



Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 05:07 PM EST

PDB ID : 7T92
EMDB ID : EMD-25750
Title : Structure of the peroxisomal retro-translocon formed by a heterotrimeric ubiquitin ligase complex
Authors : Peiqiang, F.; Tom, R.
Deposited on : 2021-12-17
Resolution : 3.10 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.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

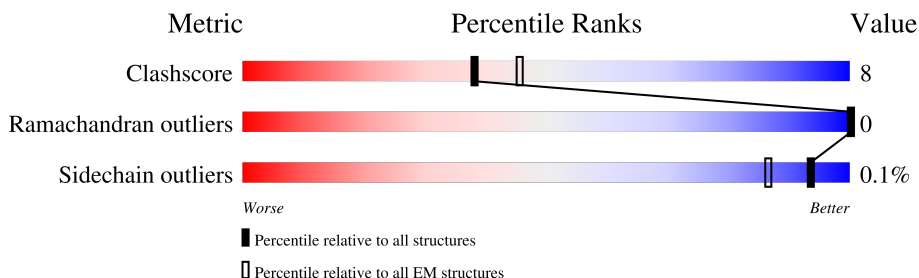
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	B	439	
2	A	347	
3	C	454	
4	H	114	
5	L	105	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	CLR	A	404	-	-	X	-

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 19360 atoms, of which 9739 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 Peroxin-12.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	B	360	Total	C	H	N	O	S	2	0
			5822	1868	2921	520	500	13		

- Molecule 2 is a protein called Peroxin-2.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	A	298	Total	C	H	N	O	S	0	0
			4766	1541	2364	430	421	10		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	157	SER	ALA	conflict	UNP G2Q1C9

- Molecule 3 is a protein called Peroxin-10.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	317	Total	C	H	N	O	S	0	0
			4989	1584	2503	458	431	13		

- Molecule 4 is a protein called Fab heavy chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	H	88	Total	C	H	N	O	S	2	0
			1380	466	660	115	137	2		

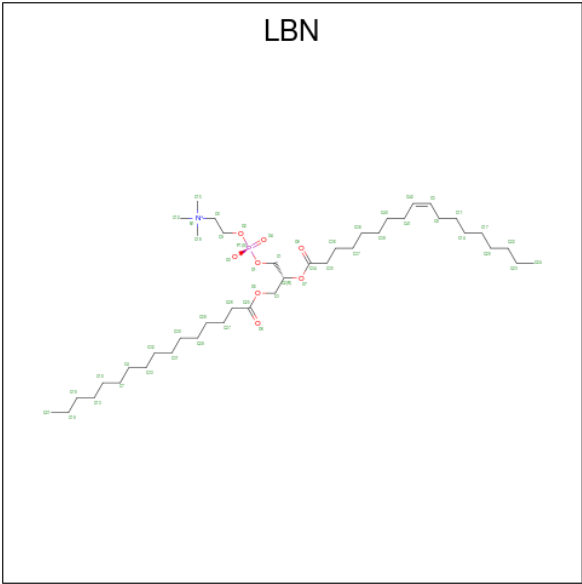
- Molecule 5 is a protein called Fab light chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	L	96	Total	C	H	N	O	S	0	0
			1428	453	708	119	145	3		

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
6	B	1	Total	Zn	0
			1	1	
6	A	2	Total	Zn	0
			2	2	
6	C	2	Total	Zn	0
			2	2	

- Molecule 7 is 1-palmitoyl-2-oleoyl-sn-glycero-3-phosphocholine (three-letter code: LBN) (formula: C₄₂H₈₂NO₈P).



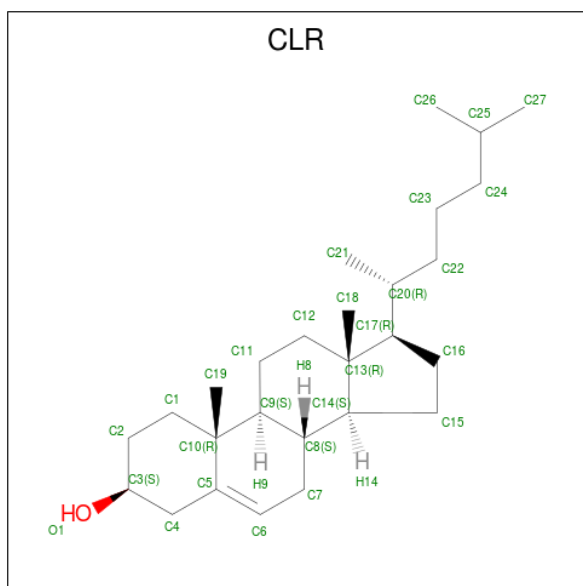
Mol	Chain	Residues	Atoms						AltConf
7	B	1	Total	C	H	N	O	P	0
			253	81	155	1	14	2	
7	B	1	Total	C	H	N	O	P	0
			253	81	155	1	14	2	
7	B	1	Total	C	H	N	O	P	0
			253	81	155	1	14	2	
7	B	1	Total	C	H	N	O	P	0
			253	81	155	1	14	2	
7	A	1	Total	C	H	N	O	P	0
			194	64	122	1	6	1	
7	A	1	Total	C	H	N	O	P	0
			194	64	122	1	6	1	
7	A	1	Total	C	H	N	O	P	0
			194	64	122	1	6	1	

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Mol	Chain	Residues	Atoms						AltConf
7	A	1	Total	C	H	N	O	P	0
			194	64	122	1	6	1	
7	A	1	Total	C	H	N	O	P	0
			194	64	122	1	6	1	
7	A	1	Total	C	H	N	O	P	0
			194	64	122	1	6	1	
7	C	1	Total	C	H	N	O	P	0
			157	48	79	1	26	3	
7	C	1	Total	C	H	N	O	P	0
			157	48	79	1	26	3	
7	C	1	Total	C	H	N	O	P	0
			157	48	79	1	26	3	
7	C	1	Total	C	H	N	O	P	0
			157	48	79	1	26	3	

- Molecule 8 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$).



Mol	Chain	Residues	Atoms				AltConf
8	A	1	Total	C	H	O	0
			144	53	89	2	
8	A	1	Total	C	H	O	0
			144	53	89	2	
8	C	1	Total	C	H	O	0
			222	81	138	3	
8	C	1	Total	C	H	O	0
			222	81	138	3	

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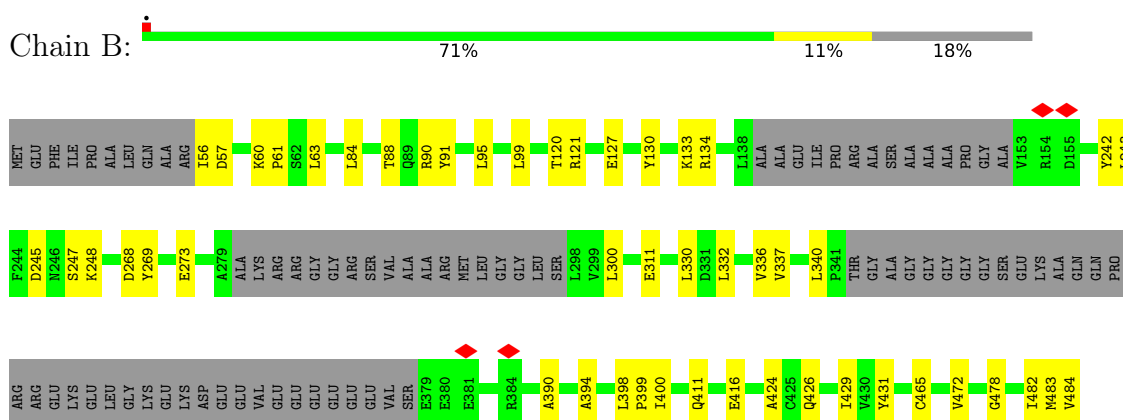
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Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	O	
8	C	1	222	81	138	3	0

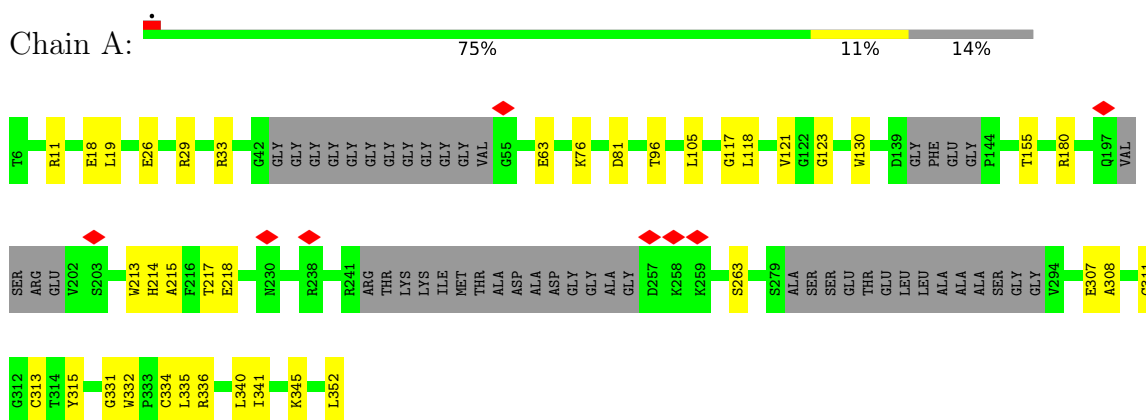
3 Residue-property plots [i](#)

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.

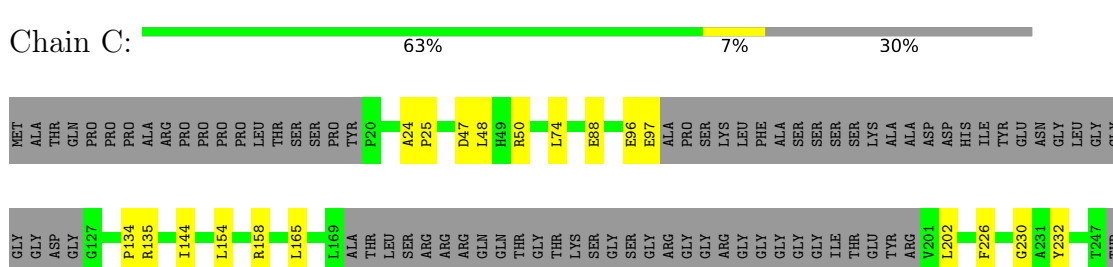
• Molecule 1: Peroxin-12

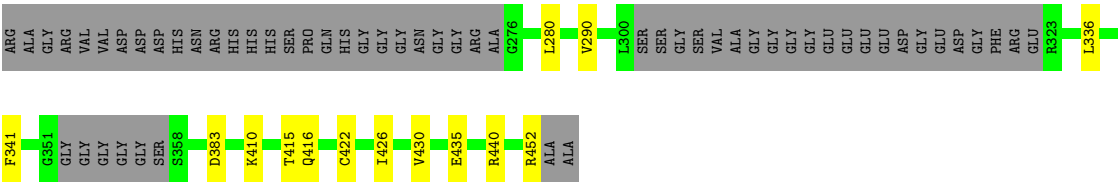


• Molecule 2: Peroxin-2

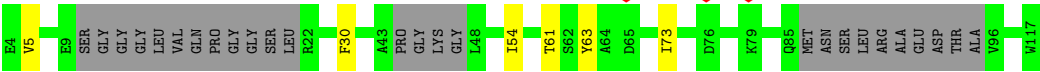


• Molecule 3: Peroxin-10

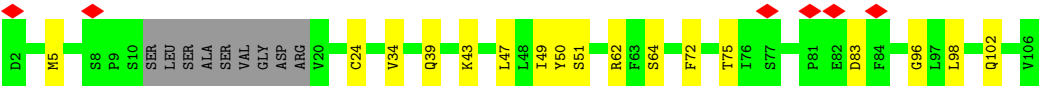




• Molecule 4: Fab heavy chain



• Molecule 5: Fab light chain



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	121644	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 ($e^-/\text{\AA}^2$)	52	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.275	Depositor
Minimum map value	-0.143	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	275.59998, 275.59998, 275.59998	wwPDB
Map dimensions	260, 260, 260	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	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: CLR, LBN, ZN

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	B	0.34	0/2981	0.54	0/4048
2	A	0.31	0/2461	0.51	0/3340
3	C	0.33	0/2539	0.54	1/3439 (0.0%)
4	H	0.31	0/746	0.49	0/1012
5	L	0.29	0/734	0.51	0/994
All	All	0.32	0/9461	0.53	1/12833 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	134	PRO	N-CA-CB	5.54	109.94	103.30

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	B	2901	2921	2915	30	0
2	A	2402	2364	2361	28	0
3	C	2486	2503	2502	26	0
4	H	720	660	670	5	0
5	L	720	708	708	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	2	0	0	0	0
6	B	1	0	0	0	0
6	C	2	0	0	0	0
7	A	72	122	0	0	0
7	B	98	155	0	0	0
7	C	78	79	0	0	0
8	A	55	89	81	34	0
8	C	84	138	132	44	0
All	All	9621	9739	9369	152	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 8.

