



## Full wwPDB EM Validation Report ⓘ

Oct 10, 2023 – 05:49 pm BST

PDB ID : 8AGC  
EMDB ID : EMD-15420  
Title : Structure of yeast oligosaccharyltransferase complex with lipid-linked oligosaccharide and non-acceptor peptide bound  
Authors : Ramirez, A.S.; de Capitani, M.; Pesciullesi, G.; Kowal, J.; Bloch, J.S.; Irobalieva, R.N.; Aebi, M.; Reymond, J.L.; Locher, K.P.  
Deposited on : 2022-07-19  
Resolution : 3.10 Å(reported)

This is a Full wwPDB EM Validation 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.dev50  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35.1

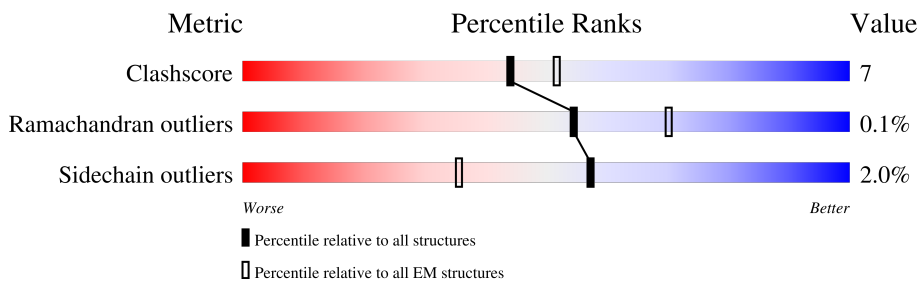
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.10 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.



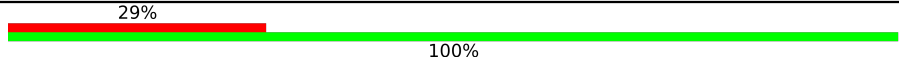

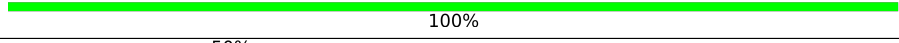

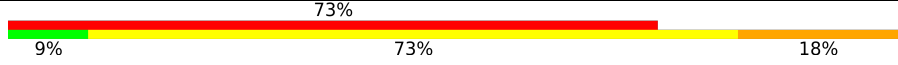
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	A	718	
2	B	65	
3	C	86	
4	D	130	
5	E	476	
6	F	283	
7	G	430	
8	H	350	

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Mol	Chain	Length	Quality of chain
9	P	7	 29% 100%
10	I	7	 14% 86%
11	J	2	 100%
11	K	2	 50% 100%
12	L	11	 9% 73% 18%

## 2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 17764 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 Dolichyl-diphosphooligosaccharide--protein glycotransferase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	697	5594	3709	890	969	26	0	0

- Molecule 2 is a protein called OST4 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	33	251	161	37	49	4	0	0

There are 29 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	37	ARG	-	expression tag	UNP A0A8H8UM72
B	38	THR	-	expression tag	UNP A0A8H8UM72
B	39	LEU	-	expression tag	UNP A0A8H8UM72
B	40	GLN	-	expression tag	UNP A0A8H8UM72
B	41	VAL	-	expression tag	UNP A0A8H8UM72
B	42	ASP	-	expression tag	UNP A0A8H8UM72
B	43	GLY	-	expression tag	UNP A0A8H8UM72
B	44	GLY	-	expression tag	UNP A0A8H8UM72
B	45	SER	-	expression tag	UNP A0A8H8UM72
B	46	GLY	-	expression tag	UNP A0A8H8UM72
B	47	GLY	-	expression tag	UNP A0A8H8UM72
B	48	SER	-	expression tag	UNP A0A8H8UM72
B	49	LEU	-	expression tag	UNP A0A8H8UM72
B	50	GLU	-	expression tag	UNP A0A8H8UM72
B	51	VAL	-	expression tag	UNP A0A8H8UM72
B	52	LEU	-	expression tag	UNP A0A8H8UM72
B	53	PHE	-	expression tag	UNP A0A8H8UM72
B	54	GLN	-	expression tag	UNP A0A8H8UM72
B	55	GLY	-	expression tag	UNP A0A8H8UM72
B	56	PRO	-	expression tag	UNP A0A8H8UM72
B	57	THR	-	expression tag	UNP A0A8H8UM72

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Chain	Residue	Modelled	Actual	Comment	Reference
B	58	GLU	-	expression tag	UNP A0A8H8UM72
B	59	THR	-	expression tag	UNP A0A8H8UM72
B	60	SER	-	expression tag	UNP A0A8H8UM72
B	61	GLN	-	expression tag	UNP A0A8H8UM72
B	62	VAL	-	expression tag	UNP A0A8H8UM72
B	63	ALA	-	expression tag	UNP A0A8H8UM72
B	64	PRO	-	expression tag	UNP A0A8H8UM72
B	65	ALA	-	expression tag	UNP A0A8H8UM72

- Molecule 3 is a protein called Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit OST5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	85	666	448	99	118	1	0	0

- Molecule 4 is a protein called Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit OST2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	109	883	595	141	141	6	0	0

- Molecule 5 is a protein called Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	438	3537	2294	565	671	7	0	0

- Molecule 6 is a protein called Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	258	1892	1242	313	334	3	0	0

- Molecule 7 is a protein called Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit WBP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	394	3201	2053	528	616	4	0	0

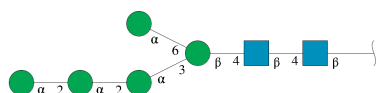
- Molecule 8 is a protein called OST3 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	131	1050	712	159	173	6	0	0

- Molecule 9 is a protein called PEPTIDE.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
9	P	7	43	26	8	9	0	1

- Molecule 10 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[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
			Total	C	N	O		
10	I	7	83	46	2	35	0	0

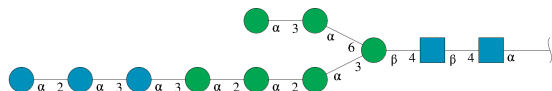
- Molecule 11 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
11	J	2	28	16	2	10	0	0
11	K	2	28	16	2	10	0	0

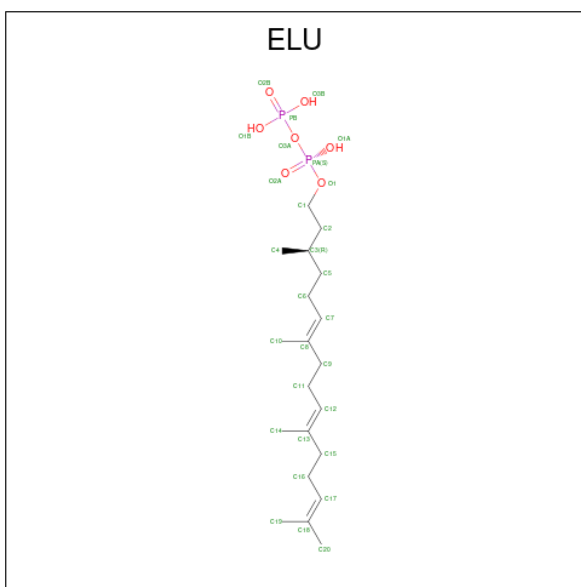
- Molecule 12 is an oligosaccharide called alpha-D-glucopyranose-(1-2)-alpha-D-glucopyranos

e-(1-3)-alpha-D-glucopyranose-(1-3)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose.



