



## wwPDB EM Validation Summary Report ⓘ

Nov 13, 2025 – 02:32 PM EST

PDB ID : 9YGY / pdb\_00009ygy  
EMDB ID : EMD-72945  
Title : Structure of a GRP94 folding intermediate engaged with a CCDC134- and FKBP11-bound secretory translocon  
Authors : Yamsek, M.; Jha, R.; Keenan, R.J.  
Deposited on : 2025-09-29  
Resolution : 4.10 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](mailto: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>.

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

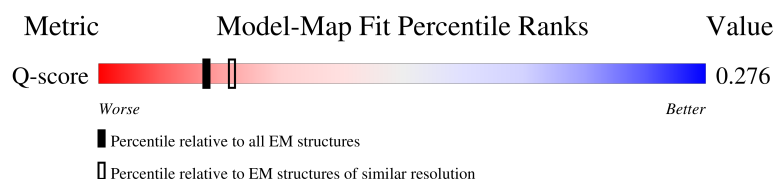
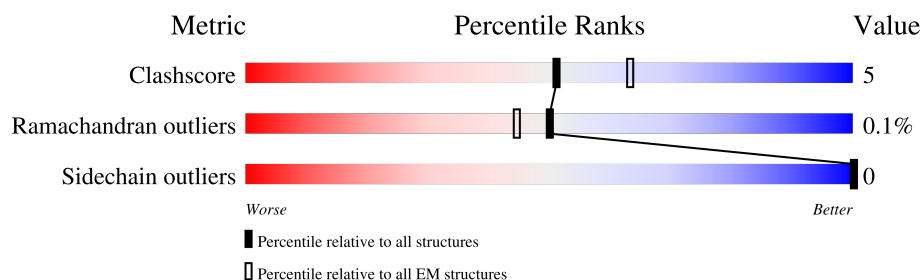
EMDB validation analysis : 0.0.1.dev129  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
EM percentile statistics : 202505.v01 (Using data in the EMDB 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) : 2.46

# 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 4.10 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	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	6458 ( 3.60 - 4.60 )

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  $\geq 3$ , 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	5	286	<div> <div>41%</div> <div>44%</div> <div>5%</div> <div>51%</div> </div>
2	6	183	<div> <div>77%</div> <div>73%</div> <div>15%</div> <div>11%</div> </div>
3	7	185	<div> <div>69%</div> <div>79%</div> <div>18%</div> <div>.</div> </div>
4	8	173	<div> <div>74%</div> <div>73%</div> <div>13%</div> <div>13%</div> </div>

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Mol	Chain	Length	Quality of chain
5	A	201	
6	B	229	
7	D	476	
8	E	96	
9	F	68	
10	G	66	
11	I	705	
12	J	149	
13	K2	37	
14	L2	79	
15	M2	113	
16	N	136	
17	N2	456	
18	O2	607	
19	P2	631	
20	y3	846	
21	K	8	
22	C	2	
23	H	8	
24	L	2	

## 2 Entry composition

There are 25 unique types of molecules in this entry. The entry contains 74558 atoms, of which 37397 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 Translocon-associated protein subunit alpha.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	5	140	Total	C	H	N	O	S	0	0
			2192	723	1071	179	217	2		

- Molecule 2 is a protein called Translocon-associated protein subunit beta.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	6	162	Total	C	H	N	O	S	0	0
			2500	808	1241	212	237	2		

- Molecule 3 is a protein called Translocon-associated protein subunit gamma.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	7	179	Total	C	H	N	O	S	0	0
			2938	946	1487	239	263	3		

- Molecule 4 is a protein called Translocon-associated protein subunit delta.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	8	150	Total	C	H	N	O	S	0	0
			2333	755	1148	199	228	3		

- Molecule 5 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP11.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	A	167	Total	C	H	N	O	S	0	0
			2695	842	1390	230	228	5		

- Molecule 6 is a protein called Coiled-coil domain-containing protein 134.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	B	197	Total	C	H	N	O	S	0	0
			3279	1046	1646	289	294	4		

- Molecule 7 is a protein called Protein transport protein Sec61 subunit alpha isoform 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	D	454	Total	C	H	N	O	S	0	0
			7189	2324	3661	564	616	24		

- Molecule 8 is a protein called Protein transport protein Sec61 subunit beta.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	E	32	Total	C	H	N	O	S	0	0
			523	171	273	40	37	2		

- Molecule 9 is a protein called Protein transport protein Sec61 subunit gamma.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	F	67	Total	C	H	N	O	S	0	0
			1112	353	574	93	87	5		

- Molecule 10 is a protein called Stress-associated endoplasmic reticulum protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	G	56	Total	C	H	N	O	S	0	0
			904	280	467	82	71	4		

- Molecule 11 is a protein called Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit STT3A.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	I	701	Total	C	H	N	O	S	0	0
			11260	3701	5611	913	998	37		

- Molecule 12 is a protein called Oligosaccharyltransferase complex subunit OSTC.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	J	149	Total	C	H	N	O	S	0	0
			2409	789	1227	189	192	12		

- Molecule 13 is a protein called Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit 4.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	K2	37	Total	C	H	N	O	S	0	0
			607	196	312	46	51	2		

- Molecule 14 is a protein called Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit TMEM258.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	L2	79	Total	C	H	N	O	S	0	0
			1302	440	659	92	107	4		

- Molecule 15 is a protein called Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit DAD1.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	M2	110	Total	C	H	N	O	S	0	0
			1743	573	880	135	151	4		

- Molecule 16 is a protein called Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit KCP2.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	N	117	Total	C	H	N	O	S	0	0
			1816	591	925	138	156	6		

- Molecule 17 is a protein called Dolichyl-diphosphooligosaccharide--protein glycosyltransferase 48 kDa subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	N2	410	Total	C	H	N	O	S	0	0
			6385	2079	3161	531	608	6		

- Molecule 18 is a protein called Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	O2	580	Total	C	H	N	O	S	0	0
			9341	2978	4686	785	883	9		

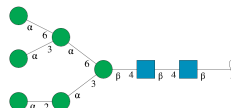
- Molecule 19 is a protein called Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	P2	607	Total	C	H	N	O	S	0	0
			9445	3020	4724	783	909	9		

- Molecule 20 is a protein called Endoplasmin.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	y3	275	Total	C	H	N	O	S	0	0
			4069	1284	2011	355	415	4		

- Molecule 21 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



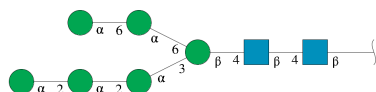
Mol	Chain	Residues	Atoms						AltConf	Trace
21	K	8	Total	C	H	N	O		0	0
			173	52	79	2	40			

- Molecule 22 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms						AltConf	Trace
22	C	2	Total	C	H	N	O		0	0
			53	16	25	2	10			

- Molecule 23 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



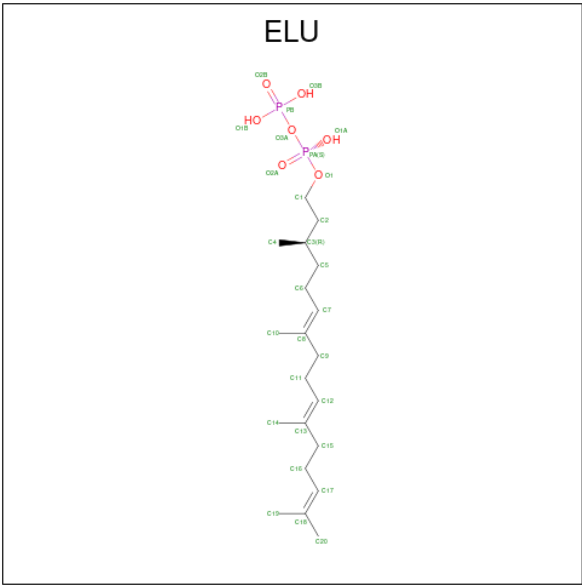
Mol	Chain	Residues	Atoms						AltConf	Trace
23	H	8	Total	C	H	N	O		0	0
			173	52	79	2	40			

- Molecule 24 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
24	L	2	53	16	25	2	10	0	0

- Molecule 25 is phosphono [(3 {R},6 {E},10 {E})-3,7,11,15-tetramethylhexadeca-6,10,14-trienyl] hydrogen phosphate (CCD ID: ELU) (formula: C<sub>20</sub>H<sub>38</sub>O<sub>7</sub>P<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



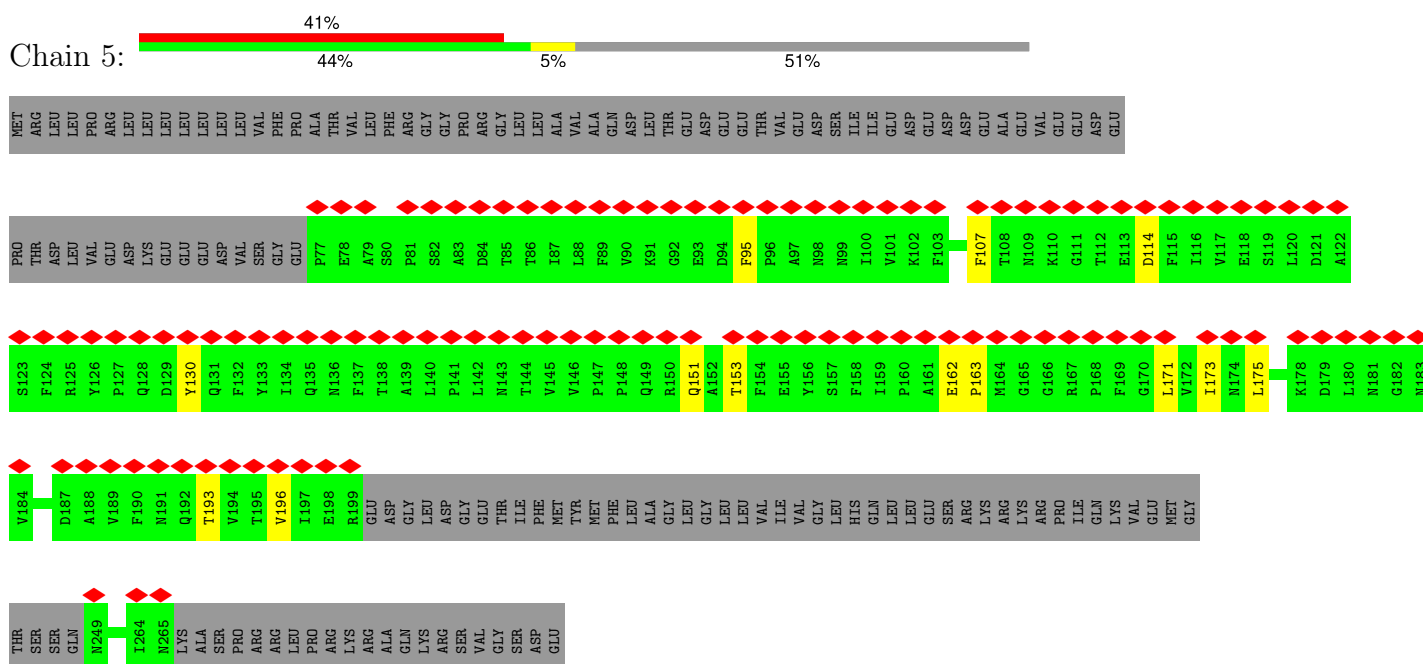
Mol	Chain	Residues	Atoms					AltConf
			Total	C	H	O	P	
25	I	1	64	20	35	7	2	0



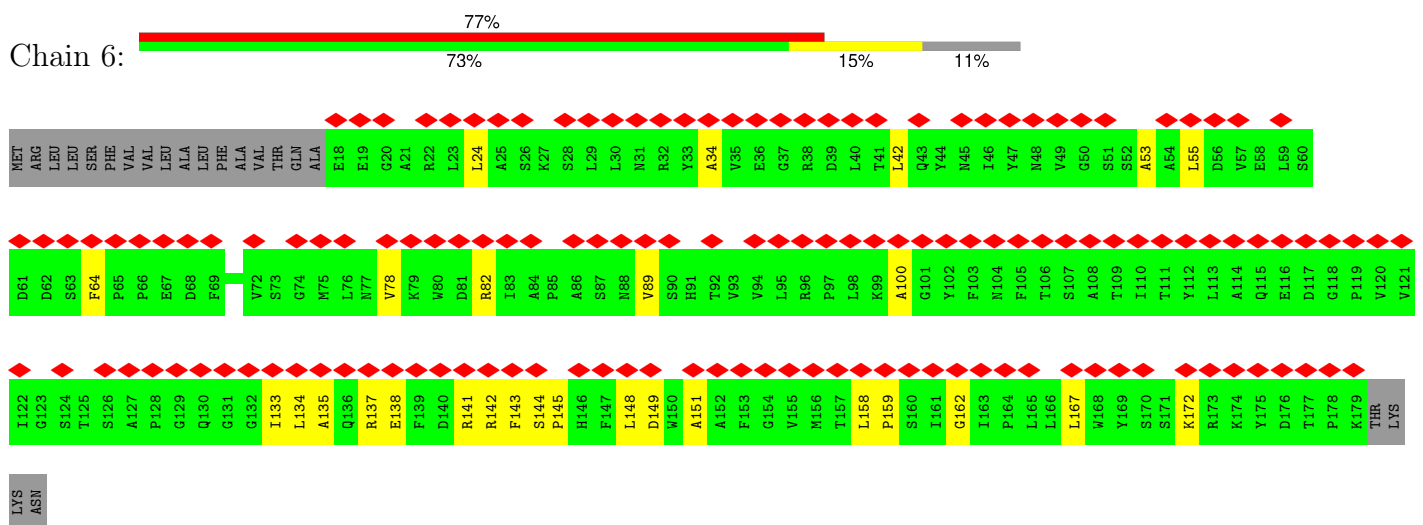
### 3 Residue-property plots [i](#)

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.