All (152) 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)
8:C:508:CLR:C10	8:C:508:CLR:C9	1.89	1.50
8:C:509:CLR:C9	8:C:509:CLR:C10	1.89	1.50
8:A:404:CLR:C10	8:A:404:CLR:C9	1.89	1.50
8:A:405:CLR:C10	8:A:405:CLR:C9	1.89	1.46
8:C:508:CLR:C10	8:C:508:CLR:C8	2.24	1.11
8:A:404:CLR:H192	8:C:503:CLR:H12	1.28	1.09
8:A:404:CLR:C10	8:A:404:CLR:C8	2.23	1.01
8:A:405:CLR:C10	8:A:405:CLR:C8	2.25	1.00
8:C:509:CLR:C10	8:C:509:CLR:C8	2.24	0.97
8:A:404:CLR:C19	8:C:503:CLR:H112	2.10	0.81
2:A:130:TRP:HE1	2:A:155:THR:HG21	1.45	0.81
1:B:130:TYR:OH	1:B:311:GLU:OE2	1.97	0.80
1:B:127:GLU:OE2	1:B:134:ARG:NH1	2.17	0.78
8:A:404:CLR:H193	8:C:503:CLR:H112	1.66	0.77
4:H:54:ILE:HG22	4:H:61:THR:HG22	1.66	0.77
8:C:509:CLR:C9	8:C:509:CLR:C5	2.64	0.74
1:B:426:GLN:N	1:B:426:GLN:OE1	2.21	0.73
3:C:435:GLU:OE2	3:C:440:ARG:NH1	2.22	0.73
3:C:97:GLU:OE2	3:C:232:TYR:OH	2.07	0.73
2:A:332:TRP:CZ2	2:A:335:LEU:HD13	2.24	0.72
2:A:263:SER:OG	2:A:336:ARG:O	2.07	0.72
1:B:84:LEU:O	1:B:88:THR:HG23	1.91	0.71
8:C:509:CLR:H192	8:C:509:CLR:O1	1.92	0.70
5:L:39:GLN:NE2	5:L:43:LYS:O	2.24	0.70
1:B:133:LYS:NZ	1:B:268:ASP:OD2	2.17	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:290:VAL:CG2	8:C:503:CLR:H212	2.22	0.69
8:A:404:CLR:H193	8:C:503:CLR:C11	2.22	0.69
1:B:426:GLN:NE2	1:B:478:GLY:O	2.26	0.69
8:A:405:CLR:C9	8:A:405:CLR:C5	2.64	0.69
8:A:404:CLR:C9	8:A:404:CLR:C5	2.65	0.68
3:C:47:ASP:OD1	3:C:50:ARG:NH2	2.25	0.68
8:C:508:CLR:C9	8:C:508:CLR:C5	2.65	0.68
3:C:74:LEU:HD12	3:C:144:ILE:HD11	1.76	0.67
2:A:334:CYS:HB2	2:A:341:ILE:HD11	1.77	0.67
1:B:398:LEU:HD12	1:B:399:PRO:HD2	1.77	0.66
8:C:508:CLR:H182	8:C:508:CLR:H111	1.76	0.66
8:C:508:CLR:H213	8:C:508:CLR:H183	1.77	0.66
2:A:117:GLY:O	2:A:121:VAL:HG12	1.94	0.66
8:C:508:CLR:H182	8:C:508:CLR:C11	2.24	0.65
8:A:404:CLR:C19	8:C:503:CLR:H12	2.15	0.65
8:C:509:CLR:H182	8:C:509:CLR:H111	1.78	0.65
5:L:64:SER:OG	5:L:75:THR:OG1	2.15	0.65
8:A:404:CLR:H211	8:C:503:CLR:H241	1.79	0.64
8:A:405:CLR:C10	8:A:405:CLR:C11	2.76	0.63
2:A:105:LEU:HD23	2:A:105:LEU:O	1.99	0.63
8:C:509:CLR:C10	8:C:509:CLR:C11	2.75	0.62
8:C:508:CLR:C10	8:C:508:CLR:C11	2.73	0.62
8:A:404:CLR:H212	8:A:404:CLR:H121	1.80	0.62
3:C:48:LEU:HB3	8:C:508:CLR:H261	1.82	0.62
8:A:404:CLR:H192	8:C:503:CLR:H112	1.82	0.61
2:A:217:THR:HG21	3:C:341:PHE:HZ	1.65	0.61
2:A:130:TRP:NE1	2:A:155:THR:HG21	2.16	0.61
2:A:307:GLU:OE2	2:A:345:LYS:NZ	2.23	0.59
8:A:404:CLR:C9	8:A:404:CLR:C1	2.78	0.59
8:C:509:CLR:H182	8:C:509:CLR:C11	2.28	0.59
8:A:404:CLR:C10	8:A:404:CLR:C11	2.74	0.59
3:C:290:VAL:HG22	8:C:503:CLR:H212	1.84	0.58
8:C:509:CLR:C11	8:C:509:CLR:C18	2.48	0.58
8:A:404:CLR:C21	8:C:503:CLR:H241	2.33	0.57
8:C:509:CLR:C9	8:C:509:CLR:C1	2.80	0.57
8:A:404:CLR:C11	8:A:404:CLR:H182	2.33	0.57
8:A:404:CLR:C11	8:A:404:CLR:C18	2.52	0.57
8:C:508:CLR:C9	8:C:508:CLR:C1	2.78	0.57
8:A:405:CLR:C9	8:A:405:CLR:C1	2.82	0.56
8:C:508:CLR:H111	8:C:508:CLR:C18	2.26	0.56
8:C:509:CLR:H121	8:C:509:CLR:H212	1.85	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:102:GLN:N	5:L:102:GLN:OE1	2.39	0.55
1:B:340:LEU:HD11	1:B:429:ILE:HD11	1.87	0.55
2:A:33:ARG:NH1	2:A:63:GLU:OE2	2.40	0.55
3:C:74:LEU:HD12	3:C:144:ILE:CD1	2.37	0.55
8:A:404:CLR:H192	8:C:503:CLR:C1	2.19	0.54
8:C:503:CLR:H213	8:C:503:CLR:H183	1.89	0.53
8:C:508:CLR:H121	8:C:508:CLR:H231	1.91	0.53
8:A:405:CLR:C11	8:A:405:CLR:H182	2.37	0.53
3:C:226:PHE:O	3:C:230:GLY:N	2.41	0.53
2:A:213:TRP:O	2:A:217:THR:HG22	2.08	0.53
8:A:404:CLR:H182	8:A:404:CLR:H111	1.89	0.53
4:H:63:TYR:CE2	4:H:73:ILE:HG22	2.44	0.53
1:B:88:THR:HG22	1:B:95:LEU:CB	2.39	0.52
8:A:404:CLR:C19	8:C:503:CLR:C11	2.83	0.52
1:B:88:THR:HG22	1:B:95:LEU:HB3	1.92	0.52
8:C:509:CLR:C9	8:C:509:CLR:C19	2.84	0.51
8:A:405:CLR:C9	8:A:405:CLR:C19	2.83	0.51
8:C:509:CLR:H111	8:C:509:CLR:C18	2.29	0.51
2:A:315:TYR:OH	2:A:334:CYS:SG	2.69	0.50
3:C:290:VAL:HG21	8:C:503:CLR:H212	1.92	0.50
1:B:61:PRO:O	1:B:242:TYR:OH	2.22	0.49
8:A:404:CLR:C9	8:A:404:CLR:C19	2.84	0.49
8:A:404:CLR:H193	8:C:503:CLR:C12	2.41	0.49
2:A:26:GLU:OE1	2:A:29:ARG:NH1	2.46	0.49
2:A:18:GLU:OE2	2:A:180:ARG:HG3	2.13	0.48
3:C:96:GLU:OE1	3:C:135:ARG:NE	2.37	0.48
2:A:76:LYS:NZ	2:A:81:ASP:OD2	2.46	0.48
1:B:330:LEU:HD23	1:B:332:LEU:HD21	1.97	0.47
1:B:426:GLN:CD	1:B:472:VAL:HG13	2.35	0.47
8:A:404:CLR:C18	8:A:404:CLR:H111	2.37	0.47
5:L:34:VAL:HG21	5:L:72:PHE:CE1	2.49	0.47
1:B:482:ILE:HG22	1:B:484:VAL:H	1.80	0.46
3:C:426:ILE:O	3:C:430:VAL:HG22	2.16	0.46
1:B:424:ALA:HB2	1:B:482:ILE:HD11	1.97	0.46
8:C:508:CLR:C9	8:C:508:CLR:C19	2.84	0.46
1:B:247:SER:O	1:B:248:LYS:HB3	2.15	0.46
8:A:405:CLR:H182	8:A:405:CLR:H111	1.97	0.46
1:B:120:THR:OG1	1:B:121:ARG:NH1	2.49	0.46
8:A:404:CLR:H193	8:C:503:CLR:H122	1.98	0.46
8:A:405:CLR:H111	8:A:405:CLR:C18	2.44	0.46
3:C:165:LEU:HD22	3:C:202:LEU:HD12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:49:ILE:HG22	5:L:51:SER:O	2.15	0.46
2:A:118:LEU:O	2:A:123:GLY:N	2.44	0.45
8:C:508:CLR:H213	8:C:508:CLR:C18	2.46	0.45
2:A:332:TRP:HZ2	2:A:335:LEU:HD13	1.79	0.45
3:C:48:LEU:CB	8:C:508:CLR:H261	2.46	0.45
2:A:11:ARG:NH2	3:C:88:GLU:OE1	2.47	0.45
1:B:411:GLN:NE2	1:B:416:GLU:O	2.50	0.45
1:B:340:LEU:HD12	3:C:452:ARG:HD3	1.99	0.45
3:C:422:CYS:O	3:C:426:ILE:HG22	2.17	0.45
2:A:214:HIS:ND1	2:A:218:GLU:OE2	2.51	0.44
2:A:215:ALA:HB2	3:C:280:LEU:HD22	2.00	0.44
8:A:405:CLR:C11	8:A:405:CLR:C18	2.55	0.44
3:C:415:THR:HG22	3:C:416:GLN:N	2.33	0.44
3:C:290:VAL:HG11	8:C:503:CLR:H162	1.98	0.44
4:H:54:ILE:CG2	4:H:61:THR:HG22	2.45	0.43
5:L:47:LEU:HD21	5:L:50:TYR:HB3	1.99	0.43
2:A:19:LEU:HD11	3:C:336:LEU:HD12	1.99	0.43
4:H:5:VAL:HG13	4:H:30:PHE:HD2	1.83	0.43
5:L:96:GLY:O	5:L:98:LEU:HD12	2.18	0.43
1:B:431:TYR:OH	1:B:465:CYS:SG	2.76	0.43
2:A:308:ALA:CB	2:A:341:ILE:HD13	2.48	0.43
4:H:54:ILE:HG21	4:H:73:ILE:HG12	2.00	0.43
1:B:88:THR:HG21	1:B:99:LEU:HB2	2.01	0.43
2:A:311:CYS:HB3	2:A:313:CYS:SG	2.58	0.42
1:B:394:ALA:HA	2:A:352:LEU:HD21	2.02	0.42
2:A:96:THR:HG21	2:A:105:LEU:HG	2.01	0.42
2:A:308:ALA:HB3	2:A:311:CYS:HB2	2.00	0.42
5:L:5:MET:HG3	5:L:24:CYS:SG	2.60	0.42
2:A:308:ALA:HB2	2:A:341:ILE:HD13	2.00	0.42
5:L:62:ARG:NH1	5:L:83:ASP:OD1	2.52	0.42
2:A:331:GLY:HA3	2:A:340:LEU:HD21	2.01	0.41
1:B:90:ARG:HG3	1:B:91:TYR:CE1	2.56	0.41
1:B:483:MET:O	1:B:484:VAL:C	2.59	0.41
3:C:24:ALA:N	3:C:25:PRO:HD2	2.36	0.41
8:C:509:CLR:H192	8:C:509:CLR:C3	2.50	0.41
3:C:74:LEU:CD1	3:C:144:ILE:HD11	2.47	0.41
1:B:269:TYR:O	1:B:273:GLU:HG2	2.20	0.41
1:B:390:ALA:HB1	1:B:400:ILE:O	2.20	0.41
1:B:63:LEU:HD22	1:B:243:LEU:HD21	2.03	0.41
3:C:383:ASP:HA	3:C:410:LYS:HA	2.03	0.41
3:C:154:LEU:HD13	3:C:158:ARG:NH2	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:336:VAL:HG12	1:B:337:VAL:N	2.35	0.40
1:B:56:ILE:HG23	1:B:57:ASP:N	2.36	0.40
8:A:404:CLR:C8	8:A:404:CLR:C19	2.97	0.40
1:B:60:LYS:NZ	1:B:245:ASP:OD1	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	354/439 (81%)	340 (96%)	14 (4%)	0	100	100
2	A	286/347 (82%)	274 (96%)	12 (4%)	0	100	100
3	C	305/454 (67%)	294 (96%)	11 (4%)	0	100	100
4	H	82/114 (72%)	78 (95%)	4 (5%)	0	100	100
5	L	92/105 (88%)	87 (95%)	5 (5%)	0	100	100
All	All	1119/1459 (77%)	1073 (96%)	46 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	300/354 (85%)	299 (100%)	1 (0%)	92	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	A	247/275 (90%)	247 (100%)	0	100	100
3	C	255/347 (74%)	255 (100%)	0	100	100
4	H	75/90 (83%)	75 (100%)	0	100	100
5	L	82/89 (92%)	82 (100%)	0	100	100
All	All	959/1155 (83%)	958 (100%)	1 (0%)	93	98

