



Full wwPDB EM Validation Report ⓘ

Mar 18, 2025 – 04:07 pm GMT

PDB ID : 8QC1
EMDB ID : EMD-18325
Title : Respiratory complex I from *Paracoccus denitrificans* in MSP2N2 nanodiscs
(ND4 & ND5 focus refinement)
Authors : Ivanov, B.S.; Bridges, H.R.; Hirst, J.
Deposited on : 2023-08-25
Resolution : 2.50 Å(reported)
Based on initial model : .

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev117
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41

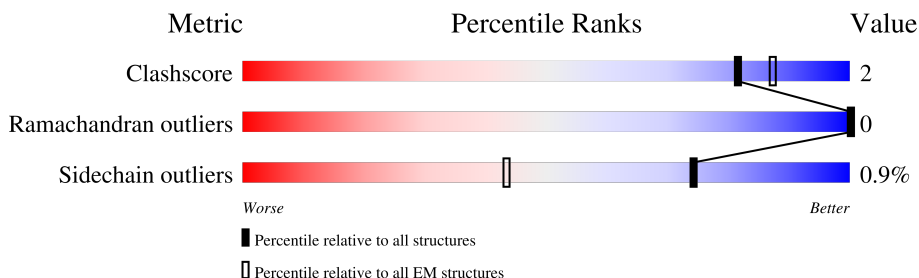
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.50 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	M	513	 92% 6%
2	L	703	 82% 6% 13%

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 9431 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.

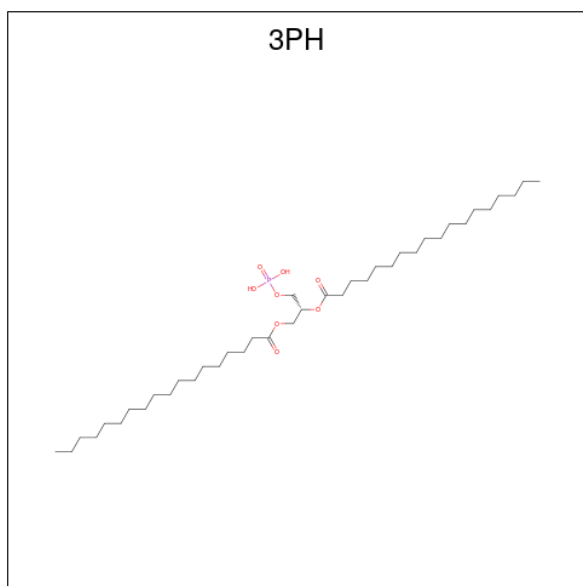
- Molecule 1 is a protein called NADH dehydrogenase subunit M.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	M	503	Total	C	N	O	S	0	0
			3913	2614	610	657	32		

- Molecule 2 is a protein called NADH dehydrogenase subunit L.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L	615	Total	C	N	O	S	0	0
			4856	3236	789	802	29		

- Molecule 3 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (three-letter code: 3PH) (formula: $C_{39}H_{77}O_8P$).



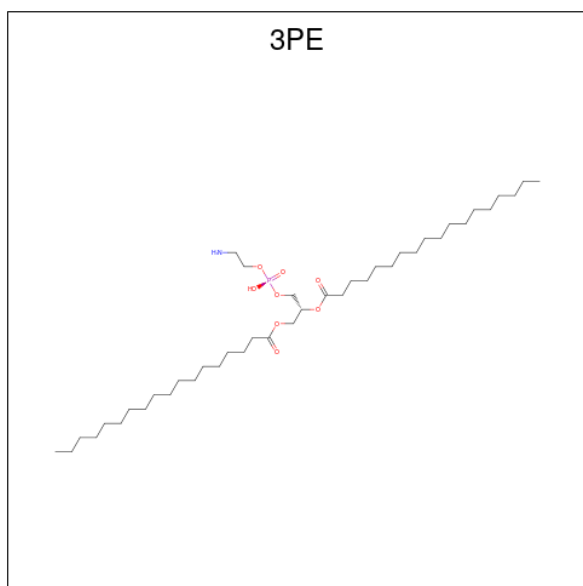
Mol	Chain	Residues	Atoms				AltConf
3	M	1	Total	C	O	P	0
			46	37	8	1	
3	M	1	Total	C	O	P	0
			36	27	8	1	

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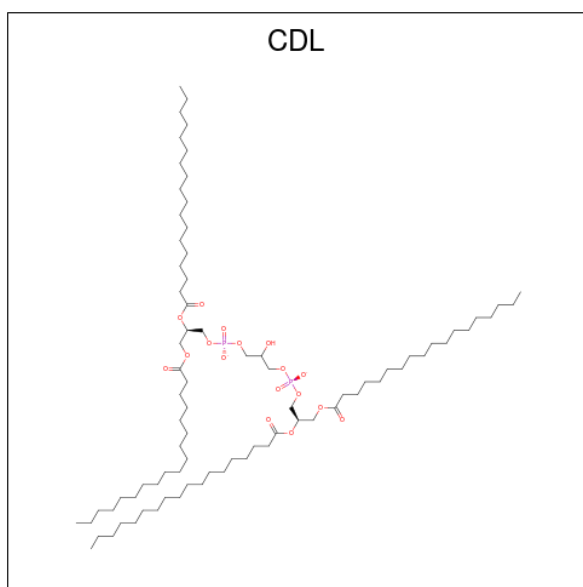
Mol	Chain	Residues	Atoms				AltConf
3	M	1	Total	C	O	P	0
			31	22	8	1	
3	M	1	Total	C	O	P	0
			33	24	8	1	
3	M	1	Total	C	O	P	0
			31	22	8	1	
3	M	1	Total	C	O	P	0
			33	24	8	1	
3	L	1	Total	C	O	P	0
			45	36	8	1	
3	L	1	Total	C	O	P	0
			29	20	8	1	

- Molecule 4 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
4	M	1	Total	C	N	O	P	0
			42	32	1	8	1	
4	M	1	Total	C	N	O	P	0
			41	31	1	8	1	
4	M	1	Total	C	N	O	P	0
			29	19	1	8	1	
4	L	1	Total	C	N	O	P	0
			45	35	1	8	1	

- Molecule 5 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).

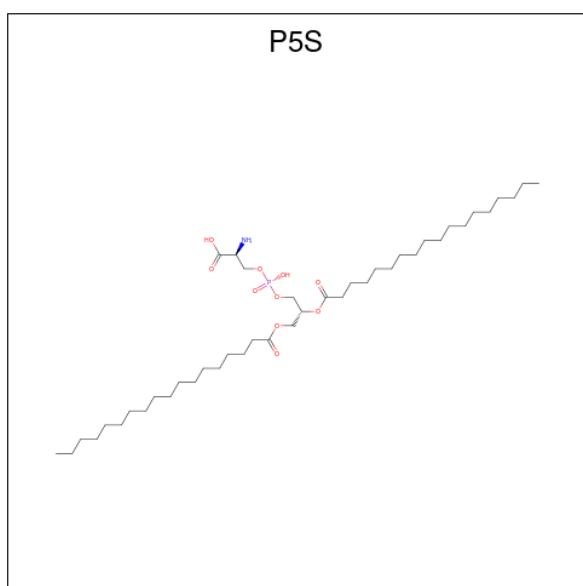


Mol	Chain	Residues	Atoms				AltConf
5	M	1	Total	C	O	P	0
			65	46	17	2	

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
6	M	1	Total	Ca	0
			1	1	

- Molecule 7 is O-[(R)-{[(2R)-2,3-bis(octadecanoyloxy)propyl]oxy}(hydroxy)phosphoryl]-L-serine (three-letter code: P5S) (formula: C₄₂H₈₂NO₁₀P).



Mol	Chain	Residues	Atoms					AltConf
7	L	1	Total	C	N	O	P	0
			40	28	1	10	1	

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		AltConf
8	M	67	Total	O	0
			67	67	
8	L	48	Total	O	0
			48	48	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	146603	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 ($e^-/\text{\AA}^2$)	40.0	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.073	Depositor
Minimum map value	-0.033	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0212	Depositor
Map size (Å)	476.8, 476.8, 476.8	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.745, 0.745, 0.745	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: P5S, CDL, 3PE, 3PH, CA

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	M	0.28	0/4018	0.46	0/5470
2	L	0.29	0/5021	0.46	0/6839
All	All	0.28	0/9039	0.46	0/12309

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

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	M	3913	0	4025	20	0
2	L	4856	0	4800	24	0
3	L	74	0	97	0	0
3	M	210	0	264	1	0
4	L	45	0	64	0	0
4	M	112	0	149	2	0
5	M	65	0	74	0	0
6	M	1	0	0	0	0
7	L	40	0	46	0	0
8	L	48	0	0	6	0
8	M	67	0	0	4	0
All	All	9431	0	9519	45	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 2.

All (45) 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)
2:L:368:GLU:O	2:L:374:TYR:OH	1.85	0.93
1:M:331:ALA:O	8:M:701:HOH:O	1.98	0.82
2:L:69:HIS:O	8:L:901:HOH:O	2.00	0.80
1:M:21:LEU:O	1:M:24:ARG:NH2	2.16	0.78
2:L:435:ALA:O	8:L:902:HOH:O	2.04	0.74
1:M:112:GLU:OE2	8:M:702:HOH:O	2.05	0.74
1:M:405:GLU:OE1	8:M:703:HOH:O	2.08	0.71
2:L:621:LYS:O	8:L:903:HOH:O	2.15	0.65
1:M:440:ARG:NH2	8:M:704:HOH:O	2.29	0.64
1:M:326:MET:HB3	1:M:412:VAL:HG21	1.82	0.61
1:M:289:PHE:HB3	1:M:419:VAL:HG21	1.86	0.57
2:L:238:LYS:NZ	8:L:908:HOH:O	2.35	0.57
2:L:268:VAL:HB	2:L:325:LEU:HD11	1.87	0.56
1:M:247:VAL:HG21	1:M:311:LYS:HG3	1.89	0.54
1:M:333:GLN:NE2	1:M:337:ASP:OD2	2.38	0.53
2:L:193:LEU:HD12	2:L:227:LEU:HD11	1.90	0.53
2:L:265:ALA:O	2:L:269:THR:OG1	2.23	0.51
4:M:607:3PE:O12	4:M:607:3PE:N	2.33	0.51
2:L:315:ARG:NH1	8:L:911:HOH:O	2.43	0.49
1:M:387:MET:SD	2:L:154:LEU:HD21	2.53	0.48
2:L:140:GLN:OE1	8:L:904:HOH:O	2.20	0.48
2:L:376:GLY:O	2:L:450:PHE:HA	2.13	0.48
1:M:184:MET:HG2	1:M:221:LEU:HD13	1.96	0.48
2:L:626:GLU:N	2:L:626:GLU:OE1	2.47	0.47
2:L:457:ASP:OD2	2:L:457:ASP:O	2.33	0.47
2:L:32:THR:O	2:L:36:LEU:HD23	2.14	0.47
1:M:292:SER:HB2	1:M:326:MET:HG3	1.96	0.46
2:L:256:THR:HG21	2:L:359:GLY:CA	2.46	0.46
1:M:366:THR:O	1:M:372:TYR:OH	2.25	0.46
4:M:607:3PE:HN2	4:M:607:3PE:P	2.39	0.45
2:L:193:LEU:HD11	2:L:214:MET:SD	2.58	0.44
2:L:256:THR:HG21	2:L:359:GLY:HA3	2.00	0.44
2:L:183:PHE:CE2	2:L:187:ILE:HD11	2.53	0.44
2:L:129:MET:SD	2:L:266:THR:O	2.76	0.44
1:M:187:MET:HE1	1:M:221:LEU:HD11	2.01	0.42
1:M:424:THR:O	1:M:427:VAL:HG22	2.20	0.42
1:M:27:ASP:OD1	1:M:27:ASP:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:20:TRP:O	2:L:24:GLY:N	2.42	0.41
2:L:98:SER:HG	2:L:118:PHE:HE2	1.68	0.41
1:M:127:VAL:HG11	1:M:264:MET:HG2	2.02	0.41
1:M:69:HIS:ND1	3:M:610:3PH:O13	2.51	0.41
1:M:337:ASP:OD1	1:M:490:VAL:HG21	2.21	0.41
2:L:595:THR:O	2:L:595:THR:HG22	2.21	0.41
2:L:191:TYR:O	2:L:195:GLY:N	2.49	0.40
1:M:152:GLY:O	1:M:159:ARG:NE	2.53	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	M	501/513 (98%)	495 (99%)	6 (1%)	0	100	100
2	L	611/703 (87%)	594 (97%)	17 (3%)	0	100	100
All	All	1112/1216 (91%)	1089 (98%)	23 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	M	411/417 (99%)	408 (99%)	3 (1%)	81	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	L	487/544 (90%)	482 (99%)	5 (1%)	73	88
All	All	898/961 (93%)	890 (99%)	8 (1%)	74	90

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	1	MET
1	M	19	MET
1	M	169	TYR
2	L	125	PHE
2	L	424	SER
2	L	458	HIS
2	L	465	HIS
2	L	605	ARG

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

Mol	Chain	Res	Type
2	L	366	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 1 is monoatomic - leaving 14 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	3PE	M	606	-	40,40,50	0.55	0	43,45,55	0.75	3 (6%)
4	3PE	L	803	-	44,44,50	0.55	0	47,49,55	0.57	1 (2%)
3	3PH	M	610	-	32,32,47	0.75	1 (3%)	36,37,52	0.71	1 (2%)
3	3PH	L	804	-	28,28,47	0.80	1 (3%)	32,33,52	0.66	0
5	CDL	M	608	-	64,64,99	0.35	0	70,76,111	0.63	1 (1%)
4	3PE	M	607	-	28,28,50	0.66	0	31,33,55	0.67	1 (3%)
7	P5S	L	802	-	38,39,53	0.62	0	42,46,60	1.07	1 (2%)
4	3PE	M	604	-	41,41,50	0.58	0	44,46,55	0.54	1 (2%)
3	3PH	M	609	-	30,30,47	0.77	1 (3%)	34,35,52	0.71	1 (2%)
3	3PH	L	801	-	44,44,47	0.64	1 (2%)	48,49,52	0.61	1 (2%)
3	3PH	M	601	-	45,45,47	0.64	1 (2%)	49,50,52	0.63	1 (2%)
3	3PH	M	605	-	32,32,47	0.75	1 (3%)	36,37,52	0.68	1 (2%)
3	3PH	M	603	-	30,30,47	0.76	1 (3%)	34,35,52	0.74	2 (5%)
3	3PH	M	602	-	35,35,47	0.73	1 (2%)	39,40,52	0.69	1 (2%)

