wwPDB EM Validation Summary Report (i)

Oct 1, 2024 – 12:40 PM JST

PDB ID	:	7VCF
EMDB ID	:	EMD-31890
Title	:	Cryo-EM structure of Chlamydomonas TOC-TIC supercomplex
Authors	:	Wu, J.; Yan, Z.; Jin, Z.; Zhang, Y.
Deposited on	:	2021-09-02
Resolution	:	2.50 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 (i) 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 (i)) were used in the production of this report:

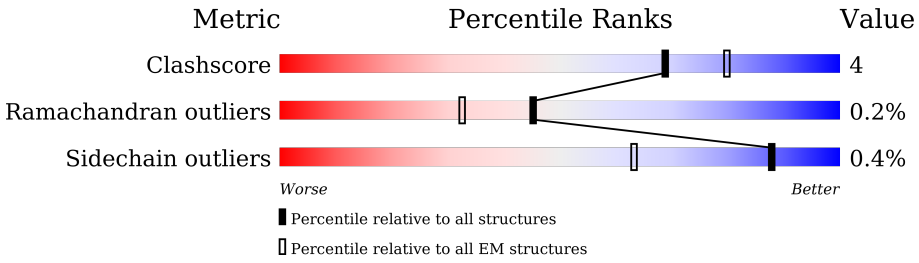
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

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 <=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	1995	68% 7% 25%
2	B	798	74% 8% 18%
3	C	477	43% 55%
4	D	124	50% 6% 44%
5	F	967	37% 58%
6	G	397	17% 82%
7	H	187	11% 35% 17% 46%
8	I	363	21% 89% 11%

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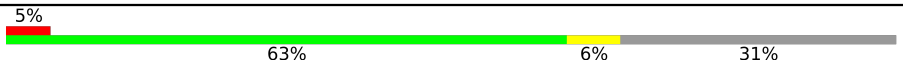
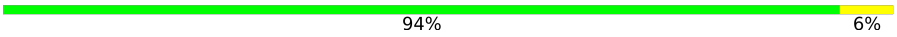
Mol	Chain	Length	Quality of chain
9	K	98	
10	M	127	
11	N	18	
12	O	329	
13	Q	244	
14	T	955	
15	W	532	

2 Entry composition (i)

There are 19 unique types of molecules in this entry. The entry contains 39626 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 Tic214.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	N	O	P	S		
1	A	1496	12577	8149	2237	2163	1	27	0	0

- Molecule 2 is a protein called Toc75.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	N	O	P	S		
2	B	651	5142	3233	890	1000	2	17	0	0

- Molecule 3 is a protein called Toc52.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	N	O	P	S		
3	C	217	1728	1089	315	317	1	6	0	0

- Molecule 4 is a protein called Tic13.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	D	69	529	333	100	96	0	0

- Molecule 5 is a protein called Toc120.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	N	O	P	S		
5	F	402	3139	1994	522	606	1	16	0	0

- Molecule 6 is a protein called Toc34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	G	70	612	383	124	104	1	0	0

- Molecule 7 is a protein called YlmG.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	H	101	Total	C	N	O	P	S	0	0
			861	576	126	149	3	7		

- Molecule 8 is a protein called Toc39.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	363	Total	C	N	O	S	0	0
			2751	1728	497	522	4		

- Molecule 9 is a protein called Toc10.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	68	Total	C	N	O	S	0	0
			549	343	103	101	2		

- Molecule 10 is a protein called Tic12.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	M	115	Total	C	N	O	S	0	0
			939	611	168	154	6		

- Molecule 11 is a protein called Unknown fragment.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	N	18	Total	C	N	O	S	0	0
			155	108	21	25	1		

- Molecule 12 is a protein called Tic35.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	O	195	Total	C	N	O	0	0
			1572	1008	278	286		

- Molecule 13 is a protein called Tic56.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Q	149	Total	C	N	O	S	0	0
			1244	805	222	208	9		

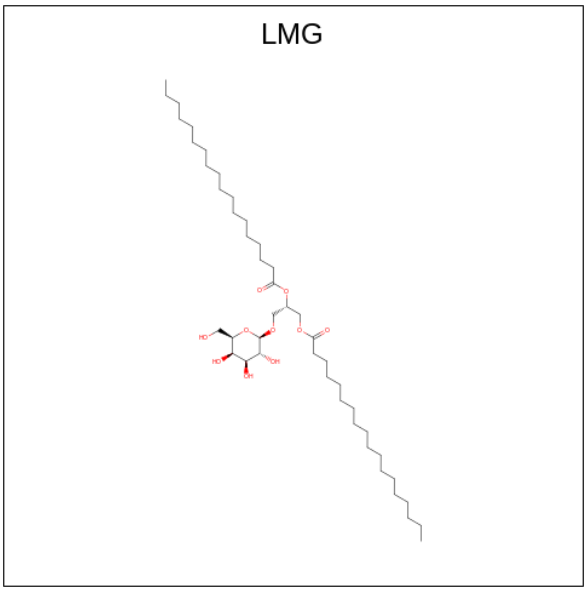
- Molecule 14 is a protein called Tic100.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	T	763	Total	C	N	O	P	S	0	0
			6185	3812	1060	1263	19	31		

- Molecule 15 is a protein called Tic20-Venus-Flag.

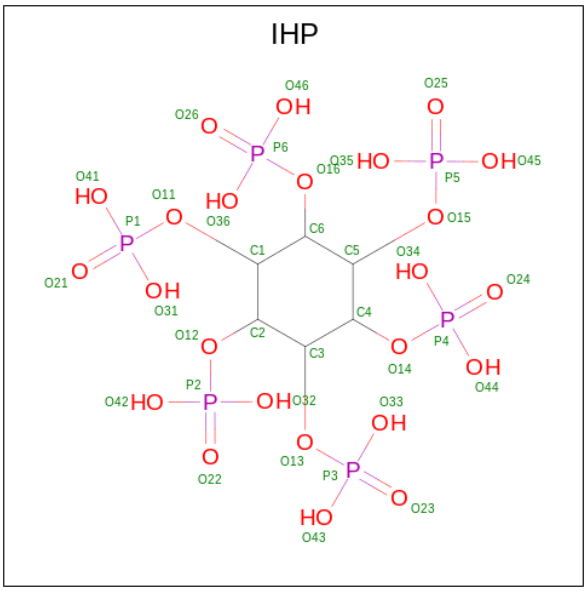
Mol	Chain	Residues	Atoms					AltConf	Trace
15	W	164	Total	C	N	O	S	0	0
			1398	955	205	226	12		

- Molecule 16 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			AltConf
16	A	1	Total	C	O	0
			49	39	10	
16	A	1	Total	C	O	0
			46	36	10	
16	A	1	Total	C	O	0
			55	45	10	
16	A	1	Total	C	O	0
			55	45	10	

- Molecule 17 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: $C_6H_{18}O_{24}P_6$).



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

- Molecule 18 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
18	F	1	Total	Mg	0
			1	1	
18	T	1	Total	Mg	0
			1	1	

- Molecule 19 is water.

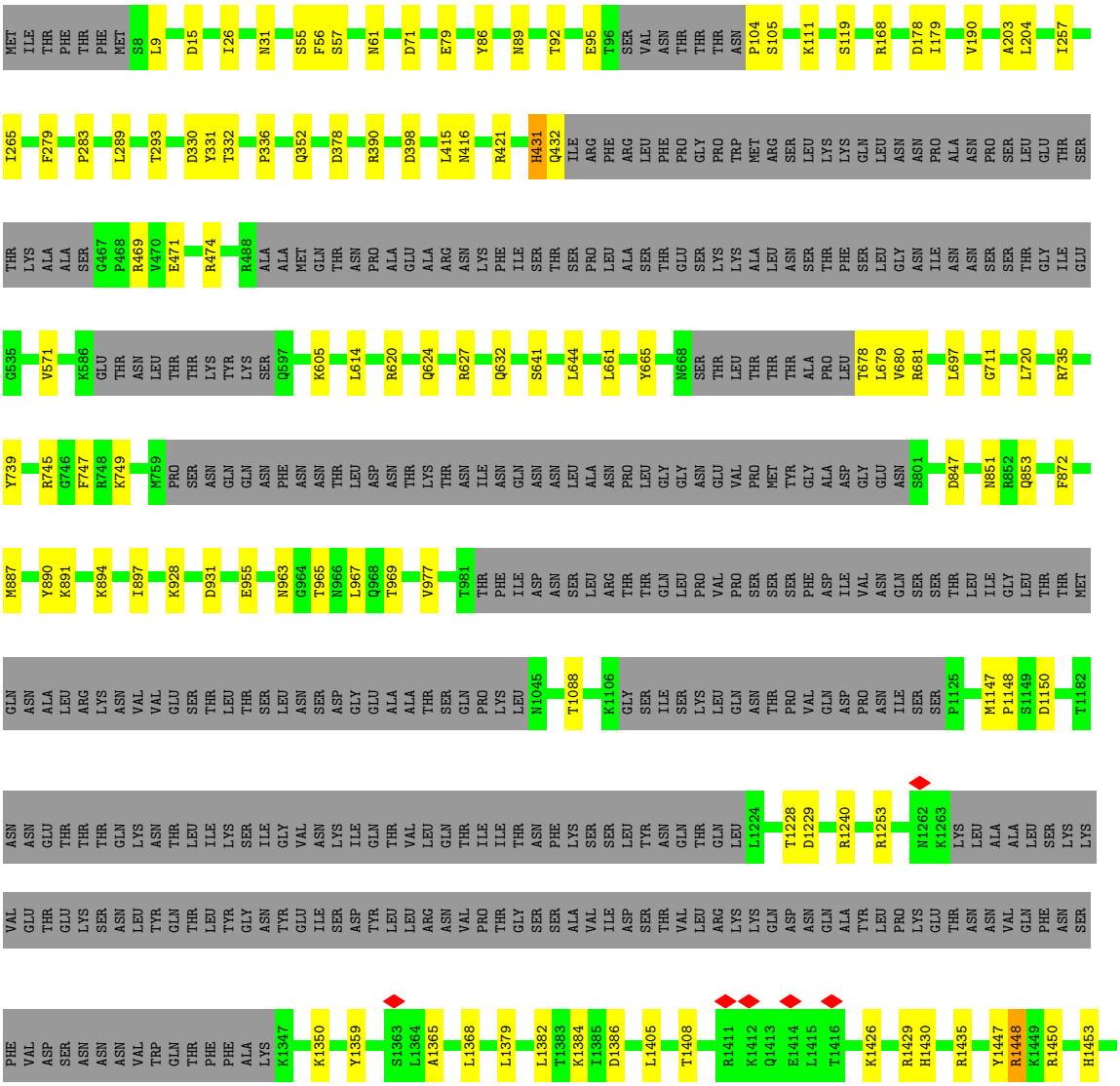
Mol	Chain	Residues	Atoms		AltConf
19	A	1	Total	O	0
			1	1	
19	O	1	Total	O	0
			1	1	

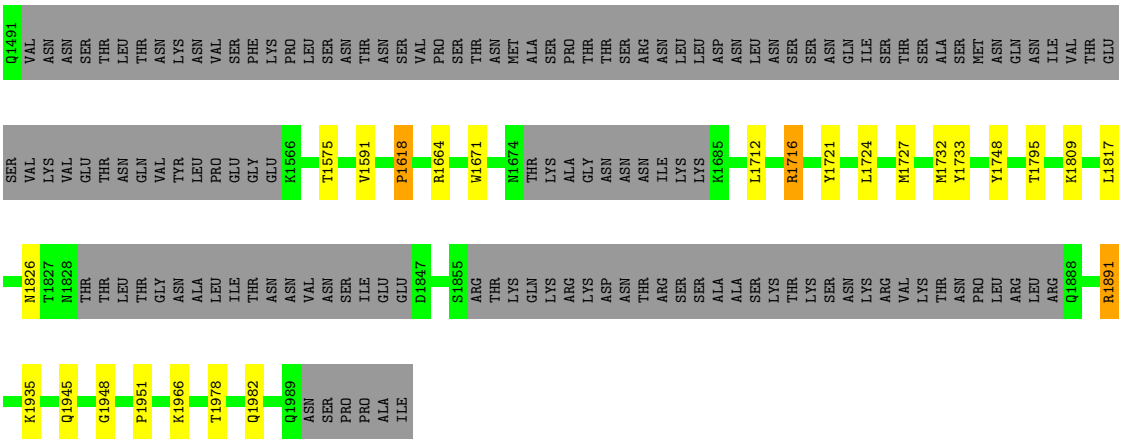
3 Residue-property plots (i)