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	300	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 25 ligands modelled in this entry, 5 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
7	LBN	B	502	-	34,34,51	1.46	4 (11%)	38,41,59	1.05	2 (5%)
7	LBN	A	409	-	7,7,51	0.29	0	6,6,59	0.73	0
7	LBN	A	403	-	12,12,51	0.33	0	11,11,59	0.69	0
7	LBN	A	407	-	12,12,51	0.34	0	11,11,59	0.66	0
7	LBN	C	507	-	18,18,51	1.39	4 (22%)	22,23,59	1.32	1 (4%)
8	CLR	A	405	-	30,30,31	14.22	18 (60%)	46,46,48	2.58	19 (41%)
8	CLR	C	503	-	31,31,31	0.86	0	48,48,48	0.81	1 (2%)
7	LBN	B	505	-	20,22,51	1.34	5 (25%)	22,24,59	1.34	2 (9%)
7	LBN	A	406	-	14,14,51	0.32	0	13,13,59	0.72	0
7	LBN	C	504	-	15,15,51	0.87	1 (6%)	15,15,59	1.08	0
7	LBN	C	505	-	19,19,51	1.29	3 (15%)	22,24,59	1.07	1 (4%)
7	LBN	B	506	-	13,13,51	0.30	0	12,12,59	0.81	0
7	LBN	C	506	-	22,22,51	1.36	5 (22%)	26,27,59	1.61	3 (11%)
8	CLR	A	404	-	31,31,31	13.94	17 (54%)	48,48,48	2.13	16 (33%)
8	CLR	C	508	-	31,31,31	13.97	17 (54%)	48,48,48	2.02	14 (29%)
7	LBN	B	503	-	13,13,51	0.27	0	12,12,59	0.88	0
7	LBN	A	408	-	13,13,51	1.02	0	12,15,59	0.50	0
7	LBN	A	410	-	8,8,51	0.29	0	7,7,59	0.75	0
8	CLR	C	509	-	31,31,31	13.95	17 (54%)	48,48,48	2.20	14 (29%)
7	LBN	B	504	-	11,11,51	0.28	0	10,10,59	0.81	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
7	LBN	B	502	-	-	15/37/37/55	-
7	LBN	A	409	-	-	2/5/5/55	-
7	LBN	A	403	-	-	2/10/10/55	-
7	LBN	A	407	-	-	4/10/10/55	-
7	LBN	C	507	-	-	12/19/19/55	-
8	CLR	A	405	-	-	9/9/67/68	0/4/4/4
8	CLR	C	503	-	-	3/10/68/68	0/4/4/4
7	LBN	B	505	-	-	10/21/24/55	-
7	LBN	A	406	-	-	5/12/12/55	-
7	LBN	C	504	-	-	7/13/13/55	-
7	LBN	C	505	-	-	9/22/22/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	LBN	B	506	-	-	4/11/11/55	-
7	LBN	C	506	-	-	5/24/24/55	-
8	CLR	A	404	-	-	4/10/68/68	0/4/4/4
8	CLR	C	508	-	-	7/10/68/68	0/4/4/4
7	LBN	B	503	-	-	5/11/11/55	-
7	LBN	A	408	-	-	6/13/13/55	-
7	LBN	A	410	-	-	1/6/6/55	-
8	CLR	C	509	-	-	2/10/68/68	0/4/4/4
7	LBN	B	504	-	-	4/9/9/55	-

All (91) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	405	CLR	C12-C13	-54.77	0.55	1.54
8	C	508	CLR	C12-C13	-54.63	0.56	1.54
8	C	509	CLR	C12-C13	-54.43	0.56	1.54
8	A	404	CLR	C12-C13	-54.19	0.56	1.54
8	A	404	CLR	C8-C9	-45.19	0.67	1.53
8	C	508	CLR	C8-C9	-45.01	0.67	1.53
8	C	509	CLR	C8-C9	-45.00	0.67	1.53
8	A	405	CLR	C8-C9	-44.95	0.67	1.53
8	A	404	CLR	C10-C9	20.20	1.89	1.56
8	A	405	CLR	C10-C9	20.19	1.89	1.56
8	C	509	CLR	C10-C9	20.19	1.89	1.56
8	C	508	CLR	C10-C9	20.18	1.89	1.56
8	C	509	CLR	C8-C14	-13.90	1.27	1.53
8	A	405	CLR	C8-C14	-13.84	1.27	1.53
8	A	404	CLR	C8-C14	-13.81	1.27	1.53
8	C	508	CLR	C8-C14	-13.56	1.27	1.53
8	C	509	CLR	C10-C5	-12.29	1.28	1.52
8	A	405	CLR	C10-C5	-12.15	1.28	1.52
8	A	404	CLR	C10-C5	-12.03	1.29	1.52
8	C	508	CLR	C10-C5	-12.02	1.29	1.52
8	A	405	CLR	C6-C5	-9.16	1.12	1.33
8	C	509	CLR	C6-C5	-9.09	1.12	1.33
8	C	508	CLR	C6-C5	-9.05	1.13	1.33
8	A	404	CLR	C6-C5	-9.01	1.13	1.33
8	C	508	CLR	C2-C3	-6.46	1.36	1.51
8	A	404	CLR	C2-C3	-6.46	1.36	1.51
8	C	508	CLR	C12-C11	-6.29	1.40	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	404	CLR	C12-C11	-6.22	1.40	1.53
8	A	405	CLR	C2-C3	-6.16	1.36	1.51
8	C	509	CLR	C2-C3	-6.14	1.37	1.51
8	C	509	CLR	C12-C11	-6.12	1.40	1.53
8	A	405	CLR	C12-C11	-6.08	1.40	1.53
8	A	404	CLR	C7-C8	5.55	1.62	1.53
8	C	509	CLR	C7-C8	5.42	1.62	1.53
7	B	502	LBN	O7-C2	-5.42	1.40	1.46
8	C	508	CLR	C7-C8	5.38	1.62	1.53
8	A	405	CLR	C7-C8	5.36	1.62	1.53
8	C	508	CLR	C4-C5	4.30	1.61	1.51
8	C	509	CLR	C4-C5	4.29	1.61	1.51
8	A	404	CLR	C4-C5	4.26	1.60	1.51
8	A	405	CLR	C4-C5	4.09	1.60	1.51
8	C	508	CLR	C16-C17	3.80	1.62	1.54
8	C	509	CLR	C16-C17	3.72	1.62	1.54
8	A	405	CLR	C16-C17	3.69	1.62	1.54
8	A	404	CLR	C7-C6	3.68	1.58	1.50
8	A	404	CLR	C16-C17	3.67	1.62	1.54
8	C	508	CLR	C11-C9	-3.54	1.47	1.53
8	C	509	CLR	O1-C3	3.54	1.53	1.43
8	A	405	CLR	C7-C6	3.53	1.57	1.50
8	A	404	CLR	O1-C3	3.53	1.53	1.43
8	A	405	CLR	O1-C3	3.50	1.53	1.43
8	C	509	CLR	C11-C9	-3.50	1.47	1.53
8	A	404	CLR	C11-C9	-3.48	1.47	1.53
8	C	508	CLR	C7-C6	3.46	1.57	1.50
8	C	509	CLR	C7-C6	3.45	1.57	1.50
8	C	508	CLR	O1-C3	3.43	1.53	1.43
8	A	405	CLR	C11-C9	-3.35	1.48	1.53
7	B	502	LBN	O7-C34	3.28	1.40	1.33
8	A	405	CLR	C15-C14	3.22	1.61	1.54
8	C	508	CLR	C15-C14	3.12	1.60	1.54
8	C	509	CLR	C15-C14	3.01	1.60	1.54
8	A	404	CLR	C18-C13	3.00	1.59	1.54
8	A	405	CLR	C18-C13	2.99	1.59	1.54
8	A	404	CLR	C15-C14	2.92	1.60	1.54
7	C	504	LBN	O5-C25	2.83	1.40	1.30
8	A	405	CLR	C1-C10	2.78	1.59	1.54
7	C	505	LBN	O7-C2	-2.72	1.39	1.46
7	C	507	LBN	P1-O2	2.69	1.65	1.54
8	C	508	CLR	C18-C13	2.68	1.59	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	506	LBN	P1-O2	2.65	1.65	1.54
8	A	404	CLR	C1-C10	2.65	1.59	1.54
8	C	508	CLR	C1-C10	2.63	1.59	1.54
8	C	509	CLR	C18-C13	2.62	1.58	1.54
7	C	507	LBN	O7-C2	-2.56	1.40	1.46
7	C	506	LBN	O7-C2	-2.53	1.40	1.46
8	C	509	CLR	C1-C10	2.45	1.58	1.54
7	B	505	LBN	O7-C2	-2.45	1.40	1.46
7	B	505	LBN	O5-C25	2.36	1.40	1.33
7	C	506	LBN	O7-C34	2.33	1.40	1.34
7	C	506	LBN	O5-C25	2.30	1.40	1.33
7	B	502	LBN	O5-C25	2.29	1.40	1.33
7	C	505	LBN	O5-C3	-2.27	1.40	1.45
7	B	502	LBN	O5-C3	-2.26	1.40	1.45
7	C	506	LBN	O5-C3	-2.26	1.40	1.45
7	B	505	LBN	O2-C9	-2.23	1.40	1.43
7	B	505	LBN	O5-C3	-2.21	1.40	1.45
8	A	405	CLR	C13-C17	-2.18	1.50	1.55
7	C	507	LBN	O5-C3	-2.14	1.40	1.45
7	C	507	LBN	O7-C34	2.11	1.40	1.34
7	B	505	LBN	O7-C34	2.10	1.40	1.34
7	C	505	LBN	O7-C34	2.09	1.40	1.34

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	405	CLR	C16-C17-C20	7.37	123.56	112.15
8	A	405	CLR	C16-C17-C13	6.66	111.87	103.84
7	C	506	LBN	O7-C34-C35	5.92	124.26	111.50
8	A	404	CLR	C18-C13-C17	-5.45	101.55	111.71
8	C	509	CLR	C12-C13-C17	5.18	124.32	116.57
8	C	508	CLR	C14-C8-C9	4.92	115.68	109.09
8	A	404	CLR	C14-C8-C9	4.85	115.58	109.09
8	A	404	CLR	C12-C13-C17	4.77	123.71	116.57
8	C	508	CLR	C11-C12-C13	4.73	120.89	112.78
8	C	509	CLR	C14-C8-C9	4.66	115.33	109.09
8	C	509	CLR	C18-C13-C17	-4.66	103.03	111.71
8	A	404	CLR	C11-C12-C13	4.60	120.67	112.78
7	C	507	LBN	O7-C34-C35	4.54	121.28	111.50
8	C	508	CLR	C12-C13-C17	4.51	123.31	116.57
8	C	508	CLR	C18-C13-C14	-4.42	103.47	111.71
8	A	405	CLR	C11-C12-C13	4.39	120.31	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	509	CLR	C2-C3-C4	4.25	116.14	110.31
8	C	509	CLR	C11-C12-C13	4.25	120.08	112.78
8	C	509	CLR	C1-C2-C3	4.23	115.89	110.47
8	A	405	CLR	C12-C13-C14	4.22	113.82	107.27
8	A	405	CLR	C18-C13-C17	-4.03	104.20	111.71
8	C	508	CLR	C11-C9-C10	-4.01	107.79	113.08
7	B	502	LBN	O7-C34-O8	-4.00	120.47	125.57
8	A	405	CLR	C14-C8-C9	3.92	114.34	109.09
8	C	509	CLR	C18-C13-C14	-3.92	104.41	111.71
8	A	404	CLR	C11-C9-C10	-3.86	108.00	113.08
8	C	508	CLR	C18-C13-C17	-3.77	104.69	111.71
7	B	505	LBN	O7-C34-C35	3.75	119.59	111.50
8	A	405	CLR	C12-C13-C17	3.70	122.11	116.57
8	C	509	CLR	C12-C13-C14	3.70	113.01	107.27
8	C	508	CLR	C12-C13-C14	3.46	112.63	107.27
8	C	509	CLR	C11-C9-C10	-3.45	108.53	113.08
7	C	505	LBN	O7-C34-C35	3.41	120.30	110.80
8	A	405	CLR	C7-C6-C5	-3.38	118.82	125.06
8	A	404	CLR	C18-C13-C14	-3.36	105.45	111.71
8	A	405	CLR	C1-C2-C3	3.36	114.78	110.47
8	A	405	CLR	C21-C20-C17	-3.34	107.81	112.92
8	A	404	CLR	C16-C17-C20	-3.26	107.09	112.15
8	C	509	CLR	C7-C6-C5	-3.24	119.08	125.06
8	A	405	CLR	C4-C5-C10	-3.22	112.14	116.42
8	A	404	CLR	C7-C6-C5	-3.22	119.13	125.06
8	A	404	CLR	C12-C13-C14	3.21	112.26	107.27
7	C	506	LBN	O5-C25-C26	3.16	119.67	111.38
8	A	405	CLR	C4-C5-C6	3.11	125.09	120.61
8	A	405	CLR	C11-C9-C10	-3.03	109.08	113.08
8	C	509	CLR	C16-C17-C20	-3.02	107.48	112.15
8	C	509	CLR	C3-C4-C5	3.00	117.11	112.03
8	C	508	CLR	C7-C6-C5	-2.97	119.59	125.06
8	A	404	CLR	C4-C5-C6	2.92	124.82	120.61
8	C	503	CLR	C13-C17-C20	2.92	124.05	119.49
8	A	405	CLR	C18-C13-C14	-2.90	106.30	111.71
8	C	508	CLR	C21-C20-C17	2.90	117.36	112.92
7	B	505	LBN	O5-C25-C26	2.77	120.58	111.91
8	A	405	CLR	C7-C8-C9	2.70	112.98	109.71
8	A	405	CLR	C15-C14-C13	2.57	106.94	103.84
8	A	404	CLR	C4-C5-C10	-2.53	113.05	116.42
8	A	404	CLR	C21-C20-C22	-2.49	106.46	110.36
7	C	506	LBN	O7-C34-O8	-2.45	117.78	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	509	CLR	C7-C8-C9	2.40	112.62	109.71
8	A	404	CLR	C1-C10-C5	2.39	113.14	108.75
8	C	508	CLR	C4-C5-C6	2.35	123.99	120.61
8	C	508	CLR	C4-C5-C10	-2.34	113.32	116.42
8	C	508	CLR	C1-C10-C9	-2.31	105.50	108.73
8	C	508	CLR	C11-C9-C8	2.27	115.02	111.75
7	B	502	LBN	O5-C25-C26	2.25	118.96	111.91
8	A	405	CLR	C13-C14-C8	-2.20	111.12	114.38
8	C	508	CLR	C1-C2-C3	2.20	113.29	110.47
8	A	404	CLR	C16-C17-C13	2.18	106.47	103.84
8	A	405	CLR	C2-C3-C4	2.17	113.29	110.31
8	A	404	CLR	C1-C10-C9	-2.07	105.83	108.73
8	A	404	CLR	C11-C9-C8	2.05	114.71	111.75
8	C	509	CLR	C4-C5-C6	2.04	123.55	120.61
8	A	405	CLR	C15-C14-C8	2.01	122.39	119.08

There are no chirality outliers.

