



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 01:57 PM UTC

PDB ID : 8XQX / pdb_00008xqx
EMDB ID : EMD-38590
Title : Cryo-EM structure of the Ycf2-FtsHi motor complex from *Chlamydomonas reinhardtii* in apo state
Authors : Liang, K.; Zhan, X.; Wu, J.; Yan, Z.
Deposited on : 2024-01-05
Resolution : 2.80 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:

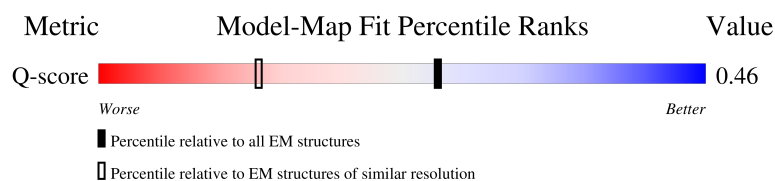
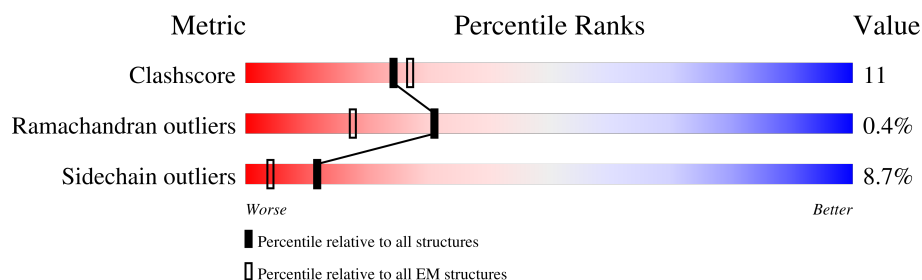
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11806 (2.30 - 3.30)

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	1182	
2	B	1112	
2	C	1112	
3	D	2971	

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Mol	Chain	Length	Quality of chain
4	E	982	
5	F	1024	
6	G	495	
7	H	555	
8	I	366	
9	J	117	
10	K	255	
11	L	303	
12	M	682	
13	N	137	
14	O	471	
15	P	691	
16	Q	365	
17	R	462	
18	S	324	
19	T	299	
20	U	156	
21	V	86	

2 Entry composition [i](#)

There are 29 unique types of molecules in this entry. The entry contains 73189 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 Fhl1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	988	Total	C	N	O	S	0	0
			7627	4839	1342	1410	36		

- Molecule 2 is a protein called Fhl3.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	751	Total	C	N	O	P	S	0	0
			5844	3675	1037	1094	3	35		
2	C	690	Total	C	N	O	S		0	0
			5324	3359	949	985	31			

- Molecule 3 is a protein called Ycf2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	1539	Total	C	N	O	S	0	0
			12719	8252	2175	2266	26		

- Molecule 4 is a protein called Ctap1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	868	Total	C	N	O	S	0	0
			6221	3881	1143	1183	14		

- Molecule 5 is a protein called Ctap6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	701	Total	C	N	O	S	0	0
			5333	3344	963	1007	19		

- Molecule 6 is a protein called ARHL.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	394	Total	C	N	O	S	0	0
			2931	1839	539	549	4		

- Molecule 7 is a protein called PcyA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	406	Total	C	N	O	S	0	0
			3246	2061	547	617	21		

- Molecule 8 is a protein called CrTam39.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	272	Total	C	N	O	S	0	0
			2119	1336	394	374	15		

- Molecule 9 is a protein called ACP.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	J	85	Total	C	N	O	P	S	0	0
			651	404	101	141	1	4		

- Molecule 10 is a protein called CrTam29.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	189	Total	C	N	O	S	0	0
			1567	1032	271	257	7		

- Molecule 11 is a protein called CrTam34.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	151	Total	C	N	O	S	0	0
			1254	844	210	196	4		

- Molecule 12 is a protein called FADL.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	390	Total	C	N	O	S	0	0
			3000	1958	510	516	16		

- Molecule 13 is a protein called CrTam15.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	115	Total	C	N	O	S	0	0
			921	585	172	161	3		

- Molecule 14 is a protein called CrTam49.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	318	Total	C	N	O	S	0	0
			1718	1044	335	337	2		

- Molecule 15 is a protein called Ctap7.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	617	Total	C	N	O	S	0	0
			4510	2802	829	868	11		

- Molecule 16 is a protein called Tic22.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	262	Total	C	N	O	S	0	0
			2078	1316	365	388	9		

- Molecule 17 is a protein called DnaJ.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	401	Total	C	N	O	P S	0	0
			3160	1981	571	585	2 21		

- Molecule 18 is a protein called CrTam35.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	117	Total	C	N	O	P S	0	0
			951	588	169	190	3 1		

- Molecule 19 is a protein called CrTam31.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	110	Total	C	N	O	P S	0	0
			868	535	147	182	2 2		

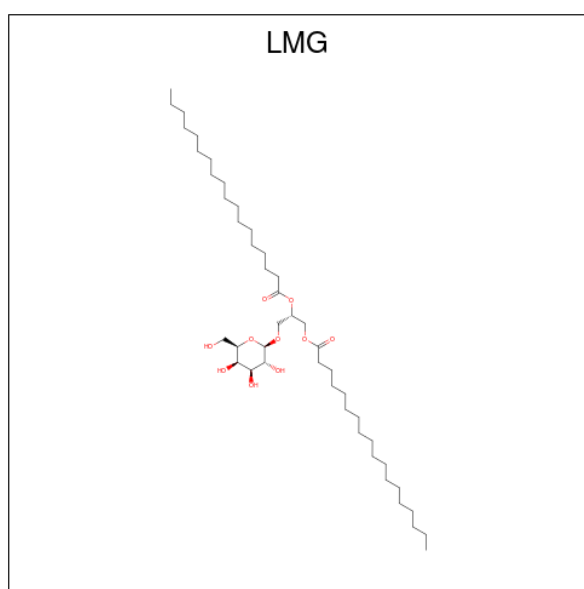
- Molecule 20 is a protein called UNK.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	U	36	Total	C	N	O	1	0
			188	115	36	37		

- Molecule 21 is a protein called UNK.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	V	68	Total	C	N	O	0	0
			340	204	68	68		

- Molecule 22 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).

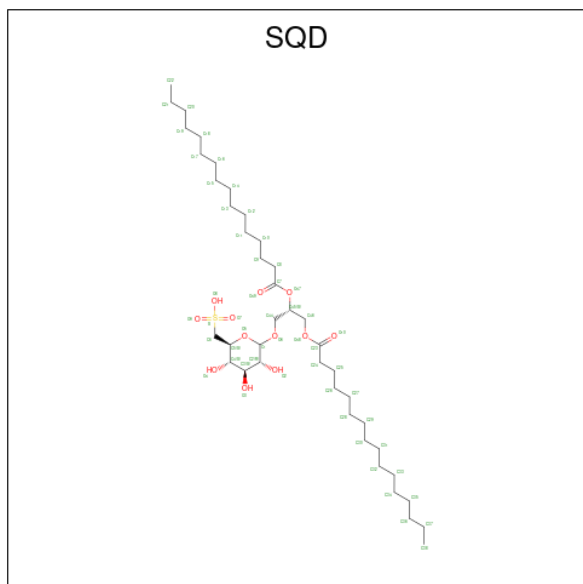


Mol	Chain	Residues	Atoms			AltConf
22	A	1	Total	C	O	0
			46	36	10	
22	C	1	Total	C	O	0
			25	20	5	
22	I	1	Total	C	O	0
			32	22	10	
22	K	1	Total	C	O	0
			41	31	10	
22	M	1	Total	C	O	0
			48	38	10	

- Molecule 23 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

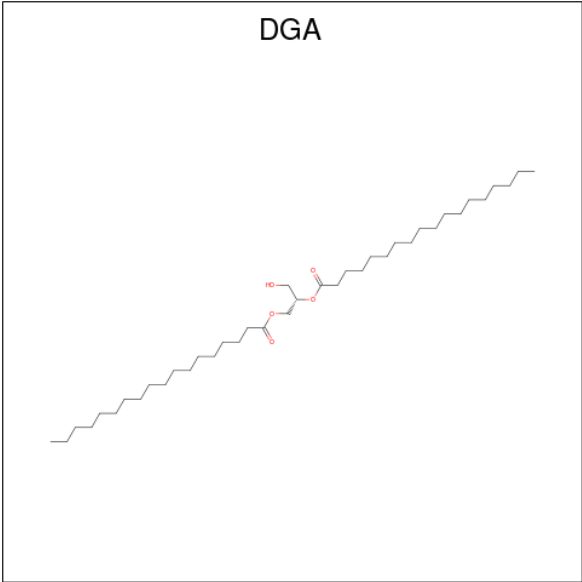
Mol	Chain	Residues	Atoms		AltConf
23	A	1	Total	Mg	0
			1	1	

- Molecule 24 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



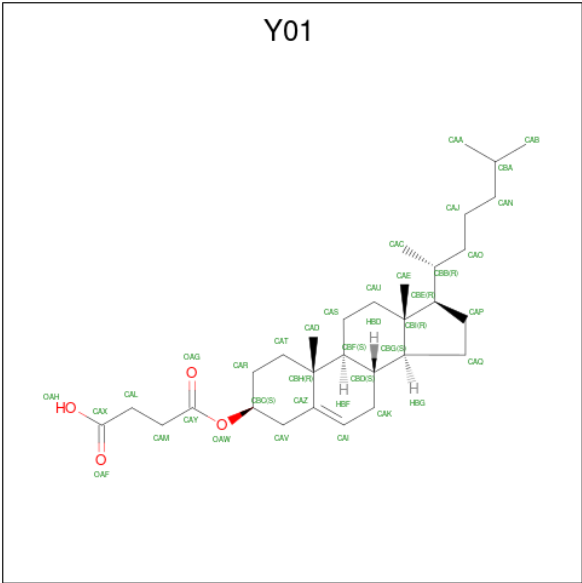
Mol	Chain	Residues	Atoms				AltConf
24	B	1	Total	C	O	S	0
			46	33	12	1	
24	I	1	Total	C	O	S	0
			49	36	12	1	
24	K	1	Total	C	O	S	0
			45	32	12	1	

- Molecule 25 is DIACYL GLYCEROL (CCD ID: DGA) (formula: $C_{39}H_{76}O_5$).



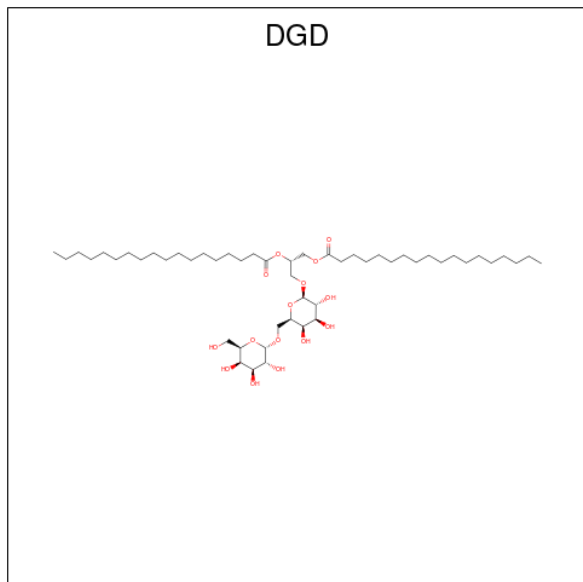
Mol	Chain	Residues	Atoms			AltConf
25	D	1	Total	C	O	0
			39	34	5	
25	L	1	Total	C	O	0
			34	29	5	

- Molecule 26 is CHOLESTEROL HEMISUCCINATE (CCD ID: Y01) (formula: C₃₁H₅₀O₄).



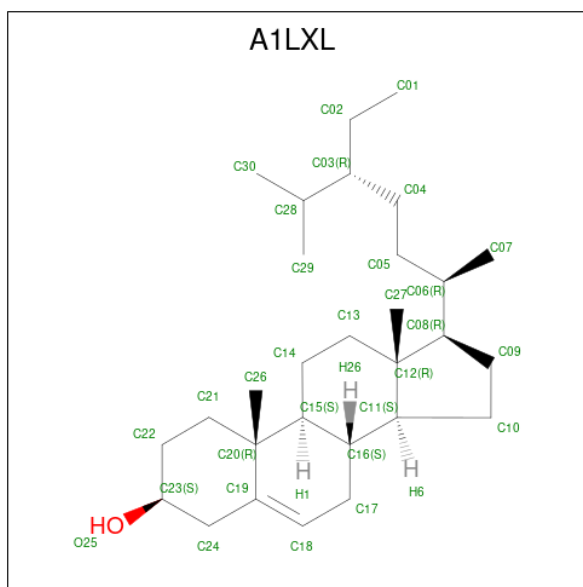
Mol	Chain	Residues	Atoms			AltConf
26	D	1	Total	C	O	0
			35	31	4	
26	M	1	Total	C	O	0
			35	31	4	

- Molecule 27 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms			AltConf
27	I	1	Total	C	O	0
			40	25	15	
27	N	1	Total	C	O	0
			41	26	15	

- Molecule 28 is Beta-Sitosterol (CCD ID: A1LXL) (formula: $C_{29}H_{50}O$).



Mol	Chain	Residues	Atoms			AltConf
28	P	1	Total	C	O	0
			30	29	1	
28	P	1	Total	C	O	0
			30	29	1	

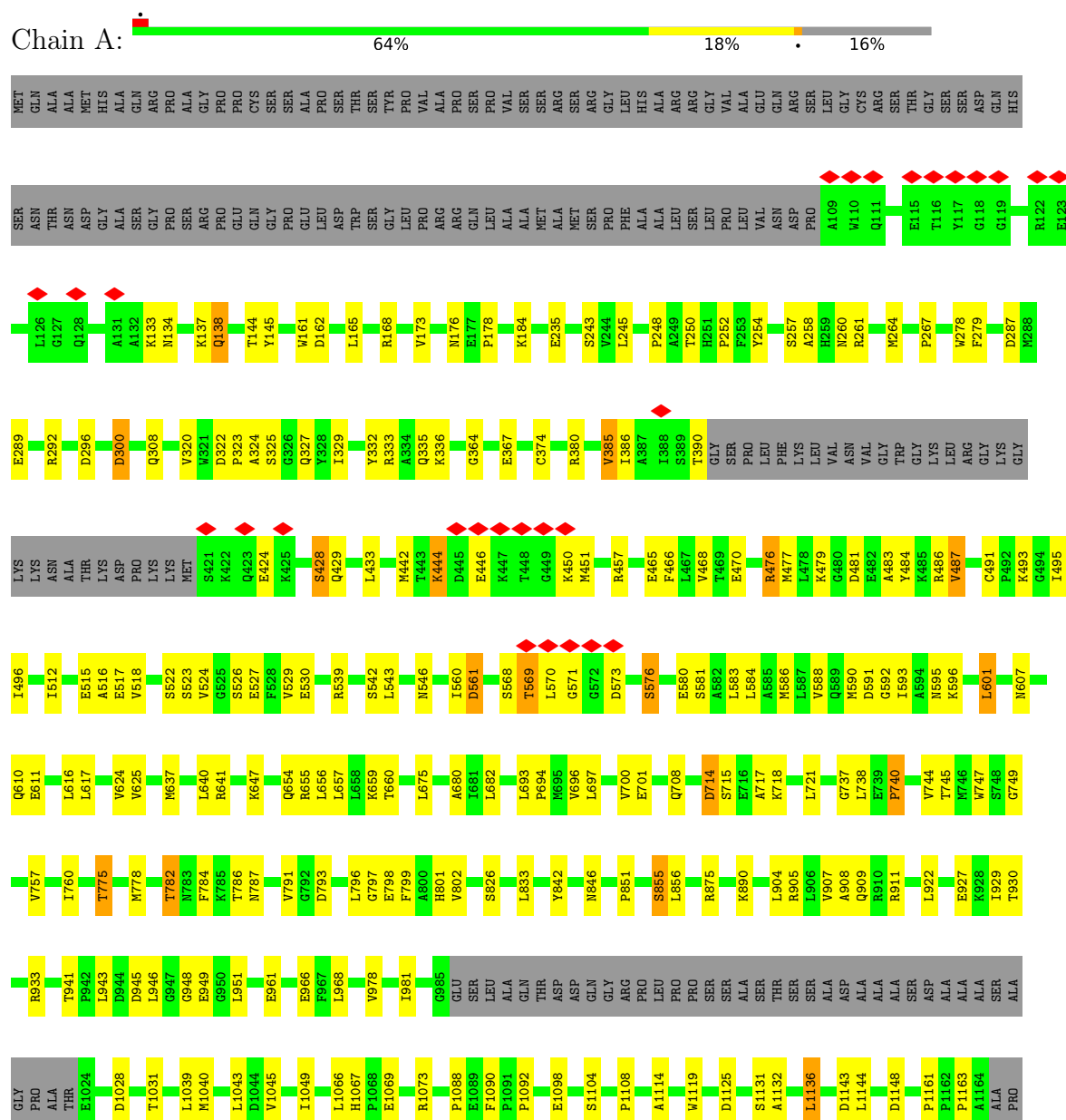
- Molecule 29 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
29	R	2	Total	Zn	0
			2	2	

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

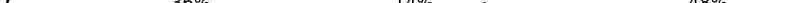
• Molecule 1: Fhl1



Chain B:

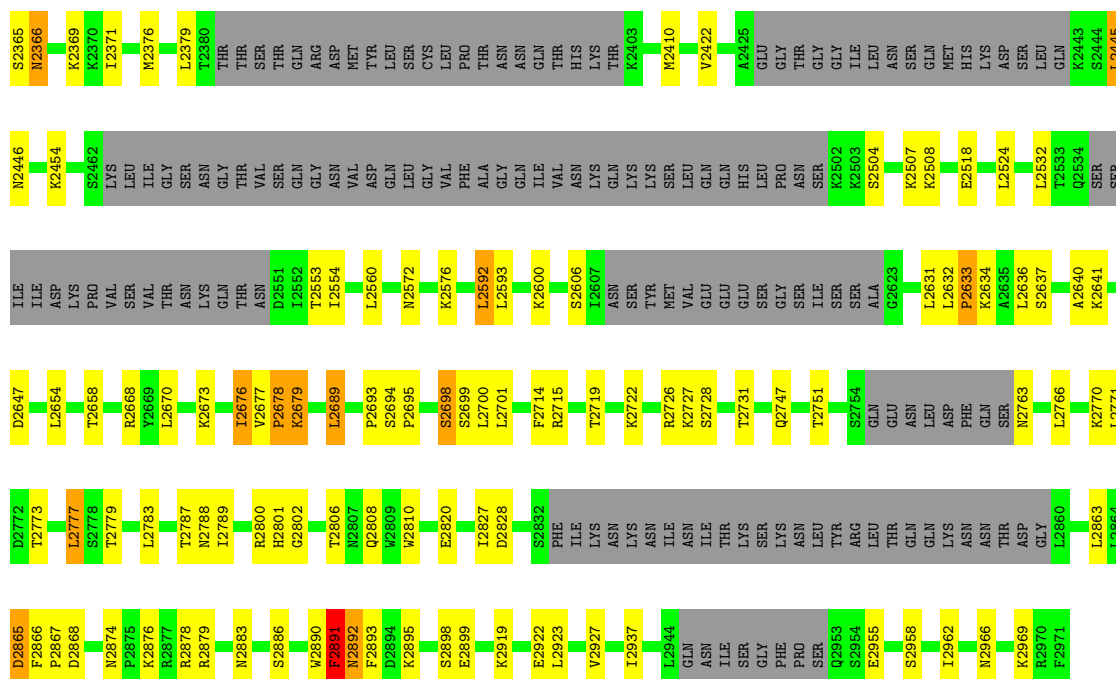


- Molecule 3: Ycf2

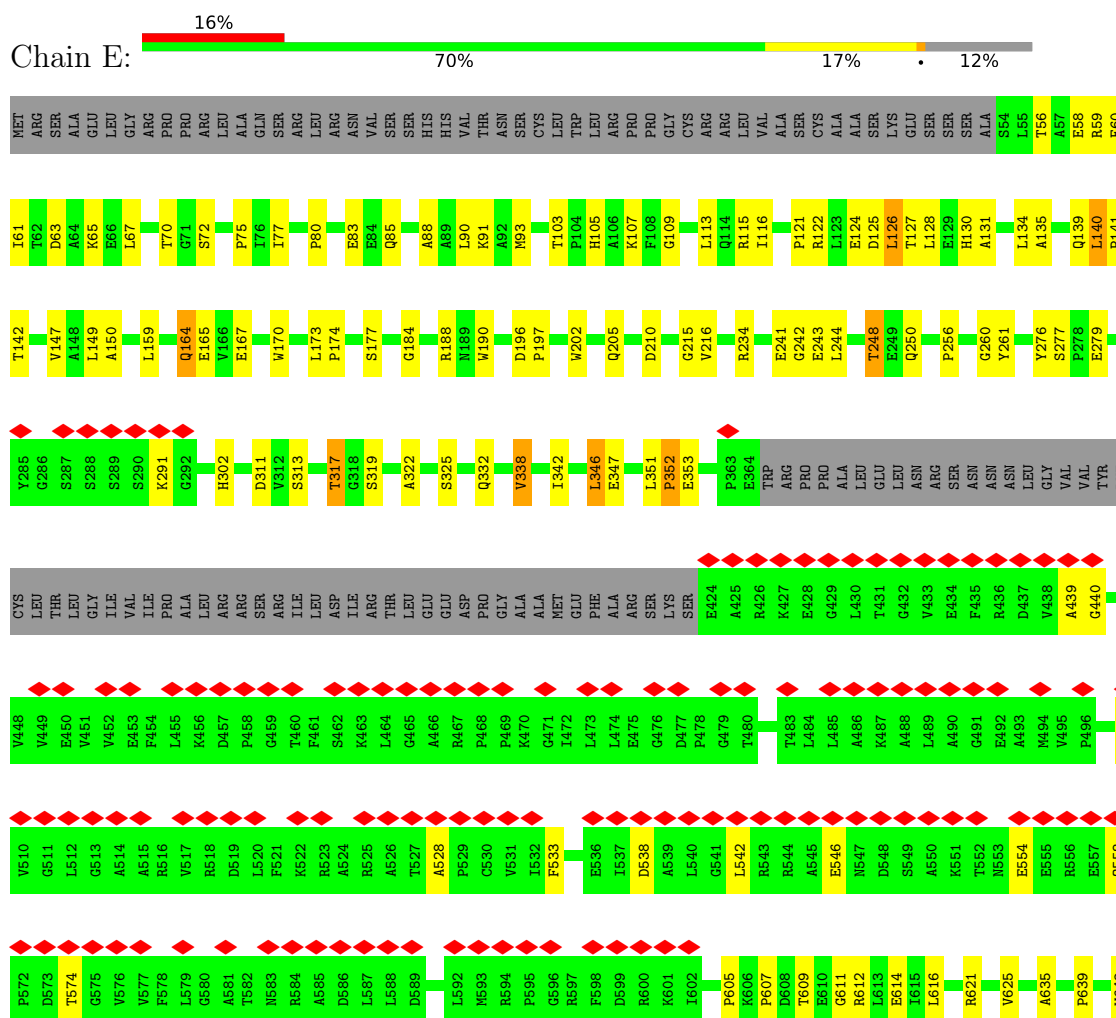
Chain D:  36% 14% 48%

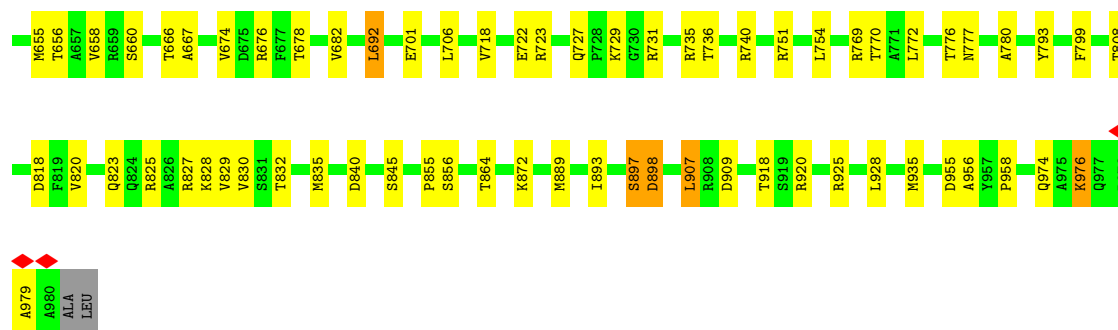




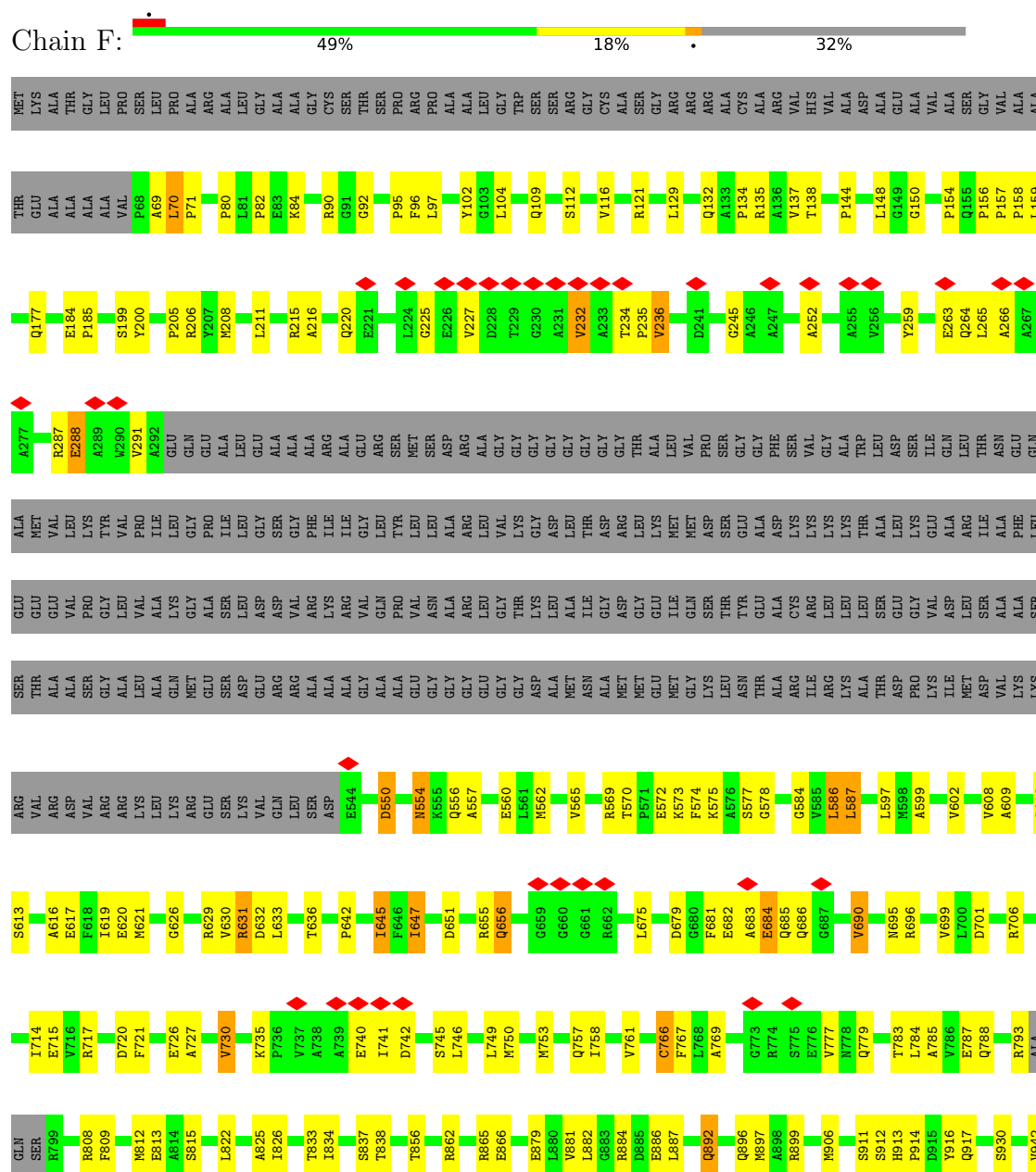


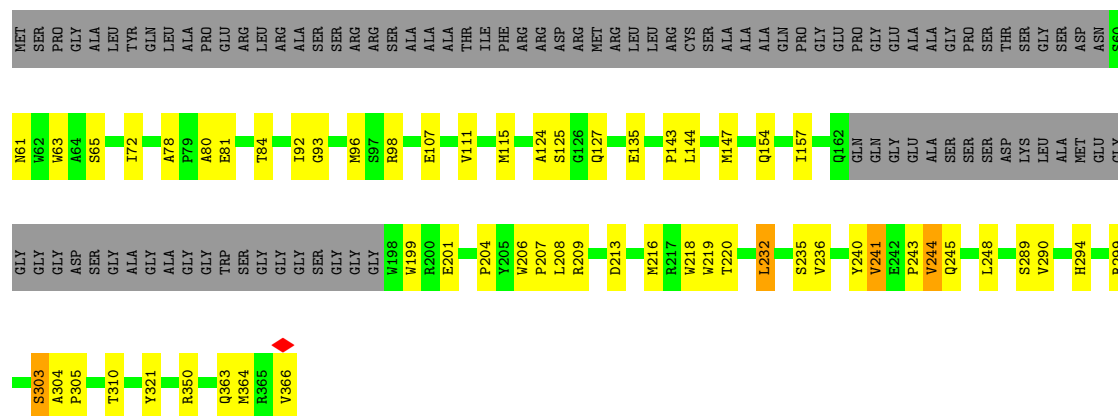
• Molecule 4: Ctap1





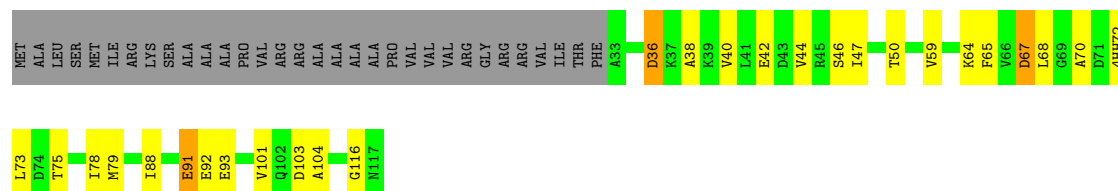
• Molecule 5: Ctap6





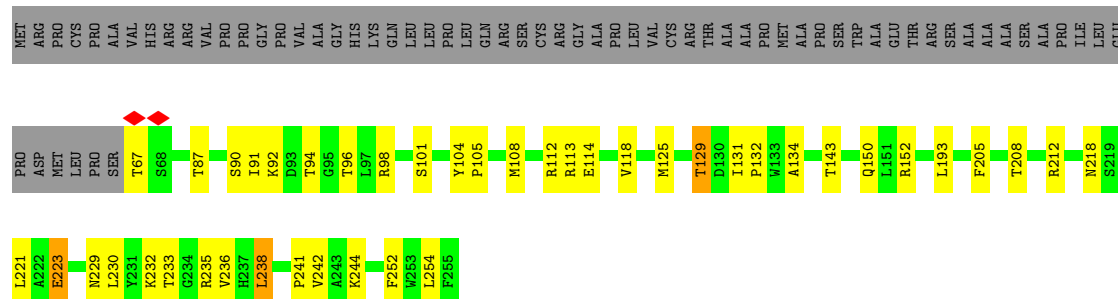
• Molecule 9: ACP

Chain J: 50% 21% • 27%



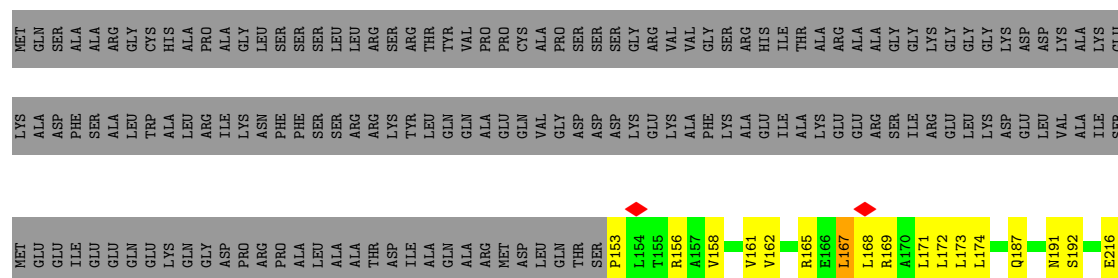
• Molecule 10: CrTam29

Chain K: 57% 16% • 26%



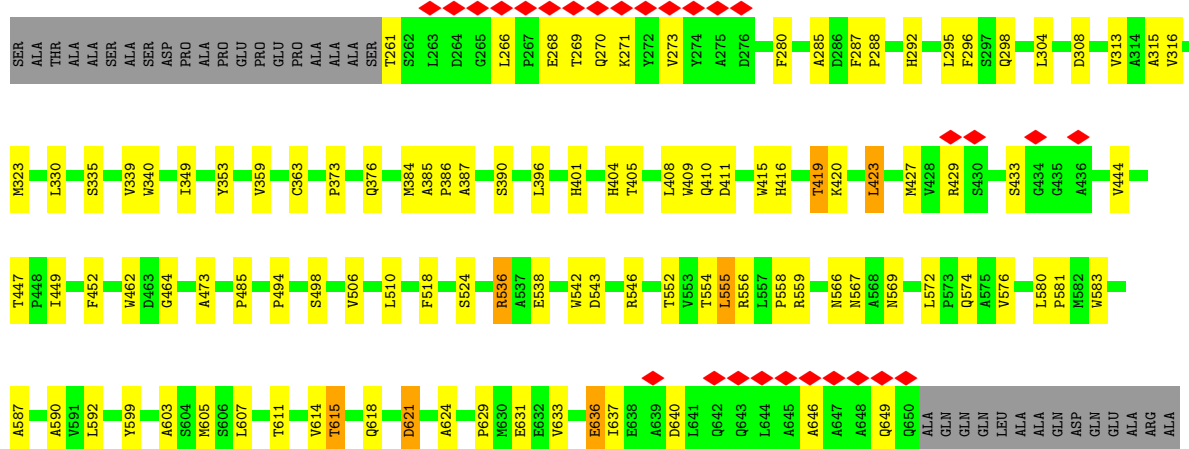
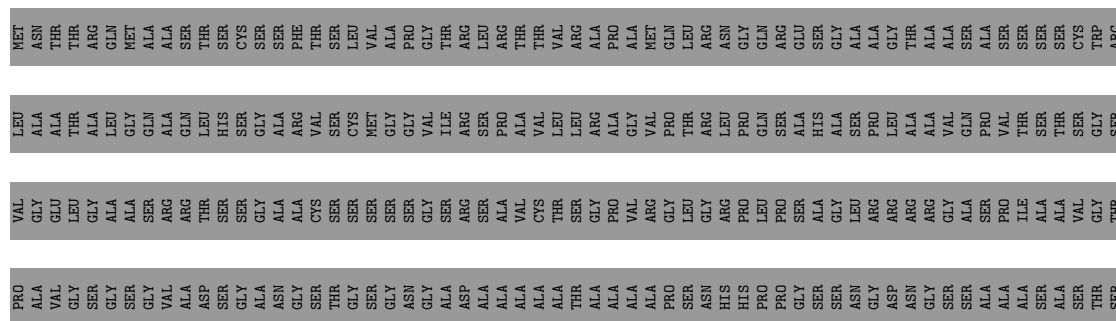
• Molecule 11: CrTam34