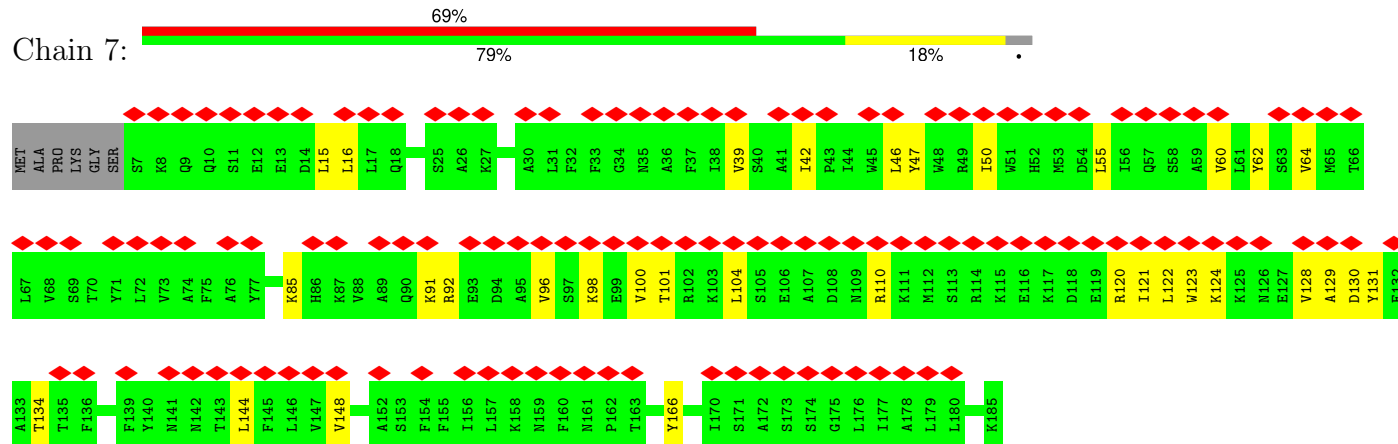
- Molecule 1: Translocon-associated protein subunit alpha



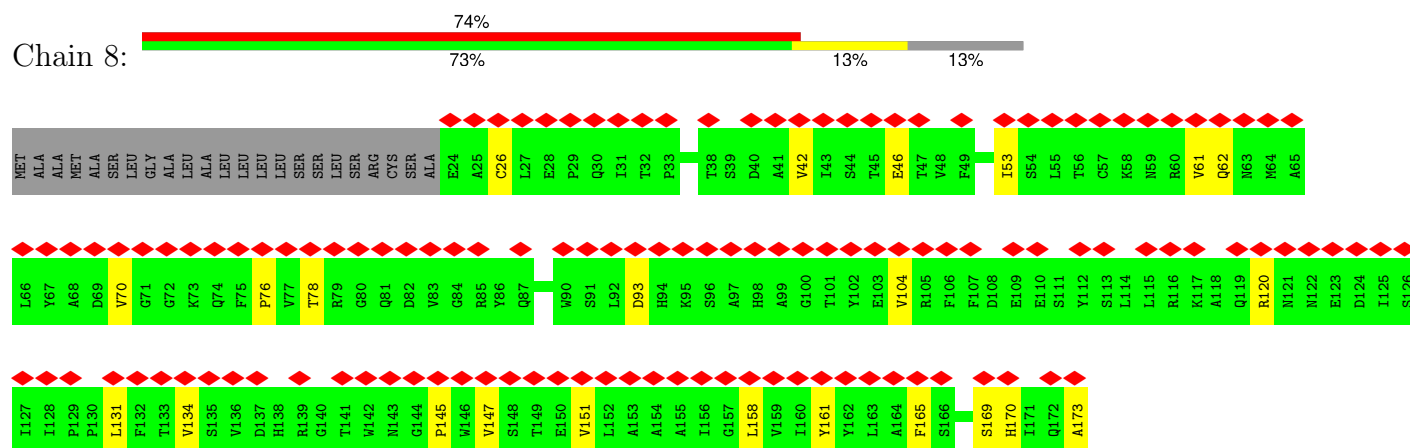
- Molecule 2: Translocon-associated protein subunit beta



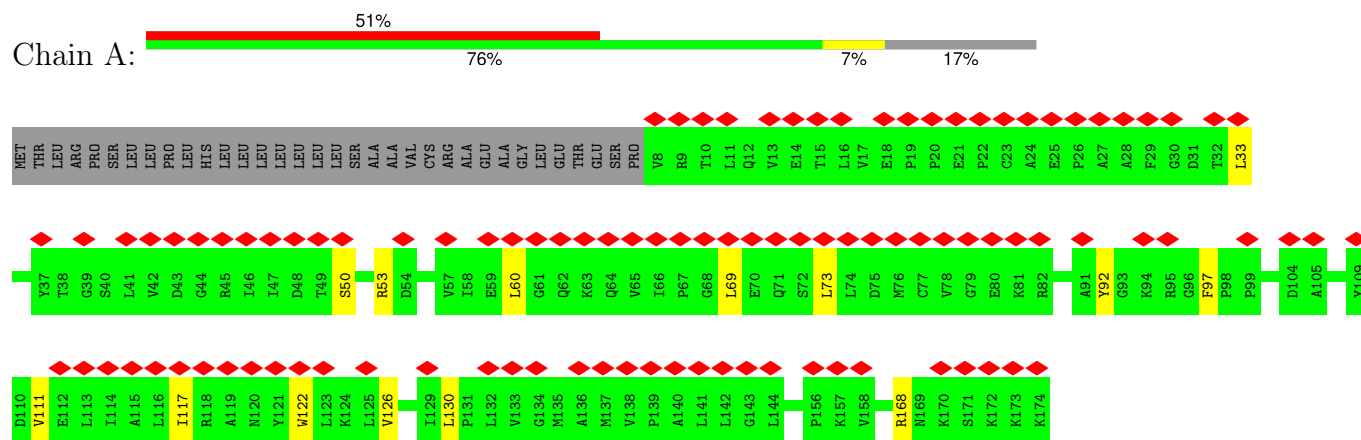
- Molecule 3: Translocon-associated protein subunit gamma



- Molecule 4: Translocon-associated protein subunit delta

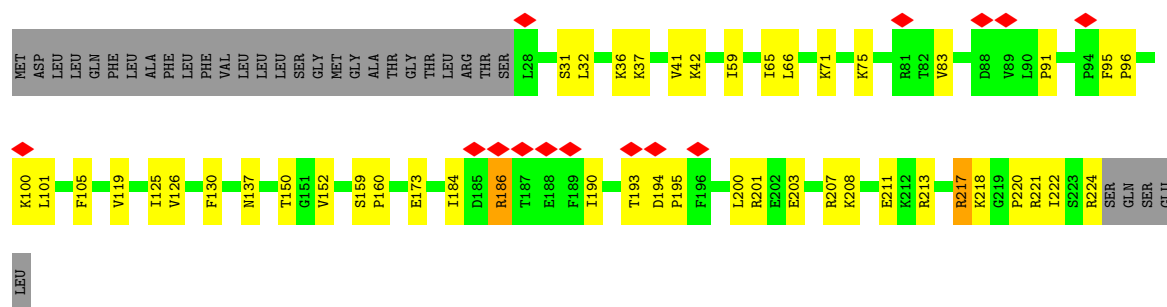


- Molecule 5: Peptidyl-prolyl cis-trans isomerase FKBP11

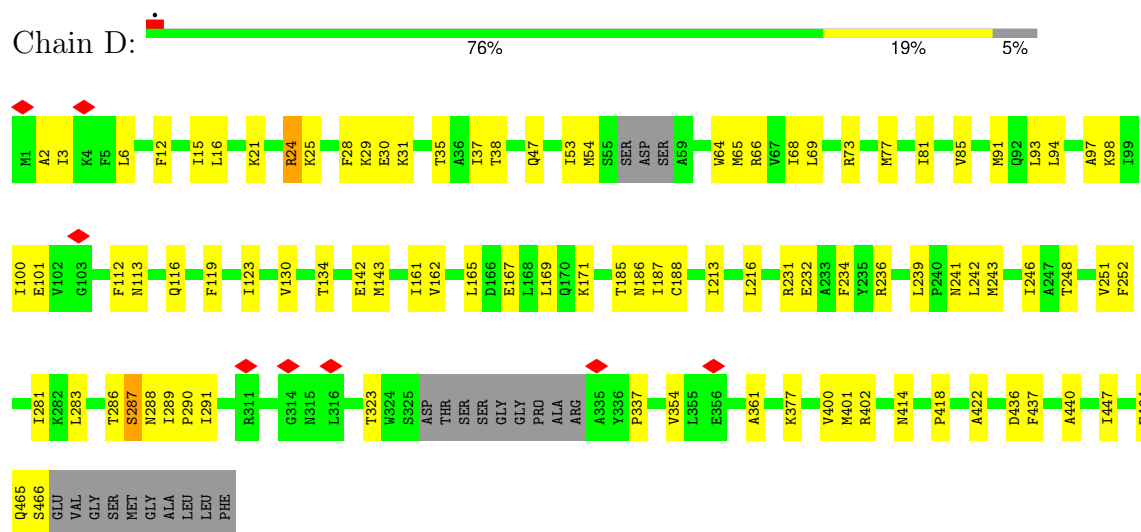


- Molecule 6: Coiled-coil domain-containing protein 134

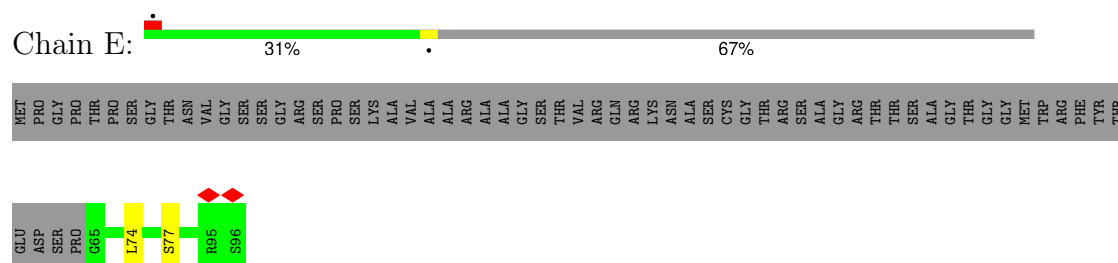




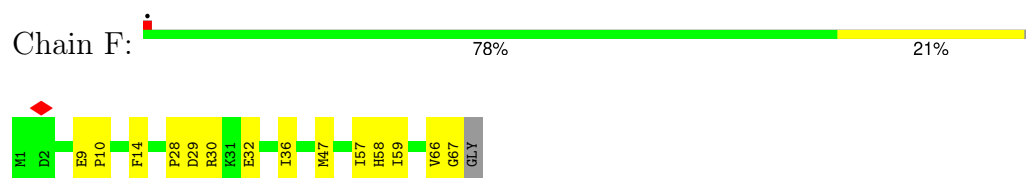
- Molecule 7: Protein transport protein Sec61 subunit alpha isoform 1



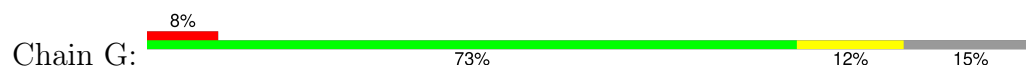
- Molecule 8: Protein transport protein Sec61 subunit beta

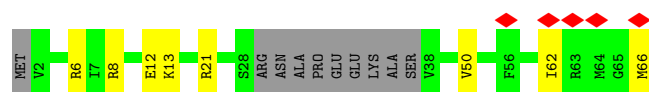


- Molecule 9: Protein transport protein Sec61 subunit gamma

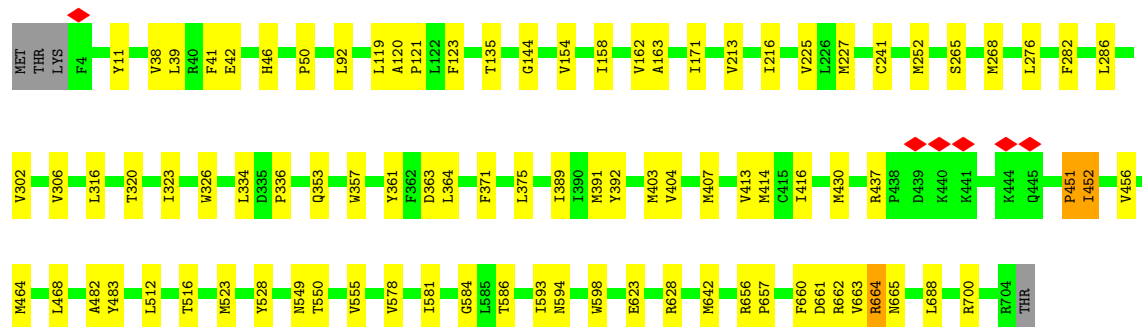
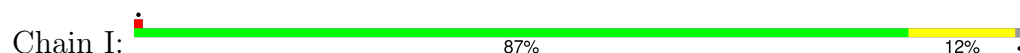


- Molecule 10: Stress-associated endoplasmic reticulum protein 1

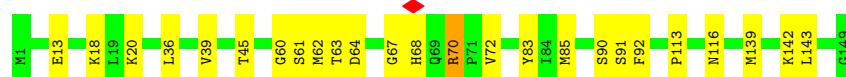
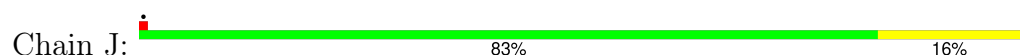




- Molecule 11: Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit STT3A



- Molecule 12: Oligosaccharyltransferase complex subunit OSTC



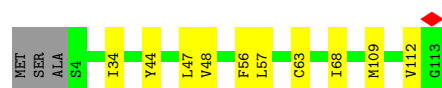
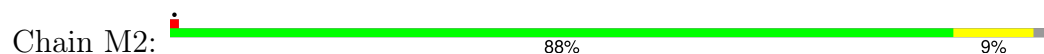
- Molecule 13: Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit 4



