



wwPDB EM Validation Summary Report ⓘ

Oct 21, 2024 – 09:39 PM JST

PDB ID : 7XZI
EMDB ID : EMD-33528
Title : Cryo-EM structure of TOC-TIC supercomplex from *Chlamydomonas reinhardtii*
Authors : Liu, H.; Li, A.J.; Liu, Z.F.
Deposited on : 2022-06-02
Resolution : 2.77 Å(reported)

This is a wwPDB EM Validation Summary 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.dev113
Mogul	:	1.8.5 (274361), 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)	:	2.39

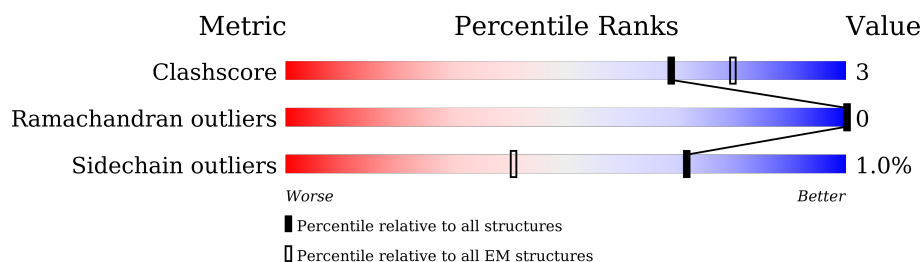
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.77 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	3	477	
2	4	363	
3	5	383	
4	7	798	
5	9	967	
6	A	1995	
7	B	259	
8	C	127	

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Mol	Chain	Length	Quality of chain
9	D	187	
10	E	955	
11	F	244	
12	G	397	
13	U	124	
14	X	21	

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 37365 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 Ctap3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	3	206	Total	C	N	O	S	0	0
			1528	965	271	286	6		

- Molecule 2 is a protein called Ctap4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	4	273	Total	C	N	O	S	0	0
			1734	1074	319	340	1		

- Molecule 3 is a protein called Ctap5.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	5	196	Total	C	N	O		0	0
			1506	973	268	265			

- Molecule 4 is a protein called Toc75.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	7	616	Total	C	N	O	S	0	0
			4249	2674	761	800	14		

- Molecule 5 is a protein called Toc90.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	9	381	Total	C	N	O	S	0	0
			2800	1790	466	529	15		

- Molecule 6 is a protein called Tic214.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	1598	Total	C	N	O	S	0	0
			12921	8361	2294	2239	27		

- Molecule 7 is a protein called Protein TIC 20.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	B	166	Total	C	N	O	S	0	0
			1409	964	206	227	12		

- Molecule 8 is a protein called Tic15.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	C	116	Total	C	N	O	S	0	0
			947	615	170	156	6		

- Molecule 9 is a protein called Simp3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	D	101	Total	C	N	O	S	0	0
			823	558	125	135	5		

- Molecule 10 is a protein called Tic100.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	E	770	Total	C	N	O	S	0	0
			6055	3784	1044	1196	31		

- Molecule 11 is a protein called Tic56.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	F	167	Total	C	N	O	S	0	0
			1361	877	245	230	9		

- Molecule 12 is a protein called Toc34.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	G	70	Total	C	N	O	0	0
			501	318	102	81		

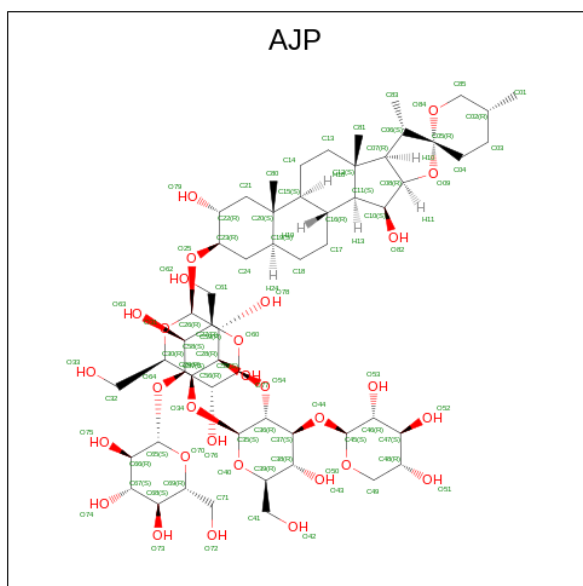
- Molecule 13 is a protein called Simp2.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	U	91	Total	C	N	O	S	0	0
			662	421	123	117	1		

- Molecule 14 is a protein called Unknown peptide.

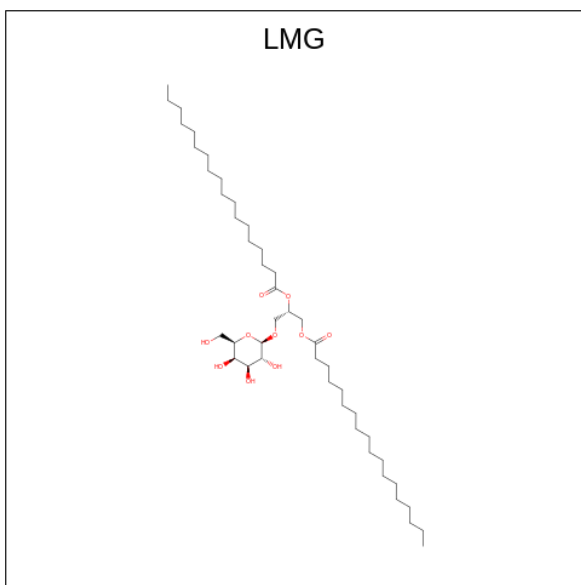
Mol	Chain	Residues	Atoms				AltConf	Trace
14	X	19	Total	C	N	O	0	0
			93	55	19	19		

- Molecule 15 is Digitonin (three-letter code: AJP) (formula: $C_{56}H_{92}O_{29}$).



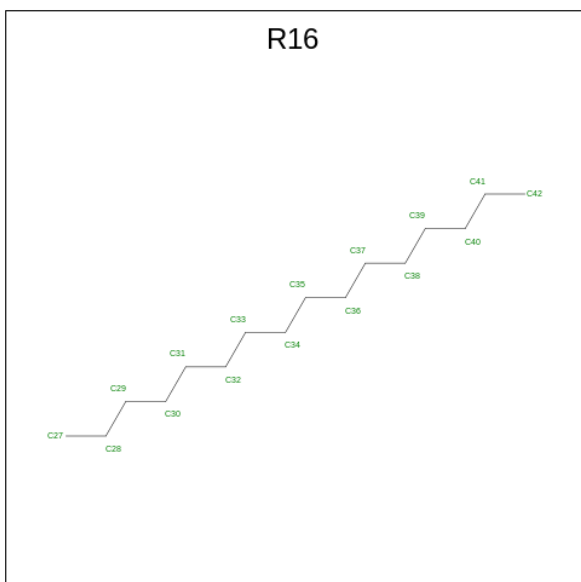
Mol	Chain	Residues	Atoms			AltConf
15	4	1	Total	C	O	0
			31	27	4	
15	5	1	Total	C	O	0
			43	33	10	
15	B	1	Total	C	O	0
			42	33	9	
15	D	1	Total	C	O	0
			32	27	5	
15	D	1	Total	C	O	0
			52	39	13	

- Molecule 16 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



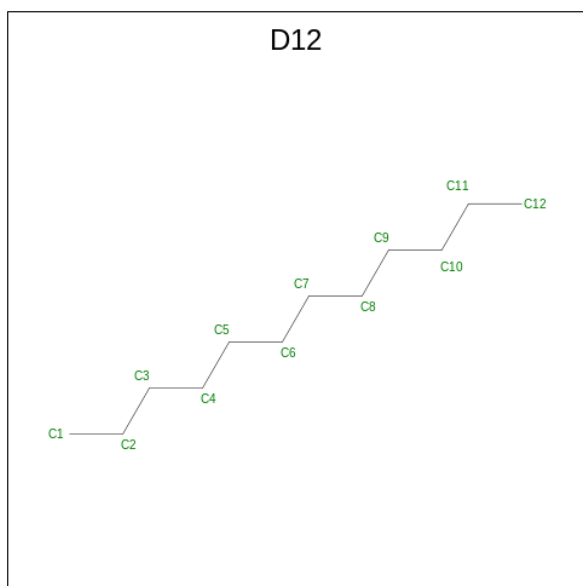
Mol	Chain	Residues	Atoms			AltConf
16	5	1	Total	C	O	0
			42	32	10	
16	A	1	Total	C	O	0
			52	42	10	
16	A	1	Total	C	O	0
			55	45	10	
16	A	1	Total	C	O	0
			39	29	10	
16	B	1	Total	C	O	0
			37	27	10	

- Molecule 17 is HEXADECANE (three-letter code: R16) (formula: $C_{16}H_{34}$).



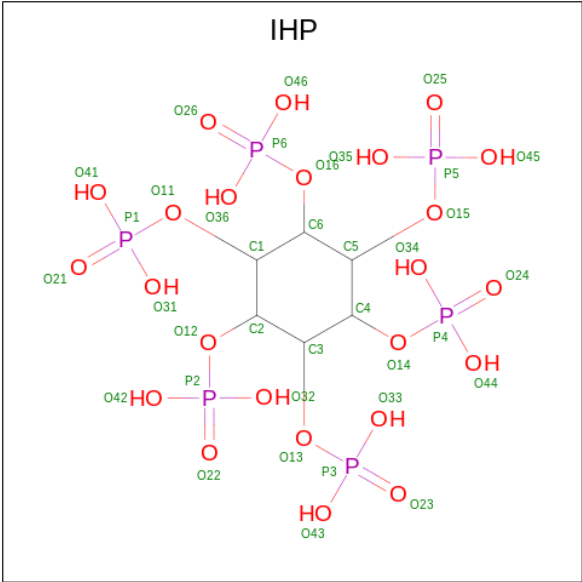
Mol	Chain	Residues	Atoms	AltConf
17	7	1	Total C 10 10	0

- Molecule 18 is DODECANE (three-letter code: D12) (formula: $C_{12}H_{26}$).



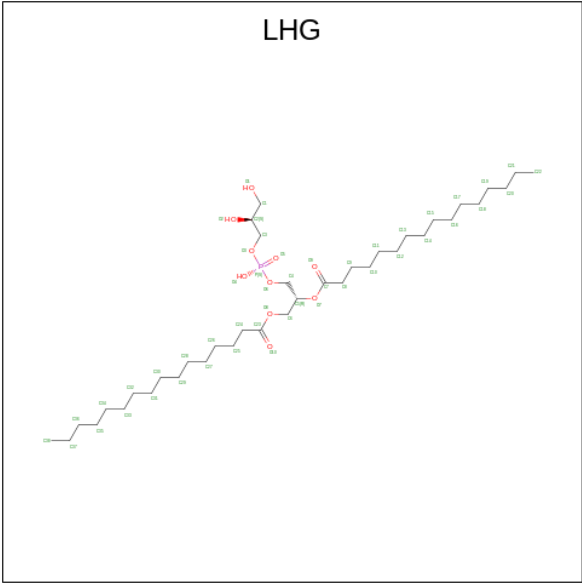
Mol	Chain	Residues	Atoms	AltConf
18	9	1	Total C 12 12	0
18	A	1	Total C 12 12	0
18	A	1	Total C 12 12	0
18	A	1	Total C 12 12	0
18	B	1	Total C 12 12	0
18	B	1	Total C 12 12	0
18	D	1	Total C 12 12	0

- Molecule 19 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: $C_6H_{18}O_{24}P_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
19	A	1	Total	C	O	P	0
			36	6	24	6	

- Molecule 20 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P) (labeled as "Ligand of Interest" by depositor).



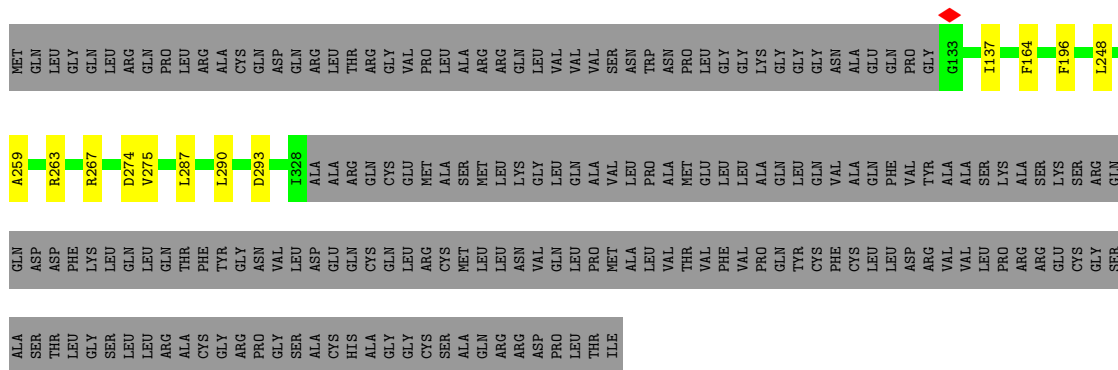
Mol	Chain	Residues	Atoms				AltConf
20	A	1	Total	C	O	P	0
			49	38	10	1	
20	B	1	Total	C	O	P	0
			36	25	10	1	

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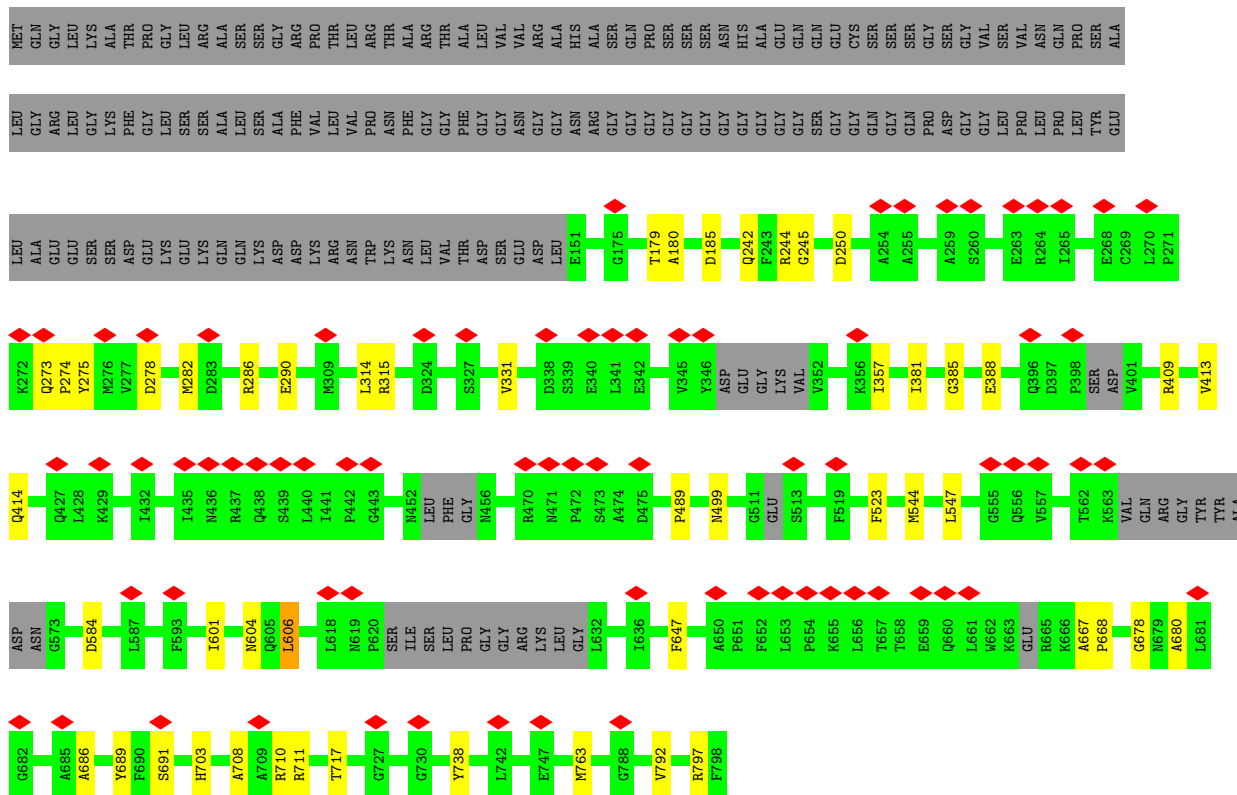
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Mol	Chain	Residues	Atoms				AltConf
20	B	1	Total	C	O	P	0
			45	34	10	1	
20	C	1	Total	C	O	P	0
			47	36	10	1	
20	F	1	Total	C	O	P	0
			44	33	10	1	