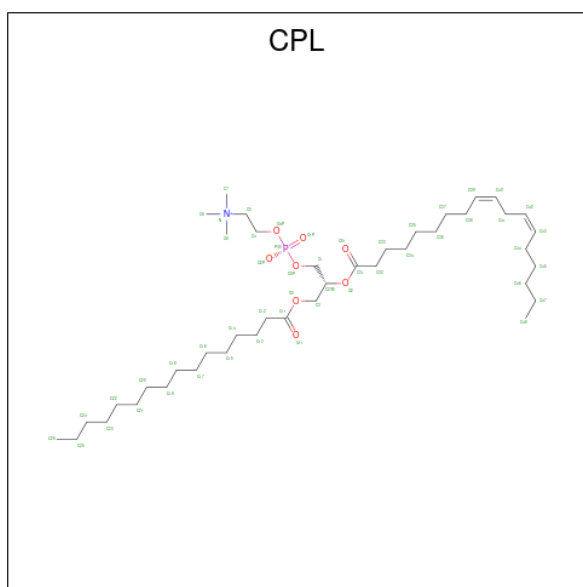
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
12	L	11	127	70	2	55	0	0

- Molecule 13 is phosphono [(3 {R},6 {E},10 {E})-3,7,11,15-tetramethylhexadeca-6,10,14-trienyl] hydrogen phosphate (three-letter code: 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).



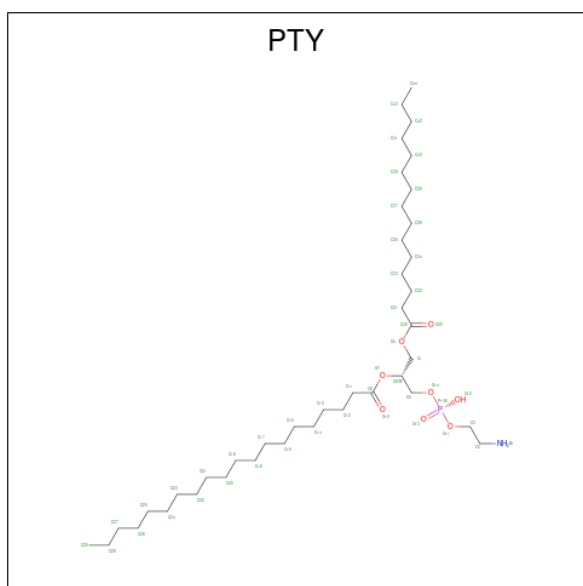
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
13	A	1	29	20	7	2	0

- Molecule 14 is 1-PALMITOYL-2-LINOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: CPL) (formula: C<sub>42</sub>H<sub>80</sub>NO<sub>8</sub>P).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
14	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
14	C	1	Total	C	N	O	P	0
			52	42	1	8	1	
14	E	1	Total	C	N	O	P	0
			52	42	1	8	1	
14	F	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 15 is PHOSPHATIDYLETHANOLAMINE (three-letter code: PTY) (formula: C<sub>40</sub>H<sub>80</sub>NO<sub>8</sub>P).



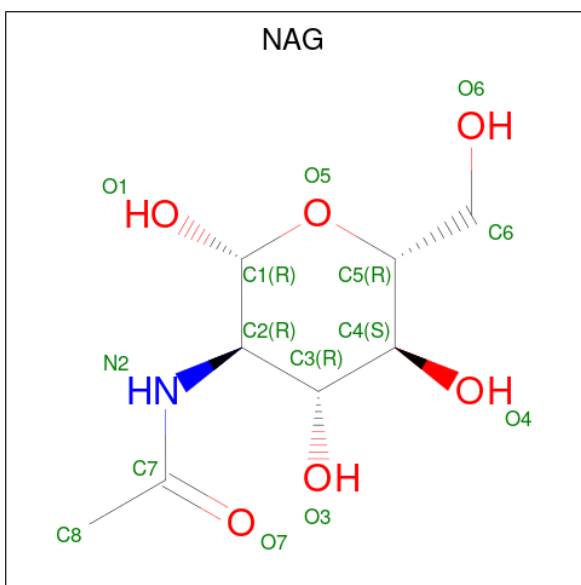


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
15	A	1	42	32	1	8	1	0
15	H	1	42	32	1	8	1	0

- Molecule 16 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

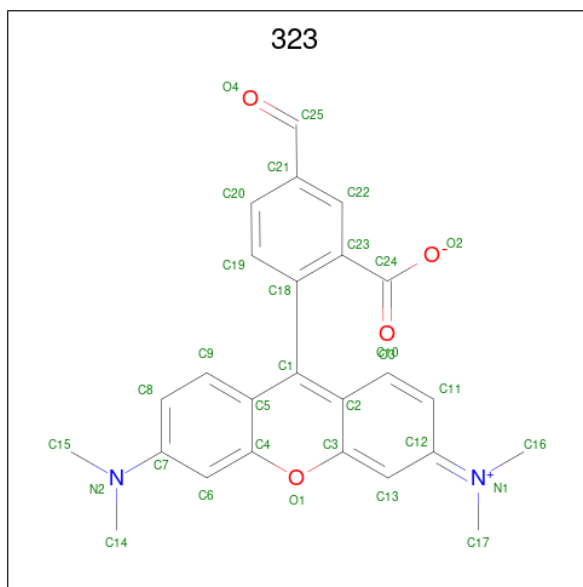
Mol	Chain	Residues	Atoms		AltConf
			Total	Mn	
16	A	1	1	1	0

- Molecule 17 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
17	G	1	14	8	1	5	0
17	G	1	14	8	1	5	0

- Molecule 18 is 2-[3,6-bis(dimethylamino)xanthen-9-yl]-5-methanoyl-benzoate (three-letter code: 323) (formula: C<sub>25</sub>H<sub>22</sub>N<sub>2</sub>O<sub>4</sub>).

