	LMT	C2B-C1B-O1B-C4'
5	B	501	DGA	CAB-CBB-CCB-CDB
4	A	602	LMT	C7-C8-C9-C10
4	C	505	LMT	C3-C4-C5-C6
5	C	502	DGA	CFA-CGA-CHA-CIA
4	D	604	LMT	C6-C7-C8-C9
3	B	502	PGT	C36-C37-C38-C39
3	D	601	PGT	C15-C16-C17-C18
4	C	508	LMT	C3'-C4'-O1B-C1B
5	C	502	DGA	CCB-CDB-CEB-CFB
5	C	502	DGA	OA1-CA1-CA2-CA3
4	B	506	LMT	C7-C8-C9-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	D	605	LMT	O5B-C1B-O1B-C4'
4	B	503	LMT	C4-C5-C6-C7
4	A	604	LMT	C4'-C5'-C6'-O6'
3	D	601	PGT	O11-C11-C12-C13
4	D	604	LMT	C5'-C4'-O1B-C1B
4	D	607	LMT	C2-C3-C4-C5
4	B	508	LMT	C5-C6-C7-C8

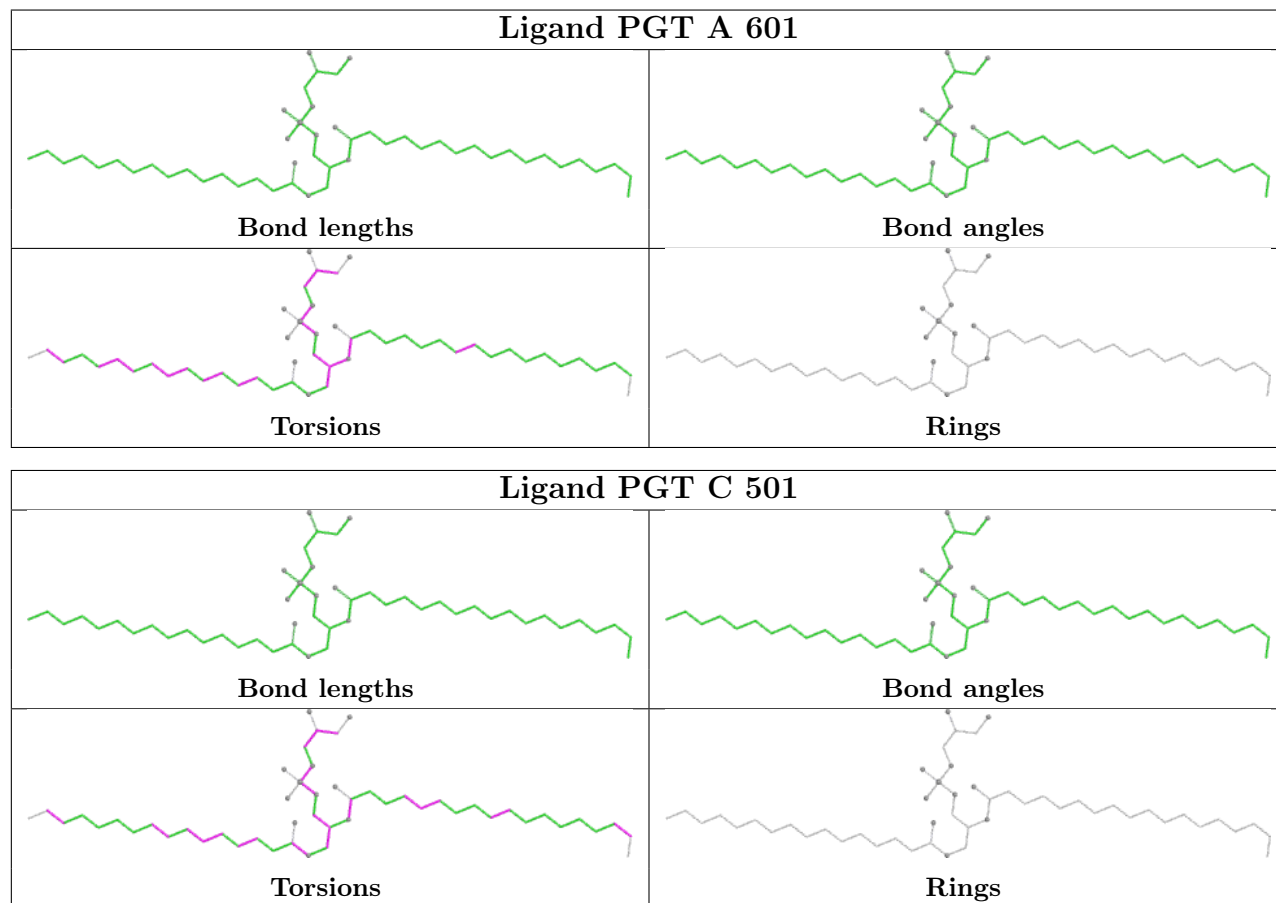
There are no ring outliers.

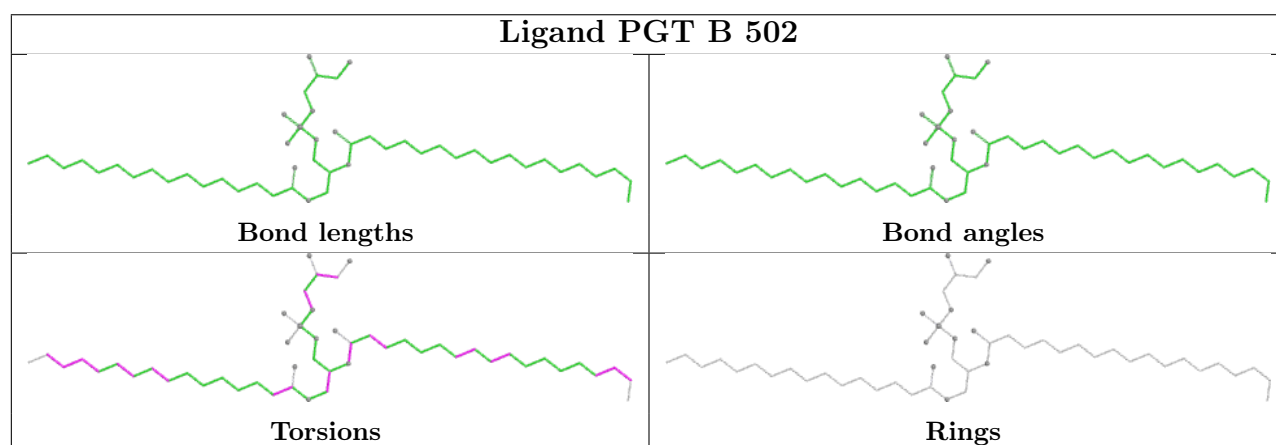
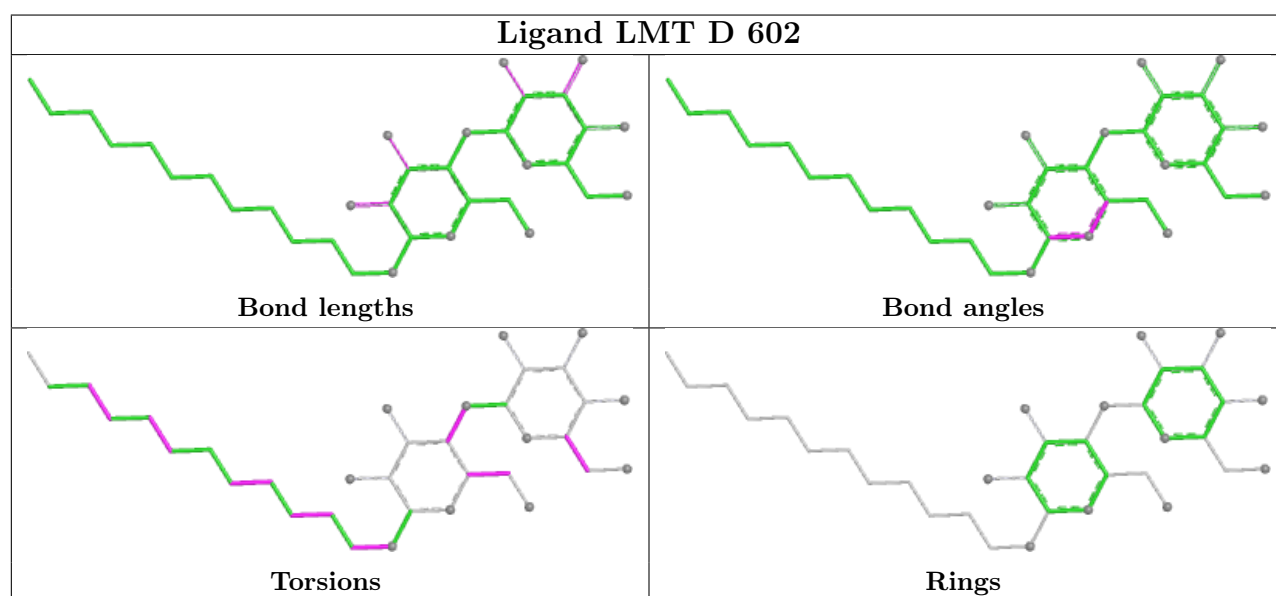
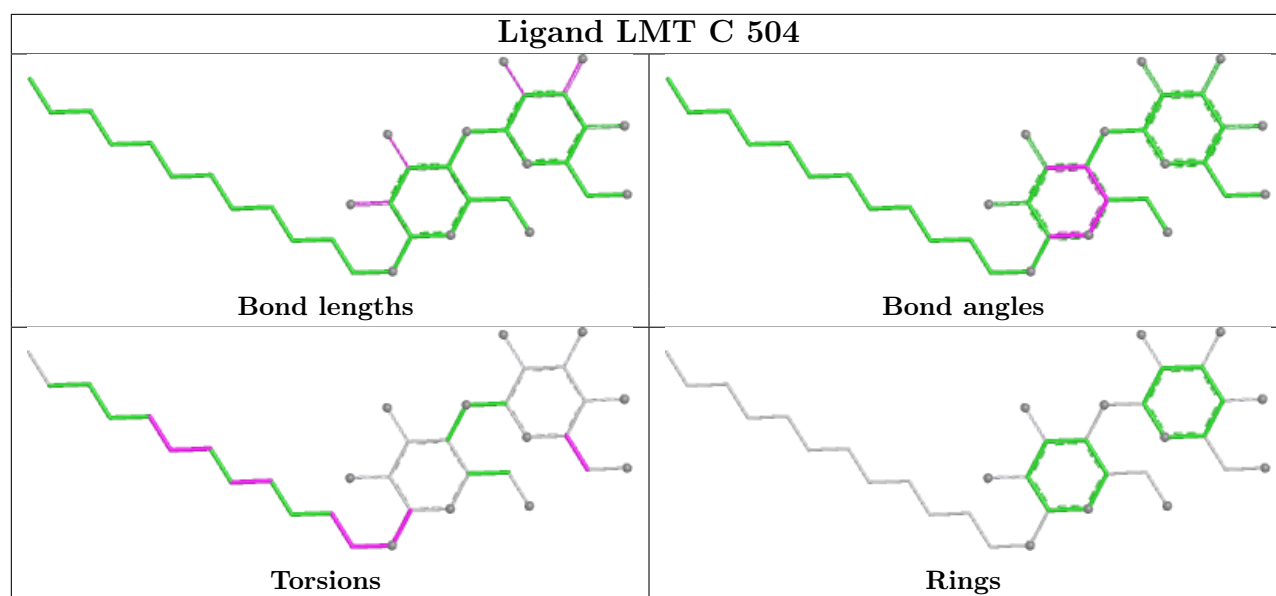
27 monomers are involved in 61 short contacts:

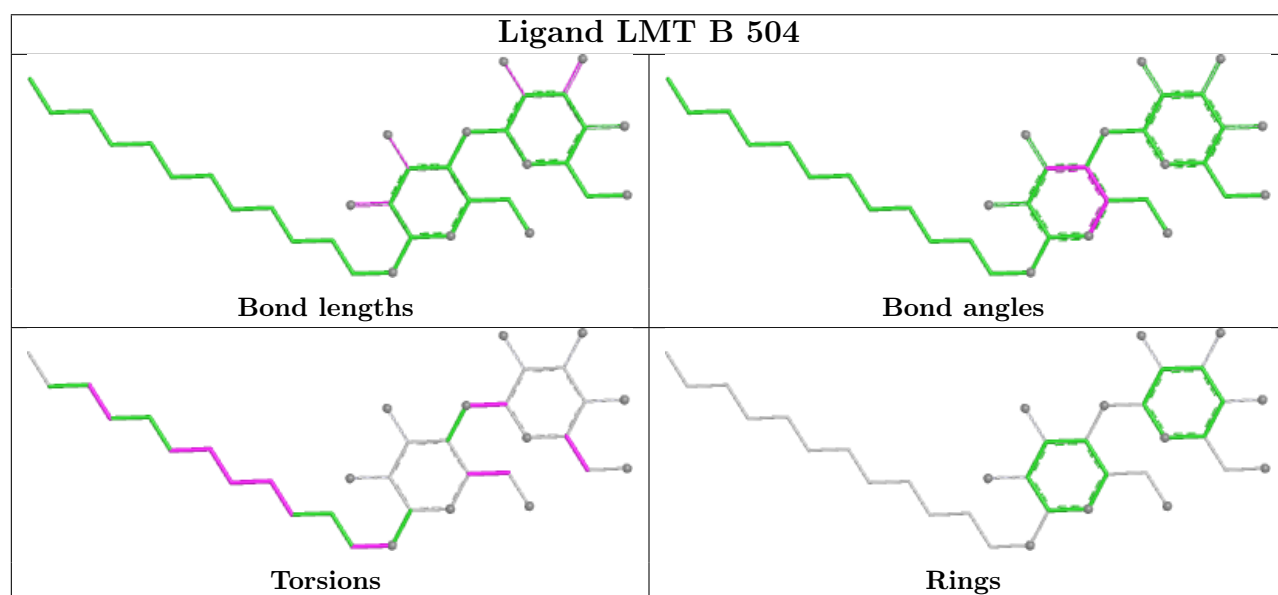
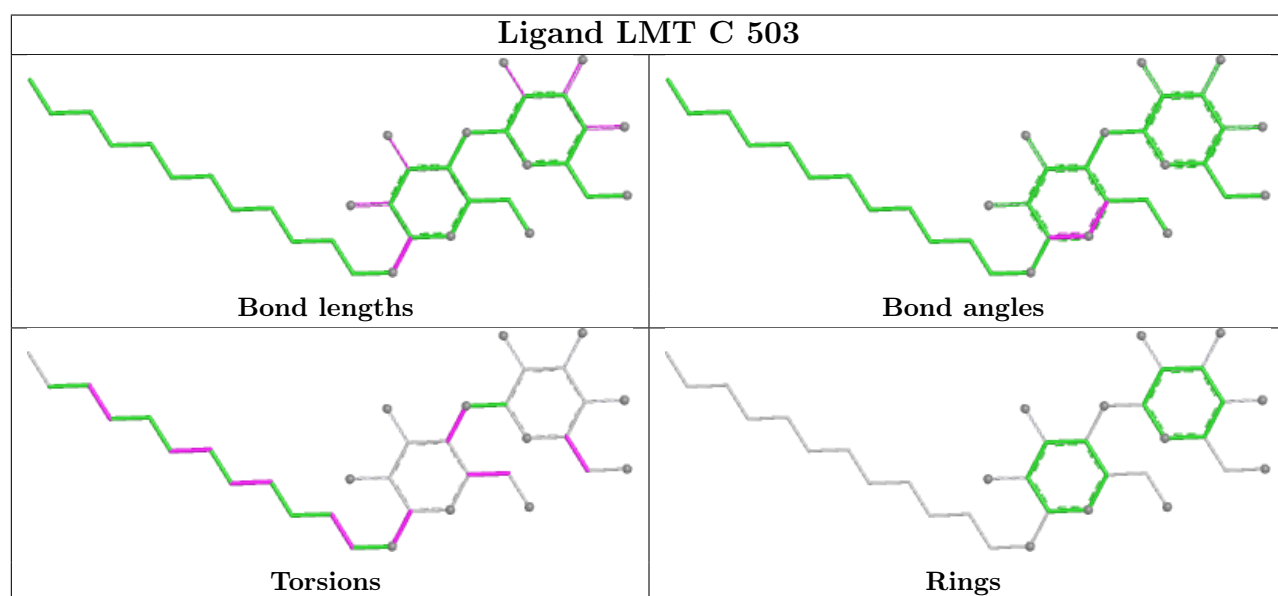
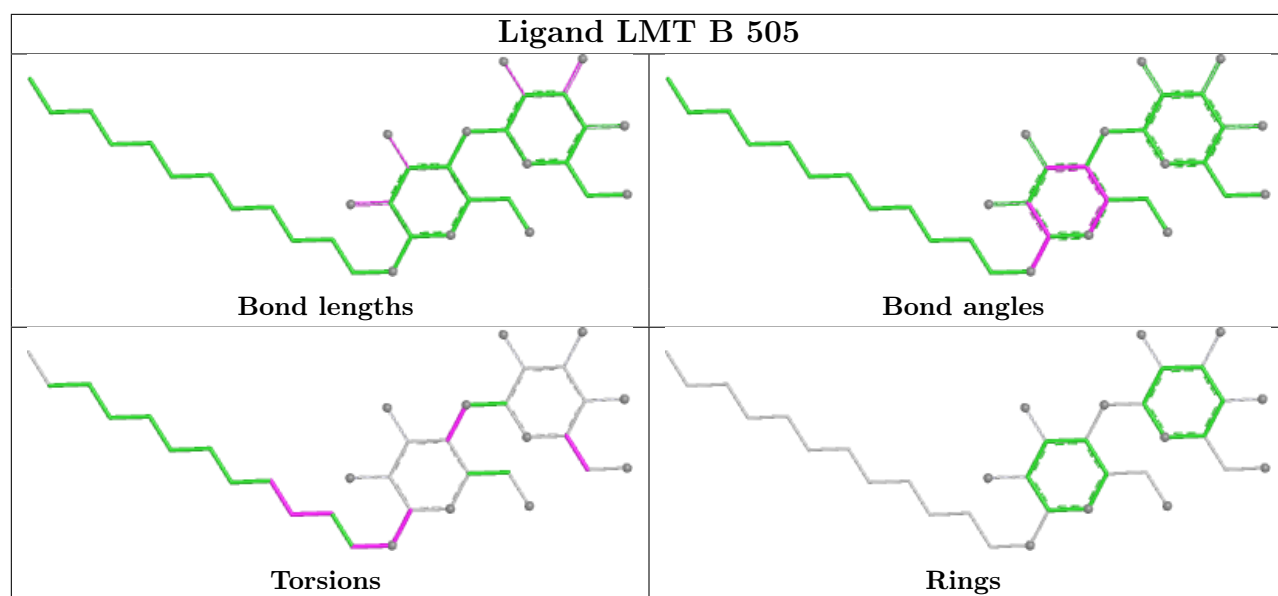
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	501	PGT	4	0
4	D	602	LMT	3	0
3	B	502	PGT	3	0
4	B	505	LMT	2	0
4	C	503	LMT	1	0
4	A	604	LMT	5	0
5	C	502	DGA	4	0
4	D	607	LMT	1	0
4	D	608	LMT	2	0
4	C	506	LMT	1	0
3	B	511	PGT	4	0
4	B	507	LMT	3	0
4	C	505	LMT	1	0
5	B	501	DGA	5	0
4	A	603	LMT	4	0
4	D	603	LMT	4	0
3	D	601	PGT	5	0
4	B	509	LMT	2	0
4	B	506	LMT	3	0
4	B	510	LMT	1	0
4	D	606	LMT	3	0
4	A	605	LMT	1	0
4	B	508	LMT	1	0
3	C	509	PGT	1	0
4	B	503	LMT	2	0
4	D	604	LMT	3	0
4	D	605	LMT	3	0

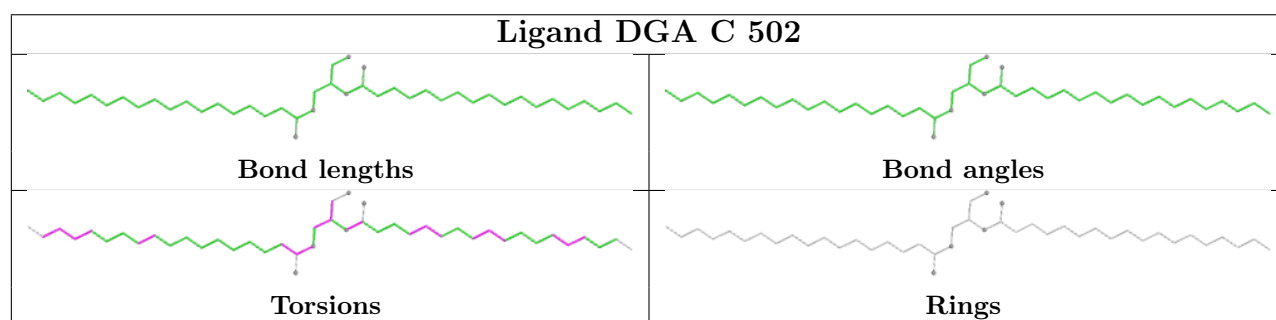
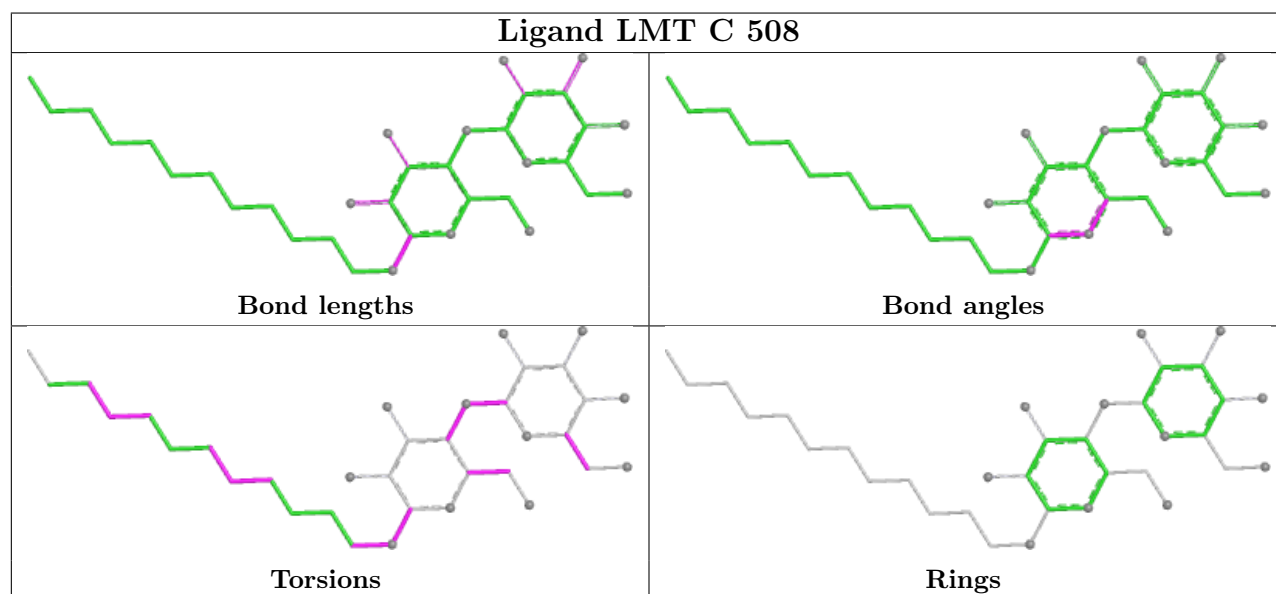
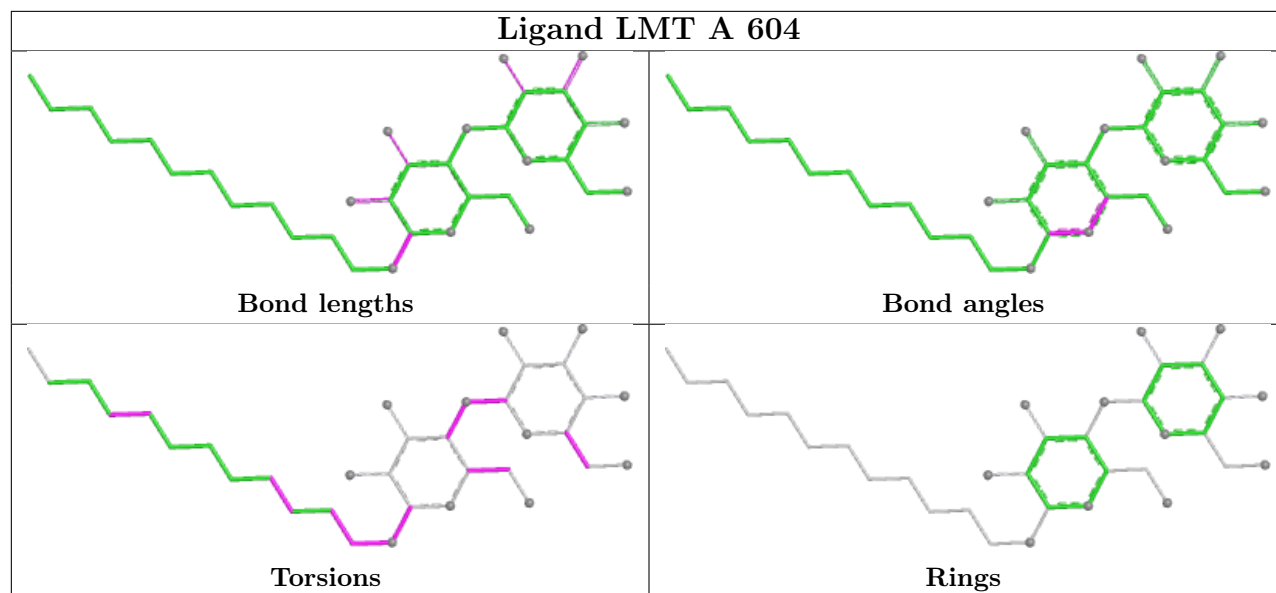
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

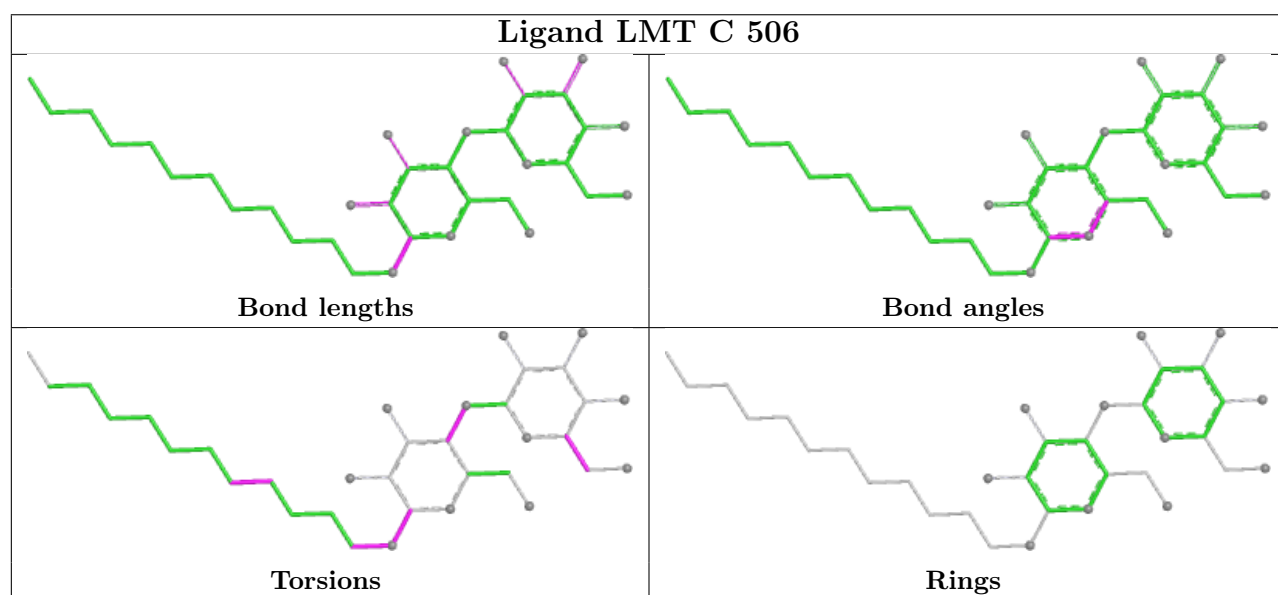
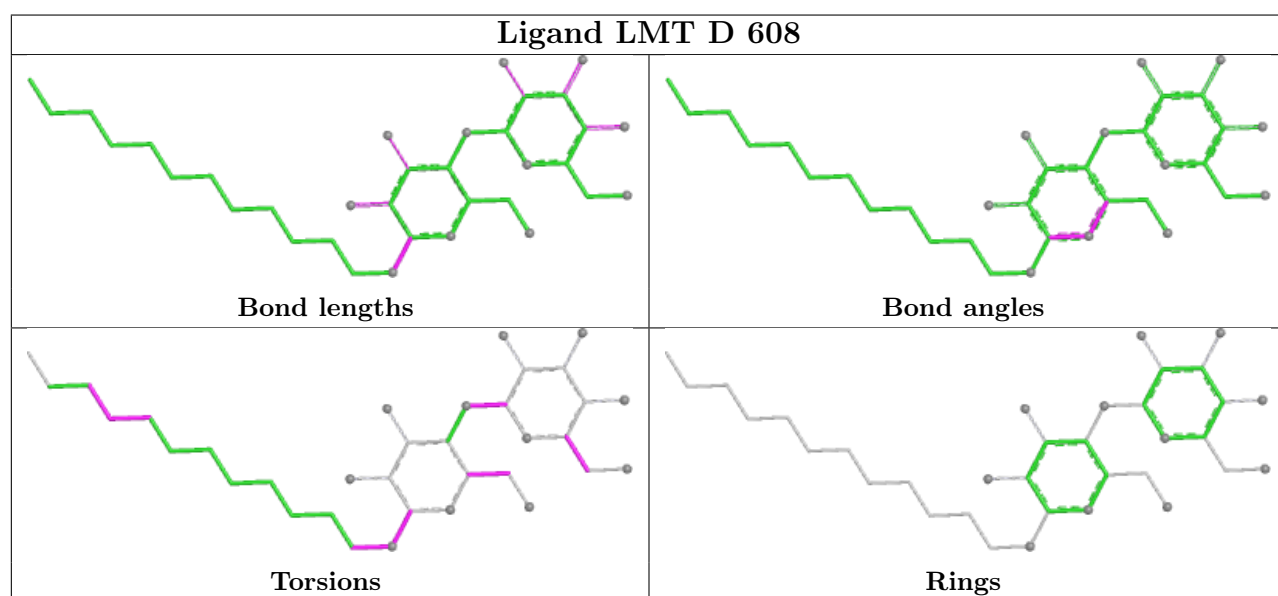
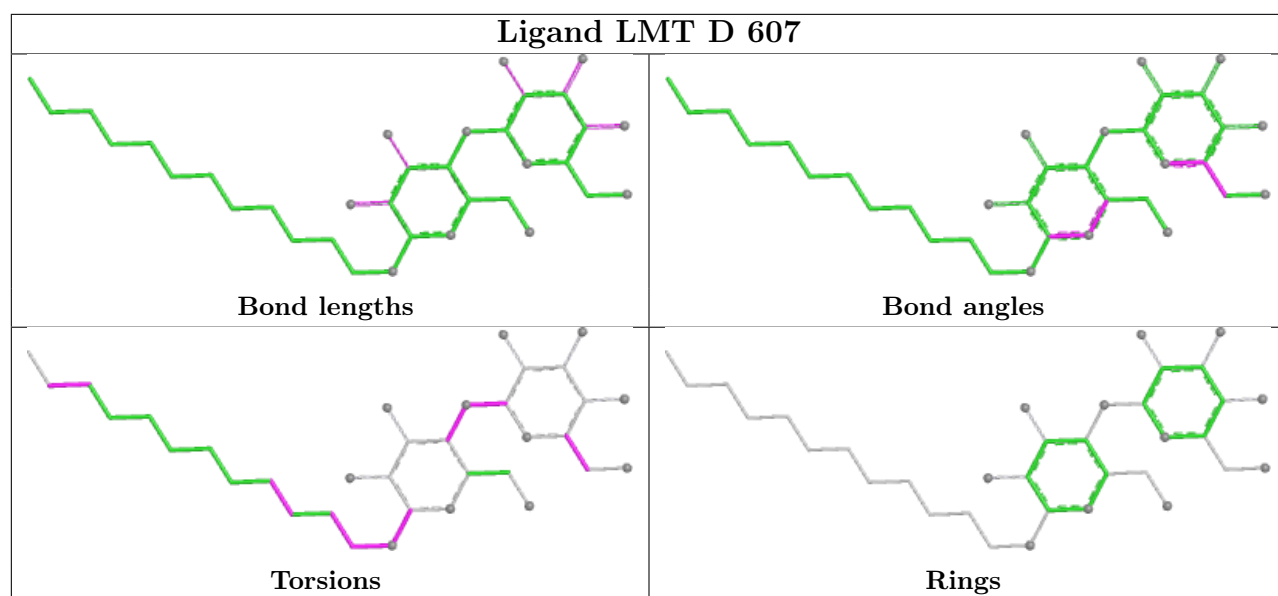
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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.

