



wwPDB EM Validation Summary Report ⓘ

Mar 10, 2026 – 04:31 AM UTC

PDB ID : 8XKS / pdb_00008xks
EMDB ID : EMD-38424
Title : The cryo-EM structure of Orf2971-FtsHi motor complex
Authors : Wang, N.; Li, M.
Deposited on : 2023-12-24
Resolution : 3.20 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

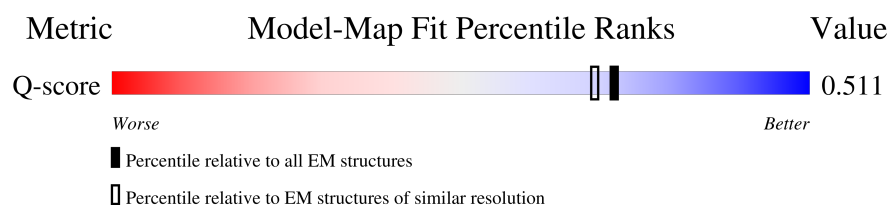
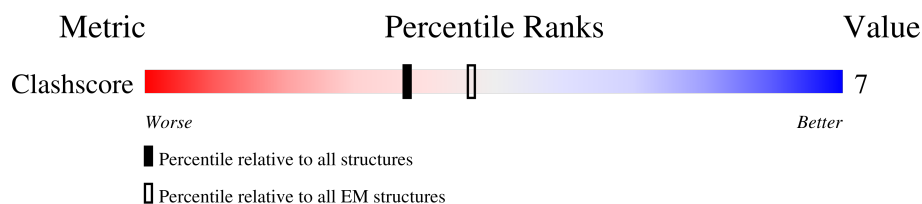
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

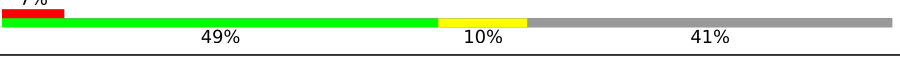
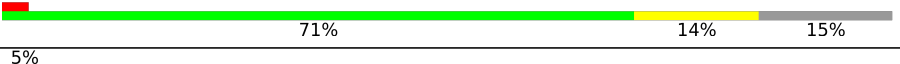
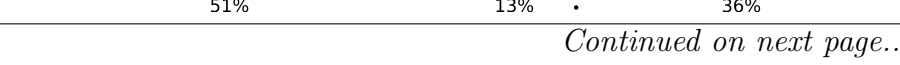
The reported resolution of this entry is 3.20 Å.

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.



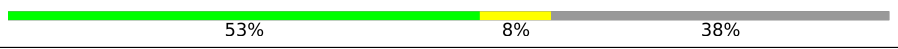
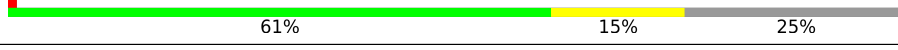
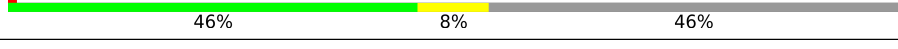
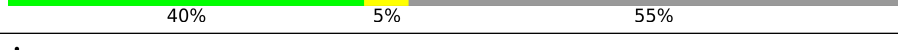
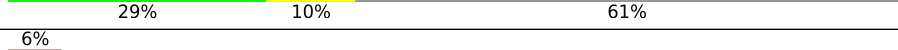
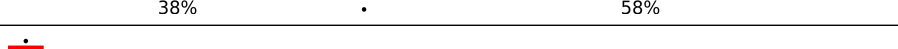
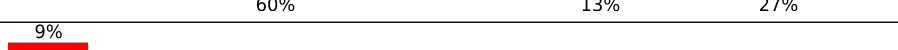
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Q-score	-	25397	15020 (2.70 - 3.70)

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	982	 5% 60% 13% 22%
2	B	1024	 7% 49% 10% 34%
3	C	462	 1% 71% 14% 14%
4	D	1178	 5% 66% 16% 13%
5	E	2971	 1% 39% 10% 50%
6	F	1058	 1% 51% 13% 35%

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Mol	Chain	Length	Quality of chain
6	G	1058	
7	H	691	
8	I	330	
9	J	365	
10	K	682	
11	L	255	
12	M	303	
13	N	324	
14	O	471	
15	P	555	
16	Q	495	
17	R	117	
18	S	137	
19	T	299	

2 Entry composition [i](#)

There are 25 unique types of molecules in this entry. The entry contains 67528 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 Ctap1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	715	Total	C	N	O	S	0	0
			5557	3504	1001	1038	14		

- Molecule 2 is a protein called Fhl2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	603	Total	C	N	O	S	0	0
			4588	2880	830	859	19		

- Molecule 3 is a protein called 4Fe-4S ferredoxin-type domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	391	Total	C	N	O	S	0	0
			3085	1940	555	569	21		

- Molecule 4 is a protein called AAA+ ATPase domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	971	Total	C	N	O	S	0	0
			7551	4796	1323	1396	36		

- Molecule 5 is a protein called Uncharacterized 341.7 kDa protein in psbD-psbC intergenic region.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	1458	Total	C	N	O	S	0	0
			12035	7819	2048	2142	26		

- Molecule 6 is a protein called AAA+ ATPase domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	676	Total	C	N	O	S	0	0
			5216	3291	927	967	31		

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	674	Total	C	N	O	S	0	0
			5260	3327	928	977	28		

- Molecule 7 is a protein called Flagellar associated protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	500	Total	C	N	O	S	0	0
			3670	2289	681	690	10		

- Molecule 8 is a protein called Tic22.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	204	Total	C	N	O	S	0	0
			1619	1035	277	298	9		

- Molecule 9 is a protein called FaxL.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	274	Total	C	N	O	S	0	0
			2101	1326	393	368	14		

- Molecule 10 is a protein called Fatty acid desaturase domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	370	Total	C	N	O	S	0	0
			2853	1866	486	485	16		

- Molecule 11 is a protein called Moc25.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	185	Total	C	N	O	S	0	0
			1541	1017	267	250	7		

- Molecule 12 is a protein called Moc29.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	135	Total	C	N	O	S	0	0
			1127	762	185	176	4		

- Molecule 13 is a protein called Moc34.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	125	Total	C	N	O	S	0	0
			1005	627	181	196	1		

- Molecule 14 is a protein called Moc45.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	197	Total	C	N	O	S	0	0
			1517	1012	246	253	6		

- Molecule 15 is a protein called PcyA1.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	406	Total	C	N	O	S	0	0
			3245	2061	547	616	21		

- Molecule 16 is a protein called ADP-ribosylglycohydrolase.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	386	Total	C	N	O	S	0	0
			2880	1811	531	534	4		

- Molecule 17 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	85	Total	C	N	O	P S	0	0
			633	393	99	137	1 3		

- Molecule 18 is a protein called Moc13.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	114	Total	C	N	O	S	0	0
			909	579	168	159	3		

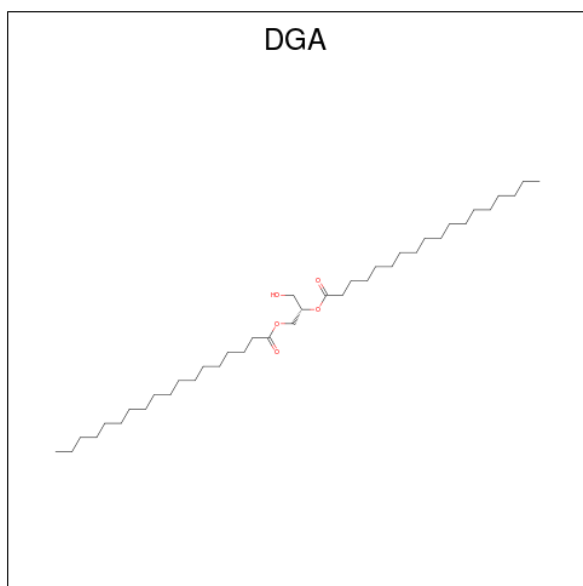
- Molecule 19 is a protein called Moc31.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	107	Total	C	N	O	S	0	0
			840	524	144	170	2		

- Molecule 20 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

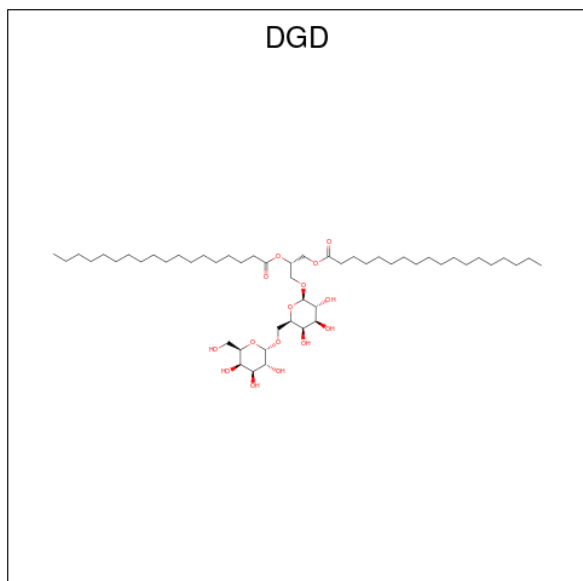
Mol	Chain	Residues	Atoms		AltConf
20	C	2	Total	Zn	0
			2	2	

- Molecule 21 is DIACYL GLYCEROL (CCD ID: DGA) (formula: $C_{39}H_{76}O_5$) (labeled as "Ligand of Interest" by depositor).



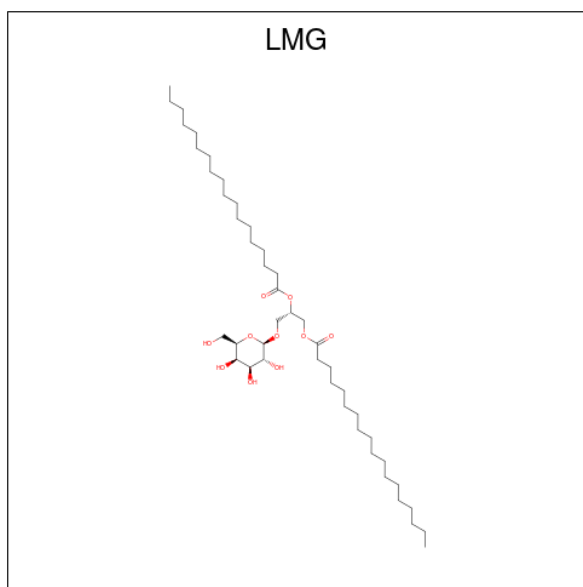
Mol	Chain	Residues	Atoms			AltConf
21	H	1	Total	C	O	0
			36	31	5	

- Molecule 22 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



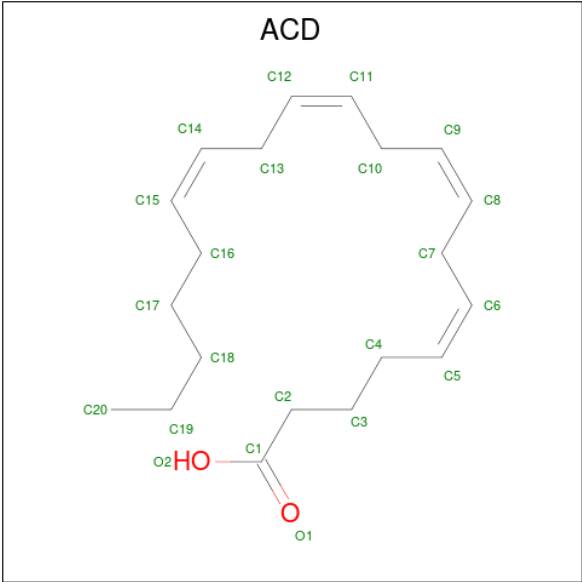
Mol	Chain	Residues	Atoms			AltConf
22	J	1	Total	C	O	0
			47	32	15	
22	L	1	Total	C	O	0
			66	51	15	

- Molecule 23 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



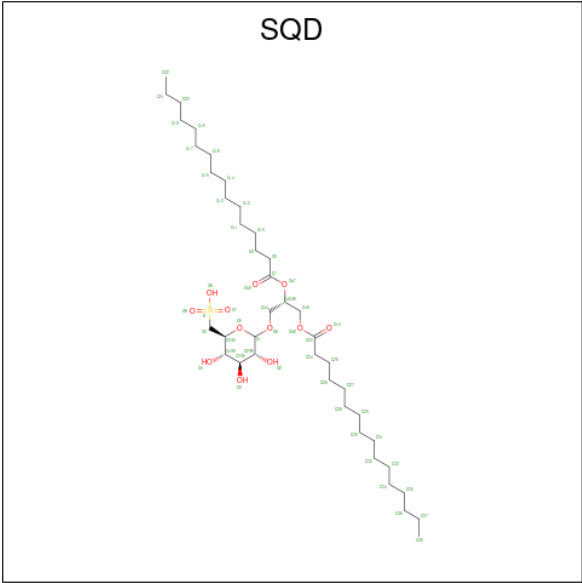
Mol	Chain	Residues	Atoms			AltConf
23	J	1	Total	C	O	0
			41	31	10	
23	L	1	Total	C	O	0
			47	37	10	

- Molecule 24 is ARACHIDONIC ACID (CCD ID: ACD) (formula: $C_{20}H_{32}O_2$) (labeled as "Ligand of Interest" by depositor).