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	3PE	M	606	-	-	20/44/44/54	-
4	3PE	L	803	-	-	12/48/48/54	-
3	3PH	M	610	-	-	11/34/34/49	-
3	3PH	L	804	-	-	13/30/30/49	-
5	CDL	M	608	-	-	36/75/75/110	-
4	3PE	M	607	-	-	12/32/32/54	-
7	P5S	L	802	-	-	19/45/45/59	-
4	3PE	M	604	-	-	23/45/45/54	-
3	3PH	M	609	-	-	15/32/32/49	-
3	3PH	L	801	-	-	13/46/46/49	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	3PH	M	601	-	-	14/47/47/49	-
3	3PH	M	605	-	-	8/34/34/49	-
3	3PH	M	603	-	-	12/32/32/49	-
3	3PH	M	602	-	-	17/37/37/49	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	602	3PH	P-O11	3.38	1.71	1.60
3	L	804	3PH	P-O11	3.30	1.70	1.60
3	M	610	3PH	P-O11	3.30	1.70	1.60
3	M	609	3PH	P-O11	3.29	1.70	1.60
3	M	605	3PH	P-O11	3.27	1.70	1.60
3	M	601	3PH	P-O11	3.24	1.70	1.60
3	L	801	3PH	P-O11	3.20	1.70	1.60
3	M	603	3PH	P-O11	3.17	1.70	1.60

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	L	802	P5S	OG-CB-CA	5.56	112.91	108.06
4	M	606	3PE	C2-O21-C21	3.26	125.81	117.79
4	M	607	3PE	O12-P-O14	2.36	123.92	112.24
4	M	604	3PE	O12-P-O14	2.36	123.89	112.24
4	L	803	3PE	O12-P-O14	2.30	123.59	112.24
3	M	602	3PH	O13-P-O11	-2.28	100.67	106.73
4	M	606	3PE	O12-P-O14	2.27	123.47	112.24
3	M	601	3PH	O13-P-O11	-2.27	100.70	106.73
3	M	605	3PH	O13-P-O11	-2.20	100.88	106.73
3	M	609	3PH	O13-P-O11	-2.18	100.93	106.73
3	M	603	3PH	O13-P-O11	-2.16	100.98	106.73
3	M	603	3PH	C3-C2-C1	2.14	116.86	111.79
3	M	610	3PH	O13-P-O11	-2.14	101.04	106.73
3	L	801	3PH	O13-P-O11	-2.03	101.33	106.73
5	M	608	CDL	CB2-C1-CA2	-2.03	106.82	112.79
4	M	606	3PE	O21-C2-C1	2.02	115.73	108.40

There are no chirality outliers.

All (225) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	M	601	3PH	C2-C1-O11-P
3	M	601	3PH	O21-C2-C3-O31
3	M	602	3PH	C1-O11-P-O13
3	M	602	3PH	C1-O11-P-O12
3	M	610	3PH	C1-O11-P-O13
3	M	610	3PH	C1-O11-P-O14
3	M	610	3PH	C1-O11-P-O12
3	L	804	3PH	C1-O11-P-O13
3	L	804	3PH	C1-O11-P-O14
3	L	804	3PH	C1-O11-P-O12
4	M	604	3PE	C1-O11-P-O12
4	M	606	3PE	C11-O13-P-O12
4	M	606	3PE	C11-O13-P-O14
4	M	606	3PE	O13-C11-C12-N
4	M	606	3PE	C22-C21-O21-C2
5	M	608	CDL	O1-C1-CA2-OA2
5	M	608	CDL	CA3-OA5-PA1-OA3
5	M	608	CDL	CA3-OA5-PA1-OA4
5	M	608	CDL	CA4-CA3-OA5-PA1
5	M	608	CDL	CB3-OB5-PB2-OB4
7	L	802	P5S	C-CA-CB-OG
7	L	802	P5S	N-CA-CB-OG
7	L	802	P5S	CB-OG-P12-O15
4	M	604	3PE	O32-C31-O31-C3
3	L	804	3PH	O32-C31-O31-C3
4	M	606	3PE	O32-C31-O31-C3
5	M	608	CDL	OA9-CA7-OA8-CA6
4	M	606	3PE	O22-C21-O21-C2
4	M	604	3PE	C32-C31-O31-C3
5	M	608	CDL	C31-CA7-OA8-CA6
3	L	804	3PH	C32-C31-O31-C3
4	M	606	3PE	C32-C31-O31-C3
3	M	603	3PH	O32-C31-O31-C3
3	M	603	3PH	C32-C31-O31-C3
3	M	610	3PH	C32-C31-O31-C3
3	L	804	3PH	C22-C21-O21-C2
4	M	604	3PE	C22-C21-O21-C2
3	M	610	3PH	O32-C31-O31-C3
5	M	608	CDL	CB2-C1-CA2-OA2
5	M	608	CDL	CA2-C1-CB2-OB2
4	M	604	3PE	O22-C21-O21-C2
3	L	801	3PH	C32-C31-O31-C3
3	M	603	3PH	O21-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
5	M	608	CDL	C36-C37-C38-C39
3	L	804	3PH	O22-C21-O21-C2
3	M	609	3PH	C2-C1-O11-P
4	M	604	3PE	C31-C32-C33-C34
4	M	607	3PE	C31-C32-C33-C34
3	M	602	3PH	C22-C21-O21-C2
3	L	801	3PH	O32-C31-O31-C3
4	M	604	3PE	C1-O11-P-O13
4	M	606	3PE	C11-O13-P-O11
5	M	608	CDL	CA3-OA5-PA1-OA2
5	M	608	CDL	CB3-OB5-PB2-OB2
7	L	802	P5S	CB-OG-P12-O16
7	L	802	P5S	C3-O16-P12-OG
3	M	602	3PH	O22-C21-O21-C2
5	M	608	CDL	C11-CA5-OA6-CA4
4	M	604	3PE	C25-C26-C27-C28
5	M	608	CDL	OA7-CA5-OA6-CA4
5	M	608	CDL	C11-C12-C13-C14
3	M	609	3PH	C26-C27-C28-C29
7	L	802	P5S	C23-C24-C25-C26
3	M	603	3PH	C34-C35-C36-C37
3	M	603	3PH	C37-C38-C39-C3A
3	M	601	3PH	C27-C28-C29-C2A
4	L	803	3PE	C22-C23-C24-C25
4	L	803	3PE	C26-C27-C28-C29
4	L	803	3PE	C34-C35-C36-C37
5	M	608	CDL	C13-C14-C15-C16
3	M	609	3PH	C32-C31-O31-C3
5	M	608	CDL	C55-C56-C57-C58
7	L	802	P5S	C25-C26-C27-C28
4	M	606	3PE	C27-C28-C29-C2A
5	M	608	CDL	C33-C34-C35-C36
7	L	802	P5S	C40-C41-C42-C43
3	L	804	3PH	C24-C25-C26-C27
3	M	610	3PH	C25-C26-C27-C28
4	M	606	3PE	C36-C37-C38-C39
3	M	609	3PH	O32-C31-O31-C3
4	M	606	3PE	C37-C38-C39-C3A
3	M	602	3PH	C32-C31-O31-C3
7	L	802	P5S	C20-C17-O19-C1
4	M	604	3PE	C24-C25-C26-C27
3	L	801	3PH	C3D-C3E-C3F-C3G

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Mol	Chain	Res	Type	Atoms
5	M	608	CDL	C51-CB5-OB6-CB4
4	M	604	3PE	O11-C1-C2-O21
5	M	608	CDL	OB7-CB5-OB6-CB4
3	M	610	3PH	C37-C38-C39-C3A
4	L	803	3PE	C27-C28-C29-C2A
5	M	608	CDL	C54-C55-C56-C57
3	M	601	3PH	O11-C1-C2-C3
4	M	606	3PE	O11-C1-C2-C3
4	M	604	3PE	C2-C3-O31-C31
3	M	602	3PH	O32-C31-O31-C3
3	M	601	3PH	C1-C2-C3-O31
3	L	804	3PH	C1-C2-C3-O31
5	M	608	CDL	C14-C15-C16-C17
3	M	601	3PH	C21-C22-C23-C24
3	M	609	3PH	C28-C29-C2A-C2B
5	M	608	CDL	CB7-C71-C72-C73
4	M	606	3PE	C1-C2-O21-C21
5	M	608	CDL	CA6-CA4-OA6-CA5
3	L	801	3PH	C2C-C2D-C2E-C2F
3	M	609	3PH	O21-C2-C3-O31
7	L	802	P5S	O18-C17-O19-C1
5	M	608	CDL	CA7-C31-C32-C33
4	M	604	3PE	C33-C34-C35-C36
3	M	603	3PH	O11-C1-C2-C3
5	M	608	CDL	OA5-CA3-CA4-CA6
7	L	802	P5S	C1-C2-C3-O16
4	M	606	3PE	C29-C2A-C2B-C2C
4	M	607	3PE	C32-C31-O31-C3
3	L	804	3PH	C2-C1-O11-P
4	M	604	3PE	C2C-C2D-C2E-C2F
3	M	602	3PH	C24-C25-C26-C27
3	M	605	3PH	C32-C31-O31-C3
3	M	603	3PH	C1-C2-C3-O31
3	L	801	3PH	C1-C2-C3-O31
4	M	607	3PE	C1-C2-C3-O31
3	M	609	3PH	C29-C2A-C2B-C2C
3	M	601	3PH	C34-C35-C36-C37
3	M	601	3PH	O11-C1-C2-O21
3	M	609	3PH	O11-C1-C2-O21
5	M	608	CDL	OA5-CA3-CA4-OA6
7	L	802	P5S	O37-C2-C3-O16
4	M	604	3PE	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
7	L	802	P5S	C42-C43-C44-C45
3	M	610	3PH	C2-C1-O11-P
4	M	606	3PE	C2-C1-O11-P
3	M	605	3PH	C21-C22-C23-C24
3	L	801	3PH	O11-C1-C2-C3
3	M	601	3PH	C25-C26-C27-C28
3	M	609	3PH	C1-O11-P-O13
7	L	802	P5S	C22-C23-C24-C25
3	M	602	3PH	C29-C2A-C2B-C2C
5	M	608	CDL	C71-CB7-OB8-CB6
3	M	602	3PH	C32-C33-C34-C35
3	M	603	3PH	C2-C1-O11-P
3	M	609	3PH	C1-C2-C3-O31
3	M	603	3PH	O11-C1-C2-O21
3	M	610	3PH	C33-C34-C35-C36
5	M	608	CDL	O1-C1-CB2-OB2
3	M	605	3PH	O32-C31-O31-C3
4	M	607	3PE	O32-C31-O31-C3
3	L	804	3PH	C22-C23-C24-C25
4	M	607	3PE	O21-C2-C3-O31
4	M	604	3PE	C28-C29-C2A-C2B
4	L	803	3PE	C33-C34-C35-C36
4	M	606	3PE	C1-O11-P-O13
4	M	607	3PE	C1-O11-P-O13
3	M	610	3PH	C34-C35-C36-C37
3	M	602	3PH	C2-C1-O11-P
5	M	608	CDL	OB9-CB7-OB8-CB6
7	L	802	P5S	C3-O16-P12-O13
7	L	802	P5S	C3-O16-P12-O15
3	M	602	3PH	O11-C1-C2-C3
4	M	604	3PE	O11-C1-C2-C3
4	M	604	3PE	C12-C11-O13-P
3	M	603	3PH	O31-C31-C32-C33
3	L	801	3PH	O11-C1-C2-O21
4	M	606	3PE	O11-C1-C2-O21
3	L	801	3PH	O21-C2-C3-O31
3	L	804	3PH	O21-C2-C3-O31
3	M	605	3PH	C24-C25-C26-C27
4	M	604	3PE	C23-C24-C25-C26
5	M	608	CDL	C38-C39-C40-C41
3	L	801	3PH	C39-C3A-C3B-C3C
3	M	609	3PH	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
4	L	803	3PE	C39-C3A-C3B-C3C
3	M	609	3PH	O11-C1-C2-C3
3	M	601	3PH	C1-O11-P-O12
3	M	602	3PH	O11-C1-C2-O21
4	L	803	3PE	C25-C26-C27-C28
4	M	607	3PE	C11-O13-P-O11
5	M	608	CDL	CA2-OA2-PA1-OA5
4	M	606	3PE	C22-C23-C24-C25
7	L	802	P5S	C2-C3-O16-P12
5	M	608	CDL	C34-C35-C36-C37
5	M	608	CDL	C32-C33-C34-C35
3	M	609	3PH	C22-C23-C24-C25
3	L	801	3PH	C23-C24-C25-C26
3	M	602	3PH	O21-C2-C3-O31
4	M	607	3PE	C33-C34-C35-C36
3	M	602	3PH	C2E-C2F-C2G-C2H
3	M	605	3PH	C23-C24-C25-C26
3	M	605	3PH	C37-C38-C39-C3A
7	L	802	P5S	C38-C39-C40-C41
4	M	606	3PE	C28-C29-C2A-C2B
3	M	601	3PH	C38-C39-C3A-C3B
3	L	801	3PH	C32-C33-C34-C35
4	M	606	3PE	C23-C24-C25-C26
4	L	803	3PE	C32-C31-O31-C3
4	L	803	3PE	O32-C31-O31-C3
4	L	803	3PE	O31-C31-C32-C33
3	L	801	3PH	C3C-C3D-C3E-C3F
4	L	803	3PE	O13-C11-C12-N
3	M	602	3PH	C1-O11-P-O14
4	M	604	3PE	C35-C36-C37-C38
3	M	603	3PH	O22-C21-O21-C2
4	M	604	3PE	C2D-C2E-C2F-C2G
3	M	601	3PH	C36-C37-C38-C39
3	M	602	3PH	C2D-C2E-C2F-C2G
3	M	609	3PH	O31-C31-C32-C33
3	M	602	3PH	C22-C23-C24-C25
3	L	801	3PH	C36-C37-C38-C39
4	M	604	3PE	O31-C31-C32-C33
3	M	610	3PH	C38-C39-C3A-C3B
4	M	604	3PE	C27-C28-C29-C2A
5	M	608	CDL	C35-C36-C37-C38
4	M	607	3PE	C11-O13-P-O14