- Molecule 3: Ctap5

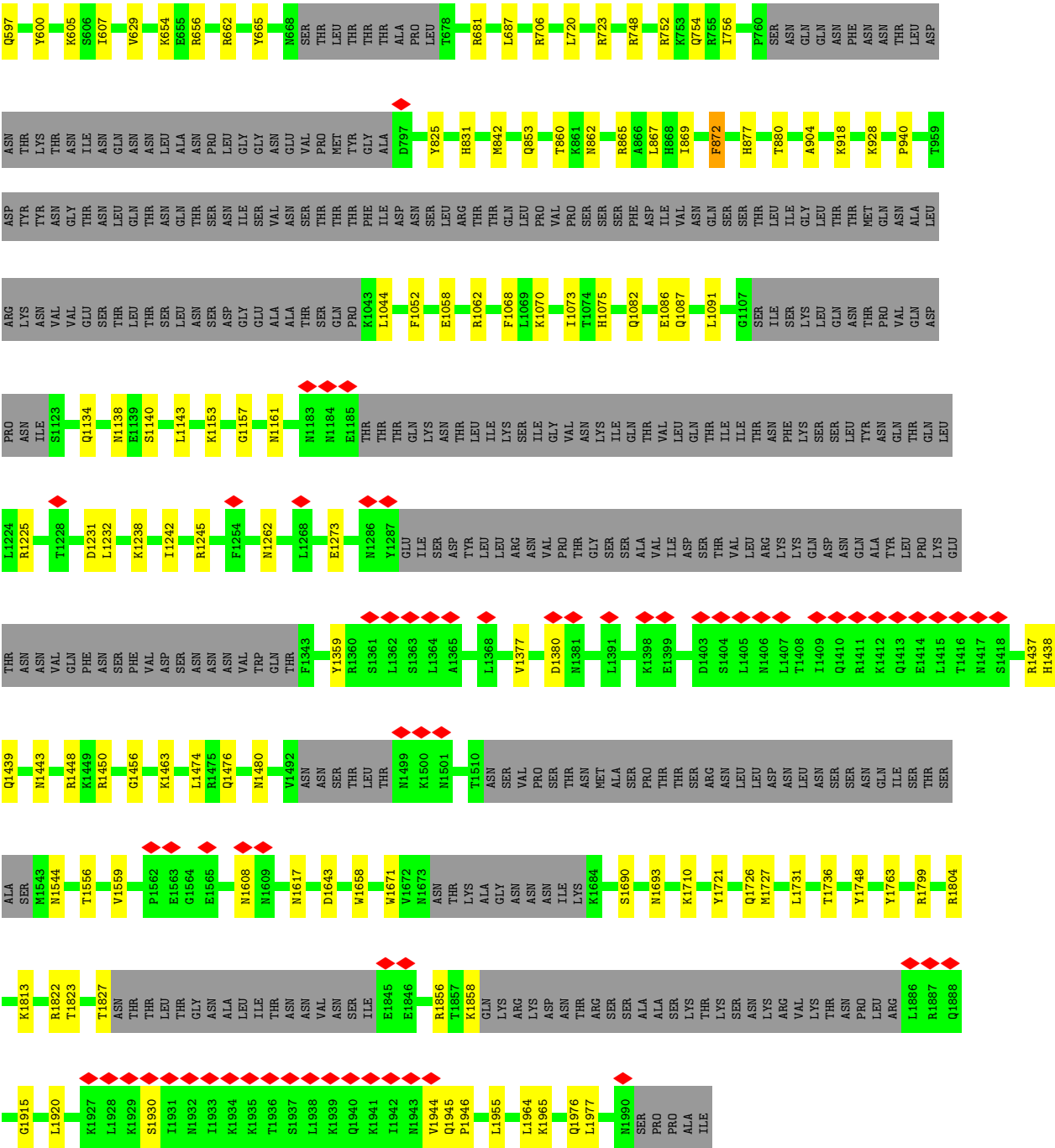


- Molecule 4: Toc75

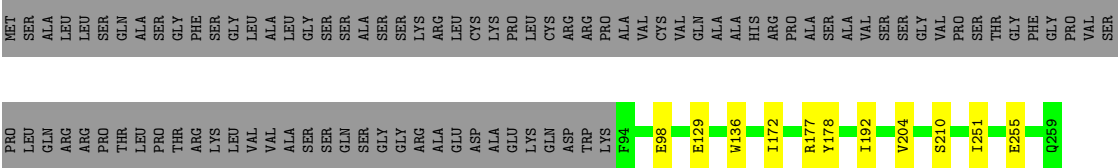


- Molecule 5: Toc90






• Molecule 7: Protein TIC 20



• Molecule 8: Tic15

Chain C:  79% 13% 9%

MET ASP GLU GLU PRO PRO PHE ASN LEU LEU H12 V13 Y14 K15 F31 N36 S61 E52 L53 H54 L63 N68 E75 N83 L87 W111 V126 Q127

• Molecule 9: Simp3

Chain D:  47% 7% 46%

MET ALA THR CYS ALA ALA VAL SER LEU ALA THR ALA VAL PHE GLN VAL SER ALA ALA LYS TYR VAL ASN LYS ALA ARG ASP ALA VAL SER ALA LEU PRO PRO SER ASN ILE ASP GLY VAL GLN ASP TRP ARG GLN VAL LYS GLU LEU LYS HIS THR ARG VAL TYR PHE ASP GLY

PHE VAL LEU PRO LEU ALA LYS ALA PHE ALA ALA GLU SER LEU THR VAL A79 R80 T81 F82 E83 R84 L94 F98 P99 R100 W111 R120 T123 L127 R131 L141 L165 G166 K169 D170 T171 F174 D179 ILE MET CYS TYR PHE ASP GLY

HIS

• Molecule 10: Tic100

Chain E:  74% 7% 19%

MET ALA SER LYS LYS THR ASP ALA L13 R25 D26 E27 F30 D54 V62 W70 P71 L83 A87 K91 A93 K94 P95 R96 P97 R98 E104 K105 T106 P116 THR VAL GLY ALA PRO VAL SER ALA ASP ALA ASP ALA ALA ALA

ARG ARG ALA LYS LYS ASP ARG LYS LYS LYS LYS ALA GLY GLY GLY GLY G152 P153 T168 D175 E213 D214 F215 D216 D226 W237 K309 Q310 V318 A330 Q333 K339 Y340 E341 Y348 K353 L359 F390 R391 D394 D427

K436 W459 D494 R498 V499 R500 P501 M517 W531 E532 G533 A552 E553 D556 L559 D566 T578 K583 Q593 D616 LYS GLY ALA LYS ASP GLU SER TYR VAL ASP ALA SER HIS PRO GLY ALA LEU L642

E645 R650 R653 R674 A680 ALA ASP GLU GLU VAL VAL LEU GLY GLY GLY VAL VAL VAL PHE R695 T708 F710 D721 R738 D757 S761 H771 Y772 P773 P783 D792 R797 T824 Y847 R856 ASP GLY ALA ALA PRO ALA GLY

GLU GLY ASP GLN ALA LEU LEU LEU THR SER THR GLY ALA ALA LYS SER VAL VAL ALA PHE ASP MET ARG GLY GLY ASN ALA SER PRO GLY SER SER GLY ARG ARG ARG GLN

ARG ALA ALA ASP VAL LEU GLY PHE ASP ALA ALA LYS SER VAL VAL MET ARG ALA ARG PRO ARG ARG ARG GLN

• Molecule 11: Tic56

Chain F:  62% 7% 32%

MET SER PRO GLY GLY PRO SER ASP GLY GLN VAL VAL THR ARG LEU ARG LYS ILE ARG MET LEU HIS VAL LYS MET ARG PRO LEU SER SER GLN GLU GLN HIS MET ASP ARG ARG LEU ALA ALA ILE LEU PRO ILE ALA ASP LEU PRO VAL PRO GLY PRO GLY SER LEU

ALA GLY SER PRO ALA ASP ALA ARG ALA VAL MET ARG ARG ARG G78 A92 H101 P102 L103 K113 E131 L160 K164 H181 K193 P197 P202 R206 R212 K228 Q239 L242 M243 R244

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	796731	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.956	Depositor
Minimum map value	-0.387	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.15	Depositor
Map size (\AA)	432.0, 432.0, 432.0	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.675, 0.675, 0.675	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: R16, LHG, IHP, LMG, AJP, D12

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	3	0.24	0/1561	0.43	0/2125
2	4	0.24	0/1757	0.47	0/2398
3	5	0.24	0/1543	0.44	0/2100
4	7	0.24	0/4336	0.46	0/5910
5	9	0.24	0/2882	0.44	0/3934
6	A	0.25	0/13218	0.46	0/17847
7	B	0.25	0/1467	0.39	0/2007
8	C	0.24	0/984	0.42	0/1338
9	D	0.25	0/854	0.43	0/1167
10	E	0.25	0/6198	0.48	0/8393
11	F	0.24	0/1400	0.46	0/1900
12	G	0.25	0/515	0.49	0/704
13	U	0.24	0/679	0.48	0/926
14	X	0.25	0/92	0.30	0/126
All	All	0.25	0/37486	0.46	0/50875

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	3	1528	0	1393	12	0
2	4	1734	0	1366	18	0
3	5	1506	0	1443	8	0
4	7	4249	0	3621	31	0
5	9	2800	0	2476	24	0
6	A	12921	0	12873	115	0
7	B	1409	0	1368	8	0
8	C	947	0	910	12	0
9	D	823	0	790	9	0
10	E	6055	0	5642	51	0
11	F	1361	0	1362	10	0
12	G	501	0	410	7	0
13	U	662	0	650	7	0
14	X	93	0	75	2	0
15	4	31	0	0	0	0
15	5	43	0	0	0	0
15	B	42	0	0	1	0
15	D	84	0	0	0	0
16	5	42	0	57	2	0
16	A	146	0	211	5	0
16	B	37	0	44	0	0
17	7	10	0	16	0	0
18	9	12	0	26	0	0
18	A	36	0	78	0	0
18	B	24	0	52	0	0
18	D	12	0	26	0	0
19	A	36	0	6	0	0
20	A	49	0	74	1	0
20	B	81	0	105	0	0
20	C	47	0	67	3	0
20	F	44	0	61	1	0
All	All	37365	0	35202	252	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 3.

The worst 5 of 252 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)
10:E:54:ASP:HB3	10:E:83:LEU:HD21	1.73	0.70
5:9:569:ALA:O	5:9:573:ASN:ND2	2.23	0.70
5:9:575:VAL:HG21	5:9:726:VAL:HG21	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:756:ILE:HD11	10:E:168:THR:HG21	1.76	0.68
1:3:406:LEU:HD13	6:A:928:LYS:HD3	1.77	0.67

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	3	204/477 (43%)	203 (100%)	1 (0%)	0	100	100
2	4	253/363 (70%)	244 (96%)	9 (4%)	0	100	100
3	5	194/383 (51%)	191 (98%)	3 (2%)	0	100	100
4	7	600/798 (75%)	587 (98%)	13 (2%)	0	100	100
5	9	375/967 (39%)	368 (98%)	7 (2%)	0	100	100
6	A	1570/1995 (79%)	1523 (97%)	47 (3%)	0	100	100
7	B	164/259 (63%)	160 (98%)	4 (2%)	0	100	100
8	C	114/127 (90%)	113 (99%)	1 (1%)	0	100	100
9	D	99/187 (53%)	96 (97%)	3 (3%)	0	100	100
10	E	762/955 (80%)	731 (96%)	31 (4%)	0	100	100
11	F	165/244 (68%)	162 (98%)	3 (2%)	0	100	100
12	G	68/397 (17%)	63 (93%)	5 (7%)	0	100	100
13	U	89/124 (72%)	87 (98%)	2 (2%)	0	100	100
14	X	17/21 (81%)	17 (100%)	0	0	100	100
All	All	4674/7297 (64%)	4545 (97%)	129 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	3	134/373 (36%)	134 (100%)	0	100	100
2	4	115/287 (40%)	115 (100%)	0	100	100
3	5	135/308 (44%)	134 (99%)	1 (1%)	81	93
4	7	349/653 (53%)	345 (99%)	4 (1%)	70	88
5	9	256/713 (36%)	252 (98%)	4 (2%)	58	83
6	A	1349/1848 (73%)	1339 (99%)	10 (1%)	81	93
7	B	149/223 (67%)	149 (100%)	0	100	100
8	C	96/106 (91%)	94 (98%)	2 (2%)	48	77
9	D	84/158 (53%)	80 (95%)	4 (5%)	21	50
10	E	613/755 (81%)	608 (99%)	5 (1%)	79	92
11	F	143/213 (67%)	140 (98%)	3 (2%)	48	77
12	G	33/336 (10%)	33 (100%)	0	100	100
13	U	64/97 (66%)	63 (98%)	1 (2%)	58	83
All	All	3520/6070 (58%)	3486 (99%)	34 (1%)	71	89

5 of 34 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	E	824	THR
10	E	847	TYR
11	F	228	LYS
6	A	872	PHE
6	A	860	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
6	A	1480	ASN
7	B	253	GLN

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Mol	Chain	Res	Type
7	B	250	GLN
9	D	128	GLN
6	A	416	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