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

- Molecule 1: Tic214

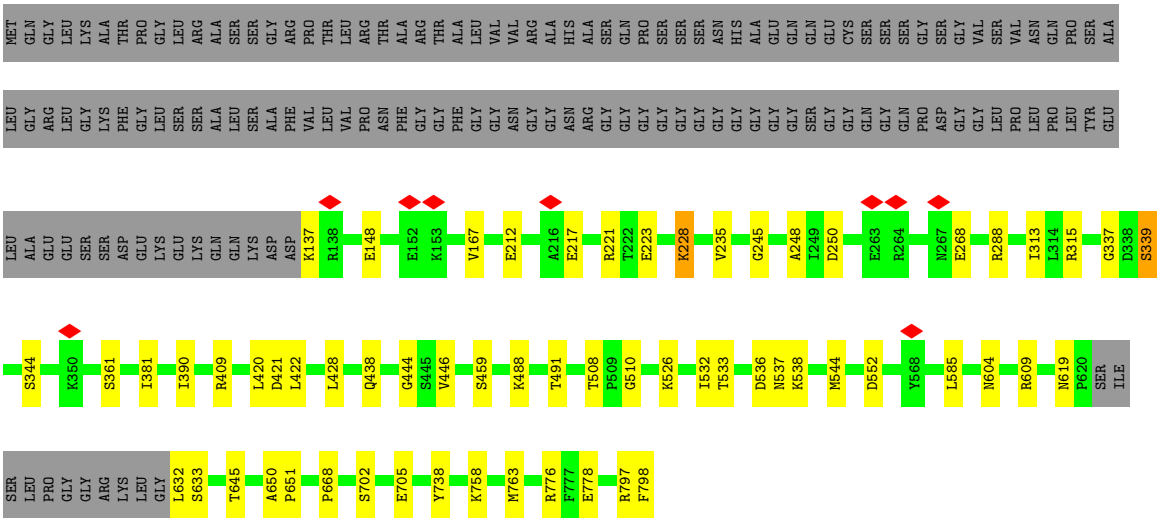
Chain A:





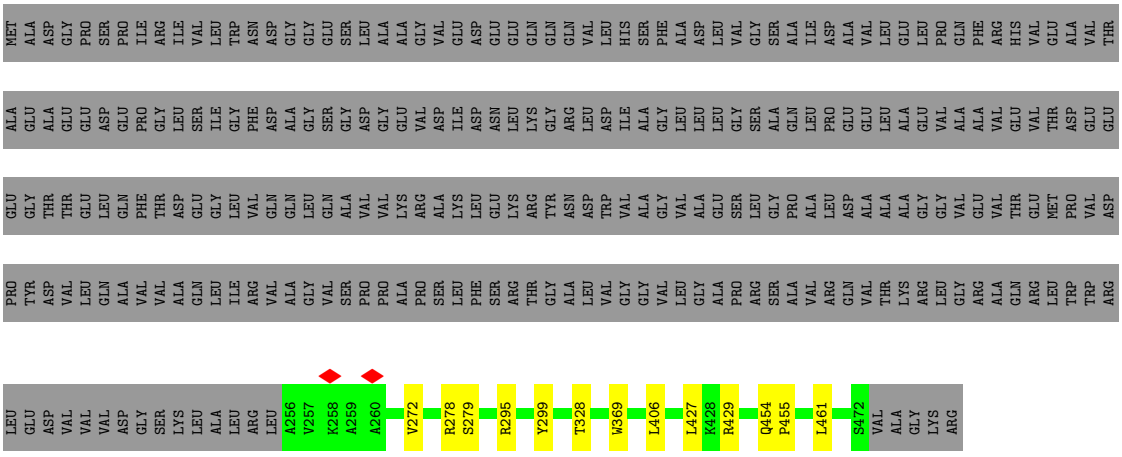
• Molecule 2: Toc75

Chain B:



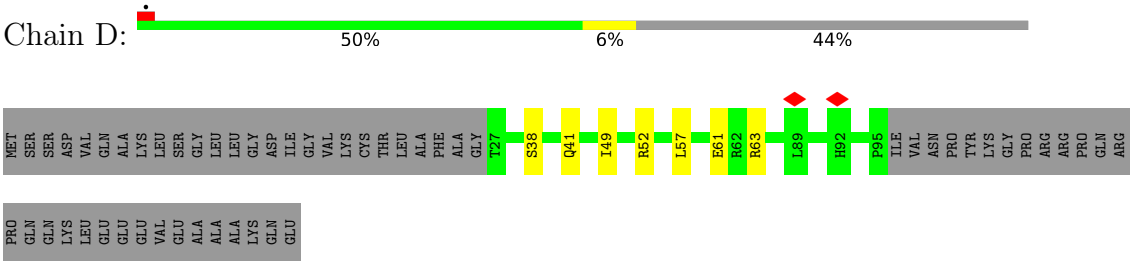
• Molecule 3: Toc52

Chain C:



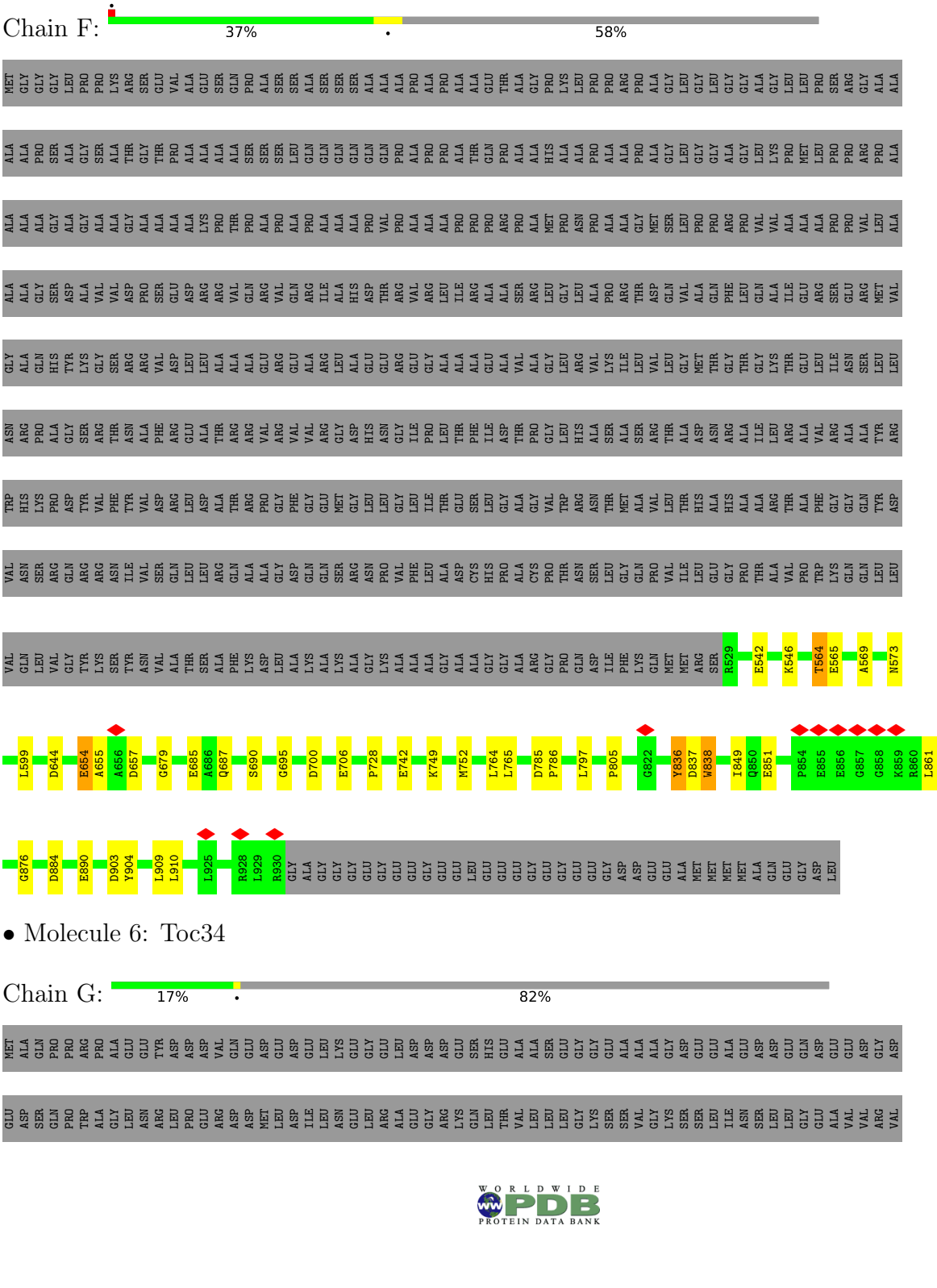
• Molecule 4: Tic13

Chain D:



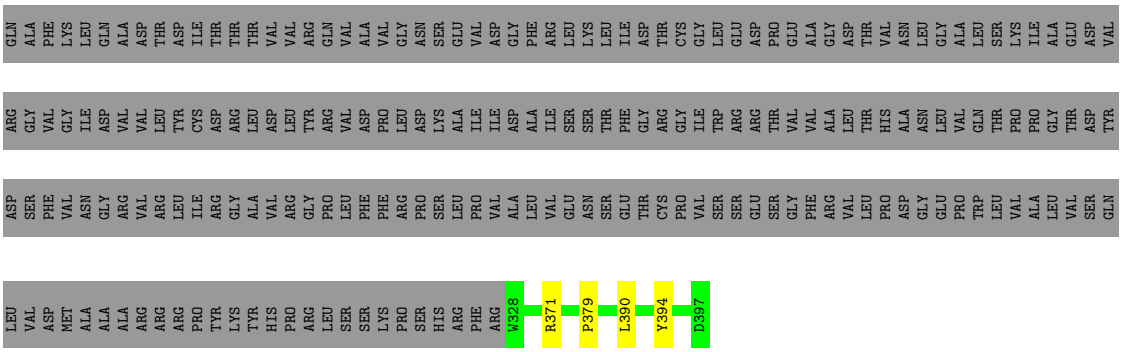
• Molecule 5: Toc120

Chain F:

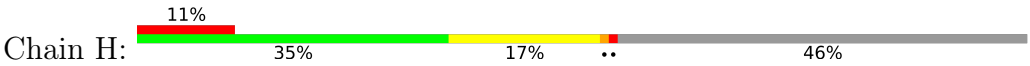


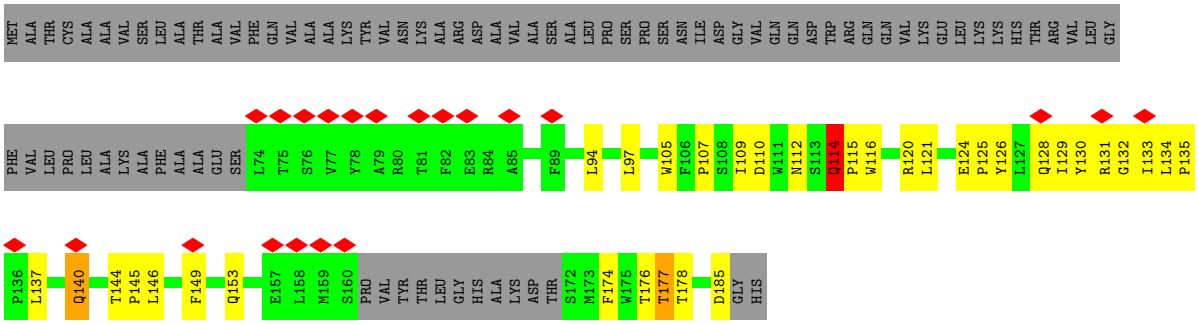
• Molecule 6: Toc34

Chain G:

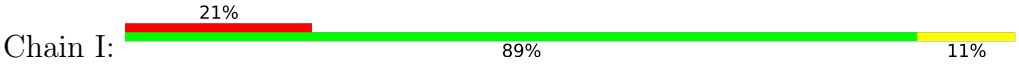


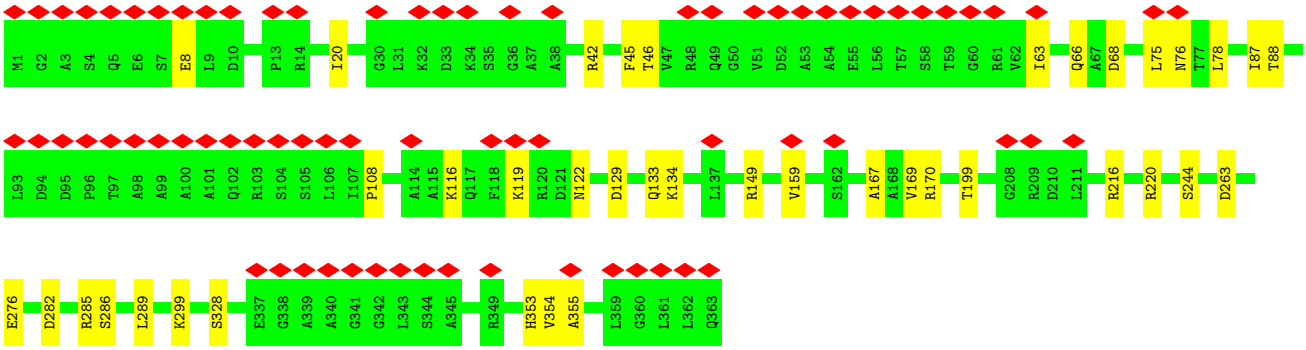
• Molecule 7: YlmG



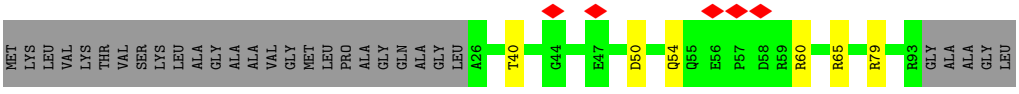


• Molecule 8: Toc39

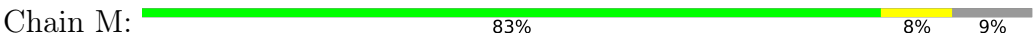




• Molecule 9: Toc10

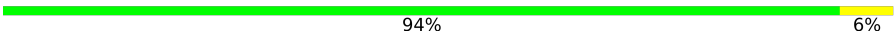


• Molecule 10: Tic12



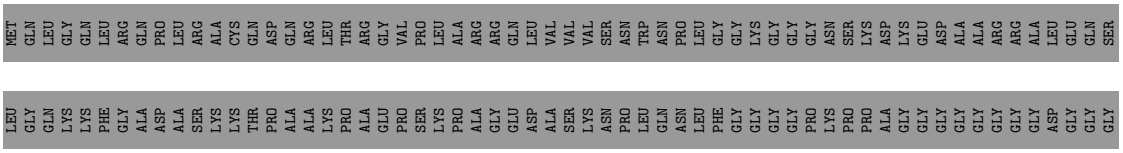
• Molecule 11: Unknown fragment

Chain N:



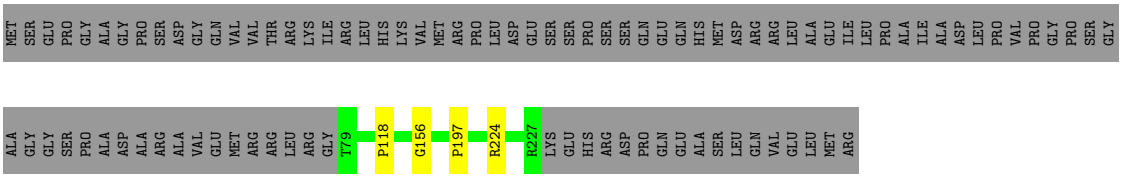
• Molecule 12: Tic35

Chain O:



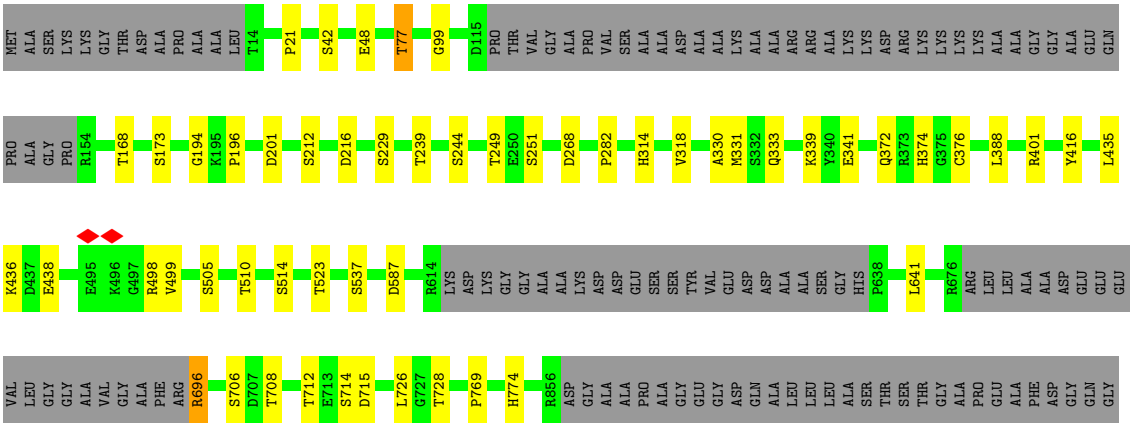
• Molecule 13: Tic56

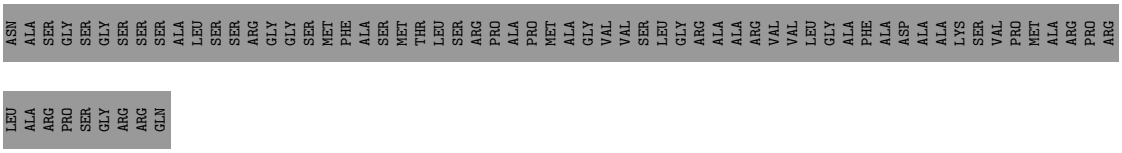
Chain Q:



• Molecule 14: Tic100

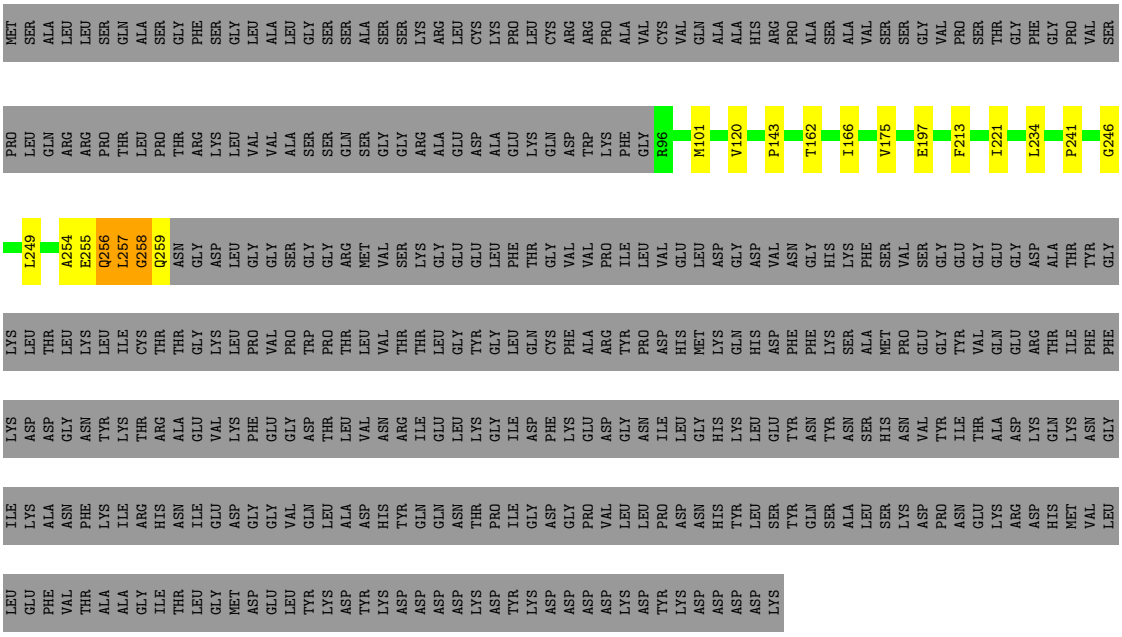
Chain T:





• Molecule 15: Tic20-Venus-Flag

Chain W: 27% 69%



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	595638	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	82000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	12.516	Depositor
Minimum map value	-2.213	Depositor
Average map value	0.037	Depositor
Map value standard deviation	0.144	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	417.40802, 417.40802, 417.40802	wwPDB
Map dimensions	384, 384, 384	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: IHP, TPO, MG, SEP, 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	0.37	0/12854	0.59	0/17304
2	B	0.31	0/5233	0.57	0/7079
3	C	0.36	0/1752	0.59	0/2369
4	D	0.28	0/544	0.52	0/742
5	F	0.34	0/3216	0.61	0/4370
6	G	0.37	0/628	0.65	0/847
7	H	0.56	0/857	0.54	0/1163
8	I	0.29	0/2804	0.58	0/3810
9	K	0.29	0/562	0.52	0/755
10	M	0.33	0/976	0.50	0/1327
11	N	0.42	0/161	0.59	0/218
12	O	0.29	0/1610	0.51	0/2182
13	Q	0.33	0/1282	0.56	0/1742
14	T	0.34	0/6112	0.57	0/8228
15	W	0.36	0/1455	0.53	0/1991
All	All	0.35	0/40046	0.57	0/54127

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	A	12577	0	12986	115	0
2	B	5142	0	4967	43	0
3	C	1728	0	1712	12	0
4	D	529	0	515	6	0
5	F	3139	0	2945	29	0
6	G	612	0	594	2	0
7	H	861	0	827	43	0
8	I	2751	0	2758	25	0
9	K	549	0	526	5	0
10	M	939	0	904	8	0
11	N	155	0	144	1	0
12	O	1572	0	1547	8	0
13	Q	1244	0	1263	4	0
14	T	6185	0	5745	30	0
15	W	1398	0	1362	17	0
16	A	205	0	305	5	0
17	A	36	0	6	1	0
18	F	1	0	0	0	0
18	T	1	0	0	0	0
19	A	1	0	0	0	0
19	O	1	0	0	0	0
All	All	39626	0	39106	278	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 4.

The worst 5 of 278 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1721:TYR:CD1	1:A:1724:LEU:HD12	1.45	1.47
1:A:1721:TYR:CD1	1:A:1724:LEU:CD1	2.27	1.15
1:A:1721:TYR:HD1	1:A:1724:LEU:CD1	1.59	1.14
7:H:110:ASP:O	7:H:116:TRP:HD1	1.42	1.01
5:F:690:SER:HB3	5:F:695:GLY:HA2	1.46	0.97

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	1465/1995 (73%)	1372 (94%)	90 (6%)	3 (0%)	44 64
2	B	645/798 (81%)	593 (92%)	52 (8%)	0	100 100
3	C	214/477 (45%)	205 (96%)	9 (4%)	0	100 100
4	D	67/124 (54%)	60 (90%)	7 (10%)	0	100 100
5	F	399/967 (41%)	370 (93%)	28 (7%)	1 (0%)	37 56
6	G	68/397 (17%)	65 (96%)	3 (4%)	0	100 100
7	H	94/187 (50%)	84 (89%)	8 (8%)	2 (2%)	5 10
8	I	361/363 (99%)	348 (96%)	13 (4%)	0	100 100
9	K	66/98 (67%)	63 (96%)	3 (4%)	0	100 100
10	M	113/127 (89%)	108 (96%)	5 (4%)	0	100 100
11	N	16/18 (89%)	14 (88%)	2 (12%)	0	100 100
12	O	193/329 (59%)	185 (96%)	8 (4%)	0	100 100
13	Q	147/244 (60%)	142 (97%)	5 (3%)	0	100 100
14	T	736/955 (77%)	707 (96%)	29 (4%)	0	100 100
15	W	162/532 (30%)	159 (98%)	1 (1%)	2 (1%)	11 21
All	All	4746/7611 (62%)	4475 (94%)	263 (6%)	8 (0%)	45 64

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	86	TYR
1	A	352	GLN
7	H	114	GLN
15	W	257	LEU
5	F	837	ASP

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	1391/1847 (75%)	1387 (100%)	4 (0%)	91 97
2	B	548/651 (84%)	547 (100%)	1 (0%)	92 97
3	C	172/372 (46%)	171 (99%)	1 (1%)	84 94
4	D	53/97 (55%)	53 (100%)	0	100 100
5	F	321/712 (45%)	317 (99%)	4 (1%)	67 86
6	G	61/336 (18%)	61 (100%)	0	100 100
7	H	88/155 (57%)	86 (98%)	2 (2%)	45 72
8	I	287/287 (100%)	287 (100%)	0	100 100
9	K	54/71 (76%)	54 (100%)	0	100 100
10	M	95/106 (90%)	95 (100%)	0	100 100
11	N	14/14 (100%)	14 (100%)	0	100 100
12	O	155/245 (63%)	154 (99%)	1 (1%)	84 94
13	Q	135/213 (63%)	135 (100%)	0	100 100
14	T	613/736 (83%)	612 (100%)	1 (0%)	92 97
15	W	149/457 (33%)	148 (99%)	1 (1%)	81 93
All	All	4136/6299 (66%)	4121 (100%)	15 (0%)	88 96