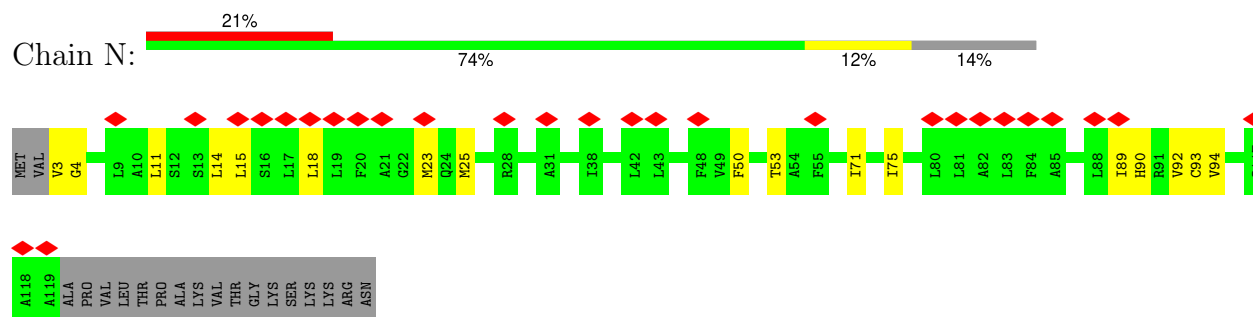
- Molecule 14: Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit TMEM258



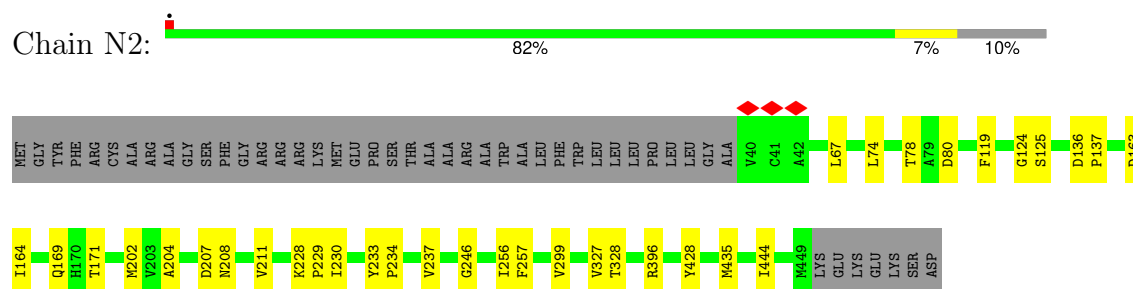
- Molecule 15: Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit DAD1



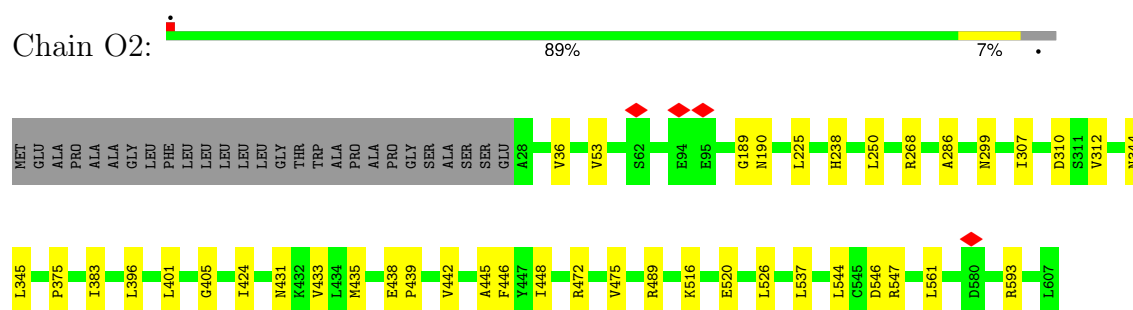
• Molecule 16: Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit KCP2



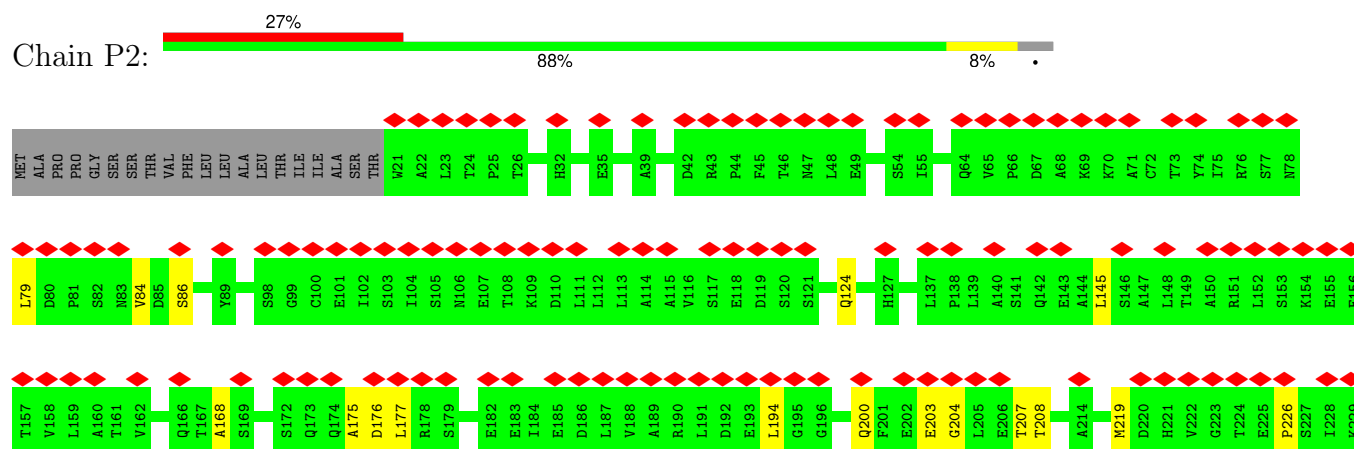
• Molecule 17: Dolichyl-diphosphooligosaccharide--protein glycosyltransferase 48 kDa subunit

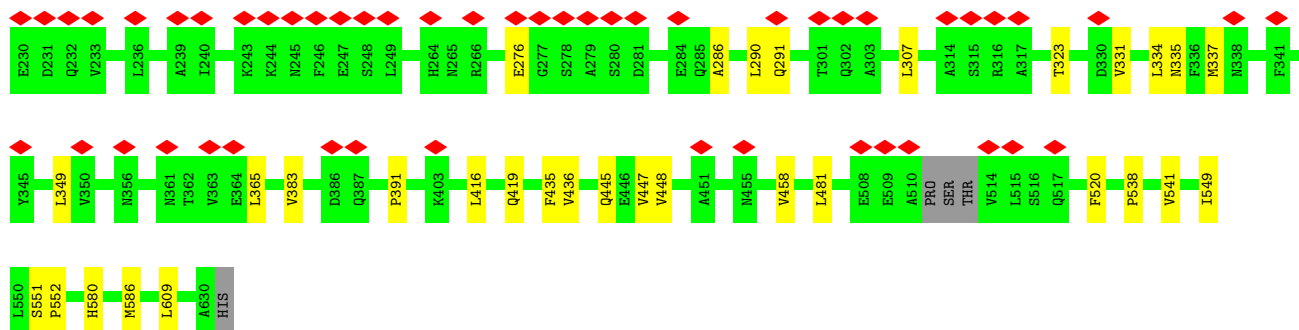


• Molecule 18: Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit 1

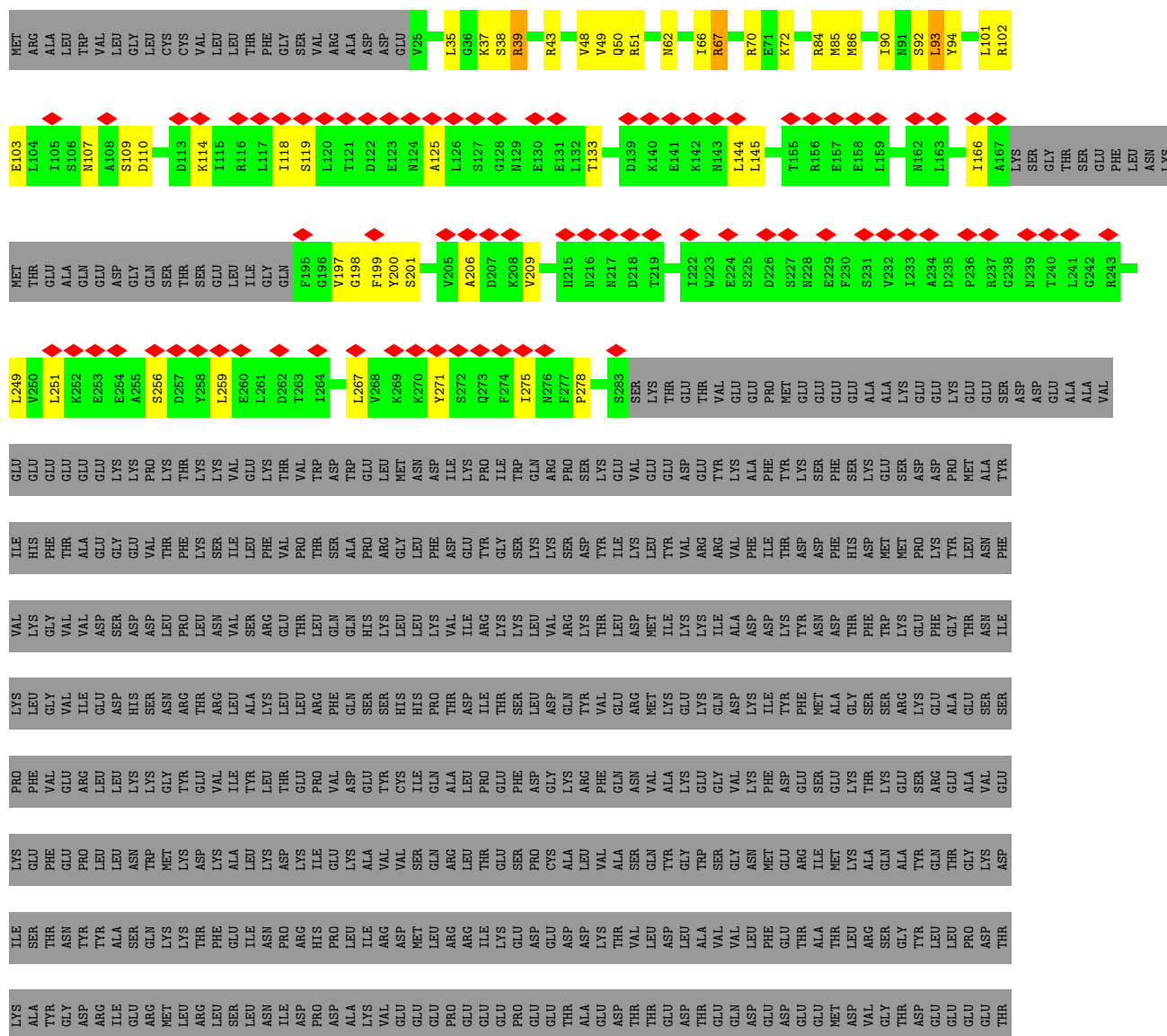


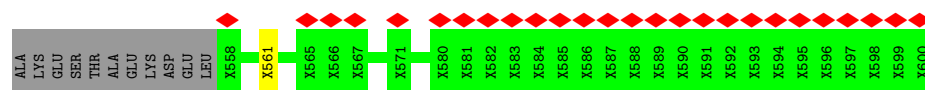
• Molecule 19: Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit 2





• Molecule 20: Endoplasmic





- Molecule 21: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K: 25% 75%



- Molecule 22: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C: 50% 50%



- Molecule 23: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H: 12% 38% 62%



- Molecule 24: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose

Chain L: 100%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	55750	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	60	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	1900	Depositor
Magnification	53000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.017	Depositor
Minimum map value	-0.005	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.00395	Depositor
Map size ( $\text{\AA}$ )	349.44, 349.44, 349.44	wwPDB
Map dimensions	416, 416, 416	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.84000003, 0.84000003, 0.84000003	Depositor



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, BMA, ELU, NAG, NDG

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	5	0.12	0/1150	0.32	0/1569
2	6	0.14	0/1291	0.44	0/1757
3	7	0.12	0/1481	0.30	0/2000
4	8	0.12	0/1214	0.35	0/1654
5	A	0.12	0/1331	0.36	0/1801
6	B	0.17	0/1670	0.37	0/2248
7	D	0.19	0/3604	0.35	0/4884
8	E	0.16	0/257	0.31	0/348
9	F	0.21	0/548	0.35	0/733
10	G	0.16	0/442	0.42	0/590
11	I	0.25	0/5806	0.39	1/7884 (0.0%)
12	J	0.22	0/1216	0.41	0/1649
13	K2	0.22	0/300	0.34	0/406
14	L2	0.18	0/663	0.29	0/903
15	M2	0.20	0/883	0.29	0/1197
16	N	0.12	0/908	0.27	0/1229
17	N2	0.17	0/3306	0.30	0/4493
18	O2	0.18	0/4752	0.31	0/6444
19	P2	0.12	0/4814	0.28	0/6553
20	y3	0.17	0/1864	0.39	0/2511
All	All	0.18	0/37500	0.34	1/50853 (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	6	0	2
3	7	0	2
4	8	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
5	A	0	2
6	B	0	6
7	D	0	5
10	G	0	3
11	I	0	4
12	J	0	1
20	y3	0	6
All	All	0	32

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	I	452	ILE	N-CA-C	6.07	121.97	109.34

There are no chirality outliers.

5 of 32 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	6	137	ARG	Sidechain
2	6	142	ARG	Sidechain
3	7	110	ARG	Sidechain
3	7	92	ARG	Sidechain
4	8	120	ARG	Sidechain

## 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	5	1121	1071	1071	8	0
2	6	1259	1241	1241	24	0
3	7	1451	1487	1487	26	0
4	8	1185	1148	1148	20	0
5	A	1305	1390	1390	9	0
6	B	1633	1646	1646	32	0
7	D	3528	3661	3661	68	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	E	250	273	272	3	0
9	F	538	574	574	13	0
10	G	437	467	467	4	0
11	I	5649	5611	5611	69	0
12	J	1182	1227	1227	24	0
13	K2	295	312	312	12	0
14	L2	643	659	659	6	0
15	M2	863	880	880	9	0
16	N	891	925	925	16	0
17	N2	3224	3161	3161	26	0
18	O2	4655	4686	4686	27	0
19	P2	4721	4724	4724	32	0
20	y3	2058	2011	1897	41	0
21	K	94	79	79	0	0
22	C	28	25	25	0	0
23	H	94	79	79	0	0
24	L	28	25	24	0	0
25	I	29	35	0	0	0
All	All	37161	37397	37246	397	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 5.