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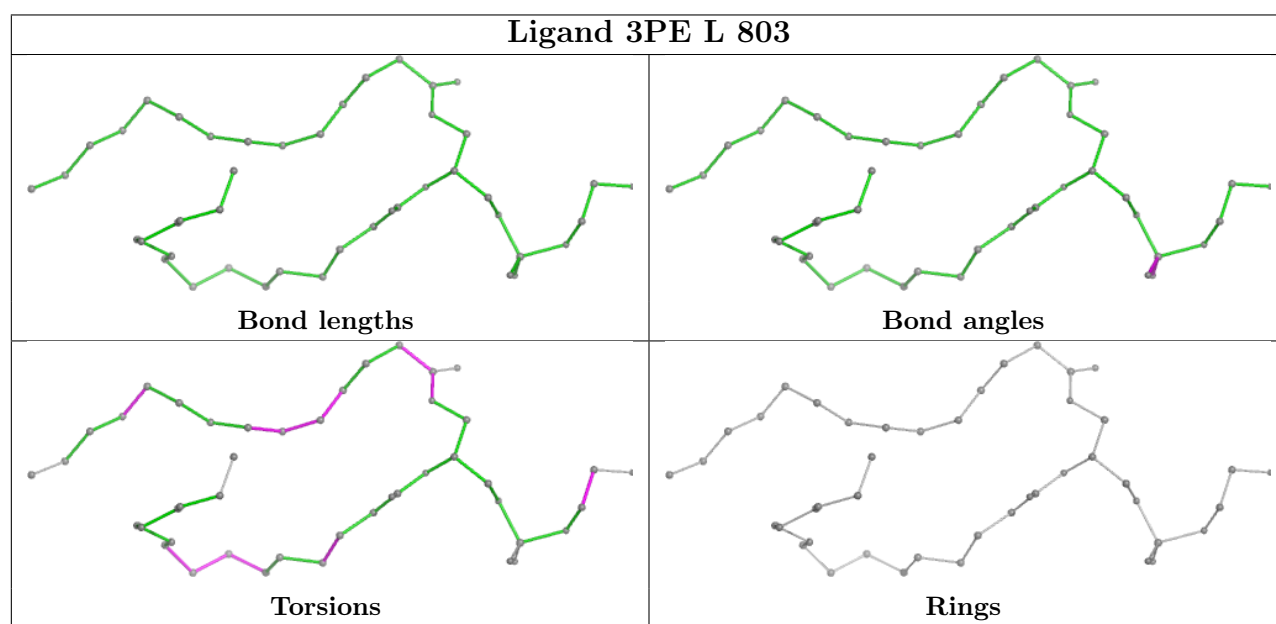
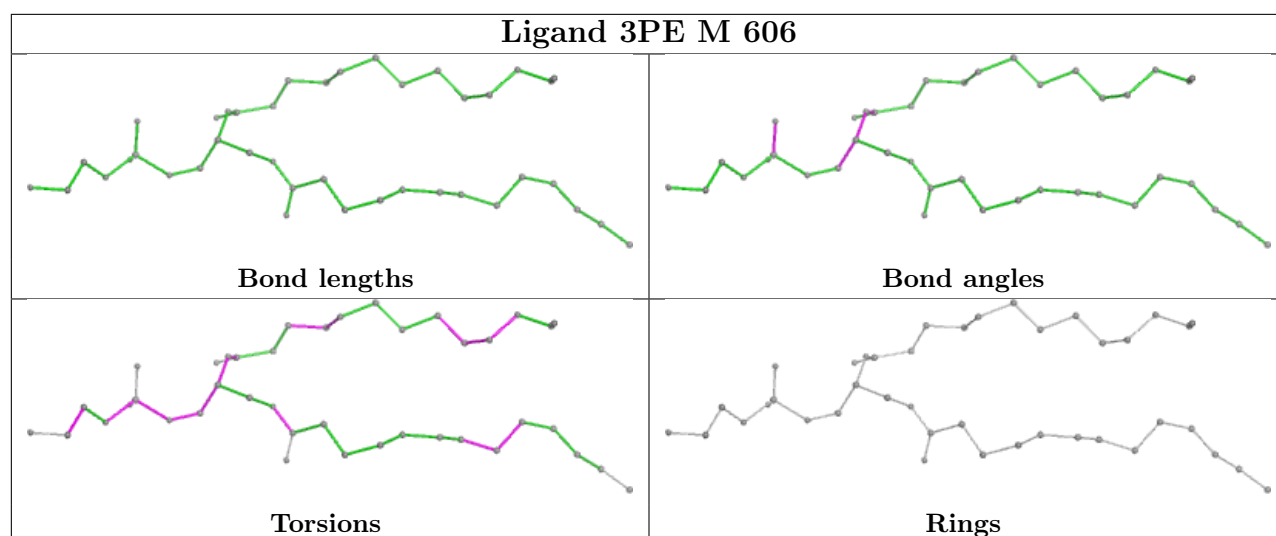
Mol	Chain	Res	Type	Atoms
5	M	608	CDL	CA2-OA2-PA1-OA3
4	M	604	3PE	O32-C31-C32-C33
3	M	605	3PH	C22-C23-C24-C25
3	L	804	3PH	C34-C35-C36-C37
3	M	603	3PH	C22-C21-O21-C2
4	M	607	3PE	C12-C11-O13-P
4	L	803	3PE	C35-C36-C37-C38
3	M	609	3PH	O32-C31-C32-C33
3	M	601	3PH	O31-C31-C32-C33
3	M	605	3PH	O21-C21-C22-C23
4	M	607	3PE	O31-C31-C32-C33
7	L	802	P5S	O19-C17-C20-C21
4	M	607	3PE	O32-C31-C32-C33
3	M	601	3PH	O32-C31-C32-C33

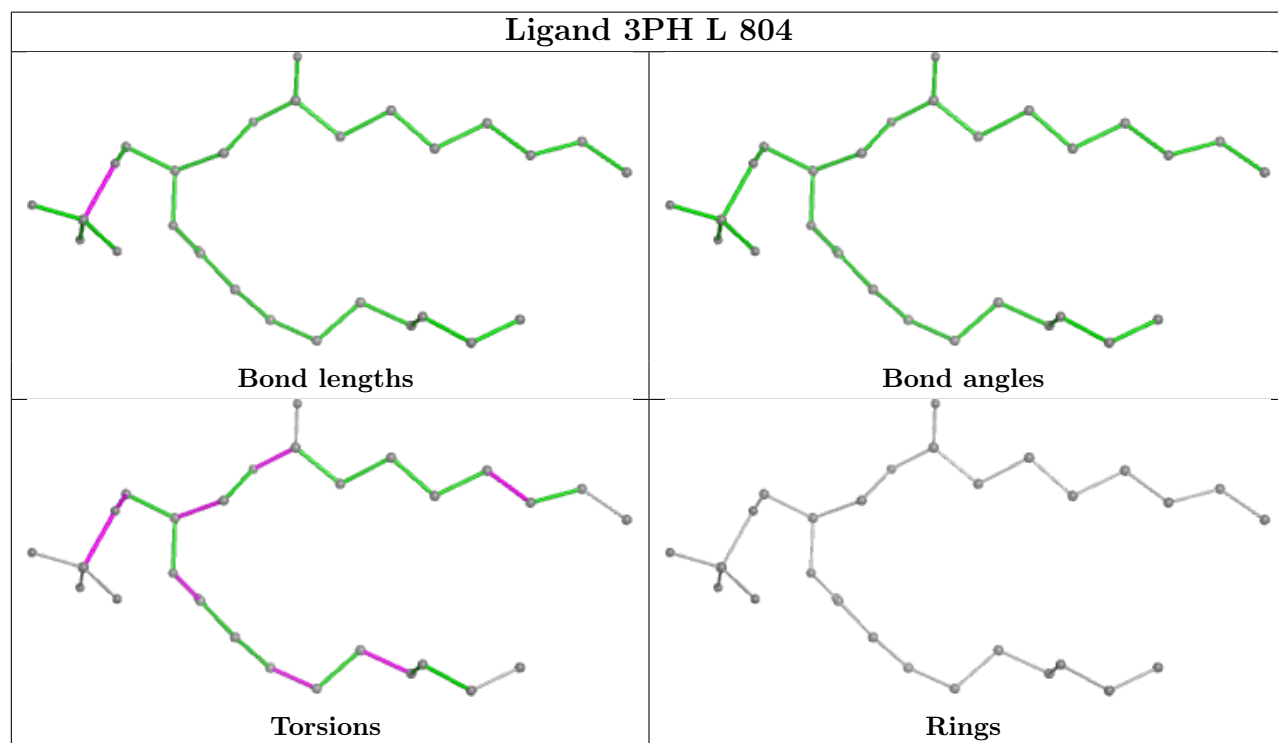
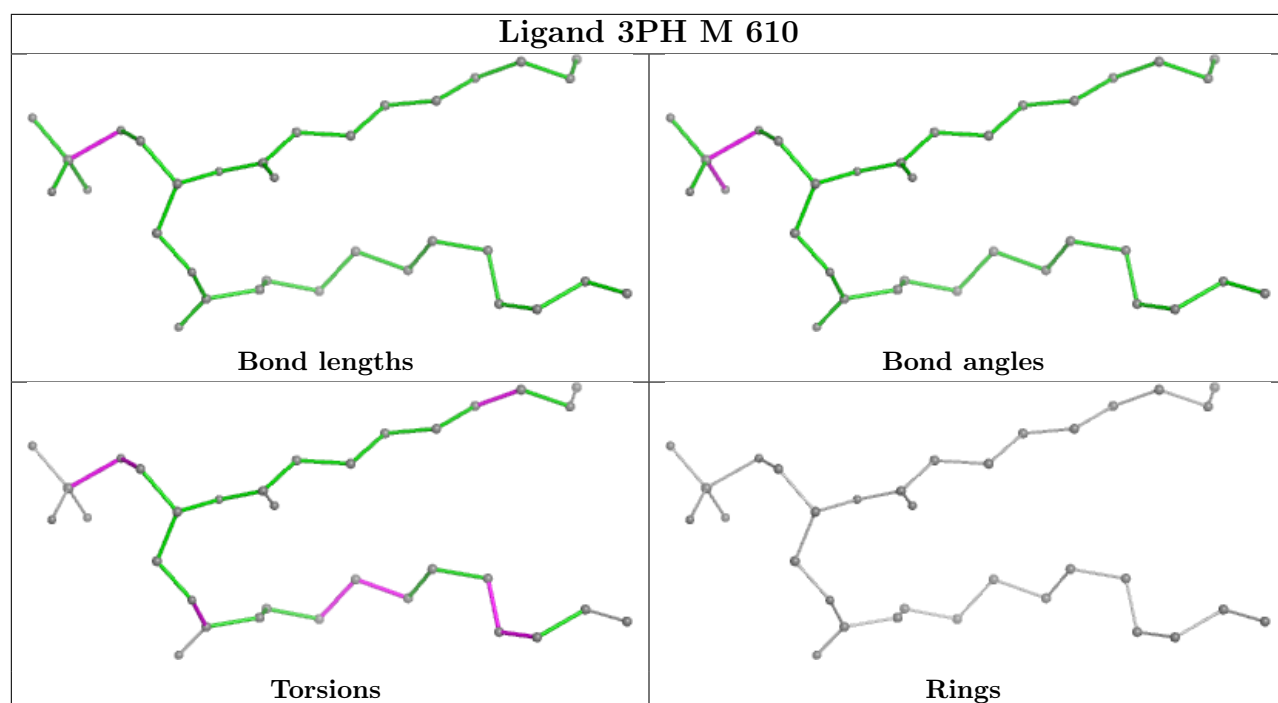
There are no ring outliers.