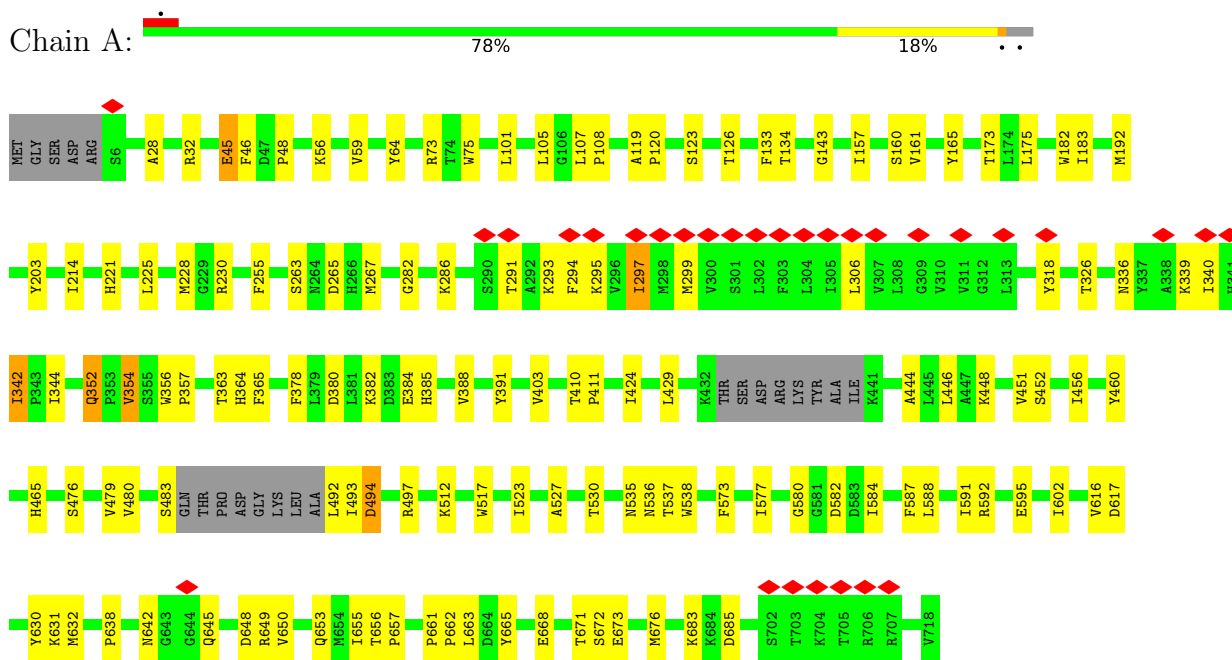


Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
18	P	1	31	25	2	4	0

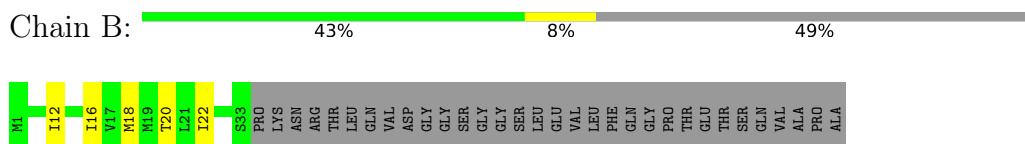
### 3 Residue-property plots [i](#)

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.

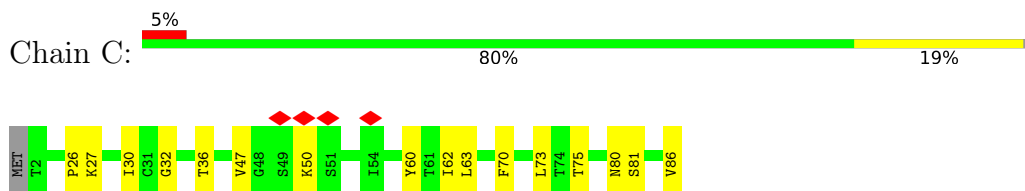
- Molecule 1: Dolichyl-diphosphooligosaccharide--protein glycotransferase



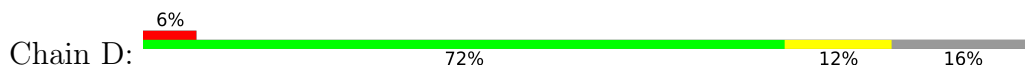
- Molecule 2: OST4 isoform 1



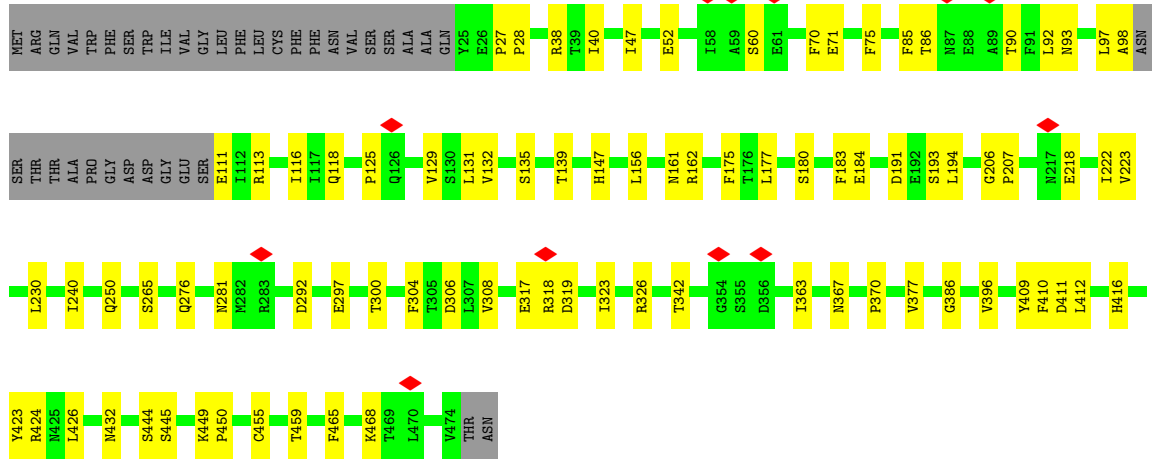
- Molecule 3: Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit OST5



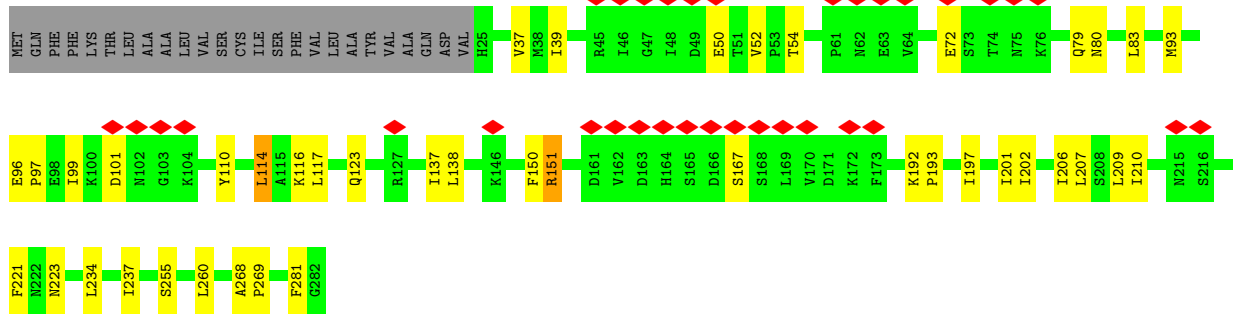
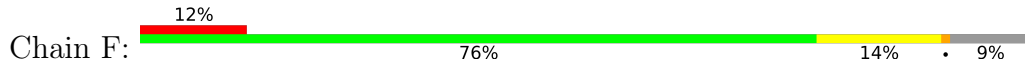
- Molecule 4: Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit OST2



