



Full wwPDB EM Validation Report ⓘ

Dec 8, 2025 – 08:11 PM JST

PDB ID : 9L0O / pdb_00009l0o
EMDB ID : EMD-62720
Title : Cryo-EM structure of human lipid phosphate phosphatase 1 complexed with LPA
Authors : Yang, M.; Qian, H.W.
Deposited on : 2024-12-12
Resolution : 2.83 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.dev129
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.47

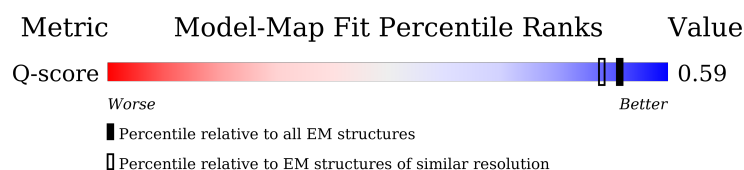
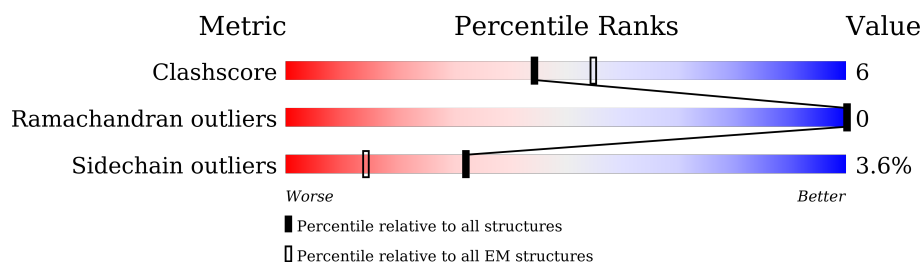
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.83 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	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	11847 (2.33 - 3.33)

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	284	 74% 14% • 11%
1	B	284	 75% 13% • 11%
1	C	284	 74% 13% • 11%
1	D	284	 73% 14% • 11%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8752 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 Phospholipid phosphatase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	252	Total 2003	C 1312	N 329	O 352	S 10	0	0
1	A	252	Total 2003	C 1312	N 329	O 352	S 10	0	0
1	B	252	Total 2003	C 1312	N 329	O 352	S 10	0	0
1	D	252	Total 2003	C 1312	N 329	O 352	S 10	0	0

There are 4 discrepancies between the modelled and reference sequences:

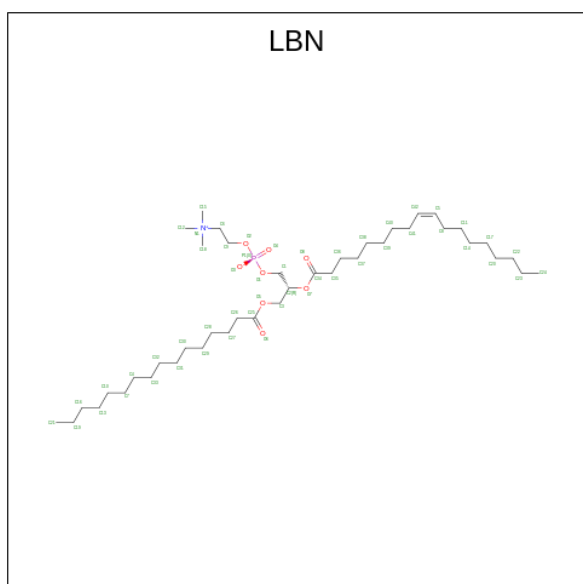
Chain	Residue	Modelled	Actual	Comment	Reference
C	171	ALA	HIS	engineered mutation	UNP O14494
A	171	ALA	HIS	engineered mutation	UNP O14494
B	171	ALA	HIS	engineered mutation	UNP O14494
D	171	ALA	HIS	engineered mutation	UNP O14494

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



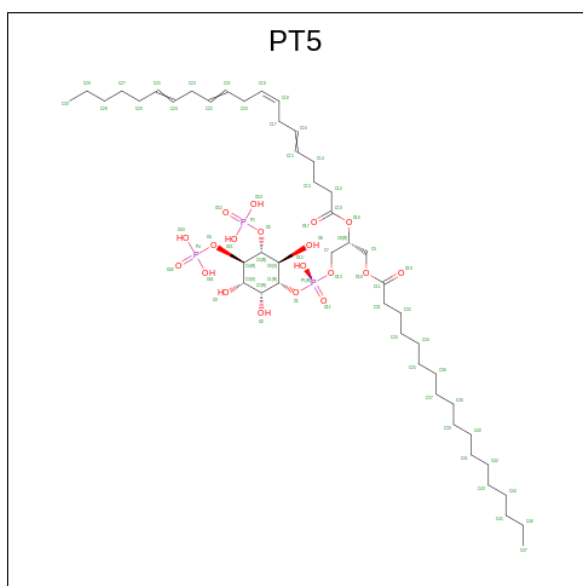
Mol	Chain	Residues	Atoms				AltConf
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	B	1	Total	C	N	O	0
			14	8	1	5	
2	D	1	Total	C	N	O	0
			14	8	1	5	

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



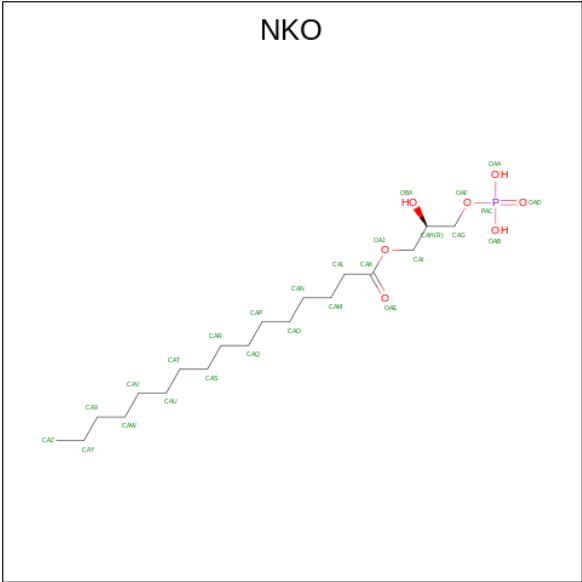
Mol	Chain	Residues	Atoms				AltConf
3	C	1	Total	C	O	P	0
			45	36	8	1	
3	A	1	Total	C	O	P	0
			45	36	8	1	
3	B	1	Total	C	O	P	0
			45	36	8	1	
3	D	1	Total	C	O	P	0
			45	36	8	1	

- Molecule 4 is [(2R)-1-octadecanoyloxy-3-[oxidanyl-[(1R,2R,3S,4R,5R,6S)-2,3,6-tris(oxidanyl)-4,5-diphosphonoxy-cyclohexyl]oxy-phosphoryl]oxy-propan-2-yl] (8Z)-icosa-5,8,11,14-tetraenoate (CCD ID: PT5) (formula: C₄₇H₈₅O₁₉P₃) (labeled as "Ligand of Interest" by depositor).



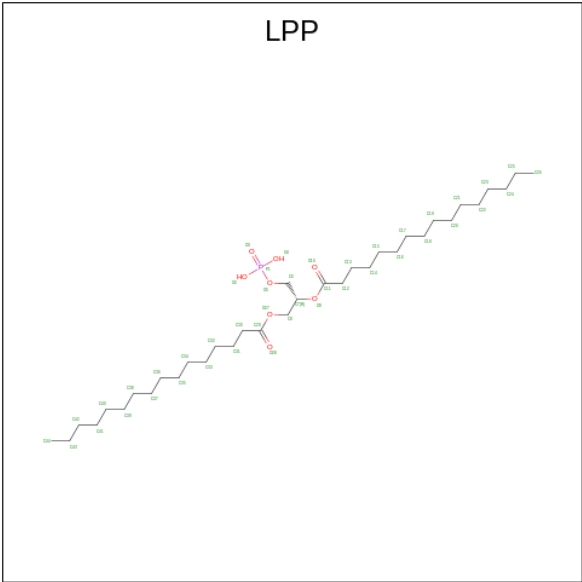
Mol	Chain	Residues	Atoms				AltConf
4	C	1	Total	C	O	P	0
			62	40	19	3	
4	A	1	Total	C	O	P	0
			62	40	19	3	
4	B	1	Total	C	O	P	0
			62	40	19	3	
4	D	1	Total	C	O	P	0
			62	40	19	3	

- Molecule 5 is (2R)-2-hydroxy-3-(phosphonoxy)propyl hexadecanoate (CCD ID: NKO) (formula: C₁₉H₃₉O₇P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
5	C	1	Total	C	O	P	0
			17	9	7	1	
5	A	1	Total	C	O	P	0
			17	9	7	1	
5	B	1	Total	C	O	P	0
			17	9	7	1	
5	D	1	Total	C	O	P	0
			17	9	7	1	

- Molecule 6 is 2-(HEXADECANOYLOXY)-1-[(PHOSPHONOXY)METHYL]ETHYL HEXADECANOATE (CCD ID: LPP) (formula: C₃₅H₆₉O₈P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
6	C	1	Total 44	C 35	O 8	P 1	0
6	A	1	Total 44	C 35	O 8	P 1	0
6	A	1	Total 44	C 35	O 8	P 1	0
6	D	1	Total 44	C 35	O 8	P 1	0

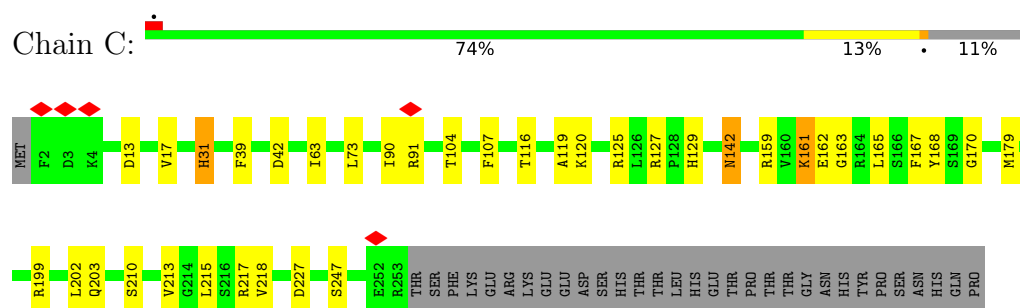
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		AltConf
7	C	3	Total 3	O 3	0
7	A	3	Total 3	O 3	0
7	B	3	Total 3	O 3	0
7	D	3	Total 3	O 3	0

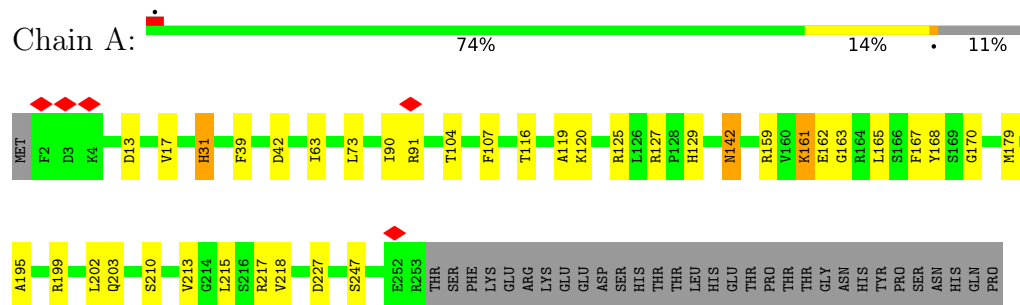
3 Residue-property plots [i](#)

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.

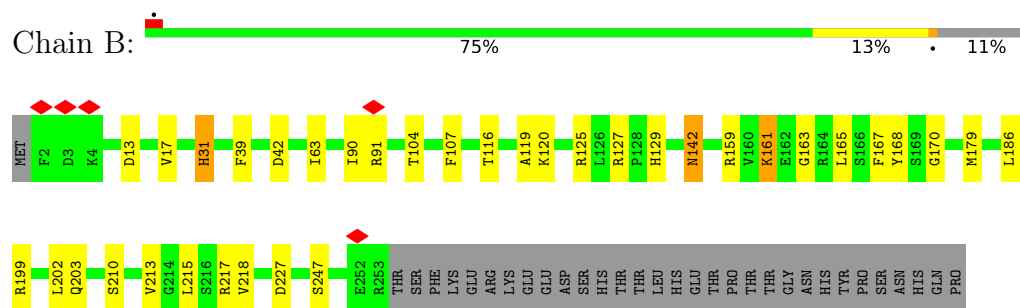
• Molecule 1: Phospholipid phosphatase 1



• Molecule 1: Phospholipid phosphatase 1

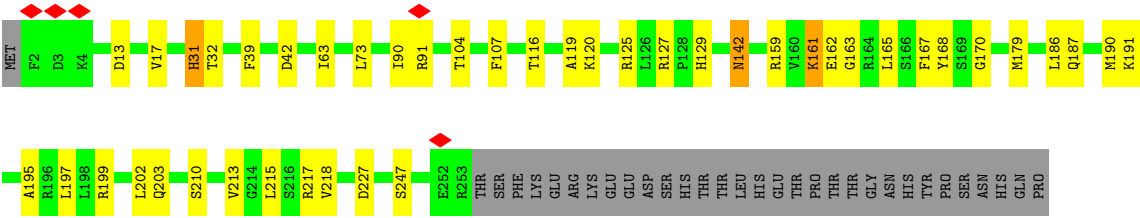


• Molecule 1: Phospholipid phosphatase 1



• Molecule 1: Phospholipid phosphatase 1





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	177681	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.708	Depositor
Minimum map value	-1.079	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.057	Depositor
Recommended contour level	0.246	Depositor
Map size (Å)	209.92, 209.92, 209.92	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.82, 0.82, 0.82	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: NKO, NAG, LPP, PT5, LBN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.27	0/2054	0.38	0/2789
1	B	0.27	0/2054	0.38	0/2789
1	C	0.27	0/2054	0.38	0/2789
1	D	0.27	0/2054	0.38	0/2789
All	All	0.27	0/8216	0.38	0/11156