All (116) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	502	LBN	C1-O1-P1-O3
7	B	502	LBN	C1-C2-O7-C34
7	B	502	LBN	C3-C2-O7-C34
7	B	502	LBN	O8-C34-O7-C2
7	B	505	LBN	C35-C34-O7-C2
7	C	505	LBN	N1-C6-C9-O2
7	C	505	LBN	C35-C34-O7-C2
7	C	506	LBN	C35-C34-O7-C2
7	C	506	LBN	O8-C34-O7-C2
7	C	507	LBN	C1-O1-P1-O2
7	C	507	LBN	C1-O1-P1-O3
7	C	507	LBN	O8-C34-O7-C2
8	A	405	CLR	C13-C17-C20-C21
7	B	505	LBN	O8-C34-O7-C2
7	C	505	LBN	O8-C34-O7-C2
7	B	505	LBN	C26-C25-O5-C3
7	C	507	LBN	C35-C34-O7-C2
8	A	405	CLR	C21-C20-C22-C23
8	A	405	CLR	C13-C17-C20-C22
8	A	405	CLR	C16-C17-C20-C21
7	B	505	LBN	O6-C25-O5-C3
8	C	503	CLR	C16-C17-C20-C22

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Mol	Chain	Res	Type	Atoms
7	B	502	LBN	C2-C1-O1-P1
8	C	508	CLR	C17-C20-C22-C23
7	B	502	LBN	C26-C25-O5-C3
7	C	507	LBN	C26-C25-O5-C3
8	C	503	CLR	C13-C17-C20-C22
8	C	508	CLR	C13-C17-C20-C22
7	B	502	LBN	O6-C25-O5-C3
8	C	509	CLR	C17-C20-C22-C23
8	C	509	CLR	C21-C20-C22-C23
7	B	502	LBN	C25-C26-C27-C28
8	A	405	CLR	C17-C20-C22-C23
8	C	503	CLR	C16-C17-C20-C21
8	C	508	CLR	C16-C17-C20-C22
8	A	404	CLR	C20-C22-C23-C24
7	B	502	LBN	C1-O1-P1-O2
7	A	408	LBN	C1-O1-P1-O2
8	A	405	CLR	C16-C17-C20-C22
8	C	508	CLR	C16-C17-C20-C21
7	B	503	LBN	C28-C29-C30-C31
7	B	503	LBN	C30-C31-C32-C33
7	B	504	LBN	C7-C10-C13-C16
7	A	406	LBN	C8-C11-C14-C17
7	A	407	LBN	C11-C14-C17-C20
7	B	504	LBN	C30-C31-C32-C33
8	C	508	CLR	C21-C20-C22-C23
7	B	505	LBN	C25-C26-C27-C28
7	C	504	LBN	C25-C26-C27-C28
7	C	507	LBN	O6-C25-O5-C3
7	B	506	LBN	C32-C33-C4-C7
7	A	407	LBN	C17-C20-C22-C23
7	B	503	LBN	C13-C10-C7-C4
7	A	410	LBN	C32-C33-C4-C7
8	C	508	CLR	C22-C23-C24-C25
7	A	403	LBN	C39-C40-C41-C42
7	A	406	LBN	C14-C11-C8-C5
8	A	404	CLR	C23-C24-C25-C27
8	A	404	CLR	C22-C23-C24-C25
8	A	404	CLR	C23-C24-C25-C26
7	C	505	LBN	C26-C25-O5-C3
7	B	505	LBN	C3-C2-O7-C34
7	C	507	LBN	C1-O1-P1-O4
7	C	507	LBN	O1-C1-C2-O7

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Mol	Chain	Res	Type	Atoms
7	B	506	LBN	C28-C29-C30-C31
7	B	506	LBN	C13-C10-C7-C4
7	B	505	LBN	C37-C38-C39-C40
7	B	505	LBN	O1-C1-C2-C3
7	C	507	LBN	C1-C2-C3-O5
8	C	508	CLR	C20-C22-C23-C24
7	B	505	LBN	C35-C36-C37-C38
7	C	504	LBN	C28-C29-C30-C31
7	B	502	LBN	C7-C10-C13-C16
7	B	505	LBN	O1-C1-C2-O7
7	B	502	LBN	C13-C16-C19-C21
7	B	502	LBN	C1-O1-P1-O4
7	A	408	LBN	C1-O1-P1-O4
7	C	505	LBN	C1-O1-P1-O3
7	B	506	LBN	C7-C10-C13-C16
7	A	408	LBN	O8-C34-O7-C2
7	C	507	LBN	O7-C2-C3-O5
7	C	504	LBN	C26-C27-C28-C29
7	A	406	LBN	C37-C38-C39-C40
7	C	507	LBN	C3-C2-O7-C34
7	C	507	LBN	O1-C1-C2-C3
7	A	408	LBN	C9-O2-P1-O1
7	C	504	LBN	C32-C33-C4-C7
7	C	505	LBN	O6-C25-O5-C3
7	A	408	LBN	C1-C2-O7-C34
7	A	403	LBN	C42-C5-C8-C11
7	B	504	LBN	C28-C29-C30-C31
7	A	407	LBN	C14-C11-C8-C5
7	B	503	LBN	C7-C10-C13-C16
7	C	504	LBN	C30-C31-C32-C33
8	A	405	CLR	C22-C23-C24-C25
7	B	502	LBN	C32-C33-C4-C7
7	C	504	LBN	C13-C10-C7-C4
7	C	504	LBN	C29-C30-C31-C32
8	A	405	CLR	C23-C24-C25-C26
7	A	406	LBN	C42-C5-C8-C11
7	A	409	LBN	C27-C28-C29-C30
7	C	506	LBN	O7-C34-C35-C36
7	A	409	LBN	C28-C29-C30-C31
7	C	506	LBN	C37-C38-C39-C40
7	A	407	LBN	C40-C41-C42-C5
7	C	505	LBN	O1-C1-C2-C3

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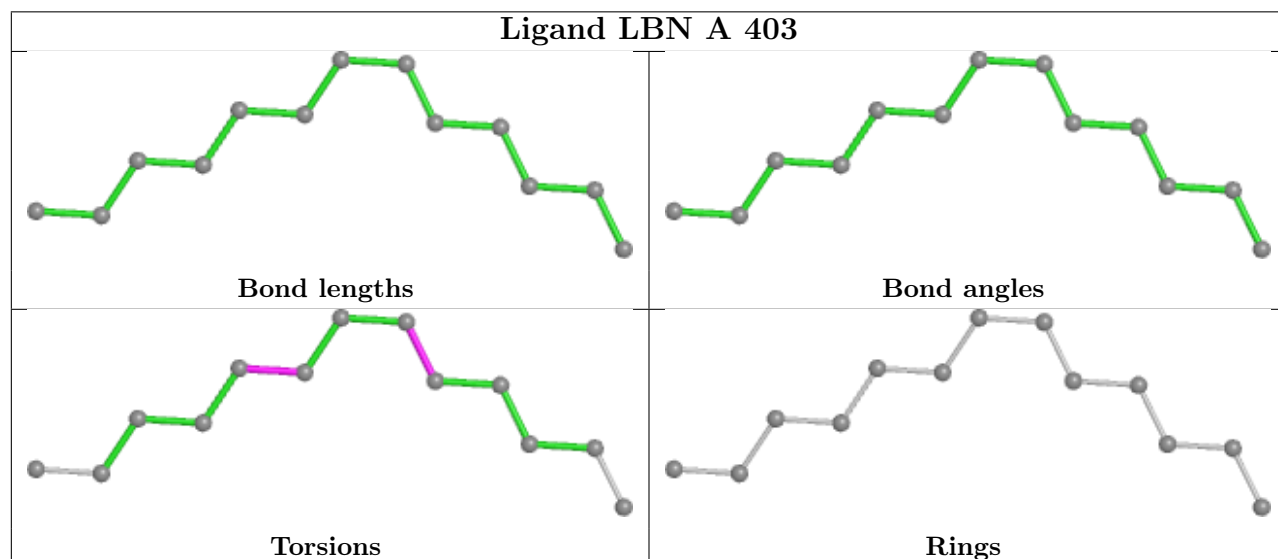
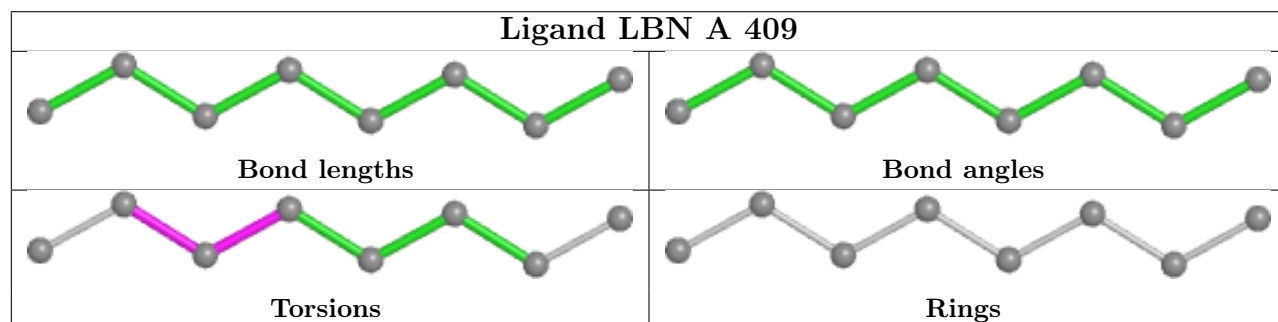
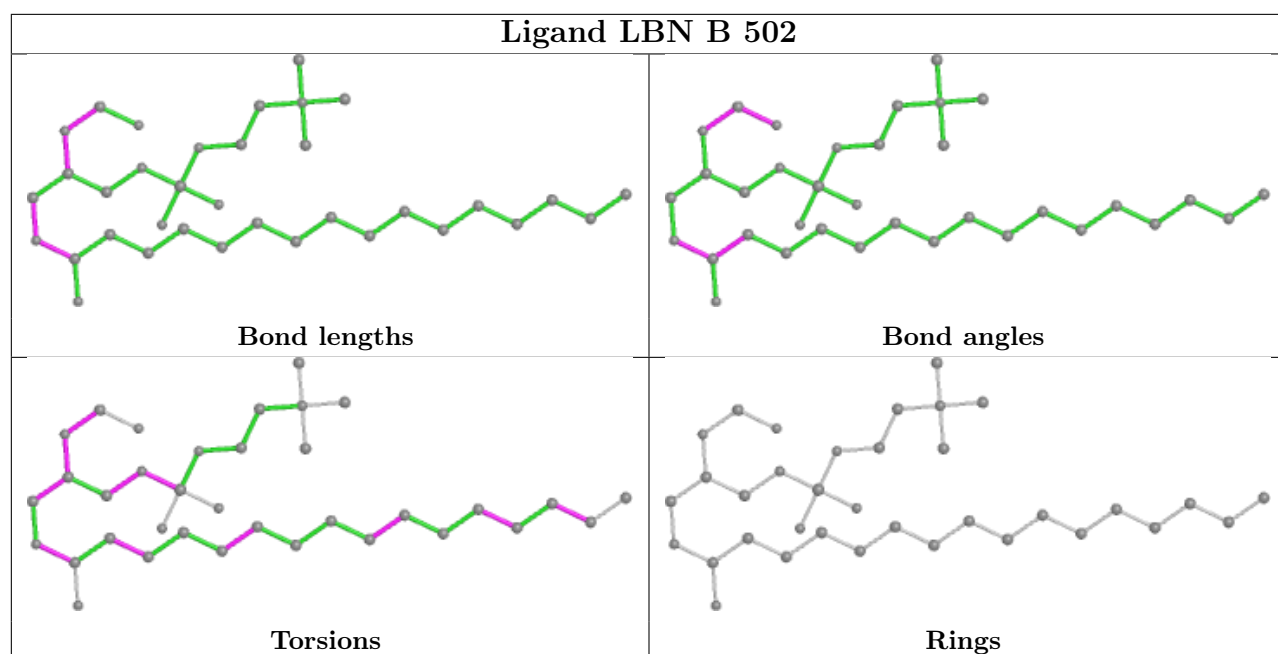
Mol	Chain	Res	Type	Atoms
7	B	502	LBN	O7-C2-C3-O5
7	C	505	LBN	O7-C34-C35-C36
7	A	408	LBN	N1-C6-C9-O2
7	C	505	LBN	O8-C34-C35-C36
7	C	506	LBN	O8-C34-C35-C36
8	A	405	CLR	C20-C22-C23-C24
7	B	502	LBN	C28-C29-C30-C31
7	A	406	LBN	C40-C41-C42-C5
7	B	503	LBN	C32-C33-C4-C7
7	B	504	LBN	C31-C32-C33-C4