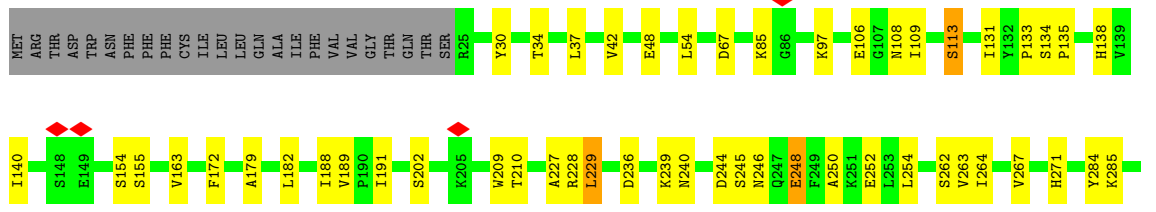
• Molecule 5: Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit 1

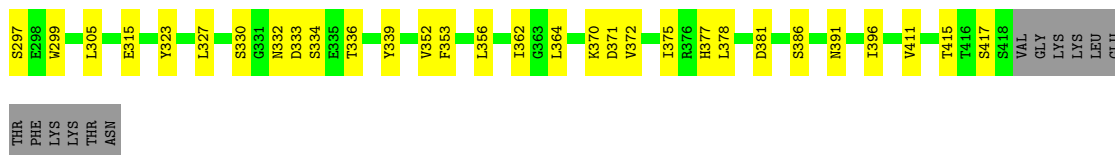


• Molecule 6: Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit 2

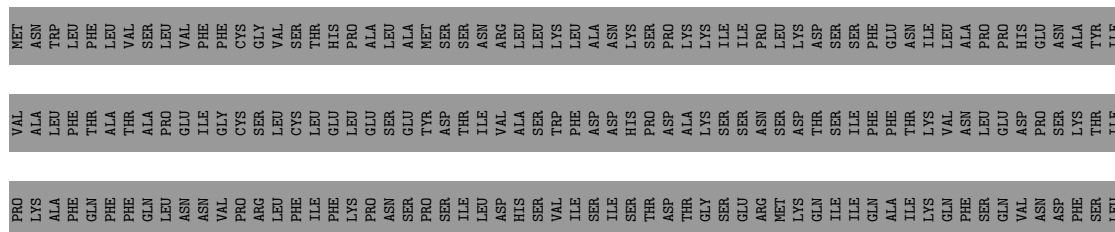


• Molecule 7: Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit WBP1





• Molecule 8: OST3 isoform 1



• Molecule 9: PEPTIDE



• Molecule 10: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[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



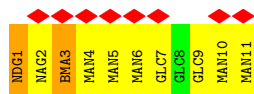
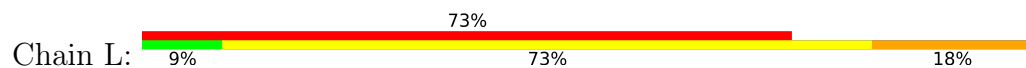
• Molecule 11: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



• Molecule 11: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 12: alpha-D-glucopyranose-(1-2)-alpha-D-glucopyranose-(1-3)-alpha-D-glucopyranose-(1-3)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	75382	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	64	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	2.198	Depositor
Minimum map value	-1.078	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.062	Depositor
Recommended contour level	0.386	Depositor
Map size ( $\text{\AA}$ )	326.40002, 326.40002, 326.40002	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.8500001, 0.8500001, 0.8500001	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: BMA, PTY, CPL, GLC, MN, ELU, DAB, 323, NAG, MAN, 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	A	0.45	0/5759	0.52	0/7837
2	B	0.38	0/253	0.43	0/342
3	C	0.38	0/684	0.45	0/926
4	D	0.40	0/905	0.48	0/1220
5	E	0.42	0/3639	0.51	0/4954
6	F	0.36	0/1934	0.51	0/2637
7	G	0.43	0/3283	0.49	0/4459
8	H	0.37	0/1080	0.46	0/1470
9	P	0.24	0/35	0.31	0/46
All	All	0.42	0/17572	0.50	0/23891

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5594	0	5565	86	0
2	B	251	0	260	4	0
3	C	666	0	677	12	0
4	D	883	0	911	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	3537	0	3412	50	0
6	F	1892	0	1831	28	0
7	G	3201	0	3102	50	0
8	H	1050	0	1085	13	0
9	P	43	0	37	0	0
10	I	83	0	70	0	0
11	J	28	0	25	0	0
11	K	28	0	25	0	0
12	L	127	0	105	2	0
13	A	29	0	0	0	0
14	A	52	0	80	2	0
14	C	52	0	80	1	0
14	E	52	0	80	1	0
14	F	52	0	80	3	0
15	A	42	0	60	1	0
15	H	42	0	60	0	0
16	A	1	0	0	0	0
17	G	28	0	26	1	0
18	P	31	0	21	1	0
All	All	17764	0	17592	245	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.