Chain L: 38% 11% 50%

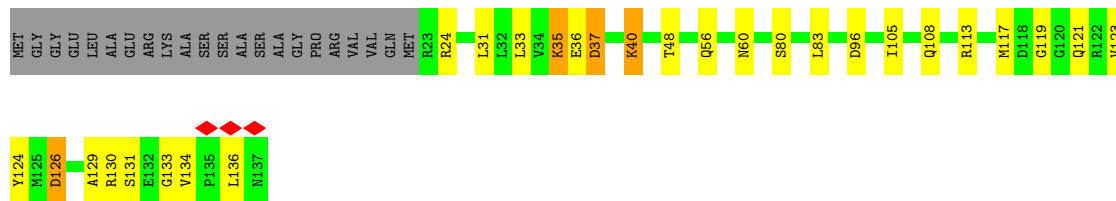




• Molecule 12: FADL

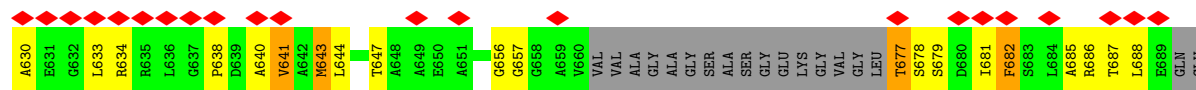
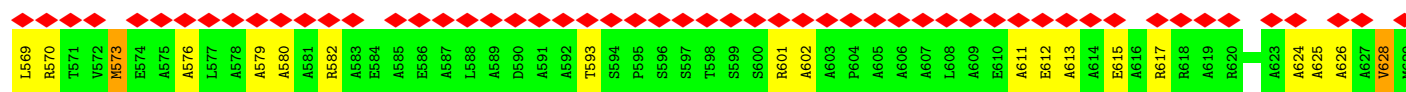


• Molecule 13: CrTam15

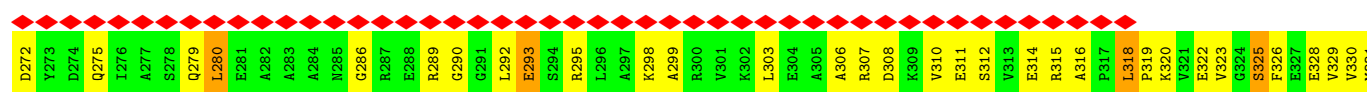
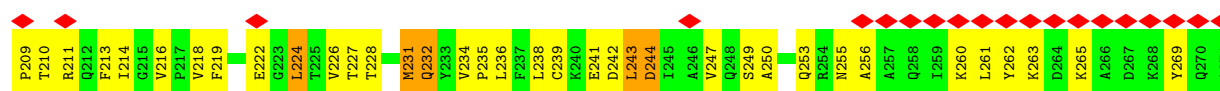
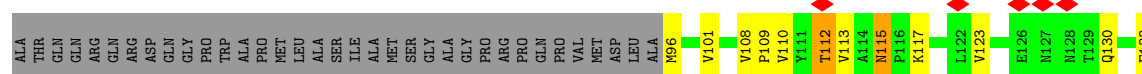
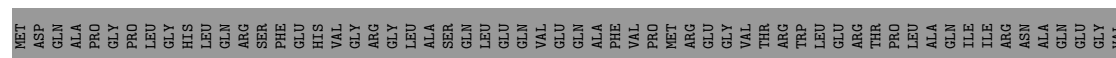


• Molecule 14: CrTam49

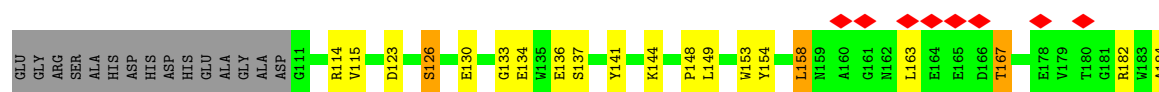




• Molecule 16: Tic22

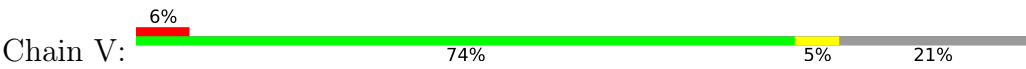


• Molecule 17: DnaJ





● Molecule 21: UNK



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	461334	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)	1400	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	5.356	Depositor
Minimum map value	-2.856	Depositor
Average map value	0.008	Depositor
Map value standard deviation	0.130	Depositor
Recommended contour level	0.35	Depositor
Map size (Å)	391.32, 391.32, 391.32	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.087, 1.087, 1.087	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 4HH, A1LXL, DGD, SQD, MG, SEP, Y01, ZN, TPO, DGA, LMG

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	0.33	0/7792	0.51	3/10575 (0.0%)
2	B	0.37	1/5925 (0.0%)	0.57	2/8024 (0.0%)
2	C	0.33	0/5432	0.50	0/7359
3	D	0.36	0/12978	0.60	14/17507 (0.1%)
4	E	0.35	0/6350	0.56	2/8655 (0.0%)
5	F	0.31	0/5432	0.49	0/7366
6	G	0.36	0/2999	0.60	2/4087 (0.0%)
7	H	0.36	0/3324	0.48	0/4515
8	I	0.36	0/2177	0.51	0/2958
9	J	0.32	0/625	0.55	0/839
10	K	0.34	0/1627	0.54	0/2223
11	L	0.32	0/1303	0.48	0/1786
12	M	0.23	0/3103	0.47	0/4258
13	N	0.29	0/945	0.50	0/1280
14	O	0.19	0/1731	0.46	0/2391
15	P	0.23	0/4601	0.53	0/6273
16	Q	0.25	0/2115	0.53	0/2857
17	R	0.29	1/3224 (0.0%)	0.53	1/4379 (0.0%)
18	S	0.17	0/936	0.47	0/1267
19	T	0.20	0/862	0.51	0/1164
20	U	0.12	0/45	0.23	0/58
All	All	0.32	2/73526 (0.0%)	0.54	24/99821 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	D	0	2
4	E	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
6	G	0	2
All	All	0	5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	794	PRO	C-O	-6.48	1.15	1.24
17	R	290	ASP	C-N	-5.46	1.23	1.33

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	2891	PHE	CA-CB-CG	-18.73	95.08	113.80
3	D	2678	PRO	N-CA-CB	-10.37	92.36	103.25
3	D	2678	PRO	N-CD-CG	-9.34	89.18	103.20
4	E	546	GLU	CB-CA-C	-8.47	100.80	111.22
3	D	971	PRO	N-CA-C	-7.59	96.84	112.47

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	962	ARG	Sidechain
3	D	979	ARG	Sidechain
4	E	676	ARG	Sidechain
6	G	257	ARG	Sidechain
6	G	265	ARG	Sidechain

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	7627	0	7581	148	0
2	B	5844	0	5785	168	0
2	C	5324	0	5301	147	0
3	D	12719	0	13029	315	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	6221	0	5650	114	0
5	F	5333	0	5318	132	0
6	G	2931	0	2867	67	0
7	H	3246	0	3152	61	0
8	I	2119	0	2069	46	0
9	J	651	0	657	18	0
10	K	1567	0	1558	24	0
11	L	1254	0	1246	22	0
12	M	3000	0	2945	63	0
13	N	921	0	917	21	0
14	O	1718	0	1100	9	0
15	P	4510	0	4451	175	0
16	Q	2078	0	2090	94	0
17	R	3160	0	3001	91	0
18	S	951	0	924	27	0
19	T	868	0	824	30	0
20	U	188	0	60	2	0
21	V	340	0	76	3	0
22	A	46	0	62	3	0
22	C	25	0	31	0	0
22	I	32	0	34	2	0
22	K	41	0	52	1	0
22	M	48	0	66	1	0
23	A	1	0	0	0	0
24	B	46	0	55	0	0
24	I	49	0	65	5	0
24	K	45	0	53	0	0
25	D	39	0	63	1	0
25	L	34	0	50	1	0
26	D	35	0	49	0	0
26	M	35	0	49	4	0
27	I	40	0	38	2	0
27	N	41	0	40	0	0
28	P	60	0	0	9	0
29	R	2	0	0	0	0
All	All	73189	0	71308	1549	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 11.

The worst 5 of 1549 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:B:760:ALA:O	2:B:763:GLU:HB2	1.68	0.94
16:Q:286:GLY:H	16:Q:289:ARG:HG2	1.31	0.93
15:P:472:THR:OG1	28:P:701:A1LXL:C17	2.22	0.88
3:D:881:LEU:HD11	3:D:990:LYS:HA	1.55	0.85
4:E:439:ALA:HB1	4:E:614:GLU:HG3	1.58	0.85

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	982/1182 (83%)	912 (93%)	70 (7%)	0	100	100
2	B	736/1112 (66%)	683 (93%)	51 (7%)	2 (0%)	36	66
2	C	682/1112 (61%)	622 (91%)	58 (8%)	2 (0%)	36	66
3	D	1471/2971 (50%)	1341 (91%)	116 (8%)	14 (1%)	12	38
4	E	864/982 (88%)	798 (92%)	64 (7%)	2 (0%)	43	72
5	F	695/1024 (68%)	646 (93%)	48 (7%)	1 (0%)	48	77
6	G	392/495 (79%)	359 (92%)	30 (8%)	3 (1%)	16	44
7	H	404/555 (73%)	384 (95%)	19 (5%)	1 (0%)	43	72
8	I	268/366 (73%)	243 (91%)	25 (9%)	0	100	100
9	J	82/117 (70%)	78 (95%)	4 (5%)	0	100	100
10	K	187/255 (73%)	167 (89%)	17 (9%)	3 (2%)	7	27
11	L	149/303 (49%)	135 (91%)	14 (9%)	0	100	100
12	M	388/682 (57%)	357 (92%)	31 (8%)	0	100	100
13	N	113/137 (82%)	107 (95%)	6 (5%)	0	100	100
14	O	312/471 (66%)	288 (92%)	24 (8%)	0	100	100
15	P	613/691 (89%)	558 (91%)	53 (9%)	2 (0%)	36	66

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	Q	260/365 (71%)	245 (94%)	15 (6%)	0	100	100
17	R	393/462 (85%)	356 (91%)	35 (9%)	2 (0%)	24	55
18	S	112/324 (35%)	101 (90%)	11 (10%)	0	100	100
19	T	106/299 (36%)	95 (90%)	10 (9%)	1 (1%)	14	41
20	U	6/156 (4%)	5 (83%)	1 (17%)	0	100	100
All	All	9215/14061 (66%)	8480 (92%)	702 (8%)	33 (0%)	31	60

5 of 33 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	971	PRO
3	D	2777	LEU
3	D	2801	HIS
3	D	2891	PHE
3	D	60	ASN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	774/936 (83%)	724 (94%)	50 (6%)	15	43
2	B	599/858 (70%)	538 (90%)	61 (10%)	7	23
2	C	548/858 (64%)	501 (91%)	47 (9%)	10	31
3	D	1443/2762 (52%)	1316 (91%)	127 (9%)	9	29
4	E	536/774 (69%)	491 (92%)	45 (8%)	10	32
5	F	542/773 (70%)	498 (92%)	44 (8%)	11	33
6	G	283/358 (79%)	251 (89%)	32 (11%)	5	19
7	H	346/451 (77%)	315 (91%)	31 (9%)	9	28
8	I	204/263 (78%)	190 (93%)	14 (7%)	14	41
9	J	64/87 (74%)	56 (88%)	8 (12%)	4	15
10	K	163/215 (76%)	147 (90%)	16 (10%)	7	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	L	124/243 (51%)	118 (95%)	6 (5%)	23	56
12	M	298/492 (61%)	276 (93%)	22 (7%)	13	37
13	N	92/107 (86%)	83 (90%)	9 (10%)	7	25
14	O	37/340 (11%)	34 (92%)	3 (8%)	11	33
15	P	431/485 (89%)	383 (89%)	48 (11%)	6	20
16	Q	218/296 (74%)	192 (88%)	26 (12%)	5	17
17	R	312/345 (90%)	290 (93%)	22 (7%)	13	39
18	S	97/226 (43%)	91 (94%)	6 (6%)	16	45
19	T	83/198 (42%)	76 (92%)	7 (8%)	10	32
20	U	1/7 (14%)	1 (100%)	0	100	100
All	All	7195/11074 (65%)	6571 (91%)	624 (9%)	12	30

5 of 624 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	K	98	ARG
16	Q	182	LEU
11	L	174	LEU
10	K	96	THR
15	P	116	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 179 such sidechains are listed below:

Mol	Chain	Res	Type
5	F	867	GLN
11	L	191	ASN
5	F	913	HIS
7	H	114	GLN
12	M	517	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

11 non-standard protein/DNA/RNA residues 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
2	TPO	B	337	2	8,10,11	1.66	1 (12%)	10,14,16	1.80	2 (20%)
19	SEP	T	28	19	8,9,10	1.61	1 (12%)	7,12,14	1.27	1 (14%)
18	SEP	S	85	18	8,9,10	1.61	1 (12%)	7,12,14	1.01	0
9	4HH	J	72	9	22,26,27	0.38	0	27,35,37	0.60	0
17	SEP	R	126	17	8,9,10	1.58	1 (12%)	7,12,14	0.95	0
19	SEP	T	18	19	8,9,10	1.60	1 (12%)	7,12,14	1.48	1 (14%)
18	SEP	S	84	18	8,9,10	1.62	1 (12%)	7,12,14	1.37	1 (14%)
17	TPO	R	167	17	8,10,11	1.07	0	10,14,16	2.26	1 (10%)
18	TPO	S	107	18	8,10,11	1.63	1 (12%)	10,14,16	1.92	1 (10%)
2	TPO	B	346	2	8,10,11	1.63	1 (12%)	10,14,16	1.92	1 (10%)
2	TPO	B	347	2	8,10,11	1.11	0	10,14,16	2.24	1 (10%)

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
2	TPO	B	337	2	-	4/9/11/13	-
19	SEP	T	28	19	-	1/6/8/10	-
18	SEP	S	85	18	-	2/6/8/10	-
9	4HH	J	72	9	-	5/33/35/37	-
17	SEP	R	126	17	-	0/6/8/10	-
19	SEP	T	18	19	-	0/6/8/10	-
18	SEP	S	84	18	-	2/6/8/10	-
17	TPO	R	167	17	-	1/9/11/13	-
18	TPO	S	107	18	-	1/9/11/13	-
2	TPO	B	346	2	-	3/9/11/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TPO	B	347	2	-	5/9/11/13	-

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	S	84	SEP	P-O1P	3.54	1.61	1.50
2	B	337	TPO	P-O1P	3.52	1.61	1.50
2	B	346	TPO	P-O1P	3.51	1.61	1.50
19	T	18	SEP	P-O1P	3.51	1.61	1.50
19	T	28	SEP	P-O1P	3.51	1.61	1.50

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	R	167	TPO	P-OG1-CB	-6.64	105.28	123.33
2	B	347	TPO	P-OG1-CB	-6.48	105.72	123.33
2	B	346	TPO	P-OG1-CB	-5.61	108.09	123.33
18	S	107	TPO	P-OG1-CB	-5.56	108.21	123.33
2	B	337	TPO	P-OG1-CB	-4.70	110.55	123.33

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	S	84	SEP	N-CA-CB-OG
18	S	84	SEP	C-CA-CB-OG
18	S	85	SEP	N-CA-CB-OG
18	S	107	TPO	O-C-CA-CB
2	B	337	TPO	C-CA-CB-CG2