The worst 5 of 397 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)
19:P2:416:LEU:HD11	19:P2:481:LEU:HD21	1.59	0.83
11:I:241:CYS:HB3	15:M2:68:ILE:HD11	1.59	0.81
7:D:85:VAL:HG11	20:y3:561:UNK:CB	2.14	0.77
19:P2:84:VAL:HG11	19:P2:124:GLN:OE1	1.87	0.74
11:I:430:MET:HE1	13:K2:27:TYR:HB2	1.70	0.73

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	5	136/286 (48%)	133 (98%)	3 (2%)	0	100	100
2	6	160/183 (87%)	153 (96%)	7 (4%)	0	100	100
3	7	177/185 (96%)	173 (98%)	4 (2%)	0	100	100
4	8	148/173 (86%)	145 (98%)	3 (2%)	0	100	100
5	A	165/201 (82%)	161 (98%)	4 (2%)	0	100	100
6	B	195/229 (85%)	190 (97%)	4 (2%)	1 (0%)	25	62
7	D	448/476 (94%)	441 (98%)	6 (1%)	1 (0%)	44	77
8	E	30/96 (31%)	30 (100%)	0	0	100	100
9	F	65/68 (96%)	65 (100%)	0	0	100	100
10	G	52/66 (79%)	51 (98%)	1 (2%)	0	100	100
11	I	699/705 (99%)	690 (99%)	8 (1%)	1 (0%)	48	82
12	J	147/149 (99%)	146 (99%)	1 (1%)	0	100	100
13	K2	35/37 (95%)	35 (100%)	0	0	100	100
14	L2	77/79 (98%)	76 (99%)	1 (1%)	0	100	100
15	M2	108/113 (96%)	108 (100%)	0	0	100	100
16	N	115/136 (85%)	115 (100%)	0	0	100	100
17	N2	408/456 (90%)	401 (98%)	7 (2%)	0	100	100
18	O2	578/607 (95%)	572 (99%)	6 (1%)	0	100	100
19	P2	603/631 (96%)	594 (98%)	9 (2%)	0	100	100
20	y3	228/846 (27%)	222 (97%)	5 (2%)	1 (0%)	30	67
All	All	4574/5722 (80%)	4501 (98%)	69 (2%)	4 (0%)	50	82

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
20	y3	93	LEU
6	B	217	ARG
7	D	287	SER
11	I	451	PRO

### 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	5	125/253 (49%)	125 (100%)	0	100	100
2	6	135/153 (88%)	135 (100%)	0	100	100
3	7	161/165 (98%)	161 (100%)	0	100	100
4	8	129/145 (89%)	129 (100%)	0	100	100
5	A	143/172 (83%)	143 (100%)	0	100	100
6	B	181/208 (87%)	181 (100%)	0	100	100
7	D	382/398 (96%)	382 (100%)	0	100	100
8	E	28/74 (38%)	28 (100%)	0	100	100
9	F	59/59 (100%)	59 (100%)	0	100	100
10	G	47/55 (86%)	47 (100%)	0	100	100
11	I	611/615 (99%)	611 (100%)	0	100	100
12	J	130/130 (100%)	130 (100%)	0	100	100
13	K2	33/33 (100%)	33 (100%)	0	100	100
14	L2	70/70 (100%)	70 (100%)	0	100	100
15	M2	96/98 (98%)	96 (100%)	0	100	100
16	N	97/113 (86%)	97 (100%)	0	100	100
17	N2	356/391 (91%)	356 (100%)	0	100	100
18	O2	519/537 (97%)	519 (100%)	0	100	100
19	P2	521/541 (96%)	521 (100%)	0	100	100
20	y3	207/725 (29%)	207 (100%)	0	100	100
All	All	4030/4935 (82%)	4030 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
16	N	57	ASN

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Mol	Chain	Res	Type
18	O2	83	HIS
20	y3	221	HIS
18	O2	57	HIS
19	P2	200	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

20 monosaccharides 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	$\# Z  > 2$
22	NAG	C	1	22,11	14,14,15	0.80	0	17,19,21	1.00	1 (5%)
22	NAG	C	2	22	14,14,15	0.75	0	17,19,21	0.88	0
23	NAG	H	1	11,23	14,14,15	0.78	0	17,19,21	0.73	0
23	NAG	H	2	23	14,14,15	0.83	0	17,19,21	0.73	0
23	BMA	H	3	23	11,11,12	0.85	0	15,15,17	1.02	1 (6%)
23	MAN	H	4	23	11,11,12	0.93	1 (9%)	15,15,17	0.99	0
23	MAN	H	5	23	11,11,12	0.88	1 (9%)	15,15,17	0.92	0
23	MAN	H	6	23	11,11,12	0.79	0	15,15,17	0.94	0
23	MAN	H	7	23	11,11,12	0.72	0	15,15,17	1.26	1 (6%)
23	MAN	H	8	23	11,11,12	0.74	0	15,15,17	1.05	1 (6%)
21	NAG	K	1	18,21	14,14,15	0.69	0	17,19,21	1.33	2 (11%)
21	NAG	K	2	21	14,14,15	0.81	0	17,19,21	0.75	0
21	BMA	K	3	21	11,11,12	0.85	0	15,15,17	1.39	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
21	MAN	K	4	21	11,11,12	0.83	0	15,15,17	1.00	1 (6%)
21	MAN	K	5	21	11,11,12	0.86	1 (9%)	15,15,17	0.94	0
21	MAN	K	6	21	11,11,12	0.78	0	15,15,17	1.08	1 (6%)
21	MAN	K	7	21	11,11,12	0.80	1 (9%)	15,15,17	0.94	1 (6%)
21	MAN	K	8	21	11,11,12	0.79	0	15,15,17	0.90	0
24	NDG	L	1	25,24	14,14,15	0.90	1 (7%)	17,19,21	1.66	3 (17%)
24	NAG	L	2	24	14,14,15	0.79	0	17,19,21	0.88	1 (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
22	NAG	C	1	22,11	-	4/6/23/26	0/1/1/1
22	NAG	C	2	22	-	0/6/23/26	0/1/1/1
23	NAG	H	1	11,23	-	2/6/23/26	0/1/1/1
23	NAG	H	2	23	-	0/6/23/26	0/1/1/1
23	BMA	H	3	23	-	0/2/19/22	0/1/1/1
23	MAN	H	4	23	-	0/2/19/22	0/1/1/1
23	MAN	H	5	23	-	2/2/19/22	0/1/1/1
23	MAN	H	6	23	-	1/2/19/22	0/1/1/1
23	MAN	H	7	23	-	2/2/19/22	0/1/1/1
23	MAN	H	8	23	-	1/2/19/22	1/1/1/1
21	NAG	K	1	18,21	-	2/6/23/26	0/1/1/1
21	NAG	K	2	21	-	1/6/23/26	0/1/1/1
21	BMA	K	3	21	-	0/2/19/22	0/1/1/1
21	MAN	K	4	21	-	0/2/19/22	0/1/1/1
21	MAN	K	5	21	-	0/2/19/22	0/1/1/1
21	MAN	K	6	21	-	2/2/19/22	0/1/1/1
21	MAN	K	7	21	-	0/2/19/22	0/1/1/1
21	MAN	K	8	21	-	0/2/19/22	0/1/1/1
24	NDG	L	1	25,24	-	2/6/23/26	0/1/1/1
24	NAG	L	2	24	-	2/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	H	4	MAN	O5-C1	-2.47	1.39	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	L	1	NDG	O5-C1	-2.33	1.39	1.43
21	K	5	MAN	O5-C1	-2.31	1.39	1.43
23	H	5	MAN	O5-C1	-2.21	1.40	1.43
21	K	7	MAN	O5-C1	-2.02	1.40	1.43

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	L	1	NDG	C1-O5-C5	4.73	118.53	112.19
21	K	3	BMA	C1-O5-C5	4.56	118.30	112.19
23	H	7	MAN	C1-O5-C5	3.80	117.28	112.19
21	K	1	NAG	C2-N2-C7	3.26	127.27	122.90
24	L	1	NDG	O5-C1-C2	3.12	116.11	111.29

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	K	6	MAN	C4-C5-C6-O6
22	C	1	NAG	C4-C5-C6-O6
21	K	6	MAN	O5-C5-C6-O6
24	L	2	NAG	O5-C5-C6-O6
23	H	7	MAN	O5-C5-C6-O6

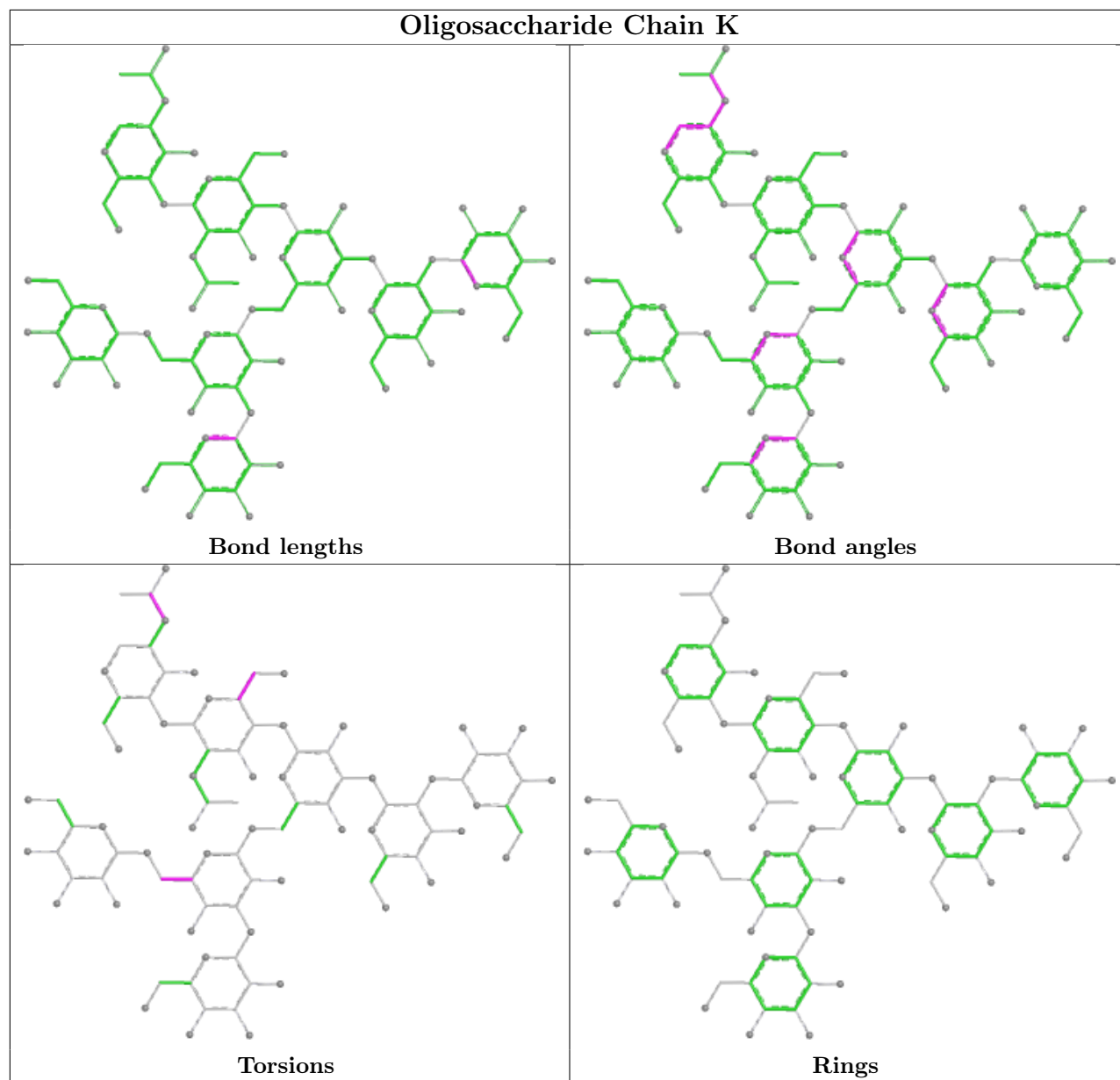
All (1) ring outliers are listed below:

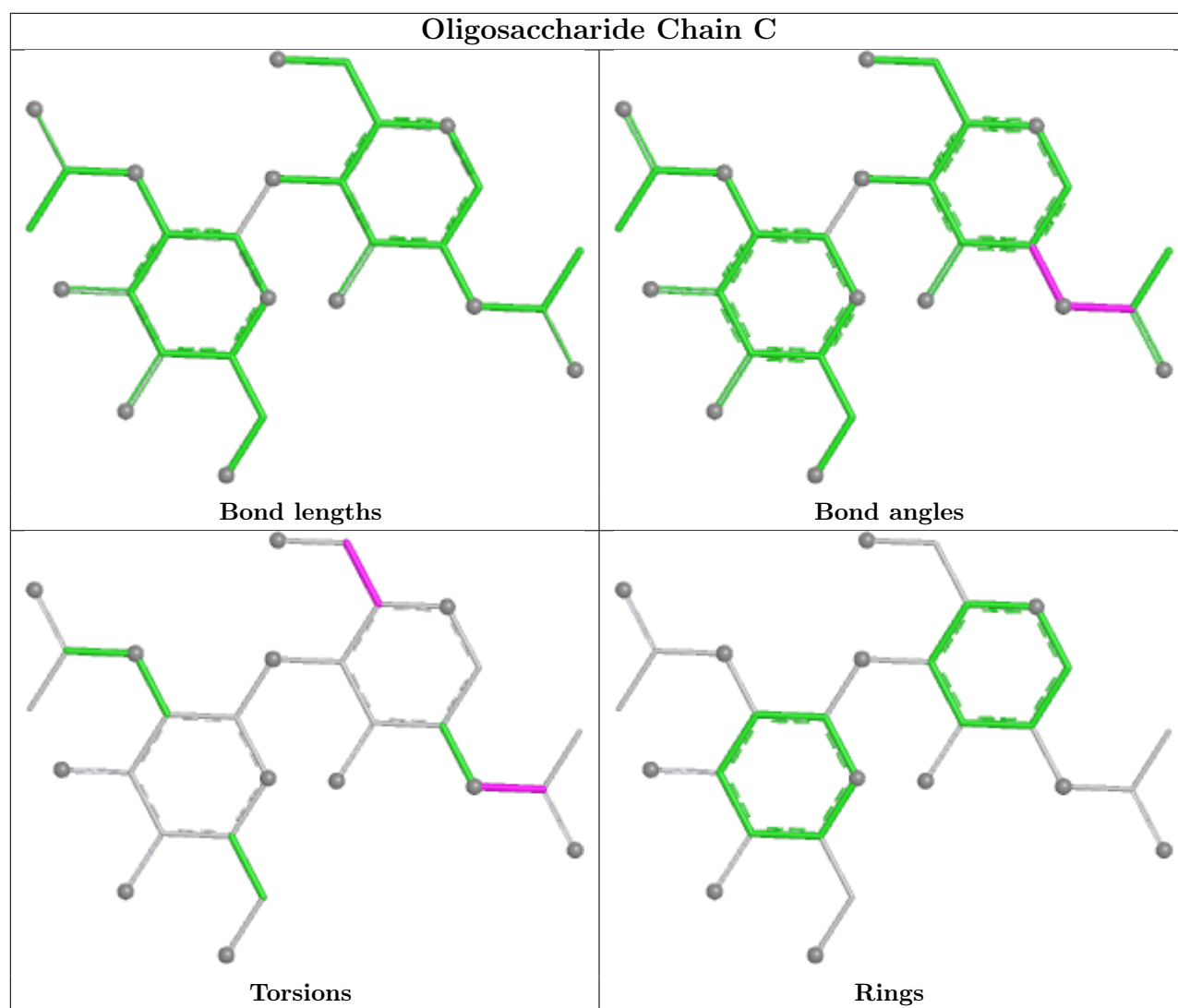
Mol	Chain	Res	Type	Atoms
23	H	8	MAN	C1-C2-C3-C4-C5-O5

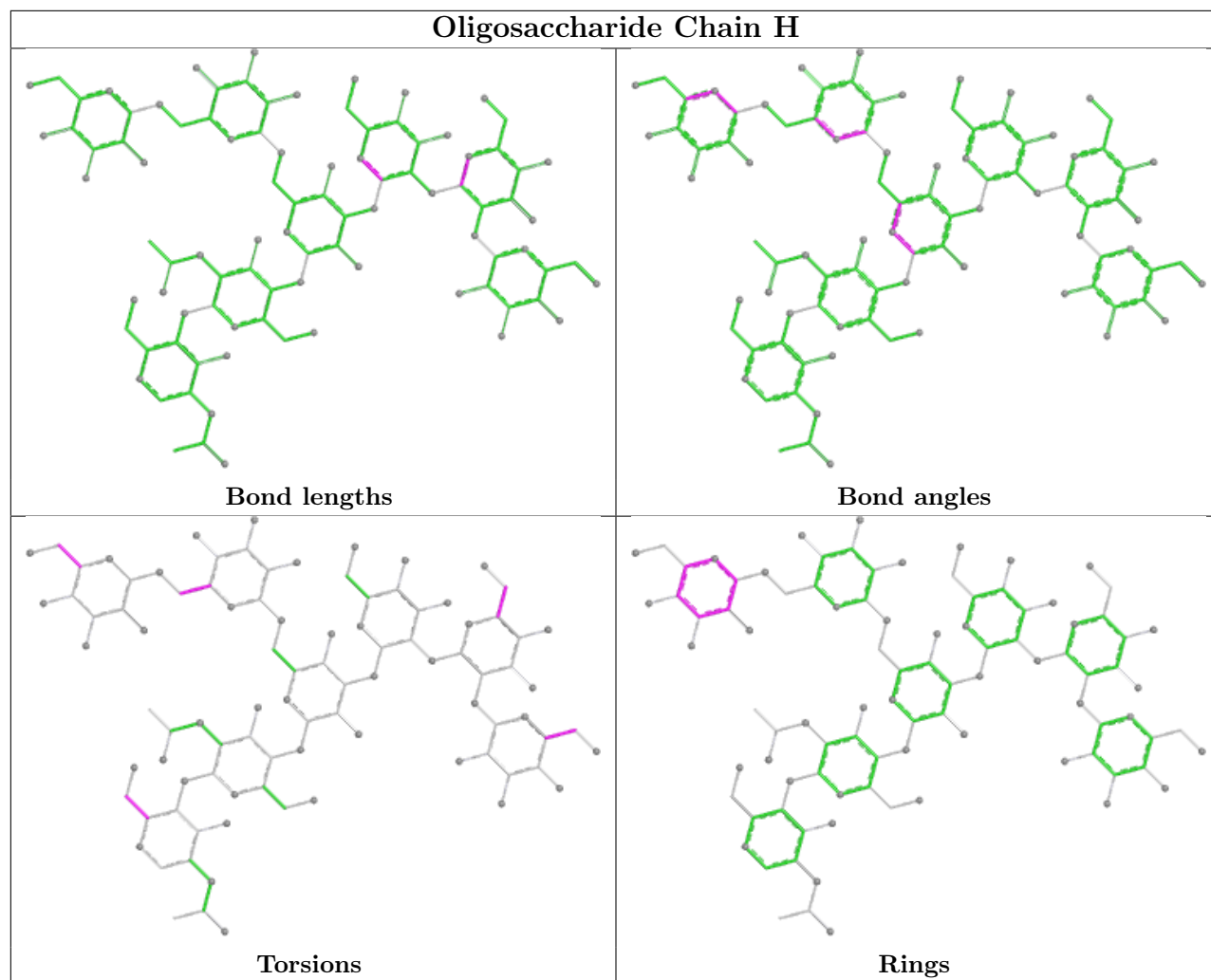
No monomer is involved in short contacts.

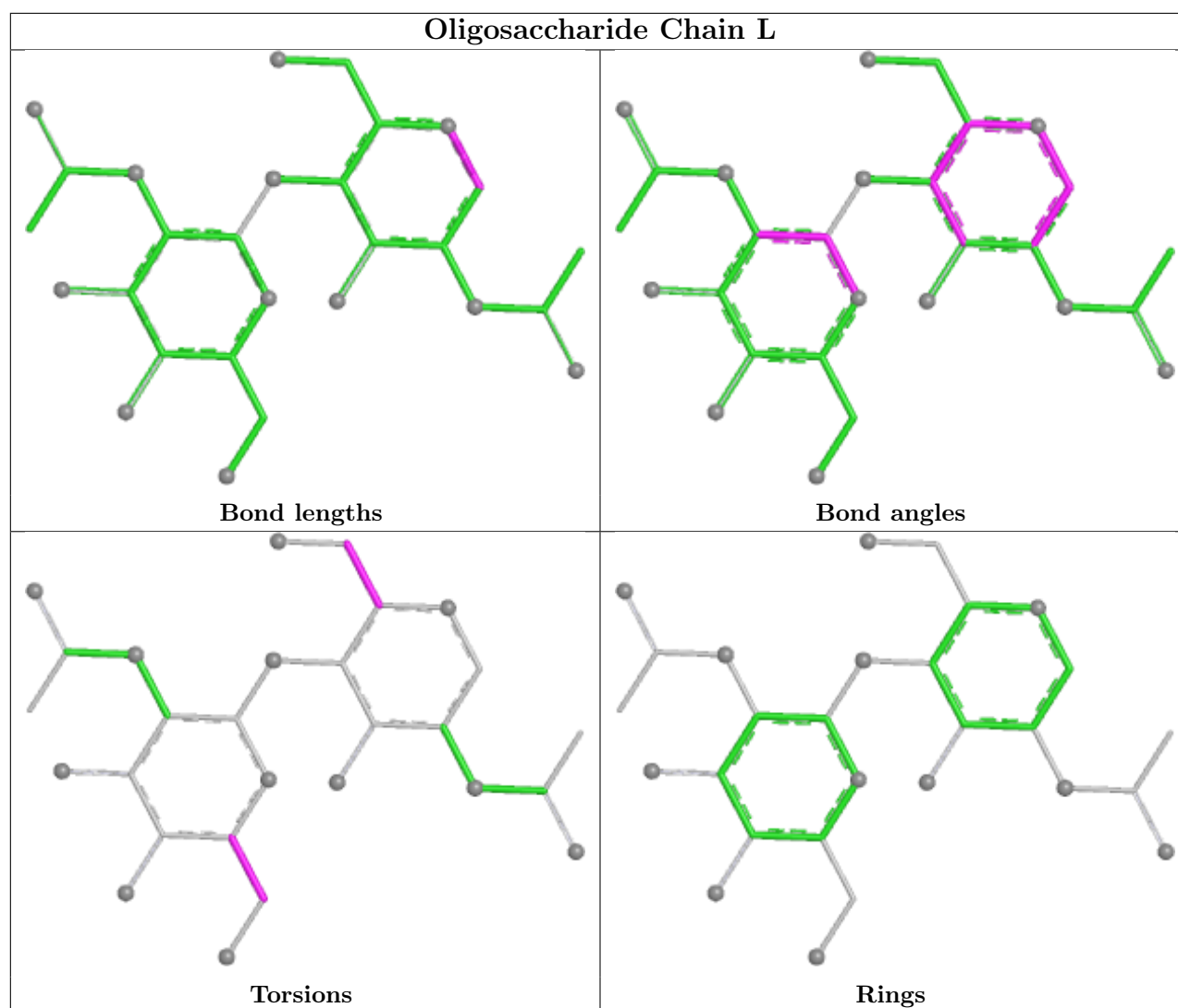
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











## 5.6 Ligand geometry [i](#)

1 ligand 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	$\# Z  > 2$
25	ELU	I	801	24	27,28,28	0.93	3 (11%)	33,37,37	1.25	5 (15%)

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	ELU	I	801	24	-	12/31/31/31	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	I	801	ELU	PA-O3A	2.92	1.62	1.59
25	I	801	ELU	PB-O2B	2.52	1.58	1.50
25	I	801	ELU	PB-O1B	-2.01	1.47	1.54

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	I	801	ELU	O1B-PB-O3A	3.19	115.33	104.64
25	I	801	ELU	O3B-PB-O1B	2.49	117.12	107.80
25	I	801	ELU	O3A-PB-O2B	-2.37	98.55	111.04
25	I	801	ELU	O1-PA-O2A	2.30	118.06	108.94
25	I	801	ELU	O3B-PB-O2B	-2.11	102.61	110.83

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

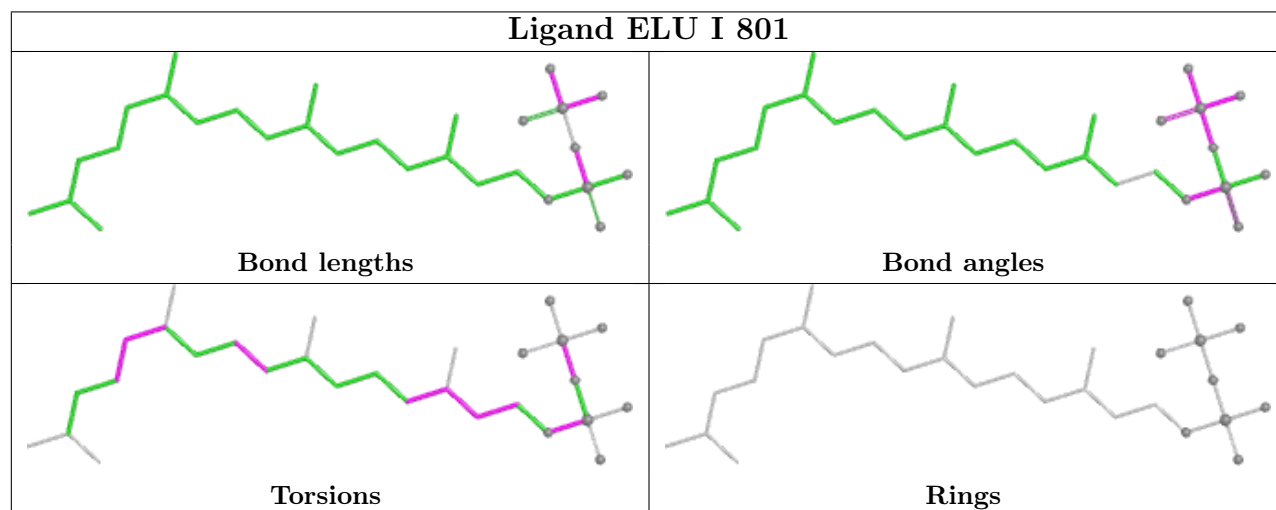
Mol	Chain	Res	Type	Atoms
25	I	801	ELU	C1-O1-PA-O2A
25	I	801	ELU	C1-O1-PA-O3A
25	I	801	ELU	PA-O3A-PB-O1B
25	I	801	ELU	C1-C2-C3-C4
25	I	801	ELU	C14-C13-C15-C16

There are no ring outliers.

No monomer is involved in short contacts.

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.

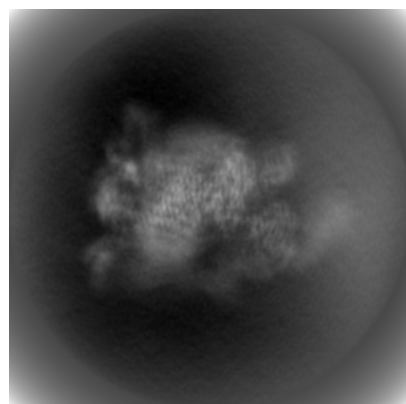
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-72945. These allow visual inspection of the internal detail of the map and identification of artifacts.