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	F	749	LYS
14	T	696	ARG
5	F	836	TYR
15	W	256	GLN
7	H	140	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
7	H	140	GLN
7	H	153	GLN
15	W	259	GLN
15	W	256	GLN
5	F	687	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

27 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	$\#\|Z\| > 2$
14	SEP	T	212	14	8,9,10	1.49	1 (12%)	8,12,14	1.71	2 (25%)
14	TPO	T	712	18,14	8,10,11	1.02	0	10,14,16	1.65	1 (10%)
14	SEP	T	714	14	8,9,10	1.41	1 (12%)	8,12,14	1.72	1 (12%)
7	TPO	H	177	7	8,10,11	1.69	3 (37%)	10,14,16	1.35	2 (20%)
14	SEP	T	173	14	8,9,10	1.38	1 (12%)	8,12,14	1.17	0
14	TPO	T	249	14	8,10,11	1.53	2 (25%)	10,14,16	1.73	1 (10%)
3	TPO	C	328	3	8,10,11	1.48	2 (25%)	10,14,16	1.56	1 (10%)
7	TPO	H	176	7	8,10,11	1.42	1 (12%)	10,14,16	1.49	1 (10%)
14	TPO	T	510	14	8,10,11	0.96	0	10,14,16	1.70	1 (10%)
14	SEP	T	229	14	8,9,10	1.43	1 (12%)	8,12,14	1.60	2 (25%)
5	TPO	F	564	5	8,10,11	1.53	1 (12%)	10,14,16	1.72	1 (10%)
2	SEP	B	339	2	8,9,10	1.48	1 (12%)	8,12,14	1.45	2 (25%)
14	SEP	T	244	14	8,9,10	1.34	1 (12%)	8,12,14	1.26	1 (12%)
14	TPO	T	708	18,14	8,10,11	0.97	0	10,14,16	1.62	1 (10%)
14	TPO	T	168	14	8,10,11	0.97	0	10,14,16	1.75	1 (10%)
2	SEP	B	344	2	8,9,10	1.54	1 (12%)	8,12,14	1.79	2 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	SEP	T	706	14	8,9,10	1.46	1 (12%)	8,12,14	2.00	2 (25%)
14	TPO	T	239	14	8,10,11	1.48	1 (12%)	10,14,16	1.55	2 (20%)
14	SEP	T	505	14	8,9,10	1.53	1 (12%)	8,12,14	1.32	1 (12%)
14	TPO	T	523	14	8,10,11	1.02	0	10,14,16	1.54	1 (10%)
14	SEP	T	537	14	8,9,10	1.49	1 (12%)	8,12,14	1.73	2 (25%)
14	SEP	T	514	14	8,9,10	1.45	1 (12%)	8,12,14	1.34	2 (25%)
7	TPO	H	178	7	8,10,11	1.27	2 (25%)	10,14,16	1.49	1 (10%)
14	SEP	T	42	14	8,9,10	1.41	1 (12%)	8,12,14	1.24	1 (12%)
14	SEP	T	251	14	8,9,10	1.47	1 (12%)	8,12,14	1.23	1 (12%)
1	TPO	A	1795	1	8,10,11	1.55	2 (25%)	10,14,16	1.45	1 (10%)
14	TPO	T	77	14	8,10,11	0.98	0	10,14,16	1.66	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
14	SEP	T	212	14	-	0/5/8/10	-
14	TPO	T	712	18,14	-	0/9/11/13	-
14	SEP	T	714	14	-	5/5/8/10	-
7	TPO	H	177	7	-	3/9/11/13	-
14	SEP	T	173	14	-	4/5/8/10	-
14	TPO	T	249	14	-	2/9/11/13	-
3	TPO	C	328	3	-	1/9/11/13	-
7	TPO	H	176	7	-	2/9/11/13	-
14	TPO	T	510	14	-	2/9/11/13	-
14	SEP	T	229	14	-	2/5/8/10	-
5	TPO	F	564	5	-	3/9/11/13	-
2	SEP	B	339	2	-	2/5/8/10	-
14	SEP	T	244	14	-	2/5/8/10	-
14	TPO	T	708	18,14	-	3/9/11/13	-
14	TPO	T	168	14	-	1/9/11/13	-
2	SEP	B	344	2	-	3/5/8/10	-
14	SEP	T	706	14	-	4/5/8/10	-
14	TPO	T	239	14	-	1/9/11/13	-
14	SEP	T	505	14	-	0/5/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	TPO	T	523	14	-	1/9/11/13	-
14	SEP	T	537	14	-	1/5/8/10	-
14	SEP	T	514	14	-	3/5/8/10	-
7	TPO	H	178	7	-	4/9/11/13	-
14	SEP	T	42	14	-	0/5/8/10	-
14	SEP	T	251	14	-	0/5/8/10	-
1	TPO	A	1795	1	-	4/9/11/13	-
14	TPO	T	77	14	-	1/9/11/13	-

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	T	505	SEP	P-O1P	3.36	1.61	1.50
2	B	344	SEP	P-O1P	3.35	1.61	1.50
14	T	212	SEP	P-O1P	3.26	1.61	1.50
14	T	537	SEP	P-O1P	3.25	1.61	1.50
14	T	706	SEP	P-O1P	3.25	1.61	1.50

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	T	168	TPO	P-OG1-CB	-5.16	107.61	123.21
14	T	249	TPO	P-OG1-CB	-4.84	108.60	123.21
14	T	77	TPO	P-OG1-CB	-4.83	108.62	123.21
5	F	564	TPO	P-OG1-CB	-4.67	109.10	123.21
14	T	510	TPO	P-OG1-CB	-4.66	109.14	123.21

There are no chirality outliers.

5 of 54 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1795	TPO	N-CA-CB-OG1
1	A	1795	TPO	O-C-CA-CB
2	B	344	SEP	CB-OG-P-O2P
2	B	344	SEP	CB-OG-P-O3P
3	C	328	TPO	O-C-CA-CB

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	H	177	TPO	1	0
5	F	564	TPO	1	0
2	B	339	SEP	1	0
14	T	77	TPO	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 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	$\#\|Z\| > 2$
16	LMG	A	2001	-	49,49,55	0.81	2 (4%)	57,57,63	1.34	8 (14%)
16	LMG	A	2003	-	55,55,55	0.83	3 (5%)	63,63,63	1.40	8 (12%)
16	LMG	A	2002	-	46,46,55	0.85	1 (2%)	54,54,63	1.29	4 (7%)
16	LMG	A	2004	-	55,55,55	0.85	4 (7%)	63,63,63	1.39	8 (12%)
17	IHP	A	2005	-	36,36,36	0.93	0	54,60,60	1.56	8 (14%)

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
16	LMG	A	2001	-	-	22/44/64/70	0/1/1/1
16	LMG	A	2003	-	-	18/50/70/70	0/1/1/1
16	LMG	A	2002	-	-	15/41/61/70	0/1/1/1
16	LMG	A	2004	-	-	22/50/70/70	0/1/1/1
17	IHP	A	2005	-	-	8/30/54/54	0/1/1/1

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	A	2004	LMG	C4-C5	2.60	1.58	1.53
16	A	2003	LMG	O7-C8	-2.45	1.40	1.46
16	A	2002	LMG	O7-C8	-2.38	1.40	1.46
16	A	2003	LMG	O1-C7	-2.37	1.39	1.43
16	A	2001	LMG	O7-C8	-2.28	1.40	1.46

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	A	2005	IHP	C6-C1-C2	3.88	118.90	110.41
17	A	2005	IHP	O12-C2-C1	3.80	117.65	108.69
16	A	2004	LMG	O1-C7-C8	-3.44	102.59	110.90
17	A	2005	IHP	C6-C5-C4	3.35	117.74	110.41
17	A	2005	IHP	O14-C4-C3	3.28	116.41	108.69

There are no chirality outliers.

5 of 85 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	A	2004	LMG	O6-C1-O1-C7
17	A	2005	IHP	C3-O13-P3-O23
17	A	2005	IHP	C4-O14-P4-O44
17	A	2005	IHP	C6-O16-P6-O26
16	A	2001	LMG	O10-C28-O8-C9

There are no ring outliers.

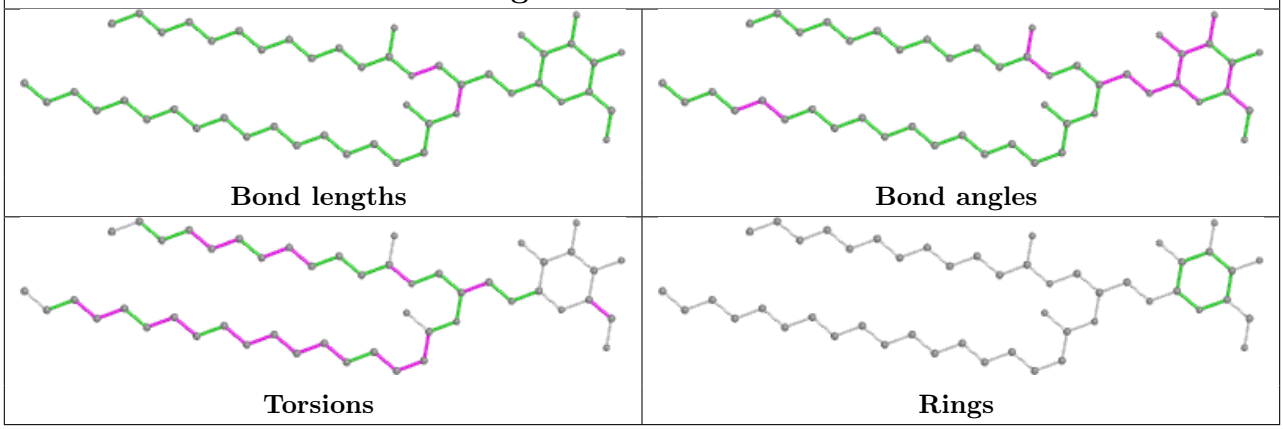
4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	A	2001	LMG	1	0
16	A	2002	LMG	1	0
16	A	2004	LMG	3	0
17	A	2005	IHP	1	0

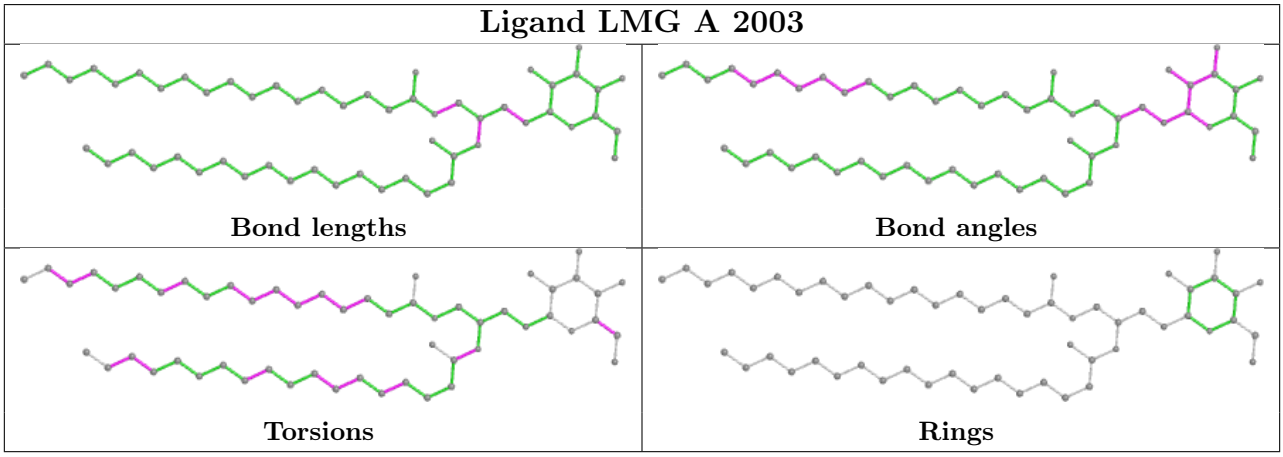
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