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	J	72	4HH	1	0
17	R	126	SEP	1	0
17	R	167	TPO	2	0
2	B	346	TPO	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 3 are monoatomic - leaving 16 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	$\# Z > 2$
22	LMG	K	301	-	41,41,55	0.82	1 (2%)	49,49,63	1.28	5 (10%)
22	LMG	M	801	-	48,48,55	0.85	2 (4%)	56,56,63	1.40	7 (12%)
25	DGA	D	3101	-	38,38,43	1.16	3 (7%)	40,40,45	1.69	3 (7%)
25	DGA	L	3001	-	33,33,43	1.23	3 (9%)	35,35,45	1.73	3 (8%)
22	LMG	I	402	-	32,32,55	0.99	2 (6%)	40,40,63	1.31	6 (15%)
26	Y01	D	3102	-	38,38,38	0.47	0	57,57,57	0.63	0
24	SQD	I	401	-	47,49,54	1.03	5 (10%)	57,60,65	1.57	12 (21%)
26	Y01	M	802	-	38,38,38	0.47	0	57,57,57	0.63	0
27	DGD	I	403	-	41,41,67	1.21	4 (9%)	55,55,81	1.45	7 (12%)
28	A1LXL	P	702	-	33,33,33	4.84	15 (45%)	51,51,51	2.25	16 (31%)
28	A1LXL	P	701	-	33,33,33	4.76	14 (42%)	51,51,51	2.39	13 (25%)
24	SQD	K	302	-	43,45,54	1.09	6 (13%)	53,56,65	1.68	10 (18%)
22	LMG	A	1201	-	46,46,55	0.85	2 (4%)	54,54,63	1.34	8 (14%)
24	SQD	B	1201	-	44,46,54	1.09	6 (13%)	54,57,65	1.65	12 (22%)
27	DGD	N	201	-	42,42,67	1.11	3 (7%)	56,56,81	1.38	8 (14%)
22	LMG	C	1201	-	24,24,55	0.73	0	26,26,63	1.09	1 (3%)

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
22	LMG	K	301	-	-	14/36/56/70	0/1/1/1
22	LMG	M	801	-	-	21/43/63/70	0/1/1/1
25	DGA	D	3101	-	-	28/40/40/45	-
25	DGA	L	3001	-	-	22/35/35/45	-
22	LMG	I	402	-	-	14/27/47/70	0/1/1/1
26	Y01	D	3102	-	-	6/19/77/77	0/4/4/4
24	SQD	I	401	-	-	20/44/64/69	0/1/1/1
26	Y01	M	802	-	-	4/19/77/77	0/4/4/4
27	DGD	I	403	-	-	12/29/69/95	0/2/2/2
28	A1LXL	P	702	-	-	5/15/73/73	0/4/4/4
28	A1LXL	P	701	-	-	10/15/73/73	0/4/4/4
24	SQD	K	302	-	-	21/40/60/69	0/1/1/1
22	LMG	A	1201	-	-	16/41/61/70	0/1/1/1
24	SQD	B	1201	-	-	17/41/61/69	0/1/1/1
27	DGD	N	201	-	-	13/30/70/95	0/2/2/2
22	LMG	C	1201	-	-	11/26/26/70	-

The worst 5 of 66 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	P	702	A1LXL	C18-C19	16.19	1.66	1.33
28	P	701	A1LXL	C18-C19	15.09	1.64	1.33
28	P	702	A1LXL	C06-C08	-10.61	1.36	1.54
28	P	701	A1LXL	C06-C08	-9.12	1.38	1.54
28	P	701	A1LXL	C17-C16	9.08	1.67	1.53

The worst 5 of 111 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	P	701	A1LXL	C17-C18-C19	-8.35	110.91	125.02
25	L	3001	DGA	CDB-CCB-CBB	-6.77	80.14	114.37
25	D	3101	DGA	CDB-CCB-CBB	-6.67	80.64	114.37
28	P	701	A1LXL	C27-C12-C13	-6.23	101.42	110.61
28	P	701	A1LXL	C20-C19-C18	-6.02	114.14	122.93

There are no chirality outliers.

5 of 234 torsion outliers are listed below:

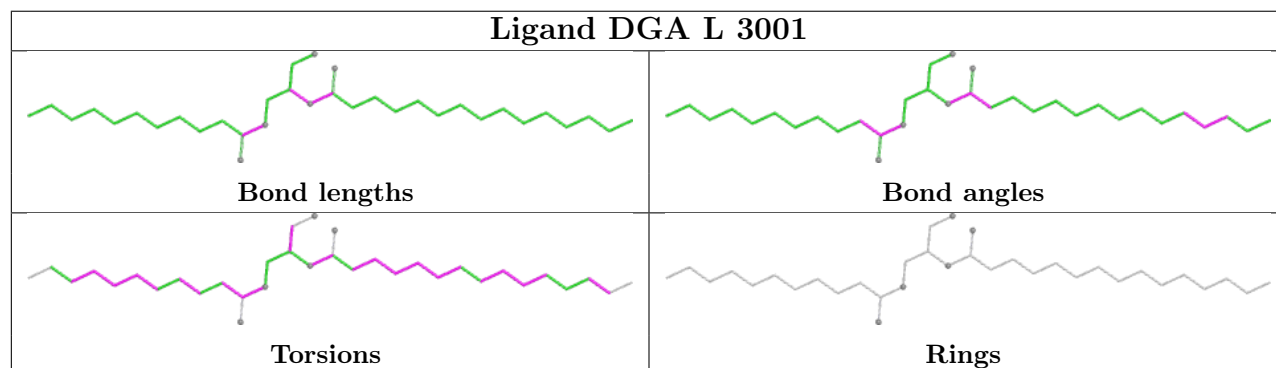
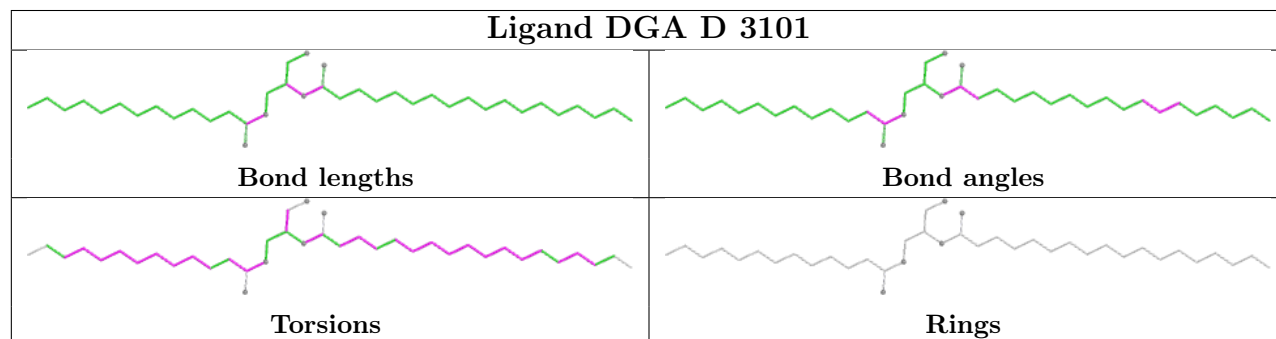
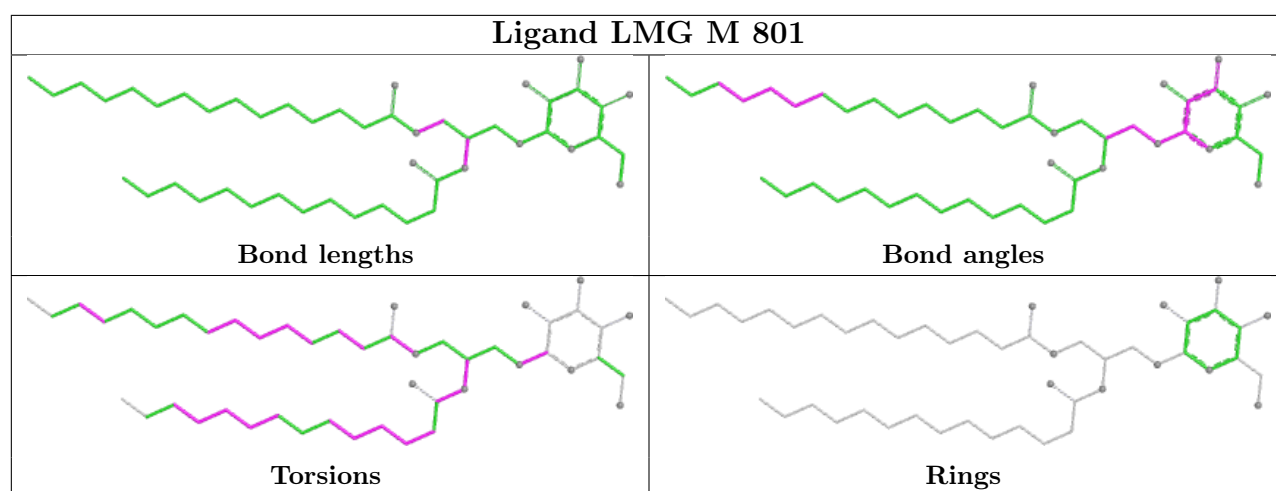
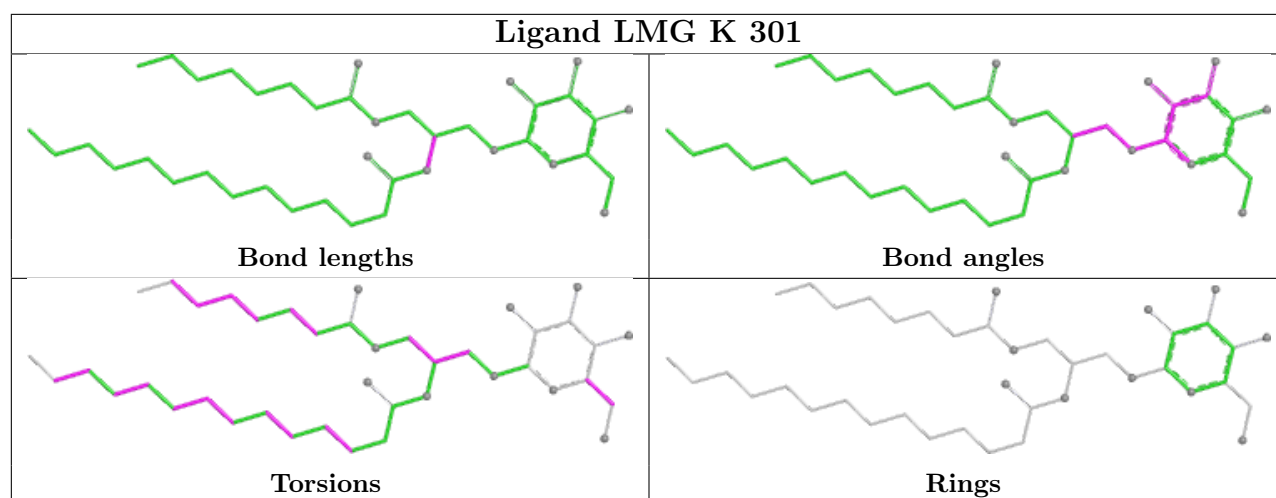
Mol	Chain	Res	Type	Atoms
22	C	1201	LMG	O1-C7-C8-O7
22	I	402	LMG	O6-C1-O1-C7
22	M	801	LMG	O6-C1-O1-C7
24	B	1201	SQD	O47-C45-C46-O48
24	B	1201	SQD	C5-C6-S-O9

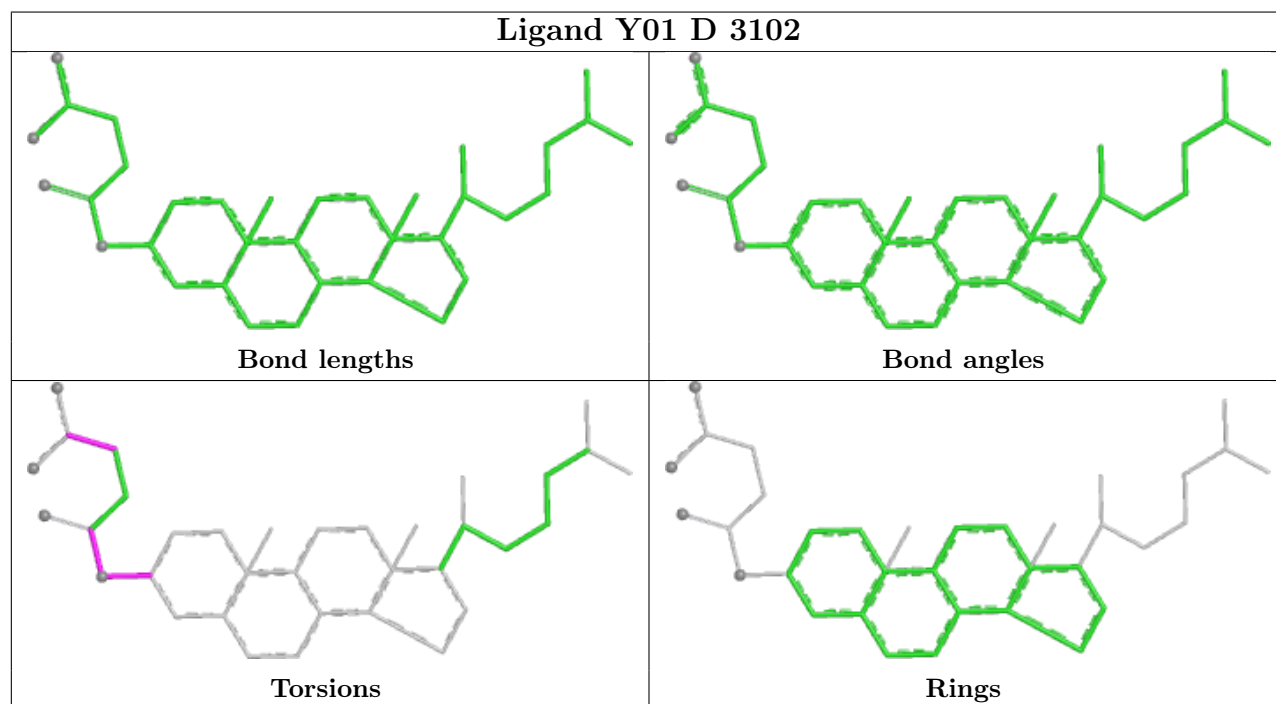
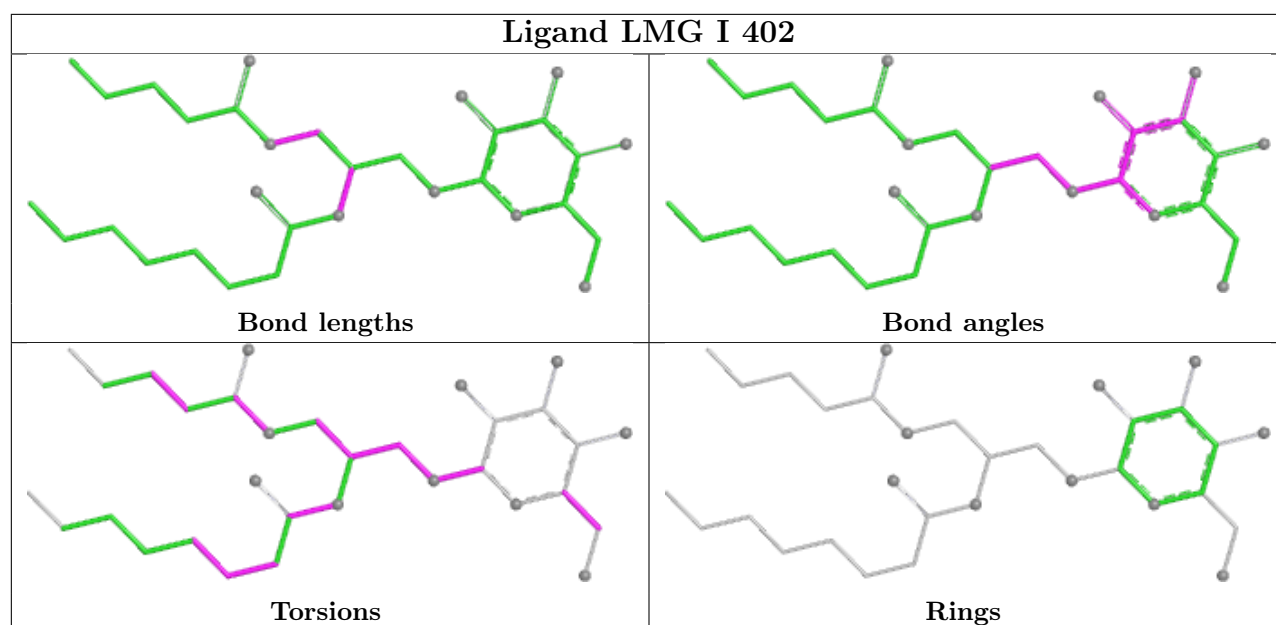
There are no ring outliers.