24 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	$\# Z > 2$
18	D12	A	2003	-	11,11,11	0.24	0	10,10,10	0.19	0
18	D12	B	303	-	11,11,11	0.24	0	10,10,10	0.20	0
15	AJP	5	501	-	49,49,95	1.10	6 (12%)	74,80,149	1.66	14 (18%)
19	IHP	A	2001	-	36,36,36	0.85	0	54,60,60	0.52	0
15	AJP	D	203	-	59,59,95	1.02	3 (5%)	89,95,149	1.58	16 (17%)
16	LMG	A	2008	-	39,39,55	0.82	0	47,47,63	1.28	6 (12%)
20	LHG	B	306	-	44,44,48	0.64	2 (4%)	47,50,54	1.29	6 (12%)
15	AJP	D	201	-	37,37,95	1.15	5 (13%)	58,62,149	1.72	11 (18%)
20	LHG	F	301	-	43,43,48	0.65	2 (4%)	46,49,54	1.21	4 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	LMG	A	2006	-	52,52,55	0.72	0	60,60,63	1.37	7 (11%)
20	LHG	B	304	-	35,35,48	0.71	1 (2%)	38,41,54	1.26	4 (10%)
16	LMG	A	2007	-	55,55,55	0.68	0	63,63,63	1.37	7 (11%)
15	AJP	4	401	-	36,36,95	1.13	4 (11%)	56,60,149	1.72	11 (19%)
18	D12	9	1001	-	11,11,11	0.24	0	10,10,10	0.19	0
17	R16	7	801	-	9,9,15	0.25	0	8,8,14	0.19	0
16	LMG	5	502	-	42,42,55	0.80	1 (2%)	50,50,63	1.33	7 (14%)
18	D12	A	2004	-	11,11,11	0.24	0	10,10,10	0.20	0
20	LHG	A	2002	-	48,48,48	0.61	1 (2%)	51,54,54	1.27	6 (11%)
18	D12	B	302	-	11,11,11	0.24	0	10,10,10	0.20	0
15	AJP	B	305	-	48,48,95	1.02	4 (8%)	73,79,149	1.61	12 (16%)
16	LMG	B	301	-	37,37,55	0.84	1 (2%)	45,45,63	1.33	7 (15%)
18	D12	A	2005	-	11,11,11	0.24	0	10,10,10	0.21	0
18	D12	D	202	-	11,11,11	0.23	0	10,10,10	0.22	0
20	LHG	C	201	-	46,46,48	0.65	1 (2%)	49,52,54	1.27	6 (12%)

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
18	D12	A	2003	-	-	0/9/9/9	-
18	D12	B	303	-	-	3/9/9/9	-
15	AJP	5	501	-	-	2/6/121/220	0/7/7/11
19	IHP	A	2001	-	-	6/30/54/54	0/1/1/1
15	AJP	D	203	-	-	5/10/141/220	1/8/8/11
16	LMG	A	2008	-	-	11/34/54/70	0/1/1/1
20	LHG	B	306	-	-	24/49/49/53	-
15	AJP	D	201	-	-	-	1/6/6/11
20	LHG	F	301	-	-	19/48/48/53	-
16	LMG	A	2006	-	-	24/47/67/70	0/1/1/1
20	LHG	B	304	-	-	13/40/40/53	-
16	LMG	A	2007	-	-	16/50/70/70	0/1/1/1
15	AJP	4	401	-	-	-	0/6/6/11
18	D12	9	1001	-	-	3/9/9/9	-
17	R16	7	801	-	-	0/7/7/13	-
16	LMG	5	502	-	-	20/37/57/70	0/1/1/1

Continued on next page...

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	D12	A	2004	-	-	2/9/9/9	-
20	LHG	A	2002	-	-	18/53/53/53	-
18	D12	B	302	-	-	2/9/9/9	-
15	AJP	B	305	-	-	2/4/119/220	0/7/7/11
16	LMG	B	301	-	-	5/32/52/70	0/1/1/1
18	D12	A	2005	-	-	4/9/9/9	-
18	D12	D	202	-	-	3/9/9/9	-
20	LHG	C	201	-	-	14/51/51/53	-

The worst 5 of 31 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	D	203	AJP	C16-C11	-3.49	1.49	1.54
15	4	401	AJP	C16-C11	-2.88	1.50	1.54
15	B	305	AJP	C16-C11	-2.79	1.50	1.54
15	5	501	AJP	C20-C15	-2.73	1.51	1.56
15	5	501	AJP	C12-C11	-2.68	1.50	1.56

The worst 5 of 124 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	5	501	AJP	C12-C11-C16	-5.27	106.26	113.82
15	D	203	AJP	C12-C11-C16	-5.26	106.28	113.82
15	B	305	AJP	C12-C11-C16	-4.99	106.66	113.82
15	D	201	AJP	C19-C24-C23	-4.98	108.97	114.46
15	4	401	AJP	C12-C11-C16	-4.95	106.71	113.82

There are no chirality outliers.

5 of 196 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	5	502	LMG	C2-C1-O1-C7
16	5	502	LMG	O6-C1-O1-C7
16	5	502	LMG	C11-C10-O7-C8
16	A	2008	LMG	C2-C1-O1-C7
16	A	2008	LMG	O6-C1-O1-C7

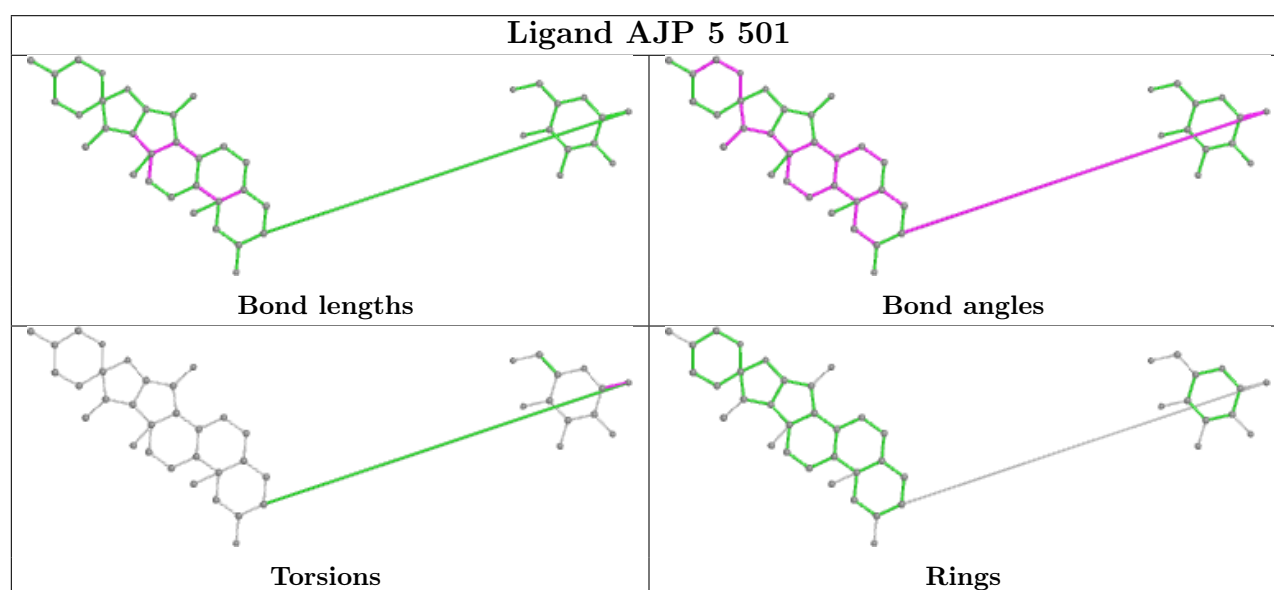
All (2) ring outliers are listed below:

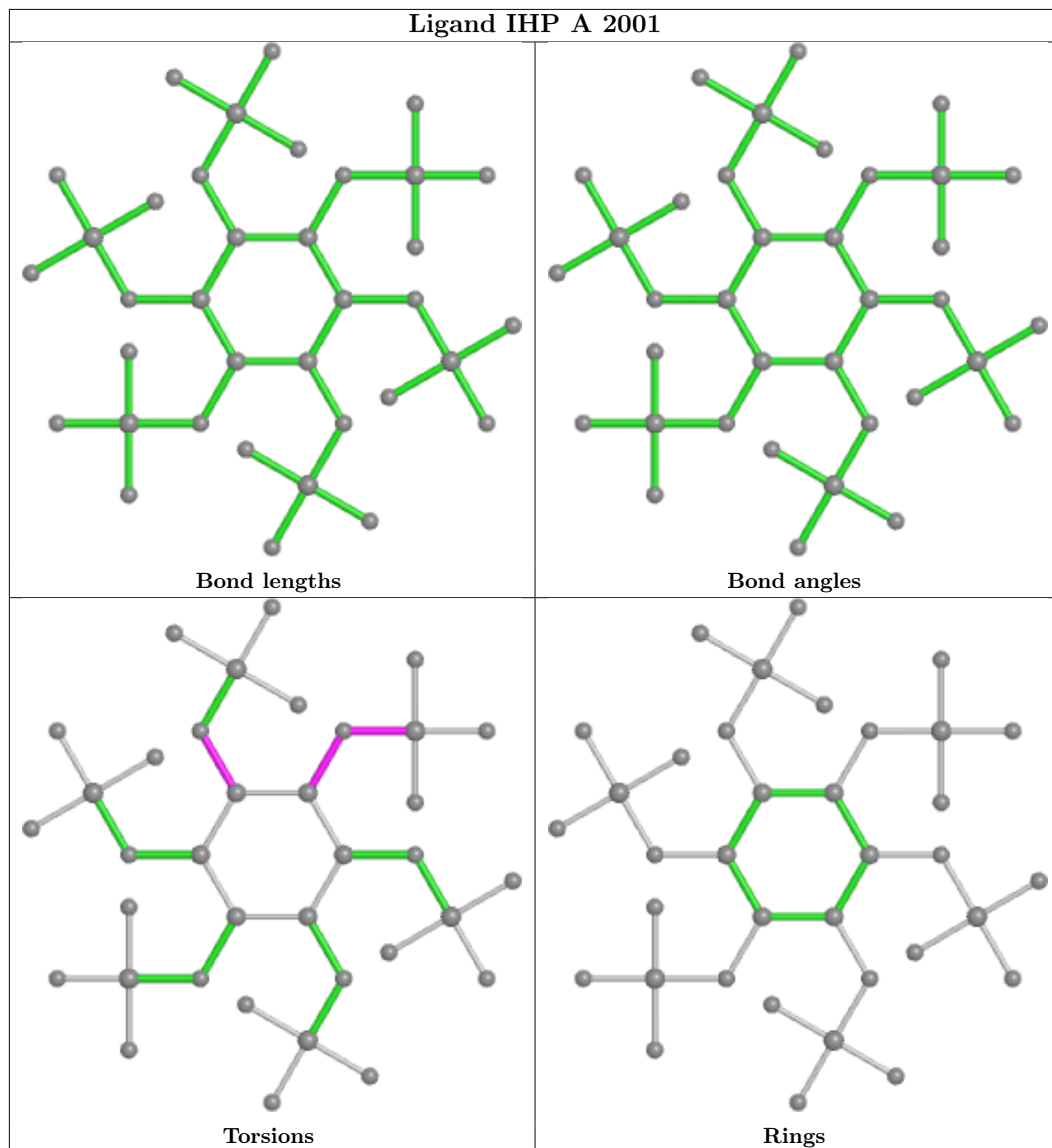
Mol	Chain	Res	Type	Atoms
15	D	201	AJP	C19-C20-C21-C22-C23-C24
15	D	203	AJP	C35-C36-C37-C38-C39-O40

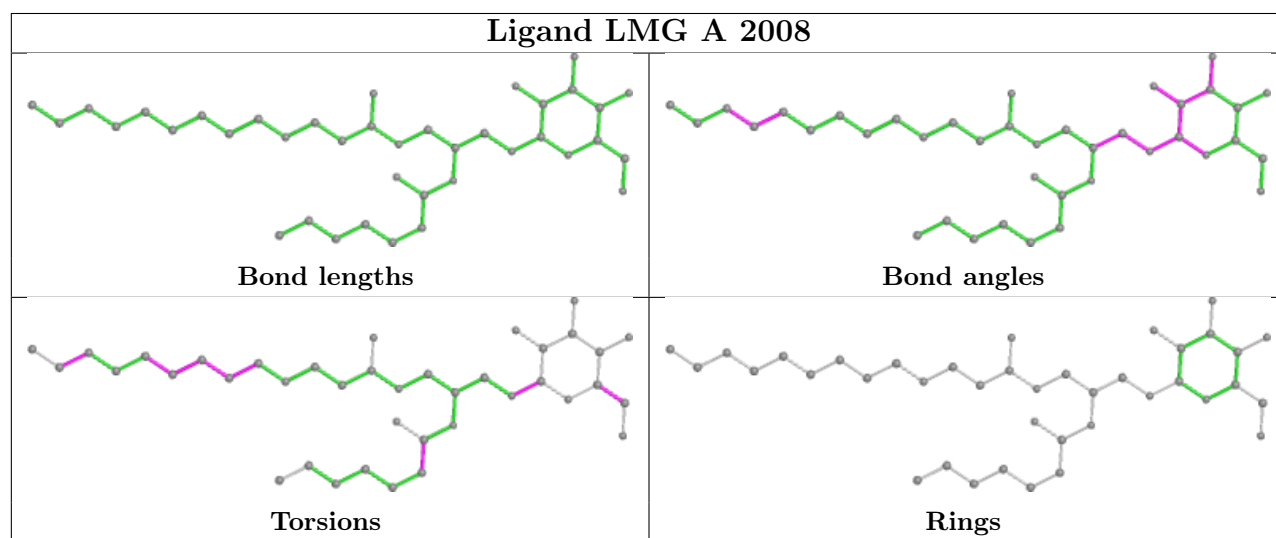
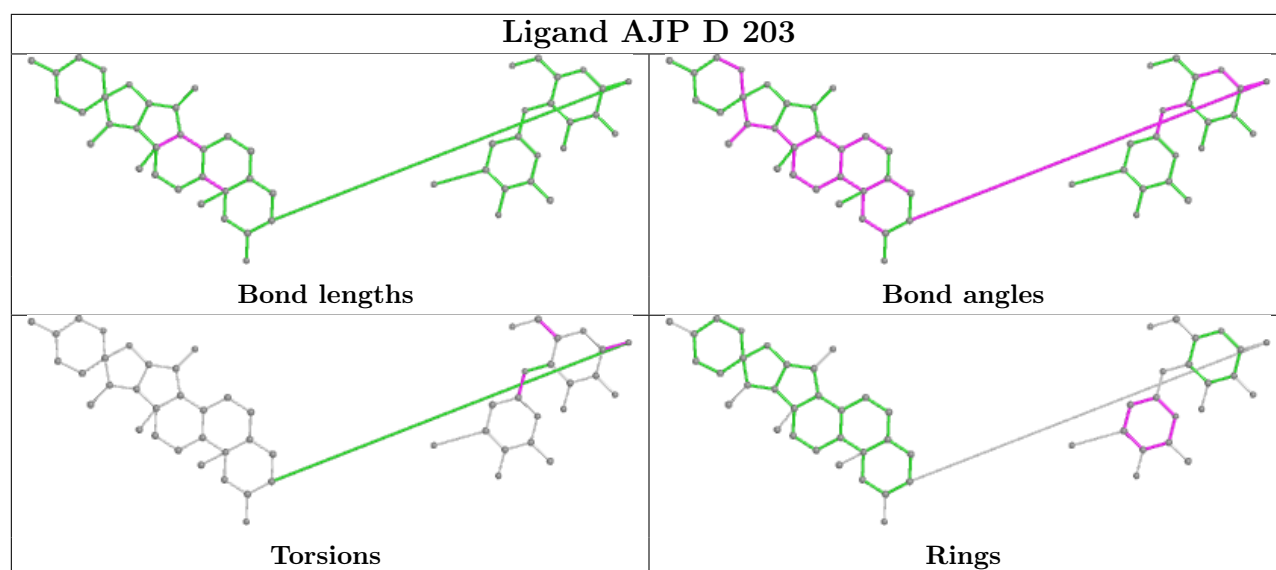
8 monomers are involved in 12 short contacts:

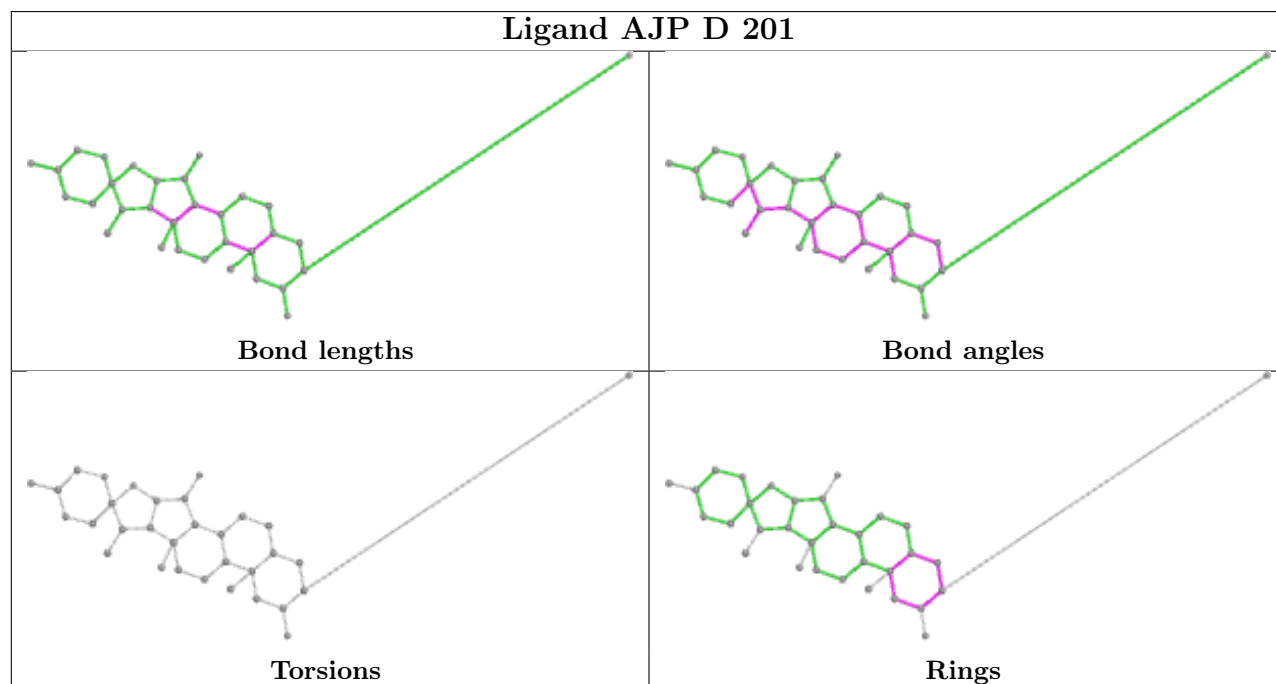
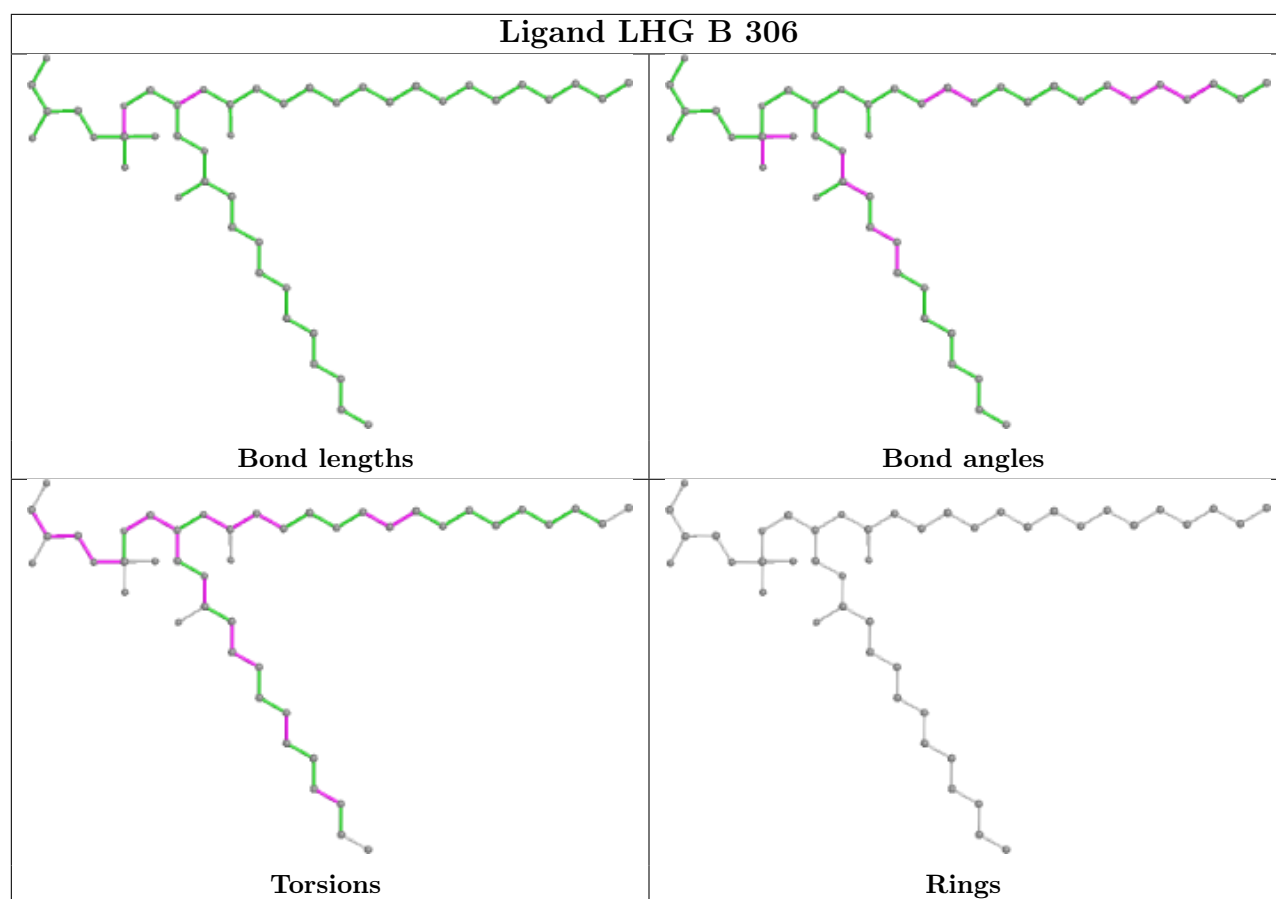
Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	A	2008	LMG	1	0
20	F	301	LHG	1	0
16	A	2006	LMG	1	0
16	A	2007	LMG	3	0
16	5	502	LMG	2	0
20	A	2002	LHG	1	0
15	B	305	AJP	1	0
20	C	201	LHG	3	0

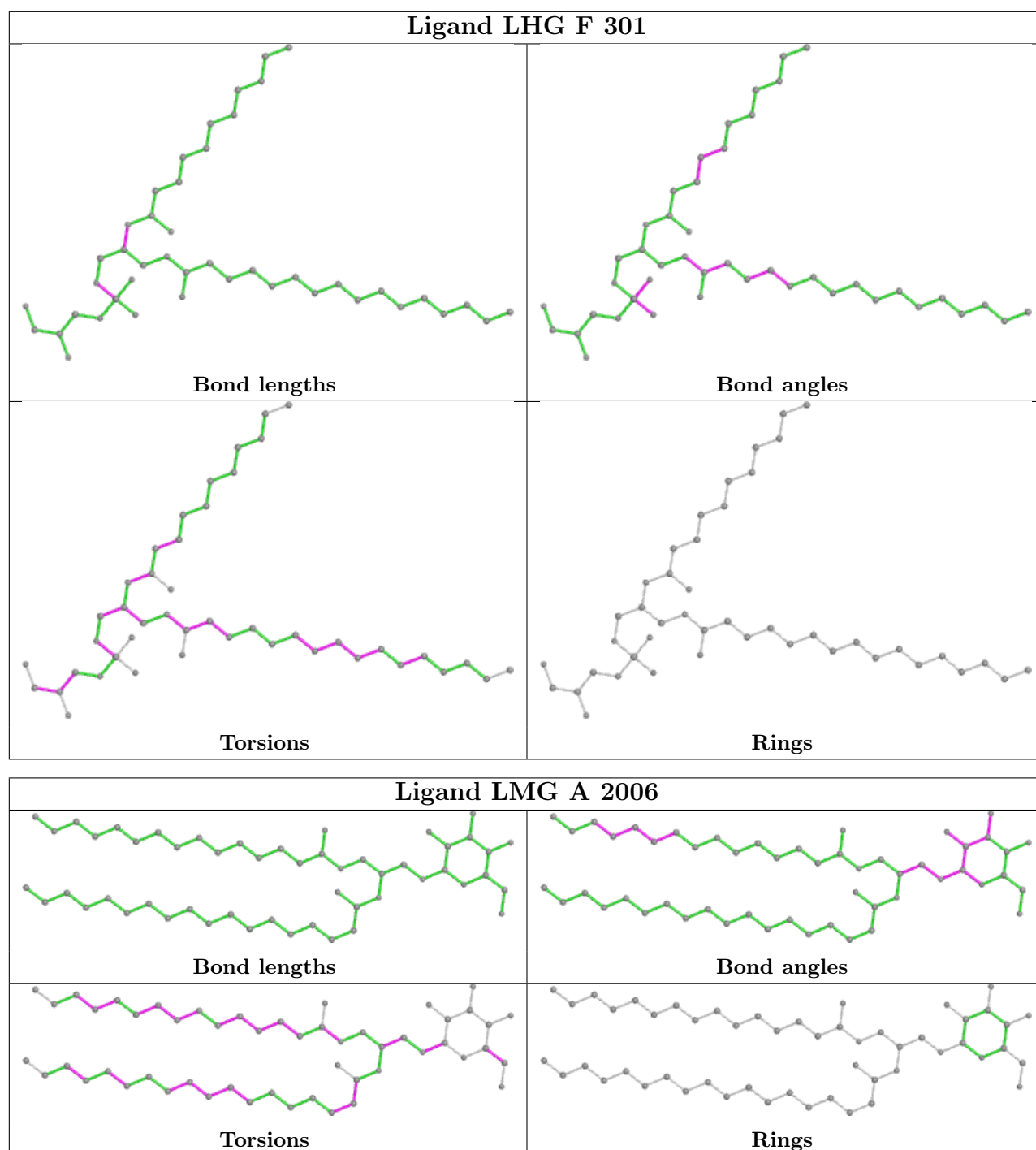
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

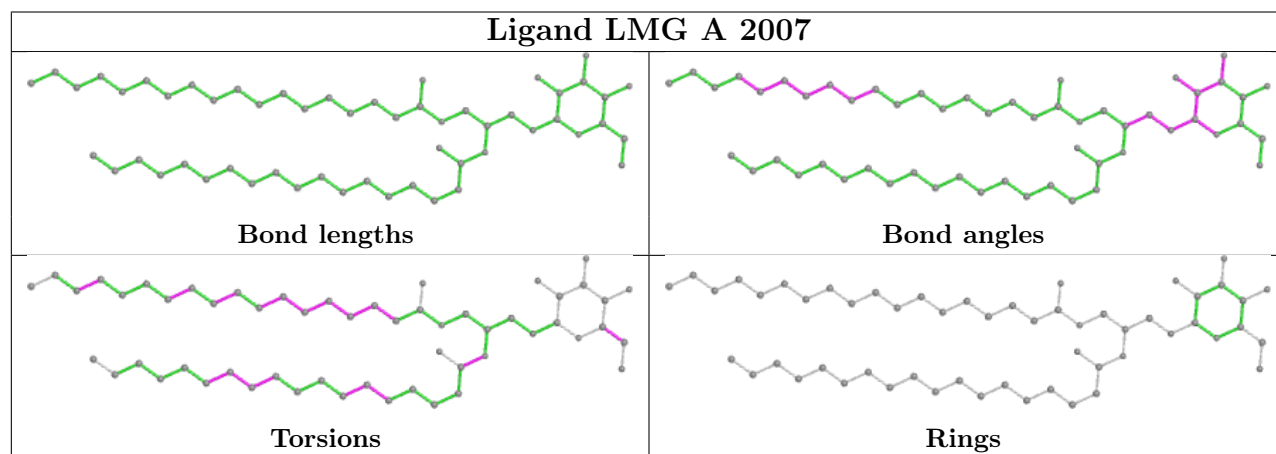
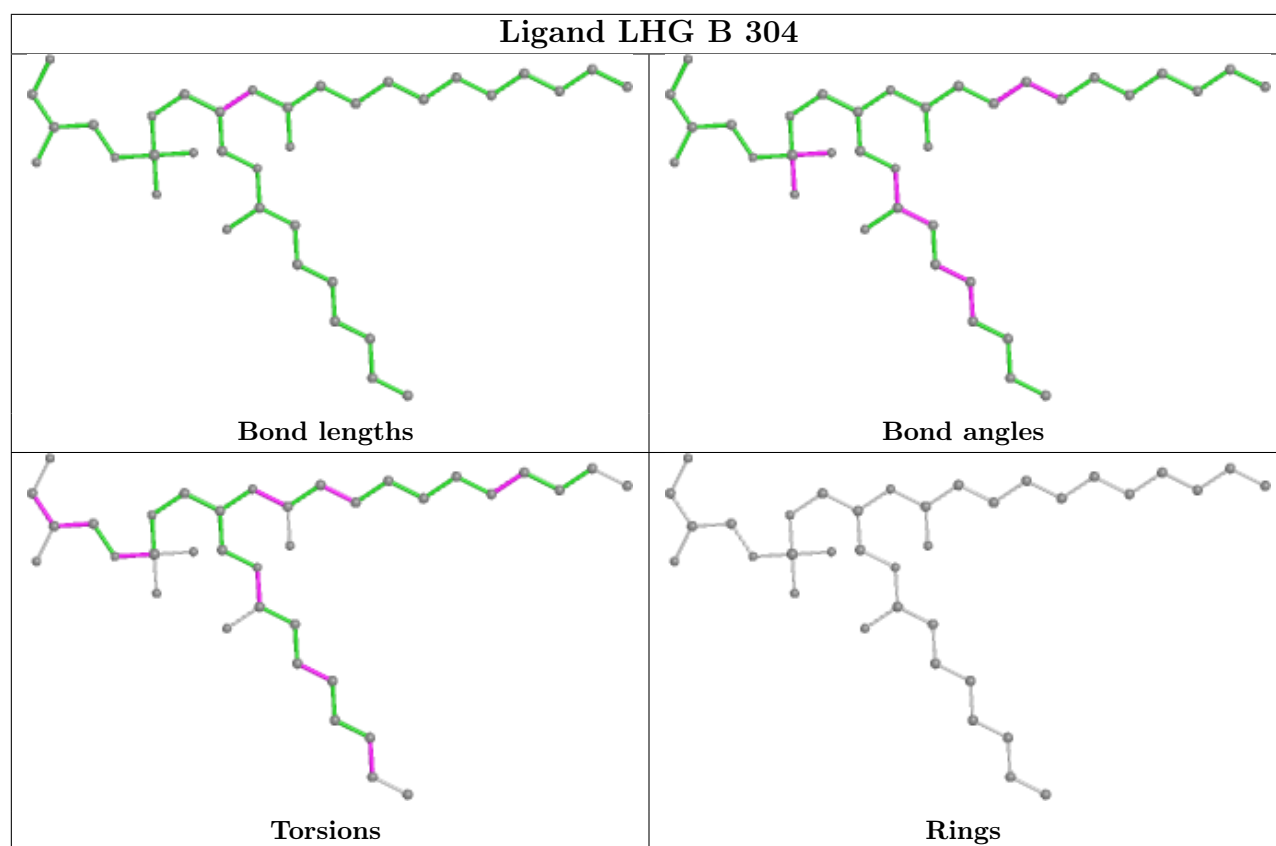