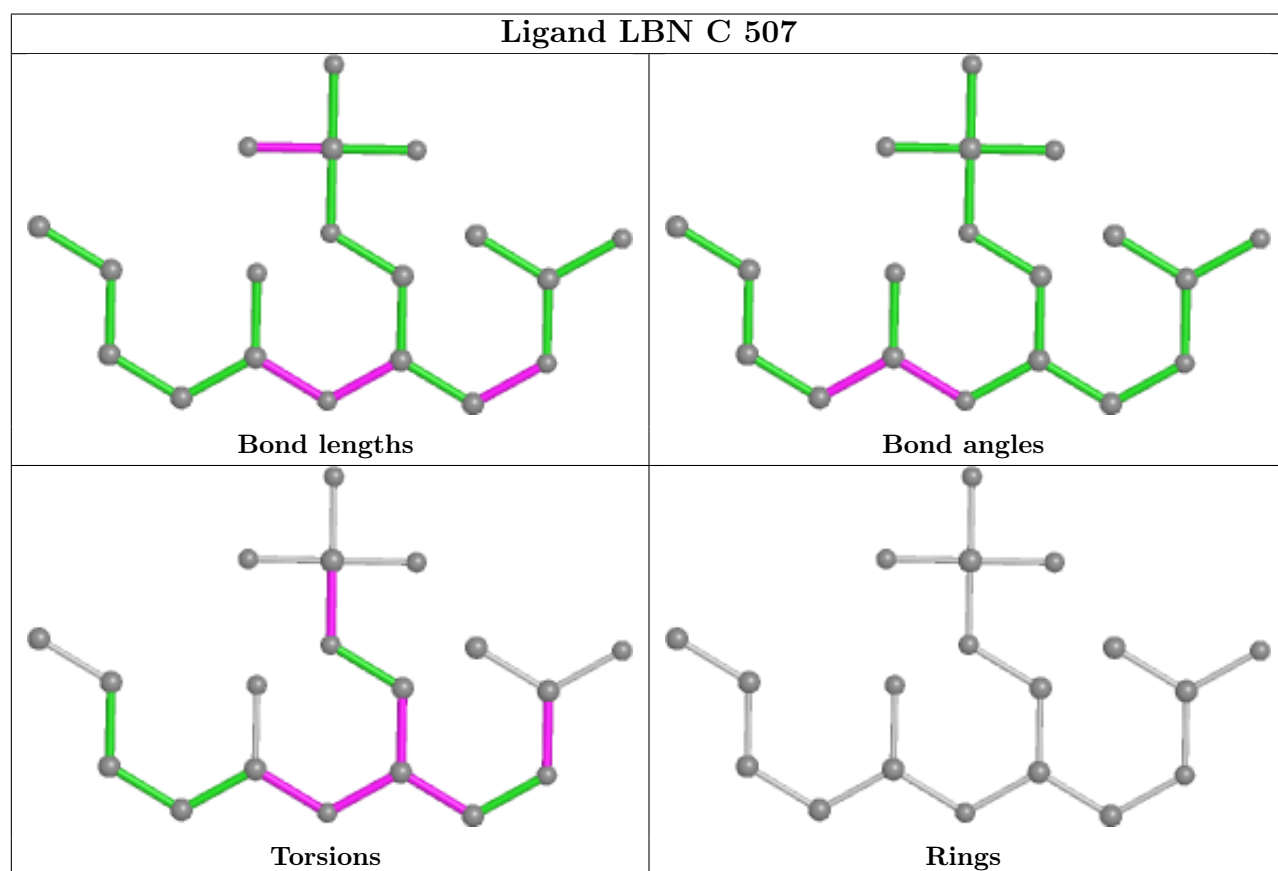
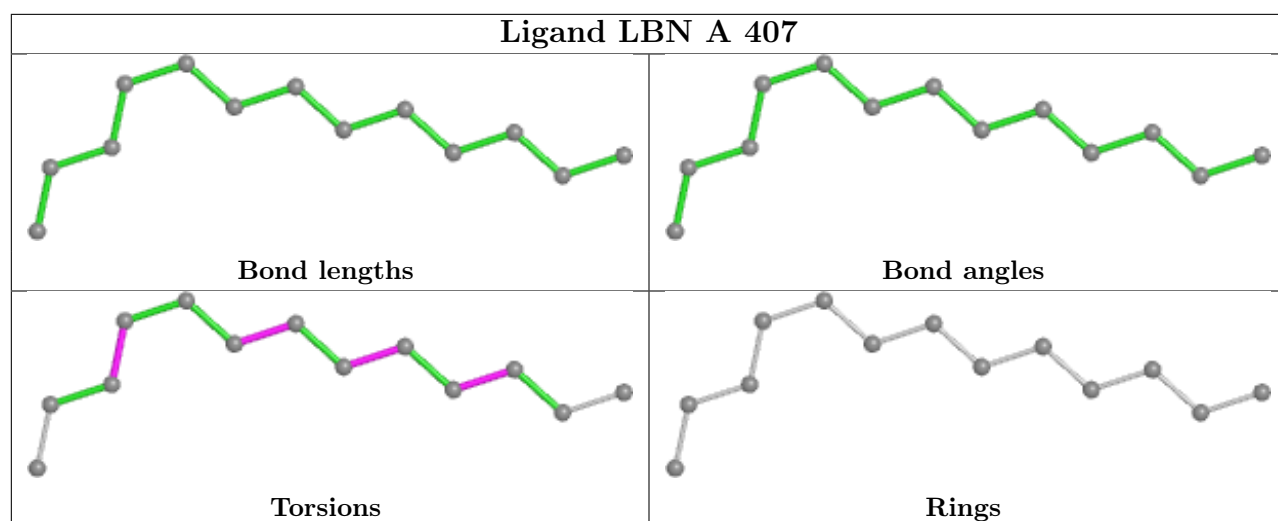
There are no ring outliers.

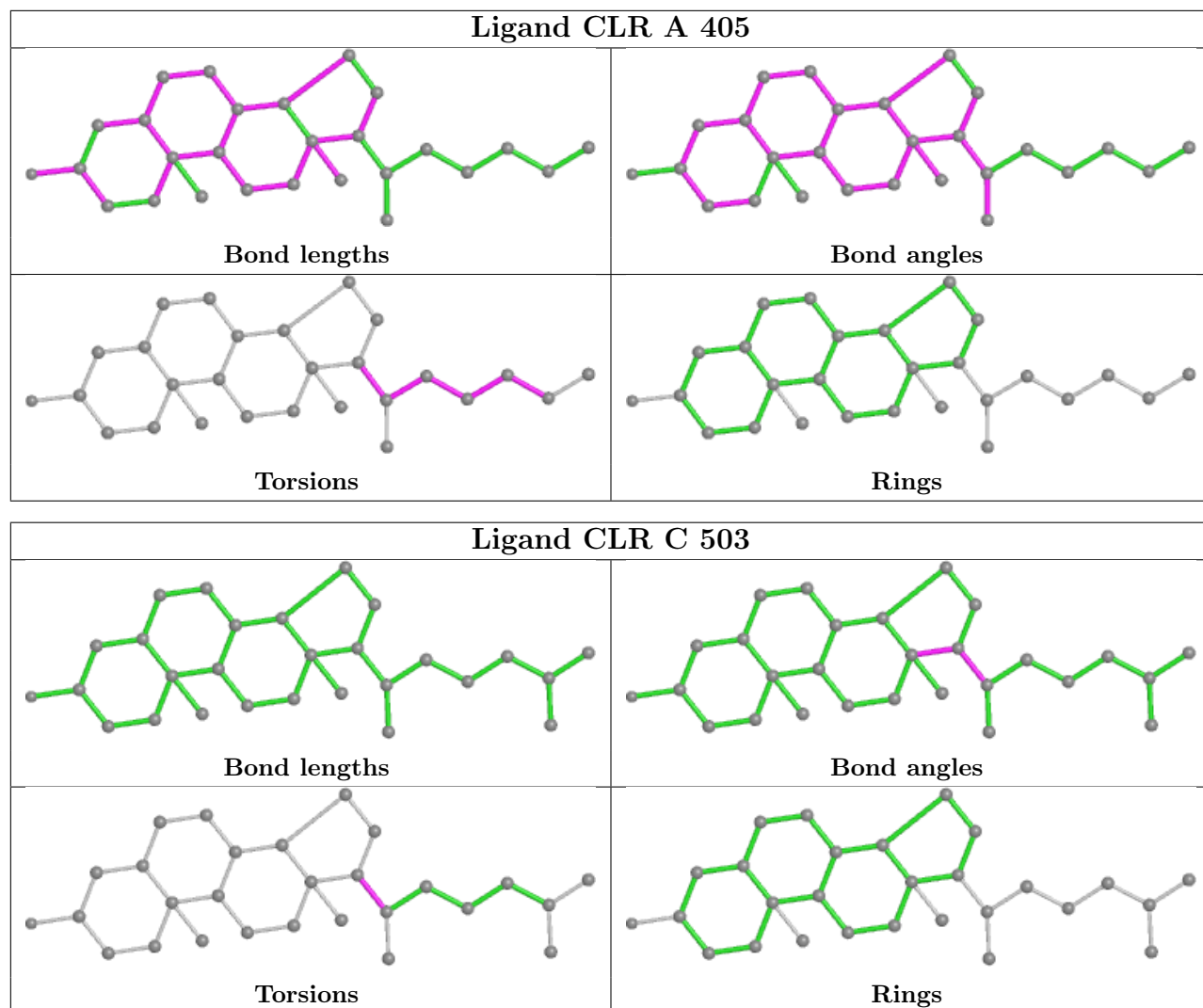
5 monomers are involved in 66 short contacts:

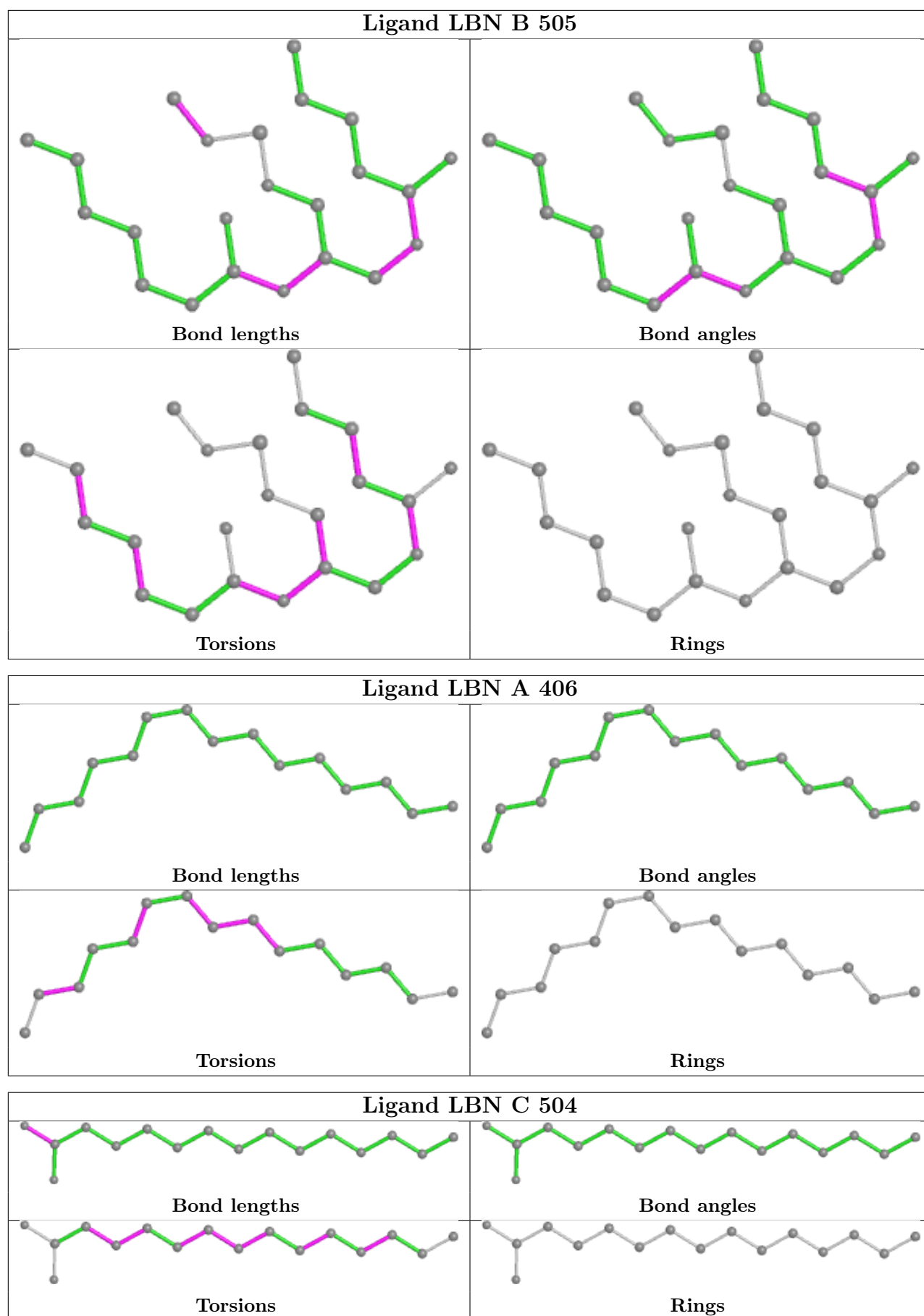
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	405	CLR	10	0
8	C	503	CLR	17	0
8	A	404	CLR	24	0
8	C	508	CLR	14	0
8	C	509	CLR	13	0