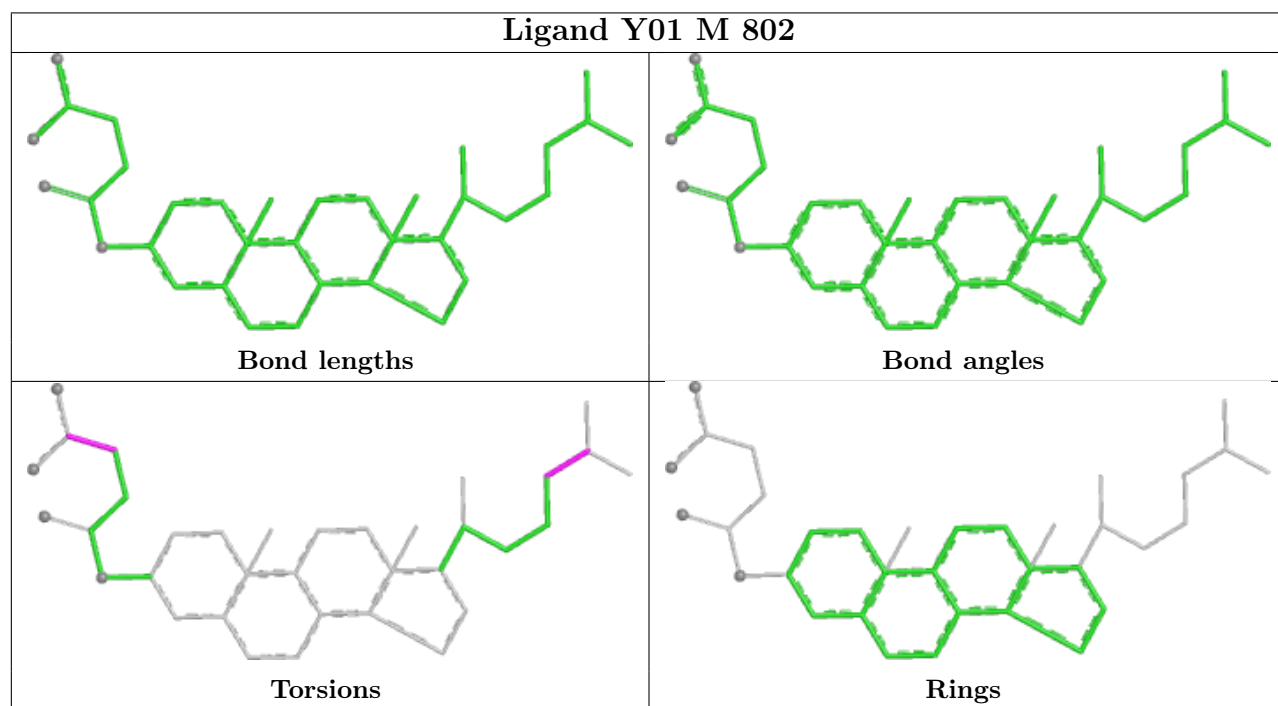
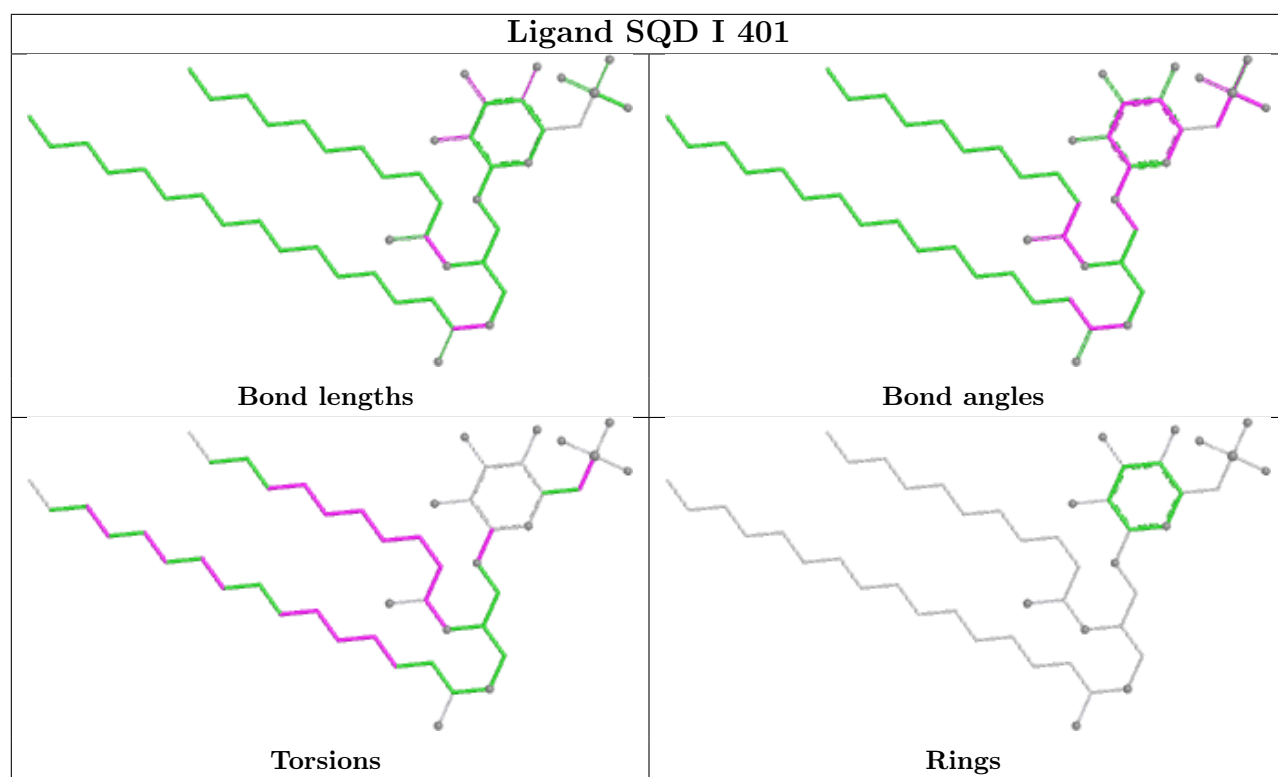
11 monomers are involved in 27 short contacts:

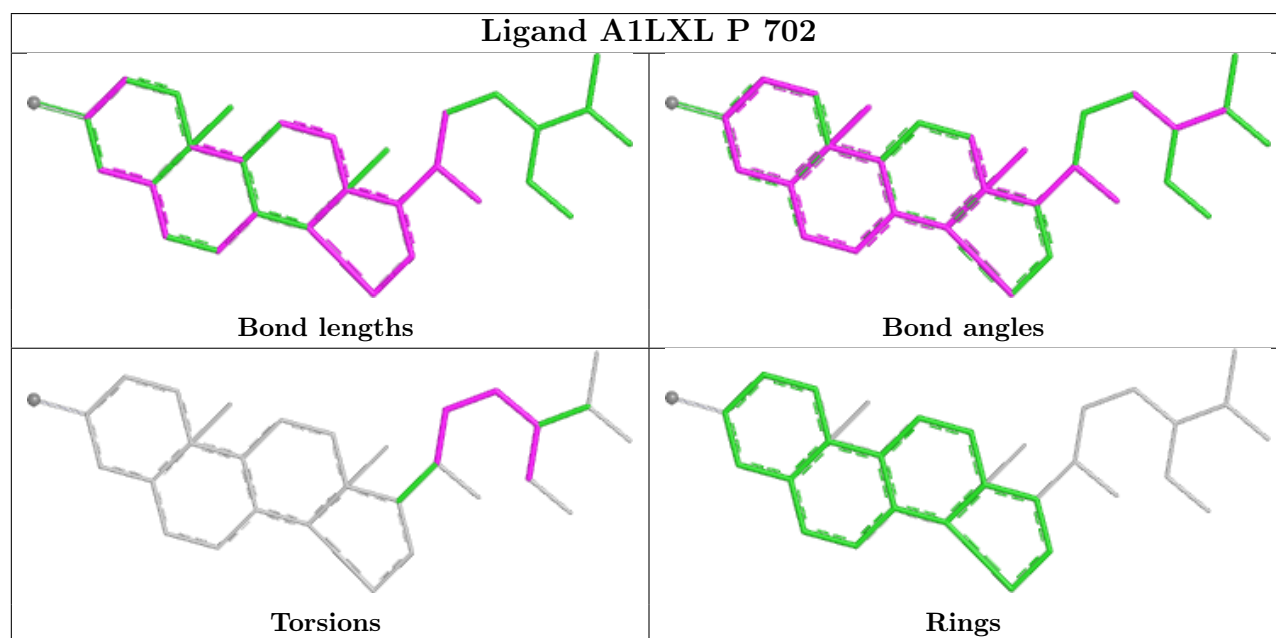
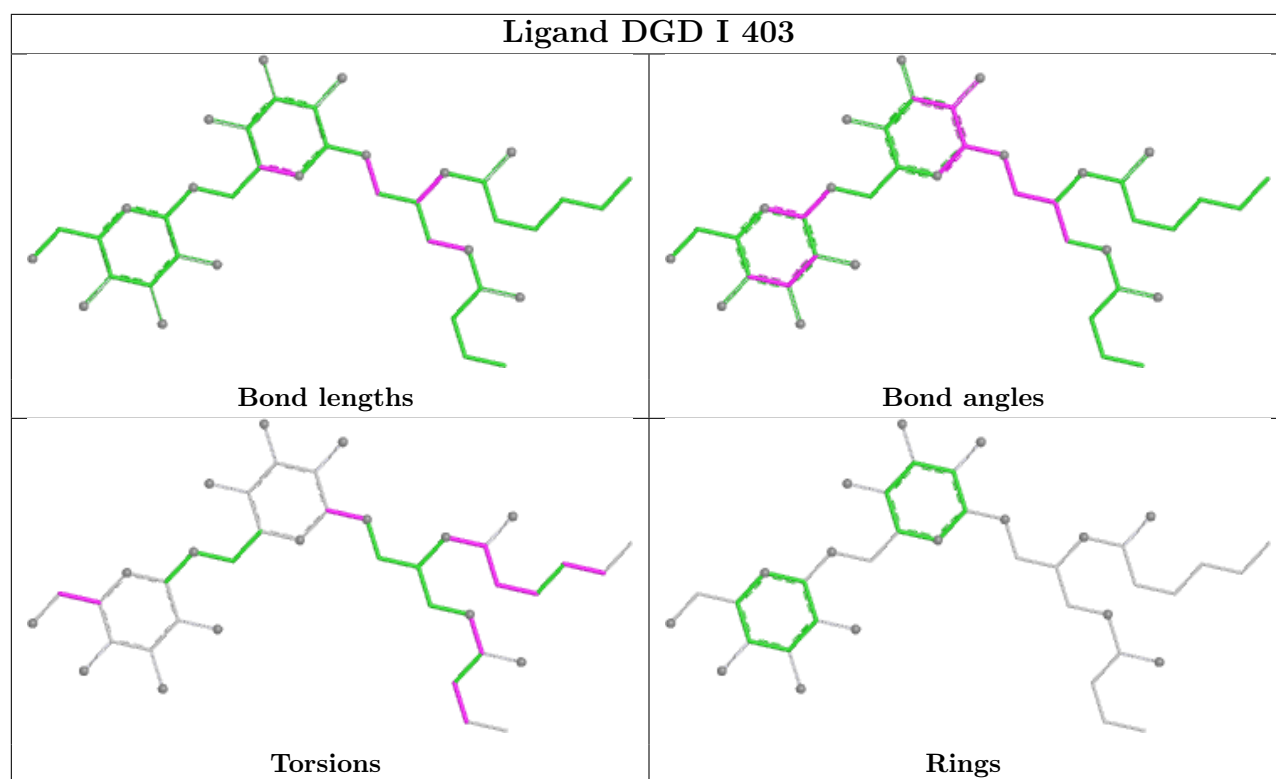
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	K	301	LMG	1	0
22	M	801	LMG	1	0
25	D	3101	DGA	1	0
25	L	3001	DGA	1	0
22	I	402	LMG	2	0
24	I	401	SQD	5	0
26	M	802	Y01	4	0
27	I	403	DGD	2	0
28	P	702	A1LXL	2	0
28	P	701	A1LXL	8	0
22	A	1201	LMG	3	0

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.