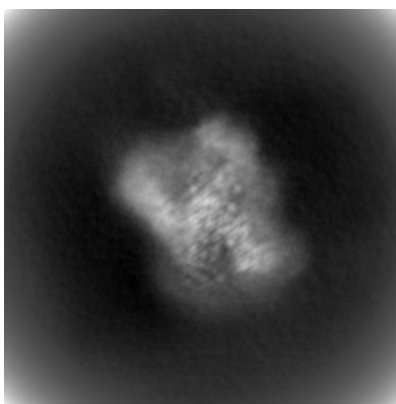
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

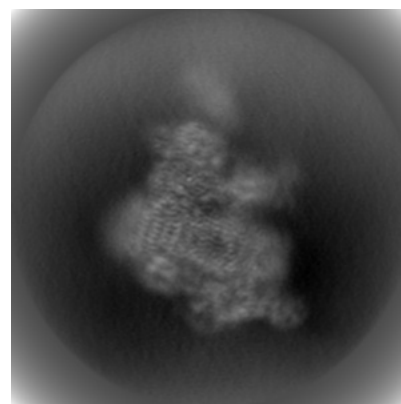
#### 6.1.1 Primary map



X

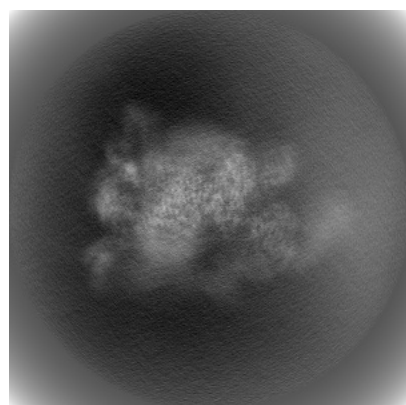


Y

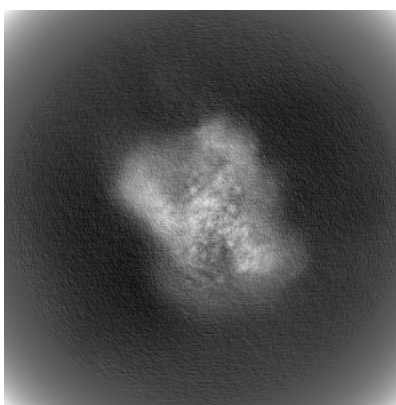


Z

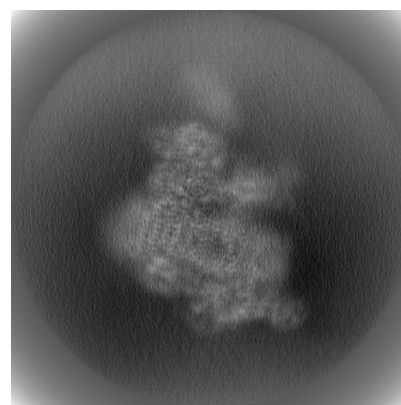
#### 6.1.2 Raw map



X



Y

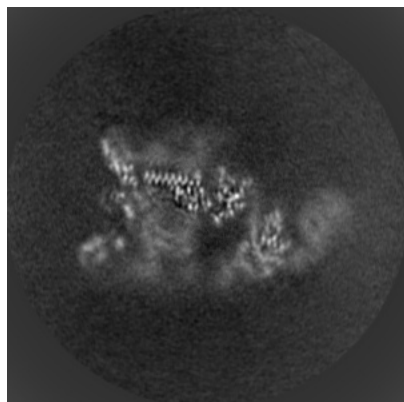


Z

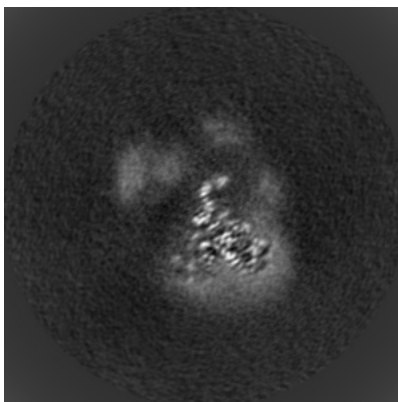
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

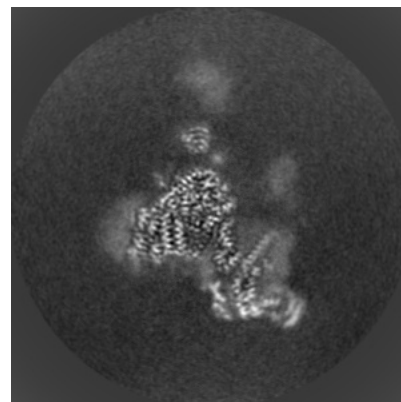
### 6.2.1 Primary map



X Index: 208

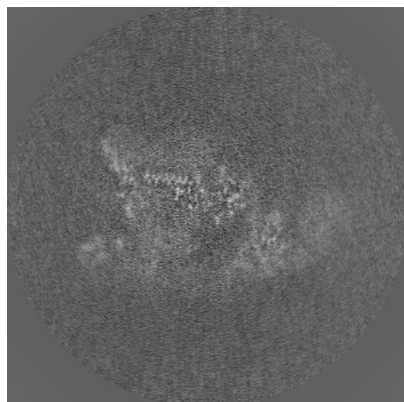


Y Index: 208

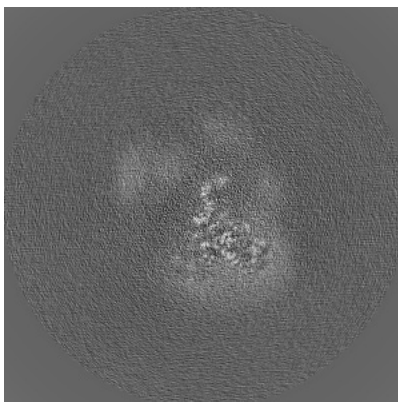


Z Index: 208

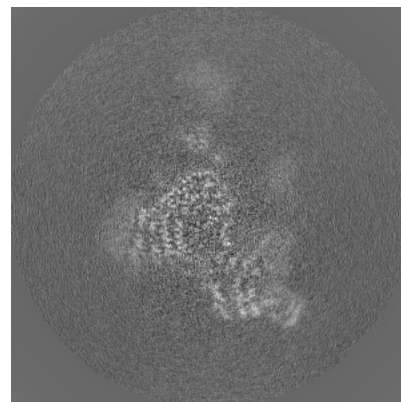
### 6.2.2 Raw map



X Index: 208



Y Index: 208



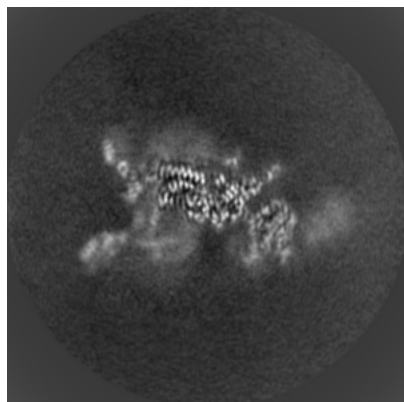
Z Index: 208

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

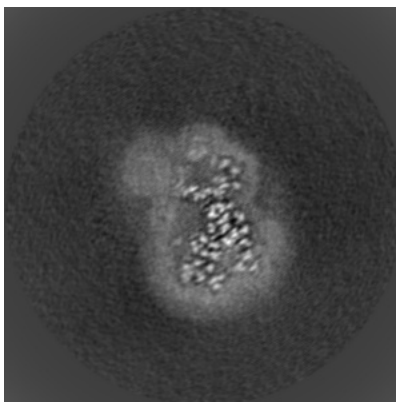


## 6.3 Largest variance slices [i](#)

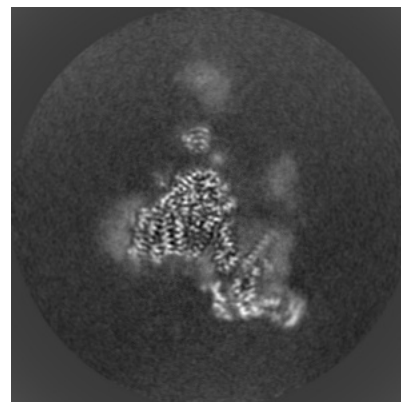
### 6.3.1 Primary map



X Index: 195

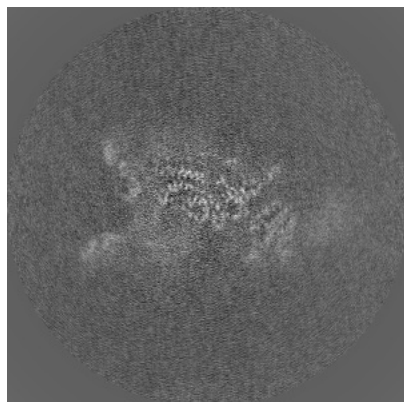


Y Index: 176

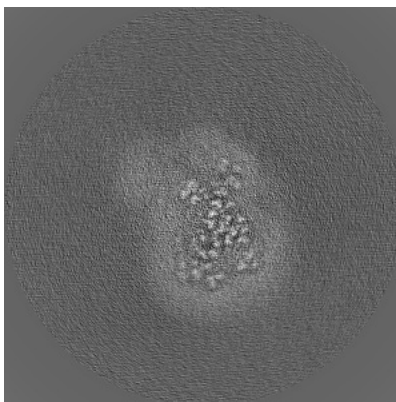


Z Index: 209

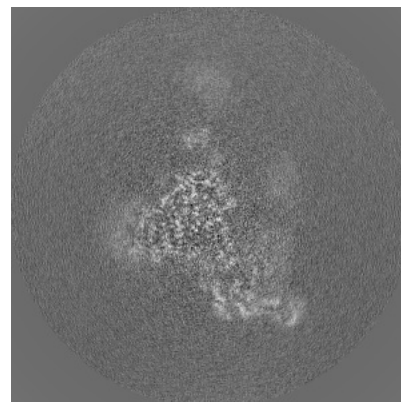
### 6.3.2 Raw map



X Index: 194



Y Index: 182

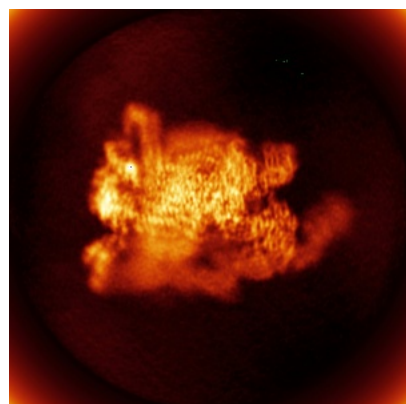


Z Index: 210

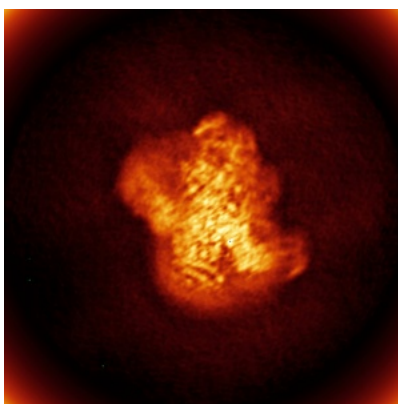
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