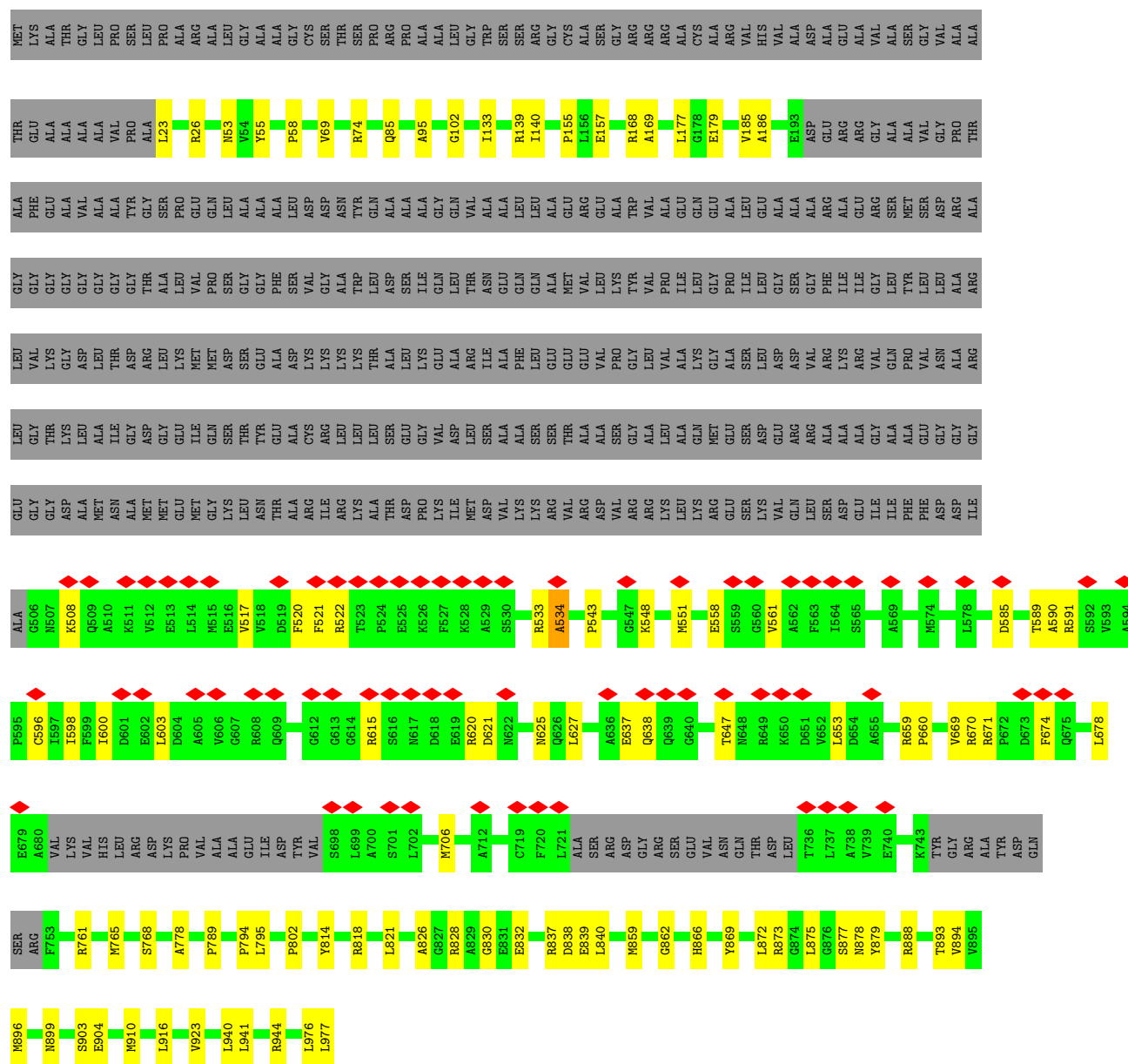


Mol	Chain	Residues	Atoms			AltConf
24	K	1	Total	C	O	0
			21	20	1	

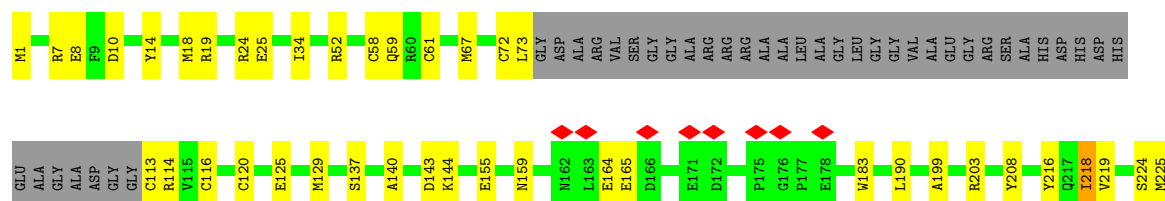
- Molecule 25 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).

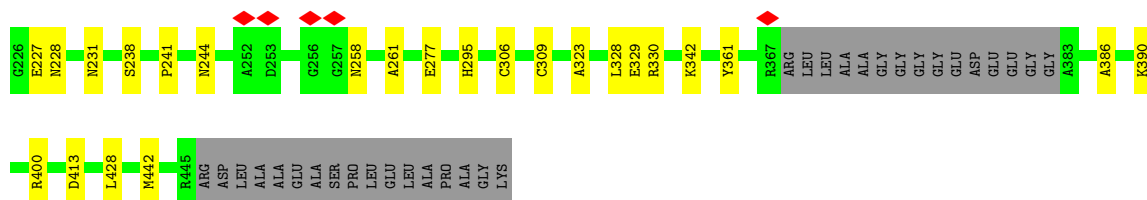


Mol	Chain	Residues	Atoms				AltConf
25	L	1	Total	C	O	S	0
			36	23	12	1	

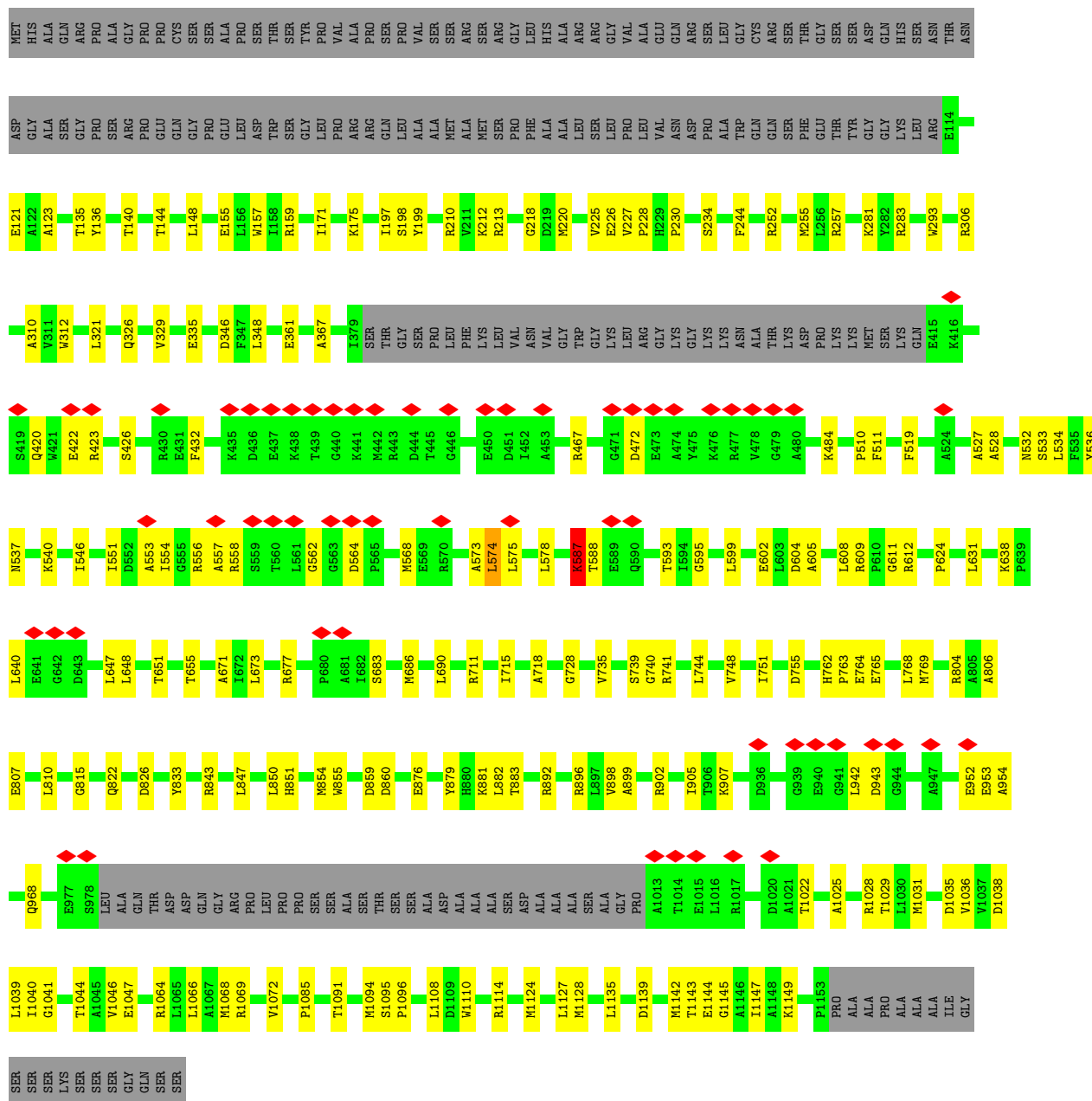


• Molecule 3: 4Fe-4S ferredoxin-type domain-containing protein

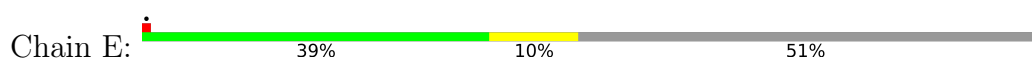




• Molecule 4: AAA+ ATPase domain-containing protein



• Molecule 5: Uncharacterized 341.7 kDa protein in psbD-psbC intergenic region









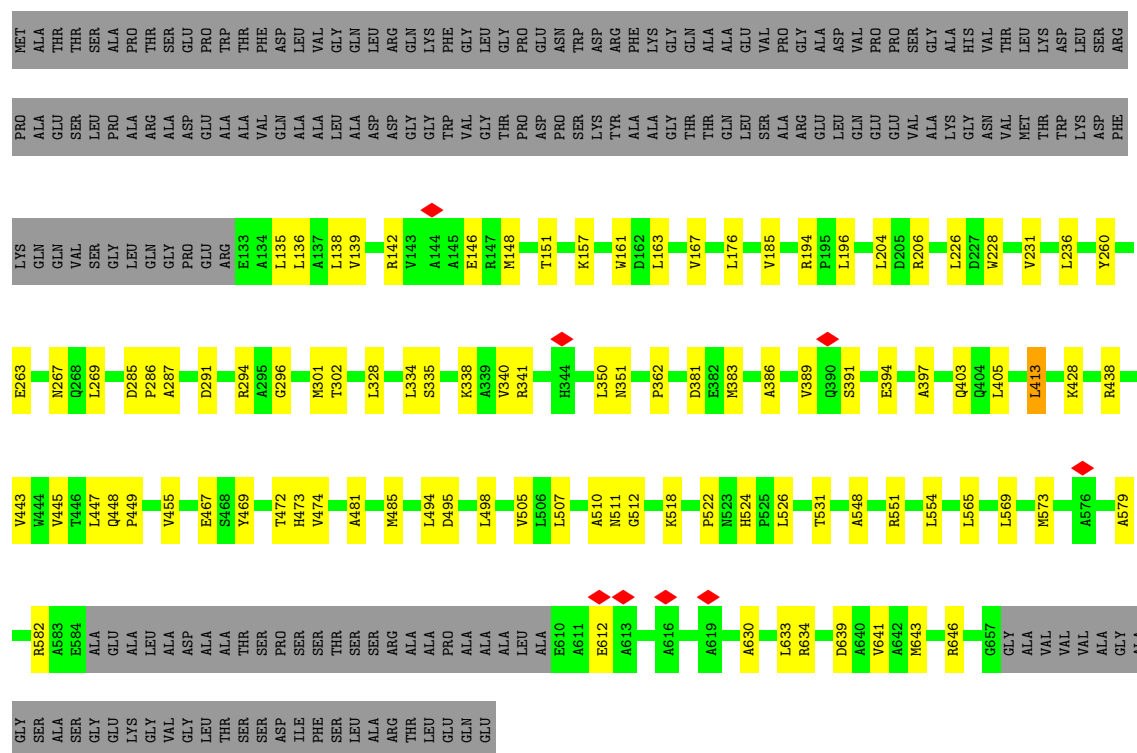
- Molecule 6: AAA+ ATPase domain-containing protein