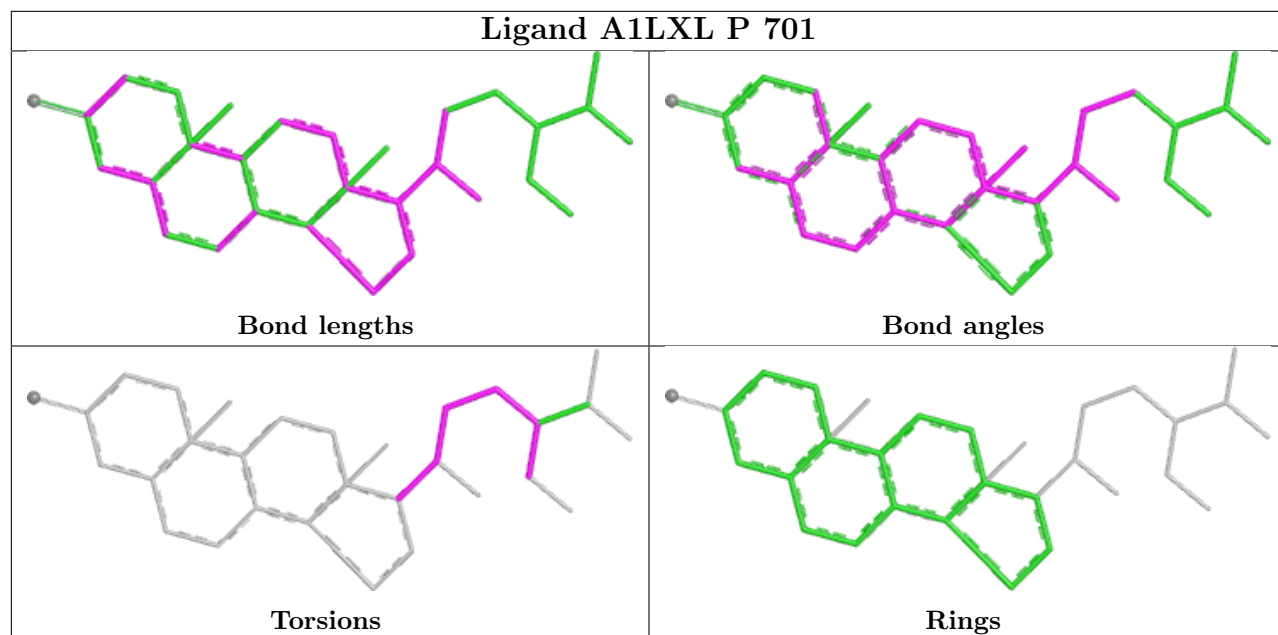




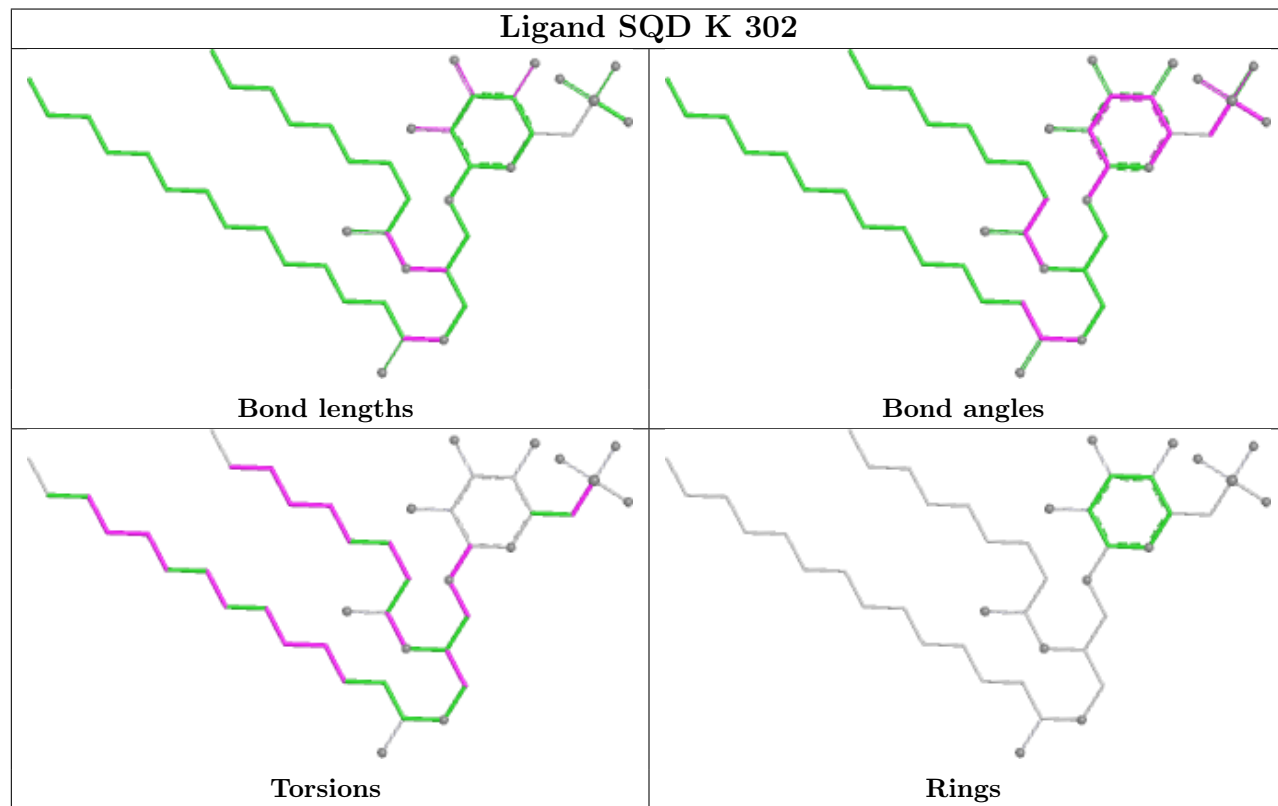


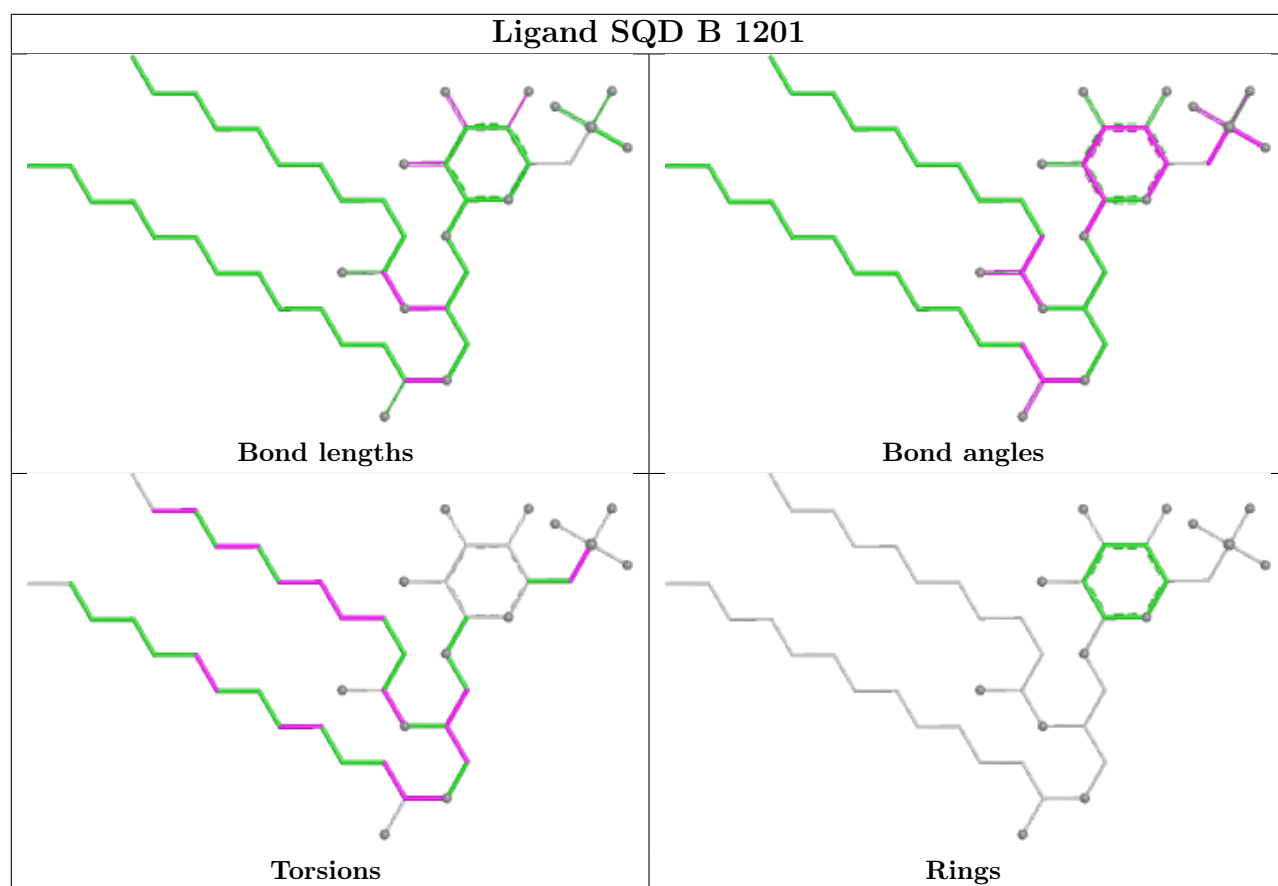
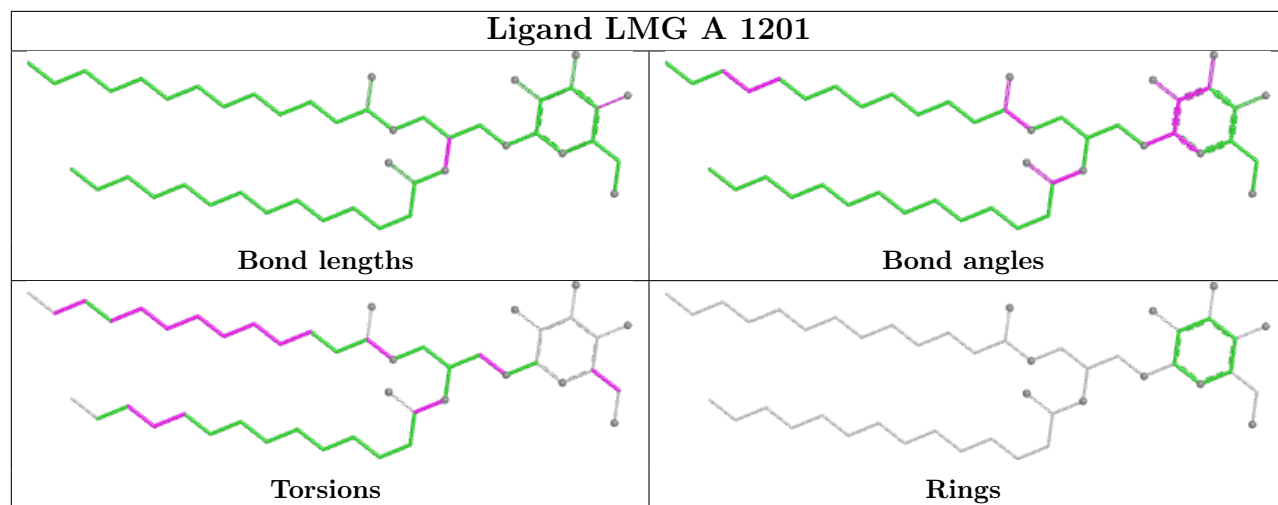


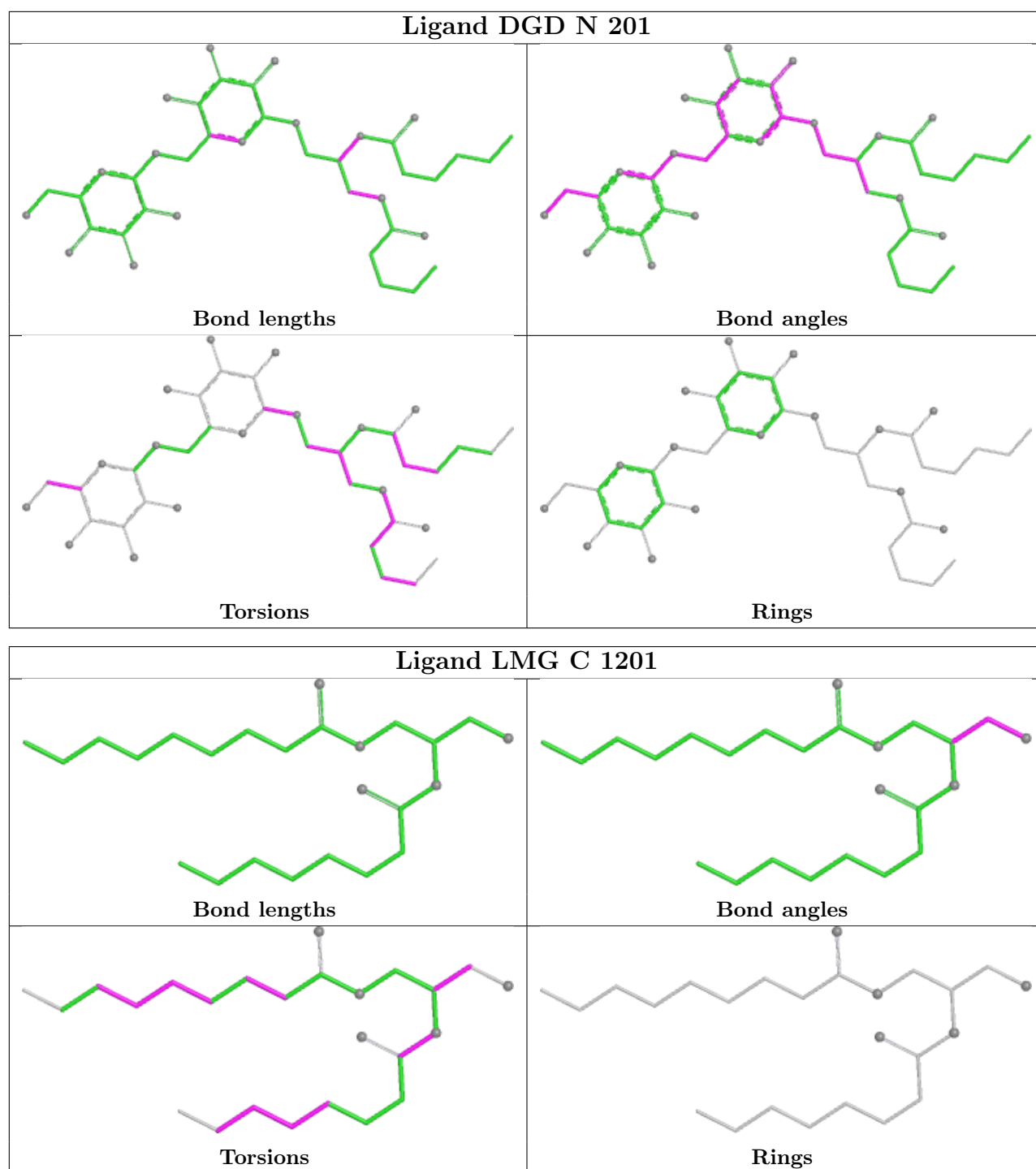
Ligand A1LXL P 701



Ligand SQD K 302







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.

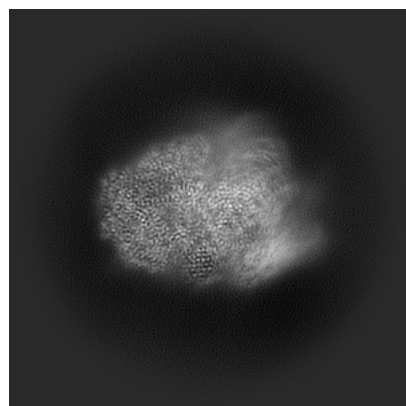
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38590. These allow visual inspection of the internal detail of the map and identification of artifacts.

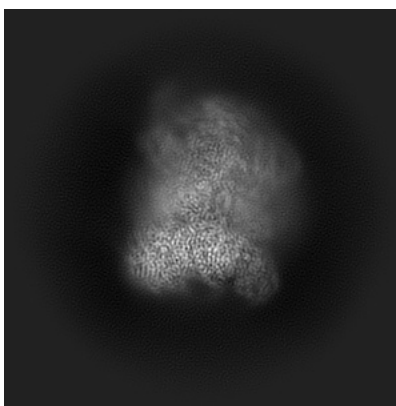
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

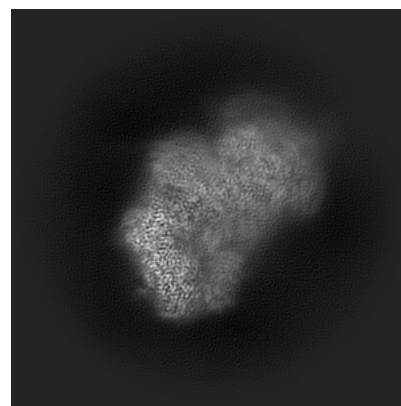
6.1.1 Primary map



X

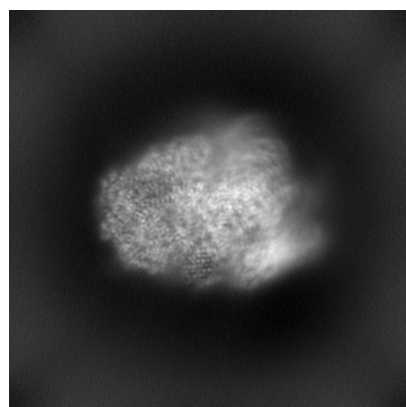


Y

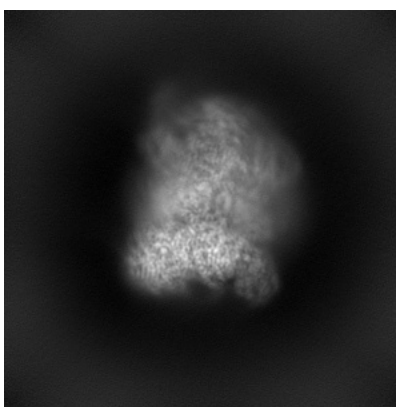


Z

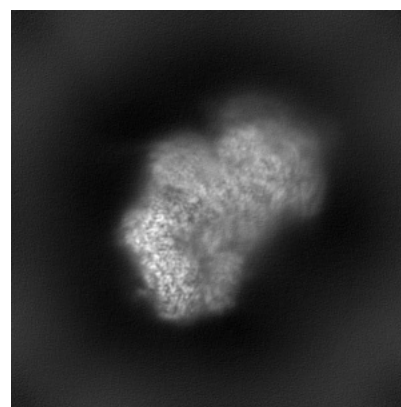
6.1.2 Raw map



X



Y

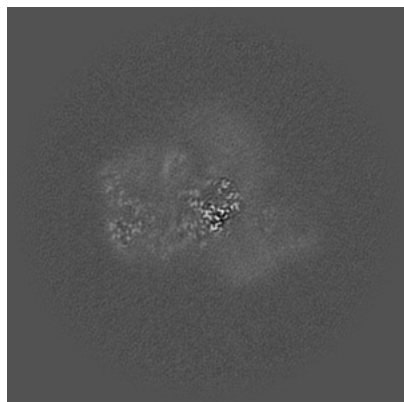


Z

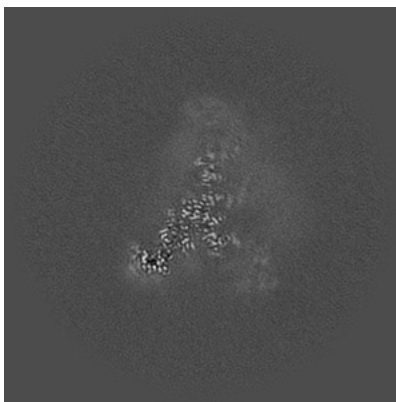
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

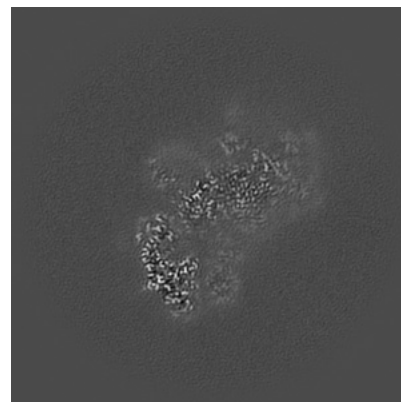
6.2.1 Primary map



X Index: 180

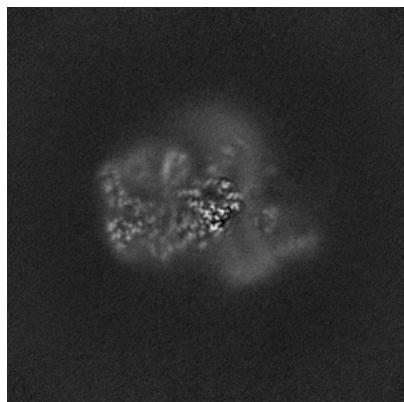


Y Index: 180

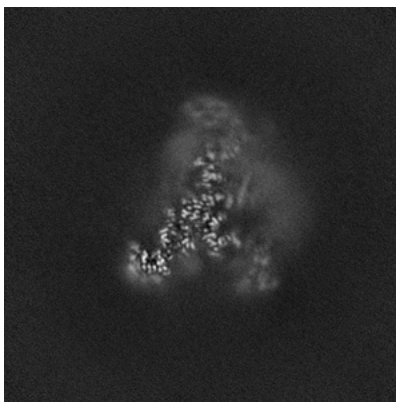


Z Index: 180

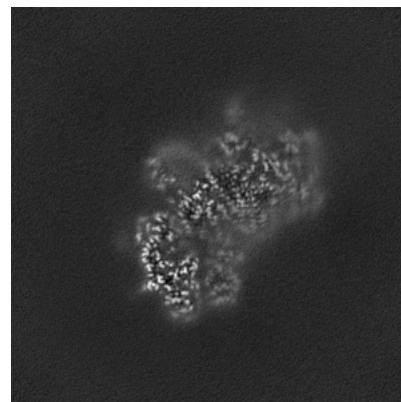
6.2.2 Raw map



X Index: 180



Y Index: 180

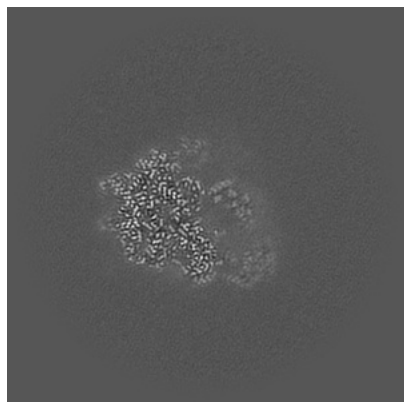


Z Index: 180

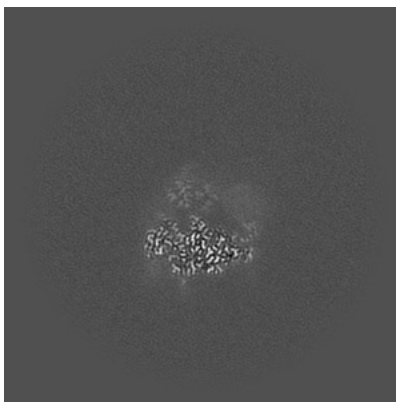
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