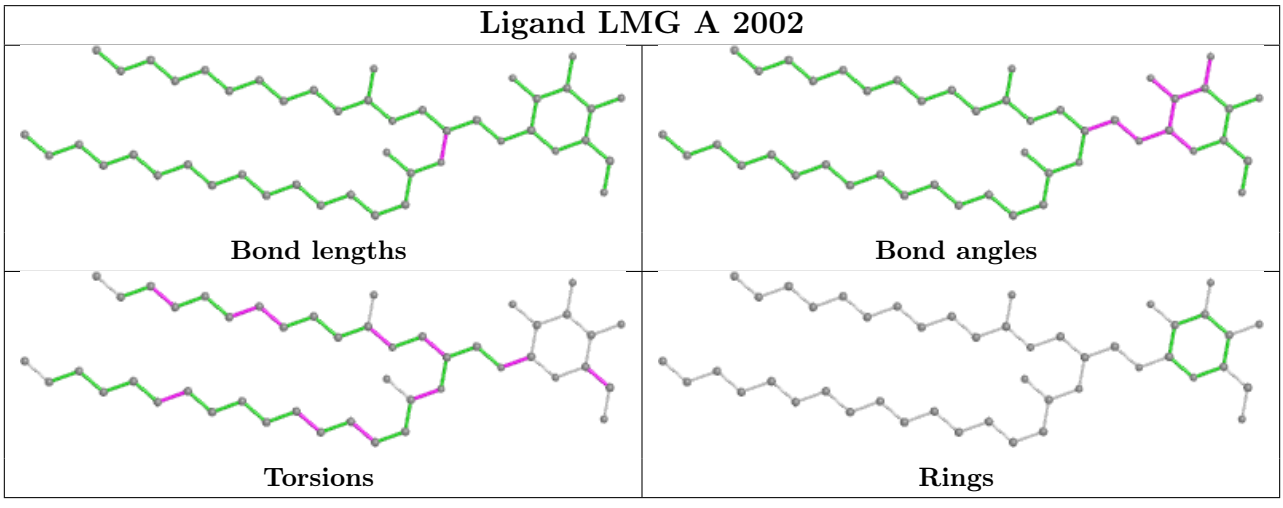
Ligand LMG A 2001

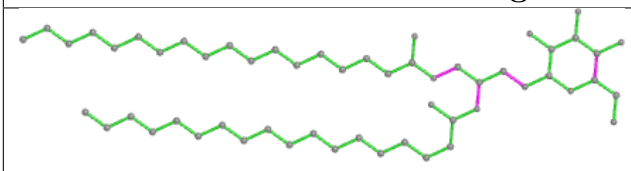
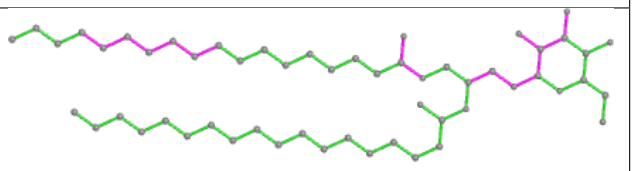
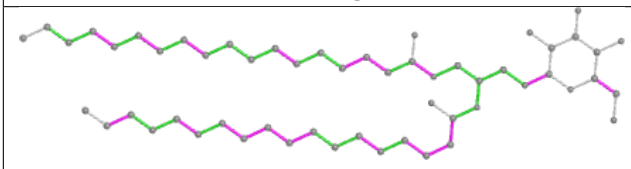
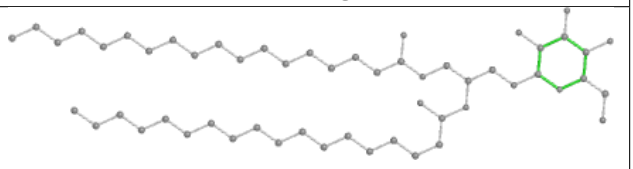


Ligand LMG A 2003

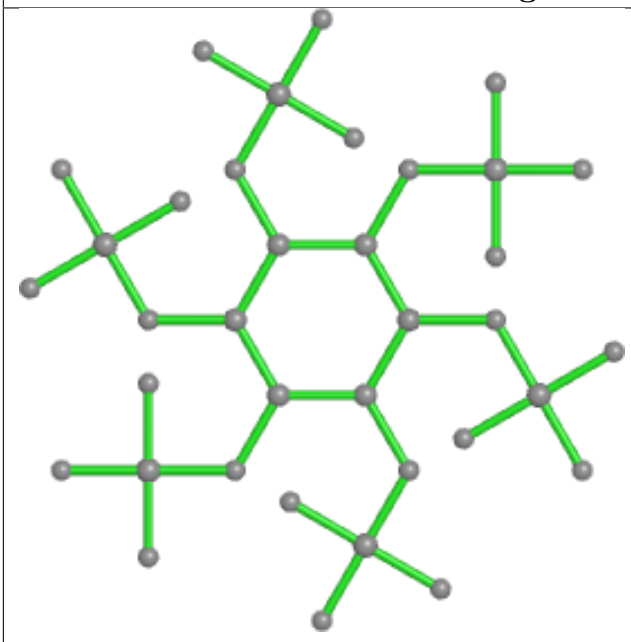


Ligand LMG A 2002

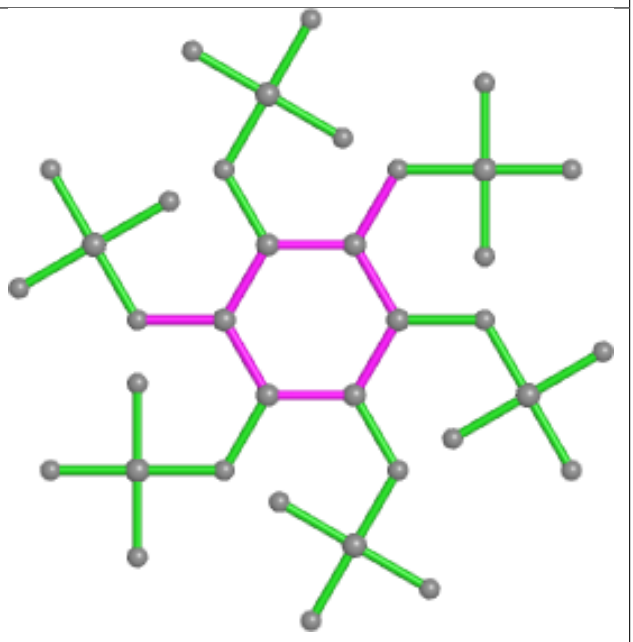


Ligand LMG A 2004	
 Bond lengths	 Bond angles
 Torsions	 Rings

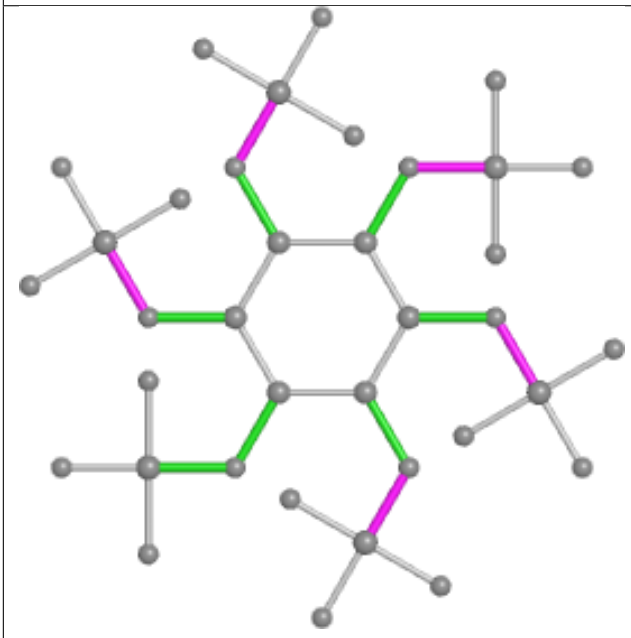
Ligand IHP A 2005



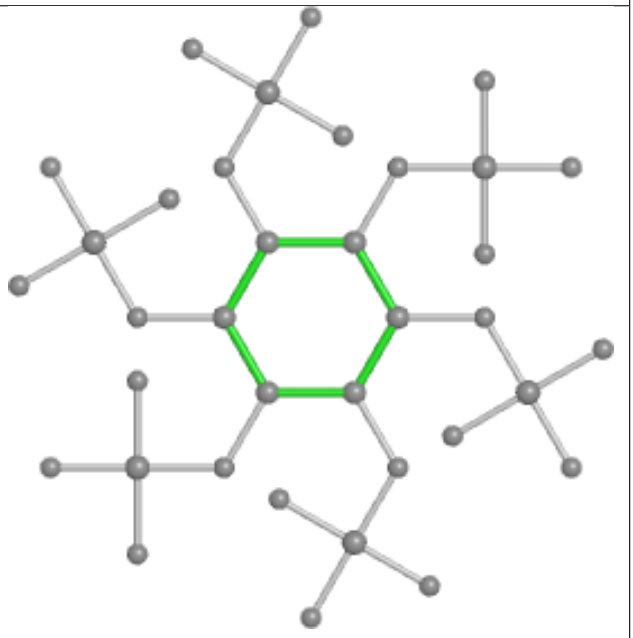
Bond lengths



Bond angles



Torsions



Rings

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.

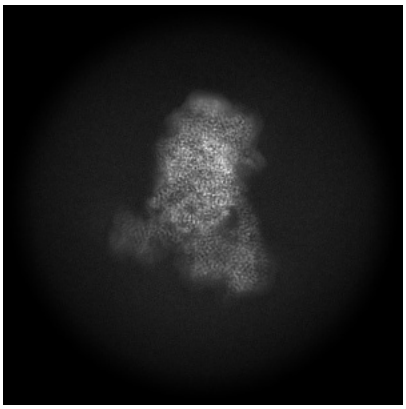
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-31890. These allow visual inspection of the internal detail of the map and identification of artifacts.

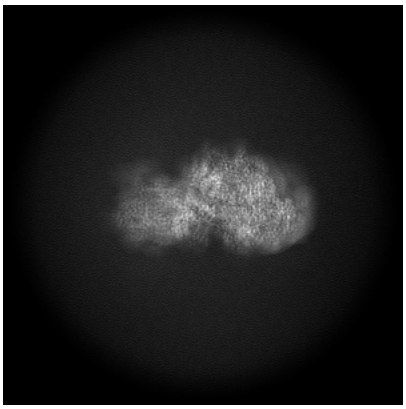
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

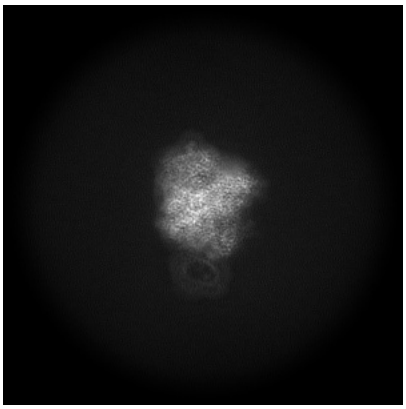
6.1.1 Primary map



X

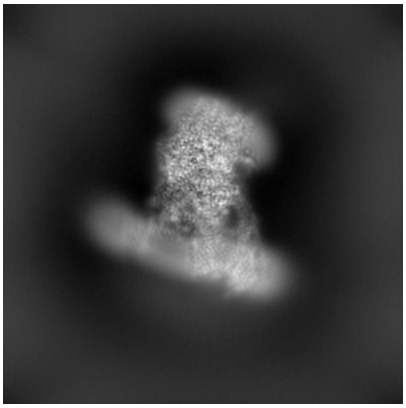


Y

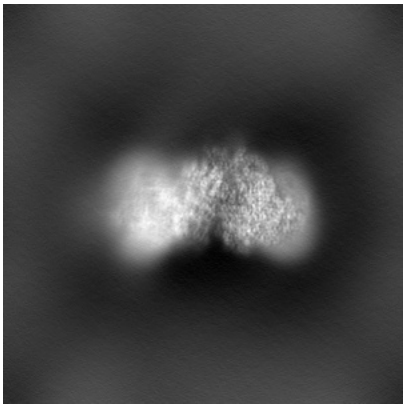


Z

6.1.2 Raw map



X



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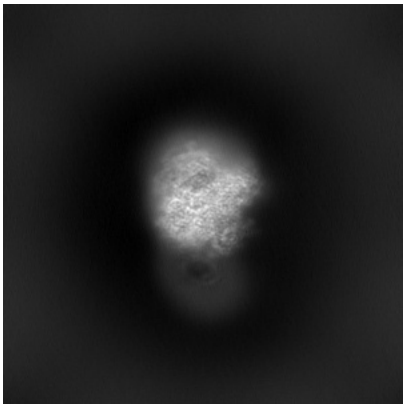
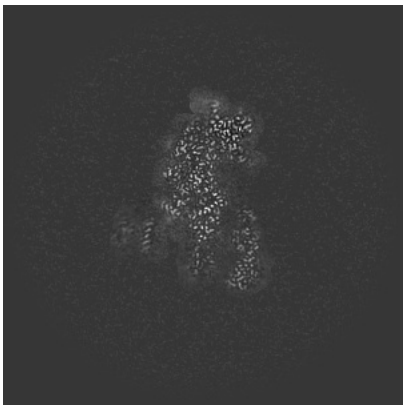