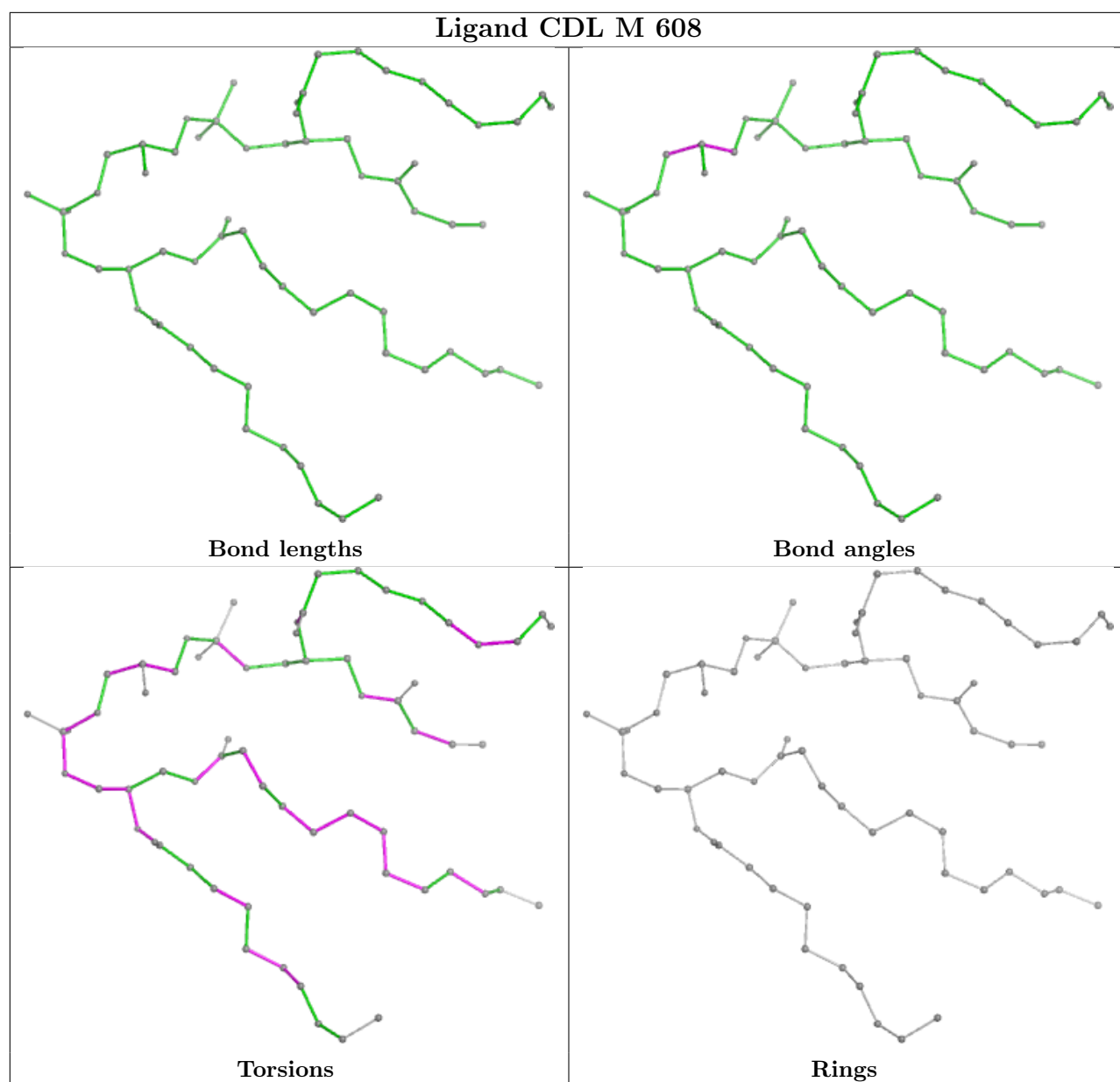
2 monomers are involved in 3 short contacts:

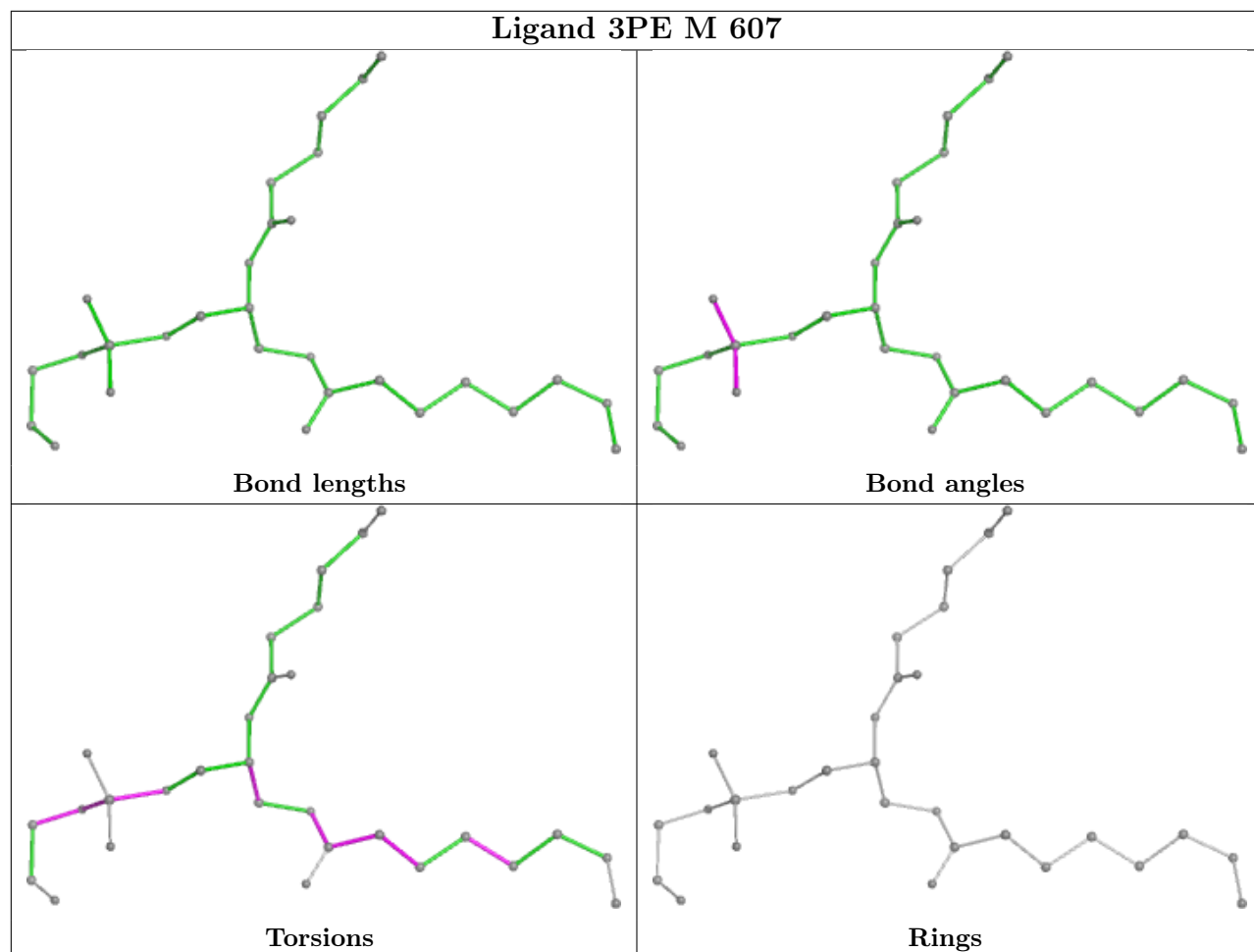
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	M	610	3PH	1	0
4	M	607	3PE	2	0

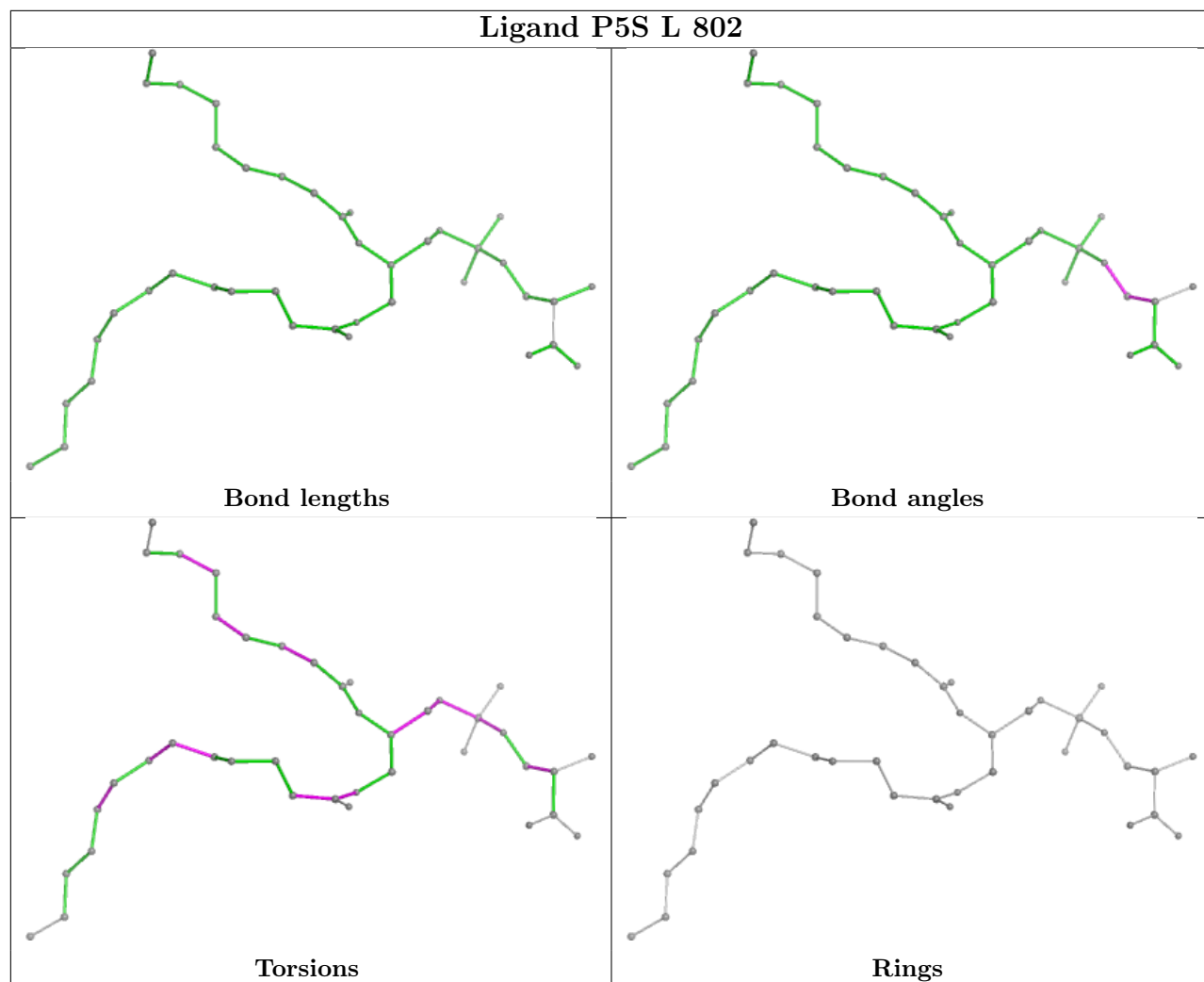
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

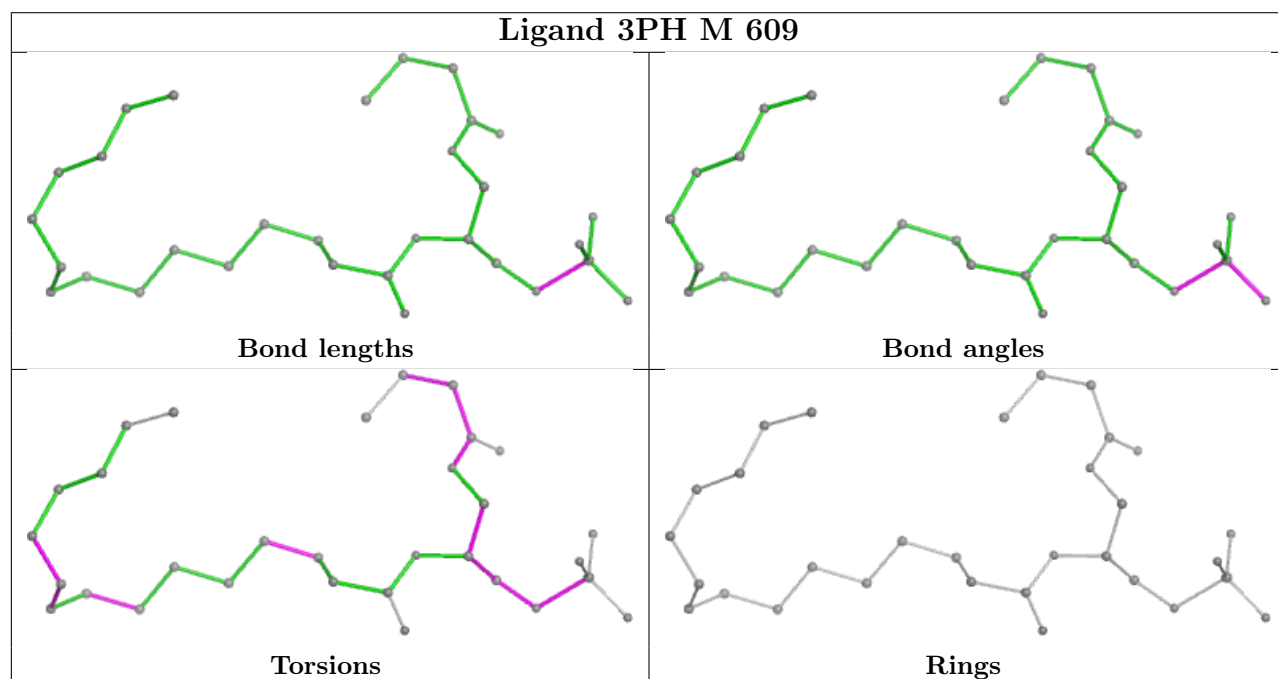
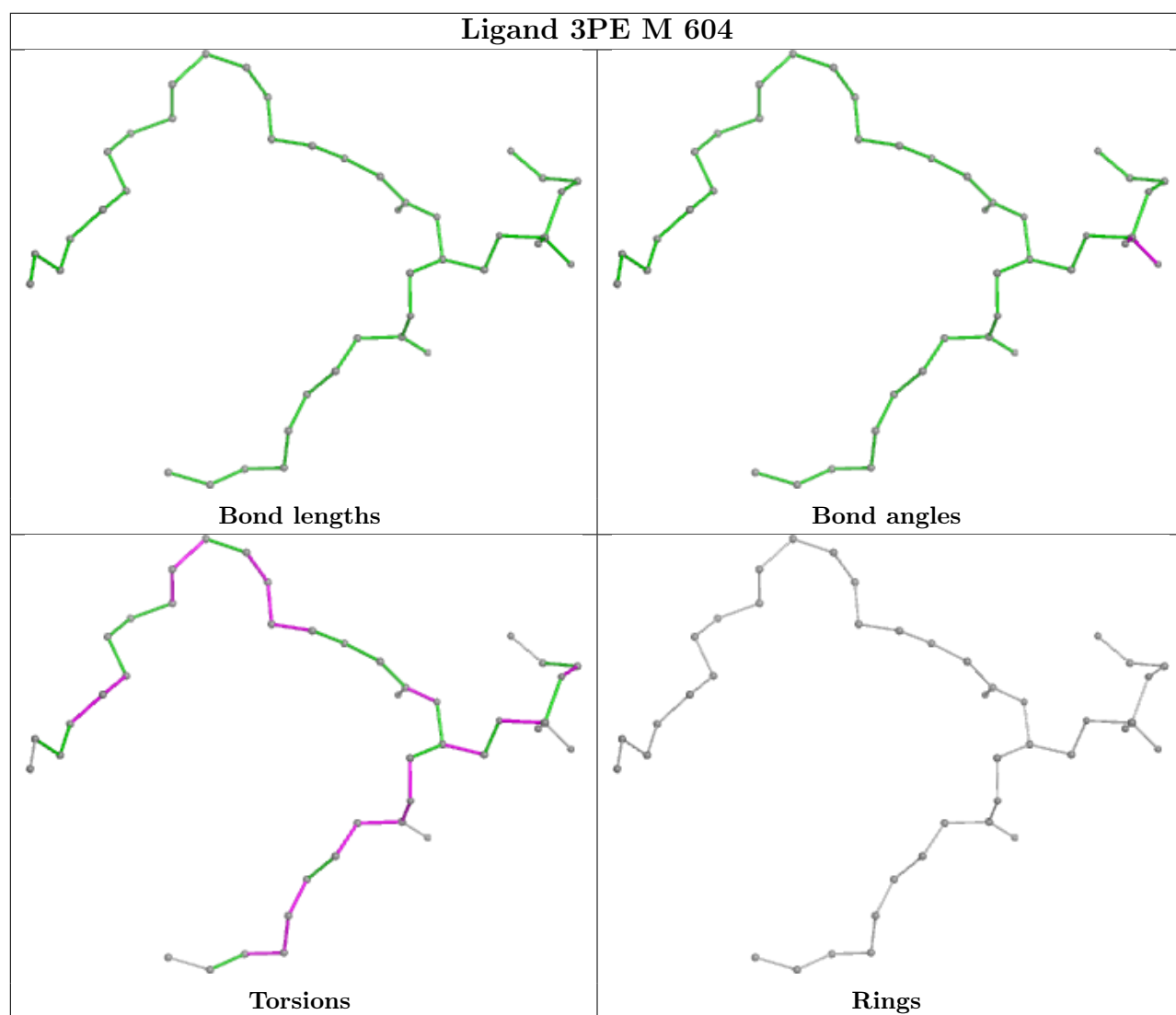