Chain G:



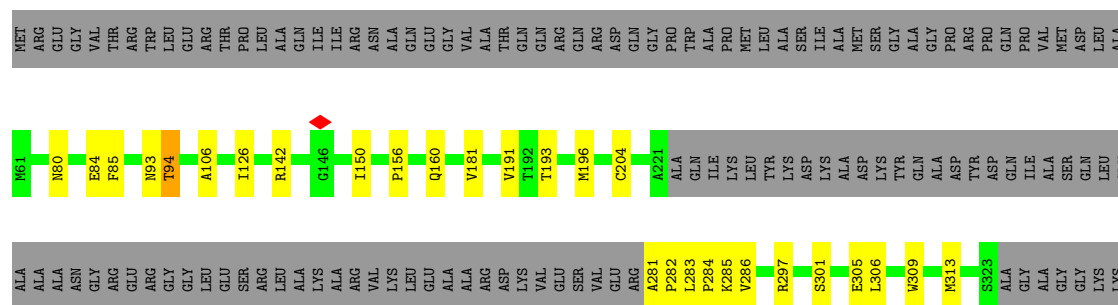
PHE	LYS	PRO	PRO	ASP	THR	PRO	PRO	GLU	GLY	GLY	SER	SER	GLY	GLY	GLY	ALA	ALA	ALA	ALA	ALA	GLU	GLY	SER	ALA	ALA	PRO	GLN	THR	PRO	ASP	LEU	SER	SER	GLY	ALA	ALA	ARG	GLY	LYS	THR	THR	TRP	PHE	ALA	ALA	ALA	THR	THR	TYR	ASP	ALA	PRO	ARG	PRO	ASN	ALA	ALA	ASP	GLY	THR	PHE	LYS	GLS	HIS	G1032	M1036	M1037	Y1058
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Chain H:  58% 14% 28%