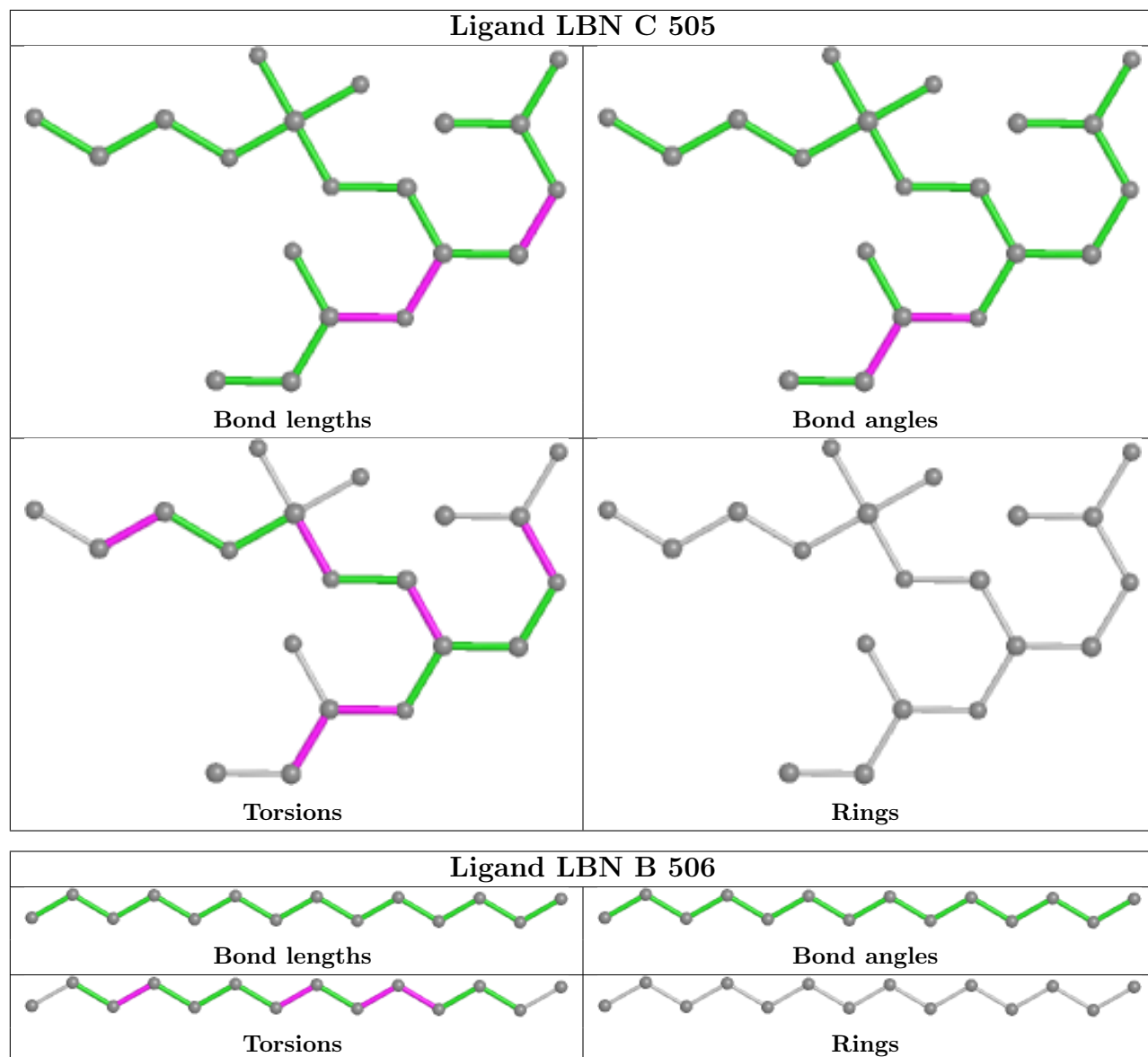
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

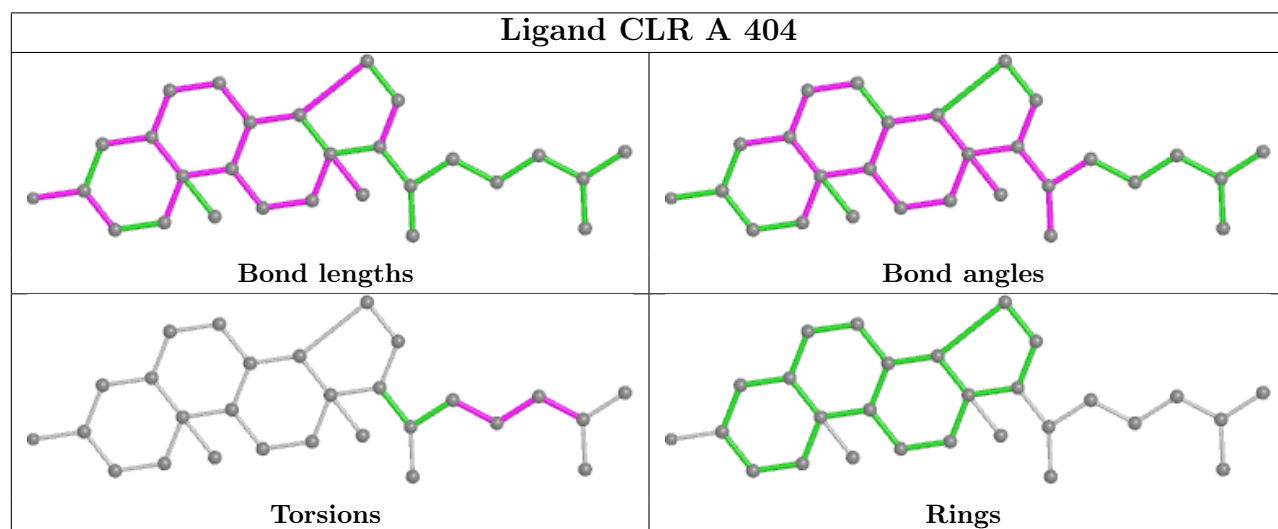
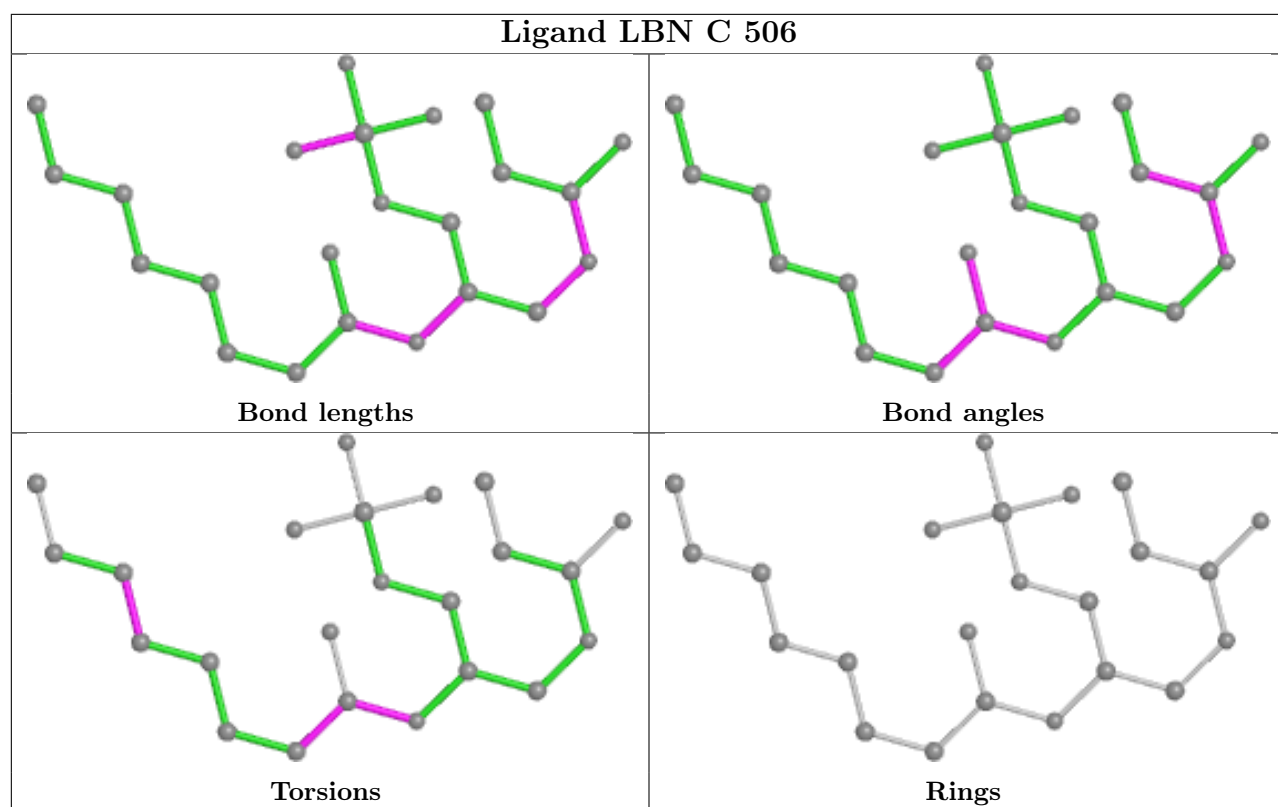


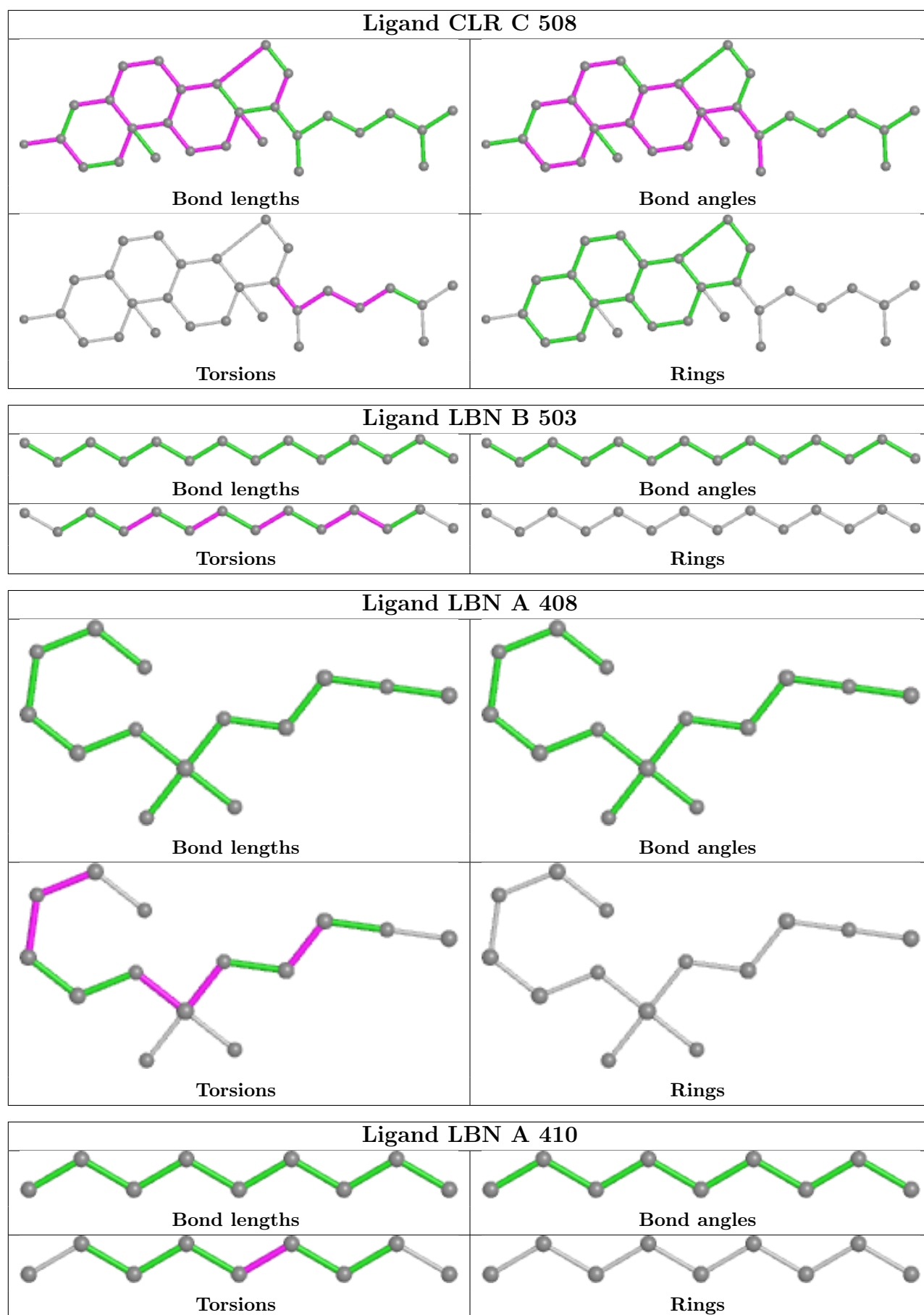


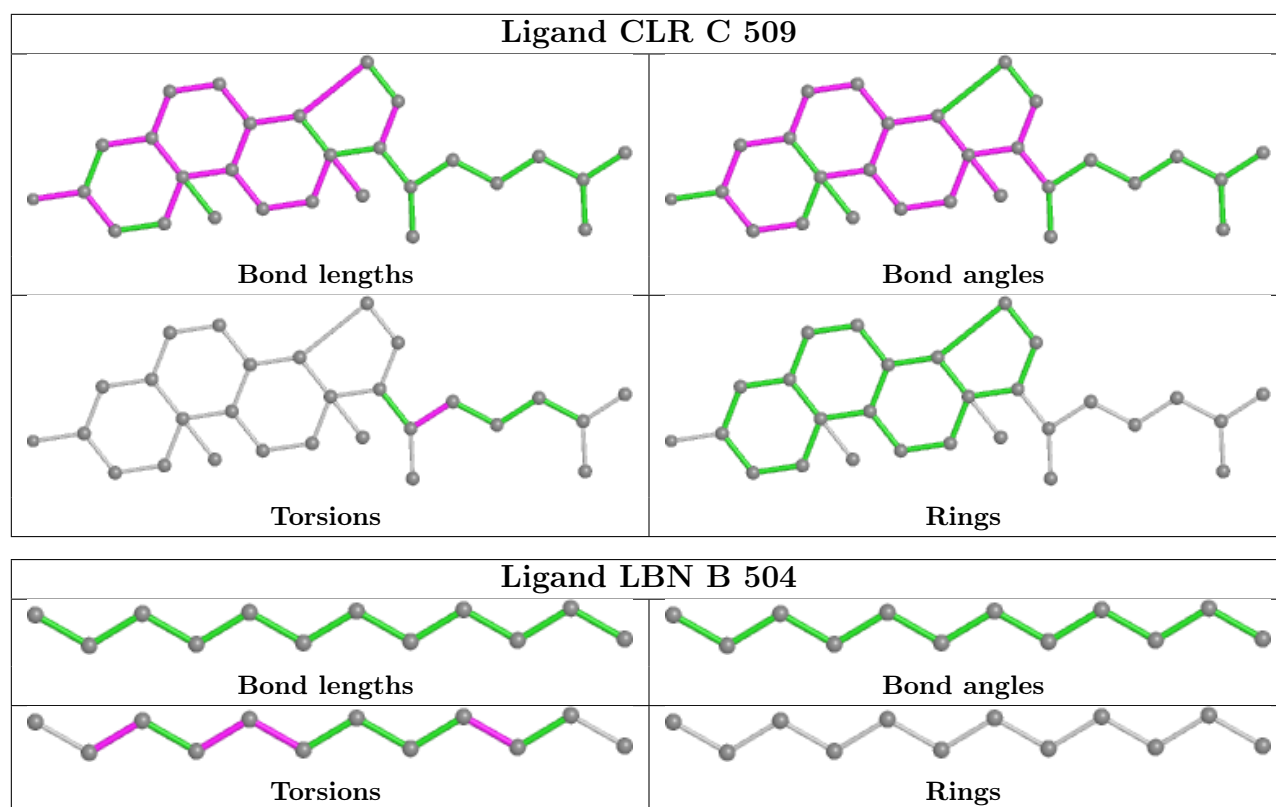












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

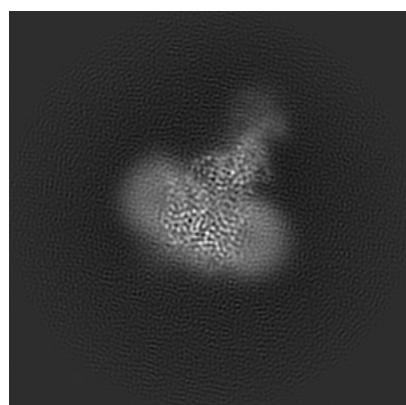
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25750. These allow visual inspection of the internal detail of the map and identification of artifacts.