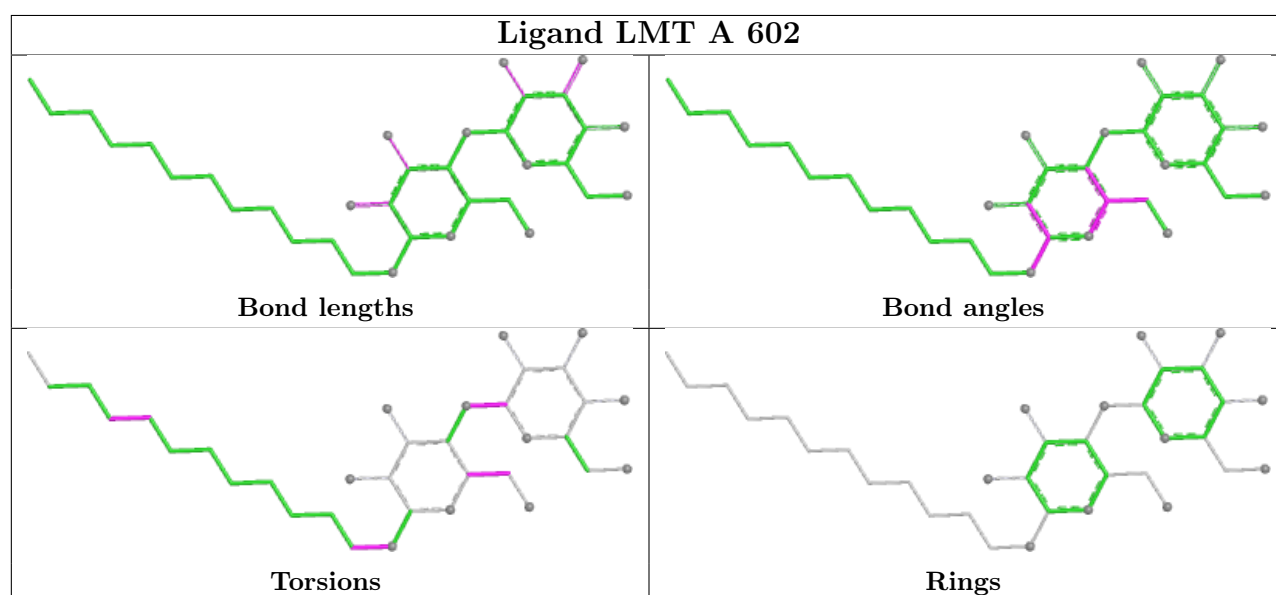
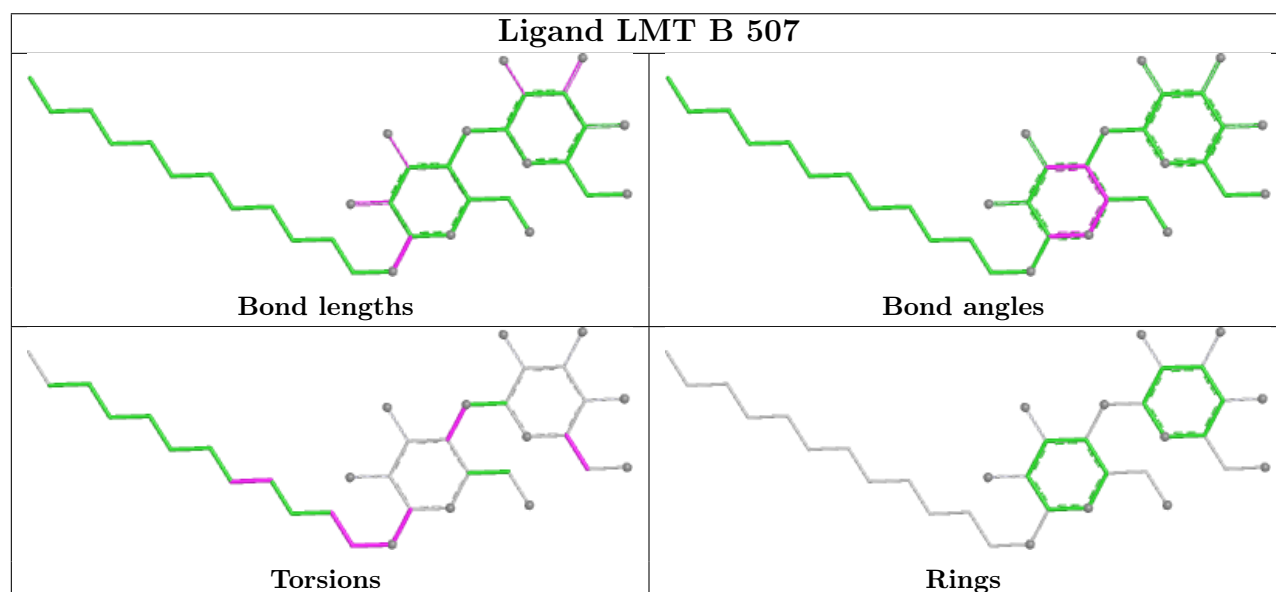
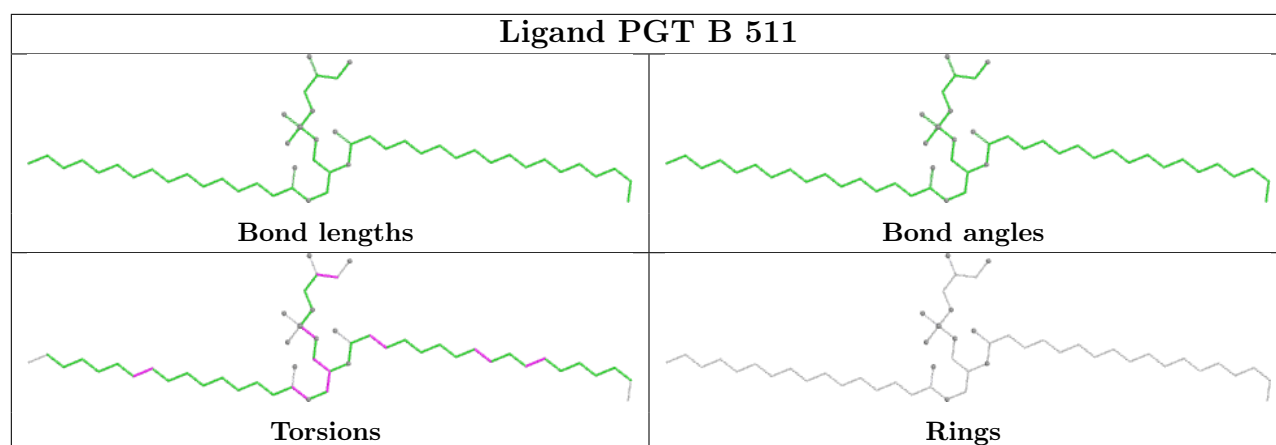


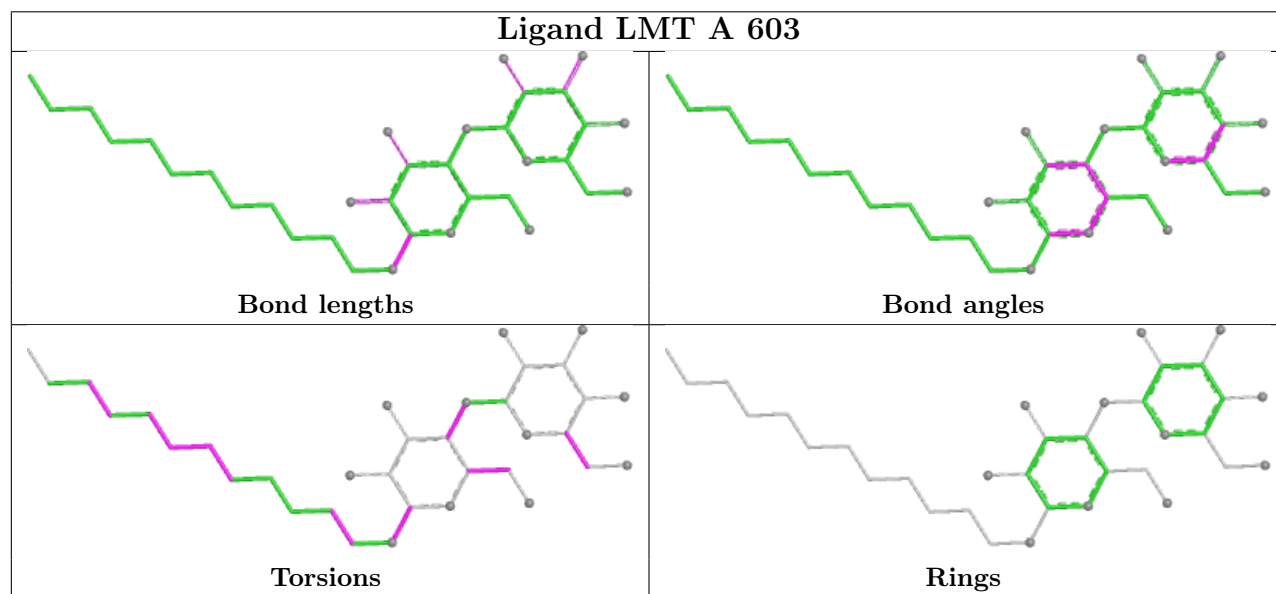
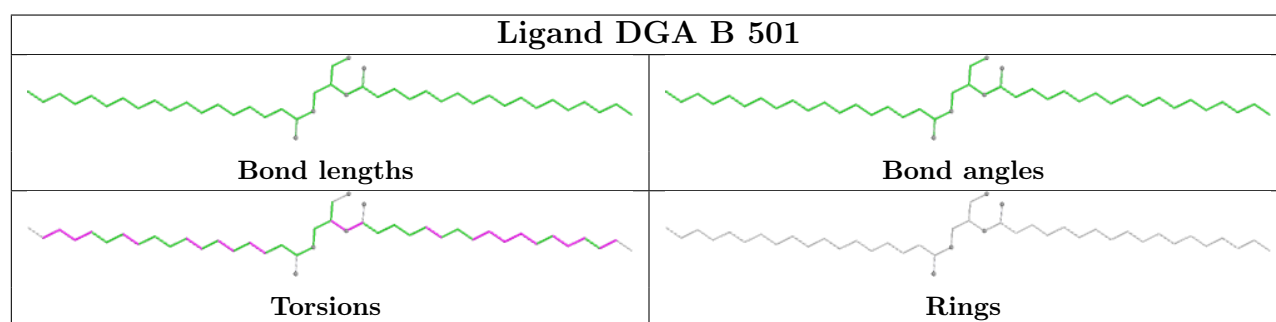
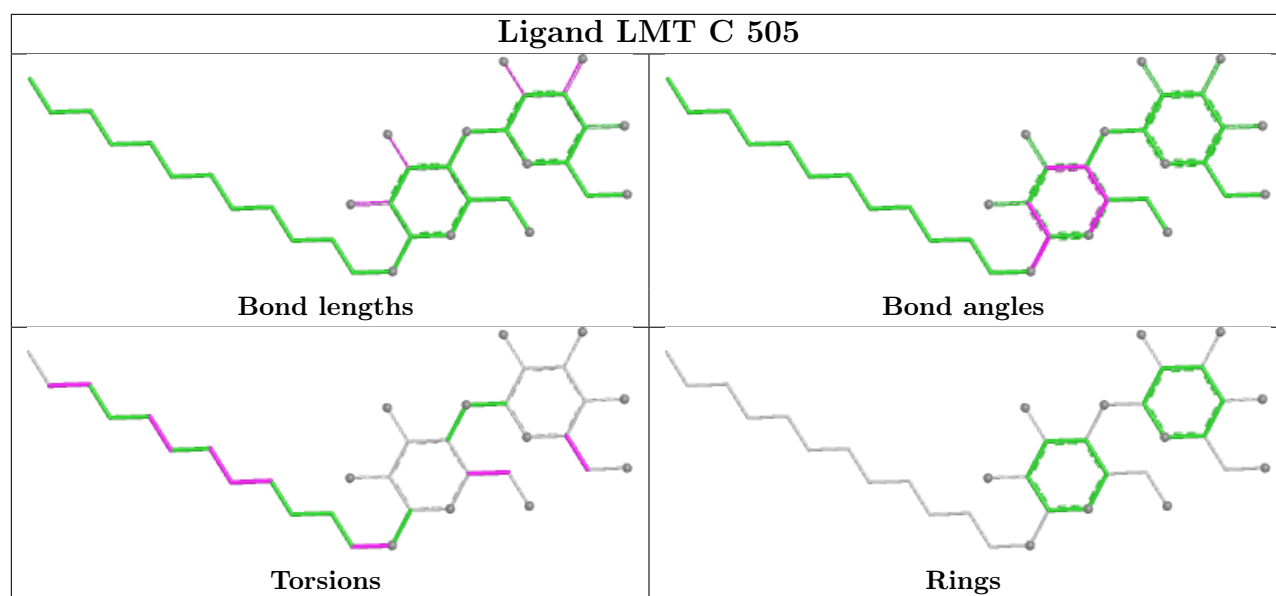