All (245) 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)
5:E:317:GLU:HG2	5:E:318:ARG:H	1.45	0.82
1:A:617:ASP:HB2	1:A:653:GLN:HE21	1.46	0.80
1:A:483:SER:HG	1:A:492:LEU:N	1.82	0.77
4:D:25:GLU:HA	4:D:28:LYS:HE3	1.66	0.77
7:G:140:ILE:HD11	7:G:179:ALA:HB2	1.67	0.77
1:A:632:MET:HG2	1:A:663:LEU:HD11	1.69	0.73
1:A:108:PRO:HD2	5:E:409:TYR:HA	1.69	0.73
1:A:32:ARG:NH1	1:A:160:SER:OG	2.24	0.70
6:F:50:GLU:HA	6:F:151:ARG:HE	1.55	0.70
7:G:333:ASP:OD1	7:G:334:SER:N	2.24	0.69
1:A:479:VAL:HG23	1:A:480:VAL:HG23	1.74	0.69
7:G:106:GLU:HA	7:G:227:ALA:HB2	1.75	0.68
6:F:223:ASN:HB2	7:G:417:SER:HB2	1.77	0.67
6:F:96:GLU:HG3	6:F:97:PRO:HD2	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:79:GLN:O	6:F:138:LEU:HA	1.95	0.66
8:H:248:VAL:HG13	8:H:252:GLY:HA2	1.78	0.65
6:F:54:THR:HA	6:F:72:GLU:HB3	1.78	0.65
15:A:1003:PTY:H201	14:F:301:CPL:H212	1.78	0.65
1:A:48:PRO:HB3	1:A:165:TYR:HB3	1.78	0.65
7:G:386:SER:HB3	7:G:396:ILE:HD11	1.77	0.64
4:D:35:PHE:HA	4:D:38:ILE:HG12	1.81	0.63
1:A:648:ASP:OD1	1:A:649:ARG:N	2.33	0.62
1:A:354:VAL:HG13	1:A:403:VAL:HG22	1.80	0.61
1:A:28:ALA:O	1:A:32:ARG:HG2	2.01	0.61
1:A:352:GLN:O	1:A:403:VAL:HG23	2.01	0.61
1:A:536:ASN:ND2	12:L:1:NDG:O3	2.33	0.60
5:E:85:PHE:CD2	5:E:92:LEU:HD11	2.36	0.60
1:A:538:TRP:HB2	12:L:3:BMA:H2	1.83	0.60
5:E:240:ILE:HD13	5:E:363:ILE:HG21	1.82	0.60
5:E:276:GLN:HA	5:E:281:ASN:ND2	2.17	0.60
3:C:75:THR:HG23	14:E:501:CPL:H192	1.83	0.60
1:A:192:MET:HB2	4:D:113:GLU:HG2	1.84	0.59
1:A:616:VAL:H	1:A:653:GLN:HE22	1.50	0.59
1:A:638:PRO:HG3	1:A:655:ILE:HG22	1.85	0.59
7:G:48:GLU:HG3	7:G:54:LEU:HD12	1.85	0.58
1:A:452:SER:O	1:A:456:ILE:HG13	2.04	0.58
5:E:97:LEU:HD22	5:E:116:ILE:HD11	1.86	0.58
7:G:332:ASN:ND2	17:G:501:NAG:H61	2.20	0.57
8:H:303:LYS:HG3	8:H:304:LYS:N	2.20	0.56
1:A:616:VAL:HG13	1:A:630:TYR:HE2	1.70	0.56
1:A:134:THR:HB	1:A:143:GLY:HA2	1.87	0.56
4:D:25:GLU:O	4:D:28:LYS:HG2	2.06	0.56
7:G:135:PRO:HG2	7:G:138:HIS:CD2	2.40	0.56
5:E:71:GLU:OE1	5:E:161:ASN:ND2	2.39	0.56
7:G:138:HIS:ND1	7:G:202:SER:HB3	2.20	0.56
5:E:250:GLN:HG2	5:E:342:THR:HG23	1.87	0.55
7:G:113:SER:O	7:G:113:SER:OG	2.24	0.55
6:F:97:PRO:HB3	6:F:110:TYR:CZ	2.42	0.55
7:G:209:TRP:HD1	7:G:210:THR:HG23	1.72	0.55
1:A:182:TRP:HE1	1:A:221:HIS:HD2	1.53	0.55
4:D:73:PRO:HB2	4:D:76:ALA:HB3	1.89	0.55
5:E:184:GLU:O	5:E:222:ILE:HG13	2.07	0.55
7:G:356:LEU:HD13	7:G:370:LYS:HG2	1.88	0.55
7:G:297:SER:HB2	7:G:336:THR:HG22	1.89	0.54
3:C:36:THR:HG22	3:C:70:PHE:HB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:411:ASP:OD2	5:E:416:HIS:HD2	1.91	0.54
1:A:588:LEU:O	1:A:592:ARG:HG3	2.07	0.53
7:G:271:HIS:HE1	7:G:371:ASP:OD2	1.91	0.53
5:E:377:VAL:HG21	5:E:426:LEU:HD12	1.89	0.53
2:B:16:ILE:O	2:B:20:THR:HG23	2.09	0.53
1:A:356:TRP:CD1	1:A:357:PRO:HD3	2.44	0.53
6:F:268:ALA:HB3	6:F:269:PRO:HD3	1.91	0.52
1:A:356:TRP:CG	1:A:357:PRO:HD3	2.44	0.52
1:A:685:ASP:OD1	1:A:685:ASP:N	2.38	0.52
7:G:250:ALA:O	7:G:254:LEU:HG	2.09	0.52
5:E:52:GLU:HG2	5:E:132:VAL:HG22	1.92	0.52
7:G:163:VAL:HG11	7:G:191:ILE:HD13	1.92	0.52
6:F:101:ASP:OD1	6:F:101:ASP:N	2.34	0.51
7:G:138:HIS:CE1	7:G:202:SER:HB3	2.45	0.51
1:A:580:GLY:HA2	1:A:650:VAL:HG11	1.93	0.51
1:A:133:PHE:HE1	1:A:183:ILE:HG13	1.74	0.51
5:E:111:GLU:N	5:E:111:GLU:OE2	2.44	0.51
6:F:197:ILE:O	6:F:201:ILE:HG12	2.11	0.51
1:A:160:SER:OG	1:A:160:SER:O	2.28	0.51
7:G:189:VAL:HG22	7:G:362:ILE:HG23	1.93	0.51
7:G:262:SER:HB3	7:G:364:LEU:HD23	1.93	0.50
1:A:668:GLU:OE2	1:A:671:THR:OG1	2.30	0.50
1:A:56:LYS:HA	1:A:59:VAL:HG12	1.93	0.50
1:A:282:GLY:O	1:A:286:LYS:N	2.44	0.50
5:E:85:PHE:HE1	5:E:129:VAL:HG13	1.77	0.50
7:G:236:ASP:HA	7:G:239:LYS:HG3	1.93	0.50
5:E:40:ILE:HB	5:E:177:LEU:HD23	1.93	0.49
7:G:353:PHE:CD1	7:G:375:ILE:HD12	2.47	0.49
3:C:32:GLY:O	3:C:36:THR:HG23	2.12	0.49
1:A:616:VAL:HG12	1:A:616:VAL:O	2.13	0.49
7:G:42:VAL:HG12	7:G:240:ASN:OD1	2.13	0.49
3:C:86:VAL:HG11	5:E:410:PHE:HD2	1.78	0.48
5:E:156:LEU:HD21	5:E:230:LEU:HD11	1.94	0.48
4:D:72:PHE:HB3	4:D:73:PRO:HD3	1.95	0.48
1:A:497:ARG:HD2	5:E:308:VAL:HG12	1.95	0.48
14:A:1002:CPL:H263	14:A:1002:CPL:H232	1.72	0.48
2:B:12:ILE:O	2:B:16:ILE:HG12	2.14	0.48
6:F:83:LEU:HA	6:F:93:MET:O	2.13	0.48
7:G:131:ILE:O	7:G:133:PRO:HD3	2.13	0.48
1:A:535:ASN:O	1:A:537:THR:HG23	2.14	0.48
7:G:109:ILE:HB	7:G:229:LEU:HD12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:377:HIS:CD2	7:G:378:LEU:H	2.32	0.48
1:A:294:PHE:HA	1:A:297:ILE:HB	1.96	0.48
1:A:460:TYR:OH	2:B:20:THR:HG22	2.14	0.48
6:F:137:ILE:HG12	6:F:150:PHE:HD1	1.79	0.48
7:G:352:VAL:HG12	7:G:372:VAL:HG12	1.95	0.48
7:G:182:LEU:HG	7:G:188:ILE:HG21	1.95	0.47
7:G:263:VAL:HG22	7:G:299:TRP:HB3	1.95	0.47
1:A:265:ASP:OD1	1:A:265:ASP:N	2.47	0.47
7:G:154:SER:OG	7:G:155:SER:N	2.47	0.47
1:A:631:LYS:HE3	1:A:661:PRO:HG2	1.96	0.47
5:E:317:GLU:CG	5:E:318:ARG:H	2.22	0.47
1:A:476:SER:HB3	18:P:101:323:H317	1.96	0.47
1:A:616:VAL:H	1:A:653:GLN:NE2	2.11	0.47
1:A:120:PRO:O	1:A:123:SER:OG	2.32	0.47
1:A:517:TRP:HE3	1:A:535:ASN:HA	1.79	0.47
1:A:107:LEU:HD12	1:A:107:LEU:O	2.15	0.47
1:A:573:PHE:O	1:A:676:MET:HA	2.14	0.47
1:A:595:GLU:HG3	1:A:602:ILE:O	2.15	0.47
1:A:672:SER:OG	1:A:673:GLU:N	2.48	0.47
1:A:126:THR:OG1	1:A:173:THR:OG1	2.28	0.47
14:A:1002:CPL:H39	14:A:1002:CPL:H362	1.60	0.47
3:C:50:LYS:HG3	3:C:50:LYS:O	2.14	0.47
1:A:45:GLU:HG2	1:A:46:PHE:H	1.80	0.47
5:E:306:ASP:OD2	5:E:326:ARG:NH2	2.48	0.47
7:G:172:PHE:HA	7:G:246:ASN:HD21	1.79	0.46
3:C:60:TYR:CE2	5:E:465:PHE:HB2	2.50	0.46