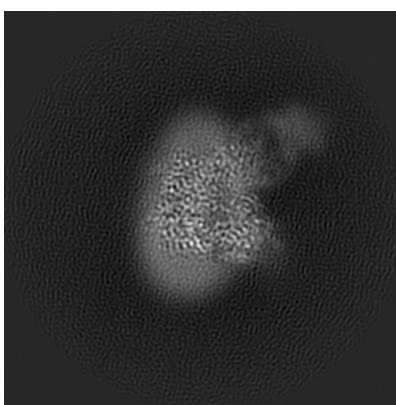
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

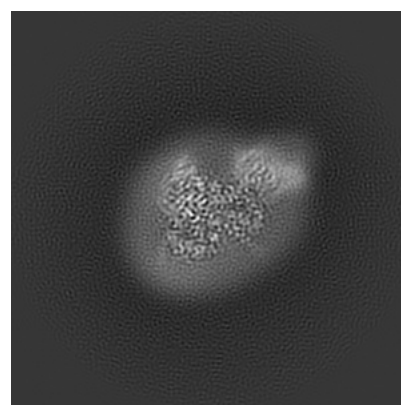
6.1.1 Primary map



X



Y

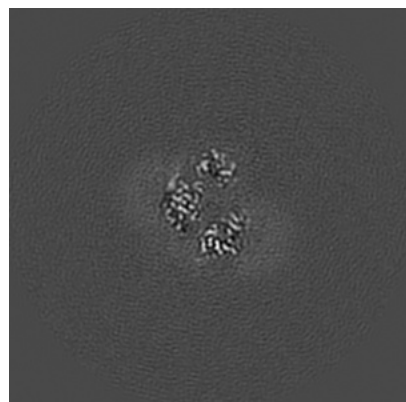


Z

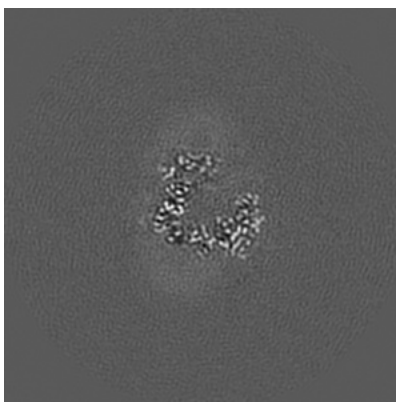
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

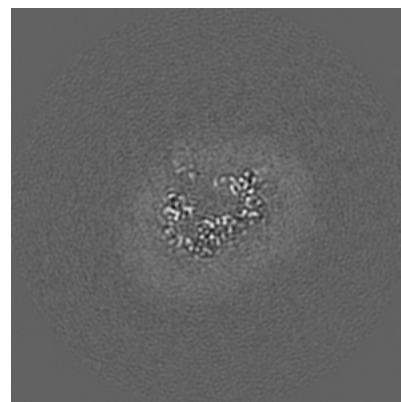
6.2.1 Primary map



X Index: 130



Y Index: 130

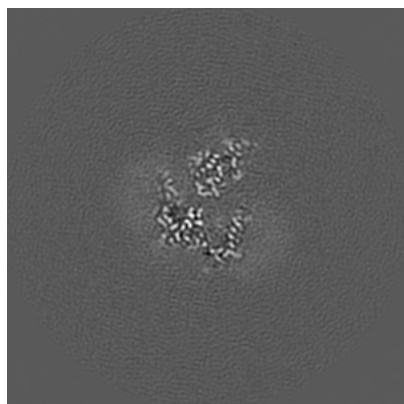


Z Index: 130

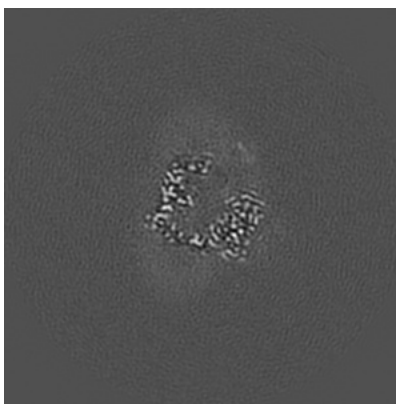
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

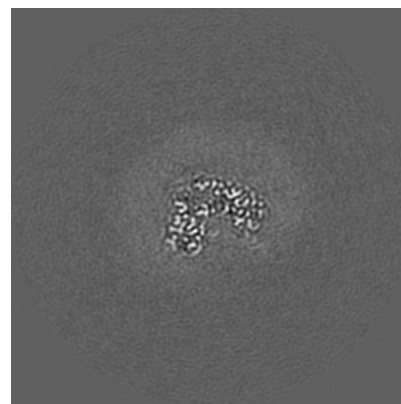
6.3.1 Primary map



X Index: 121



Y Index: 135



Z Index: 112

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

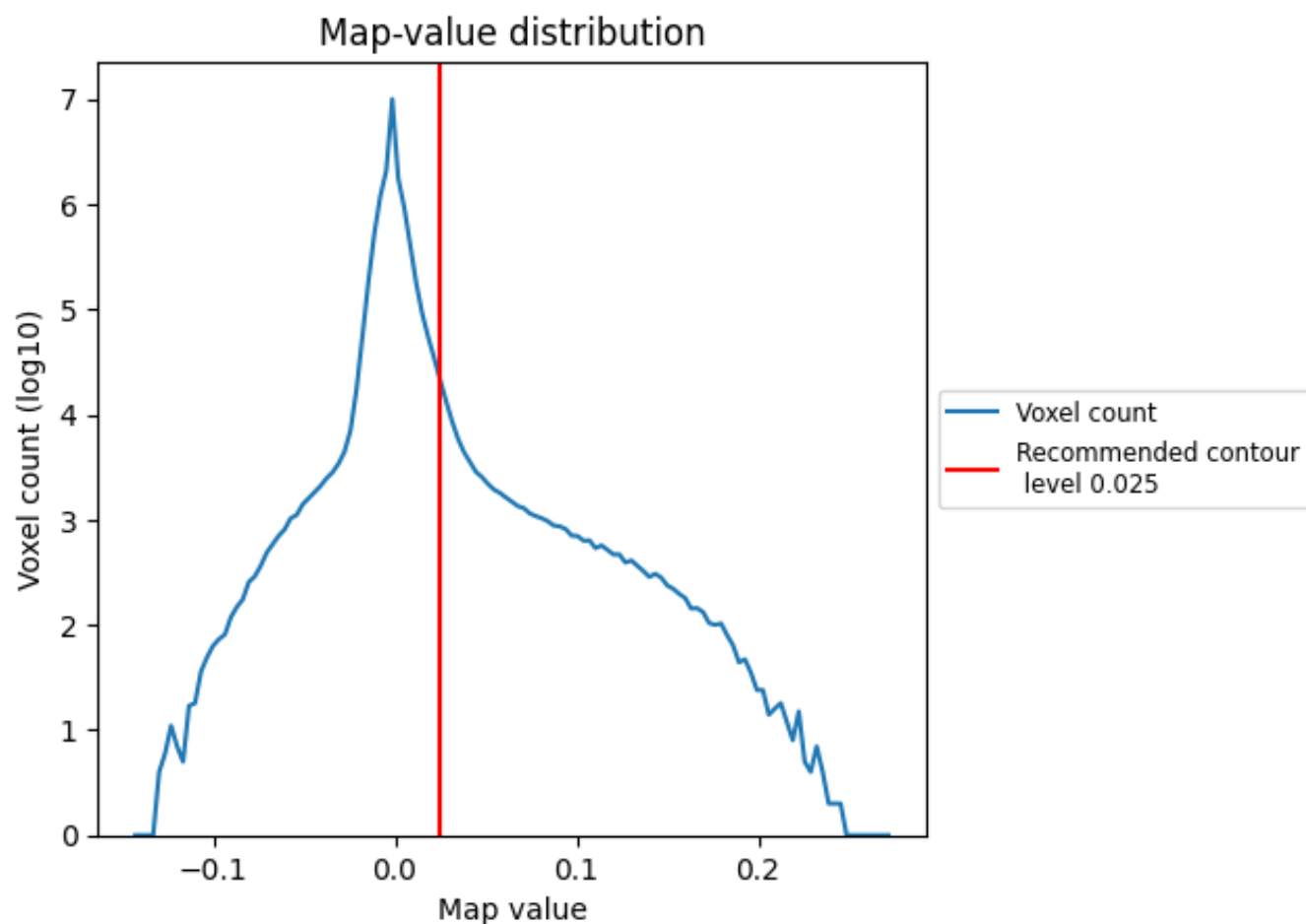
6.5 Mask visualisation

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

7 Map analysis [i](#)

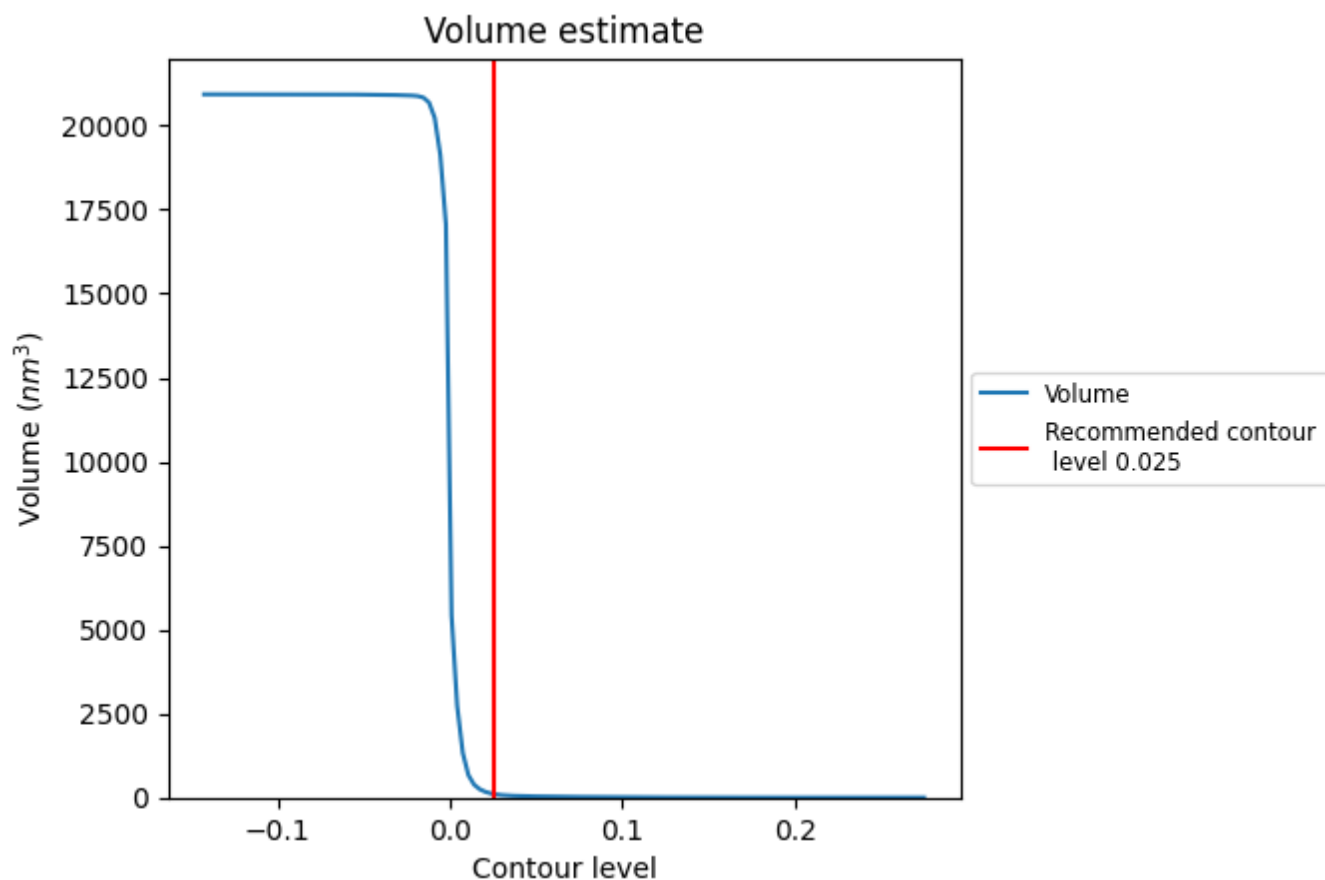
This section contains the results of statistical analysis of the map.