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	2003	0	2015	27	0
1	B	2003	0	2015	26	0
1	C	2003	0	2015	26	0
1	D	2003	0	2015	29	0
2	A	14	0	13	1	0
2	B	14	0	13	1	0
2	C	14	0	13	1	0
2	D	14	0	13	1	0
3	A	45	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	45	0	0	0	0
3	C	45	0	0	0	0
3	D	45	0	0	0	0
4	A	62	0	65	2	0
4	B	62	0	65	2	0
4	C	62	0	65	2	0
4	D	62	0	65	2	0
5	A	17	0	14	0	0
5	B	17	0	14	0	0
5	C	17	0	14	0	0
5	D	17	0	14	0	0
6	A	88	0	134	4	0
6	C	44	0	67	2	0
6	D	44	0	67	2	0
7	A	3	0	0	0	0
7	B	3	0	0	0	0
7	C	3	0	0	0	0
7	D	3	0	0	0	0
All	All	8752	0	8696	108	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (108) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:HIS:CD2	1:A:161:LYS:HD3	2.23	0.74
1:B:31:HIS:CD2	1:B:161:LYS:HD3	2.23	0.74
1:D:31:HIS:CD2	1:D:161:LYS:HD3	2.23	0.73
1:C:31:HIS:CD2	1:C:161:LYS:HD3	2.23	0.72
1:C:142:ASN:HD21	2:C:301:NAG:H62	1.57	0.69
1:A:142:ASN:HD21	2:A:303:NAG:H62	1.57	0.69
1:D:142:ASN:HD21	2:D:302:NAG:H62	1.57	0.68
1:B:142:ASN:HD21	2:B:301:NAG:H62	1.57	0.67
1:D:125:ARG:NH1	1:D:227:ASP:OD1	2.35	0.60
1:C:116:THR:HG22	1:C:120:LYS:HD2	1.84	0.60
1:B:125:ARG:NH1	1:B:227:ASP:OD1	2.35	0.60
1:A:125:ARG:NH1	1:A:227:ASP:OD1	2.35	0.59
1:D:116:THR:HG22	1:D:120:LYS:HD2	1.84	0.59
1:B:187:GLN:HA	1:B:199:ARG:HD2	1.84	0.59
1:A:187:GLN:HA	1:A:199:ARG:HD2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:THR:HG22	1:A:120:LYS:HD2	1.84	0.59
1:C:125:ARG:NH1	1:C:227:ASP:OD1	2.35	0.59
1:B:116:THR:HG22	1:B:120:LYS:HD2	1.84	0.58
6:A:301:LPP:H411	6:A:301:LPP:H261	1.85	0.58
1:D:187:GLN:HA	1:D:199:ARG:HD2	1.84	0.58
6:D:301:LPP:H411	6:D:301:LPP:H261	1.85	0.58
1:C:187:GLN:HA	1:C:199:ARG:HD2	1.84	0.57
6:A:302:LPP:H411	6:A:302:LPP:H261	1.85	0.57
6:C:305:LPP:H411	6:C:305:LPP:H261	1.85	0.57
1:A:104:THR:HG21	1:A:247:SER:HB3	1.88	0.56
1:D:104:THR:HG21	1:D:247:SER:HB3	1.88	0.56
1:C:179:MET:HG3	1:C:210:SER:HB3	1.88	0.55
1:A:179:MET:HG3	1:A:210:SER:HB3	1.88	0.55
1:C:104:THR:HG21	1:C:247:SER:HB3	1.88	0.55
1:B:104:THR:HG21	1:B:247:SER:HB3	1.88	0.55
1:B:179:MET:HG3	1:B:210:SER:HB3	1.88	0.54
1:D:179:MET:HG3	1:D:210:SER:HB3	1.88	0.54
1:A:116:THR:HG21	1:A:170:GLY:HA2	1.91	0.53
1:D:116:THR:HG21	1:D:170:GLY:HA2	1.91	0.53
1:B:116:THR:HG21	1:B:170:GLY:HA2	1.91	0.52
1:B:120:LYS:NZ	1:B:168:TYR:O	2.38	0.52
1:C:116:THR:HG21	1:C:170:GLY:HA2	1.91	0.52
1:B:127:ARG:HD3	1:B:129:HIS:CE1	2.46	0.51
1:A:127:ARG:HD3	1:A:129:HIS:CE1	2.46	0.51
1:D:127:ARG:HD3	1:D:129:HIS:CE1	2.46	0.50
1:A:120:LYS:NZ	1:A:168:TYR:O	2.38	0.50
1:C:127:ARG:HD3	1:C:129:HIS:CE1	2.46	0.49
1:A:39:PHE:HB2	1:A:42:ASP:HB2	1.94	0.49
1:C:120:LYS:NZ	1:C:168:TYR:O	2.38	0.49
1:C:39:PHE:HB2	1:C:42:ASP:HB2	1.94	0.49
1:B:39:PHE:HB2	1:B:42:ASP:HB2	1.94	0.49
1:C:119:ALA:HA	1:A:215:LEU:HD13	1.95	0.48
1:C:167:PHE:HA	1:C:168:TYR:HA	1.53	0.48
1:D:39:PHE:HB2	1:D:42:ASP:HB2	1.94	0.48
1:C:215:LEU:HD13	1:D:119:ALA:HA	1.95	0.48
1:B:119:ALA:HA	1:D:215:LEU:HD13	1.95	0.48
1:B:167:PHE:HA	1:B:168:TYR:HA	1.53	0.48
1:A:119:ALA:HA	1:B:215:LEU:HD13	1.96	0.47
1:B:190:MET:HE1	1:B:202:LEU:HD12	1.97	0.46
1:C:190:MET:HE1	1:C:202:LEU:HD12	1.97	0.46
1:D:190:MET:HE1	1:D:202:LEU:HD12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:MET:HE1	1:A:202:LEU:HD12	1.97	0.46
1:B:120:LYS:HB3	1:B:165:LEU:HD22	1.98	0.46
1:D:120:LYS:HB3	1:D:165:LEU:HD22	1.99	0.45
1:C:187:GLN:HB2	1:C:203:GLN:HE22	1.81	0.45
1:A:187:GLN:HB2	1:A:203:GLN:HE22	1.81	0.45
1:D:120:LYS:NZ	1:D:168:TYR:O	2.38	0.45
1:C:90:ILE:HD13	4:C:303:PT5:H24	1.99	0.45
1:A:167:PHE:HA	1:A:168:TYR:HA	1.53	0.45
1:D:187:GLN:HB2	1:D:203:GLN:HE22	1.81	0.45
1:C:127:ARG:NH1	1:C:162:GLU:O	2.44	0.45
1:C:120:LYS:HB3	1:C:165:LEU:HD22	1.99	0.44
1:B:90:ILE:HD13	4:B:303:PT5:H24	1.99	0.44
1:B:187:GLN:HB2	1:B:203:GLN:HE22	1.81	0.44
1:A:90:ILE:HD13	4:A:305:PT5:H24	1.99	0.44
1:C:218:VAL:HG11	6:C:305:LPP:H302	2.00	0.44
1:A:120:LYS:HB3	1:A:165:LEU:HD22	1.99	0.44
1:B:213:VAL:O	1:B:217:ARG:HG2	2.18	0.44
1:C:213:VAL:O	1:C:217:ARG:HG2	2.18	0.44
1:D:90:ILE:HD13	4:D:304:PT5:H24	1.99	0.44
1:D:218:VAL:HG11	6:D:301:LPP:H302	1.99	0.44
1:A:213:VAL:O	1:A:217:ARG:HG2	2.18	0.43
1:A:218:VAL:HG11	6:A:301:LPP:H302	2.00	0.43
1:D:127:ARG:NH1	1:D:162:GLU:O	2.44	0.43
1:D:213:VAL:O	1:D:217:ARG:HG2	2.18	0.43
1:A:13:ASP:HB3	4:A:305:PT5:H62	2.01	0.43
1:A:127:ARG:NH1	1:A:162:GLU:O	2.44	0.42
1:D:13:ASP:HB3	4:D:304:PT5:H62	2.01	0.42
1:D:187:GLN:HB2	1:D:203:GLN:NE2	2.34	0.42
1:C:187:GLN:HB2	1:C:203:GLN:NE2	2.34	0.42
1:B:13:ASP:HB3	4:B:303:PT5:H62	2.01	0.42
1:B:195:ALA:HB1	1:B:199:ARG:HB2	2.01	0.42
1:D:195:ALA:HB1	1:D:199:ARG:HB2	2.01	0.42
1:C:195:ALA:HB1	1:C:199:ARG:HB2	2.01	0.41
1:B:187:GLN:HB2	1:B:203:GLN:NE2	2.34	0.41
1:A:187:GLN:HB2	1:A:203:GLN:NE2	2.34	0.41
1:D:197:LEU:HD23	1:D:197:LEU:HA	1.87	0.41
1:C:13:ASP:HB3	4:C:303:PT5:H62	2.01	0.41
1:D:167:PHE:HA	1:D:168:TYR:HA	1.53	0.41
6:A:302:LPP:H302	1:B:218:VAL:HG11	2.01	0.41
1:A:195:ALA:HB1	1:A:199:ARG:HB2	2.01	0.41
1:A:127:ARG:HD2	1:A:163:GLY:HA2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:ARG:HD2	1:B:163:GLY:HA2	2.03	0.41
1:B:186:LEU:HD22	1:B:190:MET:HE2	2.03	0.41
1:C:17:VAL:HG22	1:C:107:PHE:HB2	2.03	0.41
1:D:31:HIS:HB3	1:D:32:THR:H	1.65	0.41
1:A:17:VAL:HG22	1:A:107:PHE:HB2	2.03	0.41
1:B:17:VAL:HG22	1:B:107:PHE:HB2	2.03	0.40
1:D:17:VAL:HG22	1:D:107:PHE:HB2	2.03	0.40
1:D:127:ARG:HD2	1:D:163:GLY:HA2	2.03	0.40
1:C:127:ARG:HD2	1:C:163:GLY:HA2	2.03	0.40
1:D:186:LEU:HD22	1:D:190:MET:HE2	2.03	0.40
1:A:186:LEU:HD22	1:A:190:MET:HE2	2.03	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	A	250/284 (88%)	248 (99%)	2 (1%)	0	100	100
1	B	250/284 (88%)	248 (99%)	2 (1%)	0	100	100
1	C	250/284 (88%)	248 (99%)	2 (1%)	0	100	100
1	D	250/284 (88%)	248 (99%)	2 (1%)	0	100	100
All	All	1000/1136 (88%)	992 (99%)	8 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	216/247 (87%)	208 (96%)	8 (4%)	29	54
1	B	216/247 (87%)	209 (97%)	7 (3%)	34	59
1	C	216/247 (87%)	208 (96%)	8 (4%)	29	54
1	D	216/247 (87%)	208 (96%)	8 (4%)	29	54
All	All	864/988 (87%)	833 (96%)	31 (4%)	32	55

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	31	HIS
1	C	63	ILE
1	C	73	LEU
1	C	91	ARG
1	C	142	ASN
1	C	159	ARG
1	C	161	LYS
1	C	191	LYS
1	A	31	HIS
1	A	63	ILE
1	A	73	LEU
1	A	91	ARG
1	A	142	ASN
1	A	159	ARG
1	A	161	LYS
1	A	191	LYS
1	B	31	HIS
1	B	63	ILE
1	B	91	ARG
1	B	142	ASN
1	B	159	ARG
1	B	161	LYS
1	B	191	LYS
1	D	31	HIS
1	D	63	ILE
1	D	73	LEU
1	D	91	ARG
1	D	142	ASN
1	D	159	ARG
1	D	161	LYS

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Mol	Chain	Res	Type
1	D	191	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	31	HIS
1	C	92	ASN
1	C	156	ASN
1	C	234	GLN
1	A	31	HIS
1	A	92	ASN
1	A	156	ASN
1	A	234	GLN
1	B	31	HIS
1	B	92	ASN
1	B	156	ASN
1	B	234	GLN
1	D	31	HIS
1	D	92	ASN
1	D	156	ASN
1	D	234	GLN

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](#)

20 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	$\# Z > 2$
4	PT5	B	303	-	62,62,69	0.88	2 (3%)	76,80,87	0.94	2 (2%)
4	PT5	D	304	-	62,62,69	0.88	2 (3%)	76,80,87	0.94	2 (2%)
6	LPP	C	305	-	43,43,43	0.91	4 (9%)	47,48,48	1.08	2 (4%)
3	LBN	B	302	-	44,44,51	1.26	7 (15%)	48,49,59	1.15	3 (6%)
2	NAG	B	301	1	14,14,15	0.29	0	17,19,21	0.92	2 (11%)
5	NKO	B	304	-	16,16,26	1.21	1 (6%)	19,20,30	1.08	2 (10%)
6	LPP	A	301	-	43,43,43	0.91	4 (9%)	47,48,48	1.08	2 (4%)
5	NKO	A	306	-	16,16,26	1.21	1 (6%)	19,20,30	1.08	2 (10%)
3	LBN	A	304	-	44,44,51	1.27	7 (15%)	48,49,59	1.15	3 (6%)
2	NAG	A	303	1	14,14,15	0.30	0	17,19,21	0.92	2 (11%)
6	LPP	A	302	-	43,43,43	0.91	4 (9%)	47,48,48	1.08	2 (4%)
2	NAG	C	301	1	14,14,15	0.29	0	17,19,21	0.92	2 (11%)
5	NKO	D	305	-	16,16,26	1.21	1 (6%)	19,20,30	1.08	2 (10%)
2	NAG	D	302	1	14,14,15	0.29	0	17,19,21	0.92	2 (11%)
4	PT5	C	303	-	62,62,69	0.88	2 (3%)	76,80,87	0.94	2 (2%)
3	LBN	D	303	-	44,44,51	1.26	7 (15%)	48,49,59	1.15	3 (6%)
6	LPP	D	301	-	43,43,43	0.90	4 (9%)	47,48,48	1.09	2 (4%)
5	NKO	C	304	-	16,16,26	1.21	1 (6%)	19,20,30	1.08	2 (10%)
4	PT5	A	305	-	62,62,69	0.88	2 (3%)	76,80,87	0.94	2 (2%)
3	LBN	C	302	-	44,44,51	1.27	7 (15%)	48,49,59	1.15	3 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PT5	B	303	-	-	17/59/83/90	0/1/1/1
4	PT5	D	304	-	-	17/59/83/90	0/1/1/1
6	LPP	C	305	-	-	16/45/45/45	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LBN	B	302	-	-	20/46/46/55	-
2	NAG	B	301	1	-	5/6/23/26	0/1/1/1
5	NKO	B	304	-	-	8/16/16/26	-
6	LPP	A	301	-	-	16/45/45/45	-
5	NKO	A	306	-	-	8/16/16/26	-
3	LBN	A	304	-	-	20/46/46/55	-
2	NAG	A	303	1	-	5/6/23/26	0/1/1/1
6	LPP	A	302	-	-	16/45/45/45	-
2	NAG	C	301	1	-	5/6/23/26	0/1/1/1
5	NKO	D	305	-	-	8/16/16/26	-
2	NAG	D	302	1	-	5/6/23/26	0/1/1/1
4	PT5	C	303	-	-	17/59/83/90	0/1/1/1
3	LBN	D	303	-	-	20/46/46/55	-
6	LPP	D	301	-	-	16/45/45/45	-
5	NKO	C	304	-	-	8/16/16/26	-
4	PT5	A	305	-	-	17/59/83/90	0/1/1/1
3	LBN	C	302	-	-	20/46/46/55	-