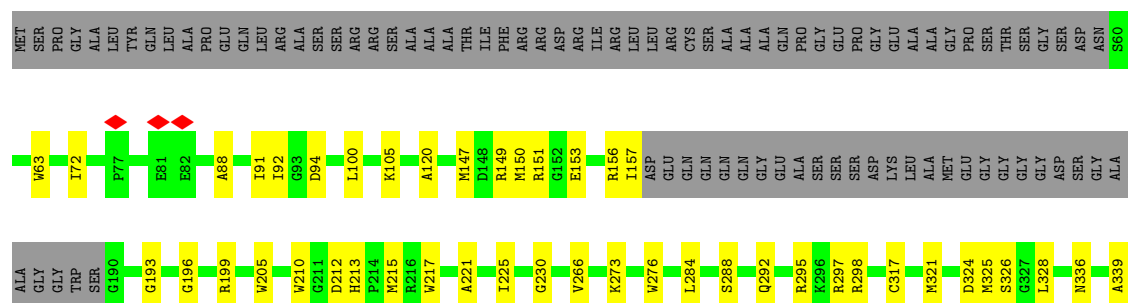
• Molecule 8: Tic22

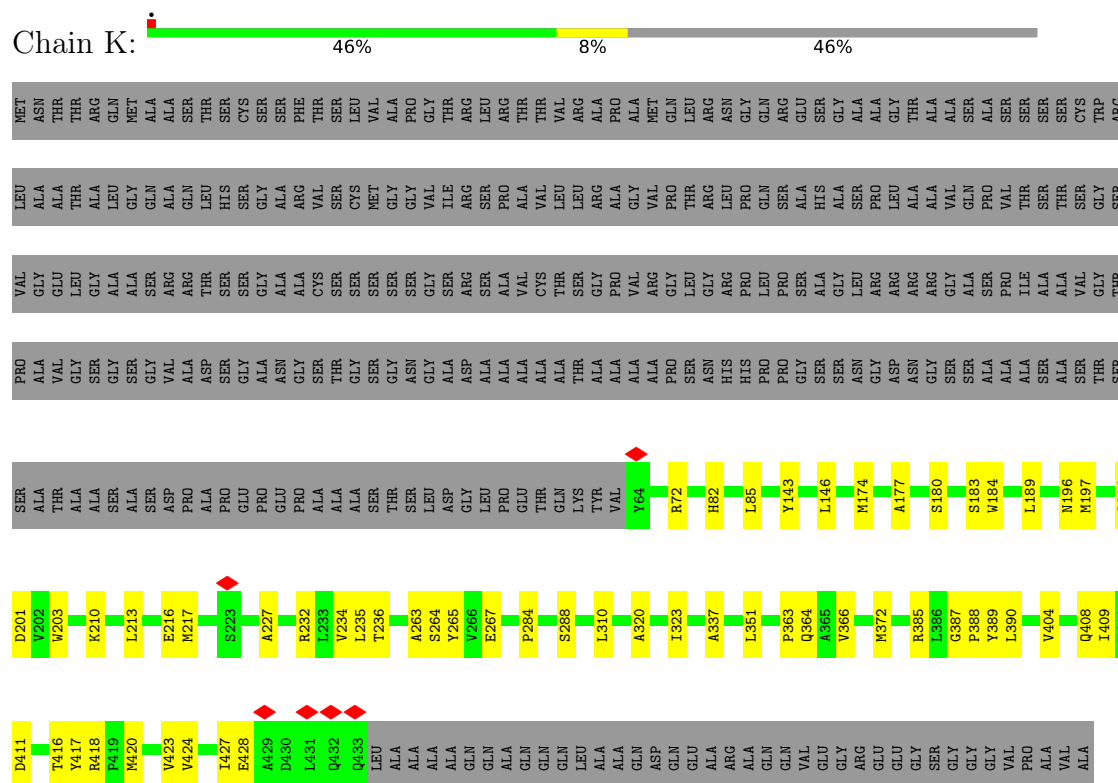
Chain I:  53% 8% 38%



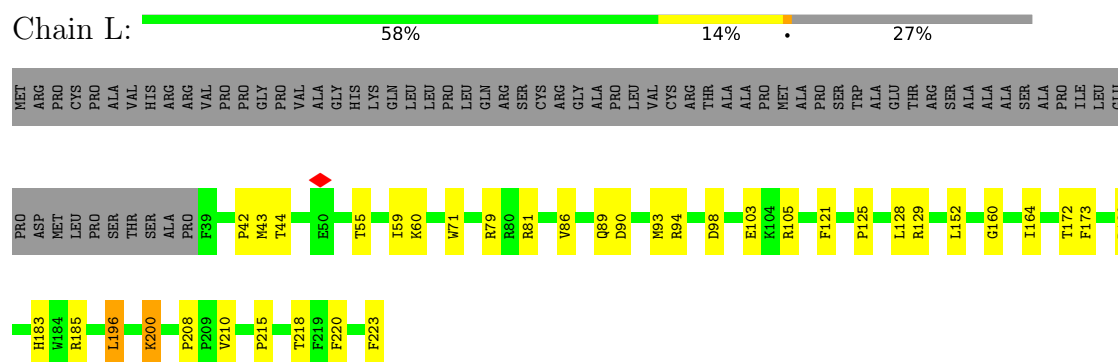
• Molecule 9: FaxL

Chain J:  61% 15% 25%

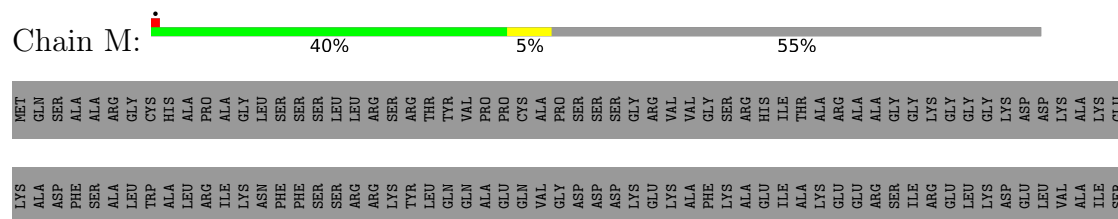


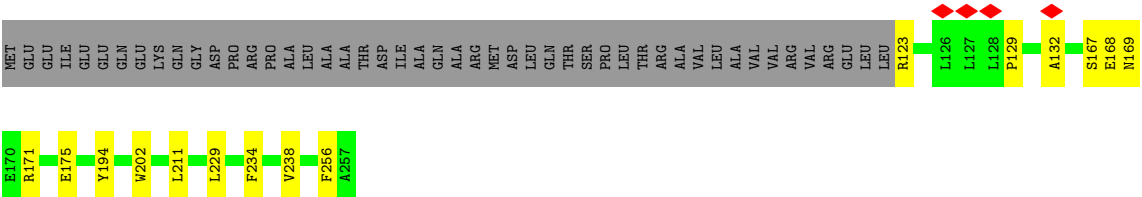


- Molecule 11: Moc25

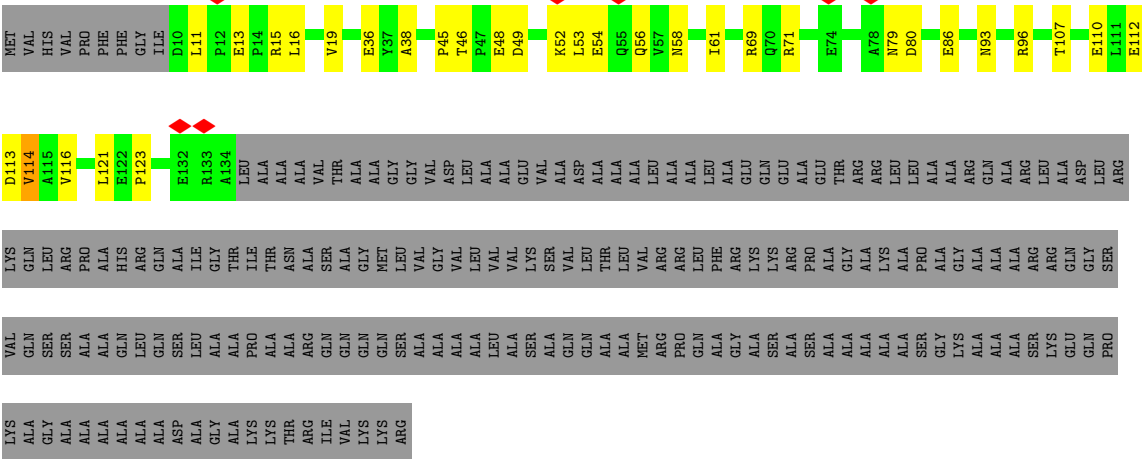


- Molecule 12: Moc29

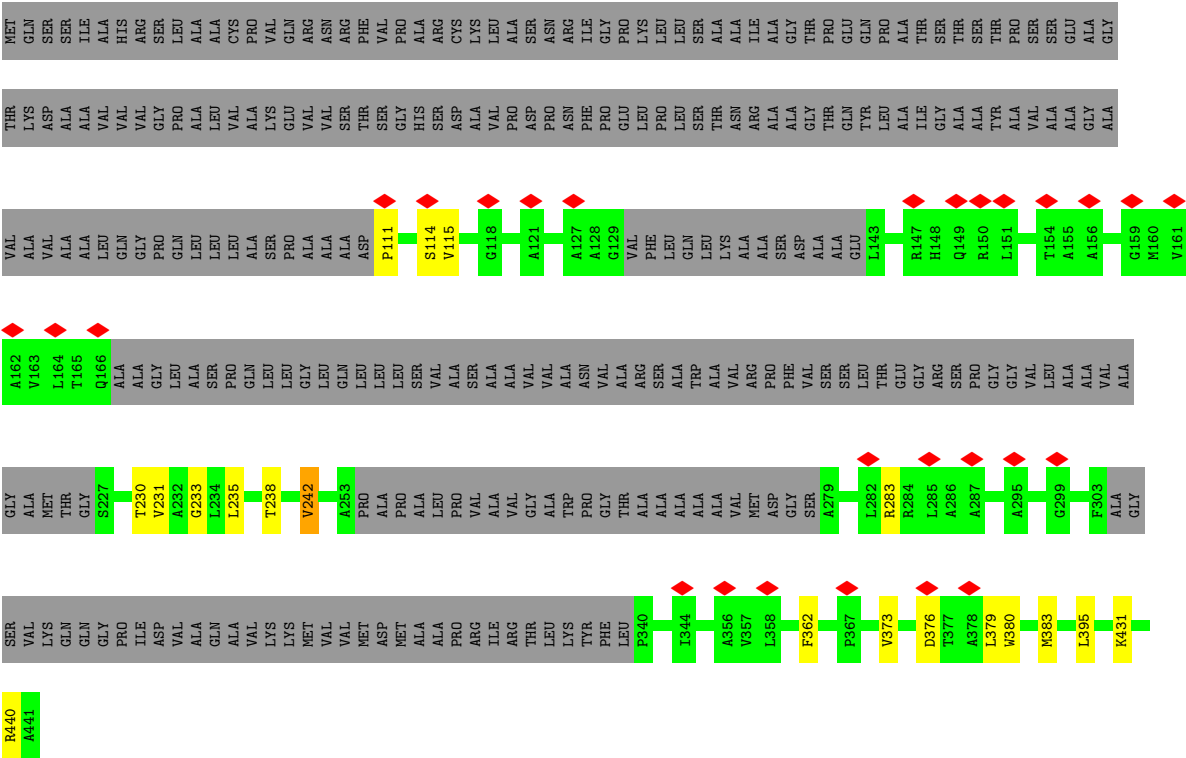




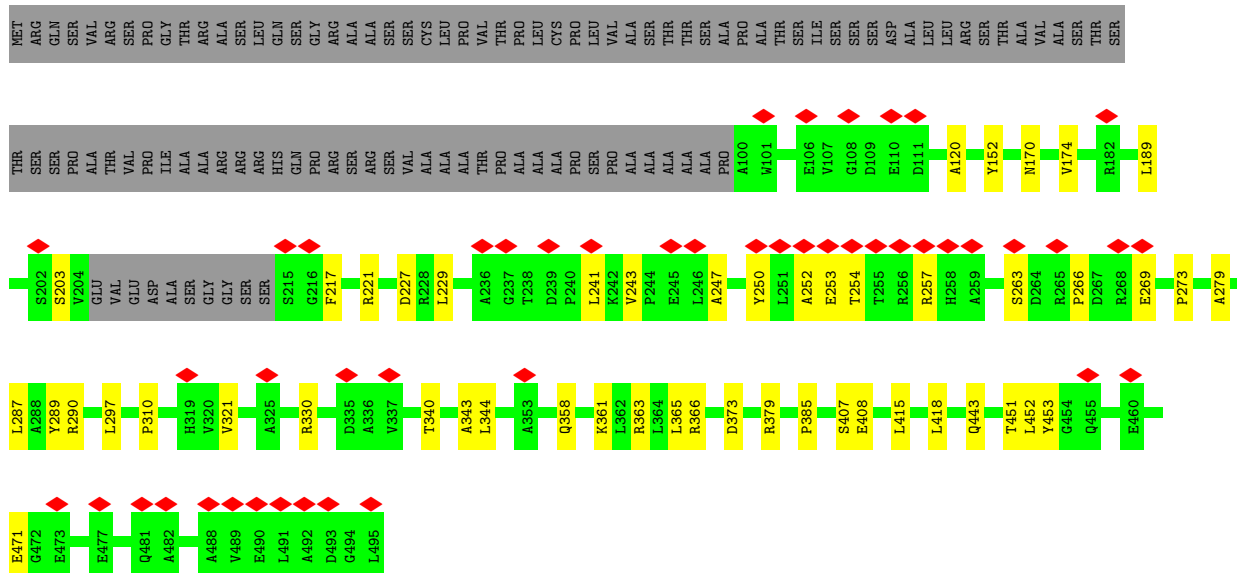
• Molecule 13: Moc34



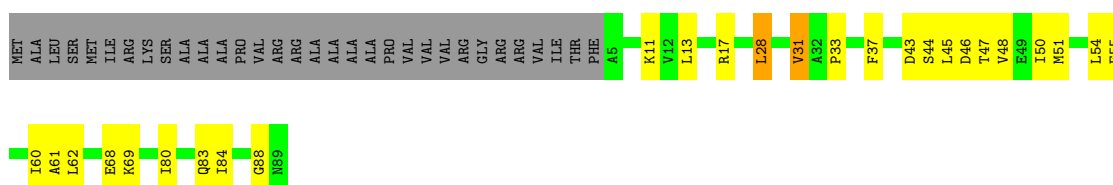
• Molecule 14: Moc45



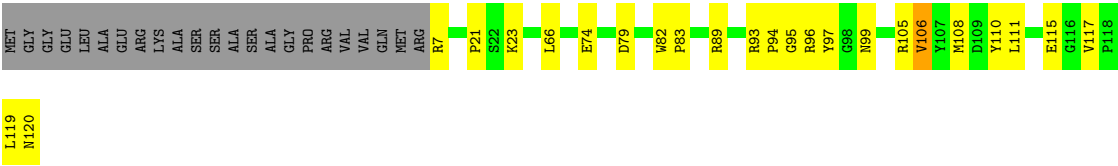
Chain P: 60% 13% 27%



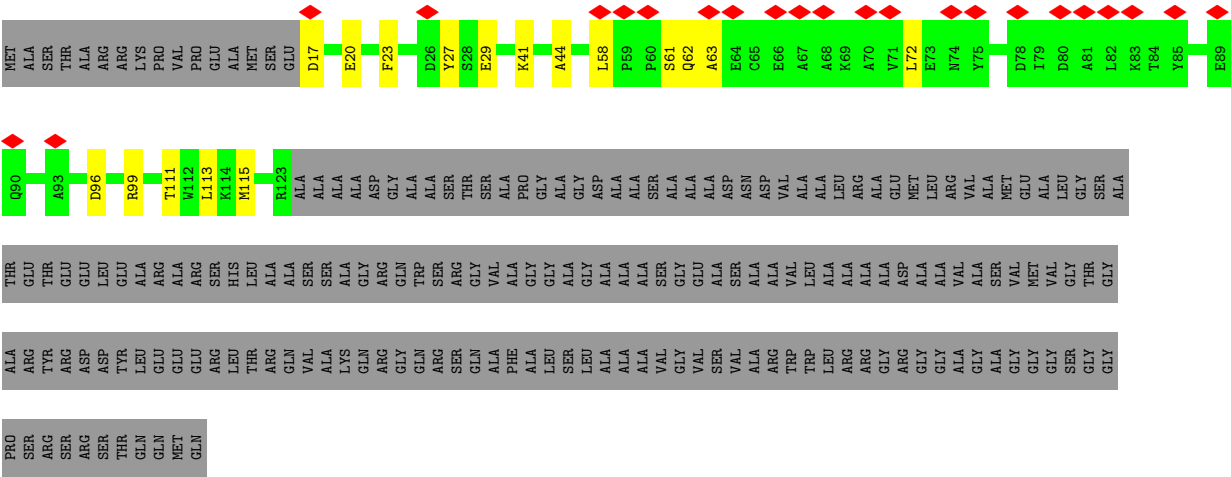
Chain R: 50% 21% • 27%



● Molecule 18: Moc13



● Molecule 19: Moc31



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	127613	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)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.099	Depositor
Minimum map value	-0.000	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.00943	Depositor
Map size (Å)	436.8, 436.8, 436.8	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ACD, DGA, DGD, SEP, SQD, ZN, 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	0.25	0/5693	0.56	6/7745 (0.1%)
2	B	0.20	0/4671	0.46	0/6328
3	C	0.23	0/3172	0.49	1/4315 (0.0%)
4	D	0.31	3/7715 (0.0%)	0.55	7/10469 (0.1%)
5	E	0.28	1/12285 (0.0%)	0.56	7/16600 (0.0%)
6	F	0.28	1/5322 (0.0%)	0.59	5/7210 (0.1%)
6	G	0.26	0/5367	0.54	1/7277 (0.0%)
7	H	0.27	1/3747 (0.0%)	0.58	0/5108
8	I	0.29	0/1652	0.57	2/2238 (0.1%)
9	J	0.28	0/2159	0.49	0/2934
10	K	0.26	0/2954	0.55	2/4054 (0.0%)
11	L	0.29	1/1600 (0.1%)	0.61	3/2186 (0.1%)
12	M	0.32	0/1175	0.53	0/1613
13	N	0.37	0/1024	0.69	1/1391 (0.1%)
14	O	0.24	0/1561	0.53	1/2135 (0.0%)
15	P	0.23	0/3323	0.50	1/4513 (0.0%)
16	Q	0.18	0/2946	0.44	0/4014
17	R	0.29	0/624	0.68	2/839 (0.2%)
18	S	0.38	1/933 (0.1%)	0.57	1/1266 (0.1%)
19	T	0.30	1/856 (0.1%)	0.55	0/1159
All	All	0.27	9/68779 (0.0%)	0.54	40/93394 (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
2	B	0	1
4	D	0	2
5	E	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
6	F	0	2
6	G	0	1
13	N	0	1
All	All	0	8

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1096	PRO	CG-CD	-10.96	1.13	1.50
4	D	1096	PRO	N-CD	6.67	1.57	1.47
7	H	413	LEU	CG-CD2	-6.56	1.30	1.52
4	D	574	LEU	CG-CD1	-5.96	1.32	1.52
18	S	106	VAL	CB-CG1	-5.75	1.33	1.52

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1096	PRO	N-CD-CG	-13.31	83.23	103.20
5	E	1186	PRO	CA-N-CD	-12.35	94.72	112.00
1	A	262	PRO	CA-N-CD	-11.27	96.22	112.00
1	A	379	PRO	CA-N-CD	-10.94	96.68	112.00
4	D	1096	PRO	N-CA-CB	-8.19	94.66	103.25

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	534	ALA	Peptide
4	D	1095	SER	Peptide
4	D	587	LYS	Peptide
5	E	970	PHE	Peptide
6	F	368	LEU	Peptide

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	5557	0	5450	87	0
2	B	4588	0	4601	73	0
3	C	3085	0	2929	53	0
4	D	7551	0	7556	137	0
5	E	12035	0	12354	254	0
6	F	5216	0	5183	108	0
6	G	5260	0	5225	101	0
7	H	3670	0	3637	72	0
8	I	1619	0	1621	20	0
9	J	2101	0	2056	50	0
10	K	2853	0	2798	42	0
11	L	1541	0	1534	31	0
12	M	1127	0	1096	18	0
13	N	1005	0	987	26	0
14	O	1517	0	1516	18	0
15	P	3245	0	3153	47	0
16	Q	2880	0	2825	32	0
17	R	633	0	636	18	0
18	S	909	0	904	27	0
19	T	840	0	810	12	0
20	C	2	0	0	0	0
21	H	36	0	57	3	0
22	J	47	0	52	2	0
22	L	66	0	96	0	0
23	J	41	0	52	6	0
23	L	47	0	64	2	0
24	K	21	0	31	1	0
25	L	36	0	36	2	0
All	All	67528	0	67259	1005	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 7.