Z

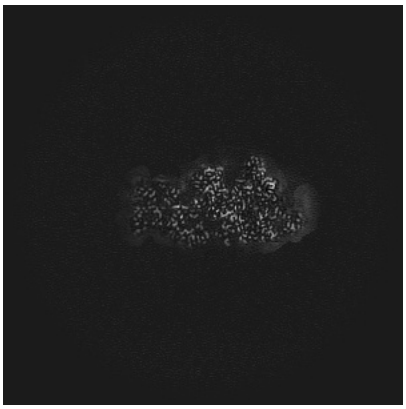
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

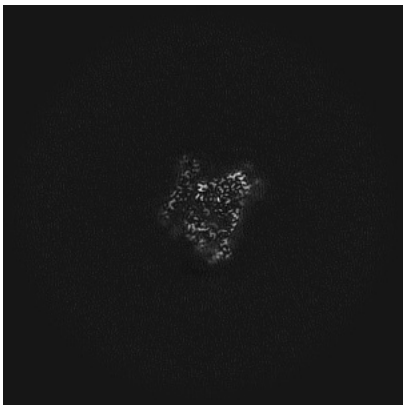
6.2.1 Primary map



X Index: 192

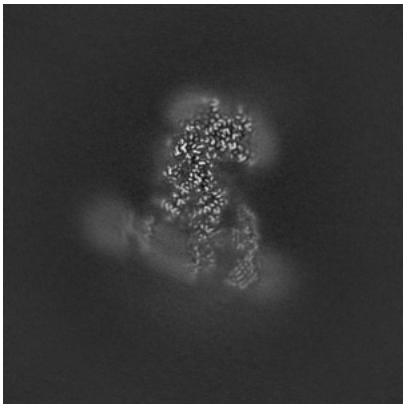


Y Index: 192

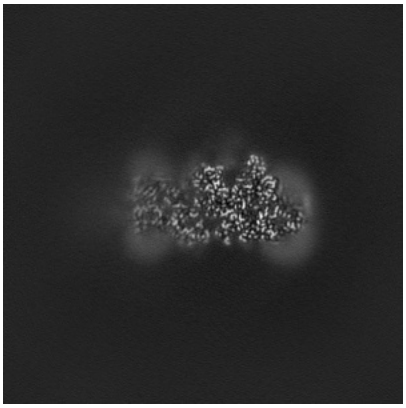


Z Index: 192

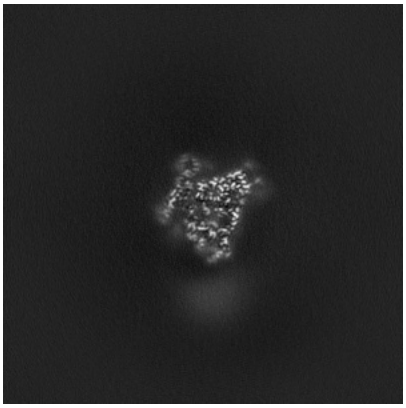
6.2.2 Raw map



X Index: 192



Y Index: 192

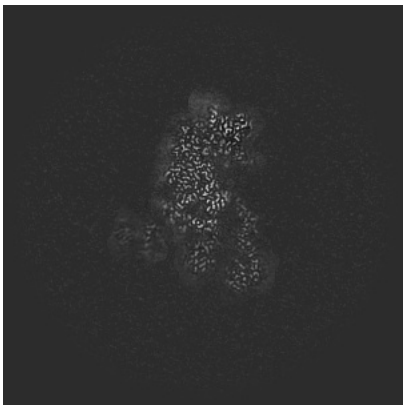


Z Index: 192

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

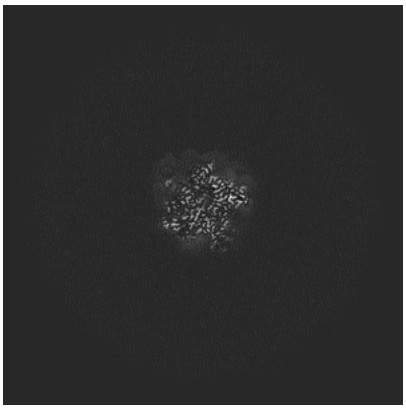
6.3 Largest variance slices (i)

6.3.1 Primary map



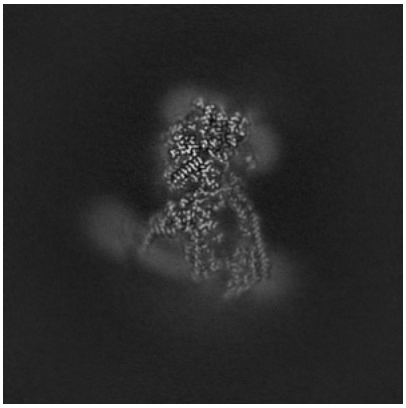
X Index: 188

Y Index: 210

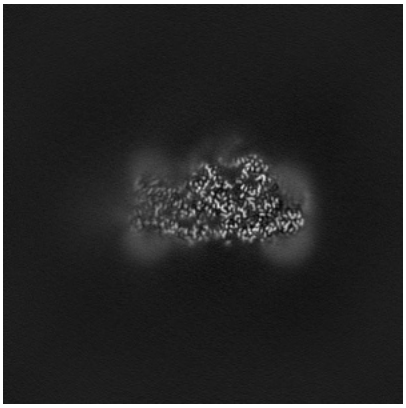


Z Index: 246

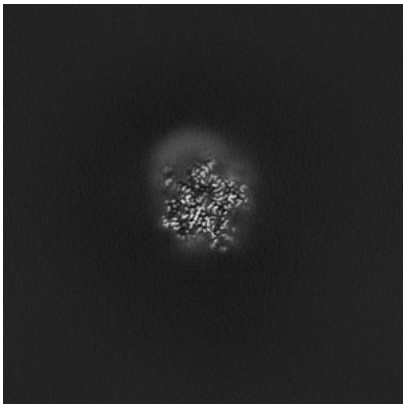
6.3.2 Raw map



X Index: 180



Y Index: 196

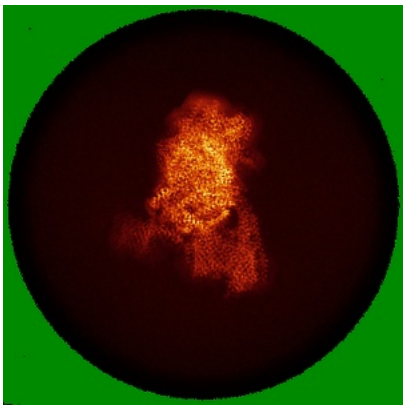


Z Index: 246

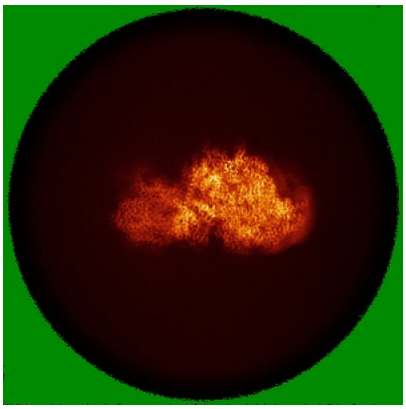
The images above show the largest variance slices of the map in three orthogonal directions.

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

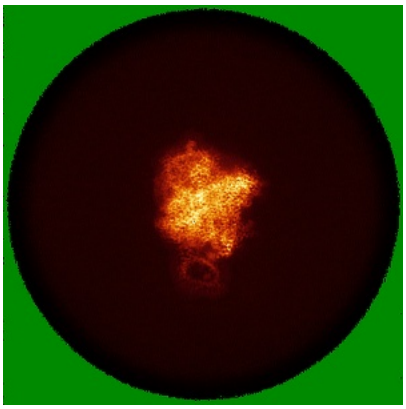
6.4.1 Primary map



X

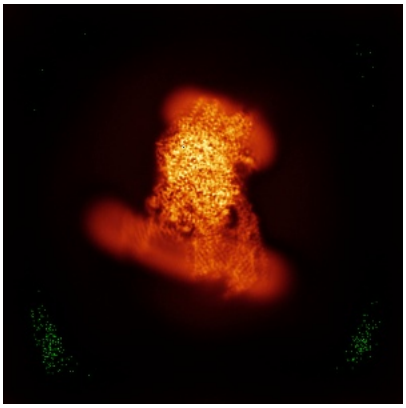


Y

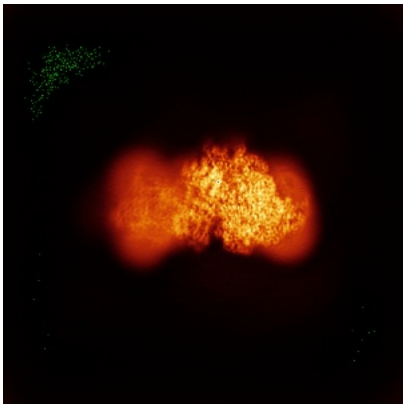


Z

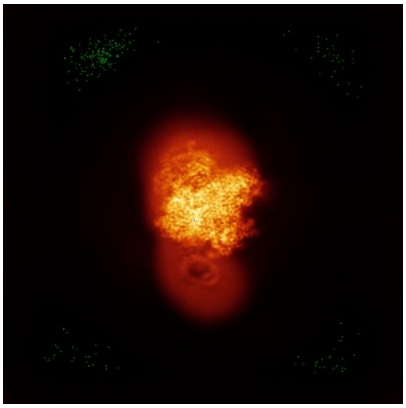
6.4.2 Raw map



X



Y

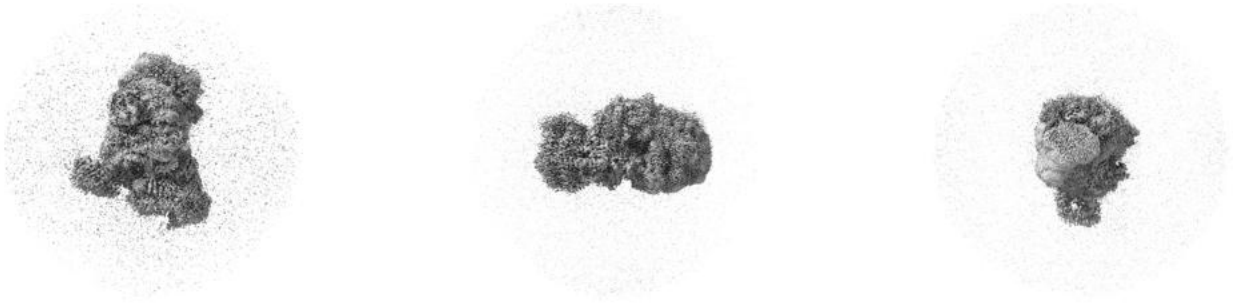


Z

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)

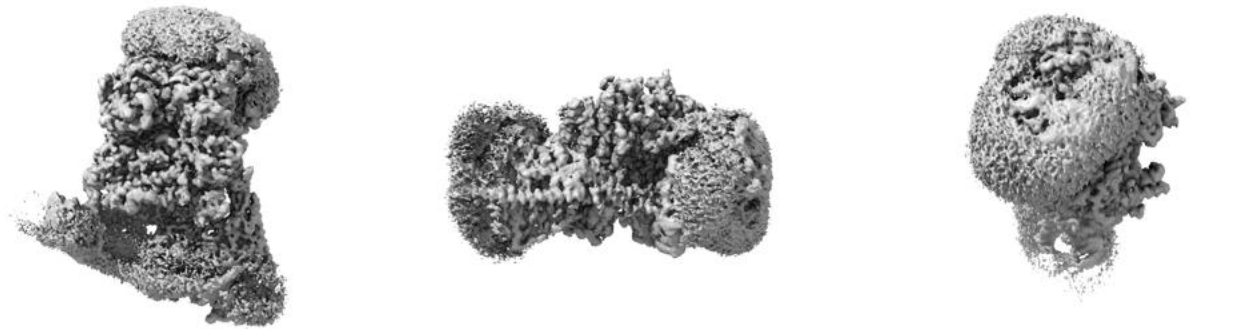
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.5. 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.