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	303	PT5	O18-C11	4.22	1.45	1.33
4	C	303	PT5	O18-C11	4.22	1.45	1.33
4	A	305	PT5	O18-C11	4.22	1.45	1.33
4	D	304	PT5	O18-C11	4.22	1.45	1.33
4	C	303	PT5	O16-C10	4.18	1.46	1.34
4	D	304	PT5	O16-C10	4.18	1.46	1.34
4	A	305	PT5	O16-C10	4.18	1.46	1.34
4	B	303	PT5	O16-C10	4.15	1.46	1.34
3	C	302	LBN	C42-C5	3.69	1.53	1.31
3	B	302	LBN	C42-C5	3.69	1.53	1.31
3	D	303	LBN	C42-C5	3.69	1.53	1.31
3	A	304	LBN	C42-C5	3.67	1.53	1.31
3	C	302	LBN	C33-C4	-3.47	1.32	1.51
3	A	304	LBN	C33-C4	-3.47	1.32	1.51
3	D	303	LBN	C33-C4	-3.47	1.32	1.51
3	B	302	LBN	C33-C4	-3.46	1.32	1.51
3	B	302	LBN	C41-C42	-3.21	1.32	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	302	LBN	C41-C42	-3.20	1.32	1.50
3	A	304	LBN	C41-C42	-3.20	1.32	1.50
3	D	303	LBN	C41-C42	-3.20	1.32	1.50
5	A	306	NKO	OAJ-CAK	2.83	1.41	1.33
5	B	304	NKO	OAJ-CAK	2.82	1.41	1.33
5	C	304	NKO	OAJ-CAK	2.82	1.41	1.33
5	D	305	NKO	OAJ-CAK	2.82	1.41	1.33
6	C	305	LPP	O9-C7	-2.66	1.39	1.46
6	A	301	LPP	O9-C7	-2.66	1.39	1.46
6	A	302	LPP	O9-C7	-2.66	1.39	1.46
6	D	301	LPP	O9-C7	-2.64	1.40	1.46
3	C	302	LBN	O7-C2	-2.60	1.40	1.46
3	A	304	LBN	O7-C2	-2.60	1.40	1.46
3	D	303	LBN	O7-C2	-2.60	1.40	1.46
3	B	302	LBN	O7-C2	-2.60	1.40	1.46
6	C	305	LPP	O27-C29	2.46	1.40	1.33
6	A	301	LPP	O27-C29	2.46	1.40	1.33
6	A	302	LPP	O27-C29	2.46	1.40	1.33
6	D	301	LPP	O27-C29	2.45	1.40	1.33
3	C	302	LBN	O5-C25	2.38	1.40	1.33
3	D	303	LBN	O5-C25	2.38	1.40	1.33
3	A	304	LBN	O5-C25	2.37	1.40	1.33
3	B	302	LBN	O5-C25	2.37	1.40	1.33
3	C	302	LBN	O5-C3	-2.16	1.40	1.45
3	A	304	LBN	O5-C3	-2.16	1.40	1.45
3	B	302	LBN	O5-C3	-2.16	1.40	1.45
3	D	303	LBN	O5-C3	-2.16	1.40	1.45
6	C	305	LPP	O9-C11	2.15	1.40	1.34
6	A	301	LPP	O9-C11	2.15	1.40	1.34
6	A	302	LPP	O9-C11	2.15	1.40	1.34
6	D	301	LPP	O9-C11	2.13	1.40	1.34
3	A	304	LBN	O7-C34	2.09	1.40	1.34
6	C	305	LPP	O27-C8	-2.08	1.40	1.45
6	A	301	LPP	O27-C8	-2.08	1.40	1.45
3	C	302	LBN	O7-C34	2.08	1.40	1.34
3	B	302	LBN	O7-C34	2.08	1.40	1.34
3	D	303	LBN	O7-C34	2.08	1.40	1.34
6	A	302	LPP	O27-C8	-2.08	1.40	1.45
6	D	301	LPP	O27-C8	-2.05	1.40	1.45

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	305	PT5	O16-C10-C12	3.83	119.75	111.50
4	B	303	PT5	O16-C10-C12	3.82	119.73	111.50
4	C	303	PT5	O16-C10-C12	3.81	119.71	111.50
3	C	302	LBN	O7-C34-C35	3.80	119.70	111.50
3	B	302	LBN	O7-C34-C35	3.80	119.70	111.50
3	D	303	LBN	O7-C34-C35	3.80	119.70	111.50
4	D	304	PT5	O16-C10-C12	3.80	119.69	111.50
3	A	304	LBN	O7-C34-C35	3.79	119.66	111.50
6	D	301	LPP	O9-C11-C12	3.73	119.53	111.50
6	C	305	LPP	O9-C11-C12	3.71	119.50	111.50
6	A	301	LPP	O9-C11-C12	3.71	119.50	111.50
6	A	302	LPP	O9-C11-C12	3.71	119.49	111.50
5	A	306	NKO	OAJ-CAK-CAL	2.65	120.24	111.91
5	B	304	NKO	OAJ-CAK-CAL	2.64	120.21	111.91
5	C	304	NKO	OAJ-CAK-CAL	2.64	120.20	111.91
5	D	305	NKO	OAJ-CAK-CAL	2.64	120.20	111.91
4	A	305	PT5	O18-C11-C31	2.56	119.96	111.91
4	C	303	PT5	O18-C11-C31	2.55	119.92	111.91
4	D	304	PT5	O18-C11-C31	2.55	119.92	111.91
4	B	303	PT5	O18-C11-C31	2.55	119.91	111.91
3	B	302	LBN	O5-C25-C26	2.50	119.74	111.91
3	A	304	LBN	O5-C25-C26	2.49	119.72	111.91
3	C	302	LBN	O5-C25-C26	2.48	119.68	111.91
3	D	303	LBN	O5-C25-C26	2.48	119.68	111.91
5	A	306	NKO	OAB-PAC-OAF	2.44	113.22	106.73
5	C	304	NKO	OAB-PAC-OAF	2.44	113.22	106.73
5	D	305	NKO	OAB-PAC-OAF	2.44	113.22	106.73
5	B	304	NKO	OAB-PAC-OAF	2.43	113.21	106.73
6	D	301	LPP	O27-C29-C30	2.32	119.19	111.91
6	C	305	LPP	O27-C29-C30	2.32	119.17	111.91
6	A	301	LPP	O27-C29-C30	2.32	119.17	111.91
6	A	302	LPP	O27-C29-C30	2.32	119.17	111.91
2	B	301	NAG	C1-O5-C5	2.23	115.22	112.19
2	C	301	NAG	C1-O5-C5	2.23	115.21	112.19
2	D	302	NAG	C1-O5-C5	2.23	115.21	112.19
2	A	303	NAG	C1-O5-C5	2.22	115.21	112.19
2	B	301	NAG	O5-C5-C6	2.18	110.62	107.20
2	C	301	NAG	O5-C5-C6	2.16	110.58	107.20
2	D	302	NAG	O5-C5-C6	2.16	110.58	107.20
2	A	303	NAG	O5-C5-C6	2.14	110.56	107.20
3	C	302	LBN	C8-C5-C42	-2.03	109.12	124.73
3	D	303	LBN	C8-C5-C42	-2.03	109.12	124.73
3	B	302	LBN	C8-C5-C42	-2.03	109.14	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	304	LBN	C8-C5-C42	-2.03	109.15	124.73

There are no chirality outliers.

All (264) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	301	NAG	C3-C2-N2-C7
2	C	301	NAG	C8-C7-N2-C2
2	C	301	NAG	O7-C7-N2-C2
2	A	303	NAG	C3-C2-N2-C7
2	A	303	NAG	C8-C7-N2-C2
2	A	303	NAG	O7-C7-N2-C2
2	B	301	NAG	C3-C2-N2-C7
2	B	301	NAG	C8-C7-N2-C2
2	B	301	NAG	O7-C7-N2-C2
2	D	302	NAG	C3-C2-N2-C7
2	D	302	NAG	C8-C7-N2-C2
2	D	302	NAG	O7-C7-N2-C2
4	C	303	PT5	C7-O13-P1-O11
4	C	303	PT5	C1-O1-P1-O12
4	A	305	PT5	C7-O13-P1-O11
4	A	305	PT5	C1-O1-P1-O12
4	B	303	PT5	C7-O13-P1-O11
4	B	303	PT5	C1-O1-P1-O12
4	D	304	PT5	C7-O13-P1-O11
4	D	304	PT5	C1-O1-P1-O12
5	C	304	NKO	OAF-CAG-CAH-CAI
5	C	304	NKO	OAE-CAK-OAJ-CAI
5	A	306	NKO	OAF-CAG-CAH-CAI
5	A	306	NKO	OAE-CAK-OAJ-CAI
5	B	304	NKO	OAF-CAG-CAH-CAI
5	B	304	NKO	OAE-CAK-OAJ-CAI
5	D	305	NKO	OAF-CAG-CAH-CAI
5	D	305	NKO	OAE-CAK-OAJ-CAI
6	C	305	LPP	C6-O5-P1-O2
6	C	305	LPP	C6-O5-P1-O4
6	A	301	LPP	C6-O5-P1-O2
6	A	301	LPP	C6-O5-P1-O4
6	A	302	LPP	C6-O5-P1-O2
6	A	302	LPP	C6-O5-P1-O4
6	D	301	LPP	C6-O5-P1-O2
6	D	301	LPP	C6-O5-P1-O4

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Mol	Chain	Res	Type	Atoms
4	C	303	PT5	O17-C10-O16-C8
4	A	305	PT5	O17-C10-O16-C8
4	B	303	PT5	O17-C10-O16-C8
4	D	304	PT5	O17-C10-O16-C8
5	C	304	NKO	CAL-CAK-OAJ-CAI
5	A	306	NKO	CAL-CAK-OAJ-CAI
5	B	304	NKO	CAL-CAK-OAJ-CAI
5	D	305	NKO	CAL-CAK-OAJ-CAI
5	C	304	NKO	OAF-CAG-CAH-OBA
5	A	306	NKO	OAF-CAG-CAH-OBA
5	B	304	NKO	OAF-CAG-CAH-OBA
5	D	305	NKO	OAF-CAG-CAH-OBA
4	C	303	PT5	C12-C10-O16-C8
4	A	305	PT5	C12-C10-O16-C8
4	B	303	PT5	C12-C10-O16-C8
4	D	304	PT5	C12-C10-O16-C8
3	C	302	LBN	C26-C25-O5-C3
3	A	304	LBN	C26-C25-O5-C3
3	B	302	LBN	C26-C25-O5-C3
3	D	303	LBN	C26-C25-O5-C3
2	C	301	NAG	O5-C5-C6-O6
2	A	303	NAG	O5-C5-C6-O6
2	B	301	NAG	O5-C5-C6-O6
2	D	302	NAG	O5-C5-C6-O6
3	C	302	LBN	C41-C42-C5-C8
3	A	304	LBN	C41-C42-C5-C8
3	B	302	LBN	C41-C42-C5-C8
3	D	303	LBN	C41-C42-C5-C8
3	C	302	LBN	O6-C25-O5-C3
3	A	304	LBN	O6-C25-O5-C3
3	D	303	LBN	O6-C25-O5-C3
3	B	302	LBN	O6-C25-O5-C3
5	C	304	NKO	CAK-CAL-CAM-CAN
5	A	306	NKO	CAK-CAL-CAM-CAN
5	B	304	NKO	CAK-CAL-CAM-CAN
5	D	305	NKO	CAK-CAL-CAM-CAN
4	C	303	PT5	C40-C41-C42-C43
4	A	305	PT5	C40-C41-C42-C43
4	B	303	PT5	C40-C41-C42-C43
4	D	304	PT5	C40-C41-C42-C43
5	C	304	NKO	CAG-CAH-CAI-OAJ
5	A	306	NKO	CAG-CAH-CAI-OAJ

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Mol	Chain	Res	Type	Atoms
5	B	304	NKO	CAG-CAH-CAI-OAJ
5	D	305	NKO	CAG-CAH-CAI-OAJ
6	C	305	LPP	C34-C35-C36-C37
6	A	301	LPP	C34-C35-C36-C37
6	A	302	LPP	C34-C35-C36-C37
6	D	301	LPP	C34-C35-C36-C37
4	C	303	PT5	C38-C39-C40-C41
4	A	305	PT5	C38-C39-C40-C41
4	B	303	PT5	C38-C39-C40-C41
4	D	304	PT5	C38-C39-C40-C41
3	C	302	LBN	C31-C32-C33-C4
3	A	304	LBN	C31-C32-C33-C4
3	B	302	LBN	C31-C32-C33-C4
3	D	303	LBN	C31-C32-C33-C4
3	C	302	LBN	C33-C4-C7-C10
3	A	304	LBN	C33-C4-C7-C10
3	B	302	LBN	C33-C4-C7-C10
3	D	303	LBN	C33-C4-C7-C10
6	C	305	LPP	C40-C41-C42-C43
6	A	301	LPP	C40-C41-C42-C43
6	A	302	LPP	C40-C41-C42-C43
6	D	301	LPP	C40-C41-C42-C43
3	C	302	LBN	C38-C39-C40-C41
3	A	304	LBN	C38-C39-C40-C41
3	B	302	LBN	C38-C39-C40-C41
3	D	303	LBN	C38-C39-C40-C41
3	C	302	LBN	C39-C40-C41-C42
3	A	304	LBN	C39-C40-C41-C42
3	B	302	LBN	C39-C40-C41-C42
3	D	303	LBN	C39-C40-C41-C42
5	C	304	NKO	OBA-CAH-CAI-OAJ
5	A	306	NKO	OBA-CAH-CAI-OAJ
5	B	304	NKO	OBA-CAH-CAI-OAJ
5	D	305	NKO	OBA-CAH-CAI-OAJ
4	C	303	PT5	C34-C35-C36-C37
4	A	305	PT5	C34-C35-C36-C37
4	B	303	PT5	C34-C35-C36-C37
4	D	304	PT5	C34-C35-C36-C37
6	A	302	LPP	C36-C37-C38-C39
6	C	305	LPP	C36-C37-C38-C39
6	A	301	LPP	C36-C37-C38-C39
6	D	301	LPP	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
3	B	302	LBN	C27-C28-C29-C30
3	C	302	LBN	C35-C34-O7-C2
3	A	304	LBN	C35-C34-O7-C2
3	B	302	LBN	C35-C34-O7-C2
3	D	303	LBN	C35-C34-O7-C2
3	C	302	LBN	C27-C28-C29-C30
3	A	304	LBN	C27-C28-C29-C30
3	D	303	LBN	C27-C28-C29-C30
3	C	302	LBN	O8-C34-O7-C2
3	A	304	LBN	O8-C34-O7-C2
3	B	302	LBN	O8-C34-O7-C2
3	D	303	LBN	O8-C34-O7-C2
3	C	302	LBN	C14-C17-C20-C22
3	A	304	LBN	C14-C17-C20-C22
3	B	302	LBN	C14-C17-C20-C22
3	D	303	LBN	C14-C17-C20-C22
6	C	305	LPP	C39-C40-C41-C42
6	A	301	LPP	C39-C40-C41-C42
6	A	302	LPP	C39-C40-C41-C42
6	D	301	LPP	C39-C40-C41-C42
3	C	302	LBN	C1-C2-C3-O5
3	A	304	LBN	C1-C2-C3-O5
3	B	302	LBN	C1-C2-C3-O5
3	D	303	LBN	C1-C2-C3-O5
4	C	303	PT5	C7-C8-O16-C10
4	A	305	PT5	C7-C8-O16-C10
4	B	303	PT5	C7-C8-O16-C10
4	D	304	PT5	C7-C8-O16-C10
6	C	305	LPP	C6-O5-P1-O3
6	A	301	LPP	C6-O5-P1-O3
6	A	302	LPP	C6-O5-P1-O3
6	D	301	LPP	C6-O5-P1-O3
4	C	303	PT5	C33-C34-C35-C36
4	A	305	PT5	C33-C34-C35-C36
4	B	303	PT5	C33-C34-C35-C36
4	D	304	PT5	C33-C34-C35-C36
4	C	303	PT5	C1-O1-P1-O13
4	A	305	PT5	C1-O1-P1-O13
4	B	303	PT5	C1-O1-P1-O13
4	D	304	PT5	C1-O1-P1-O13
5	C	304	NKO	CAM-CAN-CAO-CAP
5	A	306	NKO	CAM-CAN-CAO-CAP