The worst 5 of 1005 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)
6:F:672:MET:HE1	6:F:680:VAL:HG22	1.46	0.95
8:I:281:ALA:HB3	8:I:282:PRO:HD3	1.46	0.93
5:E:348:THR:HG23	5:E:1374:LYS:HB2	1.53	0.89
5:E:902:LYS:HD3	6:G:288:ASP:HB3	1.54	0.89
9:J:147:MET:HA	9:J:150:MET:HE2	1.56	0.86

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\# Z > 2$
17	SEP	R	44	17	8,9,10	1.64	1 (12%)	7,12,14	1.20	1 (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
17	SEP	R	44	17	-	3/6/8/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	R	44	SEP	P-O1P	3.53	1.61	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	R	44	SEP	OG-CB-CA	2.28	110.36	108.14

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	R	44	SEP	CB-OG-P-O2P
17	R	44	SEP	CB-OG-P-O3P
17	R	44	SEP	CB-OG-P-O1P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 2 are monoatomic - leaving 7 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	$\# Z > 2$
25	SQD	L	303	-	34,36,54	1.79	5 (14%)	44,47,65	2.03	13 (29%)
22	DGD	J	401	-	48,48,67	1.18	3 (6%)	62,62,81	1.30	8 (12%)
22	DGD	L	302	-	67,67,67	1.15	6 (8%)	81,81,81	1.09	8 (9%)
23	LMG	J	402	-	41,41,55	1.02	1 (2%)	49,49,63	1.12	5 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	ACD	K	501	-	19,20,21	2.57	5 (26%)	18,19,21	1.21	1 (5%)
23	LMG	L	301	-	47,47,55	0.94	1 (2%)	55,55,63	1.04	5 (9%)
21	DGA	H	701	-	35,35,43	0.70	0	37,37,45	0.91	2 (5%)

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
25	SQD	L	303	-	-	14/31/51/69	0/1/1/1
22	DGD	J	401	-	-	12/36/76/95	0/2/2/2
22	DGD	L	302	-	-	38/55/95/95	0/2/2/2
23	LMG	J	402	-	-	19/36/56/70	0/1/1/1
24	ACD	K	501	-	-	10/18/18/19	-
23	LMG	L	301	-	-	21/42/62/70	0/1/1/1
21	DGA	H	701	-	-	21/37/37/45	-

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	L	303	SQD	O9-S	5.52	1.60	1.45
24	K	501	ACD	O1-C1	5.19	1.49	1.20
25	L	303	SQD	O7-S	5.15	1.59	1.45
24	K	501	ACD	C9-C8	4.57	1.57	1.31
24	K	501	ACD	C12-C11	4.54	1.57	1.31

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	L	303	SQD	O9-S-C6	7.73	118.30	106.76
25	L	303	SQD	O8-S-C6	3.97	113.63	105.97
22	J	401	DGD	O3G-C1D-C2D	3.68	113.87	108.27
25	L	303	SQD	O7-S-C6	3.67	112.24	106.76
22	J	401	DGD	O2G-C1B-C2B	3.65	119.38	111.48

There are no chirality outliers.

5 of 135 torsion outliers are listed below:

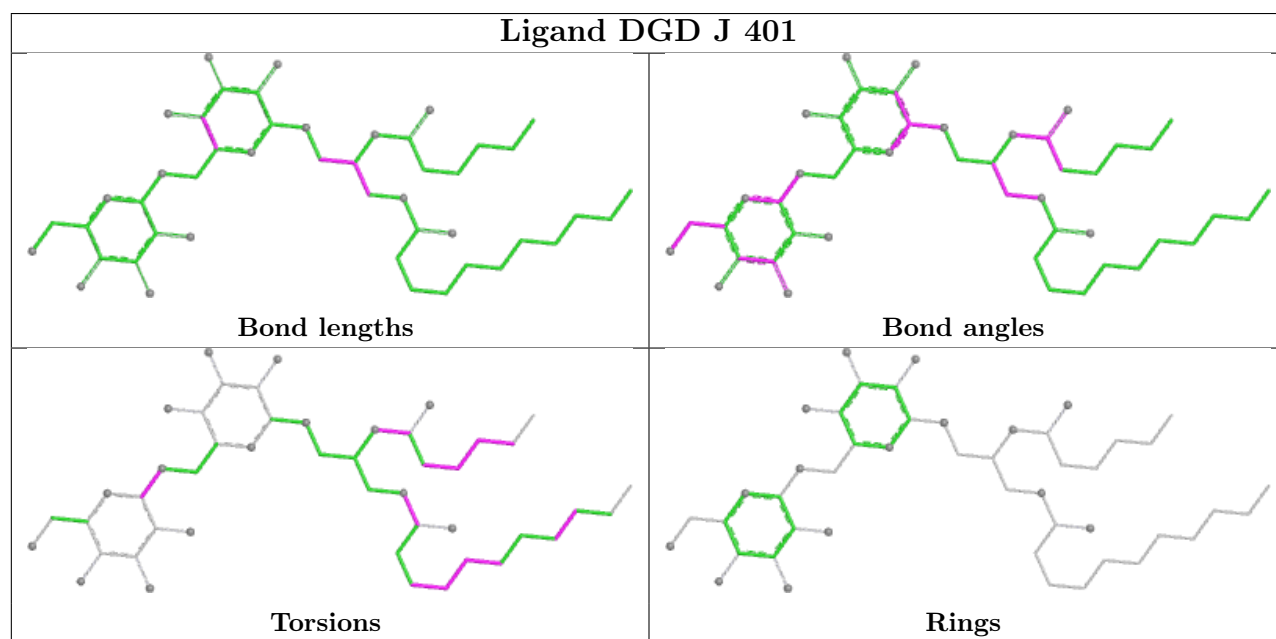
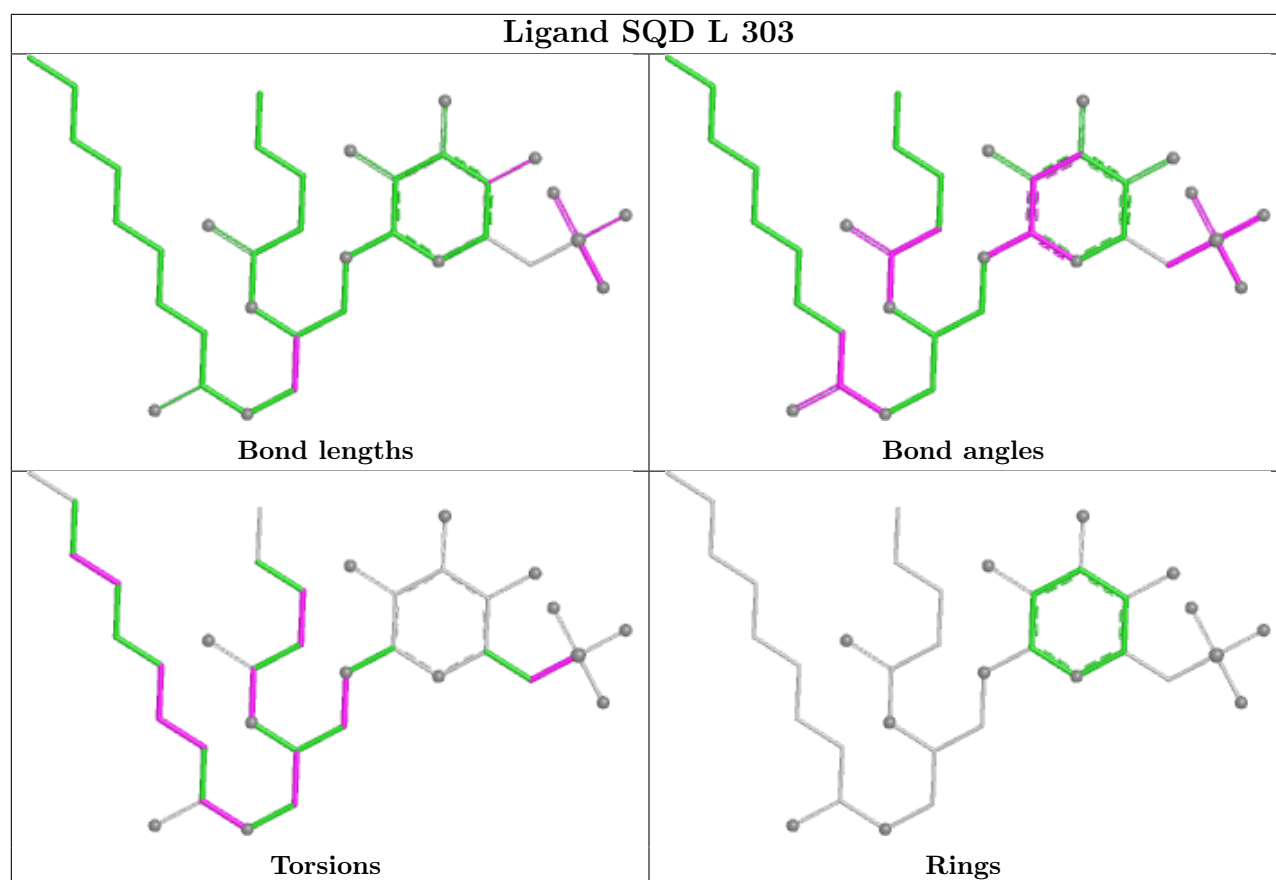
Mol	Chain	Res	Type	Atoms
21	H	701	DGA	CB2-CB1-OG2-CG2
22	J	401	DGD	C2B-C1B-O2G-C2G
22	J	401	DGD	O1B-C1B-O2G-C2G
22	L	302	DGD	C2B-C1B-O2G-C2G
22	L	302	DGD	O2G-C2G-C3G-O3G

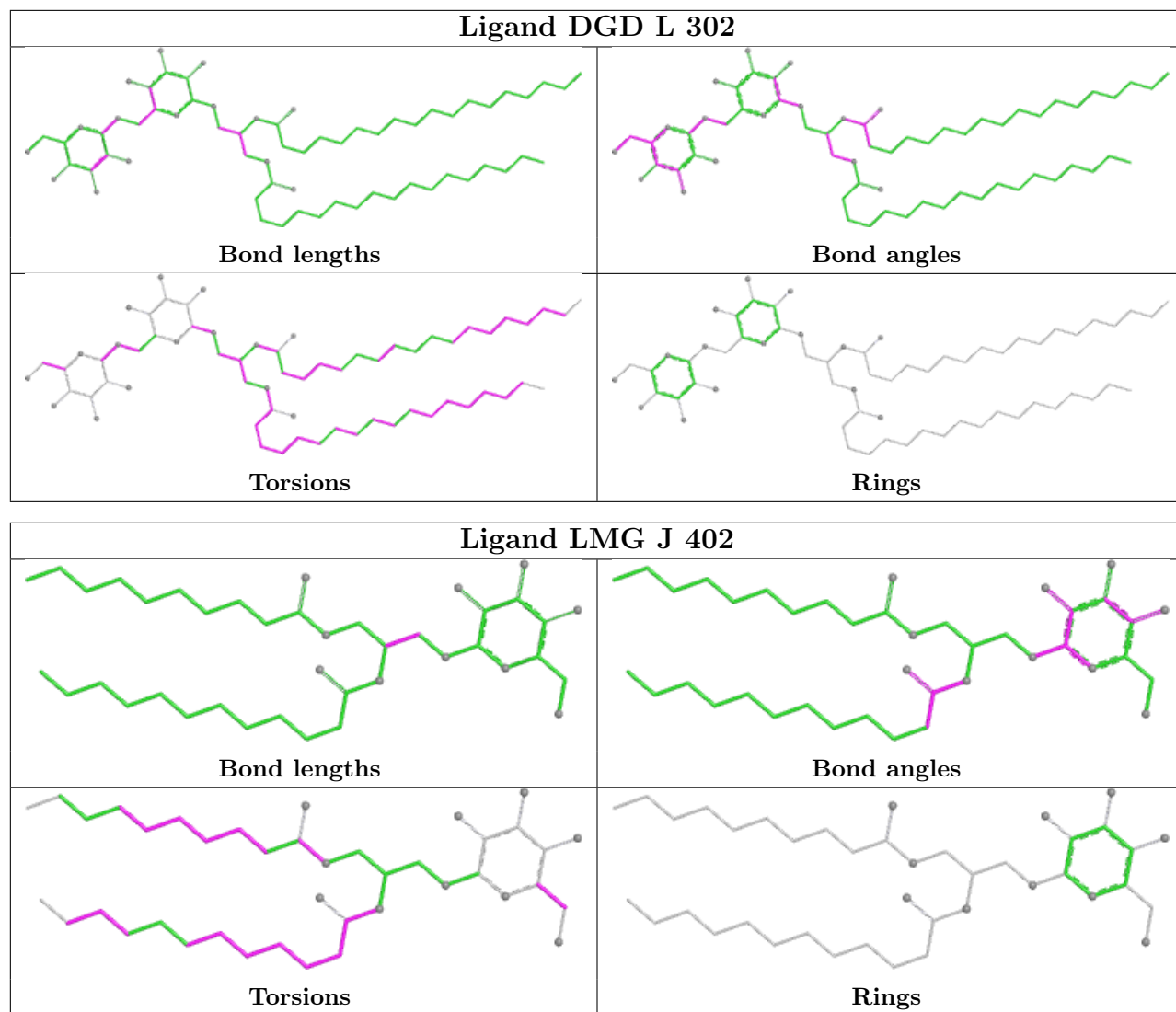
There are no ring outliers.