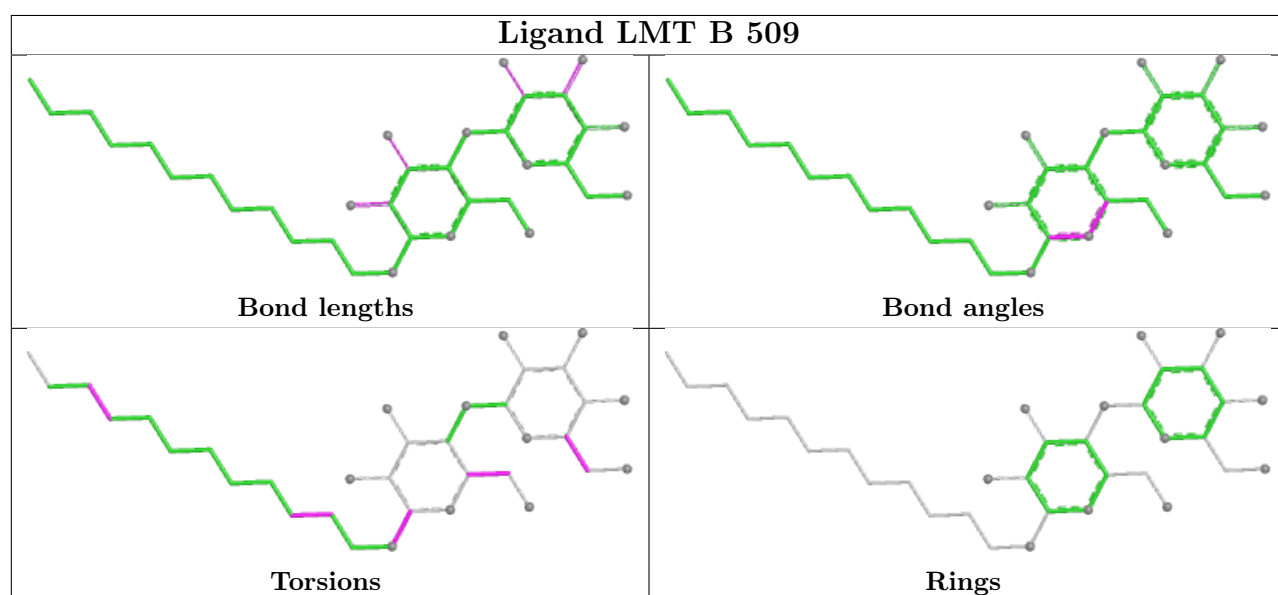
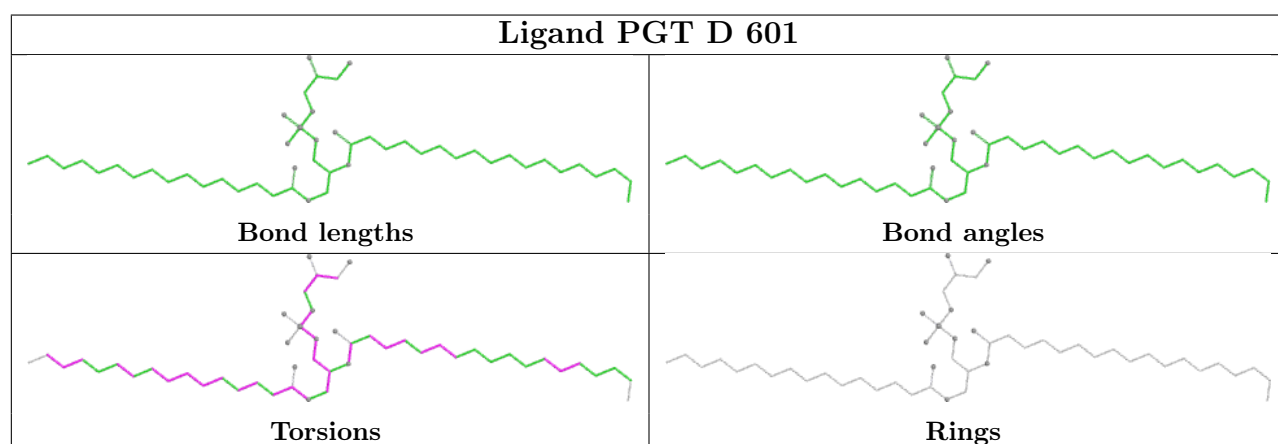
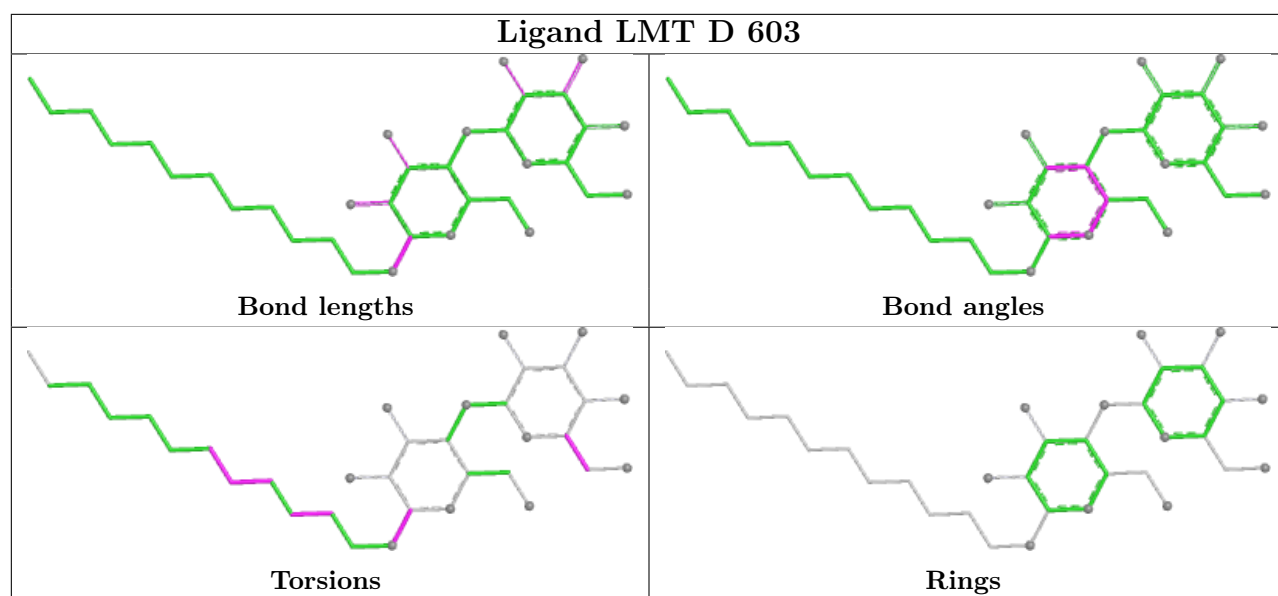


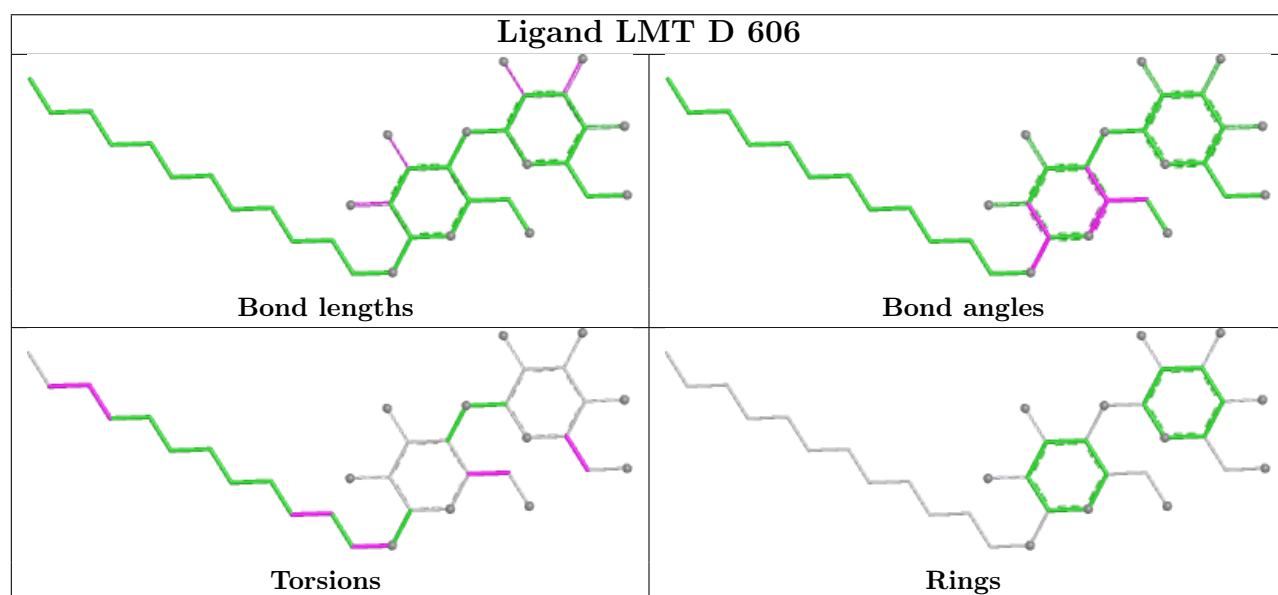
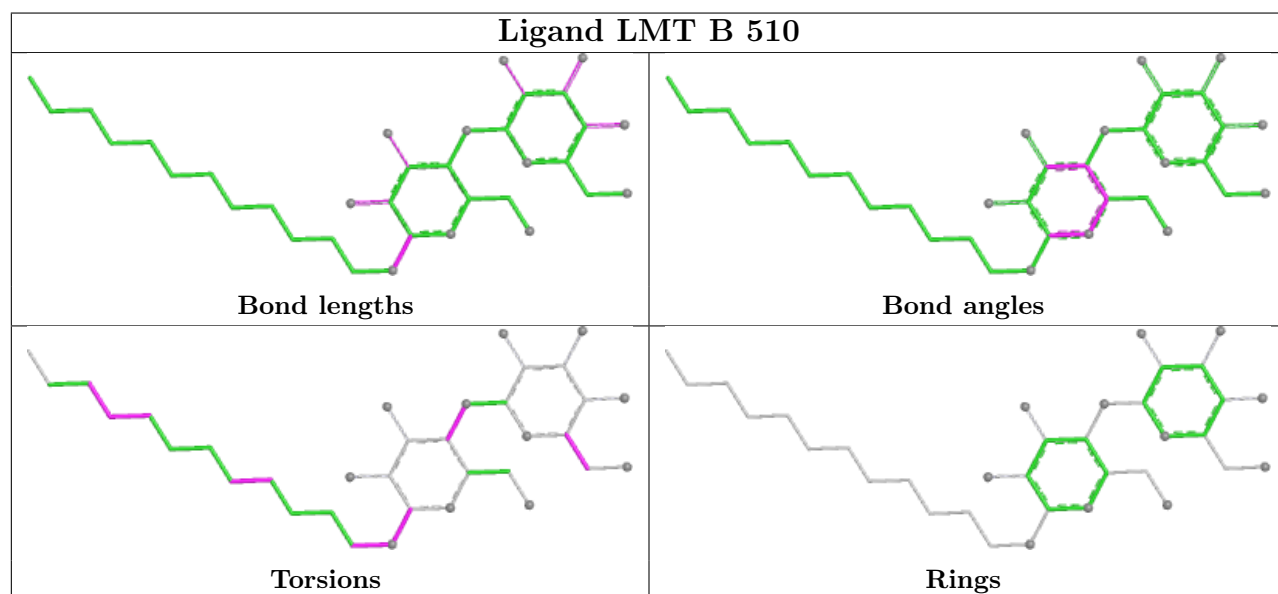
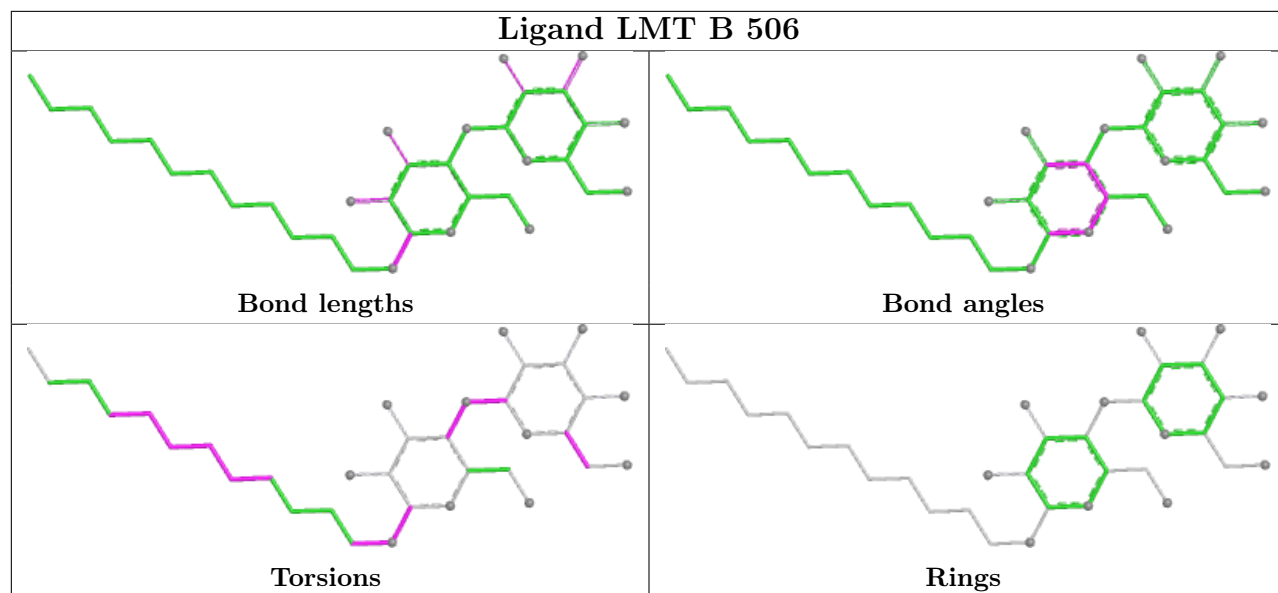