1:A:665:TYR:O	1:A:683:LYS:HG2	2.15	0.46
1:A:73:ARG:HA	1:A:530:THR:HG23	1.96	0.46
7:G:315:GLU:HA	7:G:323:TYR:O	2.15	0.46
6:F:123:GLN:HE22	6:F:167:SER:CB	2.28	0.46
4:D:53:PHE:CD1	6:F:209:LEU:HD13	2.51	0.46
1:A:512:LYS:HG3	1:A:530:THR:HB	1.98	0.45
1:A:429:LEU:HD23	1:A:429:LEU:HA	1.74	0.45
5:E:47:ILE:HG12	5:E:139:THR:O	2.16	0.45
5:E:304:PHE:CE2	5:E:323:ILE:HG23	2.51	0.45
1:A:263:SER:O	1:A:267:MET:HG2	2.17	0.45
1:A:352:GLN:HG2	8:H:241:ARG:HH22	1.81	0.45
1:A:382:LYS:HB2	1:A:385:HIS:CD2	2.50	0.45
7:G:330:SER:O	7:G:330:SER:OG	2.24	0.45
1:A:451:VAL:HG22	8:H:317:ALA:HB2	1.98	0.45
1:A:493:ILE:HD13	1:A:577:ILE:HD13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:523:ILE:HG23	1:A:527:ALA:HB3	1.98	0.45
1:A:133:PHE:CE1	1:A:183:ILE:HG13	2.51	0.45
1:A:444:ALA:O	1:A:448:LYS:HG3	2.16	0.45
5:E:367:ASN:HD22	5:E:367:ASN:HA	1.66	0.45
1:A:645:GLN:O	1:A:645:GLN:NE2	2.50	0.45
6:F:83:LEU:HD11	6:F:137:ILE:HD11	1.99	0.45
7:G:271:HIS:HD2	7:G:284:TYR:OH	2.00	0.45
1:A:380:ASP:O	1:A:385:HIS:HD2	2.00	0.45
1:A:384:GLU:O	1:A:388:VAL:HG23	2.17	0.45
6:F:207:LEU:HD23	6:F:207:LEU:HA	1.77	0.45
5:E:70:PHE:HD2	5:E:75:PHE:HD1	1.65	0.44
1:A:291:THR:HG23	1:A:293:LYS:H	1.82	0.44
14:F:301:CPL:HC82	14:F:301:CPL:HC42	1.71	0.44
8:H:339:PRO:O	8:H:341:PRO:HD3	2.17	0.44
8:H:339:PRO:HG2	8:H:340:PHE:CE2	2.53	0.44
8:H:301:GLU:O	8:H:302:THR:OG1	2.28	0.44
3:C:27:LYS:O	3:C:30:ILE:HG12	2.18	0.44
4:D:105:ILE:HG23	4:D:109:ARG:HG2	1.99	0.44
6:F:116:LYS:HB3	6:F:116:LYS:HE2	1.74	0.43
3:C:47:VAL:HG12	3:C:47:VAL:O	2.19	0.43
5:E:147:HIS:HB3	5:E:265:SER:HB3	2.00	0.43
6:F:202:ILE:O	6:F:206:ILE:HG12	2.18	0.43
7:G:30:TYR:CE1	7:G:37:LEU:HD22	2.52	0.43
1:A:364:HIS:HB3	1:A:465:HIS:CD2	2.53	0.43
5:E:85:PHE:CE1	5:E:129:VAL:HG13	2.53	0.43
5:E:183:PHE:HB3	5:E:222:ILE:HD11	2.01	0.43
1:A:342:ILE:H	1:A:342:ILE:HG12	1.44	0.43
5:E:449:LYS:HB3	5:E:450:PRO:HD3	2.00	0.43
1:A:75:TRP:HZ2	1:A:536:ASN:O	2.02	0.43
1:A:410:THR:OG1	1:A:411:PRO:HD3	2.19	0.43
5:E:38:ARG:HD3	5:E:175:PHE:HD2	1.83	0.43
6:F:192:LYS:N	6:F:193:PRO:HD2	2.33	0.43
4:D:65:ILE:HD11	4:D:71:ASN:HB3	1.99	0.43
8:H:213:ILE:HG22	8:H:214:ILE:H	1.84	0.43
1:A:336:ASN:O	1:A:340:ILE:HG13	2.19	0.43
14:C:101:CPL:H182	14:C:101:CPL:H151	1.70	0.43
8:H:236:MET:O	8:H:240:ILE:HG22	2.19	0.43
1:A:424:ILE:HD11	8:H:284:VAL:HG13	2.00	0.43
5:E:191:ASP:OD1	5:E:193:SER:N	2.51	0.43
5:E:206:GLY:HA2	5:E:207:PRO:HD3	1.82	0.43
7:G:67:ASP:OD1	7:G:67:ASP:N	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:HIS:O	1:A:365:PHE:HB3	2.18	0.43
1:A:295:LYS:NZ	1:A:299:MET:SD	2.90	0.42
4:D:120:ILE:HG12	14:F:301:CPL:H441	2.01	0.42
7:G:48:GLU:HG3	7:G:54:LEU:CD1	2.50	0.42
5:E:27:PRO:HA	5:E:28:PRO:HD3	1.91	0.42
5:E:468:LYS:HD3	5:E:468:LYS:HA	1.89	0.42
1:A:582:ASP:OD1	1:A:582:ASP:N	2.52	0.42
6:F:52:VAL:HG23	6:F:52:VAL:O	2.20	0.42
1:A:175:LEU:HD12	1:A:214:ILE:HD11	2.01	0.42
5:E:86:THR:HG22	5:E:132:VAL:HG23	2.00	0.42
7:G:327:LEU:HB3	7:G:339:TYR:HB3	2.02	0.42
6:F:223:ASN:OD1	6:F:281:PHE:HE1	2.03	0.42
5:E:317:GLU:HG2	5:E:318:ARG:N	2.23	0.42
5:E:396:VAL:HG23	5:E:423:TYR:CE1	2.54	0.42
7:G:244:ASP:OD1	7:G:245:SER:N	2.53	0.42
5:E:162:ARG:HH11	5:E:218:GLU:HG3	1.84	0.42
5:E:455:CYS:O	5:E:459:THR:HG23	2.19	0.42
6:F:234:LEU:HD23	6:F:234:LEU:HA	1.83	0.42
1:A:446:LEU:HD12	1:A:446:LEU:HA	1.90	0.42
1:A:157:ILE:O	1:A:161:VAL:HG23	2.20	0.42
5:E:60:SER:O	5:E:125:PRO:HB3	2.20	0.42
7:G:248:GLU:O	7:G:252:GLU:HG2	2.20	0.42
8:H:329:THR:O	8:H:333:ILE:HG13	2.20	0.42
1:A:119:ALA:HB3	1:A:120:PRO:HD3	2.01	0.41
3:C:62:ILE:HG13	3:C:63:LEU:N	2.34	0.41
4:D:28:LYS:O	4:D:32:ARG:HG3	2.20	0.41
5:E:386:GLY:HA3	5:E:445:SER:HB3	2.02	0.41
1:A:101:LEU:HD23	1:A:105:LEU:HD12	2.01	0.41
1:A:225:LEU:HD23	1:A:225:LEU:HA	1.84	0.41
3:C:80:ASN:HD21	3:C:86:VAL:H	1.68	0.41
5:E:98:ALA:HA	5:E:113:ARG:NH1	2.35	0.41
6:F:116:LYS:O	6:F:117:LEU:HD23	2.20	0.41
8:H:227:PHE:O	8:H:231:MET:HG2	2.20	0.41
6:F:221:PHE:HA	7:G:415:THR:HG22	2.03	0.41
1:A:64:TYR:OH	7:G:381:ASP:OD1	2.23	0.41
5:E:93:ASN:HD22	5:E:118:GLN:HG3	1.86	0.41
5:E:98:ALA:HA	5:E:113:ARG:HH11	1.84	0.41
7:G:108:ASN:HD22	7:G:228:ARG:H	1.67	0.41
6:F:114:LEU:HD13	6:F:114:LEU:HA	1.82	0.41
1:A:661:PRO:HA	1:A:662:PRO:HD3	1.94	0.41
5:E:297:GLU:HG2	5:E:319:ASP:OD2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:305:LEU:HD23	7:G:305:LEU:HA	1.86	0.41
5:E:156:LEU:O	5:E:223:VAL:HA	2.21	0.41
1:A:642:ASN:HD22	1:A:642:ASN:HA	1.63	0.41
2:B:18:MET:O	2:B:22:ILE:HG13	2.21	0.41
3:C:73:LEU:HD12	3:C:73:LEU:HA	1.79	0.41
7:G:264:ILE:HD11	7:G:364:LEU:HD22	2.03	0.41
8:H:328:THR:O	8:H:332:THR:HG23	2.21	0.41
1:A:228:MET:HE2	1:A:230:ARG:HE	1.85	0.41
6:F:99:ILE:O	6:F:99:ILE:HG13	2.20	0.41
1:A:591:ILE:HG23	1:A:602:ILE:HG22	2.04	0.40
5:E:180:SER:HB3	5:E:183:PHE:CZ	2.56	0.40
5:E:292:ASP:O	5:E:370:PRO:HD3	2.21	0.40
6:F:80:ASN:O	6:F:80:ASN:OD1	2.39	0.40
6:F:260:LEU:HD12	6:F:260:LEU:HA	1.87	0.40
5:E:162:ARG:HD3	5:E:194:LEU:HD22	2.03	0.40
1:A:480:VAL:HG22	1:A:494:ASP:OD1	2.21	0.40
1:A:517:TRP:CE3	1:A:535:ASN:HA	2.56	0.40
6:F:237:ILE:HD12	7:G:411:VAL:HG22	2.03	0.40
3:C:26:PRO:HG3	3:C:81:SER:HB2	2.04	0.40
4:D:73:PRO:HG2	7:G:391:ASN:HB2	2.03	0.40
7:G:34:THR:HG21	7:G:85:LYS:H	1.85	0.40
1:A:656:THR:HB	1:A:657:PRO:HD2	2.03	0.40
5:E:177:LEU:HD13	5:E:222:ILE:HD13	2.03	0.40
7:G:97:LYS:H	7:G:97:LYS:HG2	1.55	0.40
7:G:263:VAL:HG22	7:G:299:TRP:CB	2.51	0.40
7:G:285:LYS:HB3	7:G:285:LYS:HE2	1.68	0.40