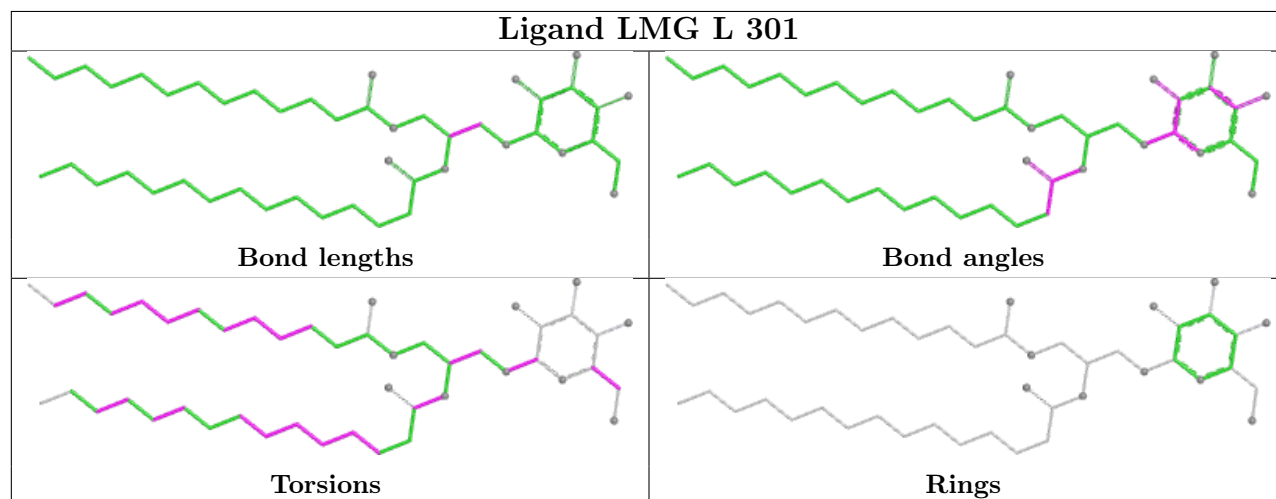
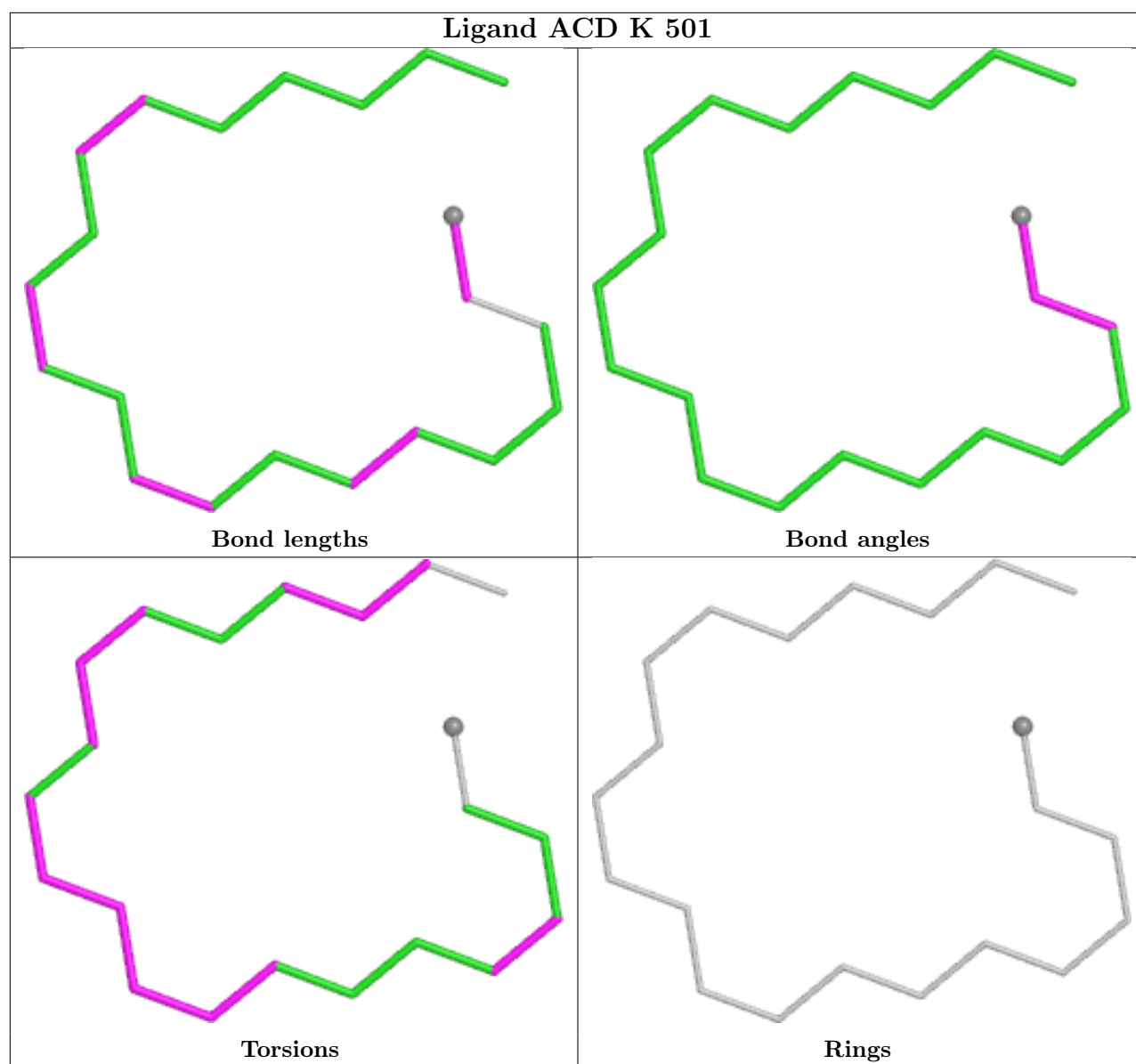
6 monomers are involved in 15 short contacts:

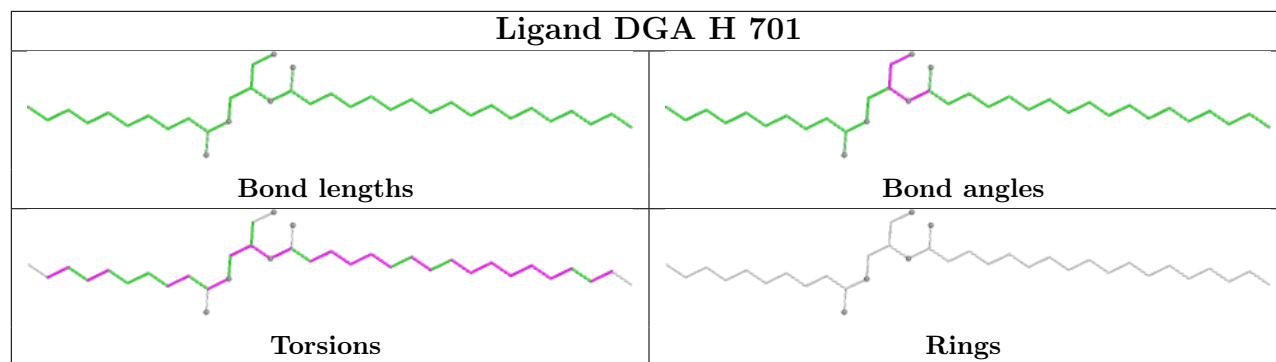
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	L	303	SQD	2	0
22	J	401	DGD	2	0
23	J	402	LMG	6	0
24	K	501	ACD	1	0
23	L	301	LMG	2	0
21	H	701	DGA	3	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

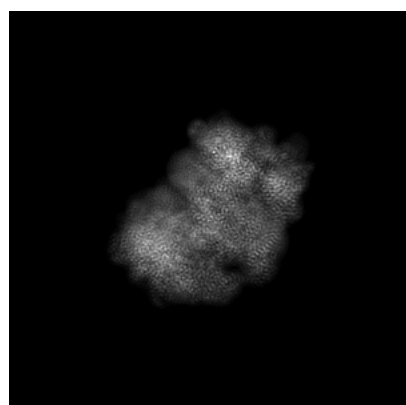
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38424. These allow visual inspection of the internal detail of the map and identification of artifacts.

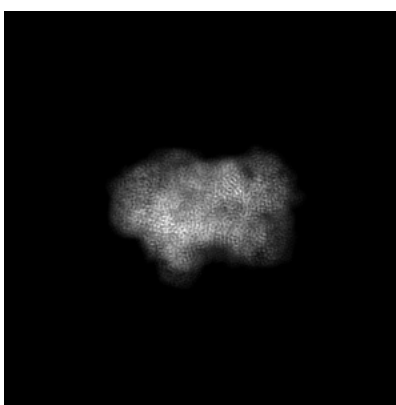
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

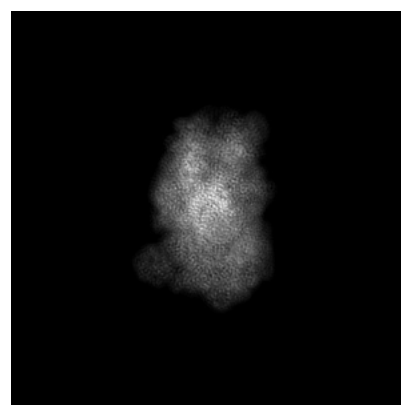
6.1.1 Primary map



X



Y

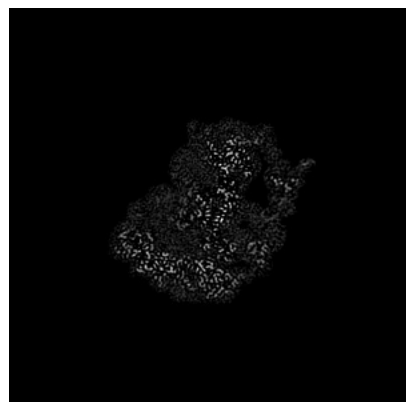


Z

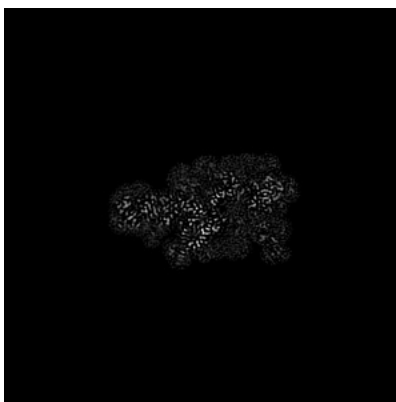
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

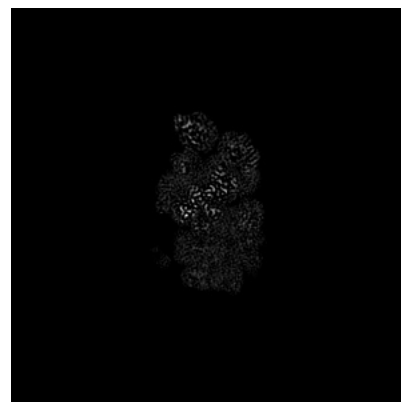
6.2.1 Primary map



X Index: 210



Y Index: 210

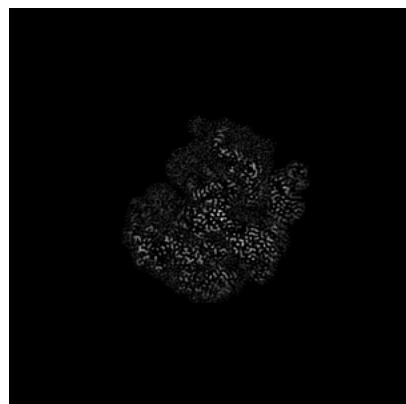


Z Index: 210

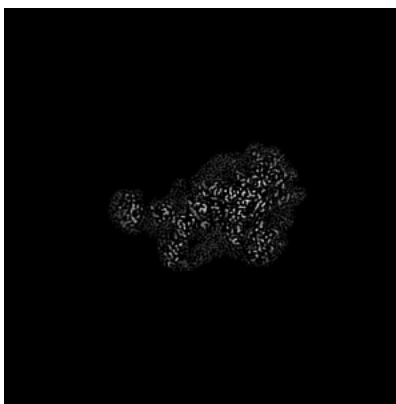
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