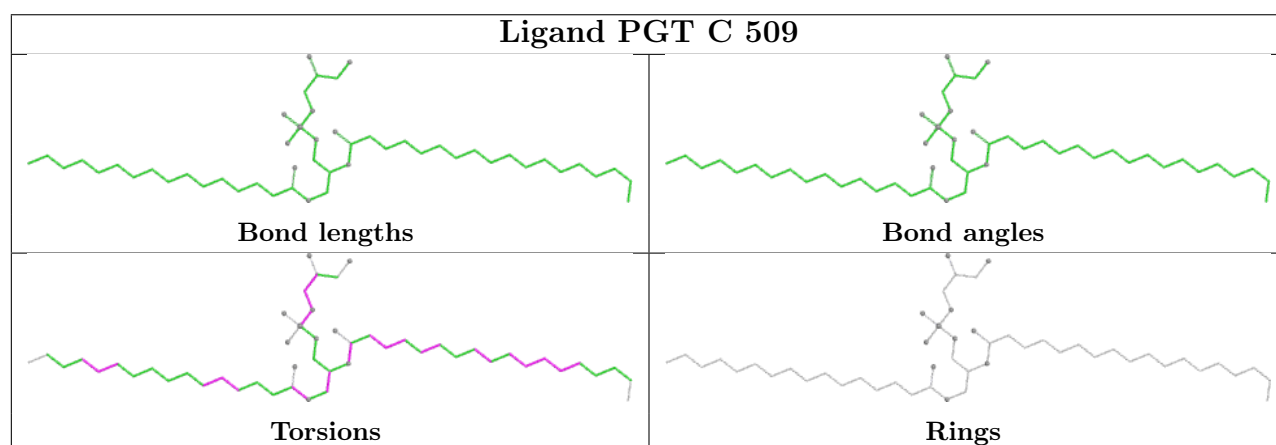
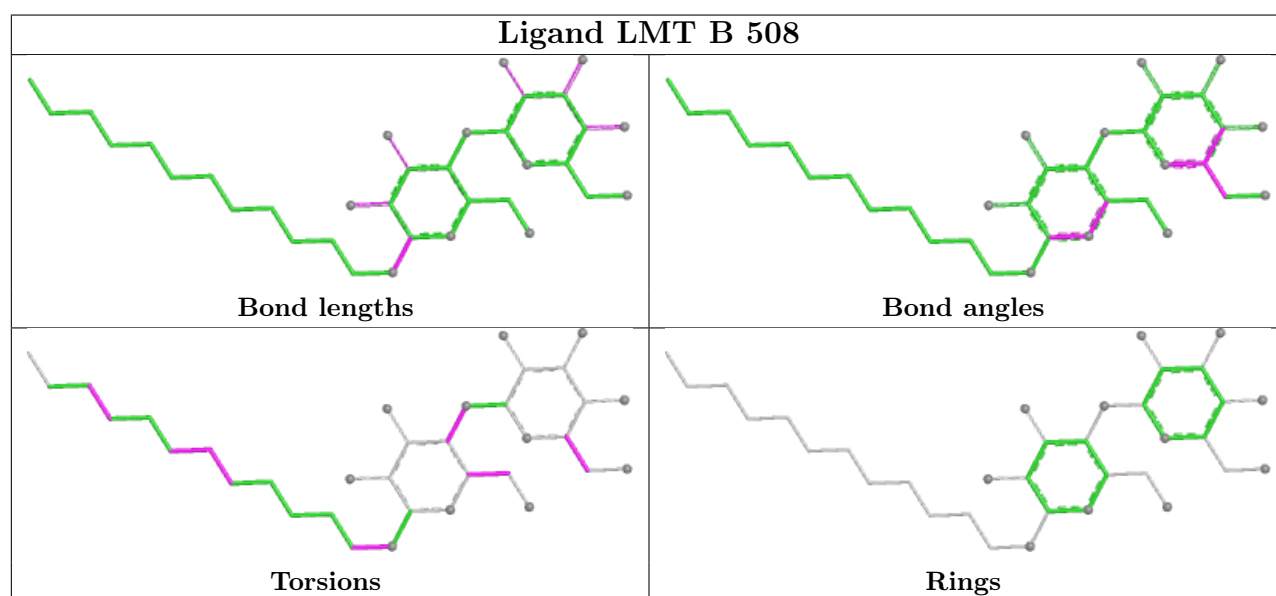
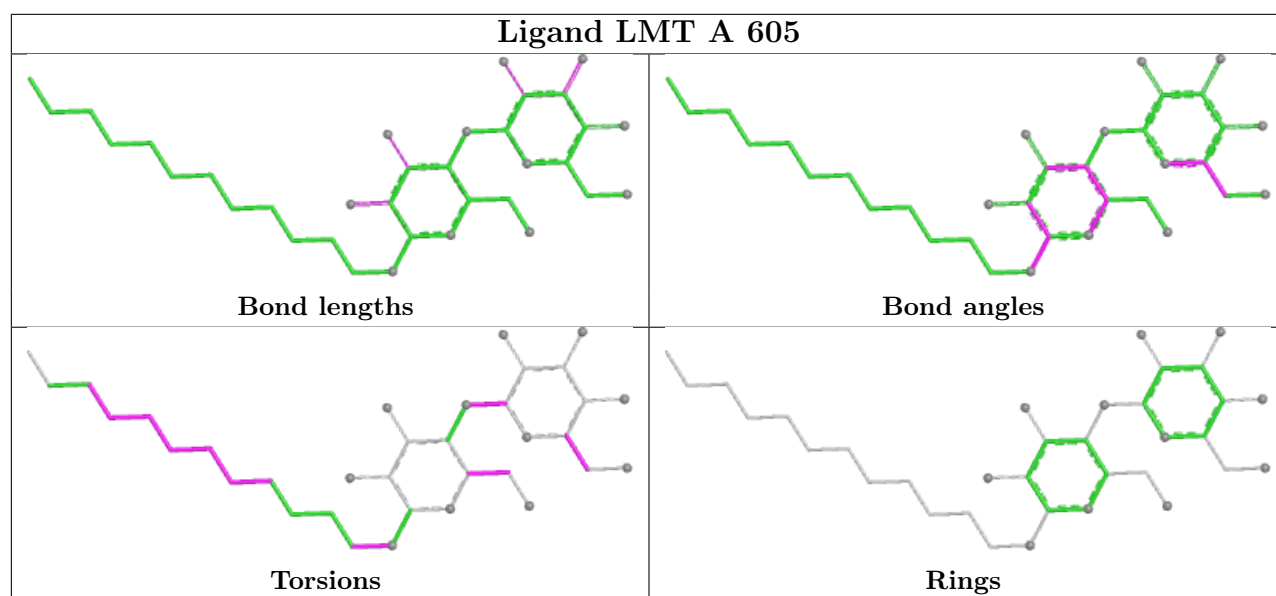


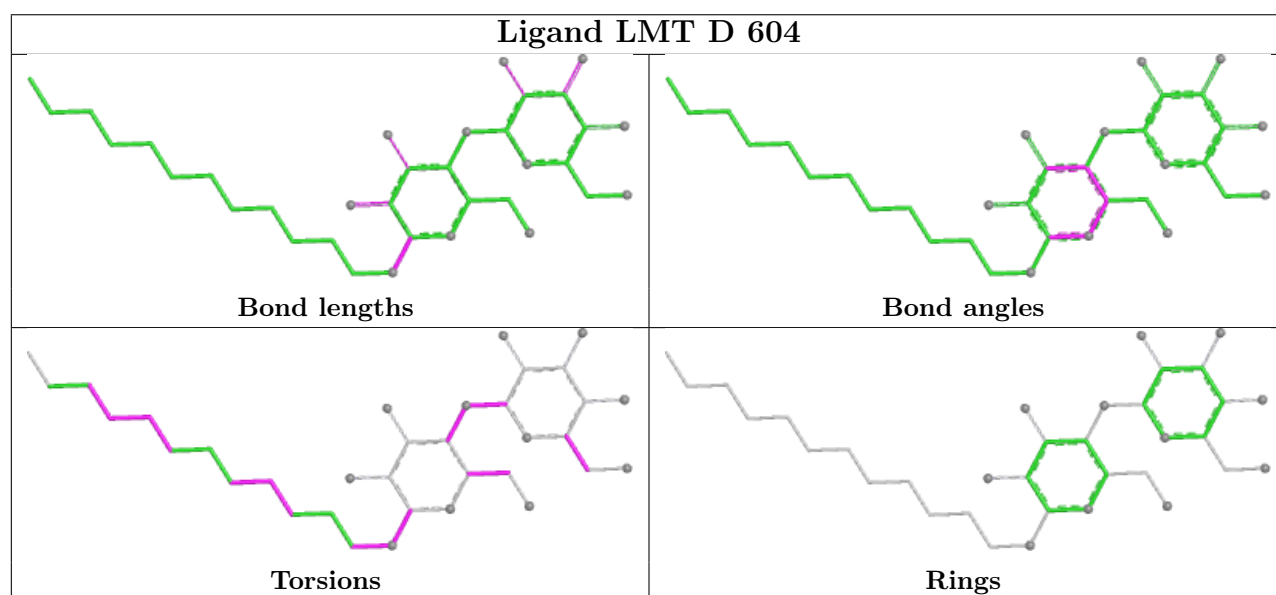
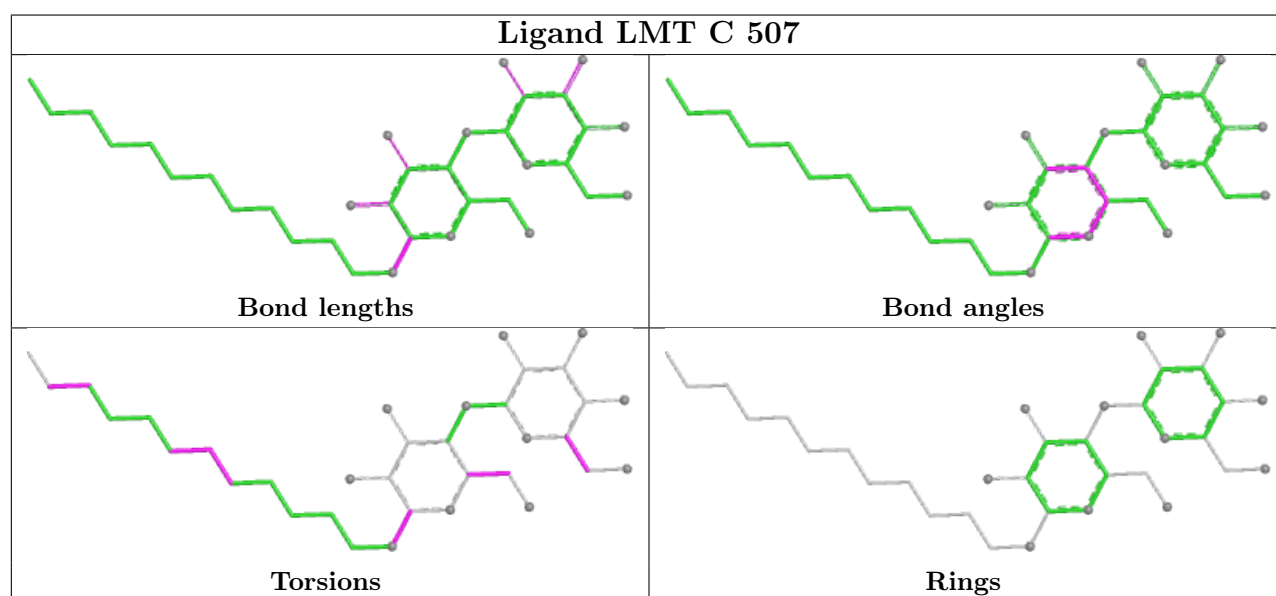
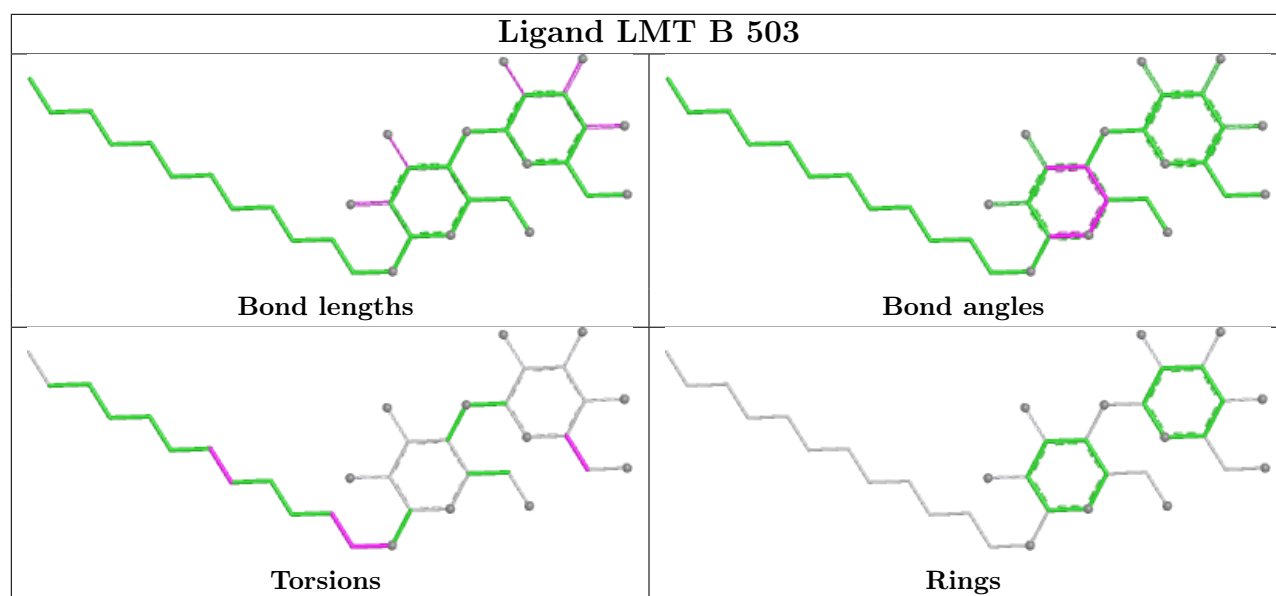