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Mol	Chain	Res	Type	Atoms
5	B	304	NKO	CAM-CAN-CAO-CAP
5	D	305	NKO	CAM-CAN-CAO-CAP
4	C	303	PT5	C1-O1-P1-O11
4	A	305	PT5	C1-O1-P1-O11
4	B	303	PT5	C1-O1-P1-O11
4	D	304	PT5	C1-O1-P1-O11
4	C	303	PT5	C15-C16-C17-C18
4	A	305	PT5	C15-C16-C17-C18
4	B	303	PT5	C15-C16-C17-C18
4	D	304	PT5	C15-C16-C17-C18
3	C	302	LBN	C28-C29-C30-C31
3	A	304	LBN	C28-C29-C30-C31
3	B	302	LBN	C28-C29-C30-C31
3	D	303	LBN	C28-C29-C30-C31
3	C	302	LBN	C29-C30-C31-C32
3	A	304	LBN	C29-C30-C31-C32
3	B	302	LBN	C29-C30-C31-C32
3	D	303	LBN	C29-C30-C31-C32
3	C	302	LBN	C30-C31-C32-C33
3	A	304	LBN	C30-C31-C32-C33
3	B	302	LBN	C30-C31-C32-C33
3	D	303	LBN	C30-C31-C32-C33
6	C	305	LPP	C6-C7-C8-O27
6	A	301	LPP	C6-C7-C8-O27
6	A	302	LPP	C6-C7-C8-O27
6	D	301	LPP	C6-C7-C8-O27
6	C	305	LPP	C35-C36-C37-C38
6	A	301	LPP	C35-C36-C37-C38
6	D	301	LPP	C35-C36-C37-C38
6	A	302	LPP	C35-C36-C37-C38
3	C	302	LBN	O7-C2-C3-O5
3	A	304	LBN	O7-C2-C3-O5
3	D	303	LBN	O7-C2-C3-O5
3	B	302	LBN	C8-C11-C14-C17
3	D	303	LBN	C8-C11-C14-C17
3	C	302	LBN	C8-C11-C14-C17
3	A	304	LBN	C8-C11-C14-C17
4	C	303	PT5	C7-O13-P1-O1
4	A	305	PT5	C7-O13-P1-O1
4	B	303	PT5	C7-O13-P1-O1
4	D	304	PT5	C7-O13-P1-O1
3	B	302	LBN	O7-C2-C3-O5

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Mol	Chain	Res	Type	Atoms
3	C	302	LBN	C40-C41-C42-C5
3	A	304	LBN	C40-C41-C42-C5
3	B	302	LBN	C40-C41-C42-C5
3	D	303	LBN	C40-C41-C42-C5
4	C	303	PT5	C7-C8-C9-O18
4	A	305	PT5	C7-C8-C9-O18
4	B	303	PT5	C7-C8-C9-O18
4	D	304	PT5	C7-C8-C9-O18
2	A	303	NAG	C4-C5-C6-O6
6	A	302	LPP	C22-C23-C24-C25
2	C	301	NAG	C4-C5-C6-O6
2	D	302	NAG	C4-C5-C6-O6
2	B	301	NAG	C4-C5-C6-O6
6	C	305	LPP	C22-C23-C24-C25
6	A	301	LPP	C22-C23-C24-C25
6	D	301	LPP	C22-C23-C24-C25
3	C	302	LBN	C14-C11-C8-C5
3	A	304	LBN	C14-C11-C8-C5
3	B	302	LBN	C14-C11-C8-C5
3	D	303	LBN	C14-C11-C8-C5
4	B	303	PT5	C39-C40-C41-C42
4	D	304	PT5	C39-C40-C41-C42
4	C	303	PT5	C39-C40-C41-C42
4	A	305	PT5	C39-C40-C41-C42
6	C	305	LPP	O5-C6-C7-C8
6	A	301	LPP	O5-C6-C7-C8
6	A	302	LPP	O5-C6-C7-C8
6	D	301	LPP	O5-C6-C7-C8
6	C	305	LPP	O9-C7-C8-O27
6	A	301	LPP	O9-C7-C8-O27
6	A	302	LPP	O9-C7-C8-O27
6	D	301	LPP	O9-C7-C8-O27
6	C	305	LPP	O9-C11-C12-C13
6	A	301	LPP	O9-C11-C12-C13
6	A	302	LPP	O9-C11-C12-C13
6	D	301	LPP	O9-C11-C12-C13
6	C	305	LPP	O10-C11-C12-C13
6	A	301	LPP	O10-C11-C12-C13
6	A	302	LPP	O10-C11-C12-C13
6	D	301	LPP	O10-C11-C12-C13
6	C	305	LPP	C21-C22-C23-C24
6	A	301	LPP	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
6	A	302	LPP	C21-C22-C23-C24
6	D	301	LPP	C21-C22-C23-C24
6	D	301	LPP	O10-C11-O9-C7
6	C	305	LPP	O10-C11-O9-C7
6	A	301	LPP	O10-C11-O9-C7
6	A	302	LPP	O10-C11-O9-C7
3	A	304	LBN	C42-C5-C8-C11
3	D	303	LBN	C42-C5-C8-C11
4	C	303	PT5	O16-C10-C12-C13
4	A	305	PT5	O16-C10-C12-C13
4	D	304	PT5	O16-C10-C12-C13
4	B	303	PT5	O16-C10-C12-C13
3	C	302	LBN	C42-C5-C8-C11
3	B	302	LBN	C42-C5-C8-C11
4	C	303	PT5	O17-C10-C12-C13
4	A	305	PT5	O17-C10-C12-C13
4	B	303	PT5	O17-C10-C12-C13
4	D	304	PT5	O17-C10-C12-C13

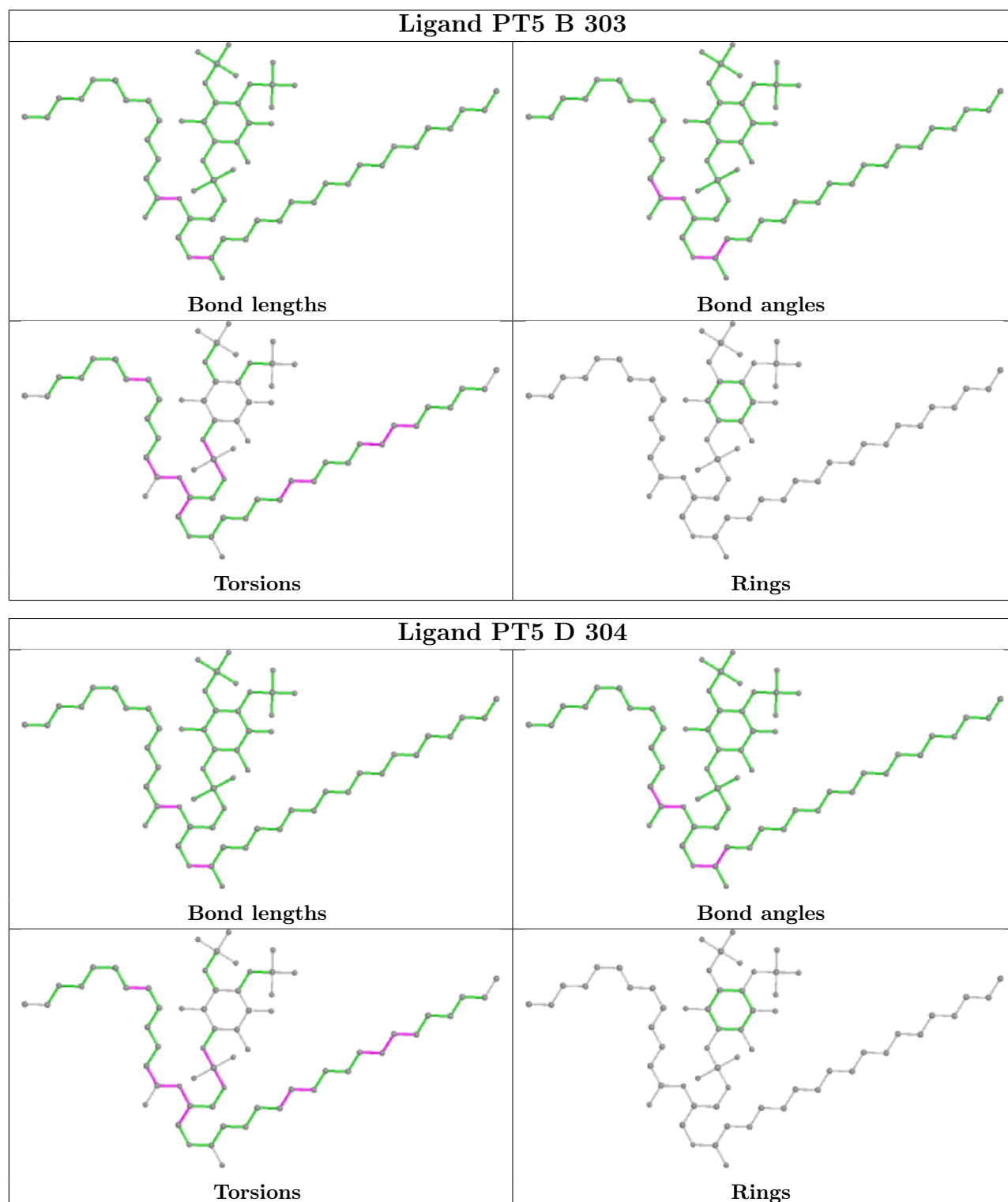
There are no ring outliers.

12 monomers are involved in 20 short contacts:

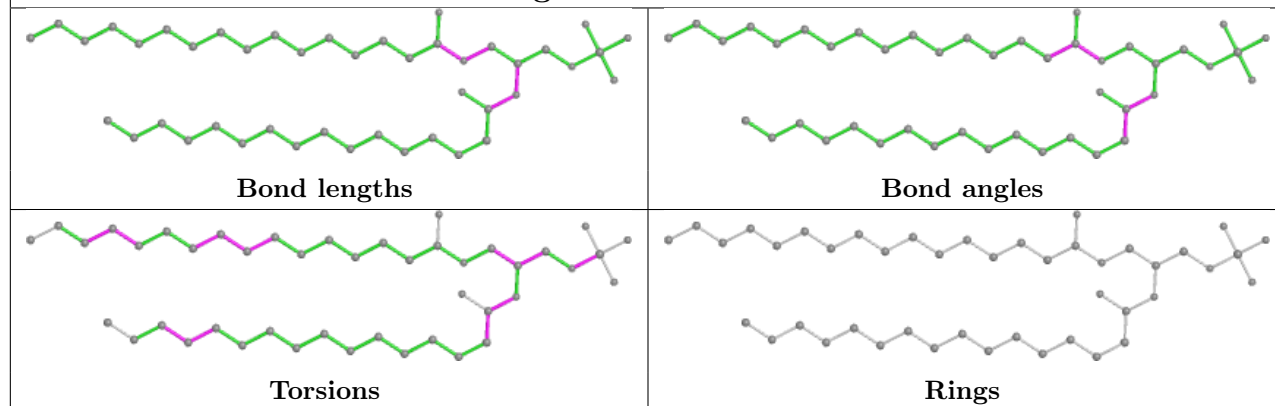
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	303	PT5	2	0
4	D	304	PT5	2	0
6	C	305	LPP	2	0
2	B	301	NAG	1	0
6	A	301	LPP	2	0
2	A	303	NAG	1	0
6	A	302	LPP	2	0
2	C	301	NAG	1	0
2	D	302	NAG	1	0
4	C	303	PT5	2	0
6	D	301	LPP	2	0
4	A	305	PT5	2	0

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

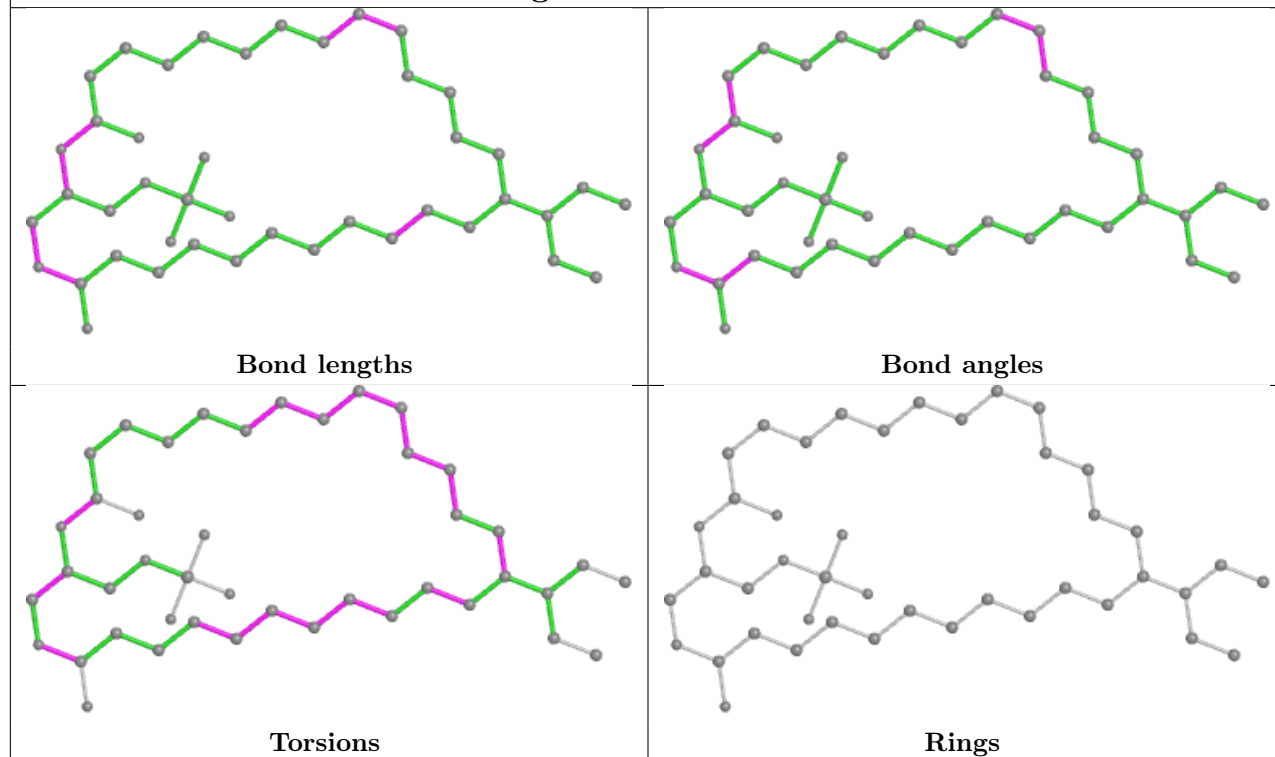
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified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