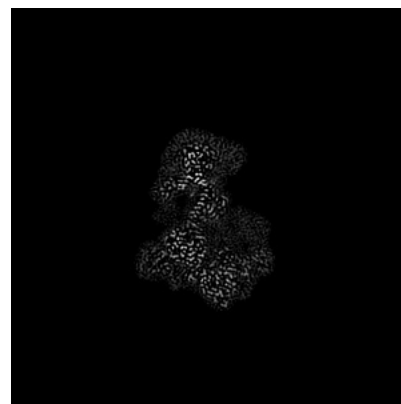
6.3.1 Primary map



X Index: 195



Y Index: 228

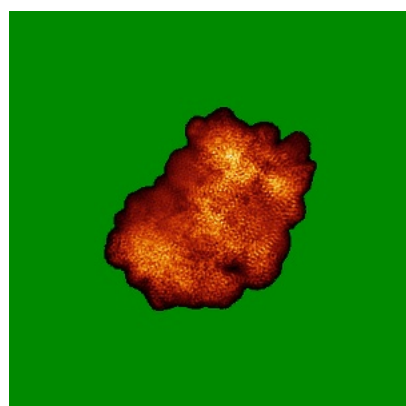


Z Index: 171

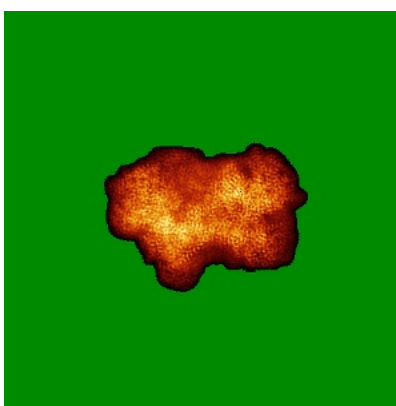
The images above show the largest variance slices of the map in three orthogonal directions.

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

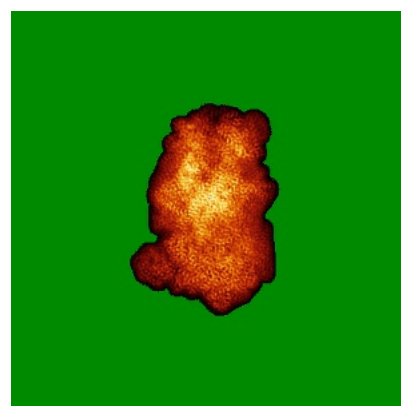
6.4.1 Primary map



X



Y

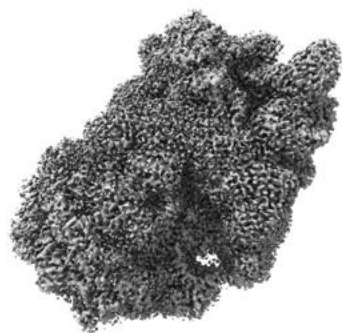


Z

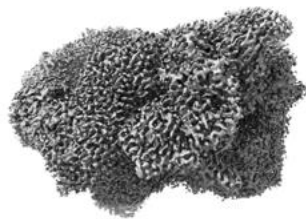
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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 0.00943. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

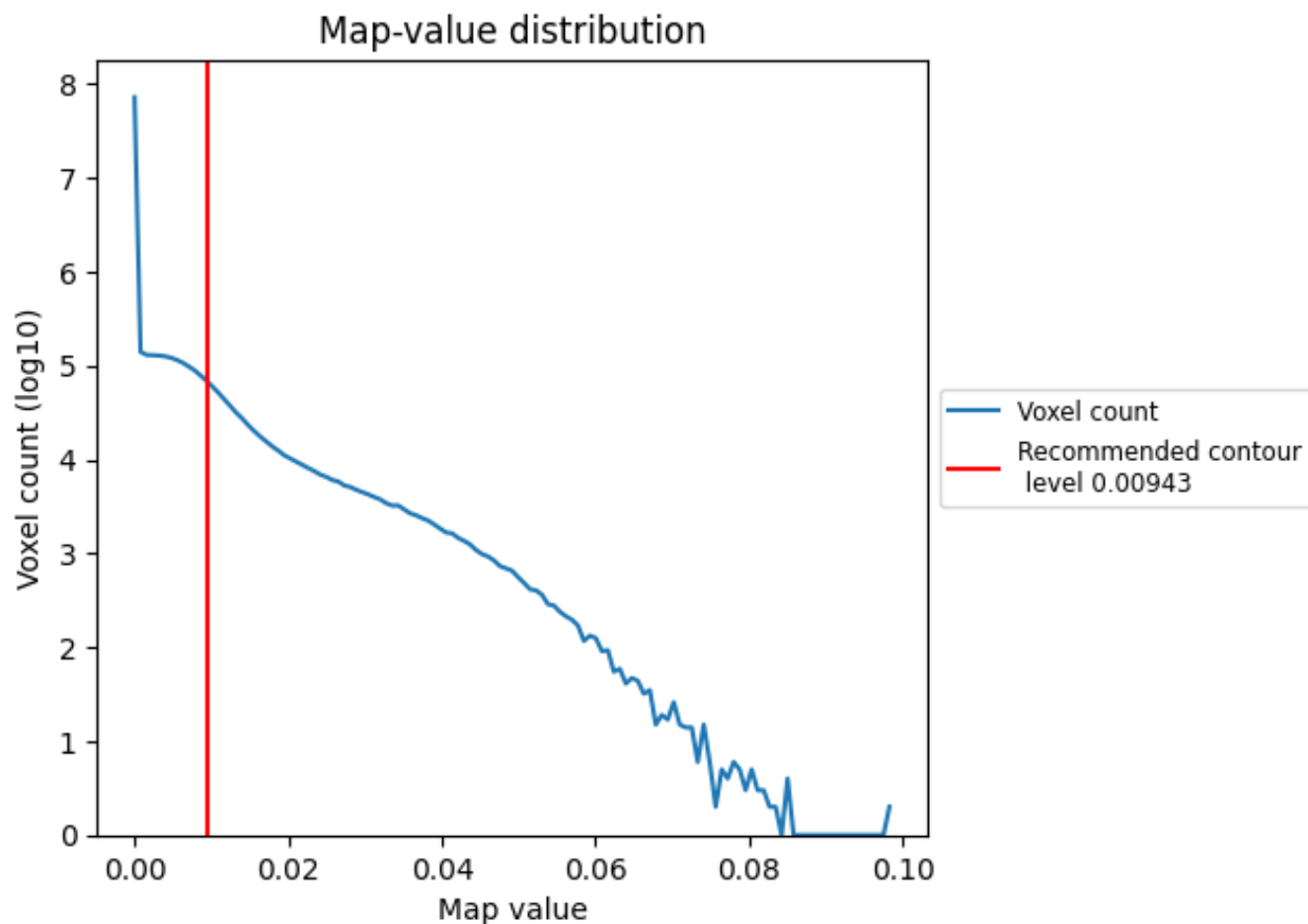
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

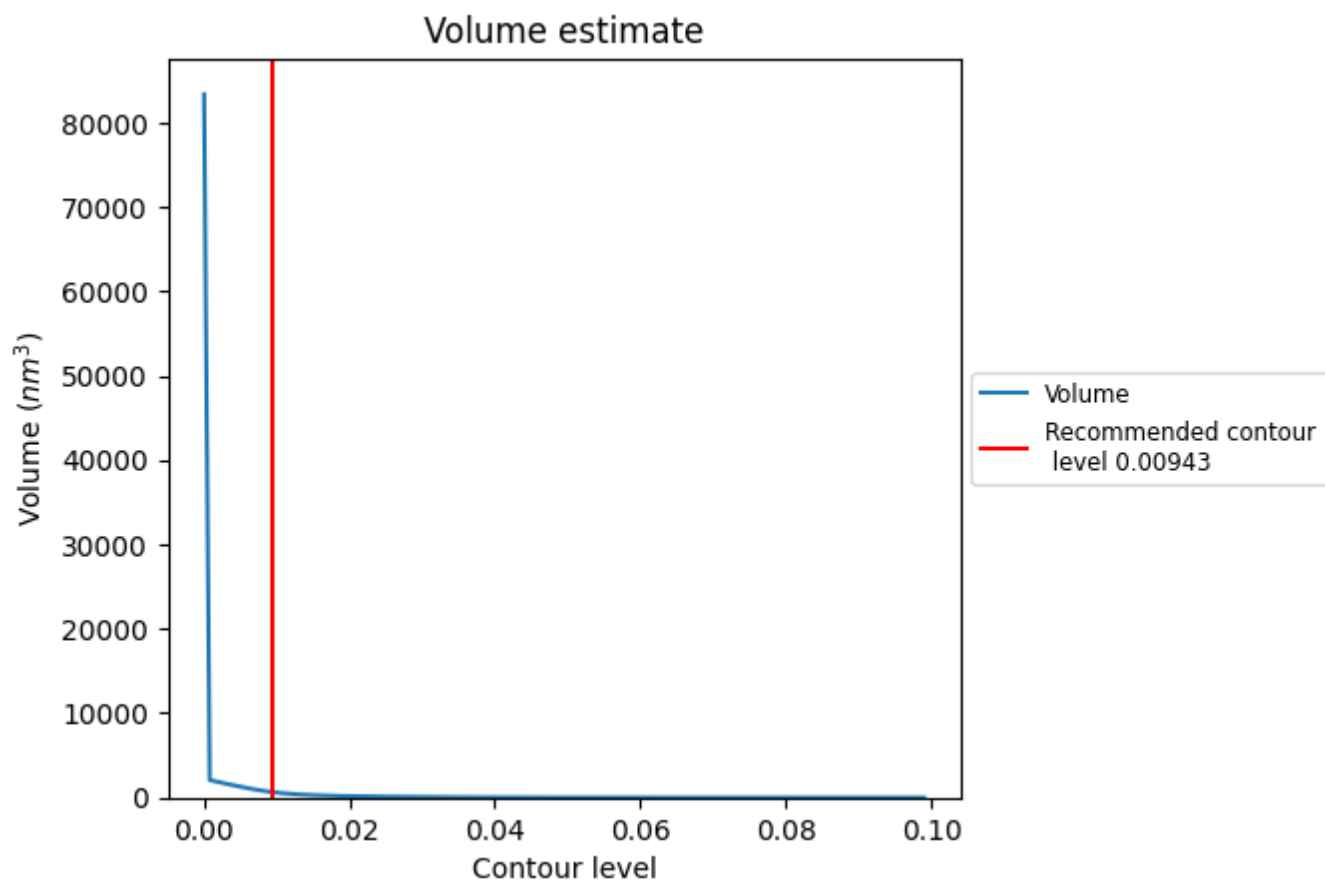
This section contains the results of statistical analysis of the map.

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.