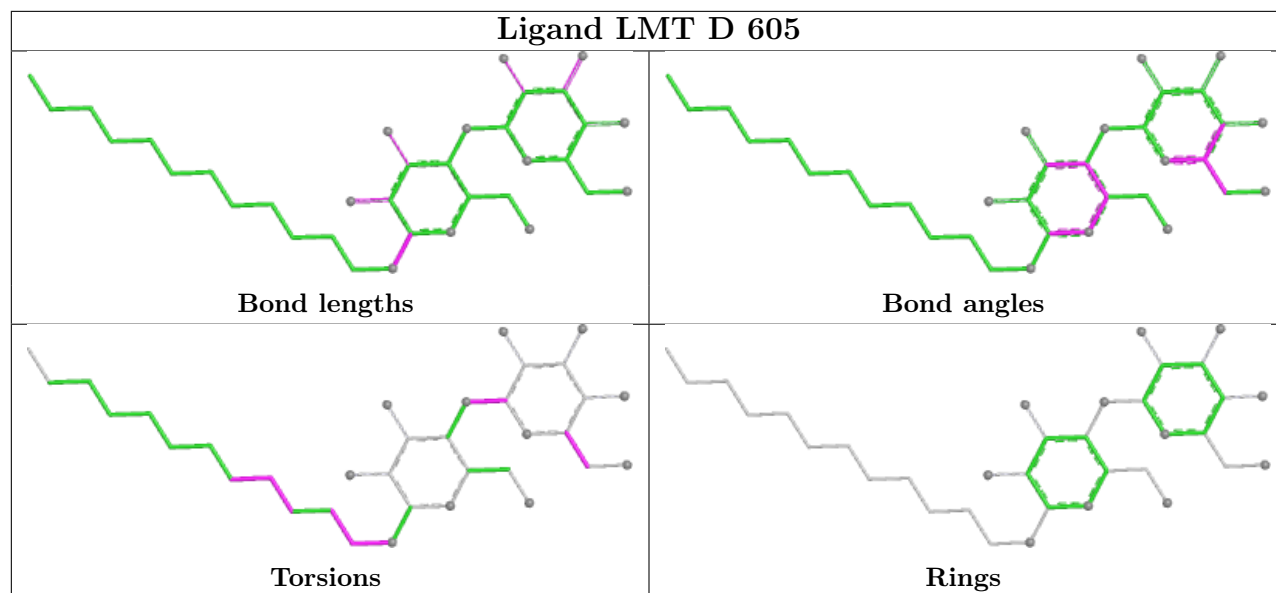












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

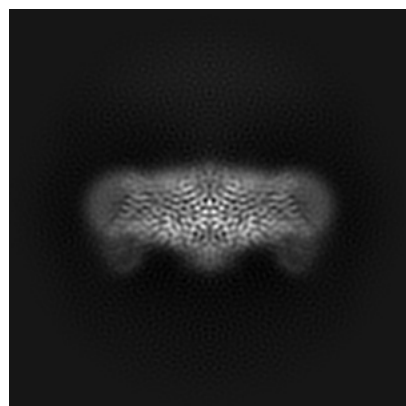
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36207. These allow visual inspection of the internal detail of the map and identification of artifacts.

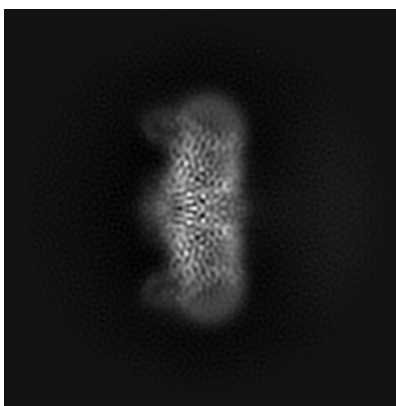
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

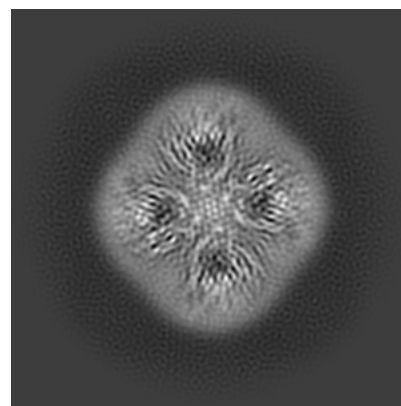
6.1.1 Primary map



X

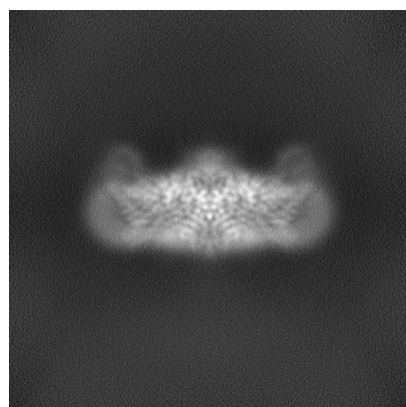


Y

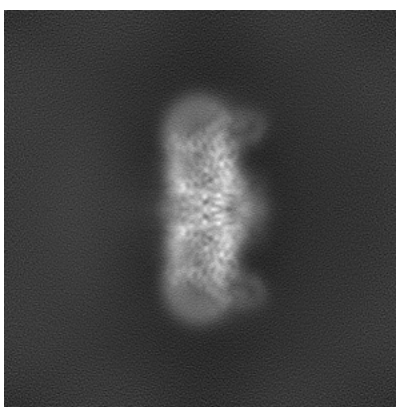


Z

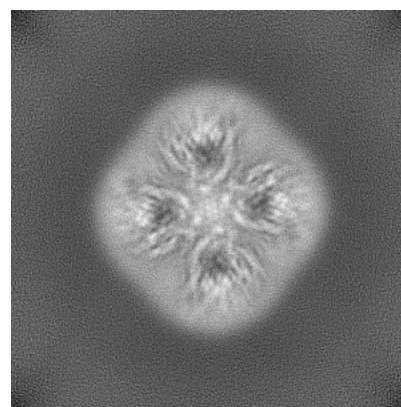
6.1.2 Raw map



X



Y

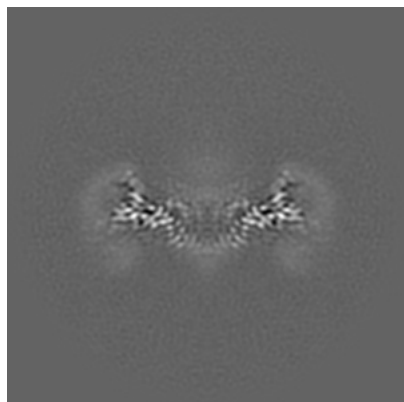


Z

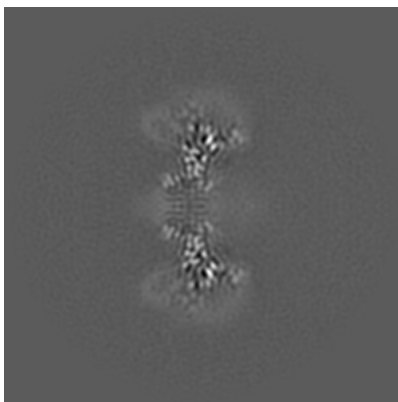
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

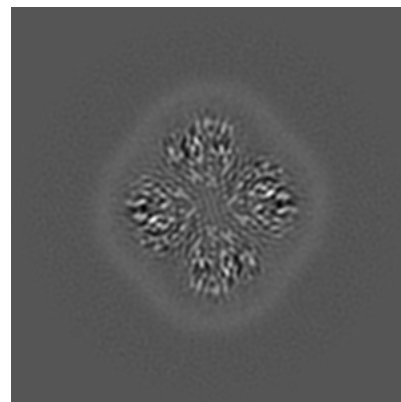
6.2.1 Primary map



X Index: 160

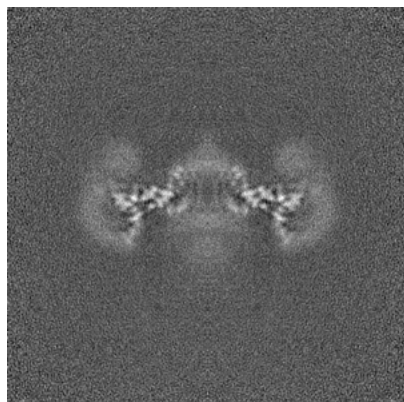


Y Index: 160

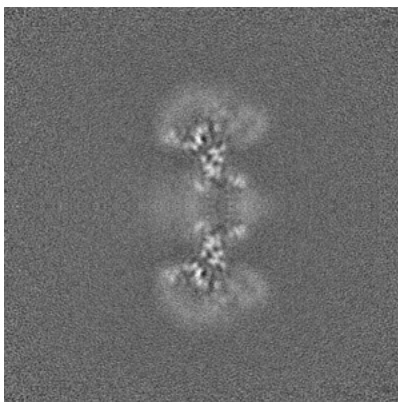


Z Index: 160

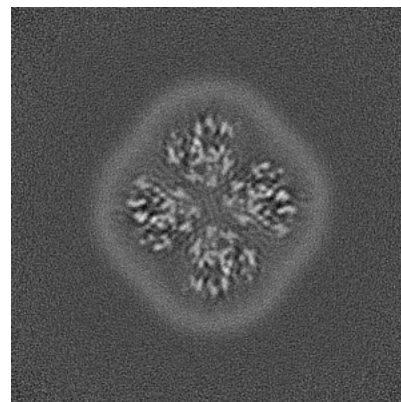
6.2.2 Raw map



X Index: 160



Y Index: 160

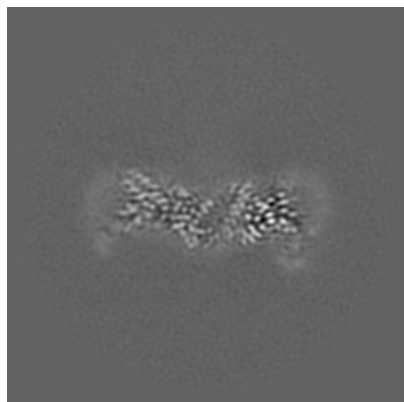


Z Index: 160

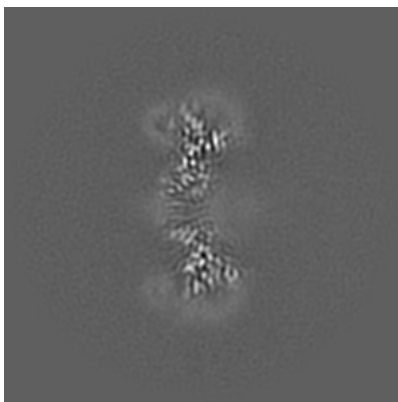
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

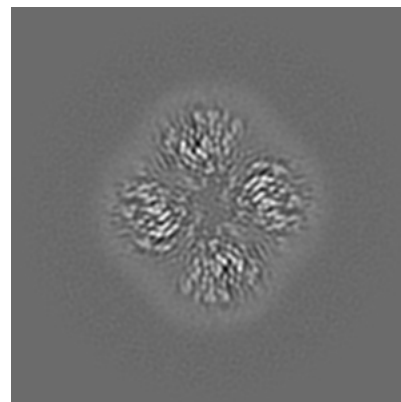
6.3.1 Primary map



X Index: 145

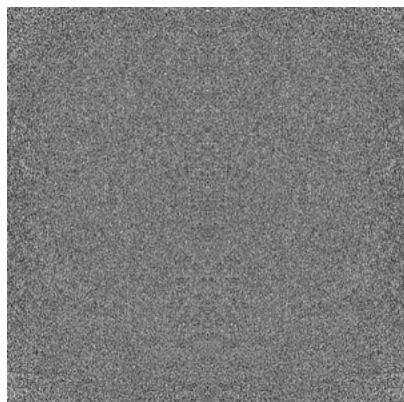


Y Index: 165

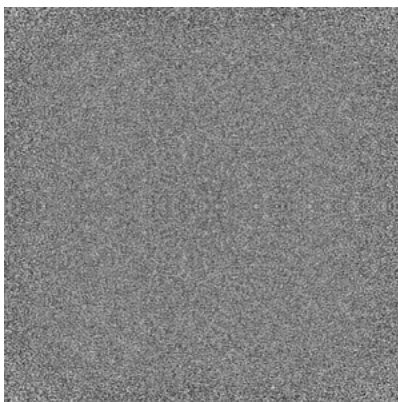


Z Index: 150

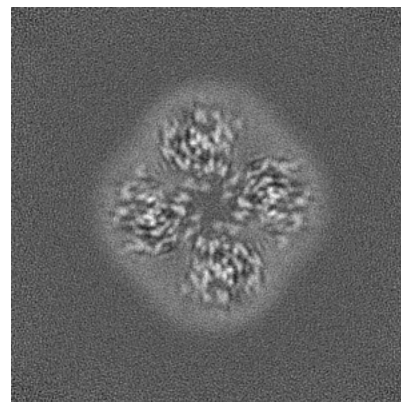
6.3.2 Raw map



X Index: 0



Y Index: 0

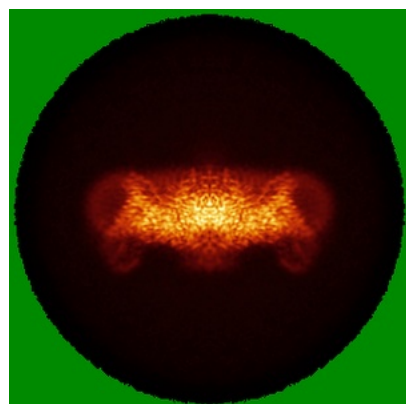


Z Index: 171

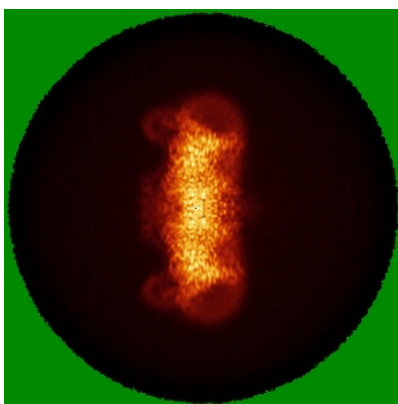
The images above show the largest variance slices of the map in three orthogonal directions.