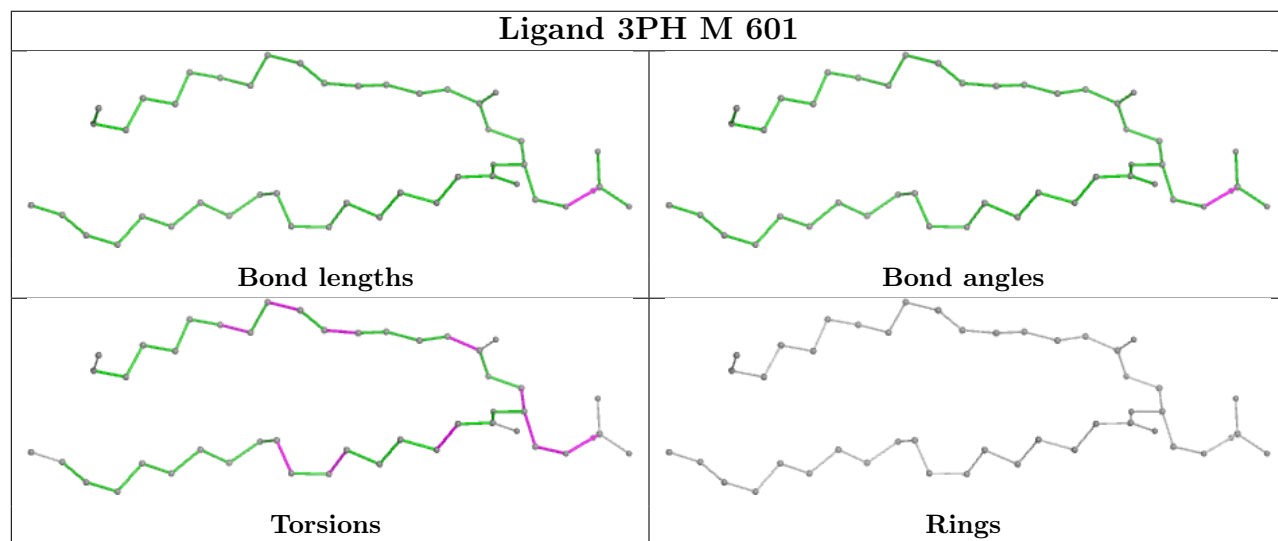
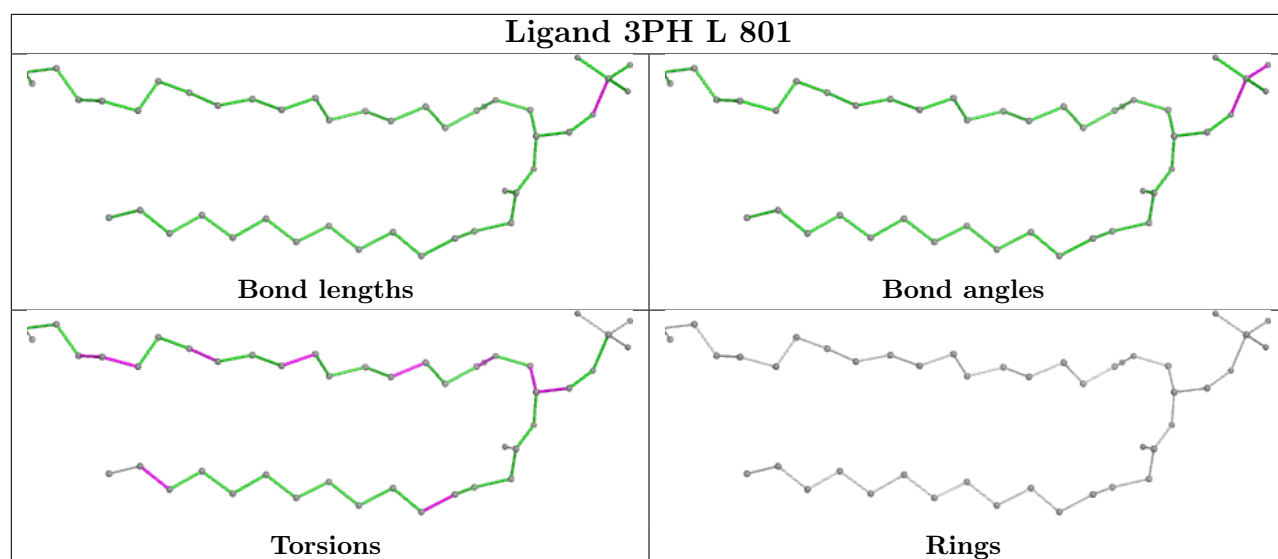


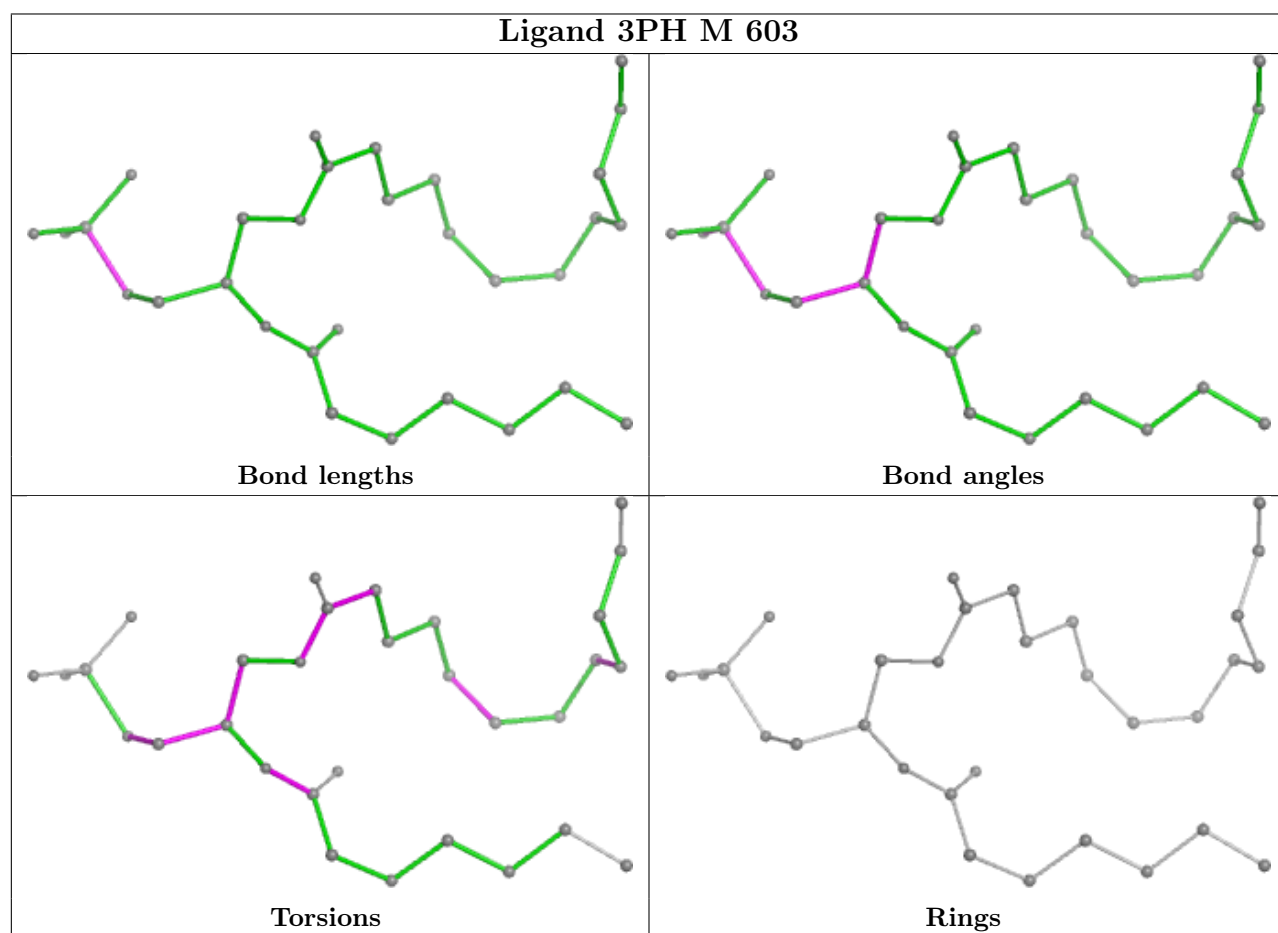
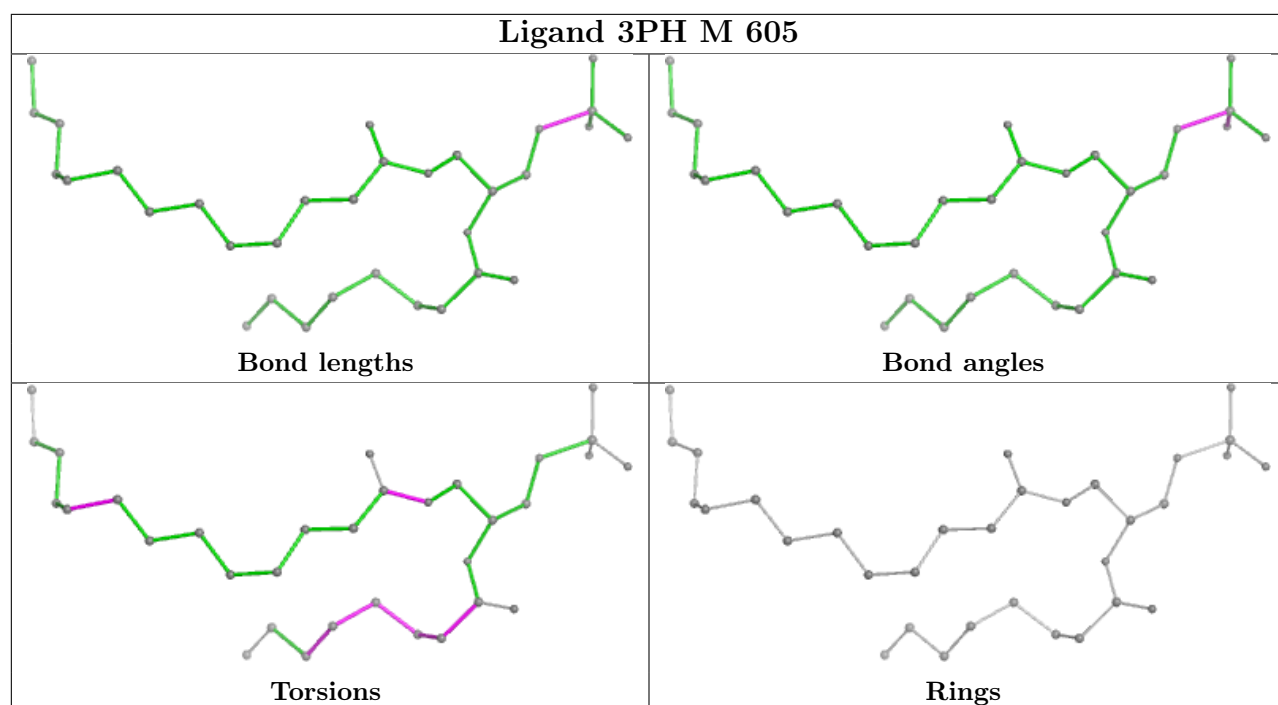