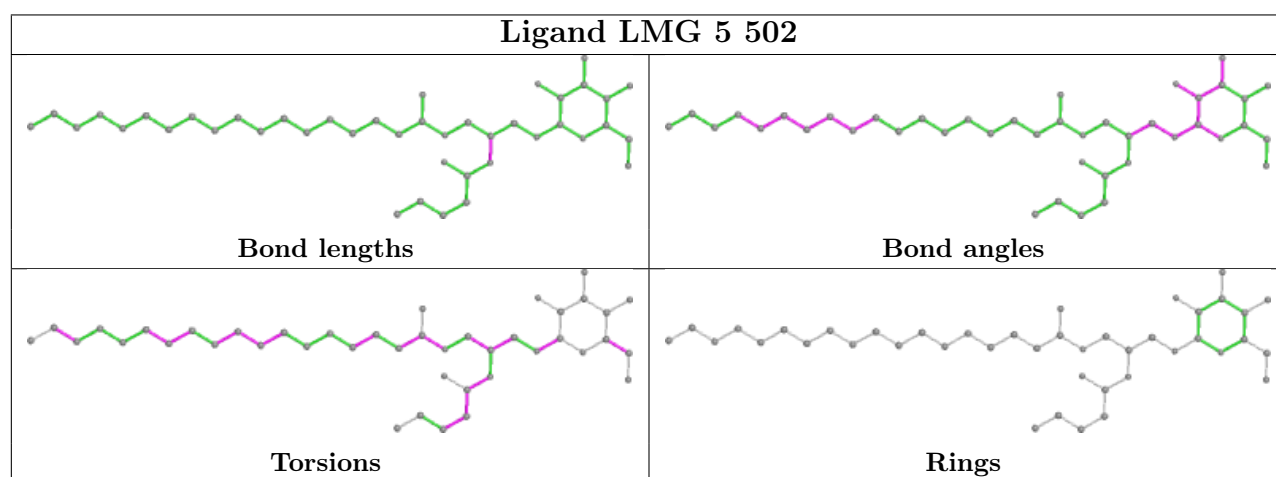
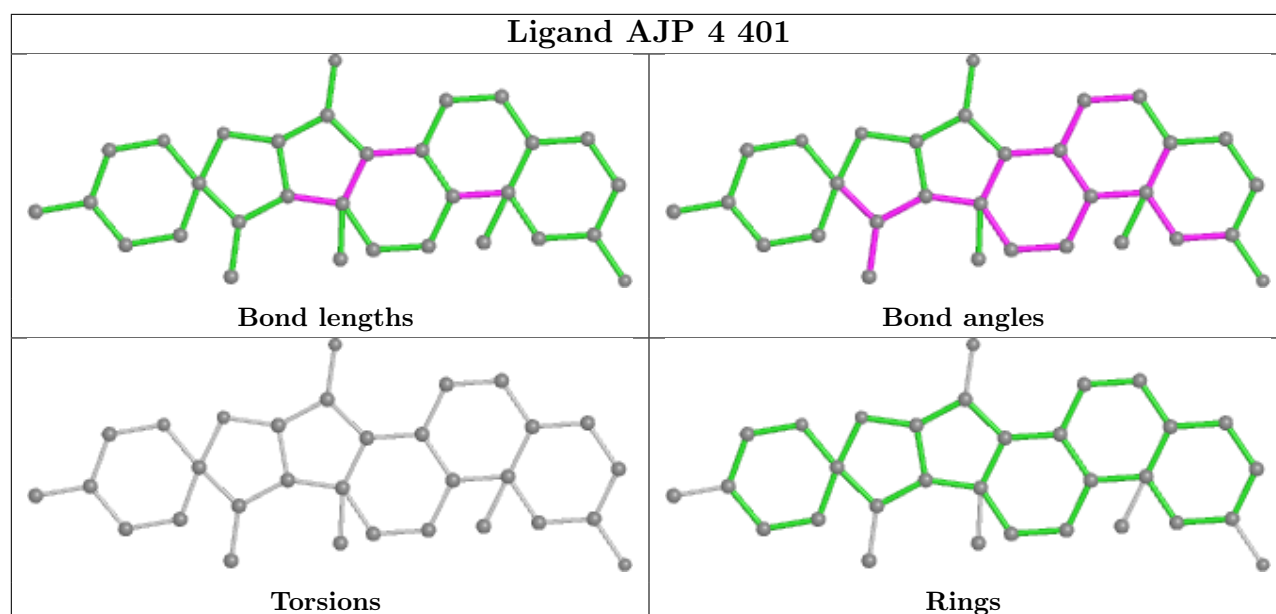


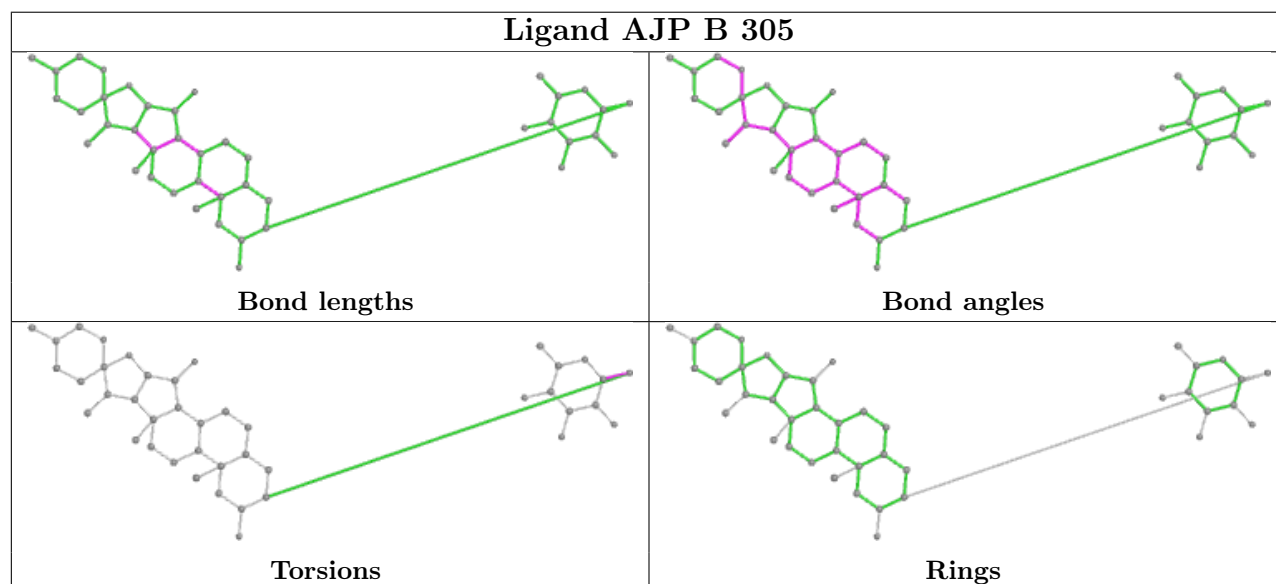
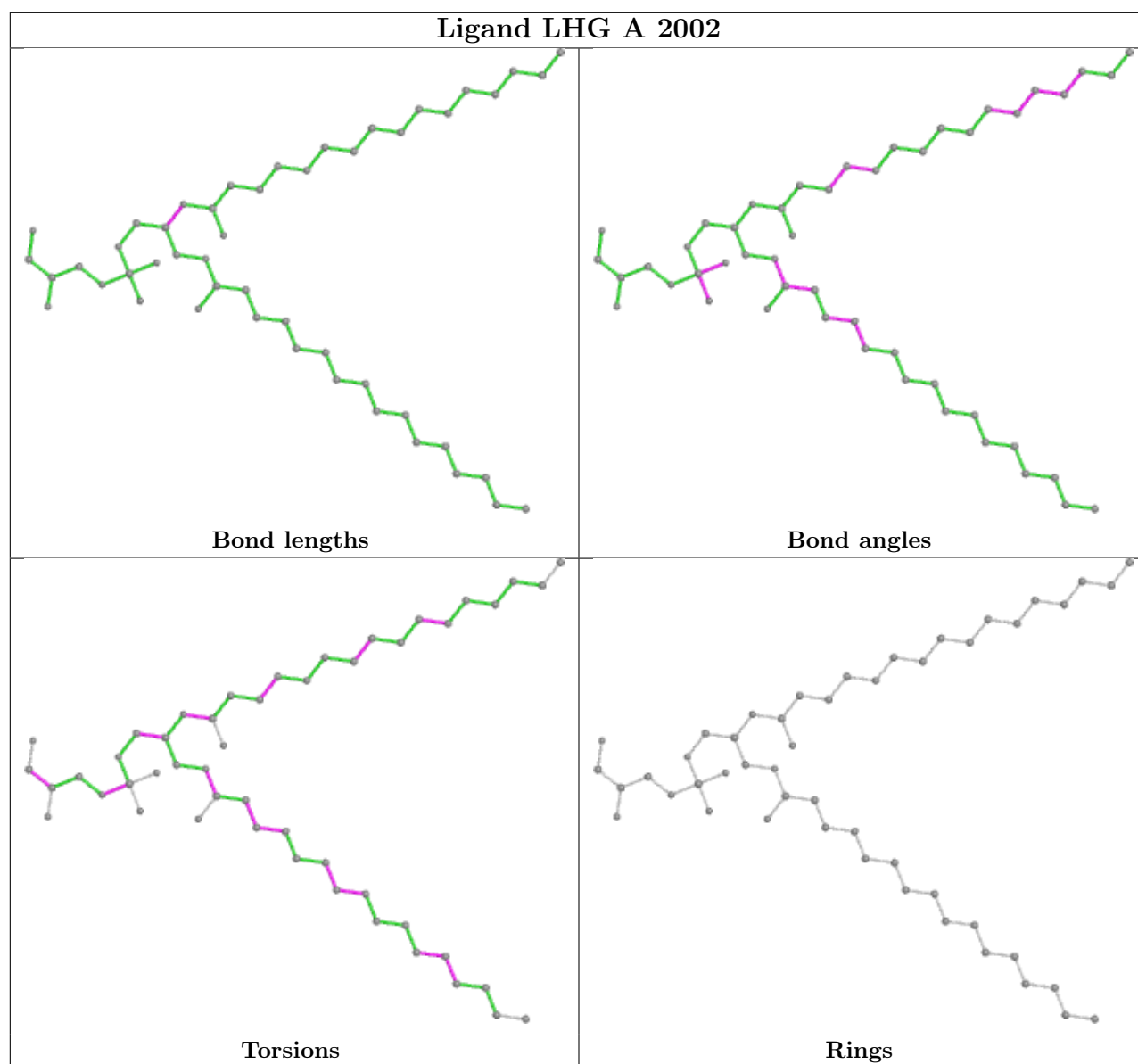