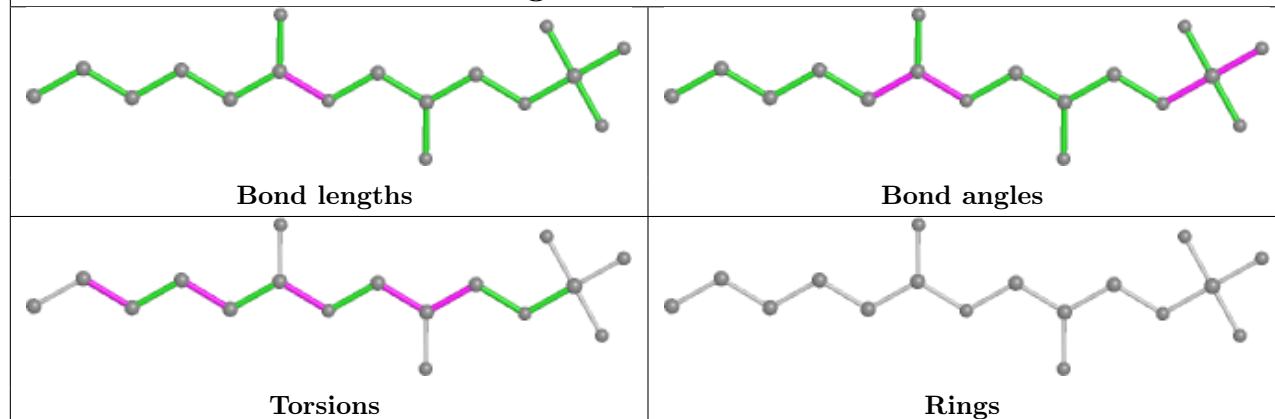
Ligand LPP C 305



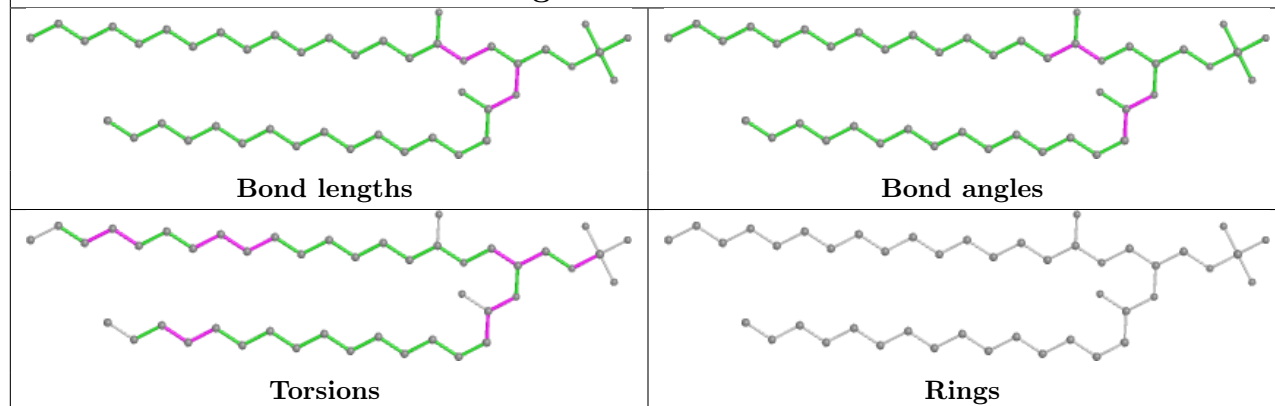
Ligand LBN B 302



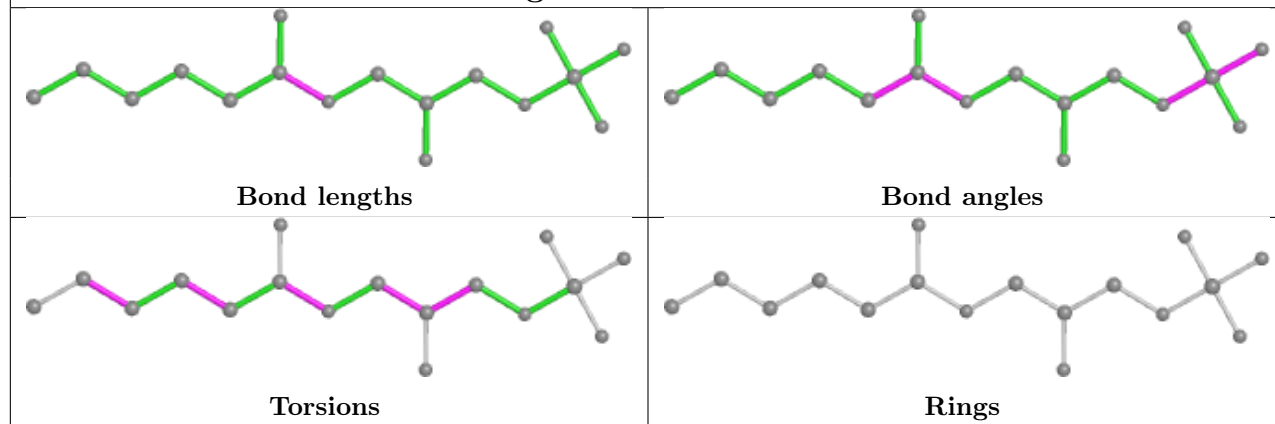
Ligand NKO B 304



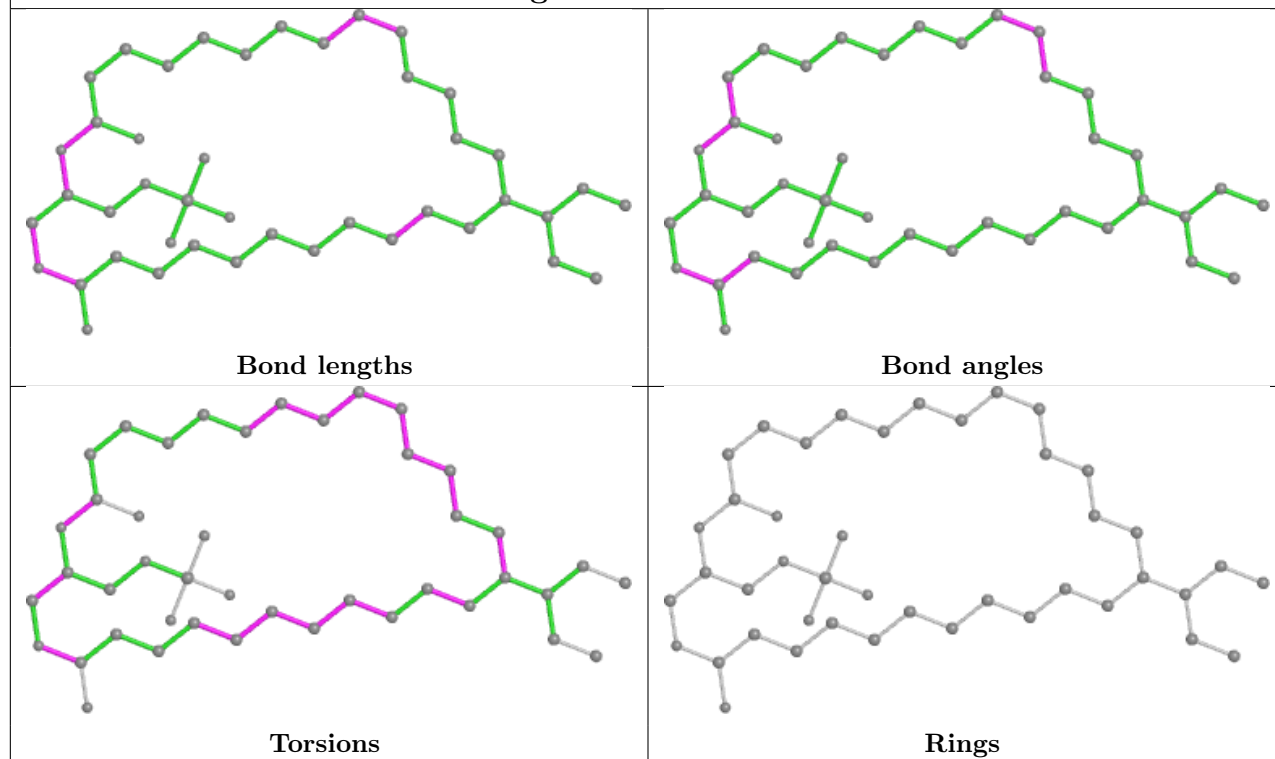
Ligand LPP A 301



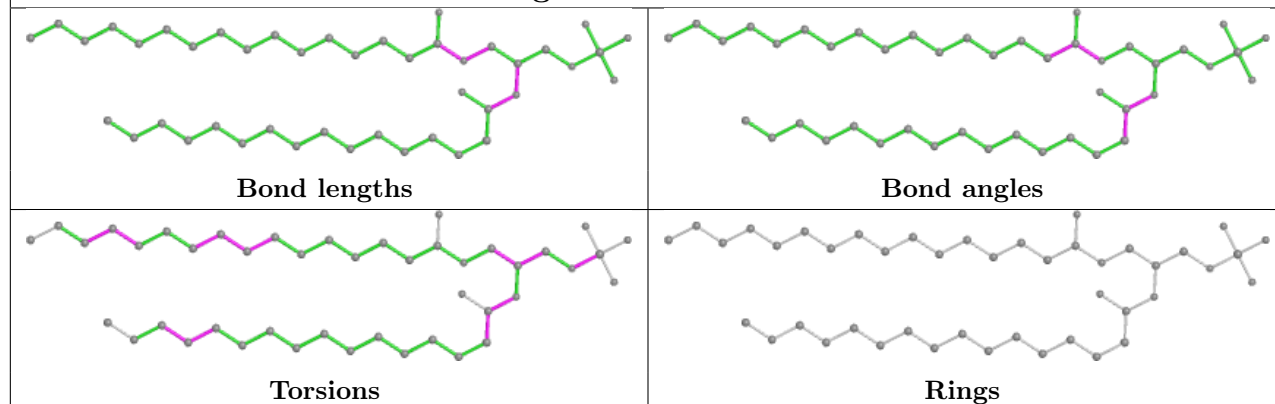
Ligand NKO A 306



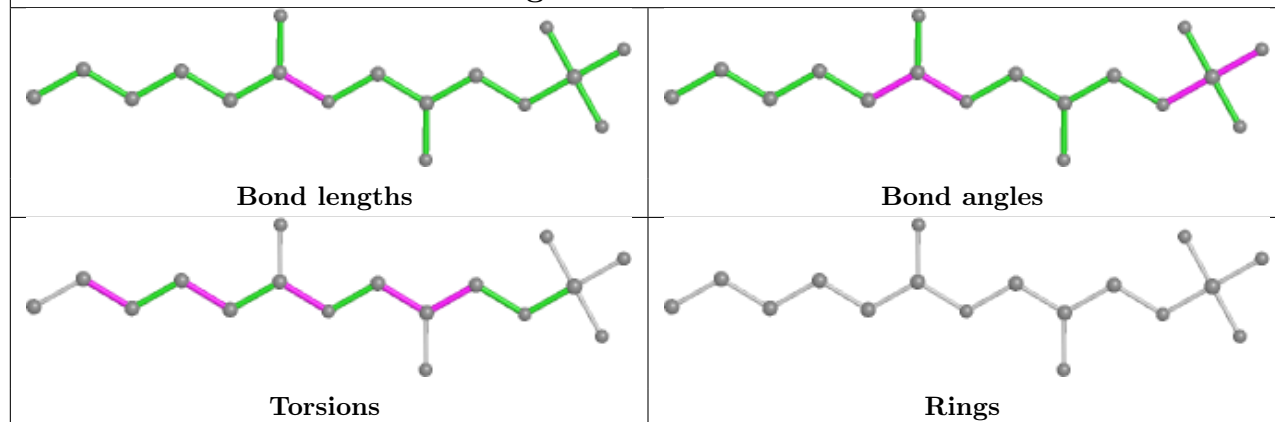
Ligand LBN A 304



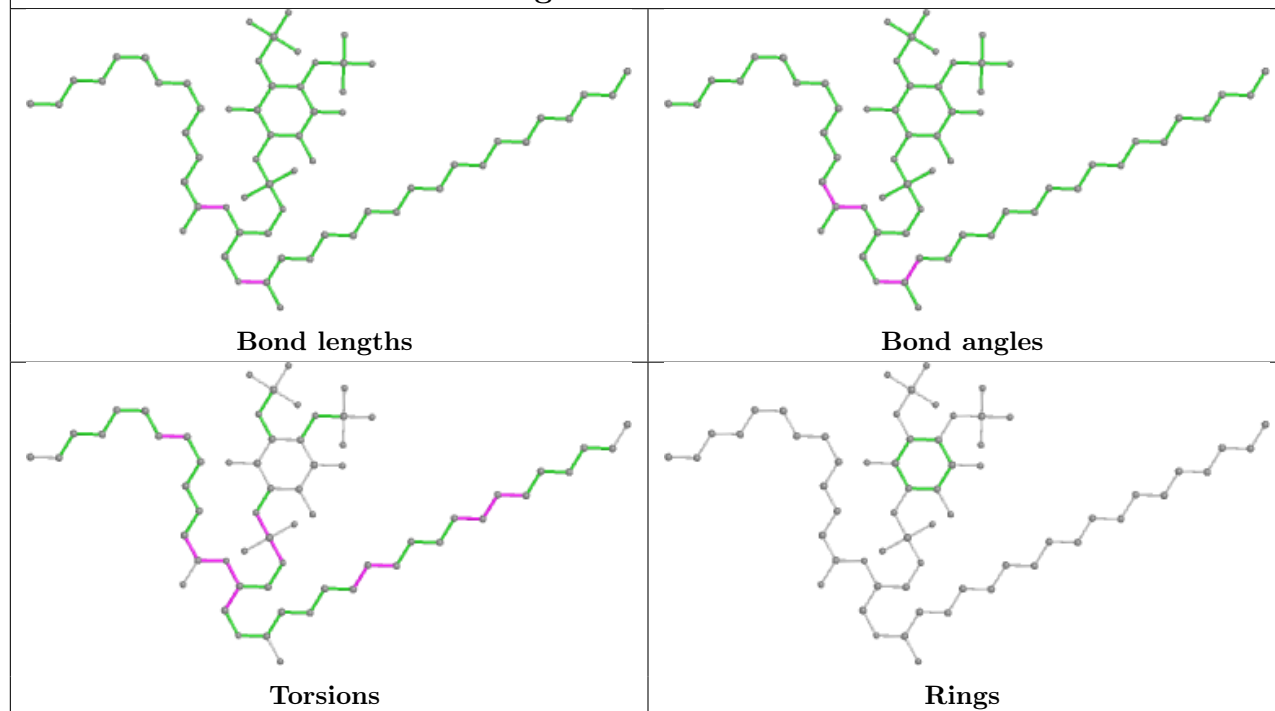
Ligand LPP A 302

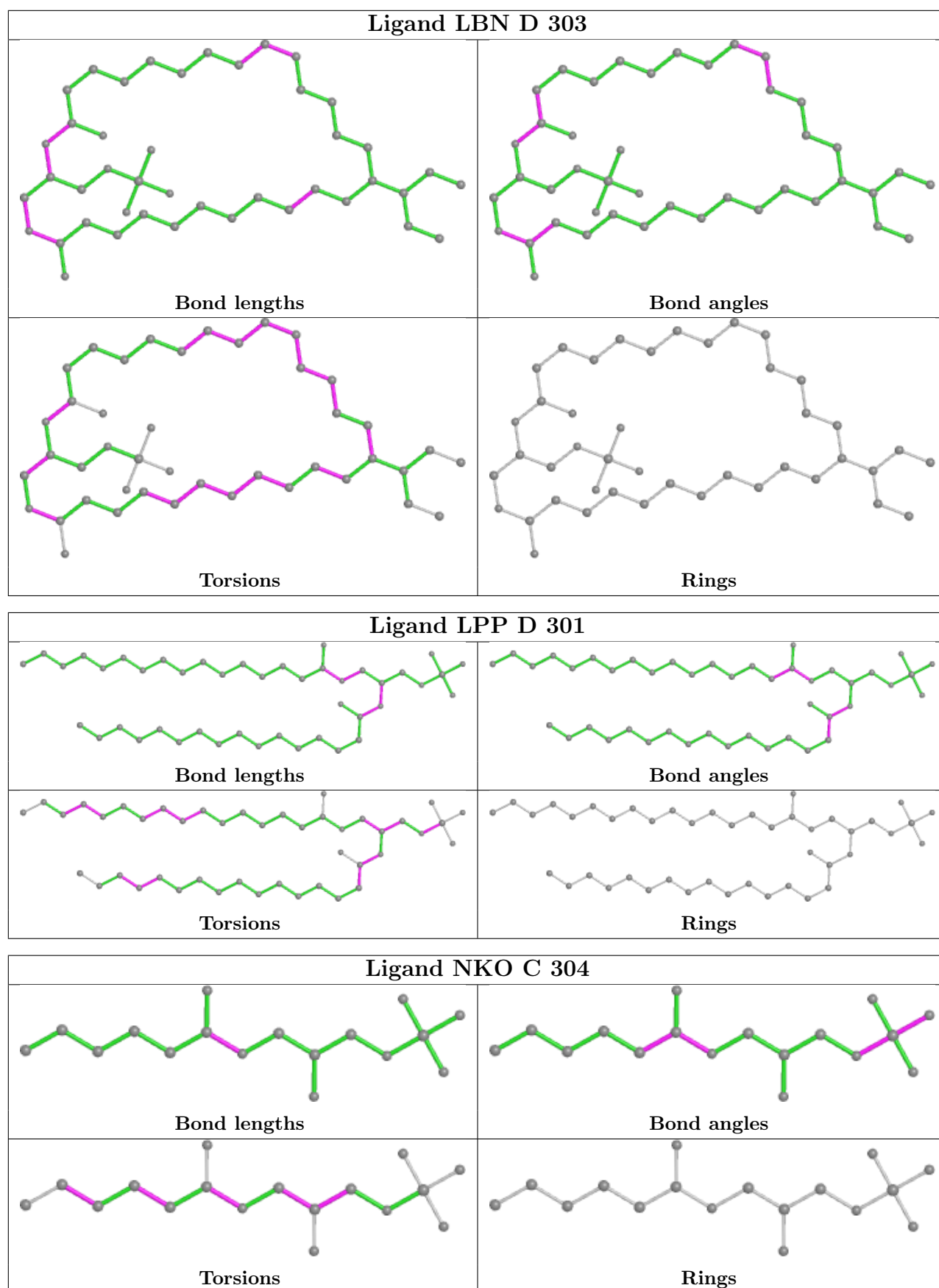


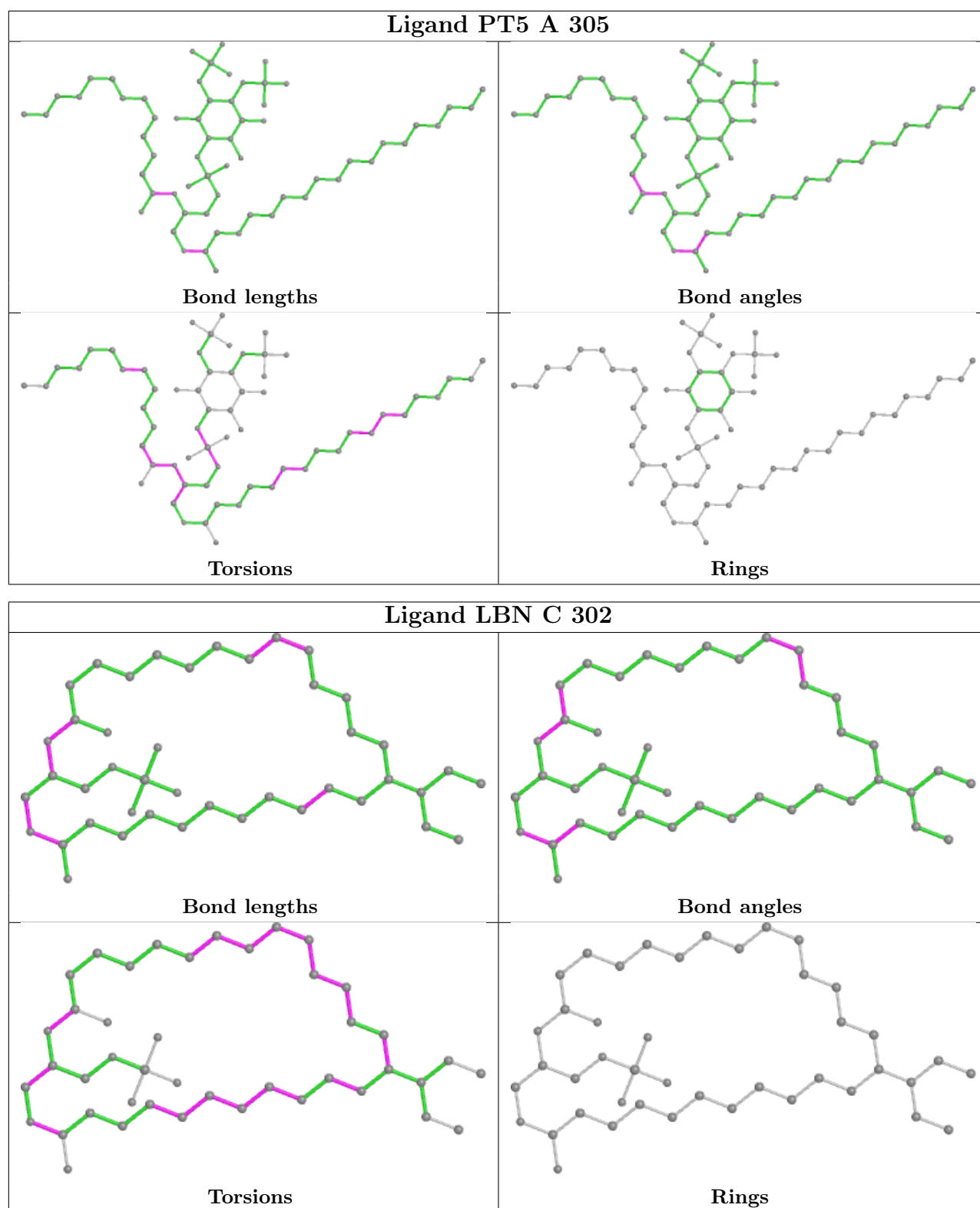
Ligand NKO D 305



Ligand PT5 C 303







5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

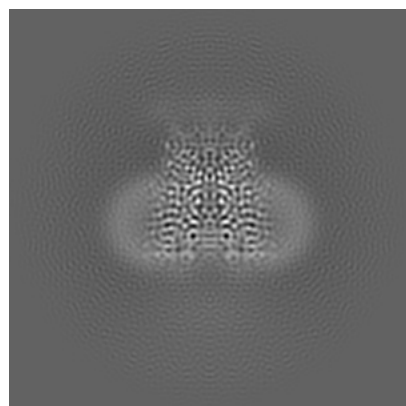
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62720. These allow visual inspection of the internal detail of the map and identification of artifacts.

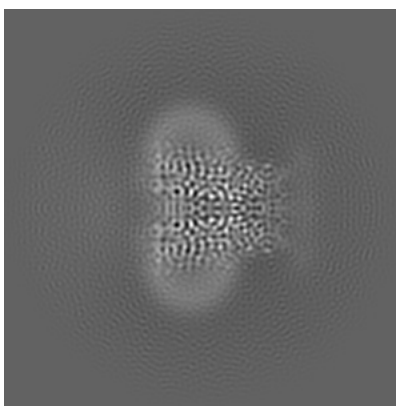
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

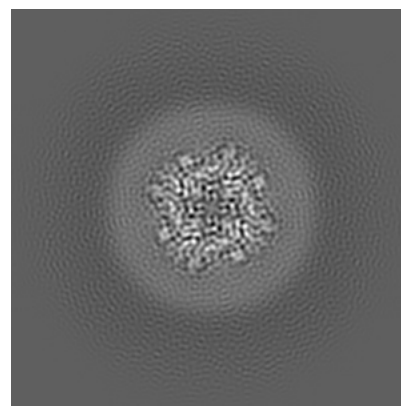
6.1.1 Primary map



X

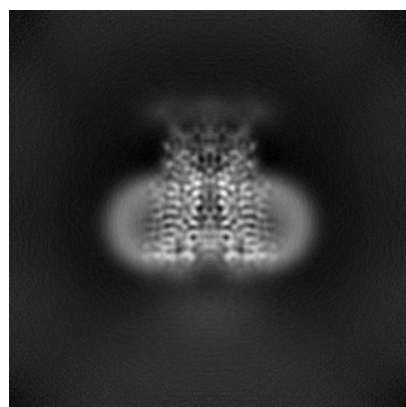


Y

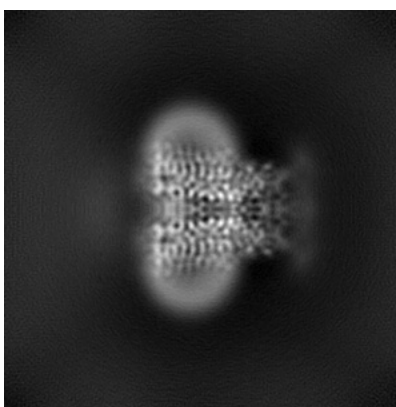


Z

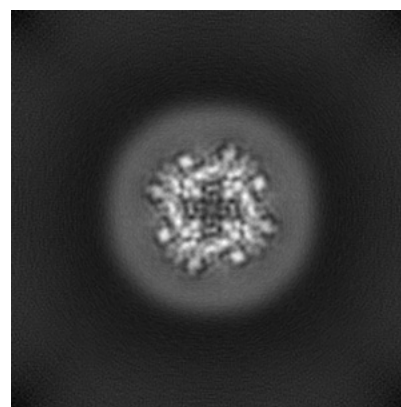