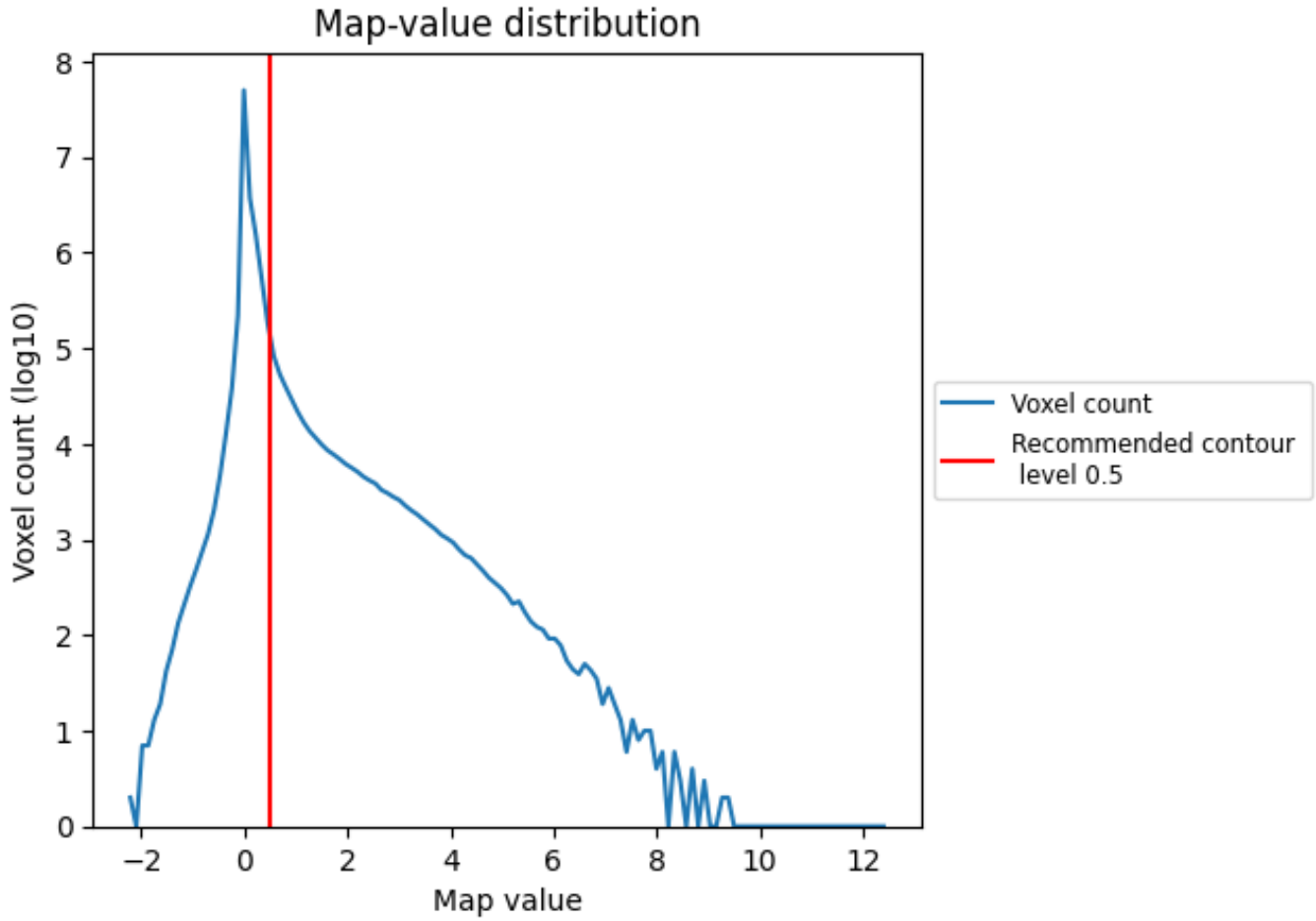
6.6 Mask visualisation (i)

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

7 Map analysis

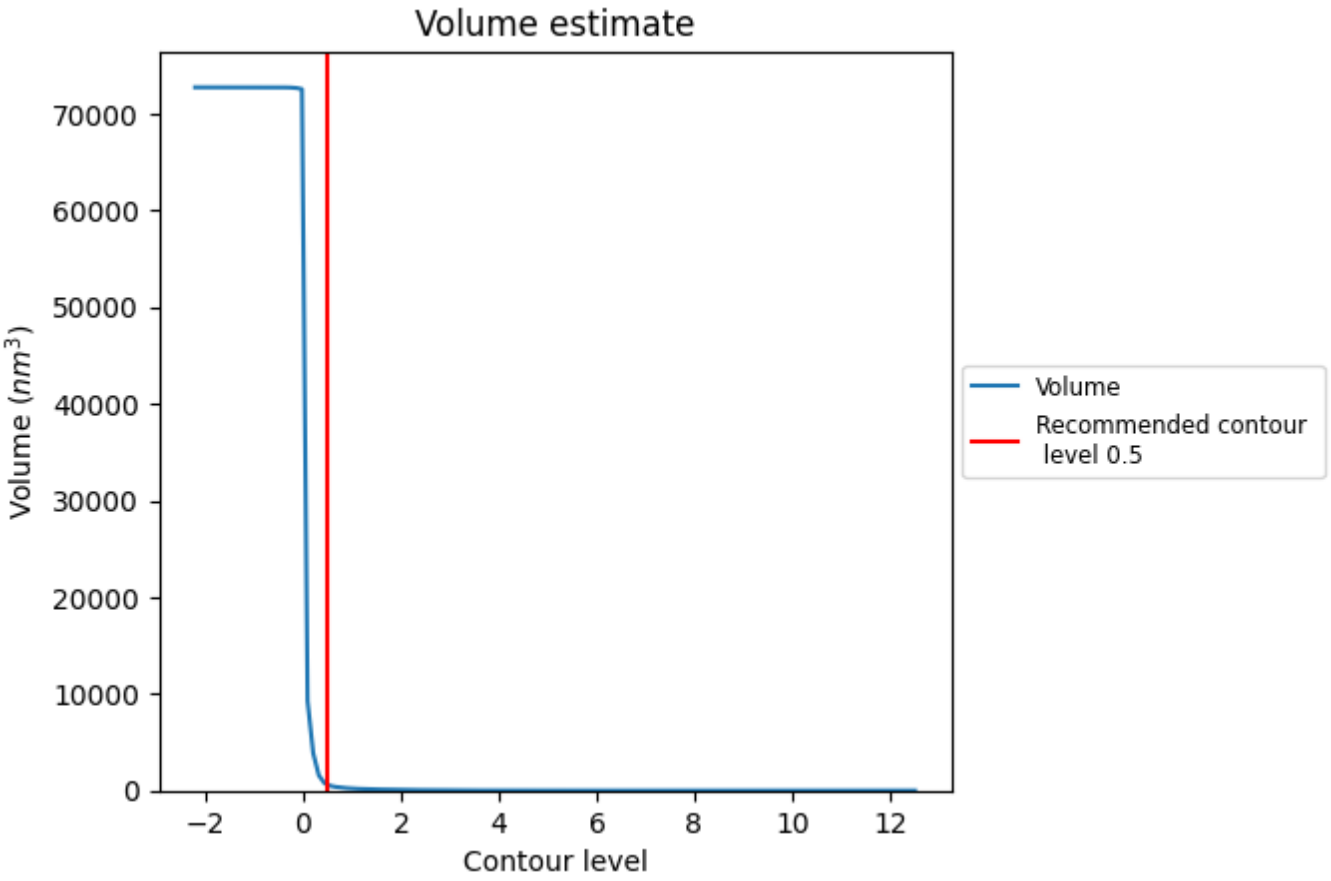
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

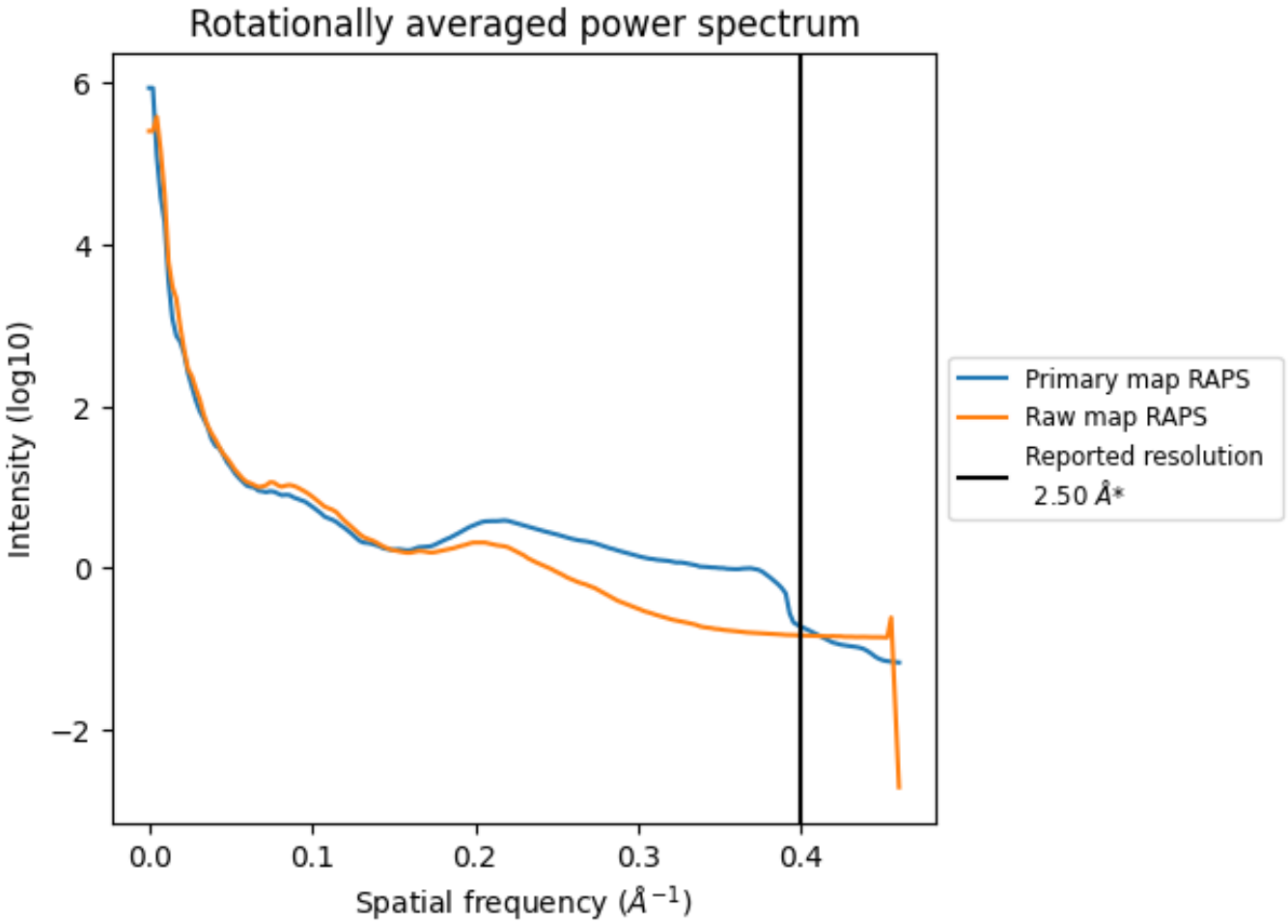
7.2 Volume estimate (i)



The volume at the recommended contour level is 608 nm^3; this corresponds to an approximate mass of 549 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 (i)