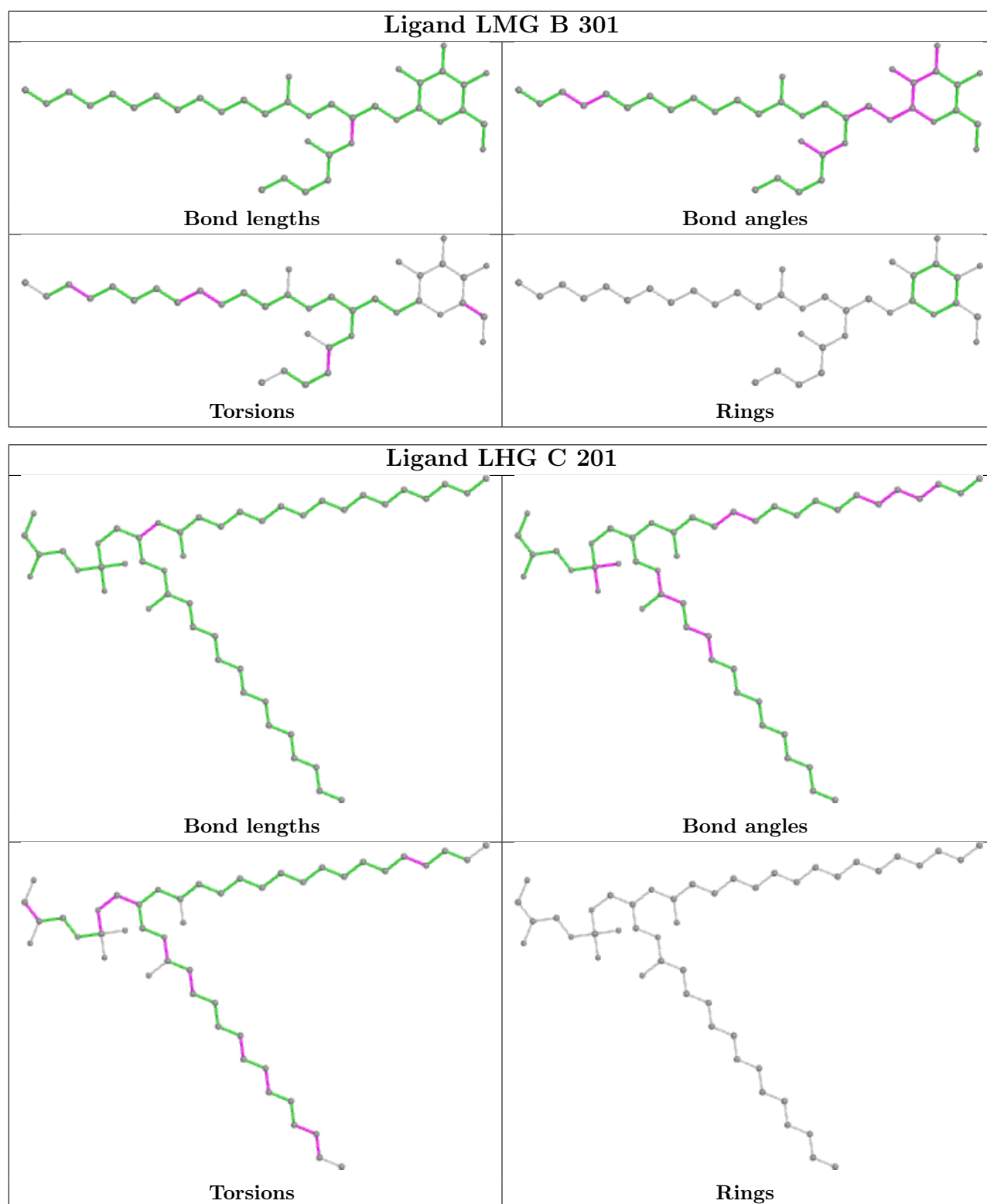












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

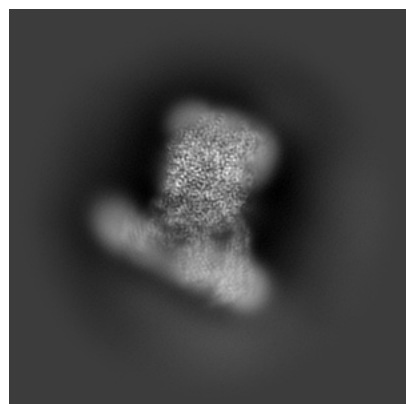
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33528. These allow visual inspection of the internal detail of the map and identification of artifacts.

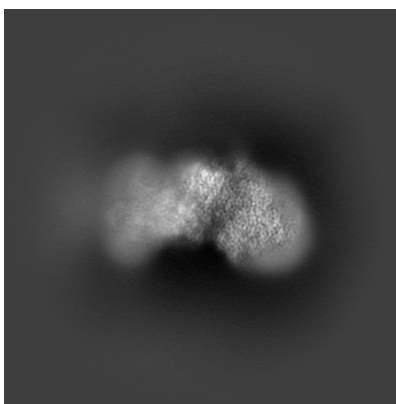
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

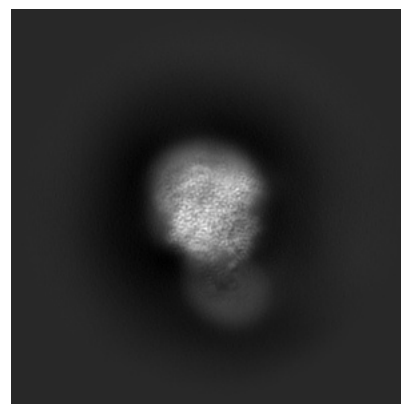
6.1.1 Primary map



X

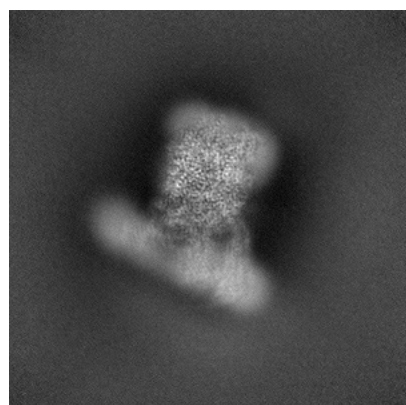


Y

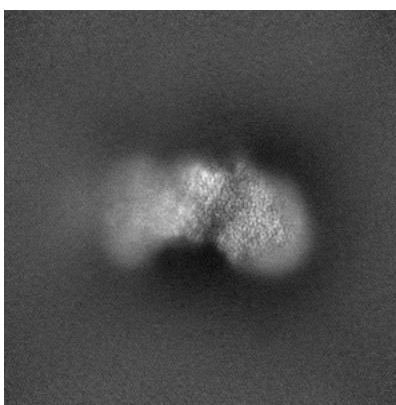


Z

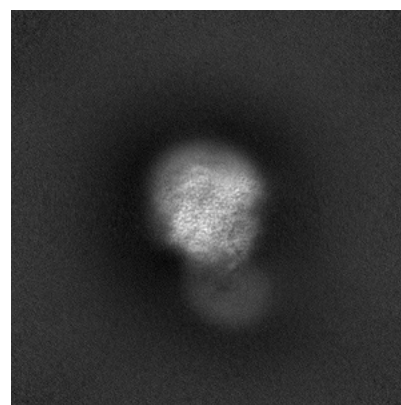
6.1.2 Raw map



X



Y

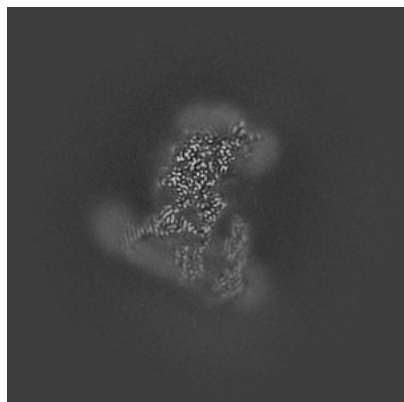


Z

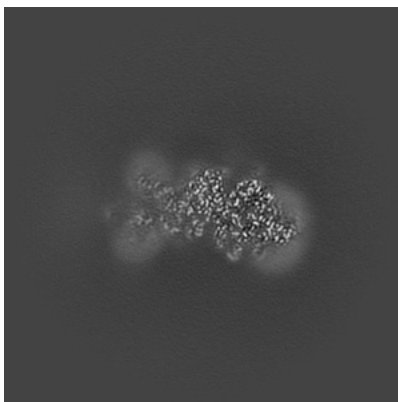
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

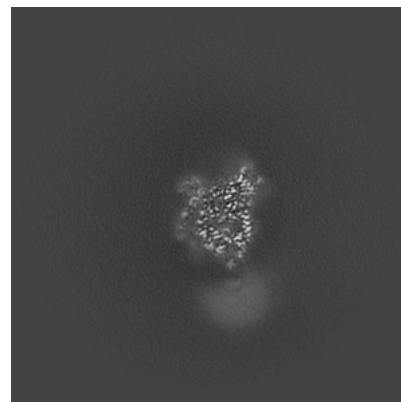
6.2.1 Primary map



X Index: 320

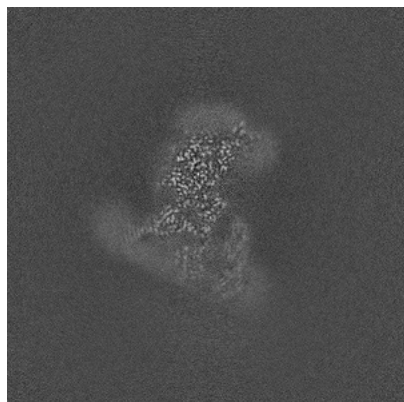


Y Index: 320

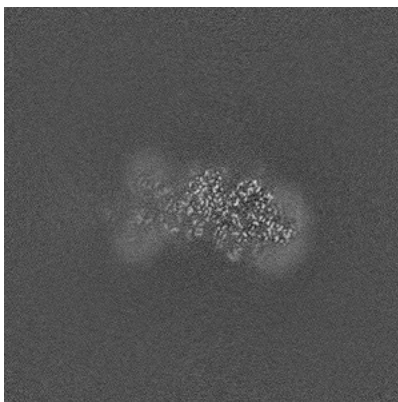


Z Index: 320

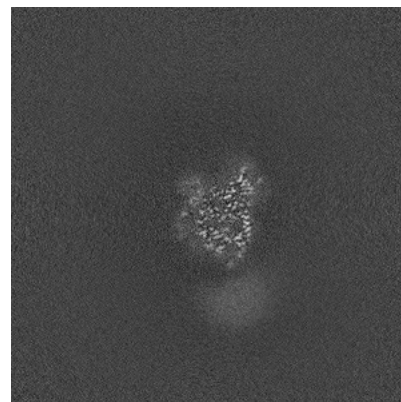
6.2.2 Raw map



X Index: 320



Y Index: 320

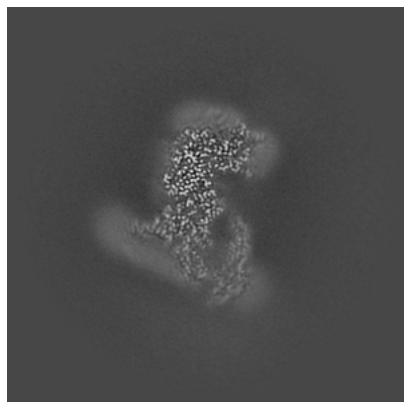


Z Index: 320

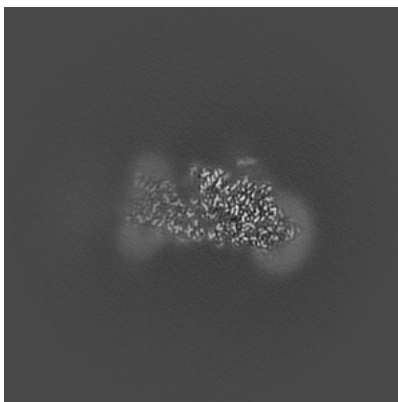
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

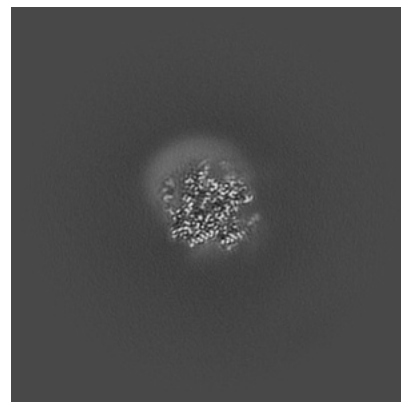
6.3.1 Primary map



X Index: 312

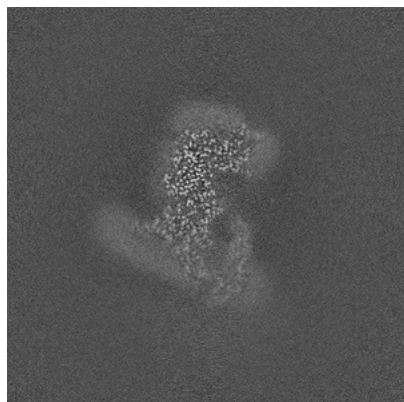


Y Index: 305

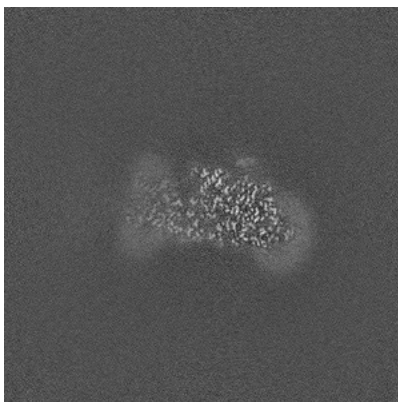


Z Index: 397

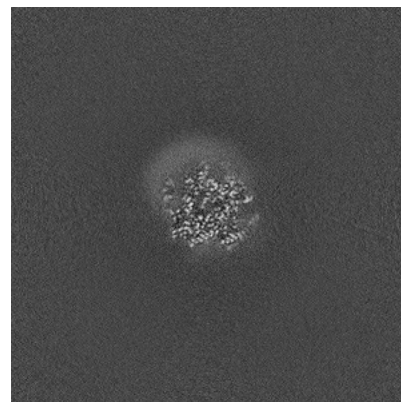
6.3.2 Raw map



X Index: 312



Y Index: 304

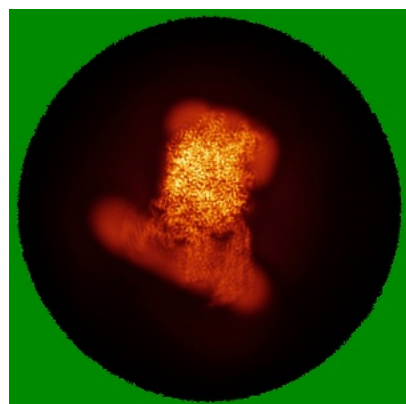


Z Index: 397

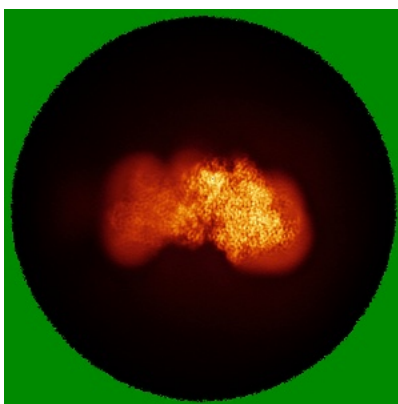
The images above show the largest variance slices of the map in three orthogonal directions.