6.1.2 Raw map



X



Y

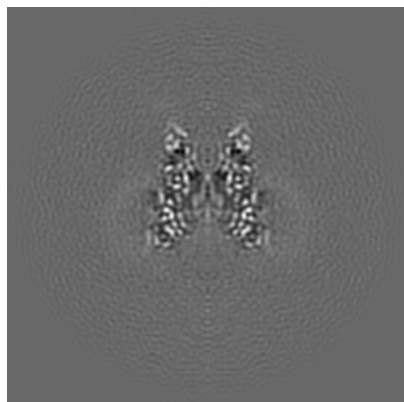


Z

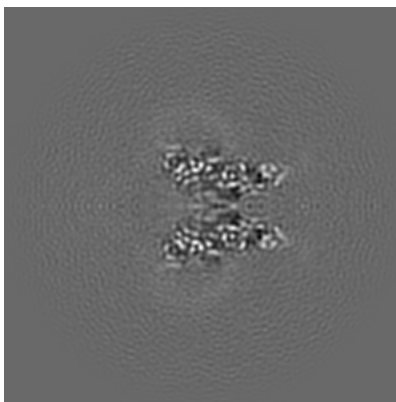
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

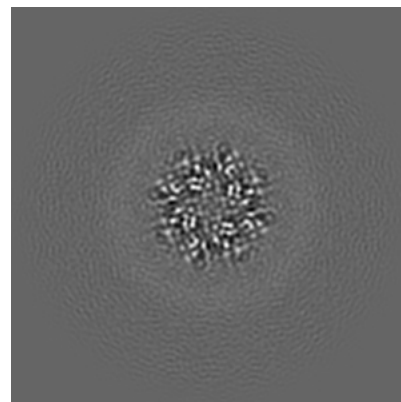
6.2.1 Primary map



X Index: 128

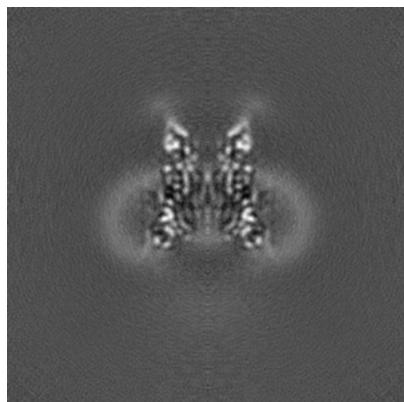


Y Index: 128

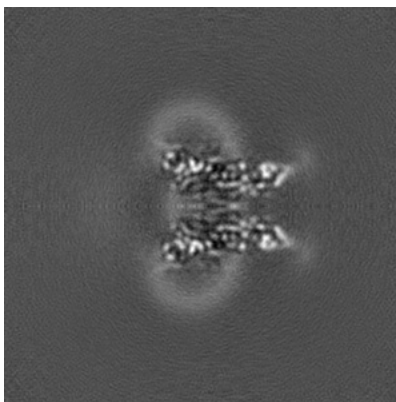


Z Index: 128

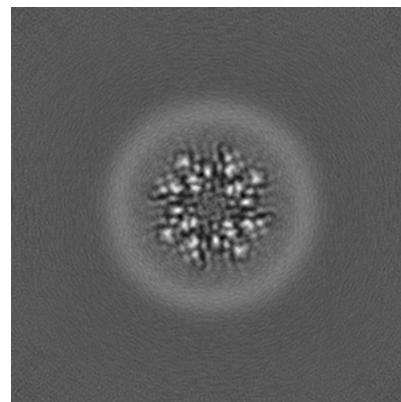
6.2.2 Raw map



X Index: 128



Y Index: 128

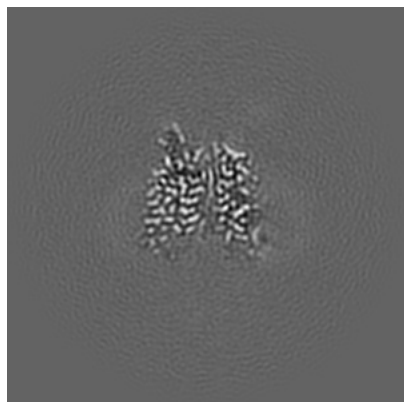


Z Index: 128

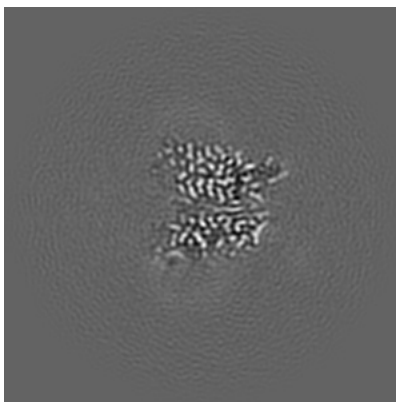
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

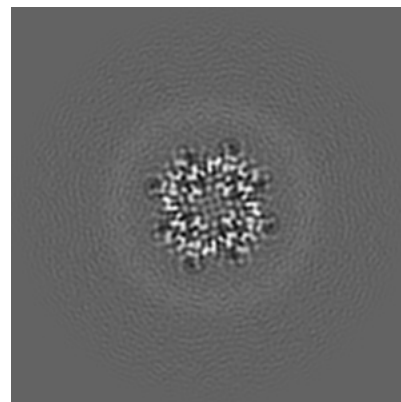
6.3.1 Primary map



X Index: 119

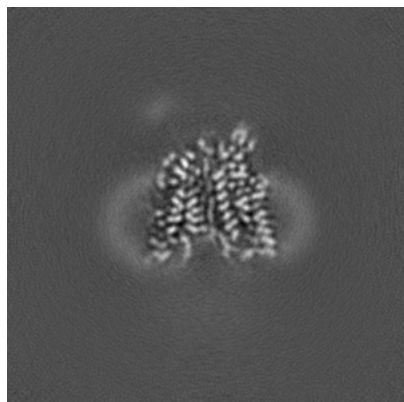


Y Index: 119

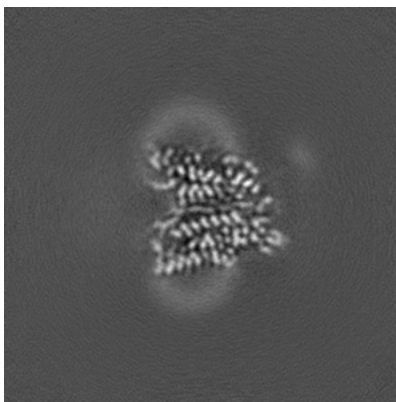


Z Index: 120

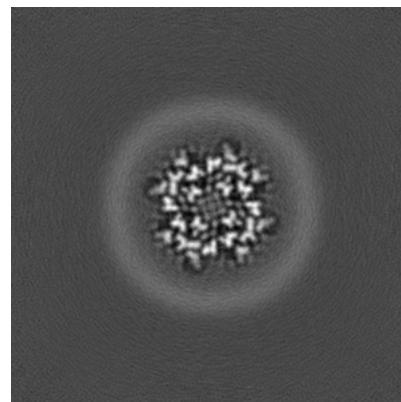
6.3.2 Raw map



X Index: 140



Y Index: 140

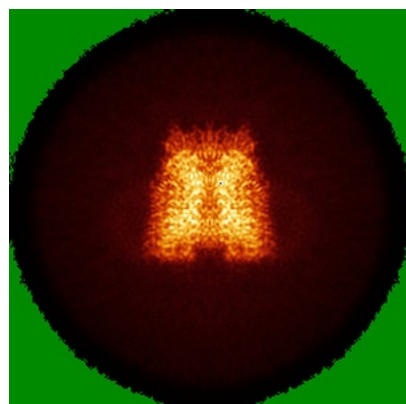


Z Index: 120

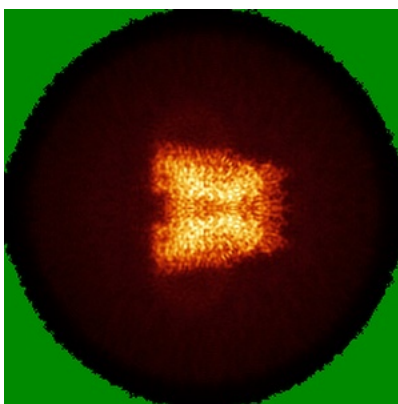
The images above show the largest variance slices of the map in three orthogonal directions.