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	691/718 (96%)	661 (96%)	29 (4%)	1 (0%)	51	83
2	B	31/65 (48%)	31 (100%)	0	0	100	100
3	C	83/86 (96%)	81 (98%)	2 (2%)	0	100	100
4	D	107/130 (82%)	105 (98%)	2 (2%)	0	100	100
5	E	434/476 (91%)	415 (96%)	19 (4%)	0	100	100
6	F	256/283 (90%)	229 (90%)	25 (10%)	2 (1%)	19	54
7	G	392/430 (91%)	373 (95%)	19 (5%)	0	100	100
8	H	129/350 (37%)	123 (95%)	6 (5%)	0	100	100
9	P	4/7 (57%)	4 (100%)	0	0	100	100
All	All	2127/2545 (84%)	2022 (95%)	102 (5%)	3 (0%)	54	83

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	39	ILE
1	A	45	GLU
6	F	37	VAL

### 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	590/613 (96%)	573 (97%)	17 (3%)	42	72
2	B	30/55 (54%)	30 (100%)	0	100	100
3	C	74/75 (99%)	74 (100%)	0	100	100
4	D	96/115 (84%)	95 (99%)	1 (1%)	76	90
5	E	394/426 (92%)	386 (98%)	8 (2%)	55	80
6	F	181/246 (74%)	177 (98%)	4 (2%)	52	78
7	G	359/392 (92%)	354 (99%)	5 (1%)	67	86
8	H	113/316 (36%)	111 (98%)	2 (2%)	59	82
9	P	3/3 (100%)	3 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1840/2241 (82%)	1803 (98%)	37 (2%)	57 80