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

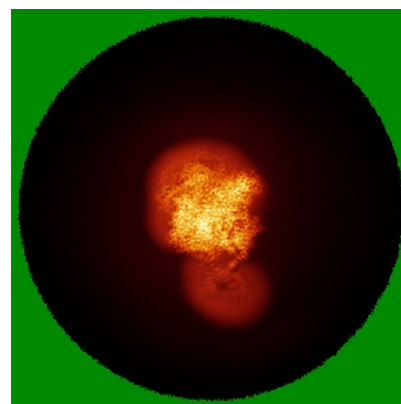
6.4.1 Primary map



X

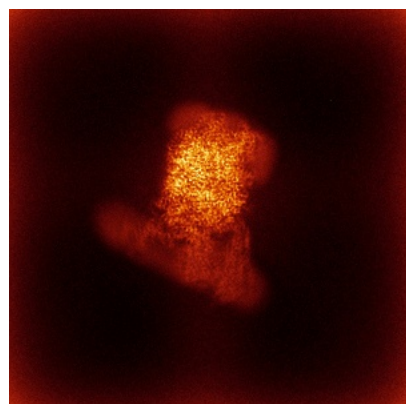


Y

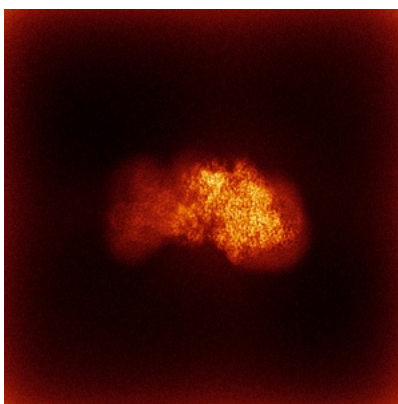


Z

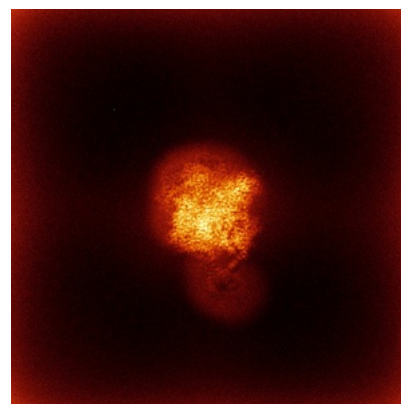
6.4.2 Raw map



X



Y

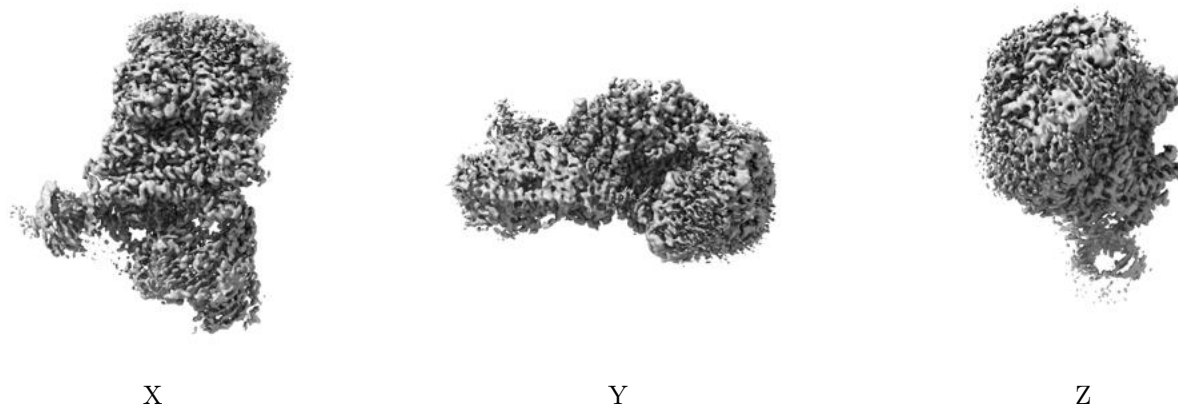


Z

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.

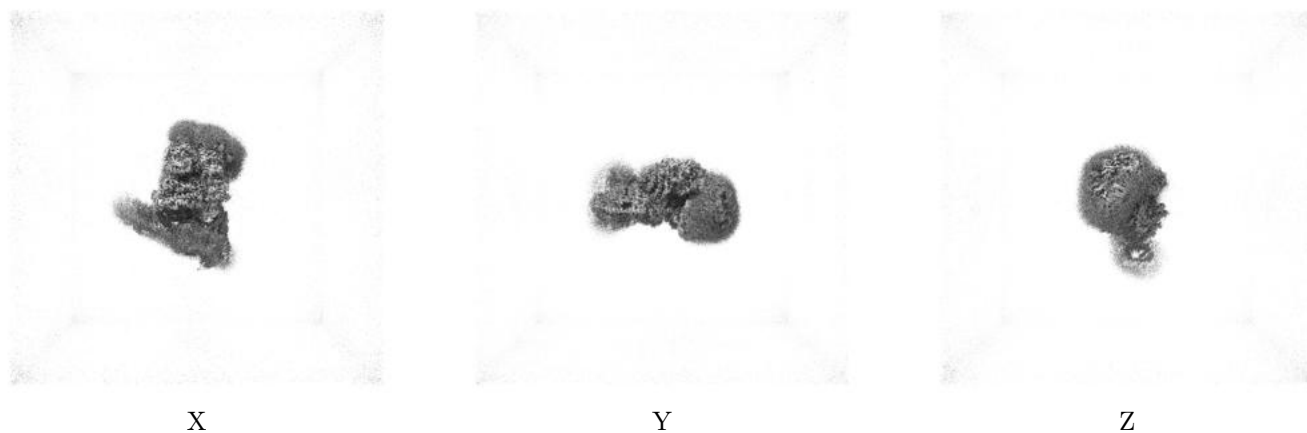
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.15. 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.

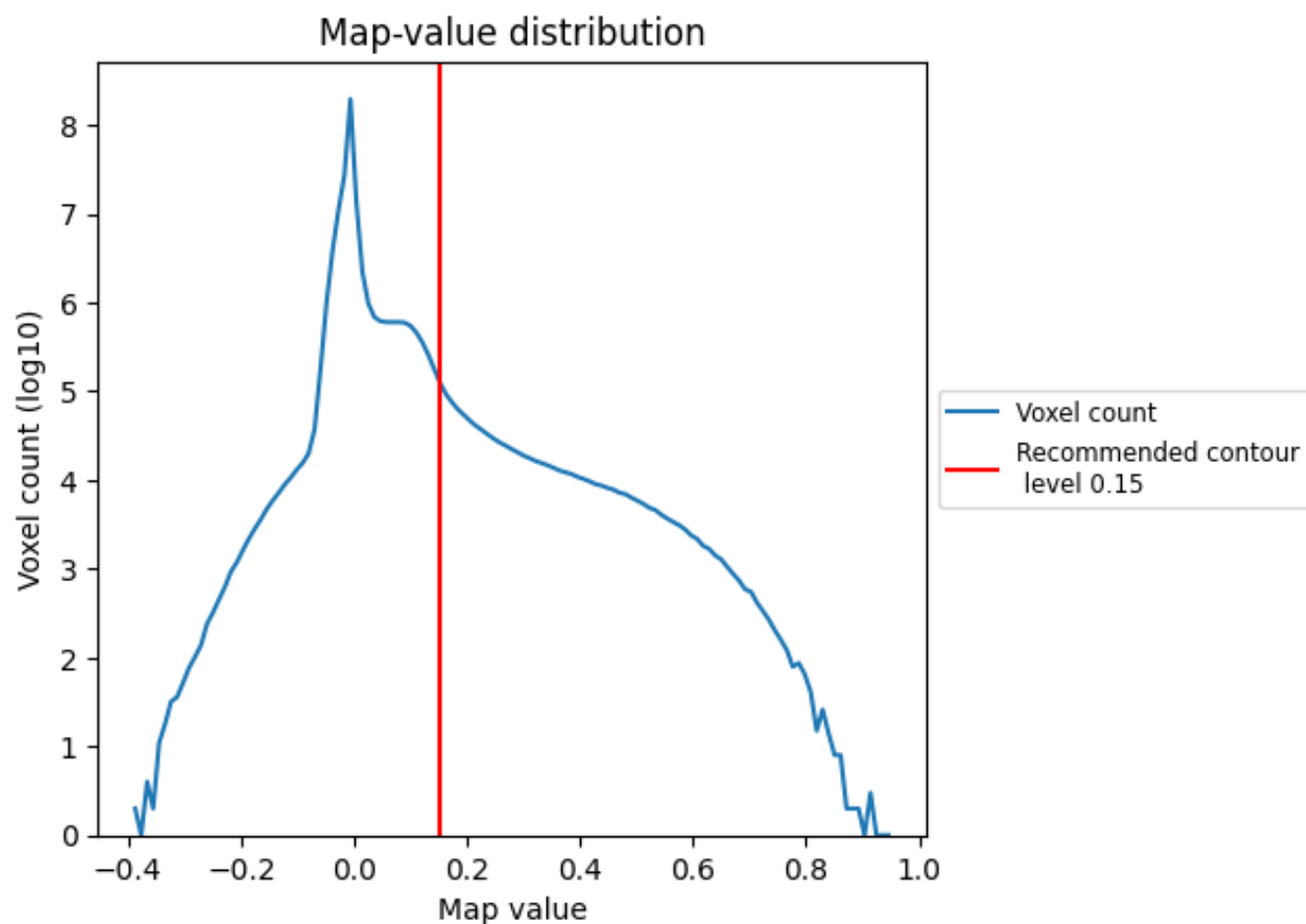
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

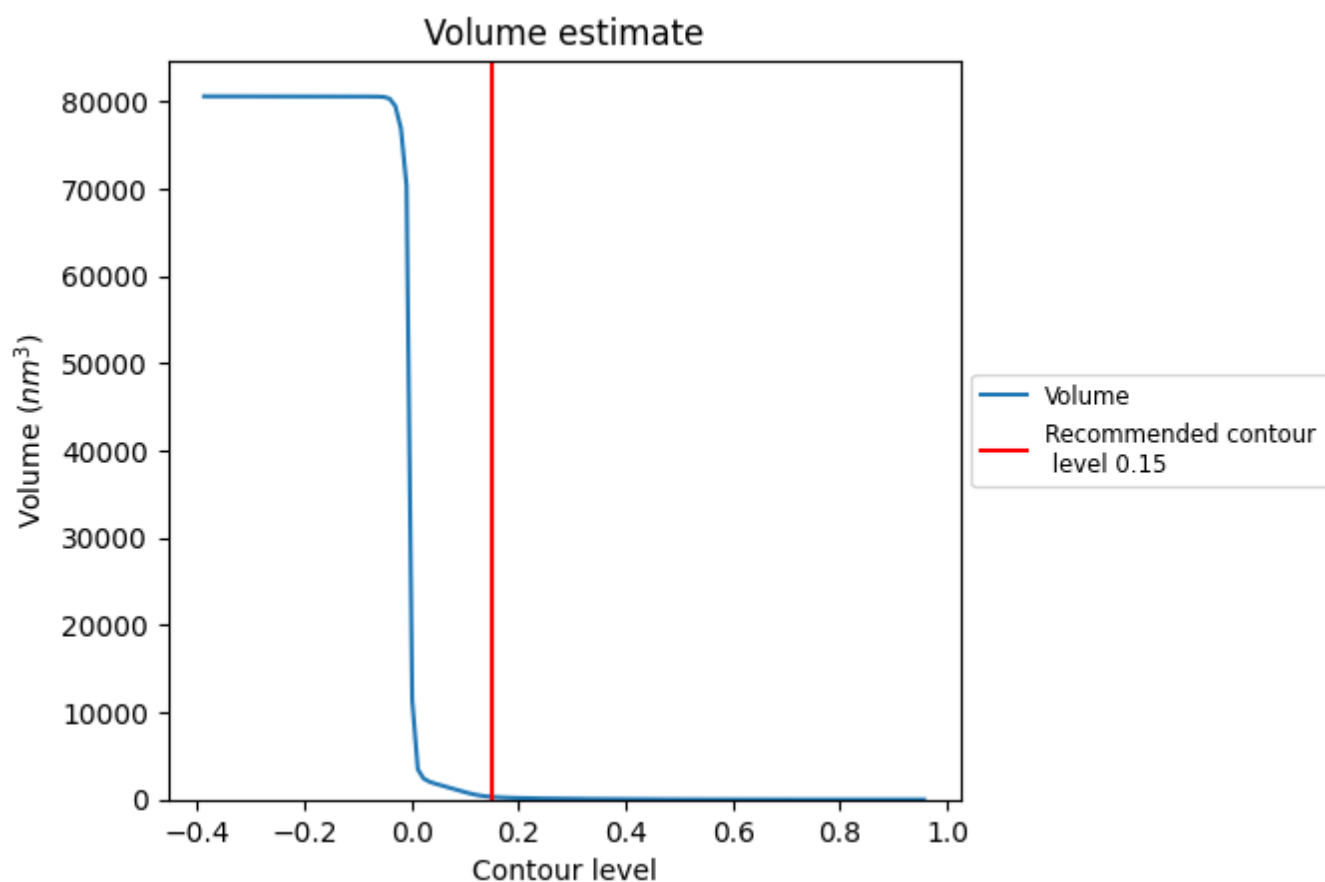
This section contains the results of statistical analysis of the map.

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.

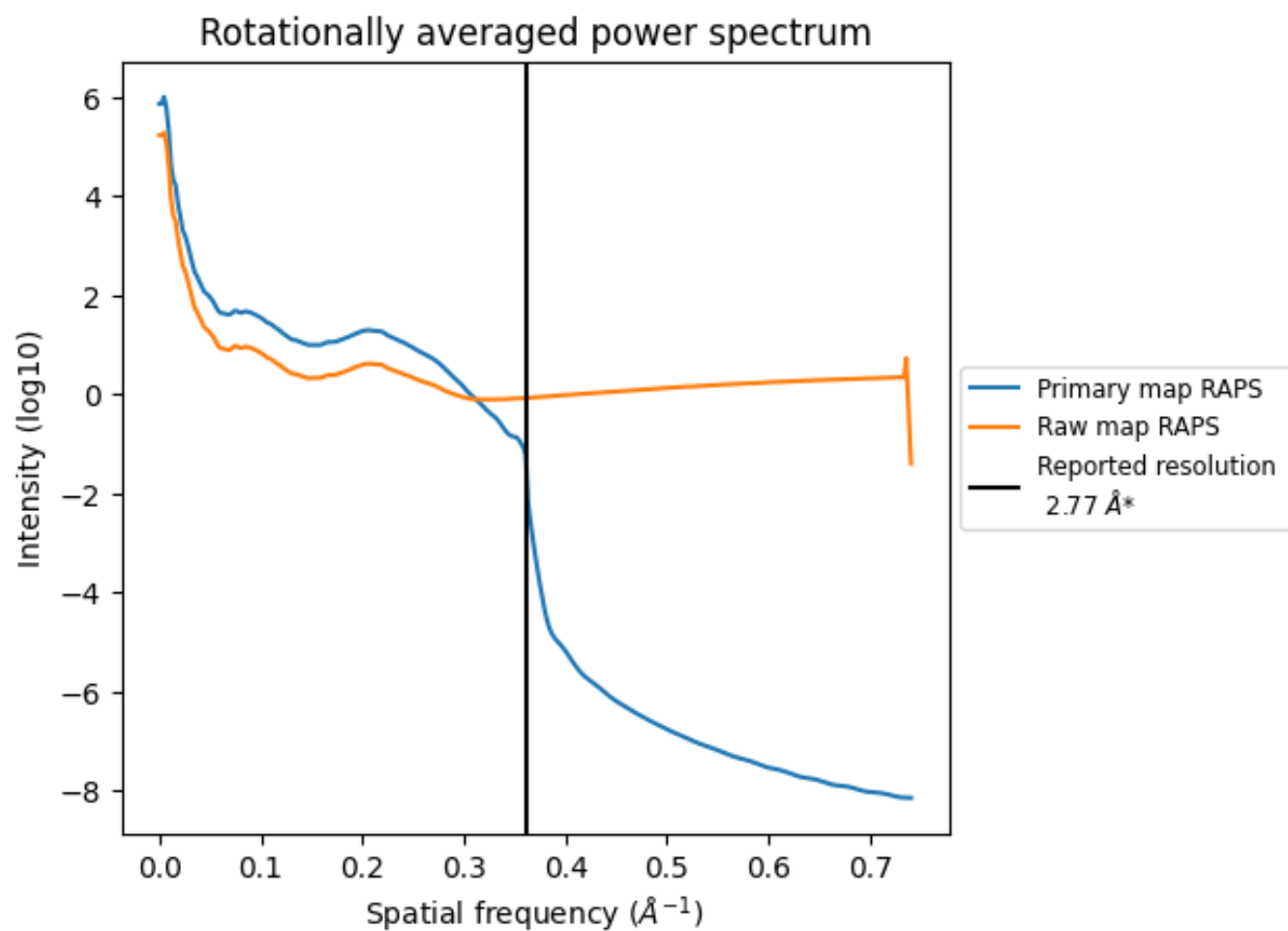
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 307 nm³; this corresponds to an approximate mass of 278 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 ⓘ