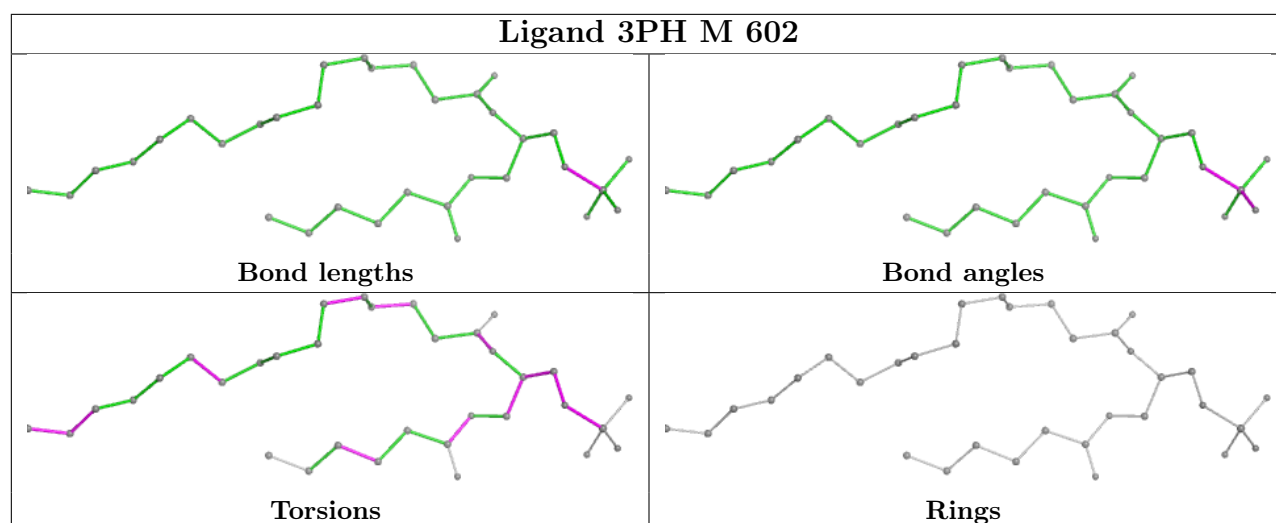












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

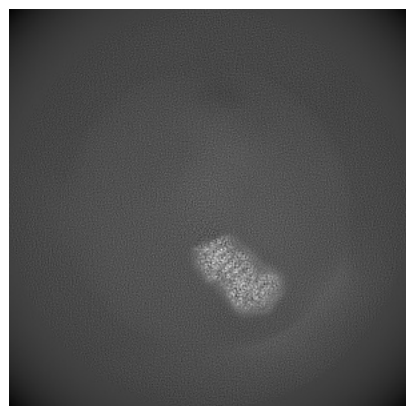
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18325. These allow visual inspection of the internal detail of the map and identification of artifacts.

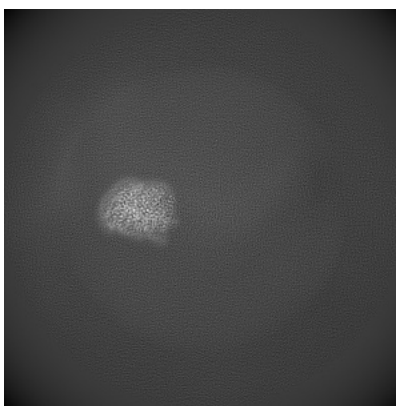
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

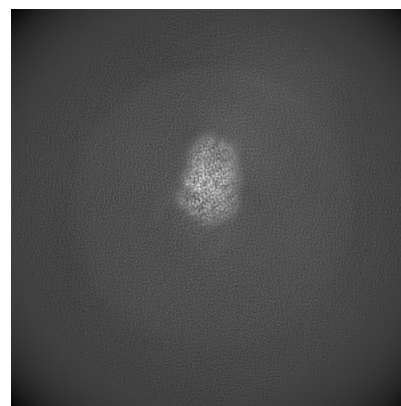
6.1.1 Primary map



X



Y

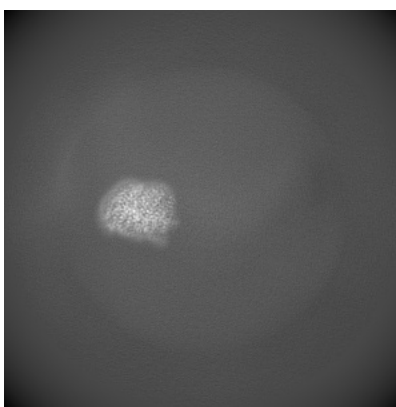


Z

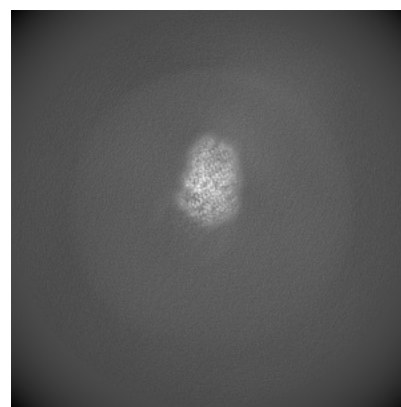
6.1.2 Raw map



X



Y

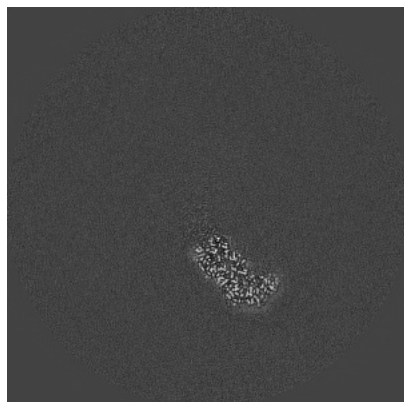


Z

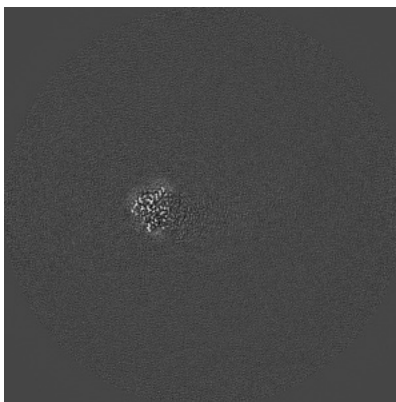
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

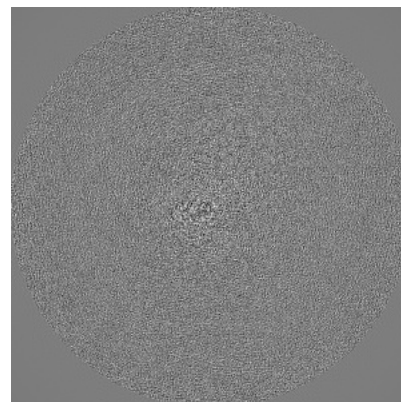
6.2.1 Primary map



X Index: 320

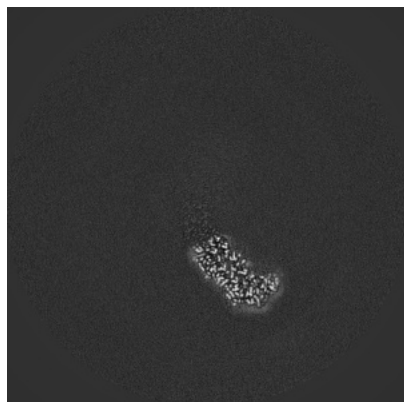


Y Index: 320

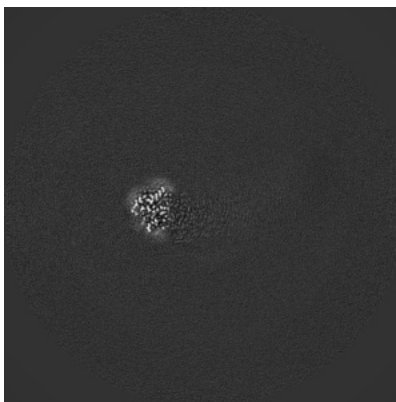


Z Index: 320

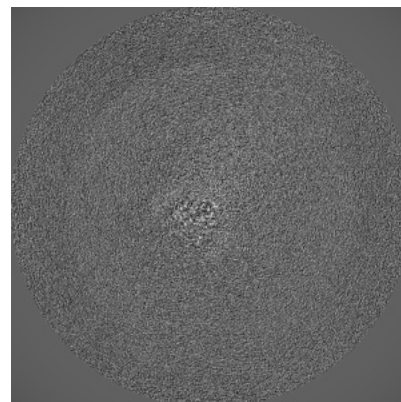
6.2.2 Raw map



X Index: 320



Y Index: 320

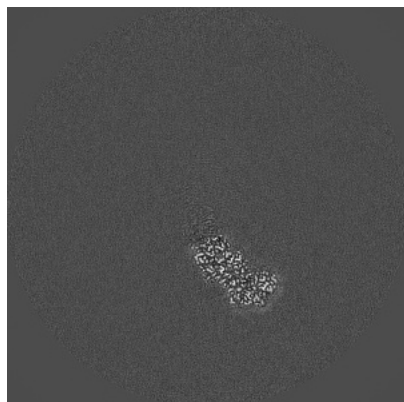


Z Index: 320

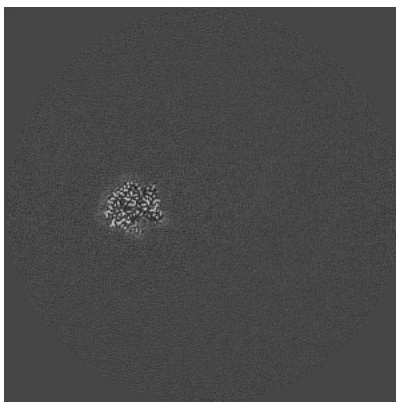
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

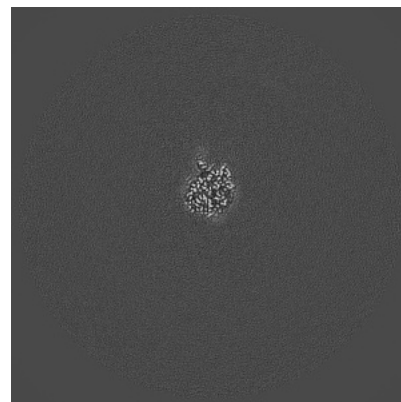
6.3.1 Primary map



X Index: 315

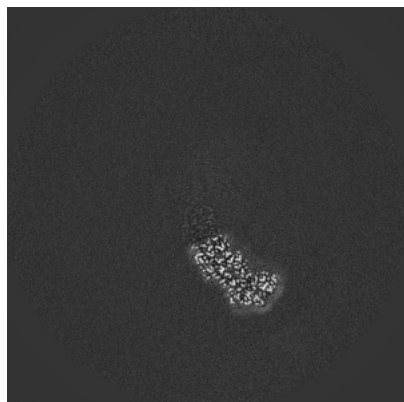


Y Index: 372

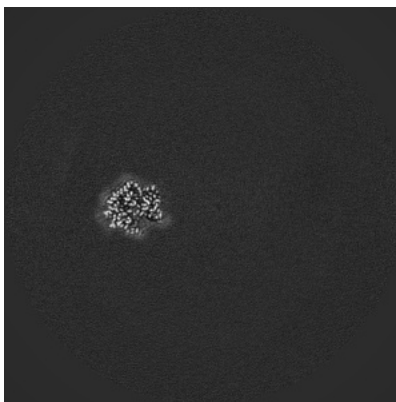


Z Index: 229

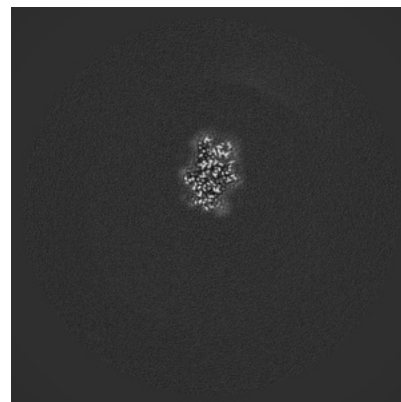
6.3.2 Raw map



X Index: 315



Y Index: 371

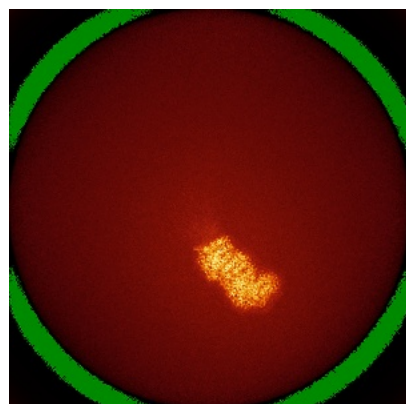


Z Index: 209

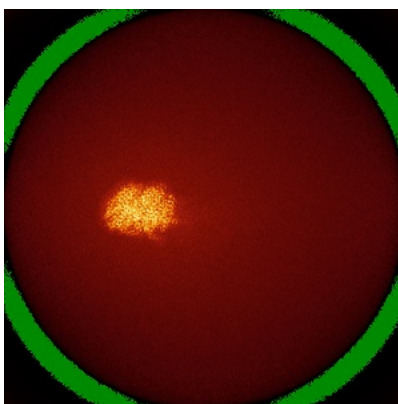
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

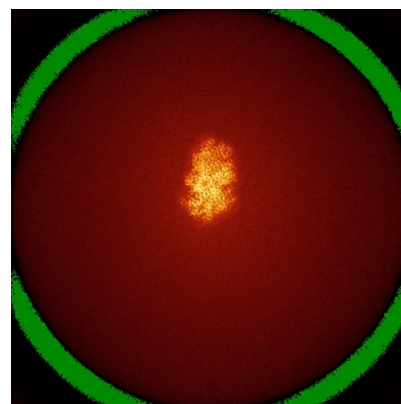
6.4.1 Primary map



X



Y

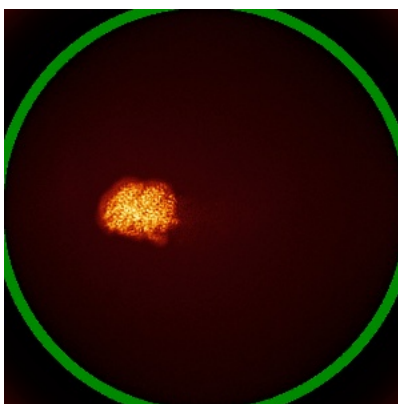


Z

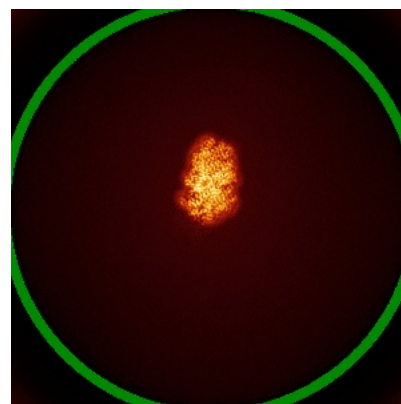
6.4.2 Raw map



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



X



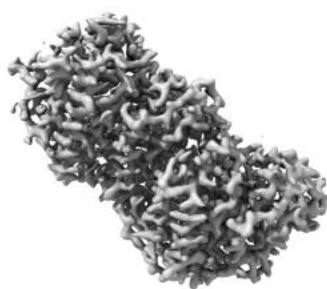
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0212. 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



X



Y



Z

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.