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.

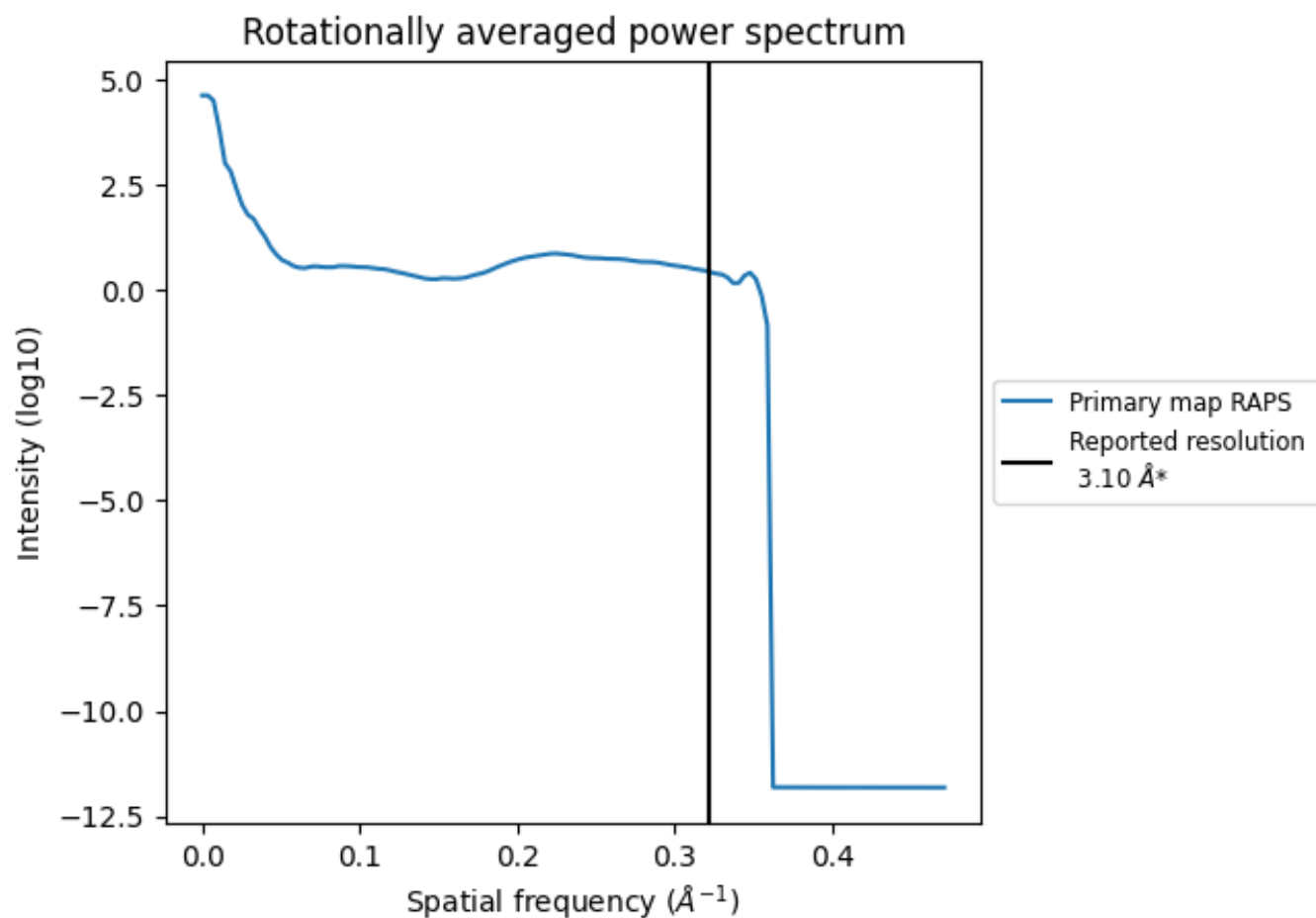
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 109 nm³; this corresponds to an approximate mass of 98 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 0.323 Å⁻¹

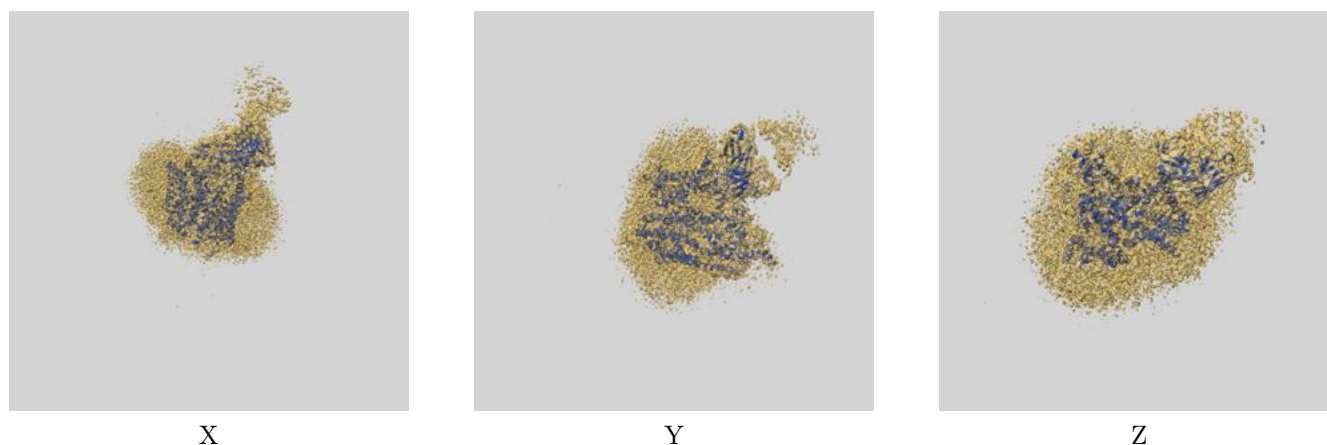
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

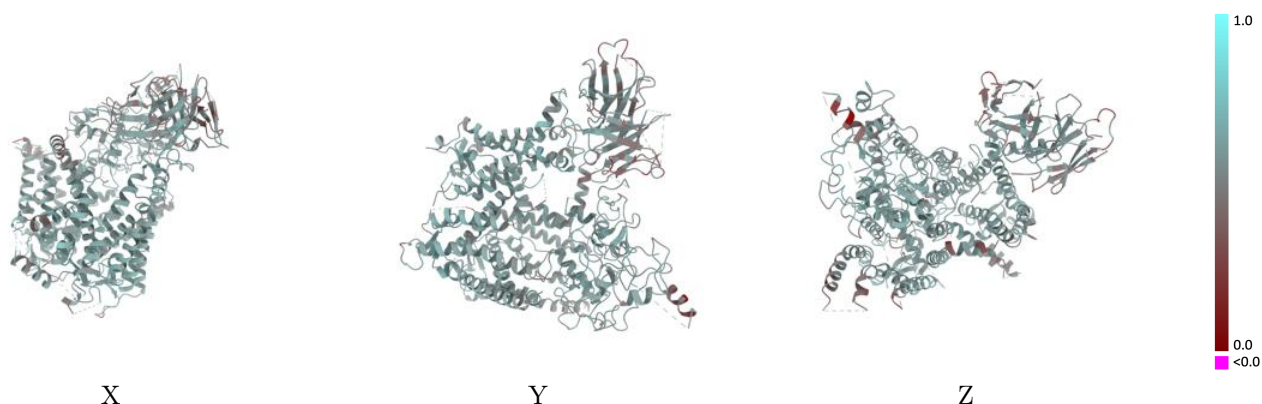
This section contains information regarding the fit between EMDB map EMD-25750 and PDB model 7T92. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

9.1 Map-model overlay [i](#)



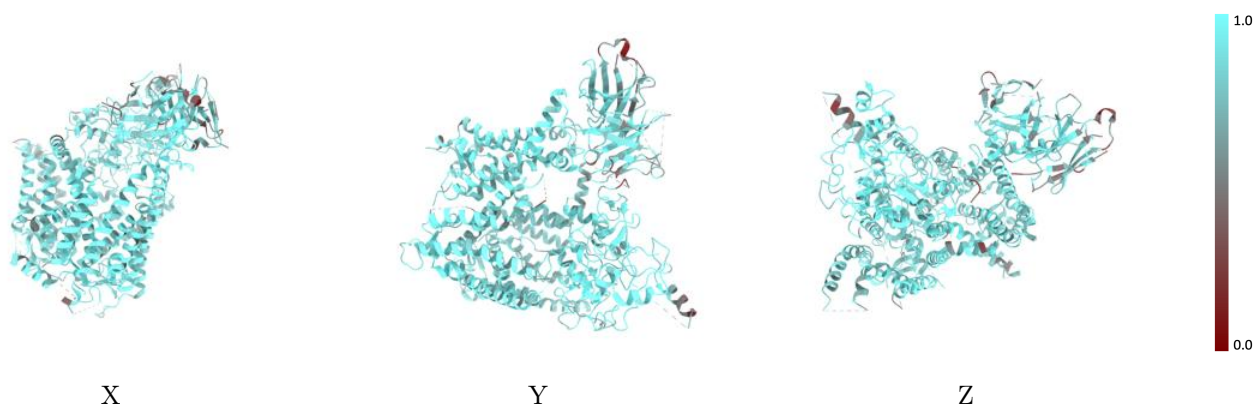
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



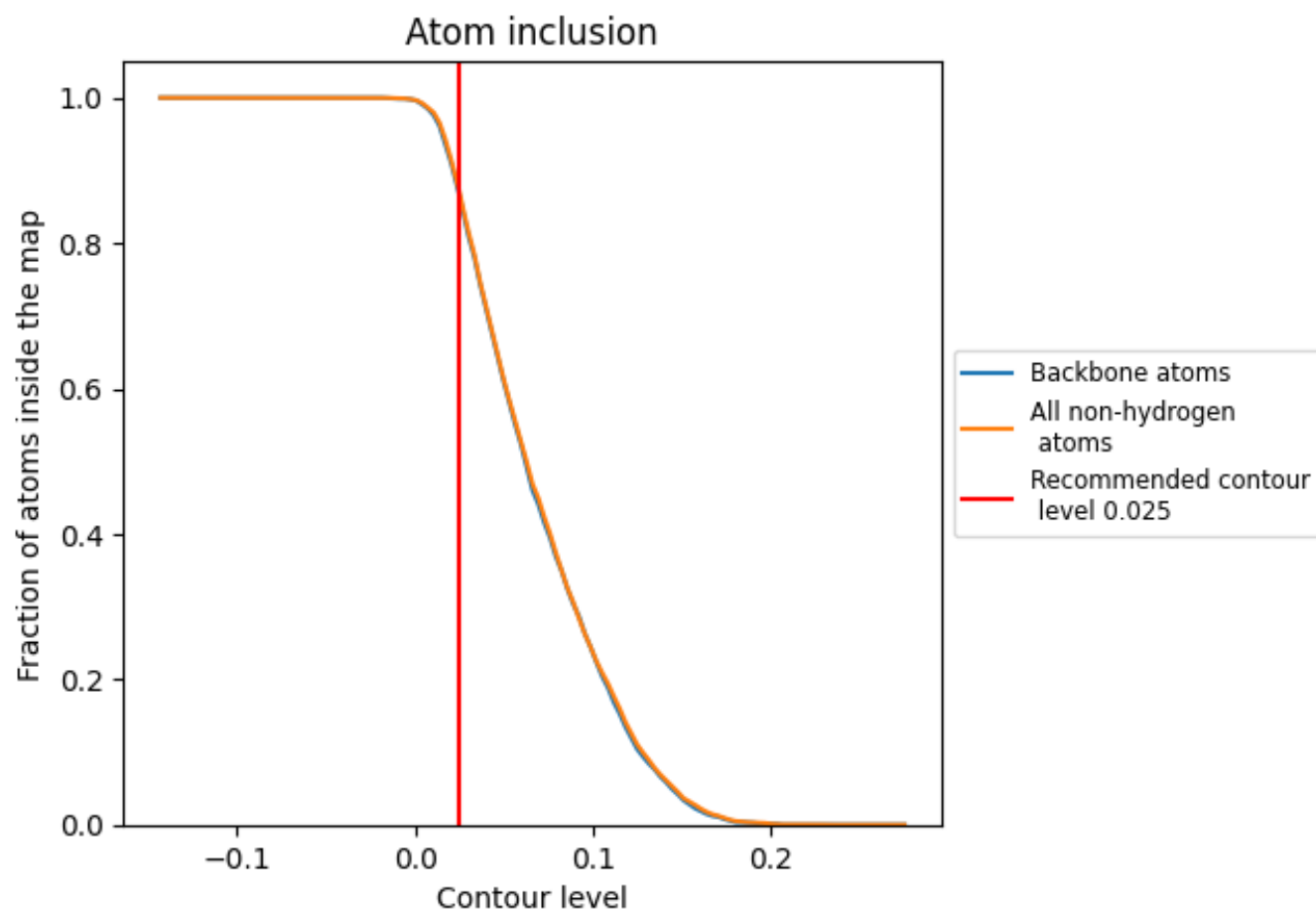
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.025).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 87% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8704	<div></div> 0.5580
A	<div></div> 0.8898	<div></div> 0.5690
B	<div></div> 0.9016	<div></div> 0.5660
C	<div></div> 0.9036	<div></div> 0.5690
H	<div></div> 0.7942	<div></div> 0.5010
L	<div></div> 0.7331	<div></div> 0.4990