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

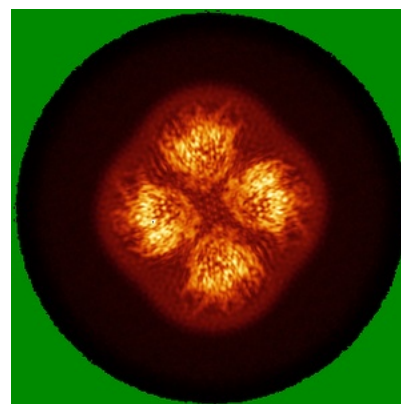
6.4.1 Primary map



X

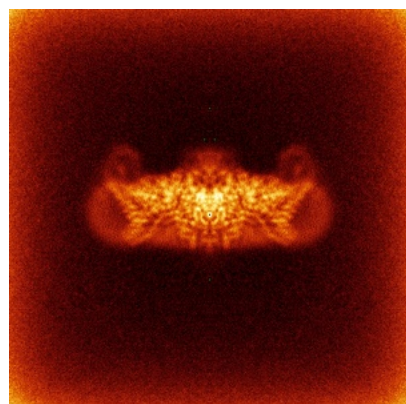


Y

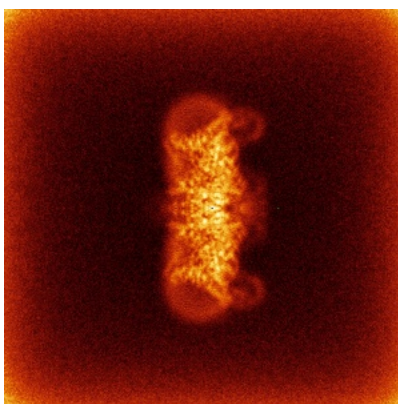


Z

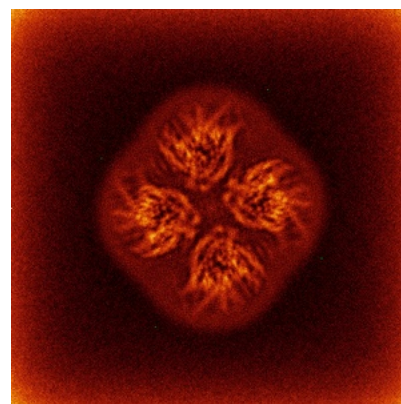
6.4.2 Raw map



X



Y

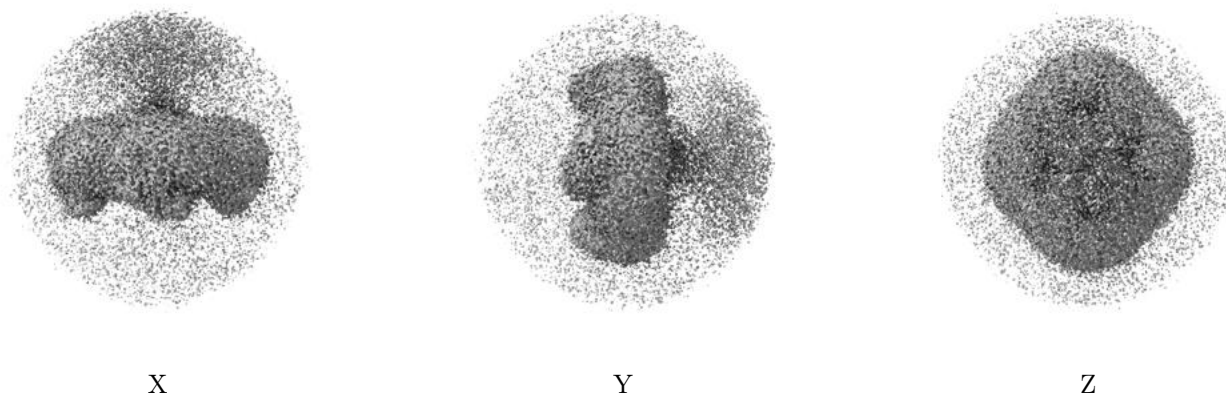


Z

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.

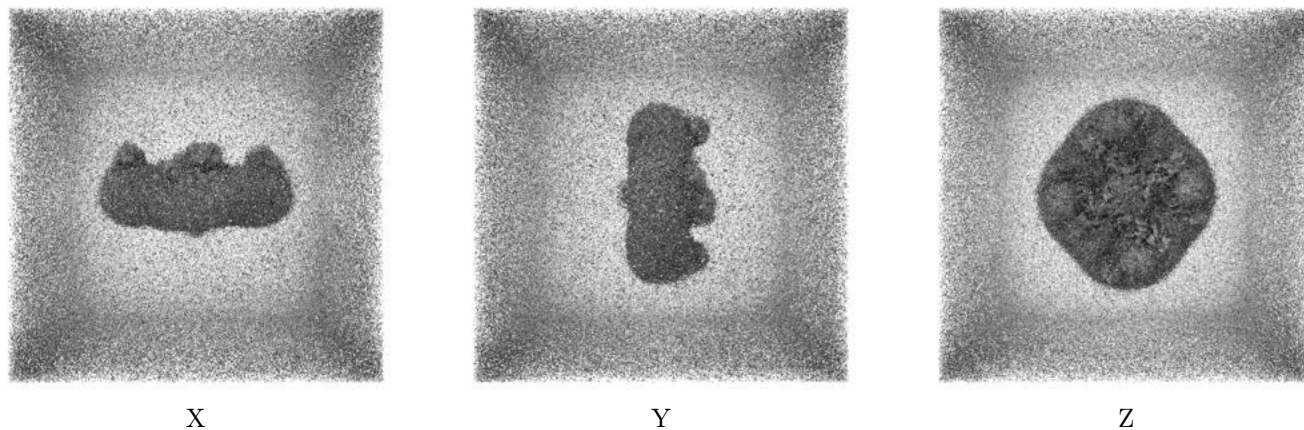
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. 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.

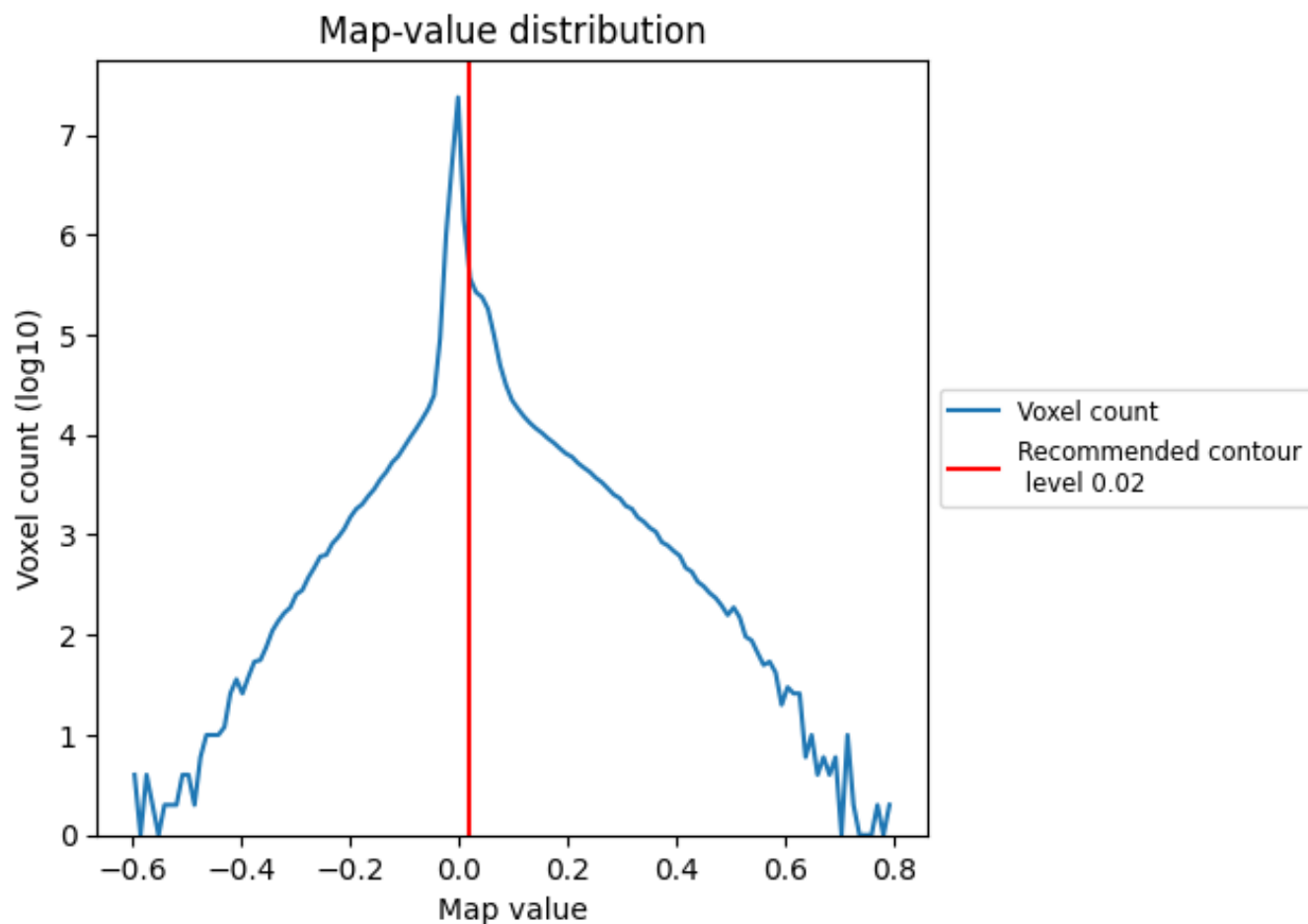
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

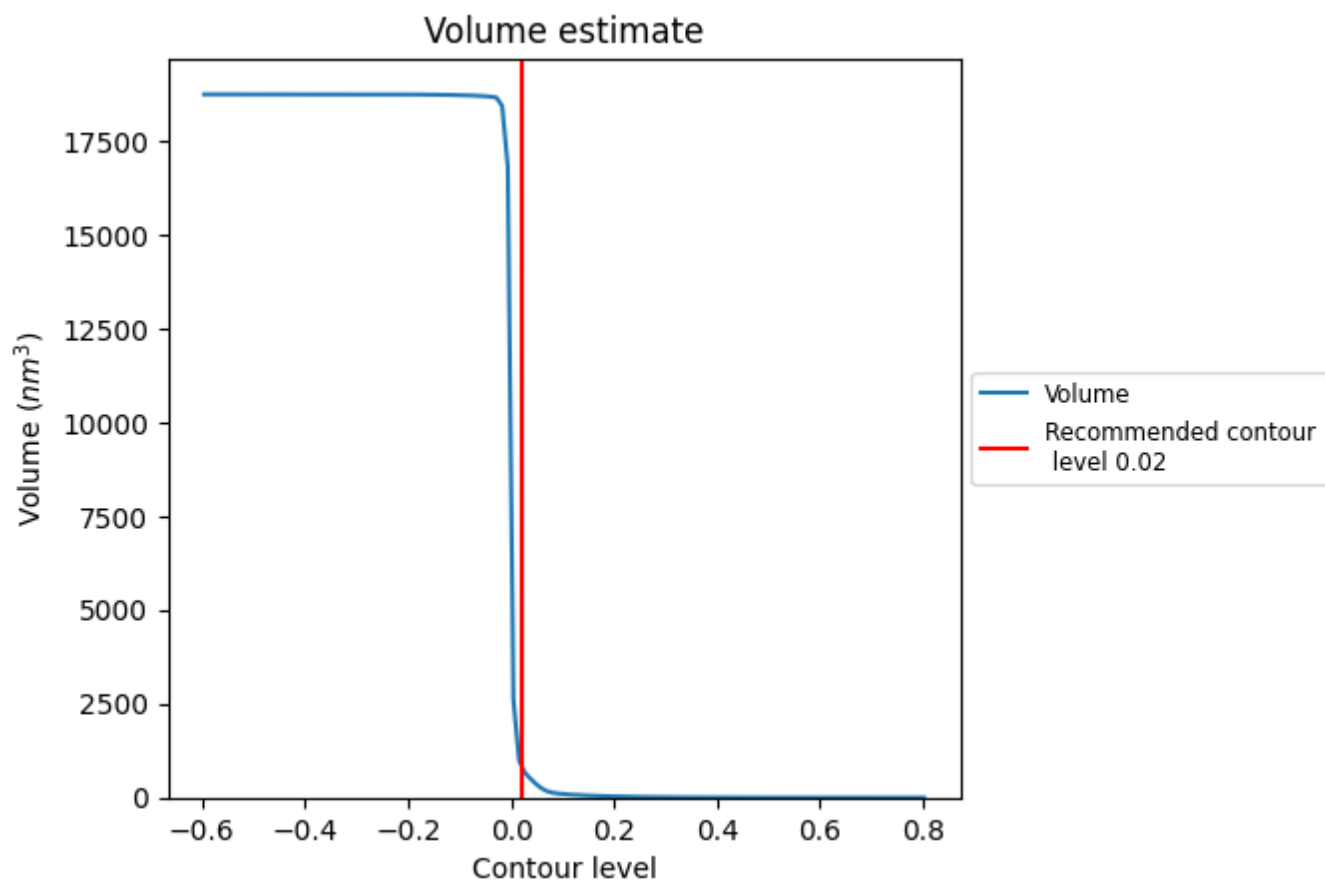
This section contains the results of statistical analysis of the map.

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.

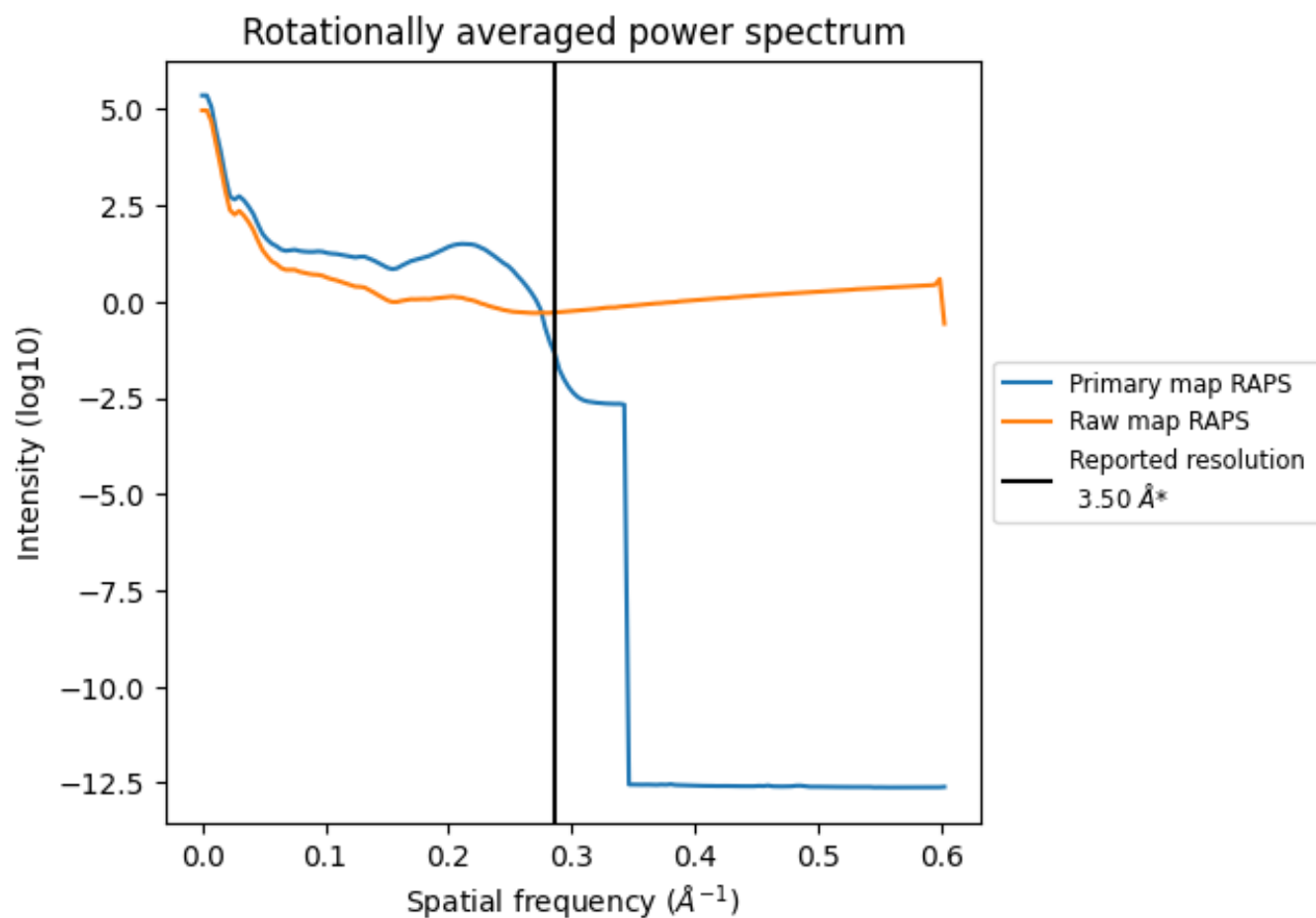
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 858 nm³; this corresponds to an approximate mass of 775 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 ⓘ