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

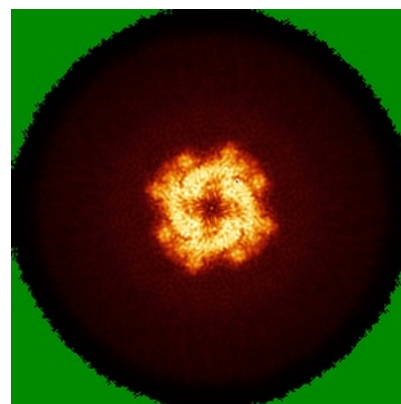
6.4.1 Primary map



X

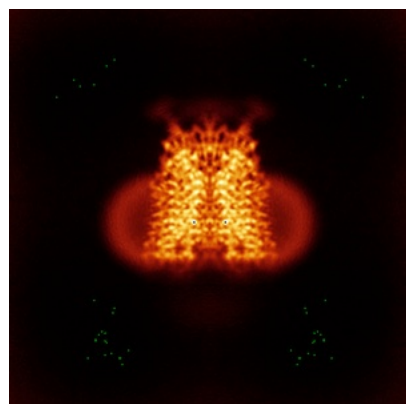


Y

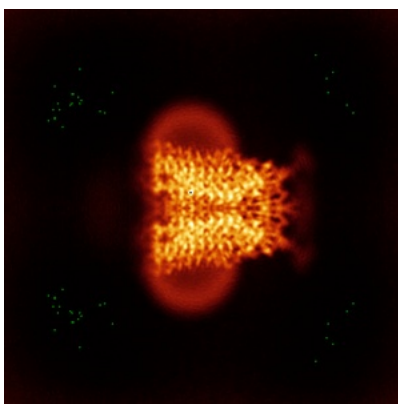


Z

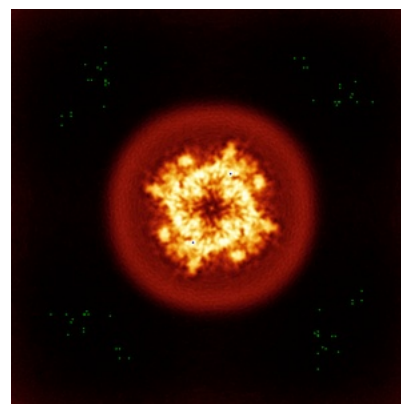
6.4.2 Raw map



X



Y

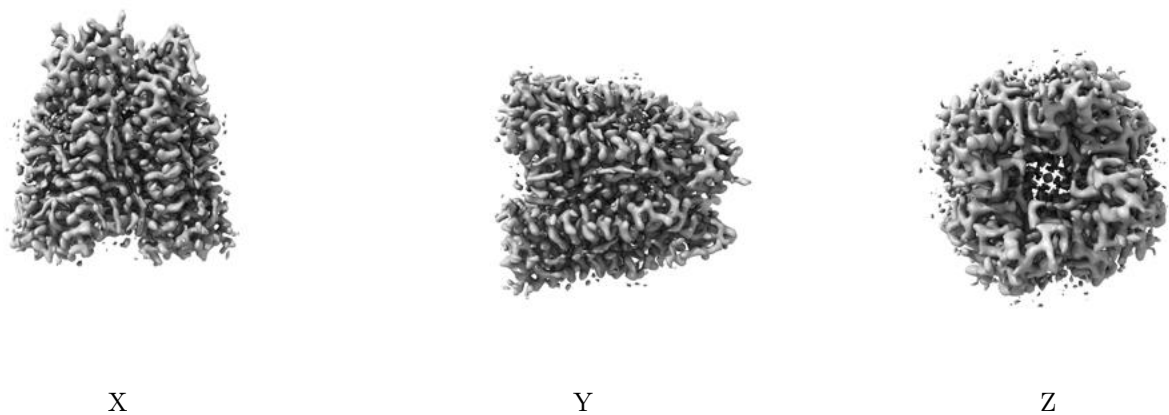


Z

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.

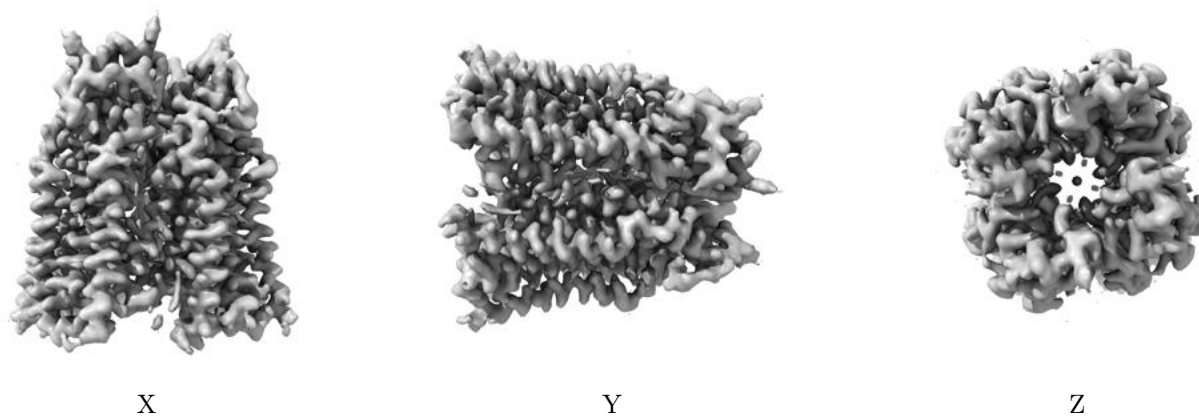
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.246. 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.

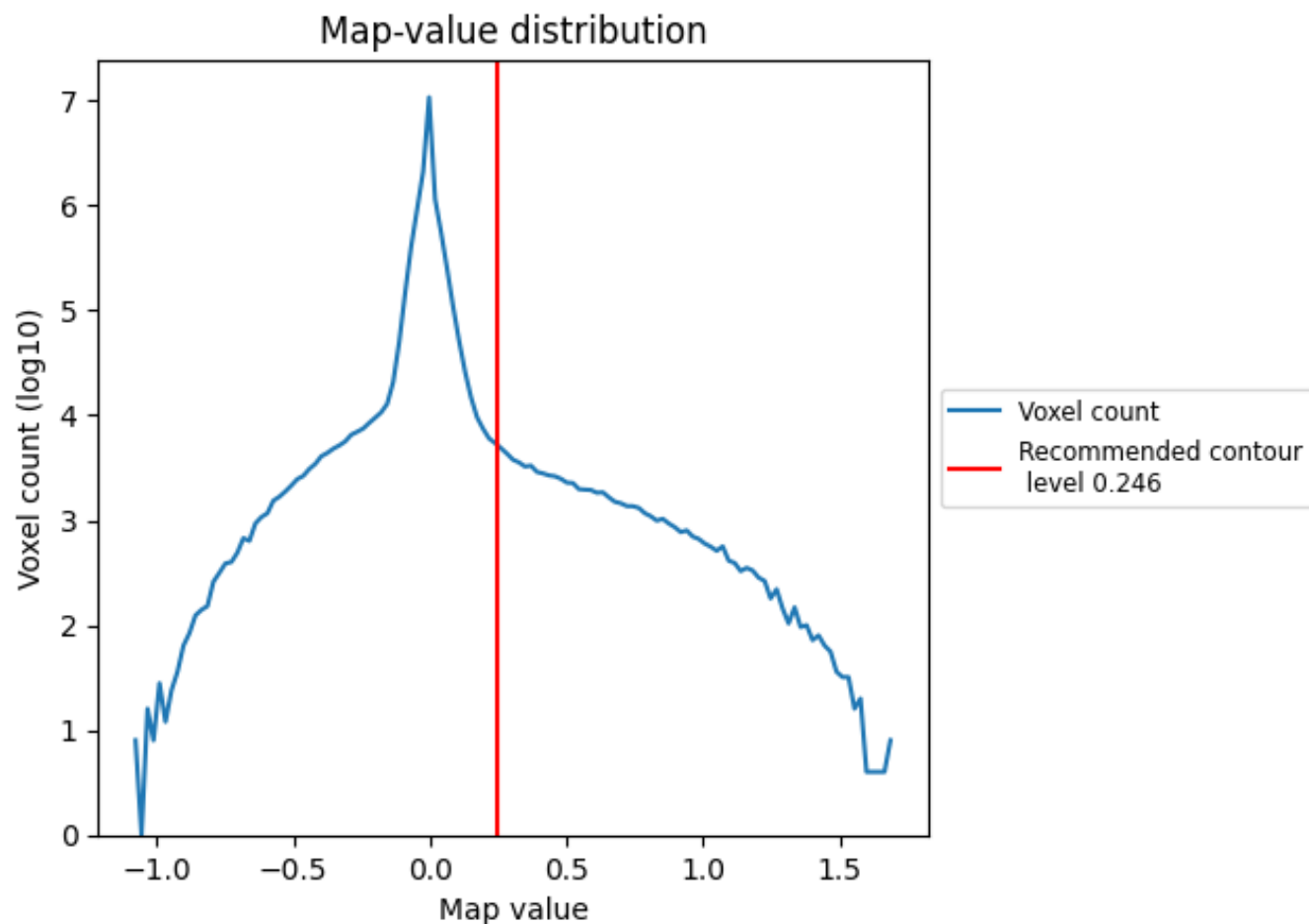
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

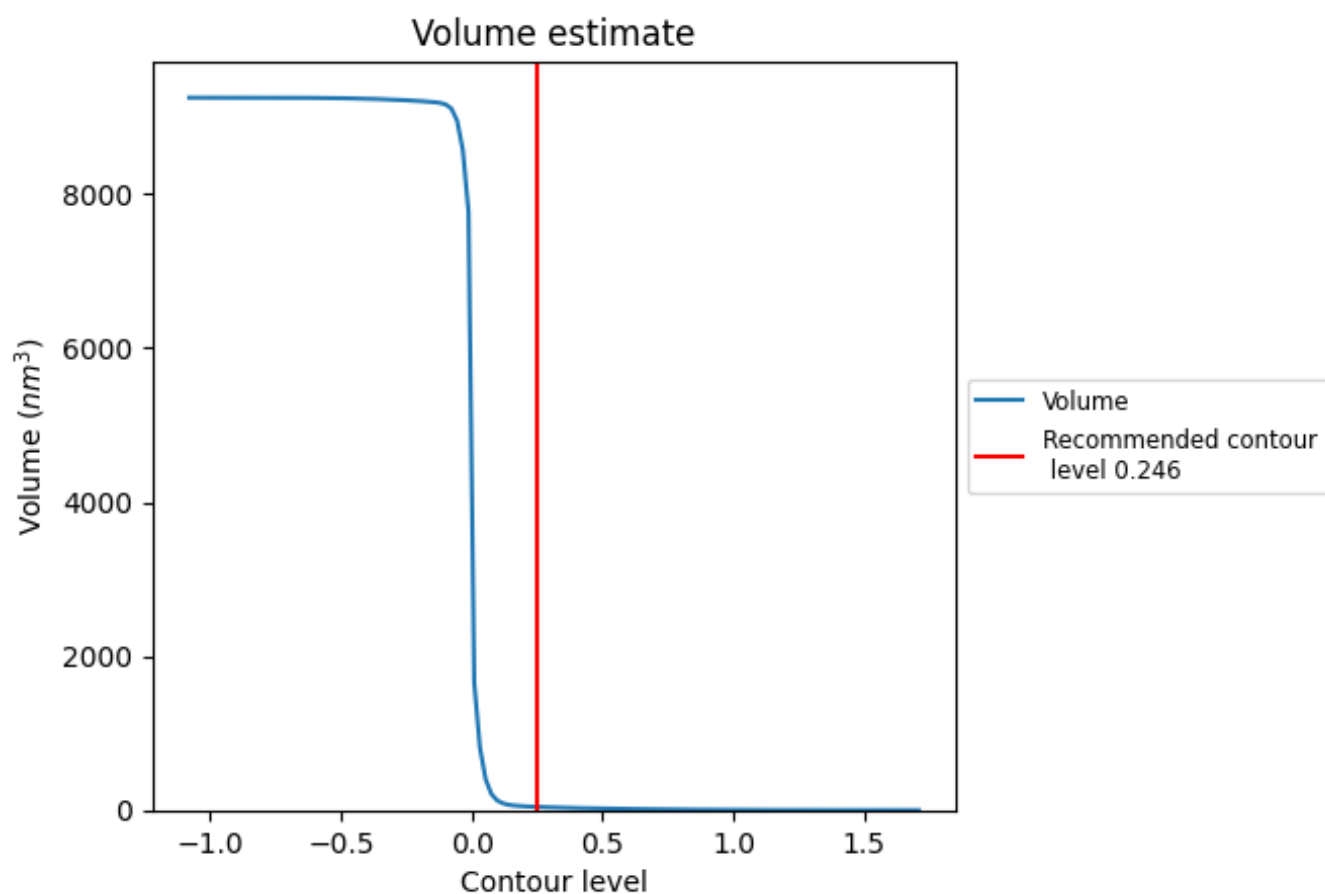
This section contains the results of statistical analysis of the map.

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.