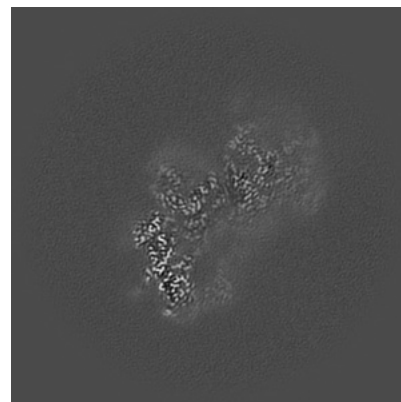
6.3.1 Primary map



X Index: 135

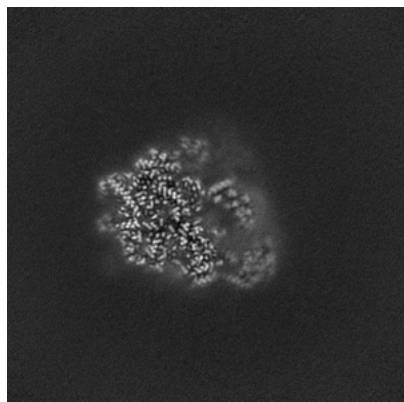


Y Index: 120

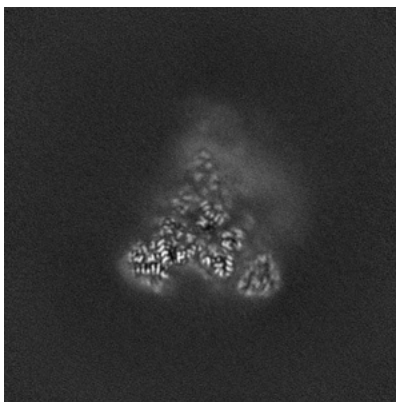


Z Index: 188

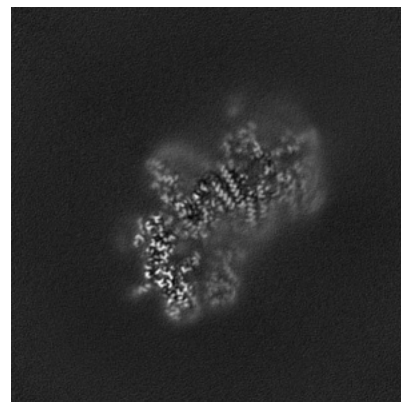
6.3.2 Raw map



X Index: 135



Y Index: 170

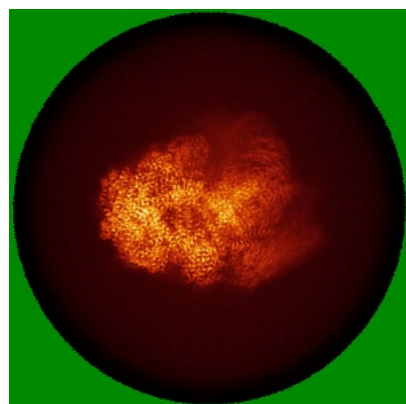


Z Index: 184

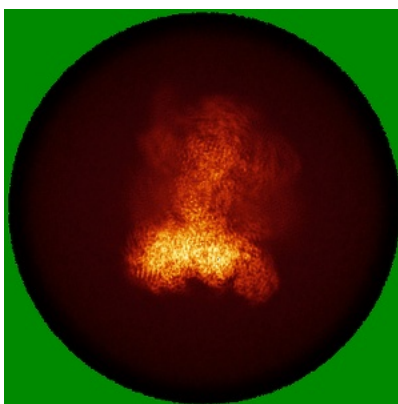
The images above show the largest variance slices of the map in three orthogonal directions.

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

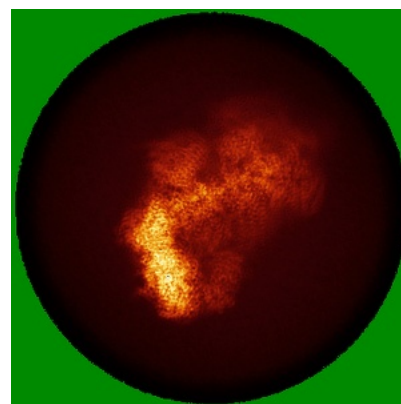
6.4.1 Primary map



X

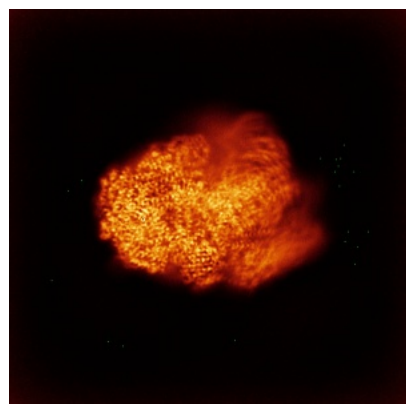


Y

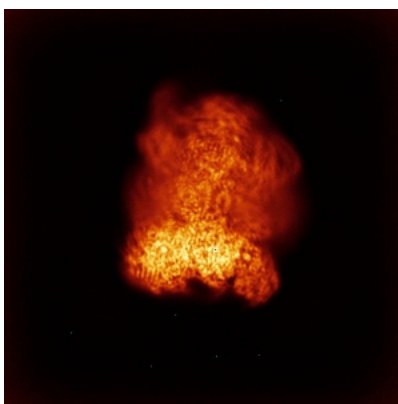


Z

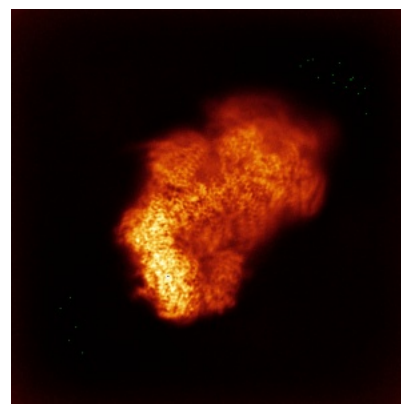
6.4.2 Raw map



X



Y

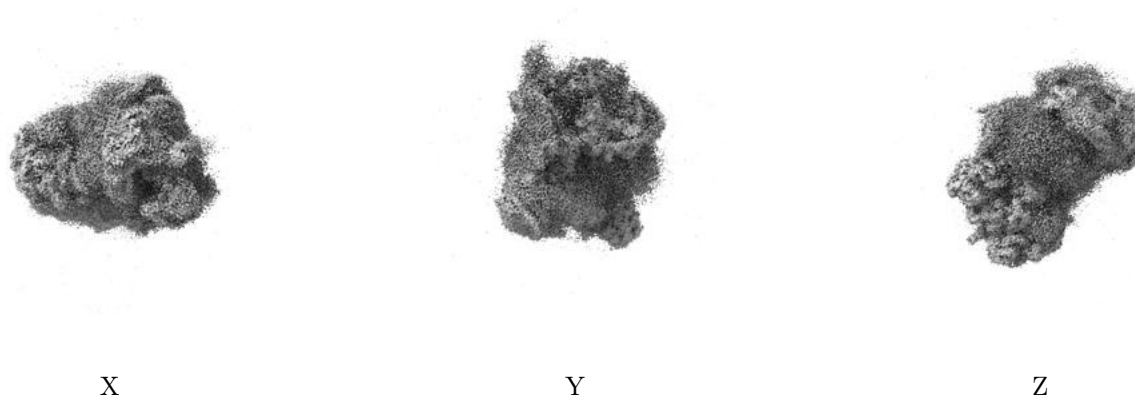


Z

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.

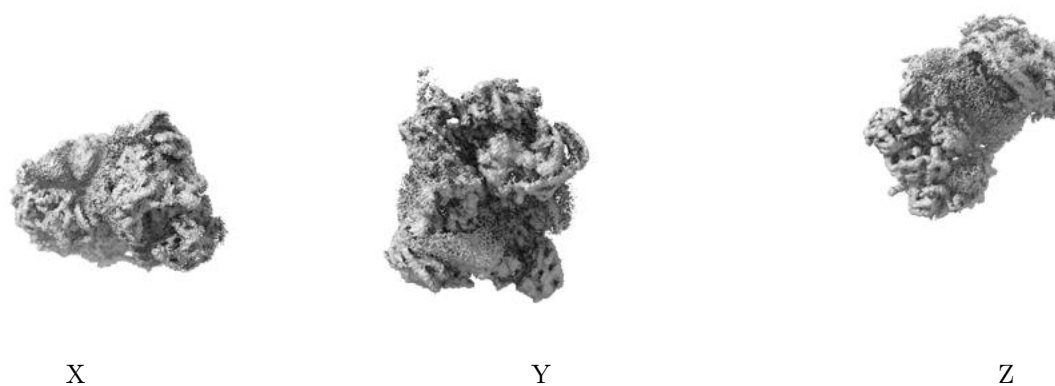
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.35. 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.

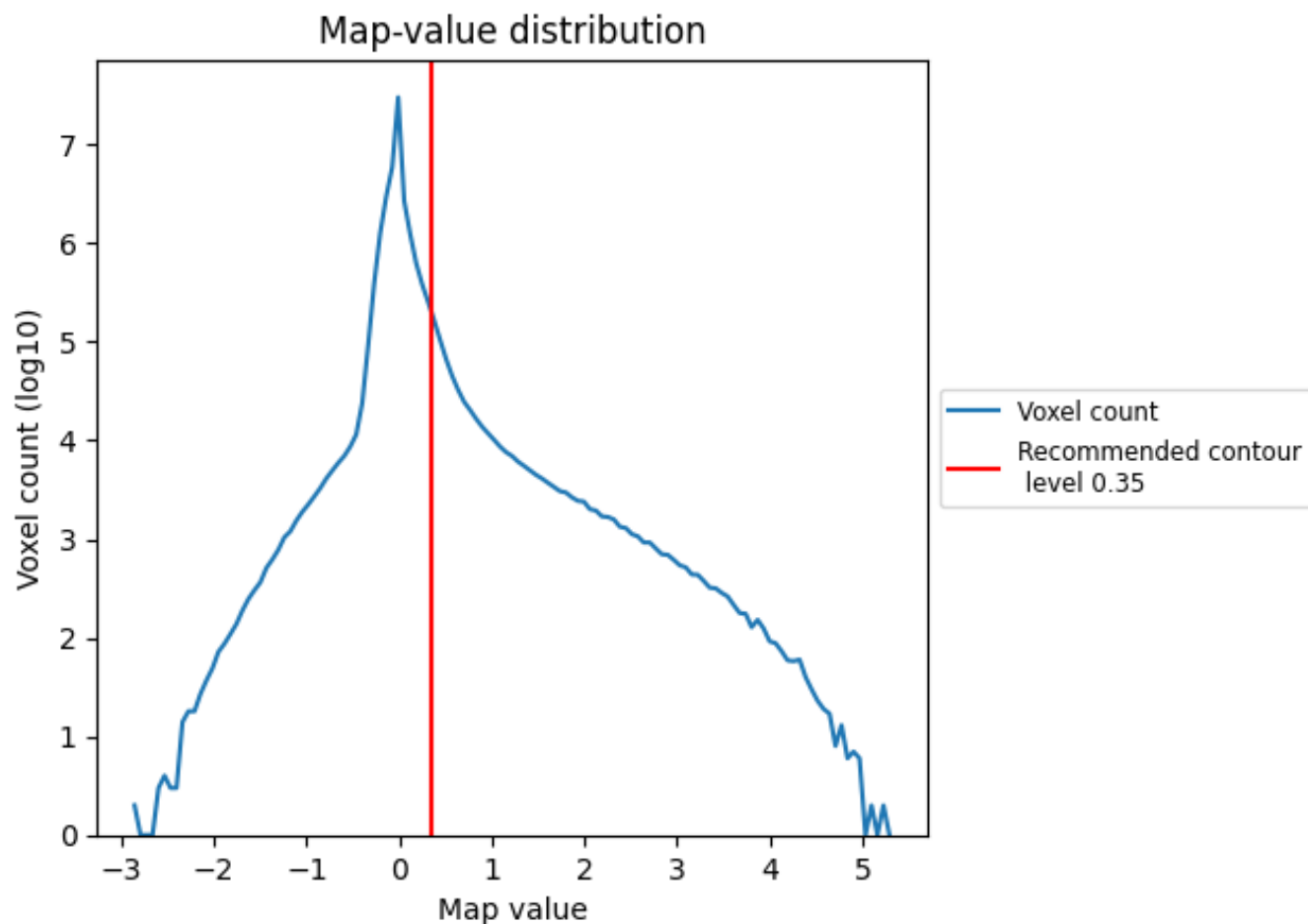
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

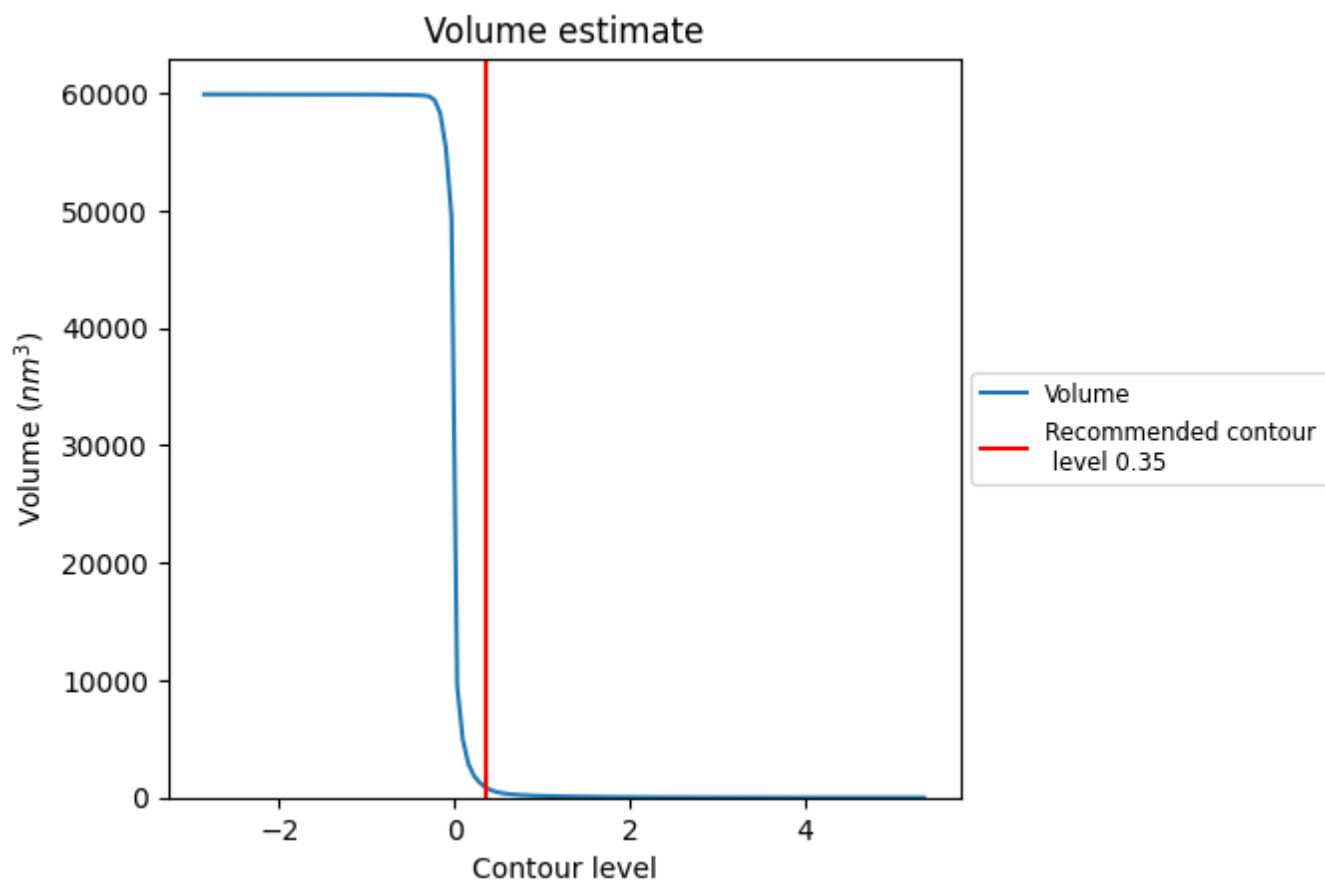
This section contains the results of statistical analysis of the map.

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.