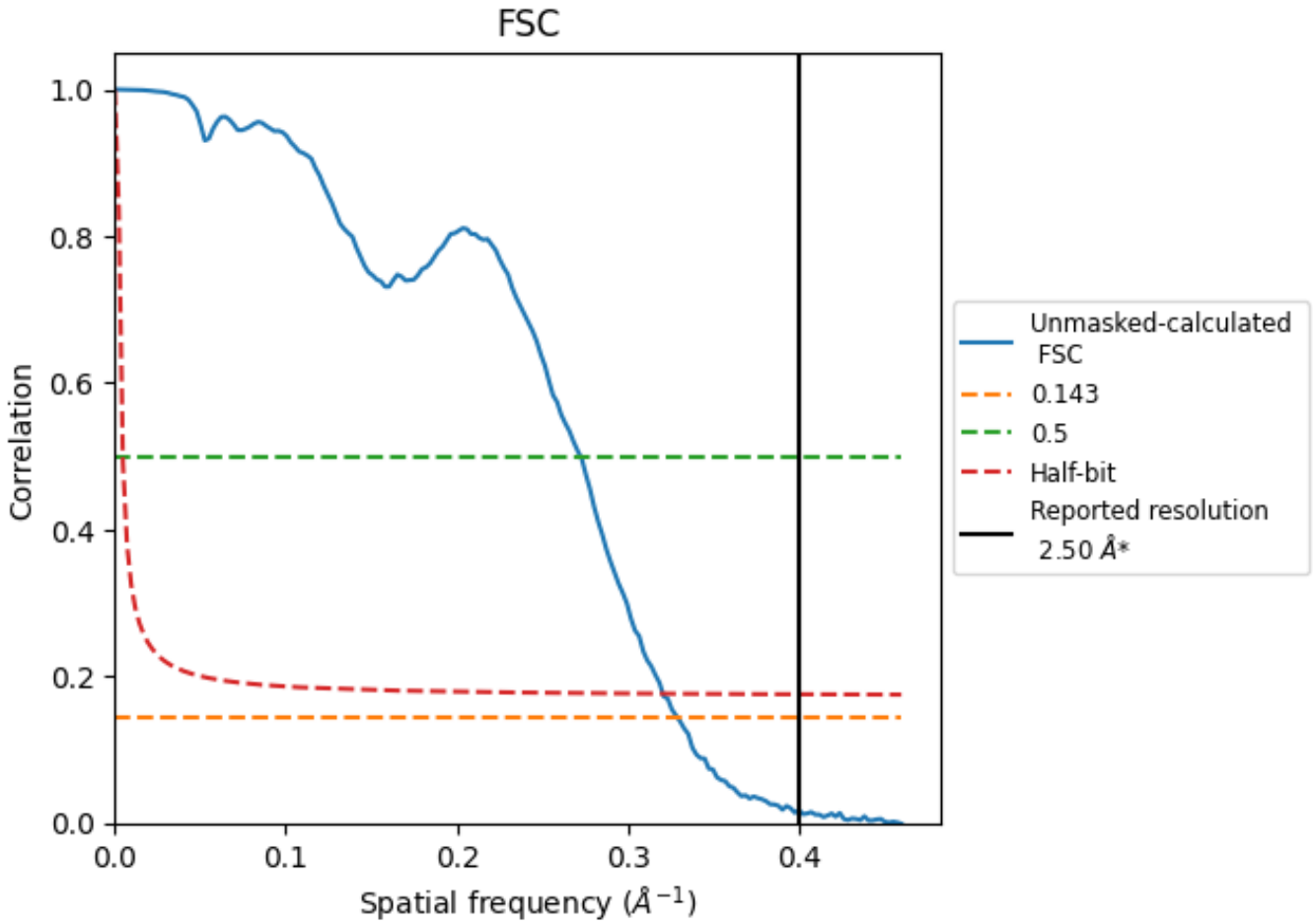


*Reported resolution corresponds to spatial frequency of 0.400 $Å^{-1}$

8 Fourier-Shell correlation

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



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

8.2 Resolution estimates (i)

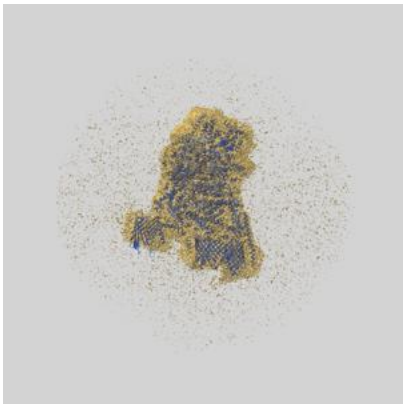
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.04	3.67	3.12

*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 3.04 differs from the reported value 2.5 by more than 10 %

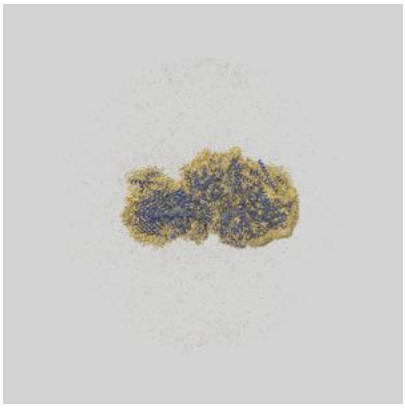
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-31890 and PDB model 7VCF. Per-residue inclusion information can be found in section 3 on page 8.

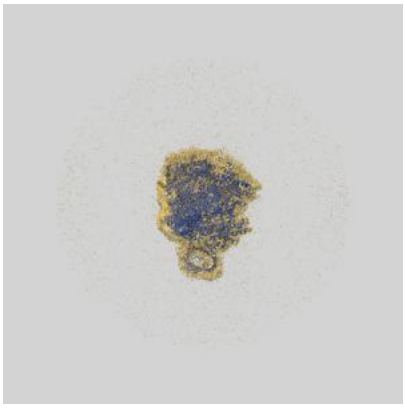
9.1 Map-model overlay



X



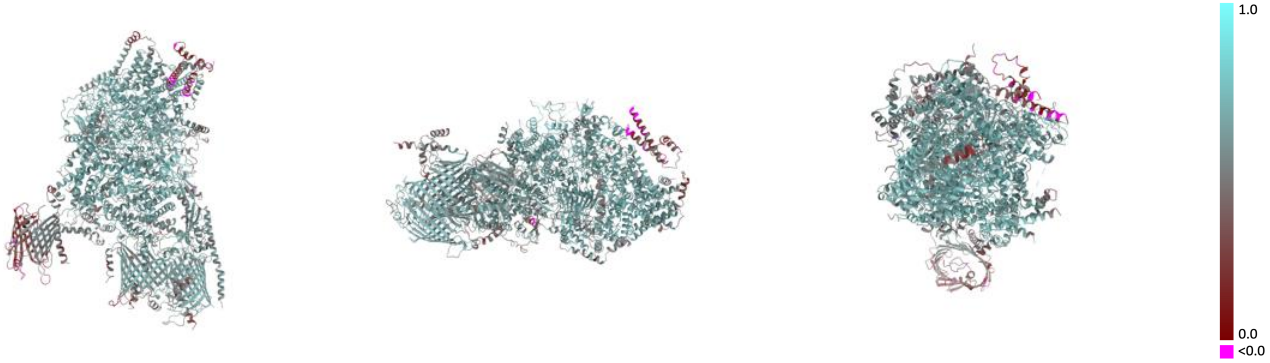
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.5 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.

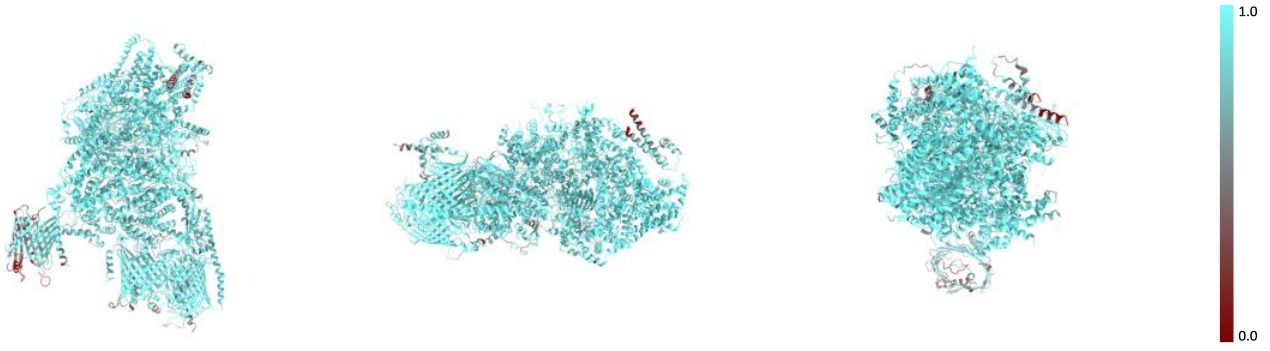
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according 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.

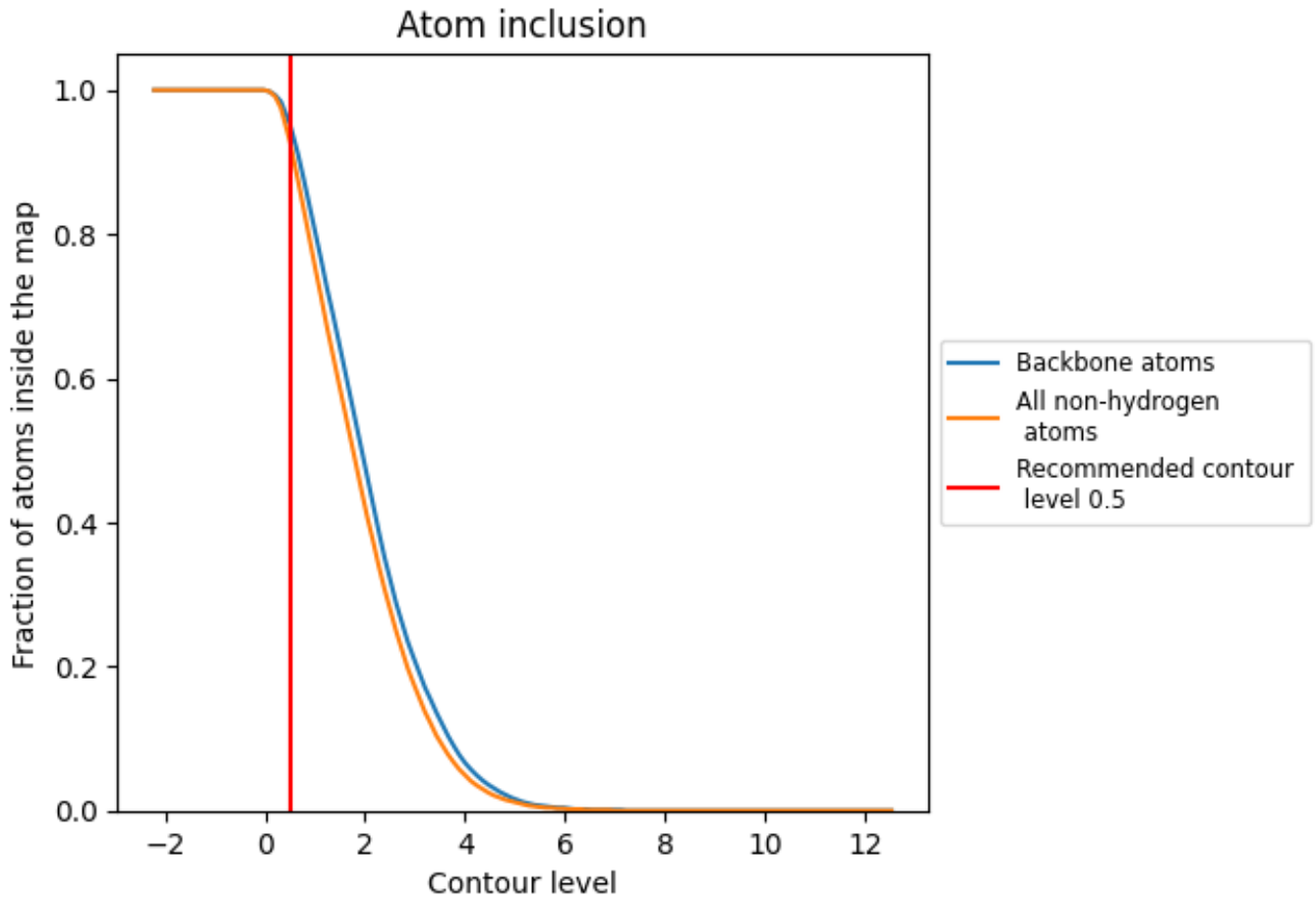
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (0.5).

9.4 Atom inclusion (i)



At the recommended contour level, 95% of all backbone atoms, 93% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9280	0.5890
A	0.9840	0.6200
B	0.9190	0.5700
C	0.9490	0.5900
D	0.8830	0.5100
F	0.9070	0.5620
G	0.9210	0.5650
H	0.6730	0.2740
I	0.6840	0.3860
K	0.8230	0.5110
M	0.9920	0.6910
N	0.8810	0.4330
O	0.9250	0.6000
Q	0.9620	0.6730
T	0.9650	0.6620
W	0.9850	0.6350