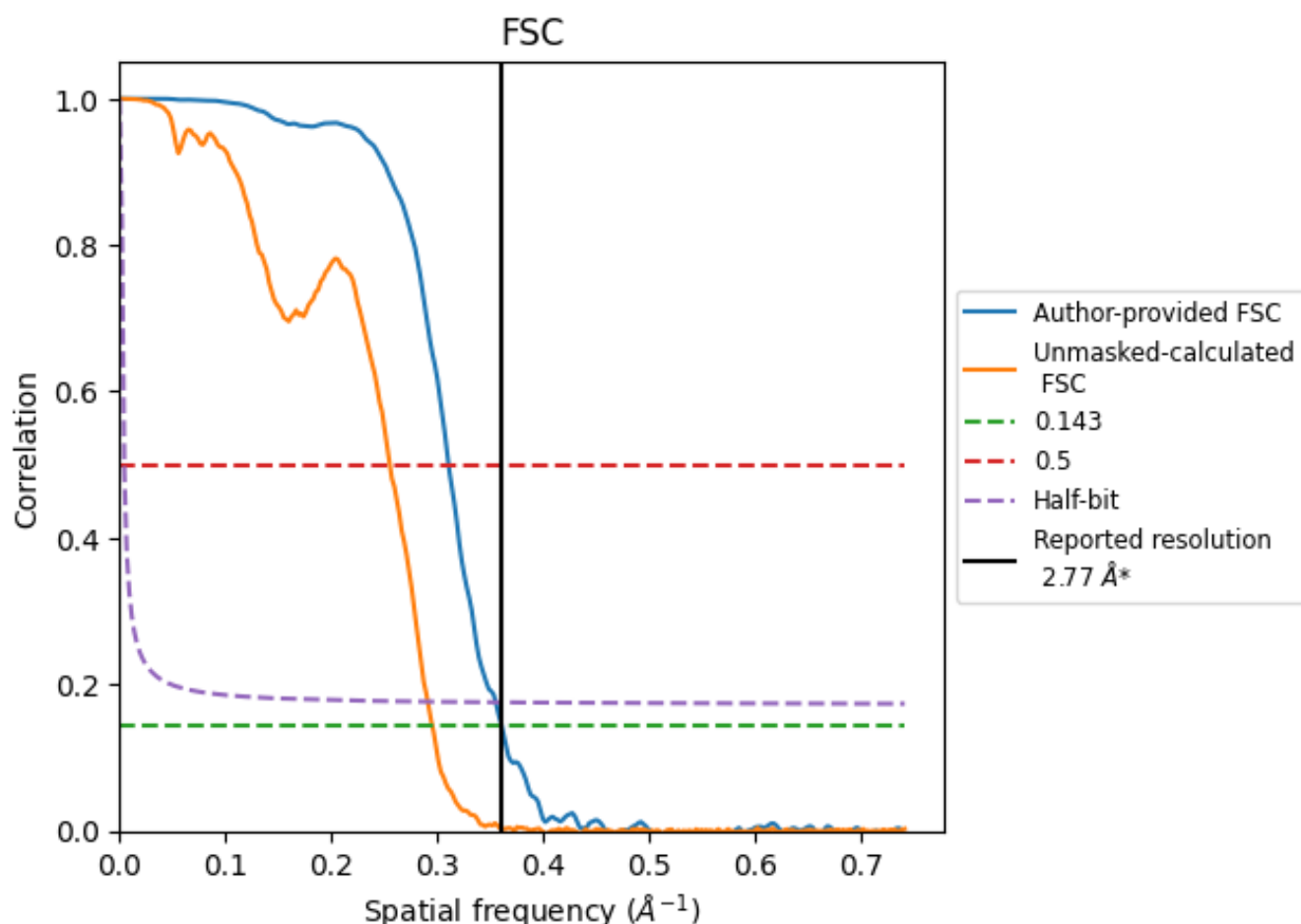


*Reported resolution corresponds to spatial frequency of 0.361 Å⁻¹

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 0.361 Å⁻¹

8.2 Resolution estimates [i](#)

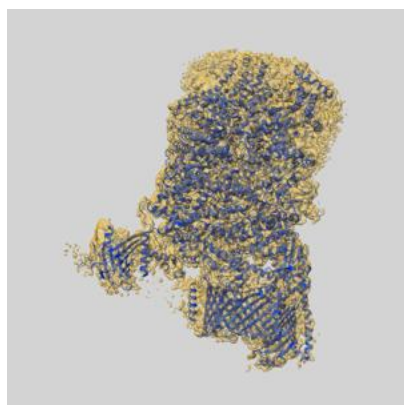
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.77	-	-
Author-provided FSC curve	2.77	3.22	2.82
Unmasked-calculated*	3.39	3.92	3.44

*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 3.39 differs from the reported value 2.77 by more than 10 %

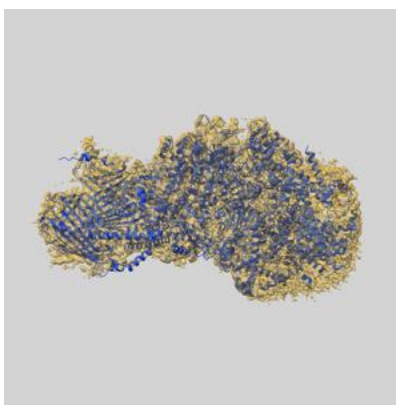
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-33528 and PDB model 7XZI. Per-residue inclusion information can be found in section [3](#) on page [11](#).

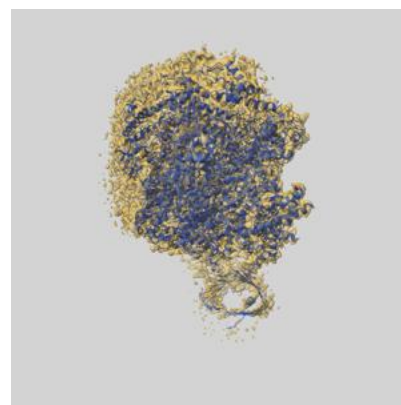
9.1 Map-model overlay [i](#)



X



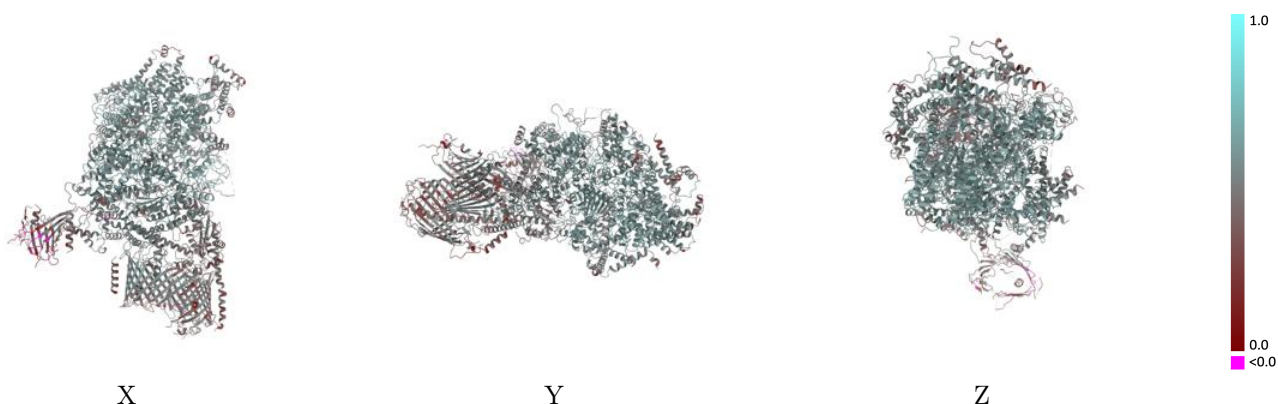
Y



Z

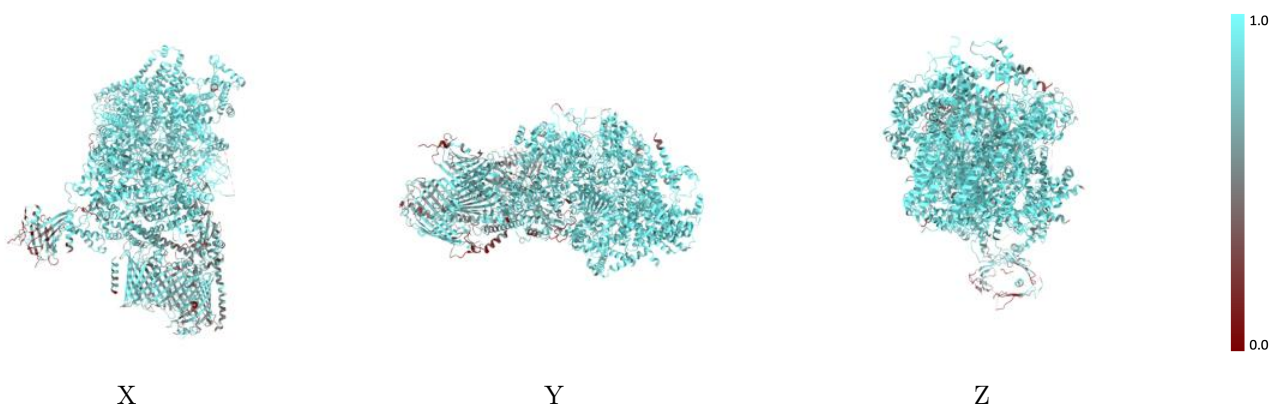
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



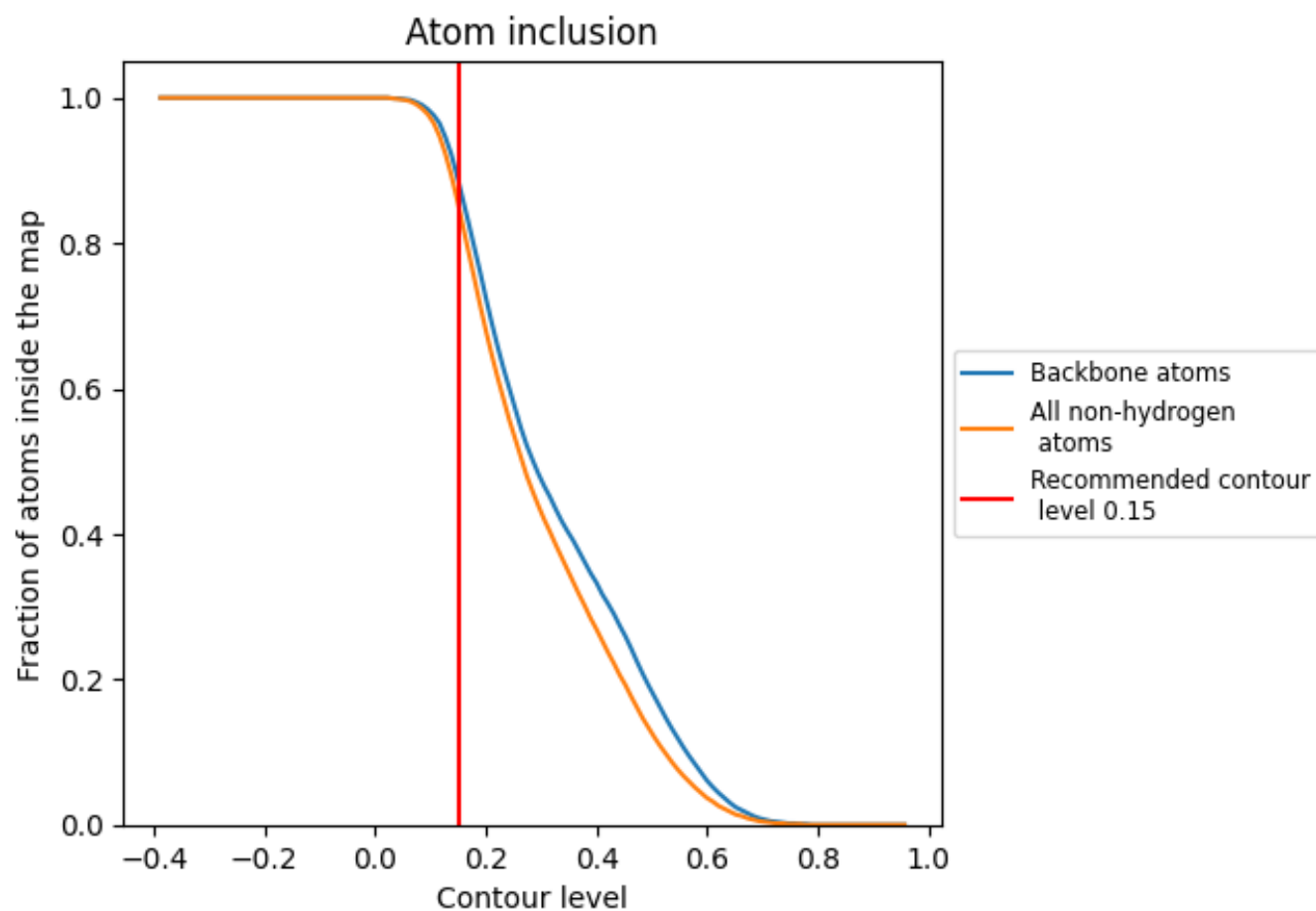
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.15).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 86% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8550	<div></div> 0.5170
3	<div></div> 0.8970	<div></div> 0.5330
4	<div></div> 0.6490	<div></div> 0.3700
5	<div></div> 0.9160	<div></div> 0.5440
7	<div></div> 0.7240	<div></div> 0.4460
9	<div></div> 0.7700	<div></div> 0.4760
A	<div></div> 0.8820	<div></div> 0.5400
B	<div></div> 0.9510	<div></div> 0.5620
C	<div></div> 0.9510	<div></div> 0.5850
D	<div></div> 0.8490	<div></div> 0.4460
E	<div></div> 0.9310	<div></div> 0.5610
F	<div></div> 0.9170	<div></div> 0.5670
G	<div></div> 0.6400	<div></div> 0.3790
U	<div></div> 0.8560	<div></div> 0.4860
X	<div></div> 0.6880	<div></div> 0.3600

1.0

0.0

<0.0