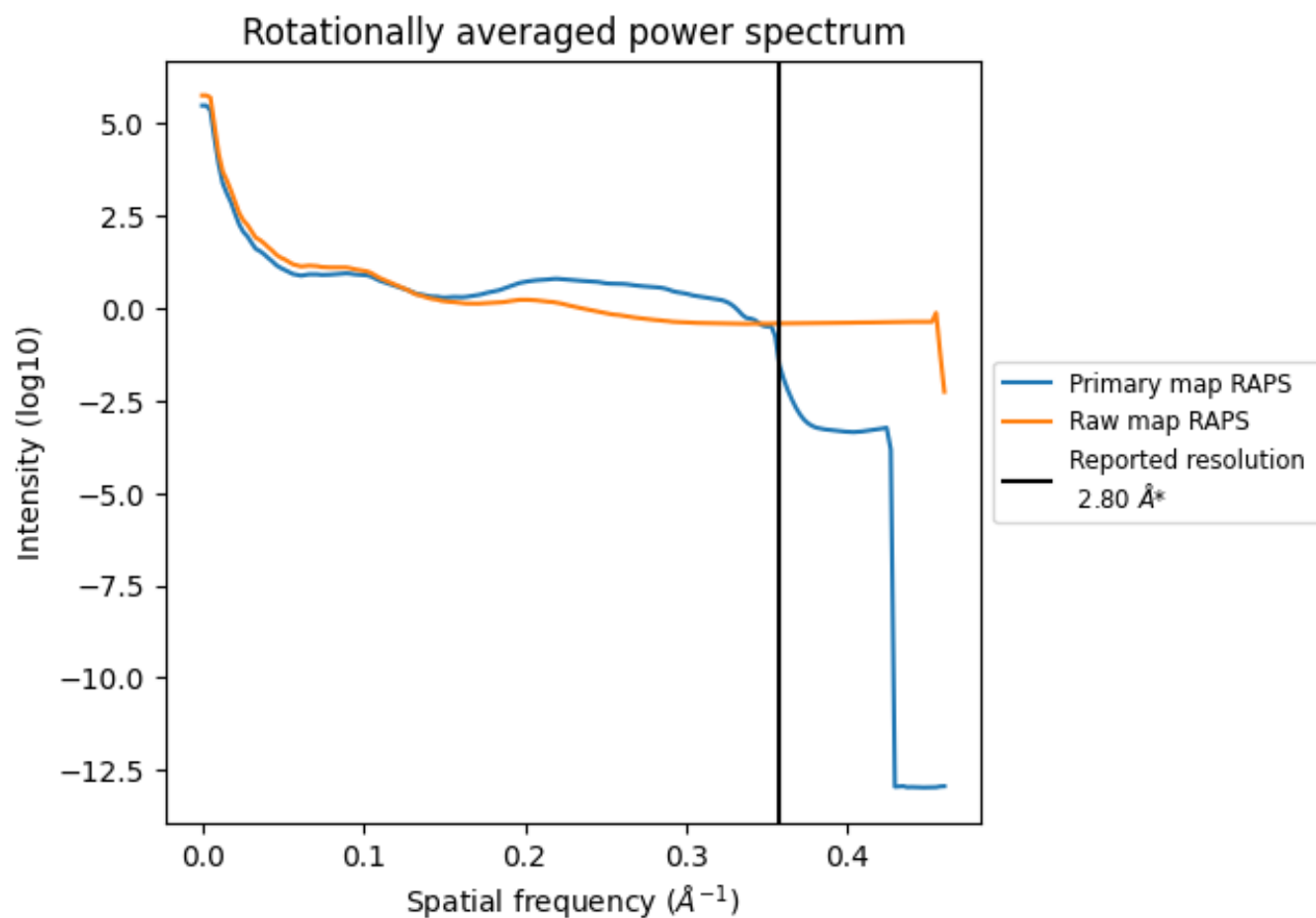
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 901 nm^3 ; this corresponds to an approximate mass of 814 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 ⓘ

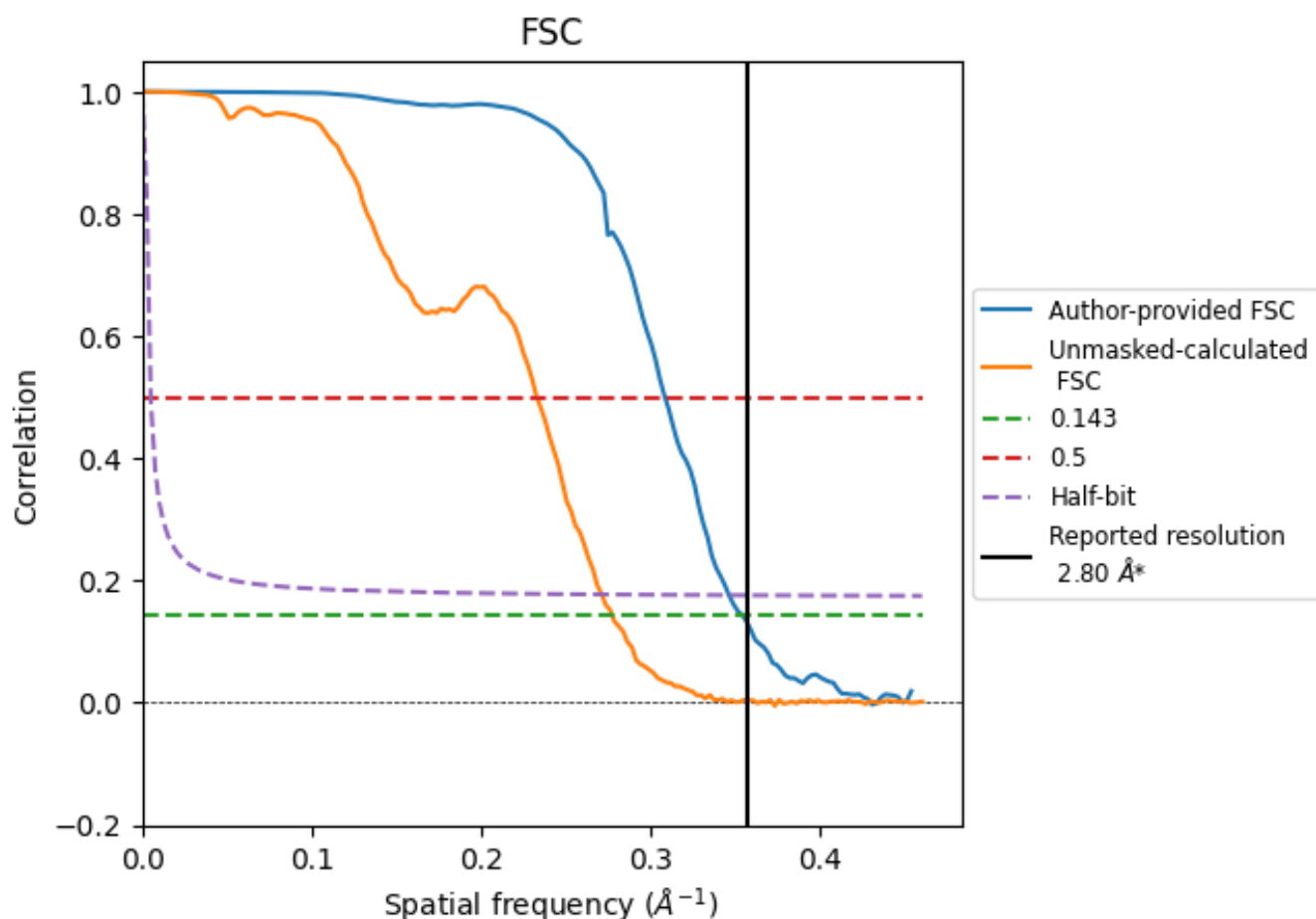


*Reported resolution corresponds to spatial frequency of 0.357 Å⁻¹

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 0.357 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

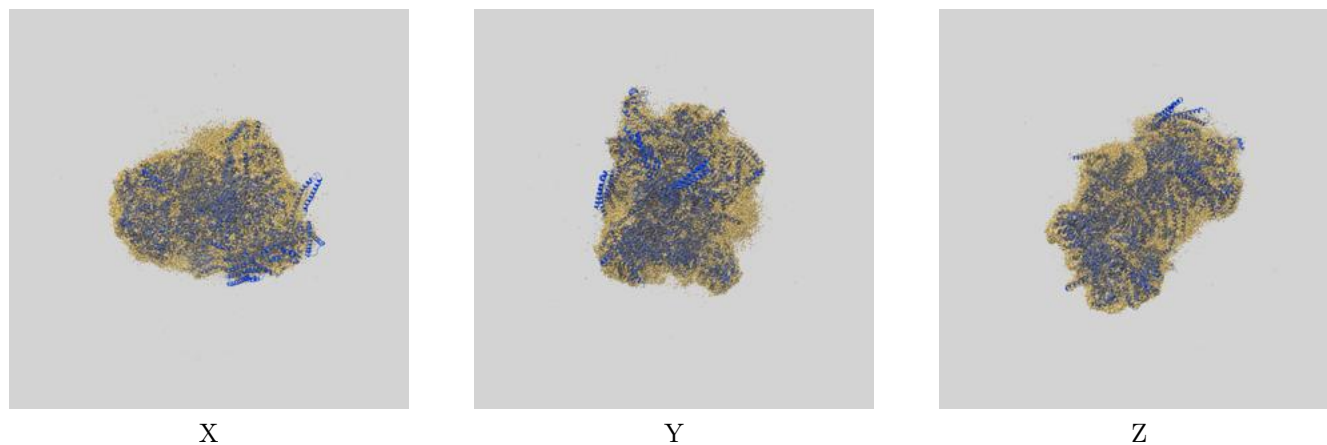
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.82	3.24	2.89
Unmasked-calculated*	3.61	4.30	3.69

*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 3.61 differs from the reported value 2.8 by more than 10 %

9 Map-model fit [i](#)

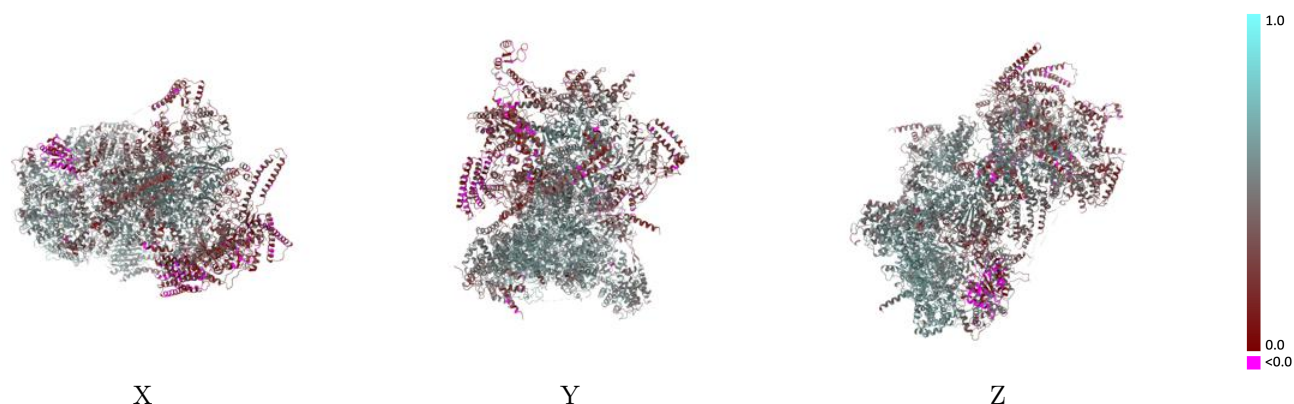
This section contains information regarding the fit between EMDB map EMD-38590 and PDB model 8XQX. Per-residue inclusion information can be found in [section 3](#) on [page 12](#).

9.1 Map-model overlay [i](#)



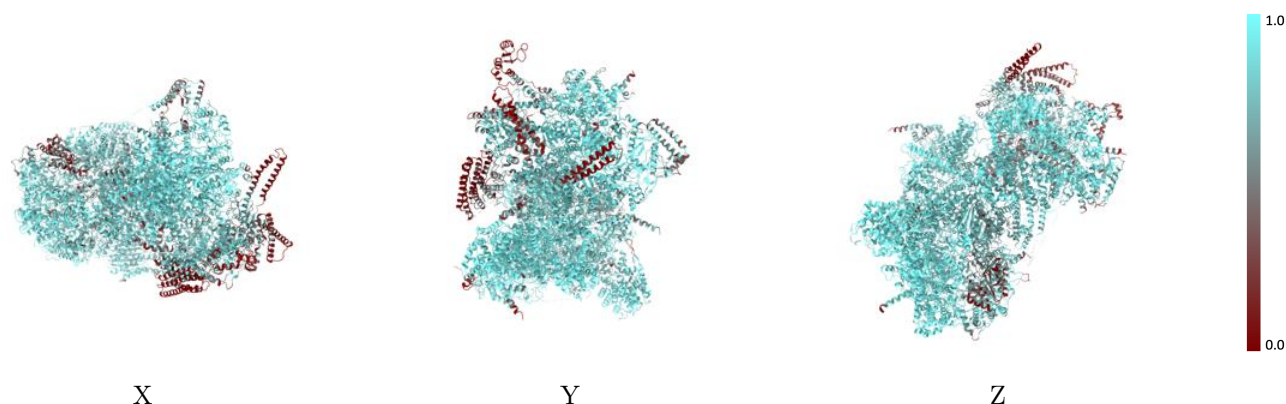
The images above show the 3D surface view of the map at the recommended contour level 0.35 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



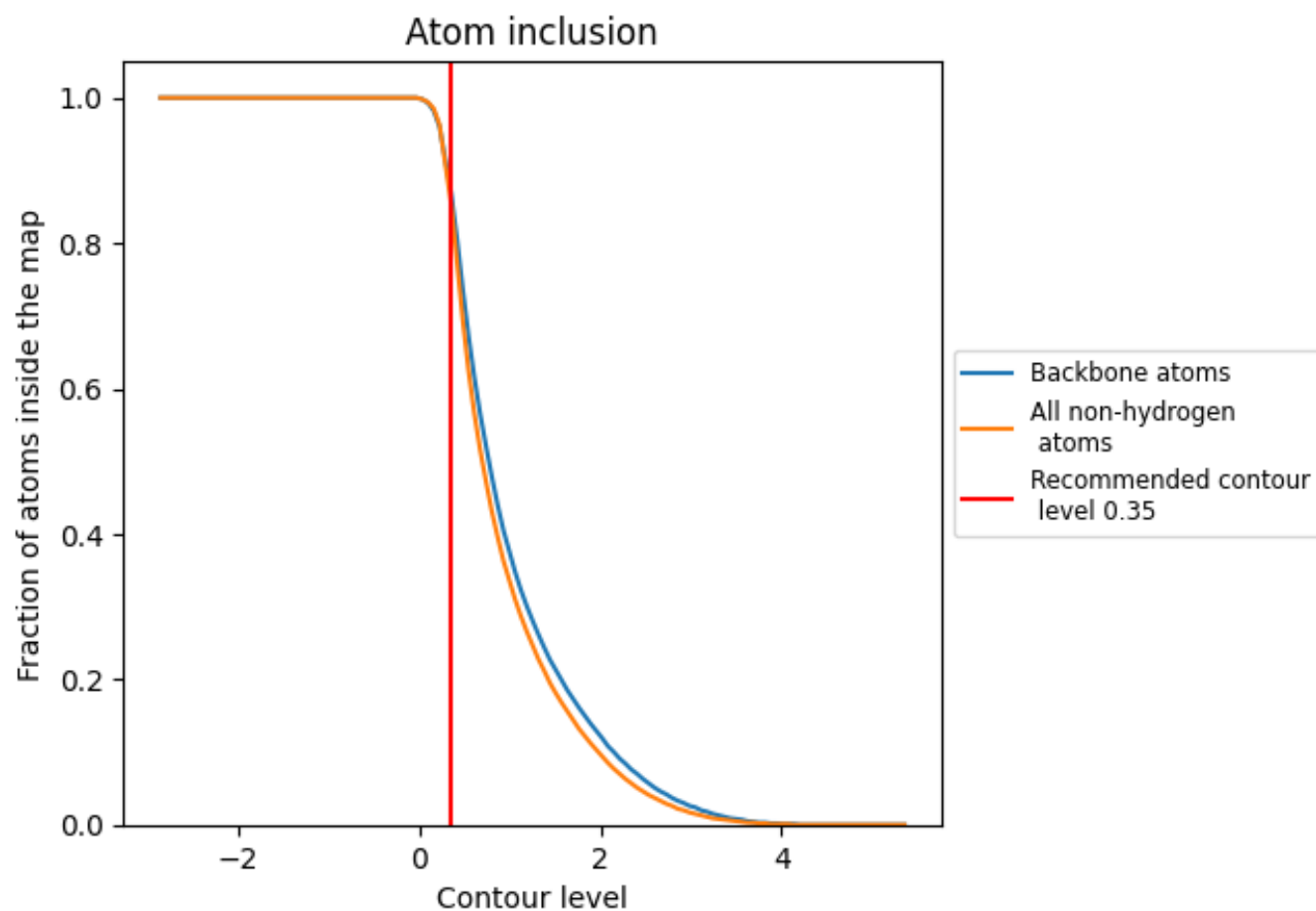
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.35).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% 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 (0.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8560	 0.4600
A	 0.9350	 0.5320
B	 0.8990	 0.4820
C	 0.9030	 0.4870
D	 0.9160	 0.4980
E	 0.8460	 0.4370
F	 0.8860	 0.4840
G	 0.8990	 0.4840
H	 0.9360	 0.5300
I	 0.9650	 0.5610
J	 0.9310	 0.4850
K	 0.9640	 0.5580
L	 0.9000	 0.5080
M	 0.8810	 0.4540
N	 0.8800	 0.4740
O	 0.3620	 0.2090
P	 0.5780	 0.2660
Q	 0.5040	 0.2680
R	 0.9010	 0.4550
S	 0.7480	 0.3570
T	 0.6910	 0.2940
U	 0.6940	 0.2890
V	 0.8380	 0.2160