X

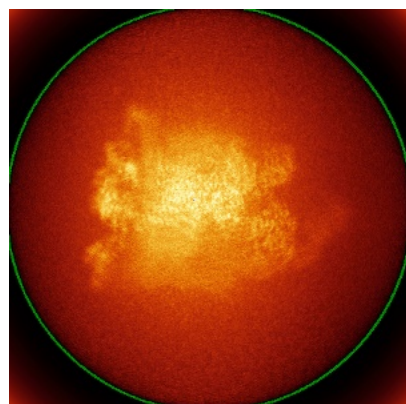


Y

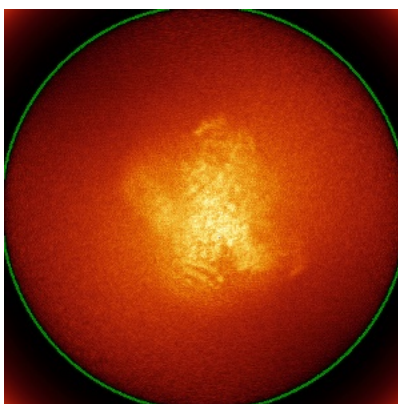


Z

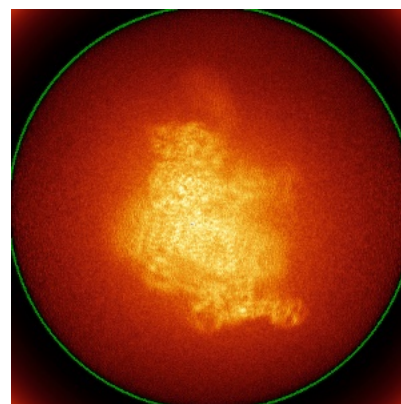
### 6.4.2 Raw map



X



Y

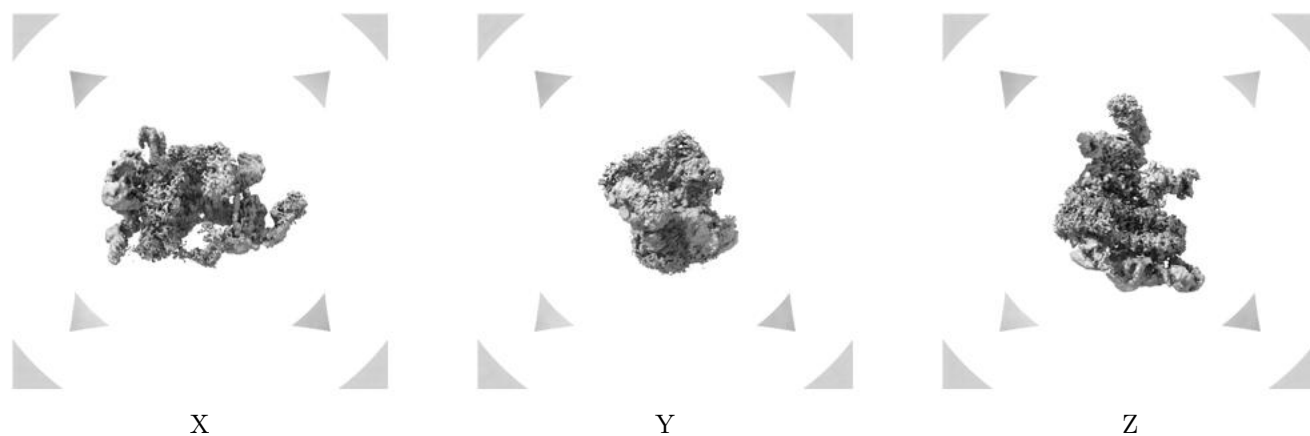


Z

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

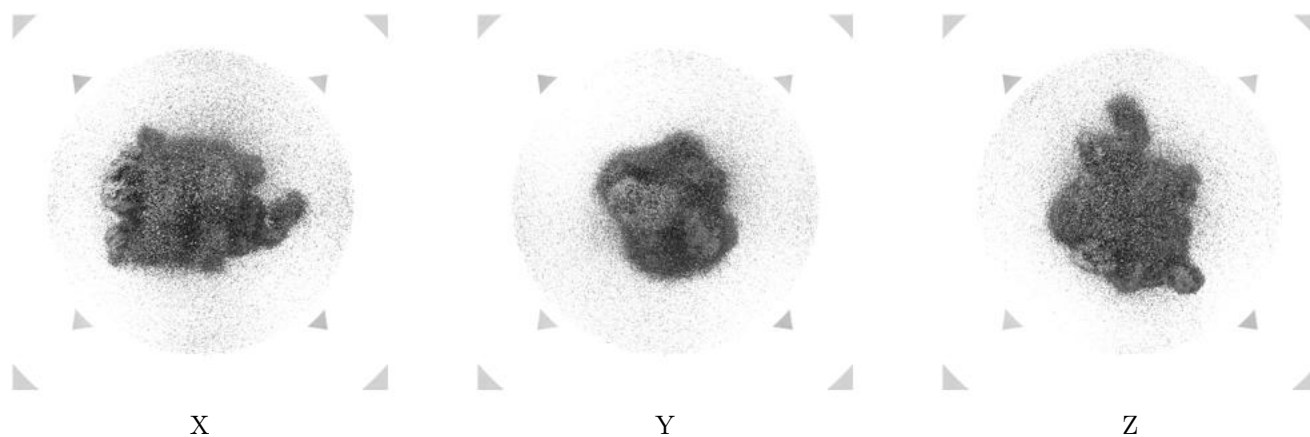
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.00395. 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.

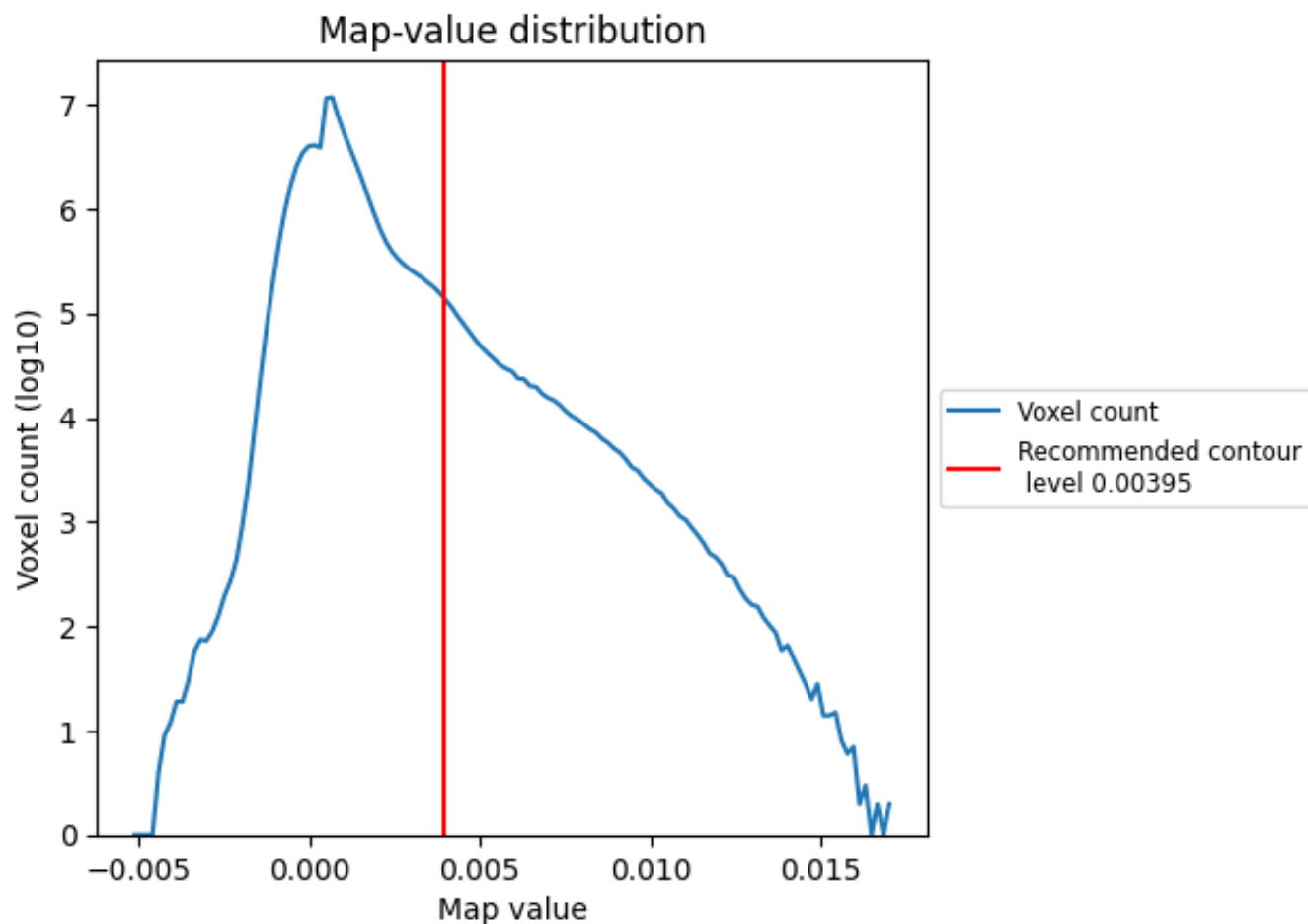
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

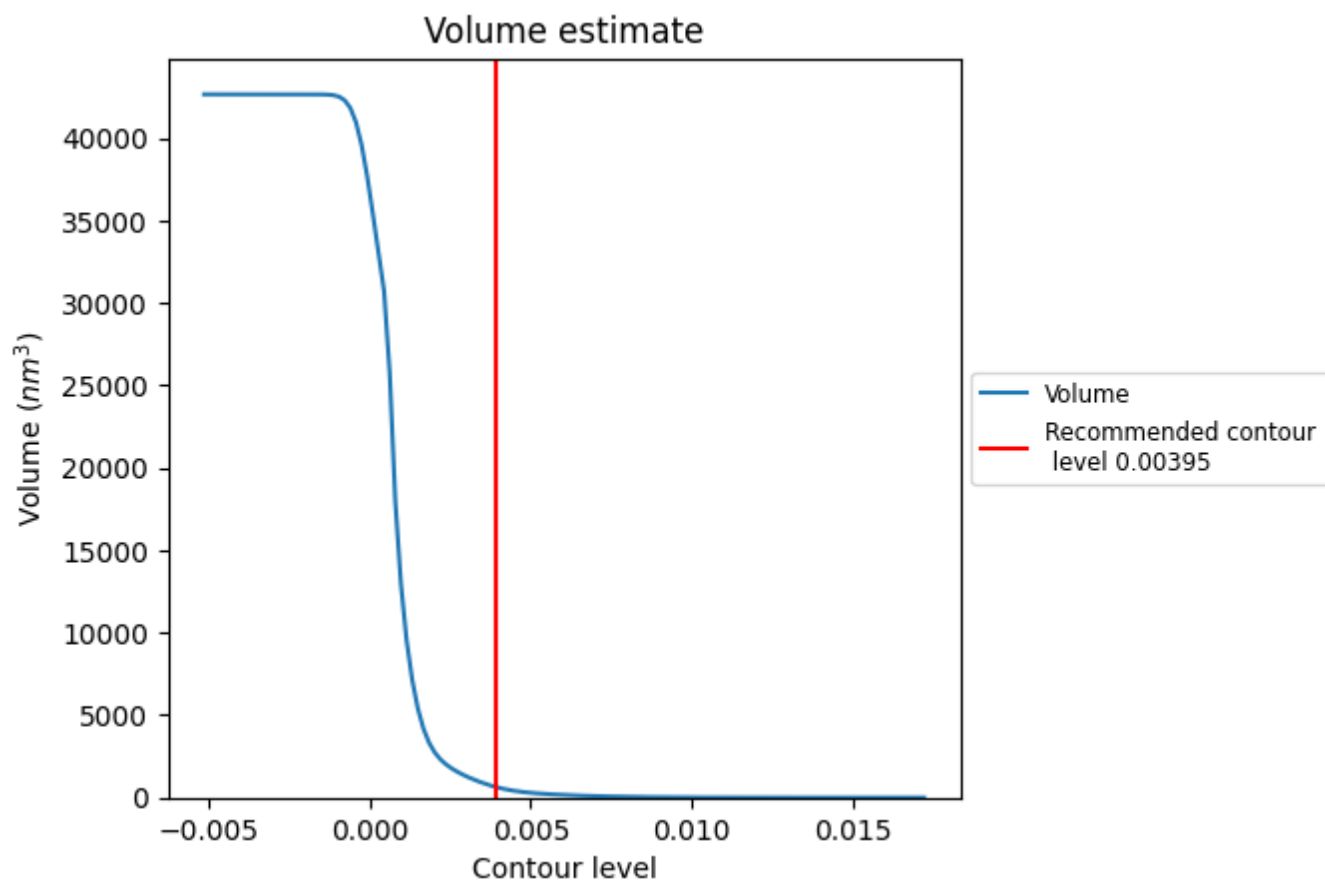
This section contains the results of statistical analysis of the map.

### 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.

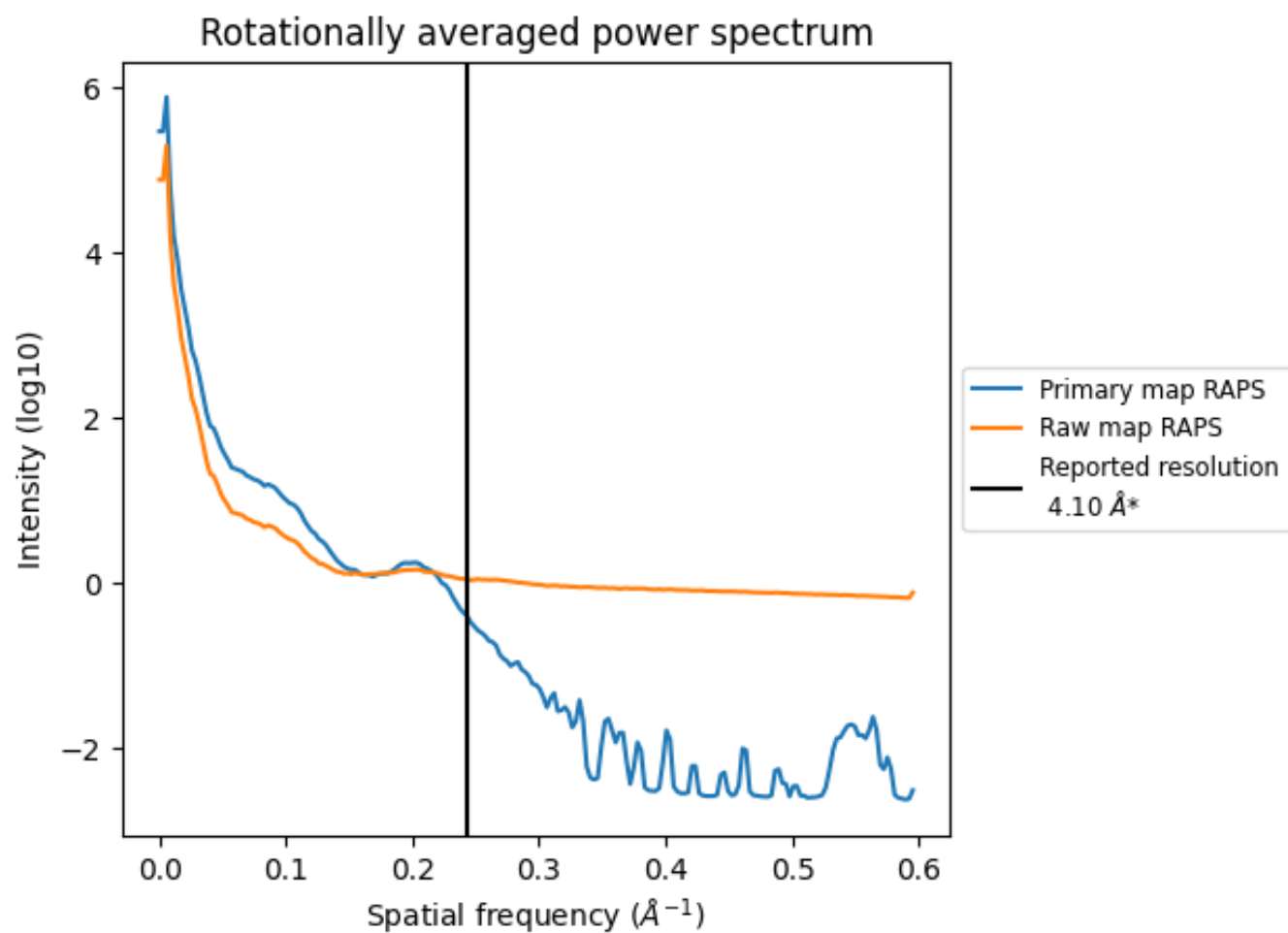
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 625 nm<sup>3</sup>; this corresponds to an approximate mass of 564 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 ⓘ