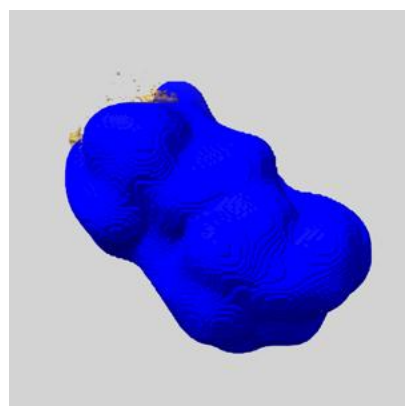
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

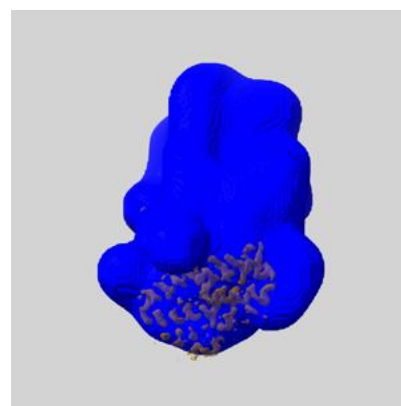
6.6.1 emd_18325_msk_1.map [i](#)



X



Y

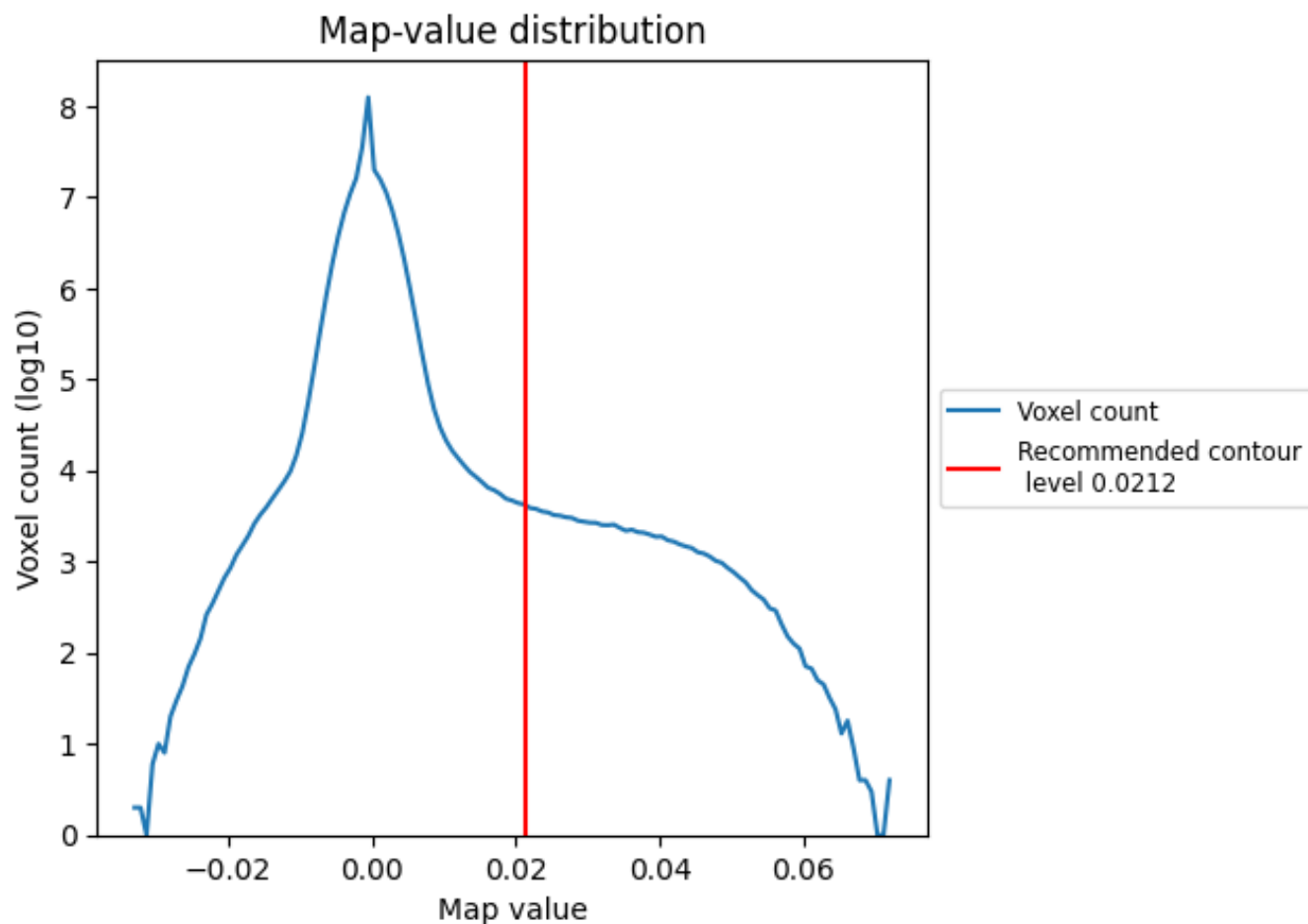


Z

7 Map analysis [i](#)

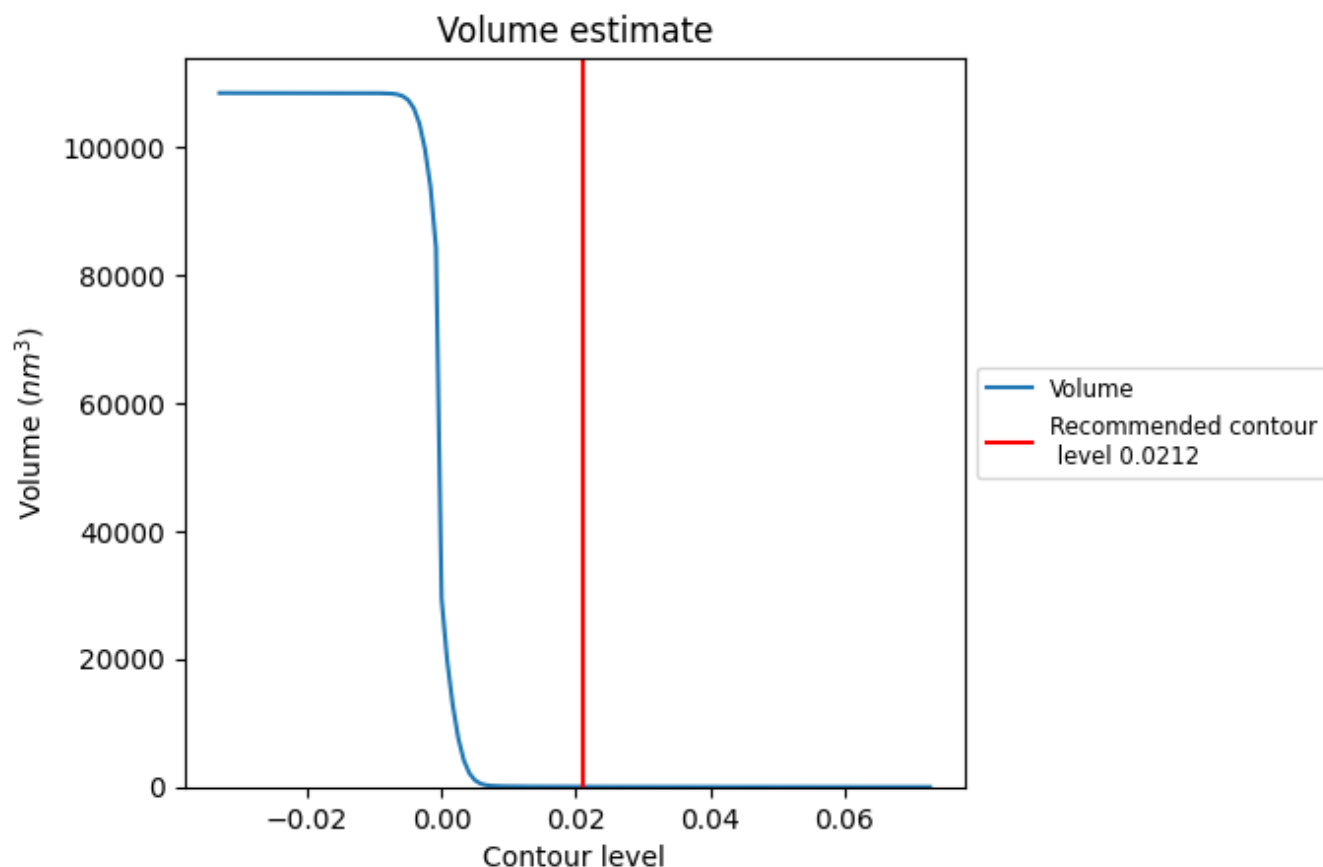
This section contains the results of statistical analysis of the map.

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.

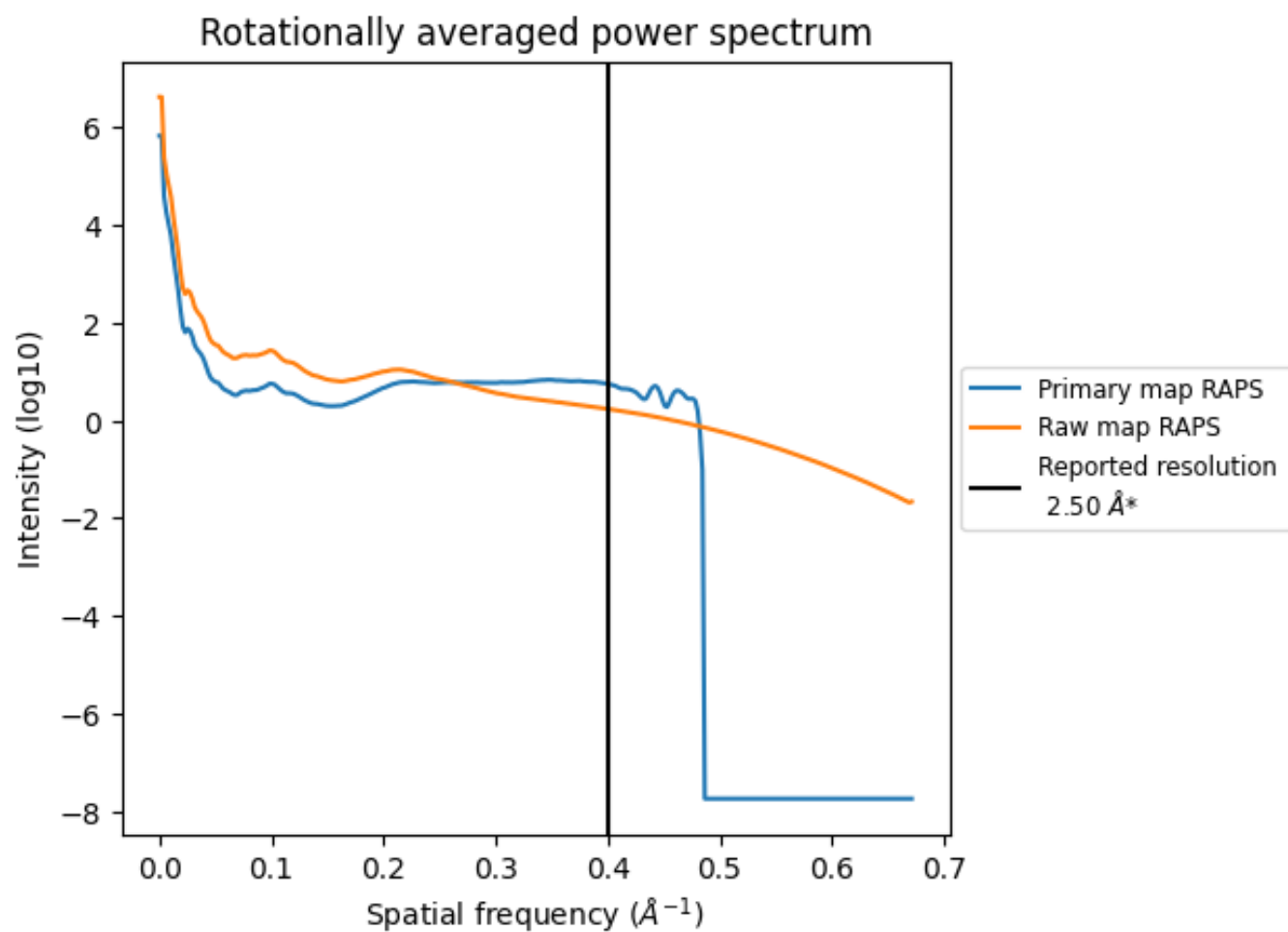
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 35 nm^3 ; this corresponds to an approximate mass of 32 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