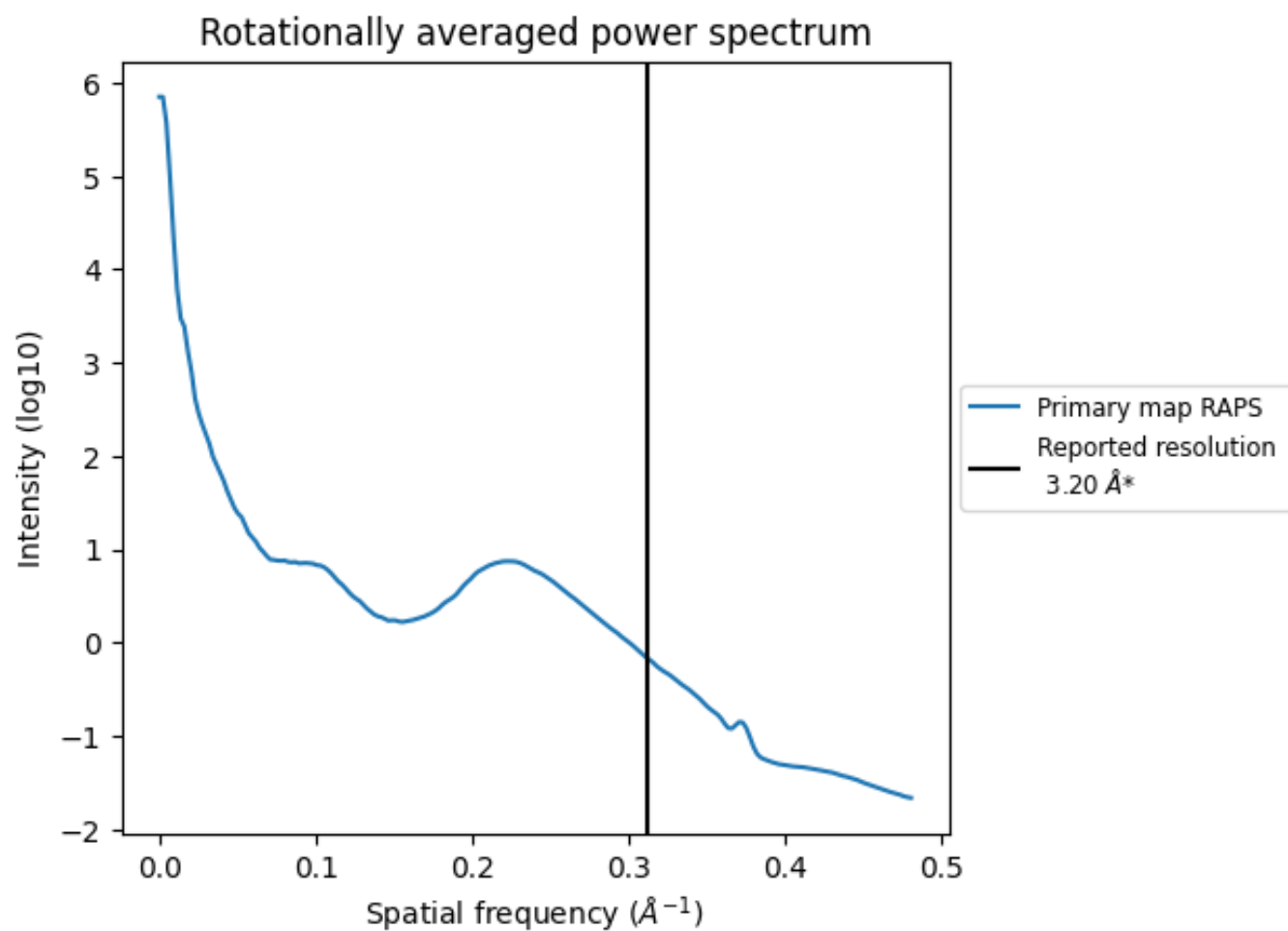
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 644 nm³; this corresponds to an approximate mass of 582 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 0.312 Å⁻¹

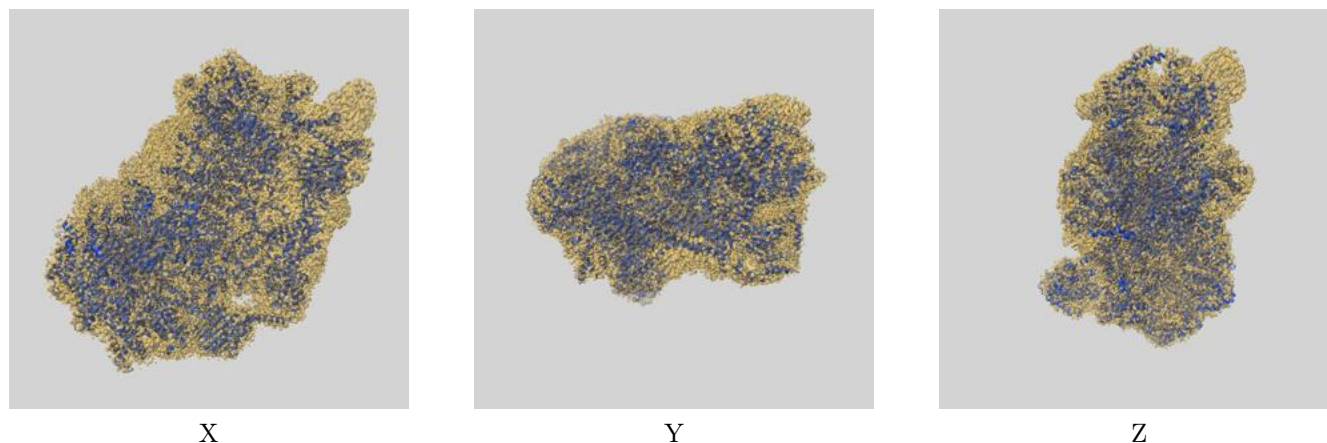
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

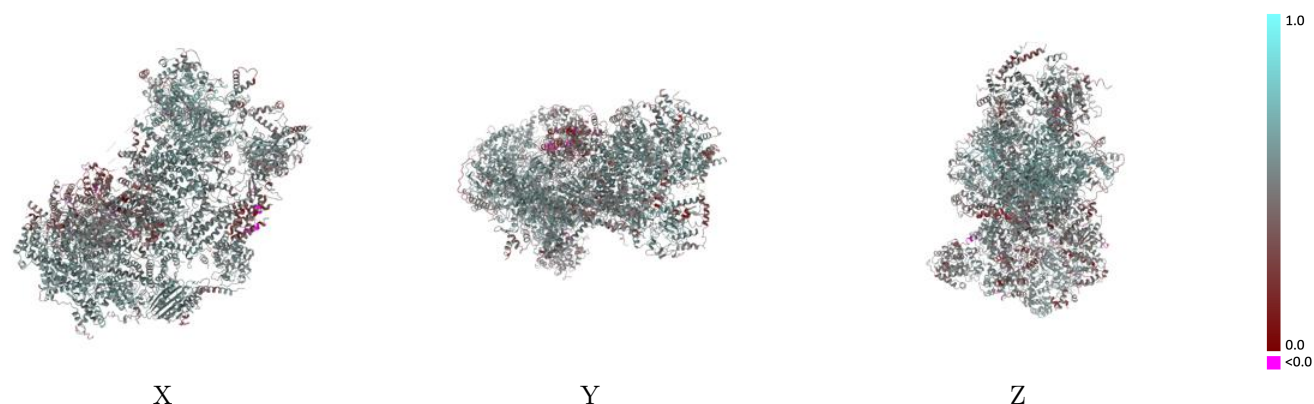
This section contains information regarding the fit between EMDB map EMD-38424 and PDB model 8XKS. Per-residue inclusion information can be found in section [3](#) on page [10](#).

9.1 Map-model overlay [i](#)



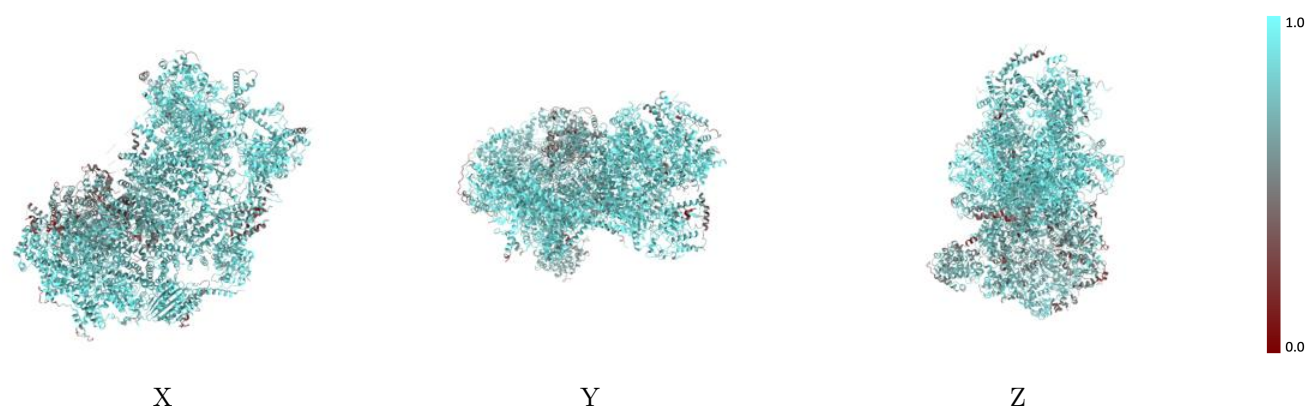
The images above show the 3D surface view of the map at the recommended contour level 0.00943 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



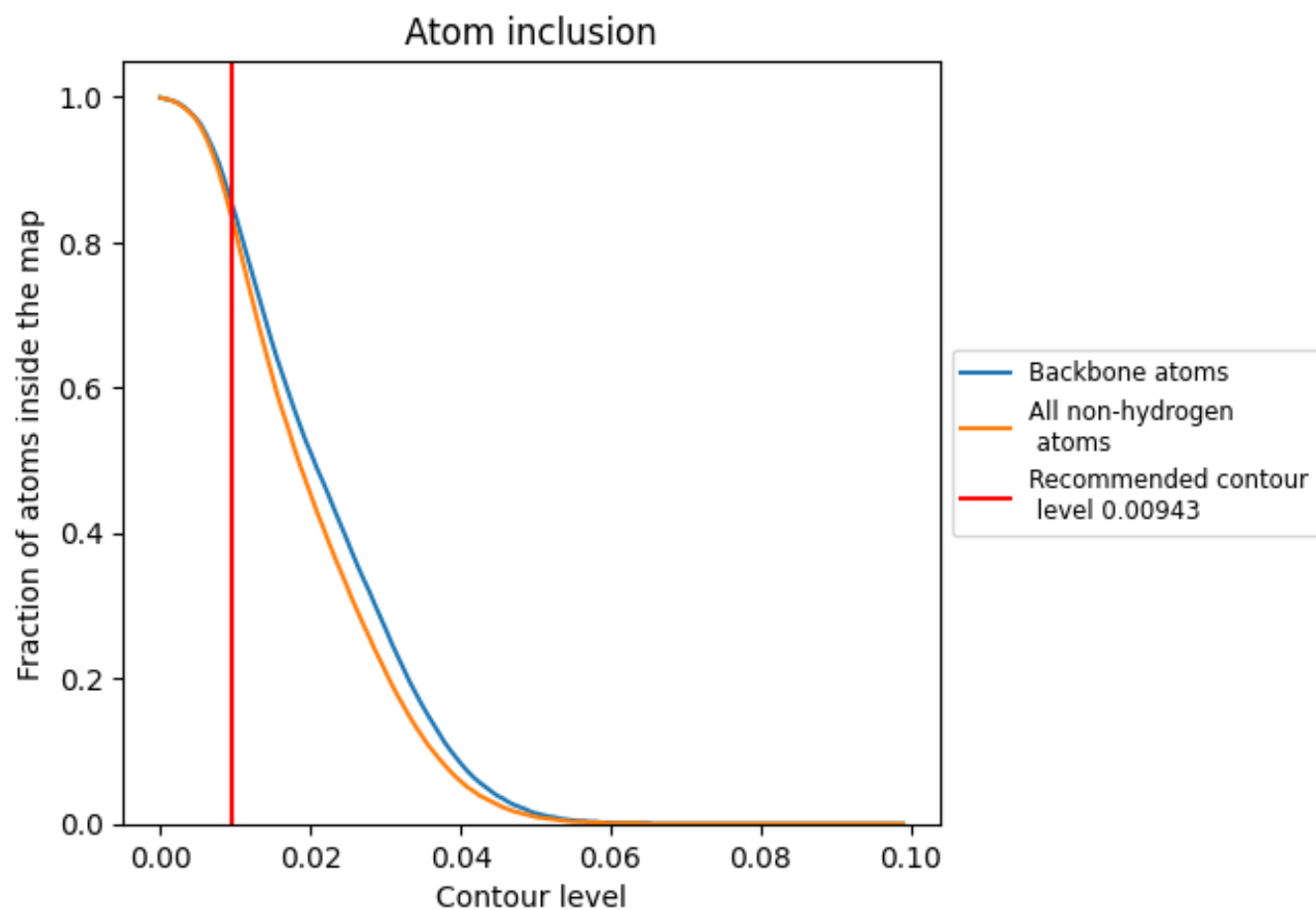
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00943).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 84% 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 (0.00943) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8370	 0.5110
A	 0.8280	 0.5030
B	 0.7880	 0.5030
C	 0.8910	 0.5550
D	 0.8360	 0.5250
E	 0.8710	 0.5370
F	 0.8080	 0.4820
G	 0.8420	 0.5100
H	 0.8520	 0.4910
I	 0.8730	 0.4820
J	 0.8950	 0.5490
K	 0.8880	 0.5240
L	 0.9040	 0.5420
M	 0.8900	 0.5450
N	 0.8020	 0.4790
O	 0.7080	 0.3800
P	 0.8280	 0.5150
Q	 0.7010	 0.4660
R	 0.8300	 0.4890
S	 0.8830	 0.5530
T	 0.6920	 0.4480