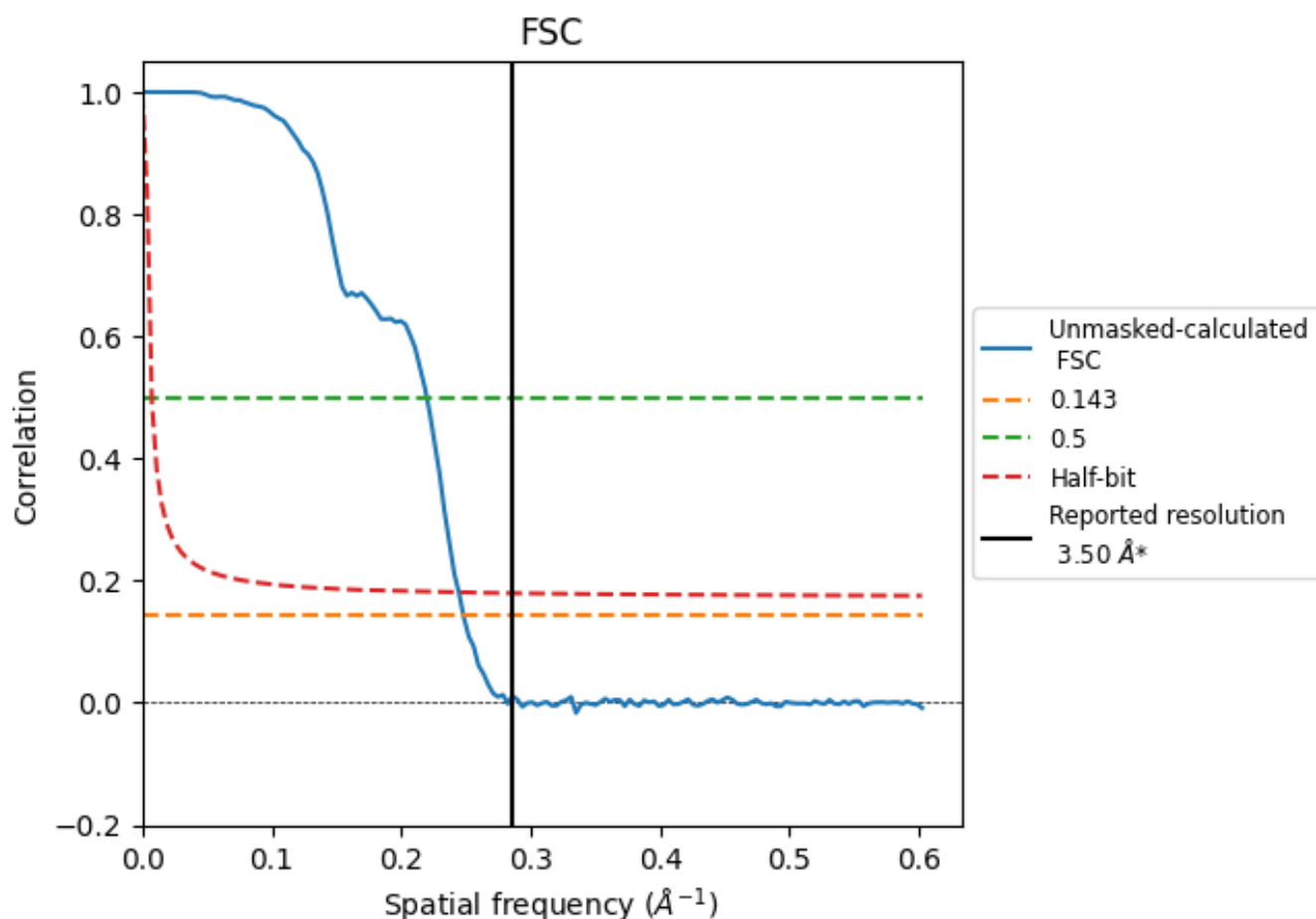


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

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 0.286 Å⁻¹

8.2 Resolution estimates [i](#)

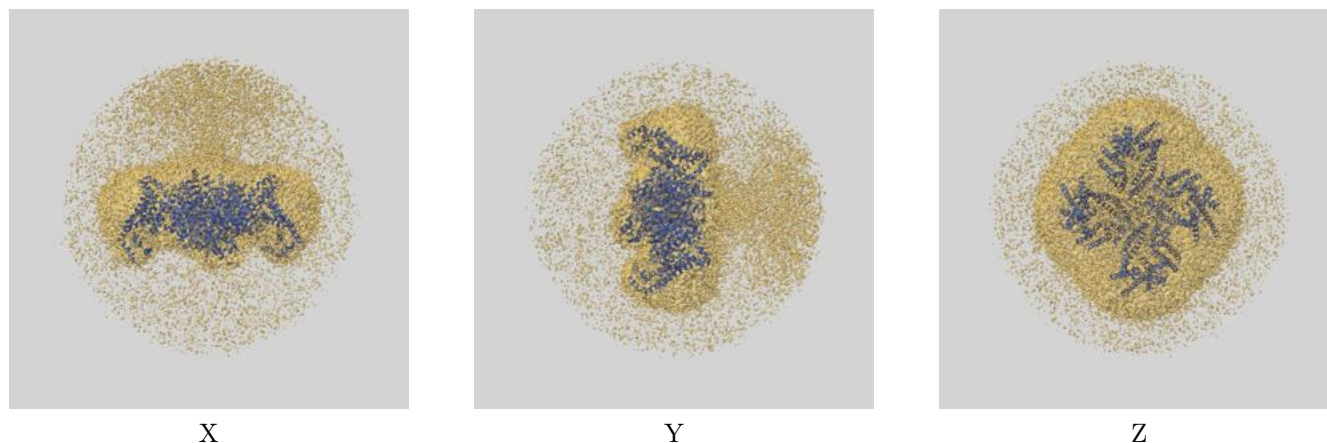
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.03	4.55	4.09

*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 4.03 differs from the reported value 3.5 by more than 10 %

9 Map-model fit [i](#)

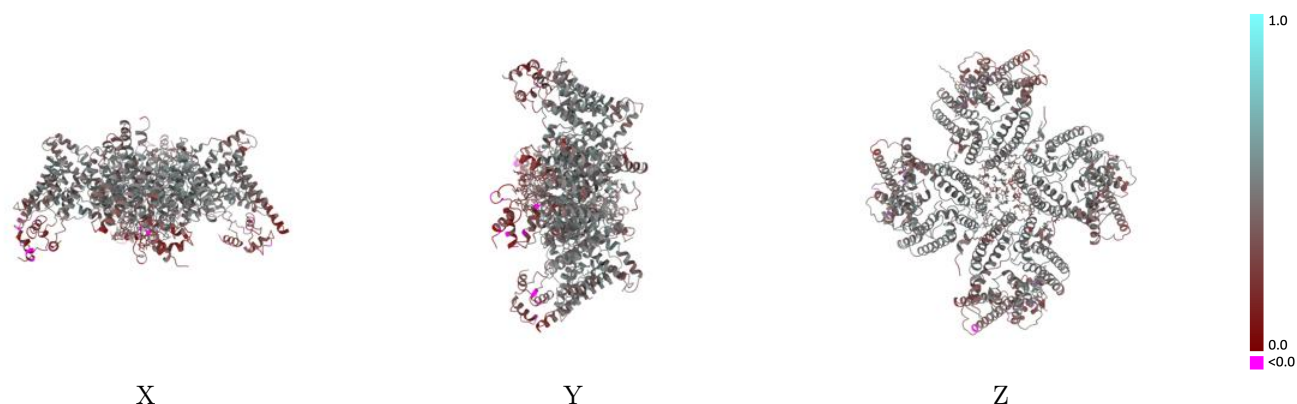
This section contains information regarding the fit between EMDB map EMD-36207 and PDB model 8JF2. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)



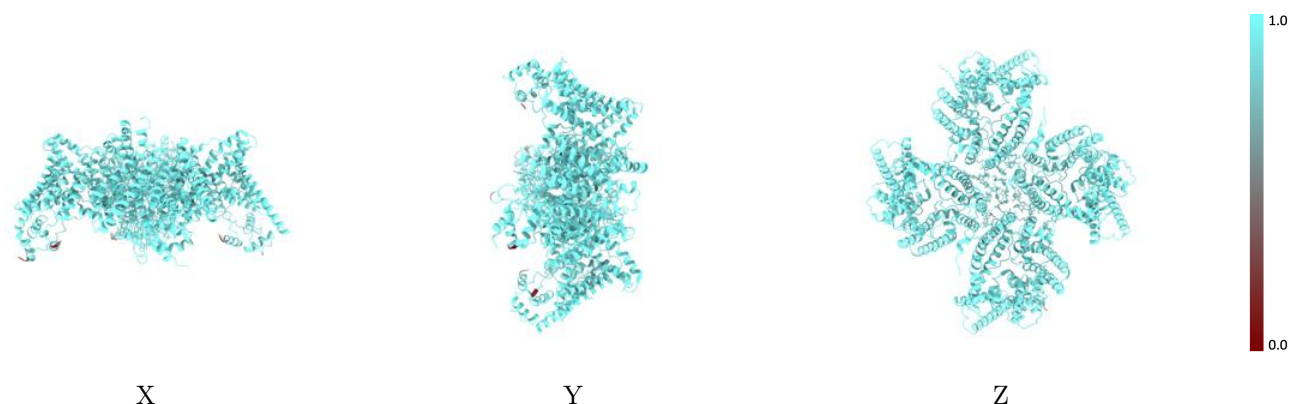
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



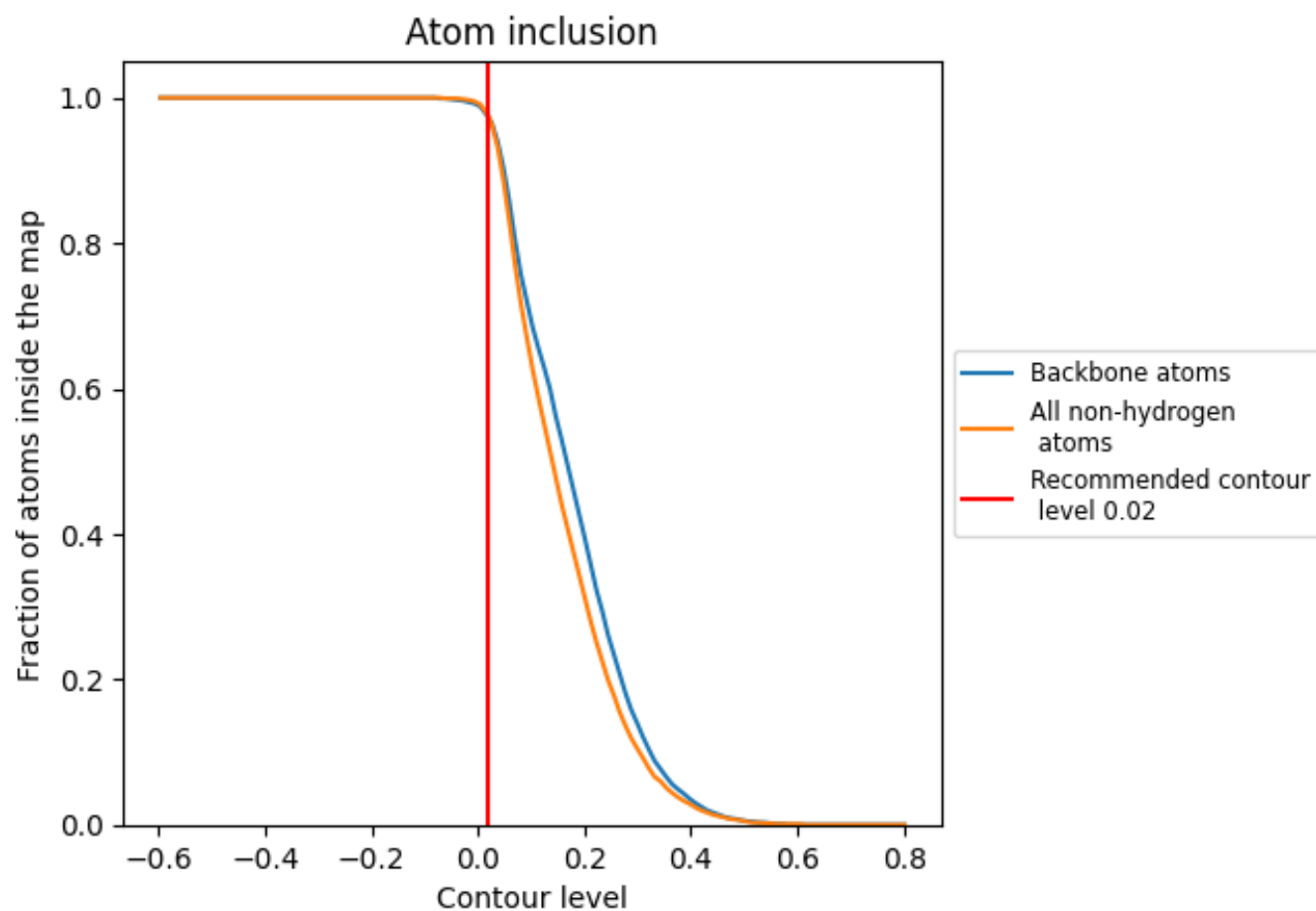
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 98% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9750	0.4240
A	0.9820	0.4490
B	0.9800	0.4610
C	0.9770	0.4480
D	0.9830	0.4670
F	0.9320	0.2060
G	0.9630	0.2520
H	0.9220	0.1940
I	0.9580	0.2620

1.0

0.0

<0.0