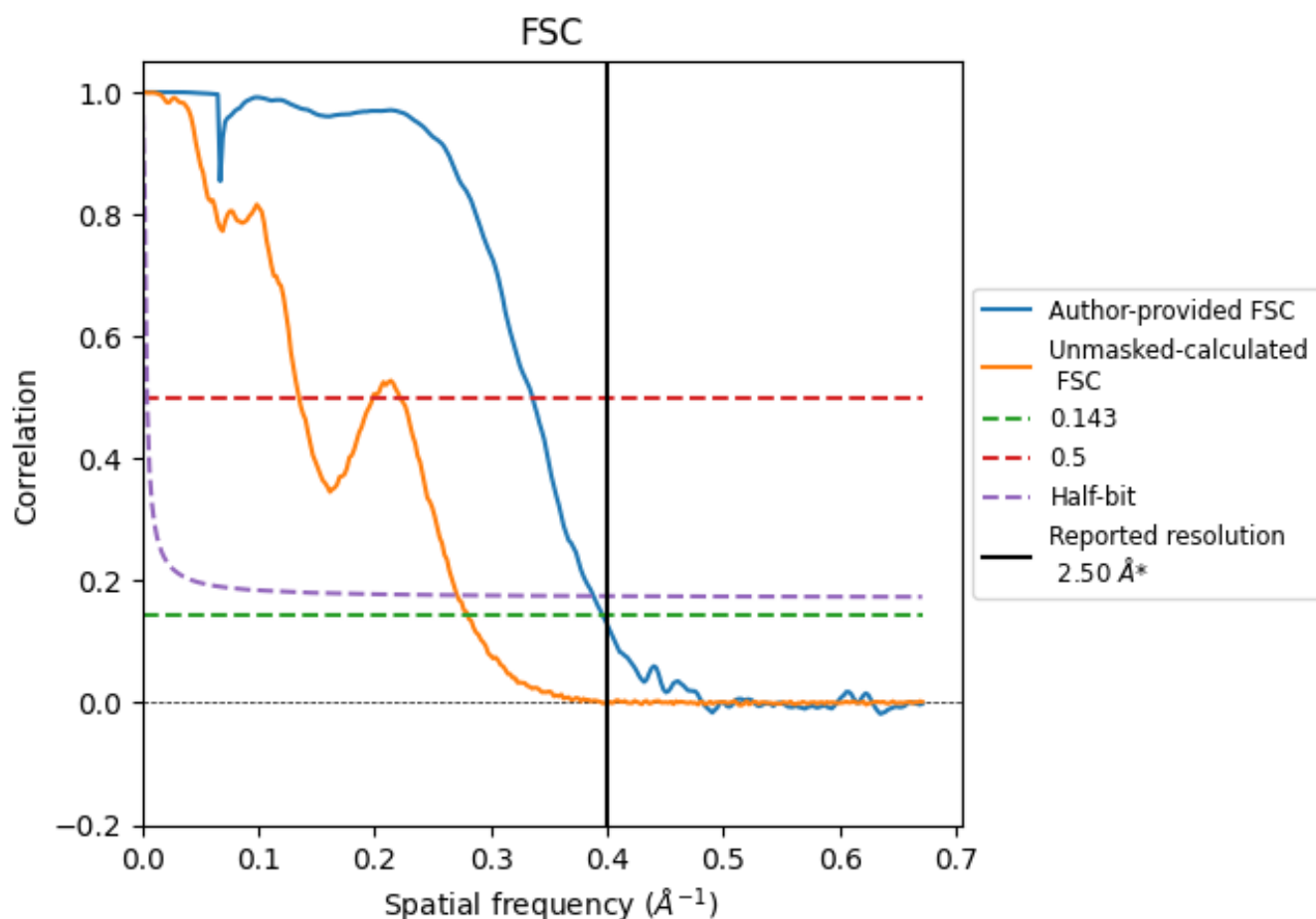


*Reported resolution corresponds to spatial frequency of 0.400 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.400 \AA^{-1}

8.2 Resolution estimates [i](#)

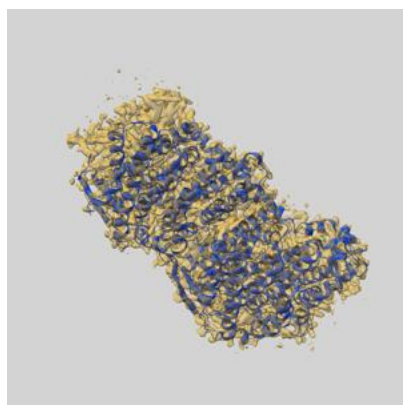
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.50	-	-
Author-provided FSC curve	2.52	2.98	2.58
Unmasked-calculated*	3.57	7.41	3.69

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.57 differs from the reported value 2.5 by more than 10 %

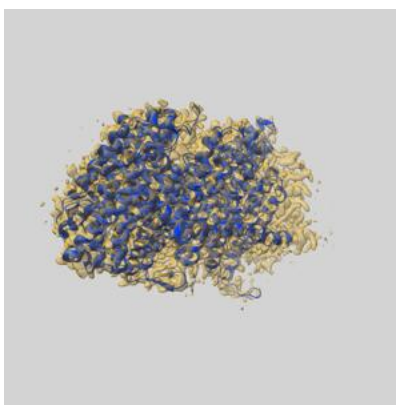
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-18325 and PDB model 8QC1. Per-residue inclusion information can be found in section [3](#) on page [7](#).

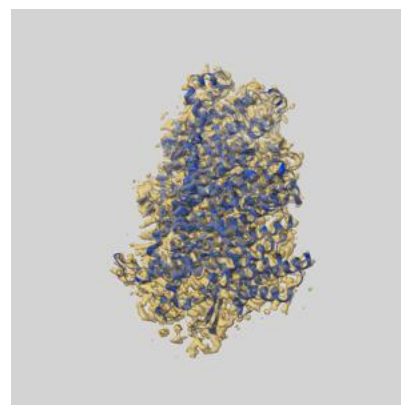
9.1 Map-model overlay [i](#)



X



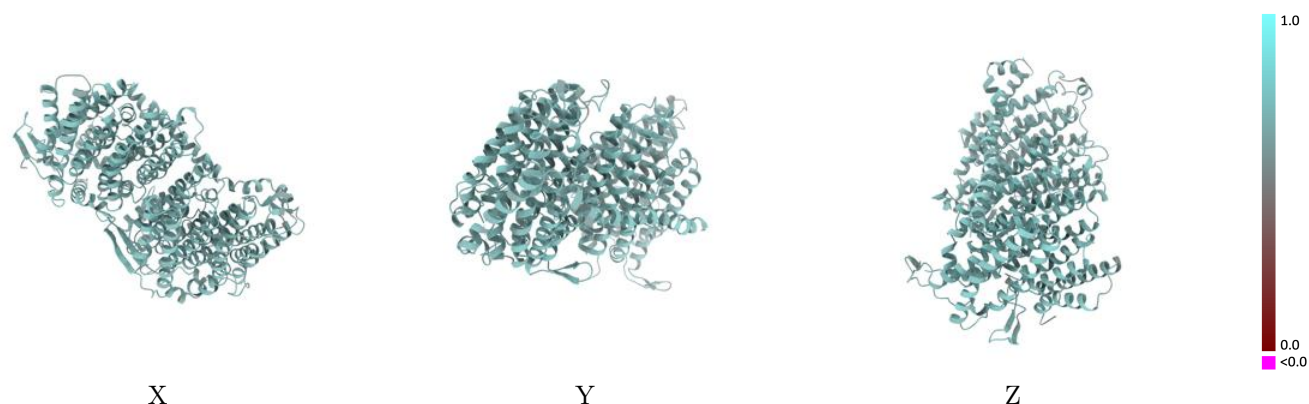
Y



Z

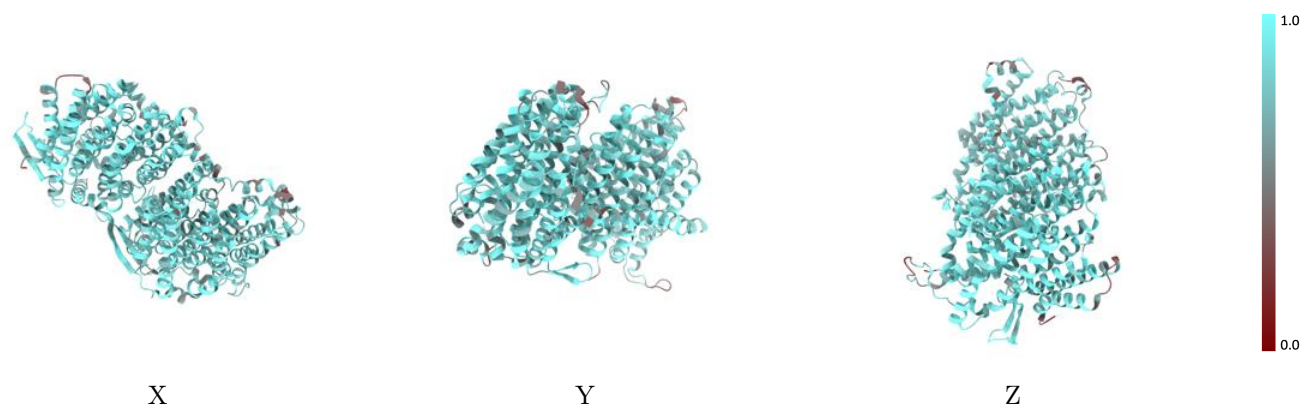
The images above show the 3D surface view of the map at the recommended contour level 0.0212 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



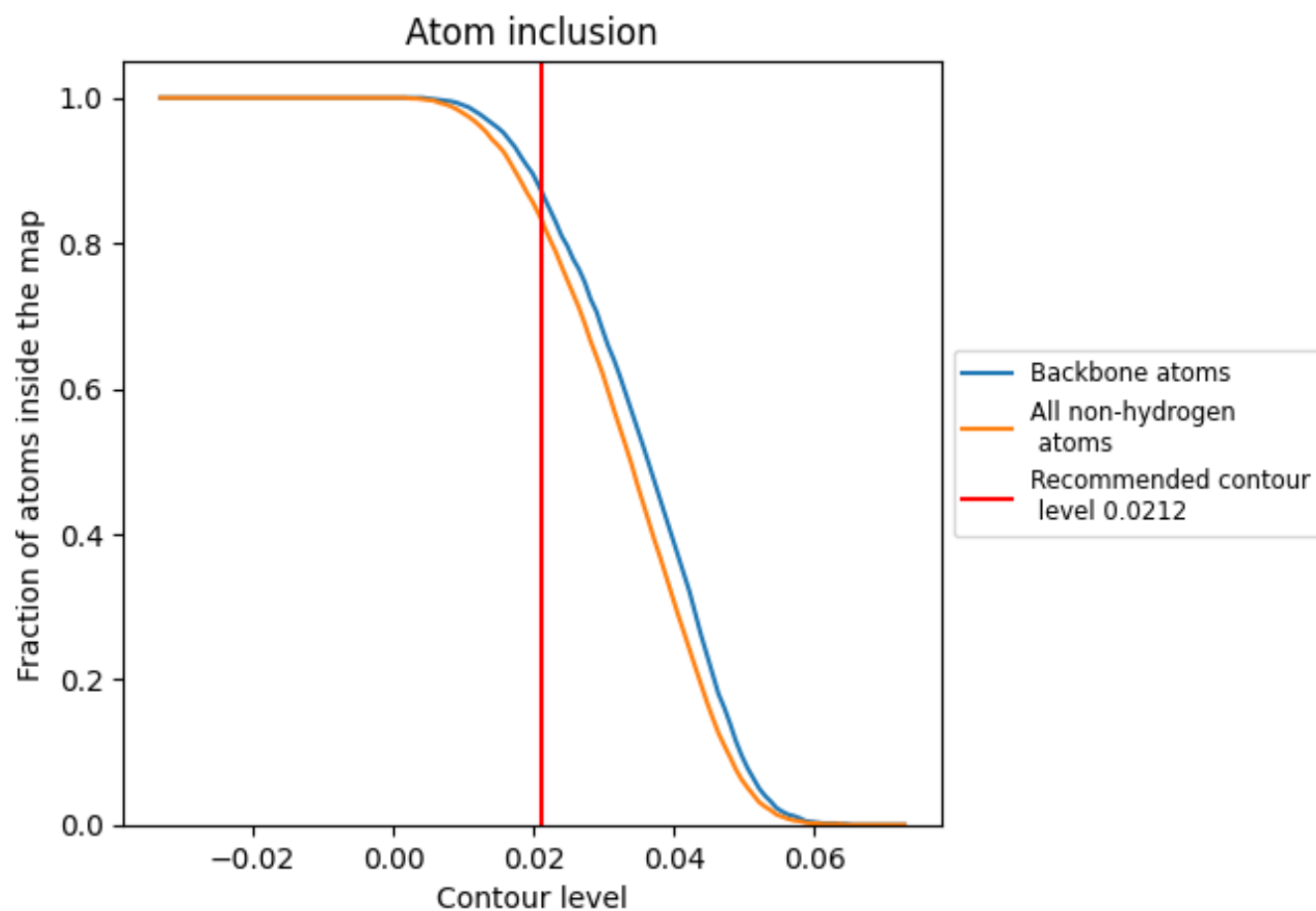
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0212).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 83% 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 (0.0212) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8310	<div></div> 0.6670
L	<div></div> 0.8370	<div></div> 0.6640
M	<div></div> 0.8300	<div></div> 0.6690