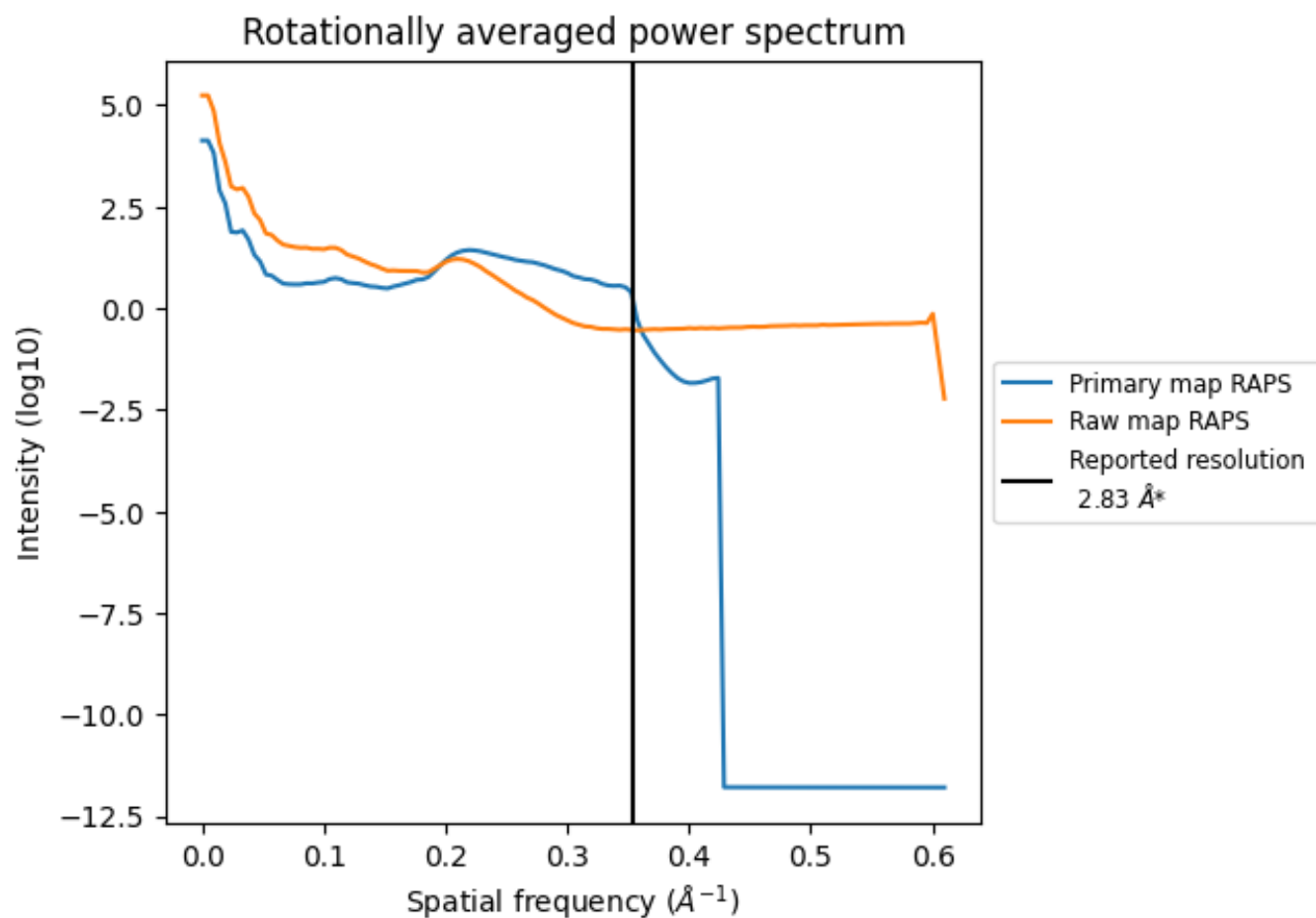
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 43 nm³; this corresponds to an approximate mass of 39 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 ⓘ

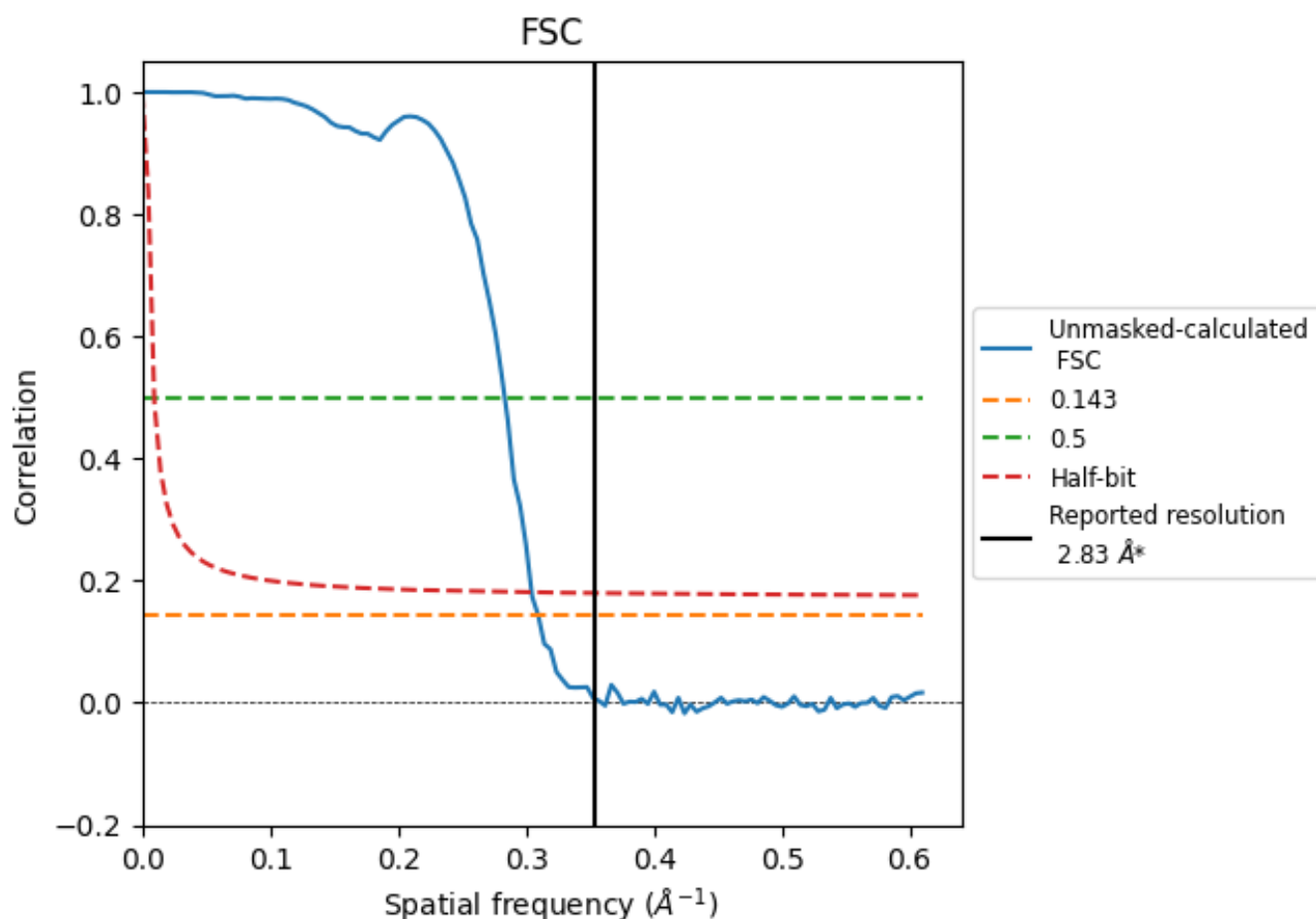


*Reported resolution corresponds to spatial frequency of 0.353 \AA^{-1}

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 0.353 \AA^{-1}

8.2 Resolution estimates [i](#)

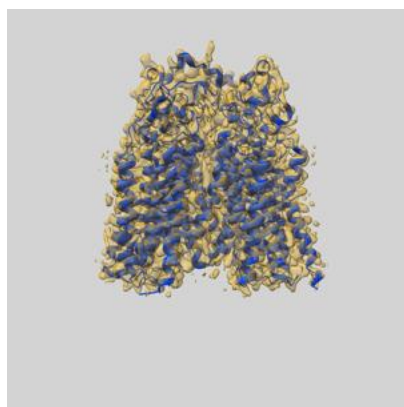
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.83	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.23	3.53	3.28

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.23 differs from the reported value 2.83 by more than 10 %

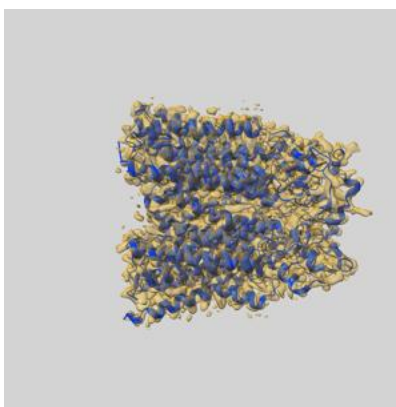
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-62720 and PDB model 9L0O. Per-residue inclusion information can be found in section [3](#) on page [8](#).

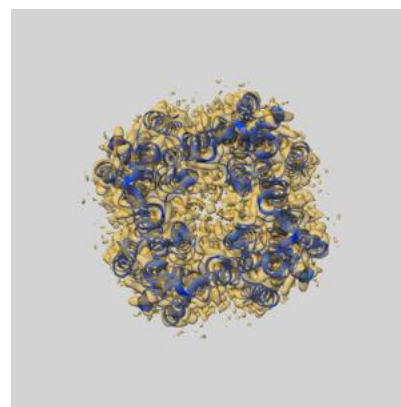
9.1 Map-model overlay [i](#)



X



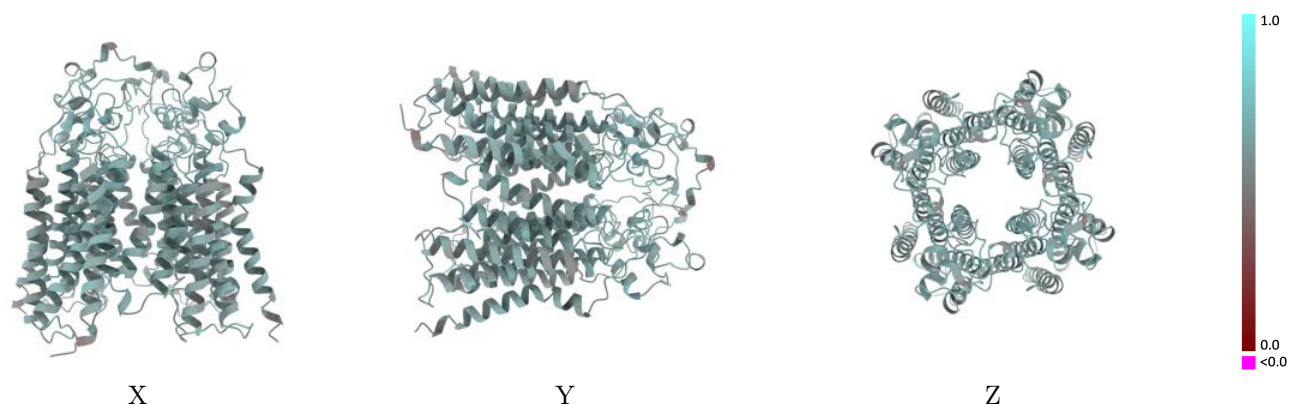
Y



Z

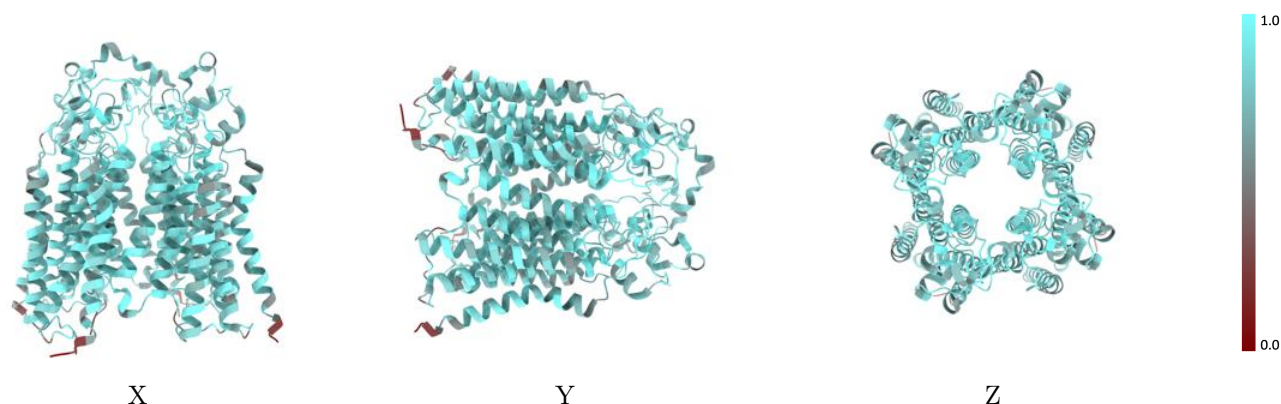
The images above show the 3D surface view of the map at the recommended contour level 0.246 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



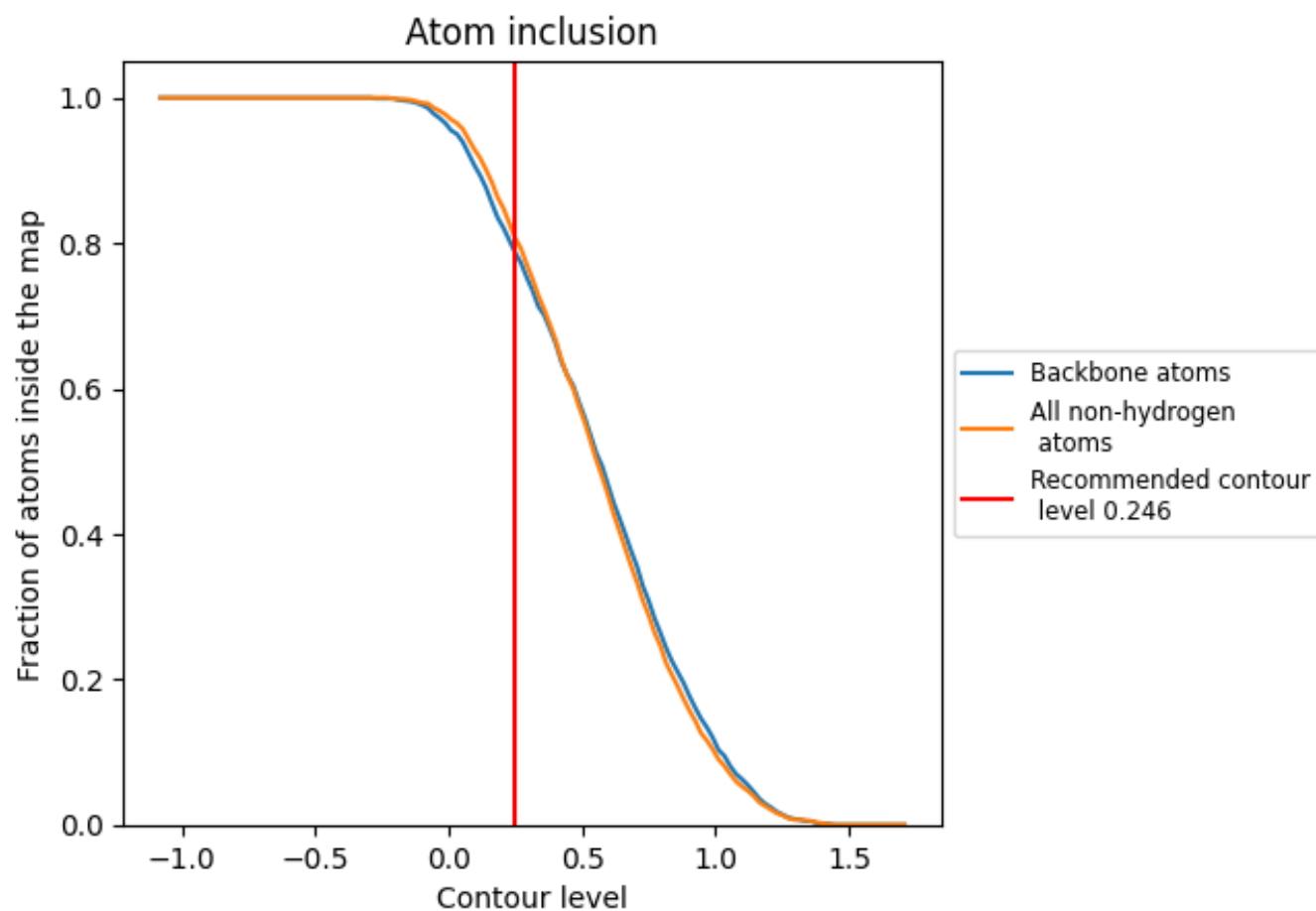
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.246).

9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 81% 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 (0.246) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8100	<div></div> 0.5900
A	<div></div> 0.8160	<div></div> 0.5910
B	<div></div> 0.8160	<div></div> 0.5900
C	<div></div> 0.8170	<div></div> 0.5900
D	<div></div> 0.8170	<div></div> 0.5900