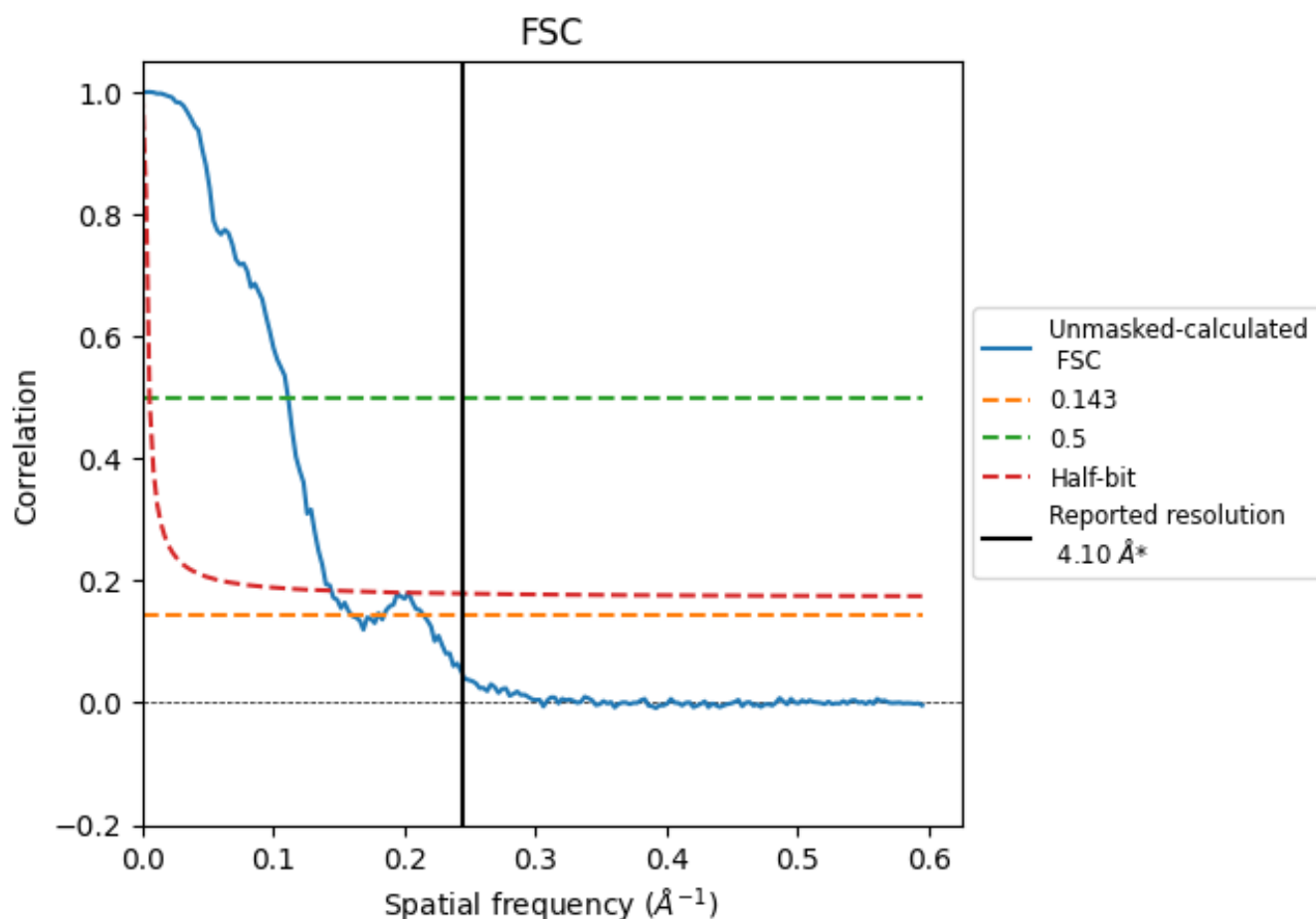


\*Reported resolution corresponds to spatial frequency of 0.244 Å<sup>-1</sup>

## 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 0.244 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.25	8.98	6.93

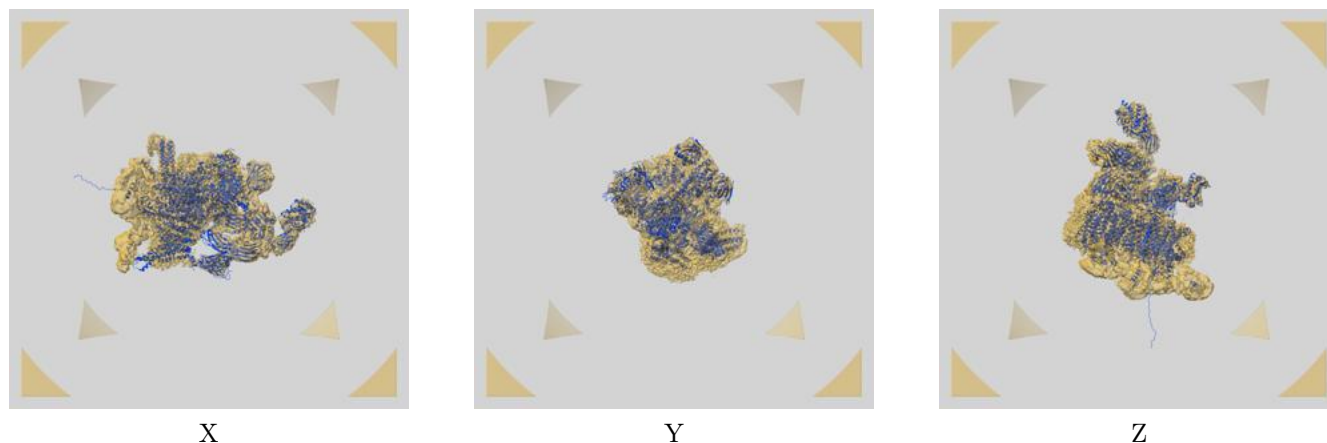
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.25 differs from the reported value 4.1 by more than 10 %



## 9 Map-model fit [i](#)

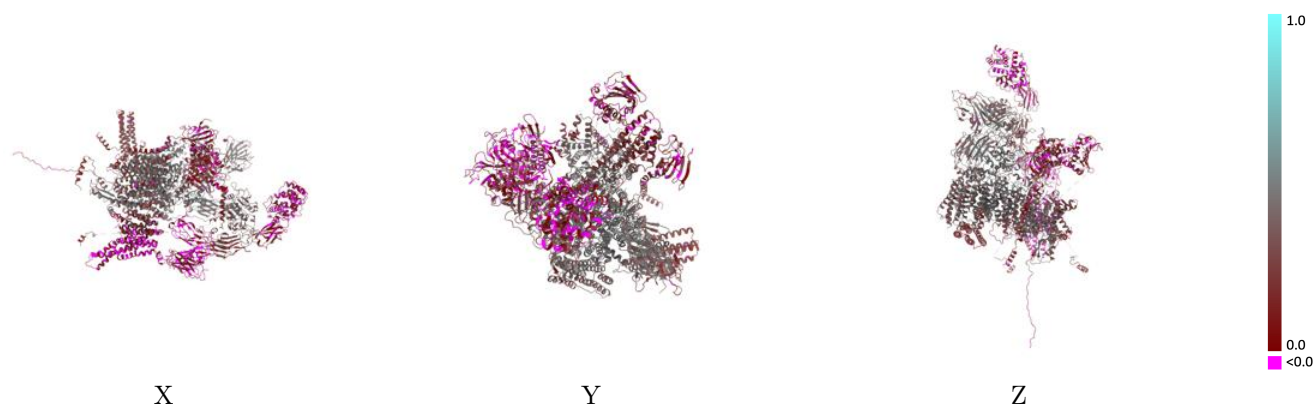
This section contains information regarding the fit between EMDB map EMD-72945 and PDB model 9YGY. Per-residue inclusion information can be found in [section 3](#) on [page 9](#).

### 9.1 Map-model overlay [i](#)



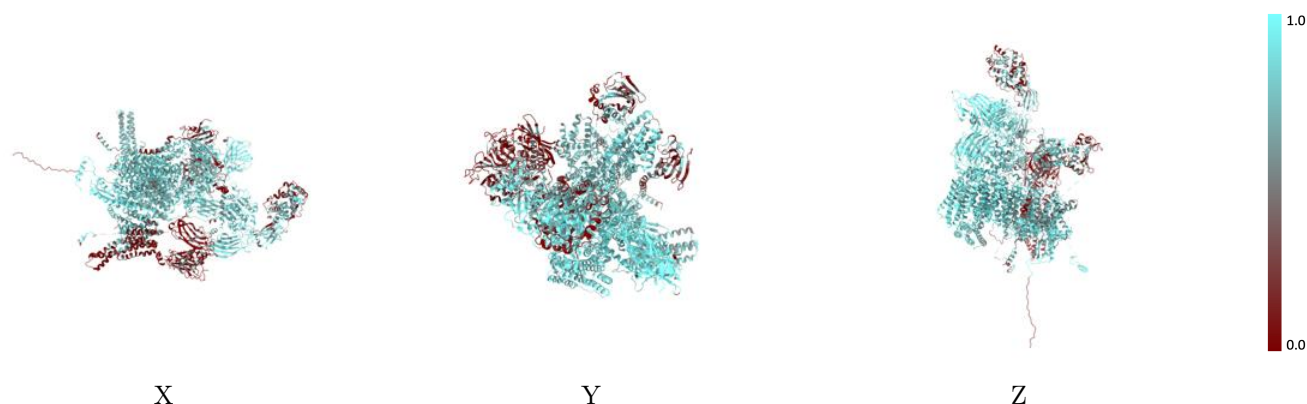
The images above show the 3D surface view of the map at the recommended contour level 0.00395 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



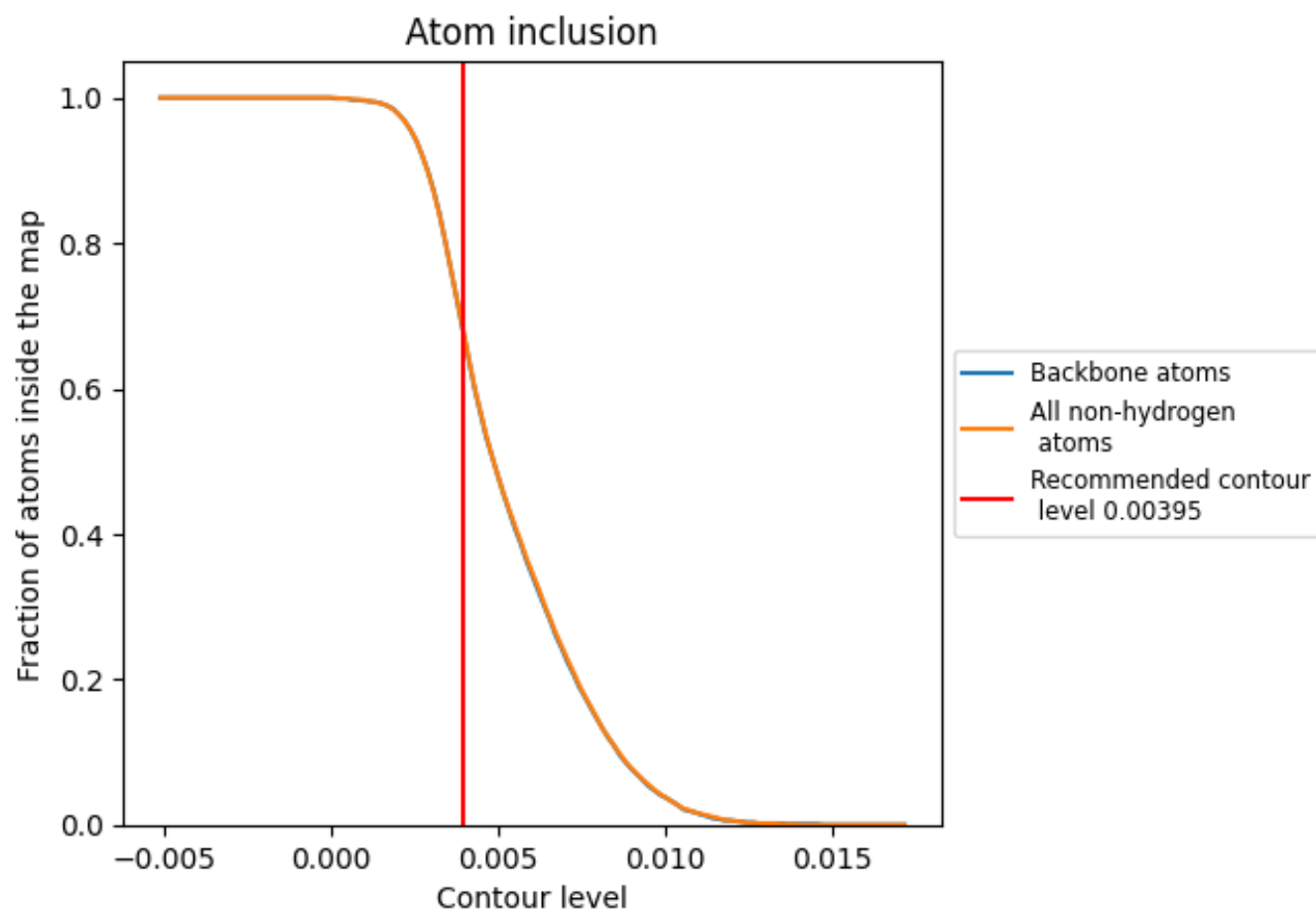
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00395).



















































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 68% of all backbone atoms, 68% 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 (0.00395) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6790	 0.2760
5	 0.1680	 0.0600
6	 0.1490	 0.0290
7	 0.2600	 0.0330
8	 0.1700	 0.0500
A	 0.3500	 0.1360
B	 0.7410	 0.2070
C	 0.8570	 0.4170
D	 0.8140	 0.3690
E	 0.7890	 0.3300
F	 0.8400	 0.3450
G	 0.7410	 0.2480
H	 0.7550	 0.4280
I	 0.8800	 0.4250
J	 0.8450	 0.3950
K	 0.8190	 0.4270
K2	 0.7880	 0.3900
L	 0.7500	 0.3960
L2	 0.8530	 0.3660
M2	 0.8510	 0.3650
N	 0.6160	 0.1900
N2	 0.8930	 0.3900
O2	 0.8540	 0.3450
P2	 0.6280	 0.1670
y3	 0.4820	 0.1830