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	203	TYR
1	A	255	PHE
1	A	297	ILE
1	A	306	LEU
1	A	318	TYR
1	A	326	THR
1	A	339	LYS
1	A	342	ILE
1	A	344	ILE
1	A	352	GLN
1	A	354	VAL
1	A	363	THR
1	A	378	PHE
1	A	391	TYR
1	A	494	ASP
1	A	584	ILE
1	A	587	PHE
4	D	50	PHE
5	E	90	THR
5	E	131	LEU
5	E	135	SER
5	E	300	THR
5	E	412	LEU
5	E	424	ARG
5	E	432	ASN
5	E	444	SER
6	F	114	LEU
6	F	151	ARG
6	F	210	ILE
6	F	255	SER
7	G	113	SER
7	G	134	SER
7	G	229	LEU
7	G	248	GLU
7	G	267	VAL
8	H	240	ILE
8	H	248	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	HIS
1	A	60	ASN
1	A	216	ASN
1	A	221	HIS
1	A	351	HIS
1	A	352	GLN
1	A	364	HIS
1	A	385	HIS
1	A	536	ASN
1	A	564	HIS
1	A	642	ASN
1	A	645	GLN
1	A	652	GLN
1	A	653	GLN
1	A	674	ASN
2	B	26	HIS
3	C	80	ASN
4	D	108	ASN
5	E	93	ASN
5	E	121	ASN
5	E	201	ASN
5	E	232	GLN
5	E	235	ASN
5	E	281	ASN
5	E	315	HIS
5	E	343	ASN
5	E	367	ASN
5	E	416	HIS
6	F	66	GLN
6	F	79	GLN
6	F	80	ASN
6	F	123	GLN
7	G	32	GLN
7	G	108	ASN
7	G	138	HIS
7	G	156	ASN
7	G	214	GLN
7	G	222	GLN
7	G	225	ASN
7	G	226	ASN
7	G	242	ASN

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Mol	Chain	Res	Type
7	G	246	ASN
7	G	247	GLN
7	G	271	HIS
7	G	318	GLN
7	G	337	GLN
8	H	238	ASN
8	H	239	GLN
8	H	244	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](#)

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	$\# Z  > 2$
9	DAB	P	4	9	5,6,7	0.86	0	1,6,8	0.40	0

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
9	DAB	P	4	9	-	1/4/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	P	4	DAB	N-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

22 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	$\# Z  > 2$
10	NAG	I	1	1,10	14,14,15	0.89	1 (7%)	17,19,21	0.62	0
10	NAG	I	2	10	14,14,15	0.30	0	17,19,21	0.61	0
10	BMA	I	3	10	11,11,12	0.66	0	15,15,17	0.87	1 (6%)
10	MAN	I	4	10	11,11,12	0.86	0	15,15,17	1.21	2 (13%)
10	MAN	I	5	10	11,11,12	0.93	1 (9%)	15,15,17	1.07	1 (6%)
10	MAN	I	6	10	11,11,12	0.54	0	15,15,17	0.95	1 (6%)
10	MAN	I	7	10	11,11,12	0.57	0	15,15,17	0.97	2 (13%)
11	NAG	J	1	5,11	14,14,15	0.55	0	17,19,21	0.70	0
11	NAG	J	2	11	14,14,15	0.24	0	17,19,21	0.64	0
11	NAG	K	1	5,11	14,14,15	0.43	0	17,19,21	0.92	2 (11%)
11	NAG	K	2	11	14,14,15	0.59	1 (7%)	17,19,21	0.54	0
12	NDG	L	1	12,13	14,14,15	0.30	0	17,19,21	0.83	1 (5%)
12	MAN	L	10	12	11,11,12	0.64	0	15,15,17	0.95	1 (6%)
12	MAN	L	11	12	11,11,12	0.61	0	15,15,17	0.90	1 (6%)
12	NAG	L	2	12	14,14,15	0.26	0	17,19,21	1.16	1 (5%)
12	BMA	L	3	12	11,11,12	0.79	0	15,15,17	0.79	1 (6%)
12	MAN	L	4	12	11,11,12	0.77	0	15,15,17	2.51	4 (26%)
12	MAN	L	5	12	11,11,12	0.76	0	15,15,17	1.45	3 (20%)
12	MAN	L	6	12	11,11,12	0.61	0	15,15,17	0.94	1 (6%)
12	GLC	L	7	12	11,11,12	0.56	0	15,15,17	0.95	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
12	GLC	L	8	12	11,11,12	0.63	0	15,15,17	0.87	0
12	GLC	L	9	12	11,11,12	0.62	0	15,15,17	0.98	1 (6%)

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
10	NAG	I	1	1,10	-	4/6/23/26	0/1/1/1
10	NAG	I	2	10	-	2/6/23/26	0/1/1/1
10	BMA	I	3	10	-	0/2/19/22	0/1/1/1
10	MAN	I	4	10	-	0/2/19/22	0/1/1/1
10	MAN	I	5	10	-	0/2/19/22	0/1/1/1
10	MAN	I	6	10	-	0/2/19/22	0/1/1/1
10	MAN	I	7	10	-	0/2/19/22	0/1/1/1
11	NAG	J	1	5,11	-	0/6/23/26	0/1/1/1
11	NAG	J	2	11	-	2/6/23/26	0/1/1/1
11	NAG	K	1	5,11	-	4/6/23/26	0/1/1/1
11	NAG	K	2	11	-	3/6/23/26	0/1/1/1
12	NDG	L	1	12,13	-	2/6/23/26	0/1/1/1
12	MAN	L	10	12	-	0/2/19/22	0/1/1/1
12	MAN	L	11	12	-	2/2/19/22	0/1/1/1
12	NAG	L	2	12	-	0/6/23/26	0/1/1/1
12	BMA	L	3	12	-	0/2/19/22	0/1/1/1
12	MAN	L	4	12	-	1/2/19/22	0/1/1/1
12	MAN	L	5	12	-	0/2/19/22	0/1/1/1
12	MAN	L	6	12	-	2/2/19/22	0/1/1/1
12	GLC	L	7	12	-	2/2/19/22	0/1/1/1
12	GLC	L	8	12	-	0/2/19/22	0/1/1/1
12	GLC	L	9	12	-	1/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	I	1	NAG	O5-C1	-3.26	1.38	1.43
10	I	5	MAN	O5-C1	-2.43	1.39	1.43
11	K	2	NAG	C1-C2	2.05	1.55	1.52

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	L	4	MAN	O2-C2-C3	-6.22	97.68	110.14
12	L	4	MAN	C1-O5-C5	5.39	119.50	112.19
12	L	2	NAG	C1-O5-C5	4.42	118.19	112.19
10	I	4	MAN	O2-C2-C3	-3.45	103.22	110.14
12	L	4	MAN	C1-C2-C3	3.36	113.79	109.67
12	L	5	MAN	C1-O5-C5	3.07	116.36	112.19
10	I	5	MAN	O2-C2-C3	-3.04	104.04	110.14
12	L	5	MAN	O2-C2-C3	-3.03	104.06	110.14
12	L	5	MAN	O5-C1-C2	2.70	114.94	110.77
12	L	4	MAN	C3-C4-C5	2.69	115.05	110.24
12	L	9	GLC	C1-O5-C5	2.62	115.74	112.19
10	I	6	MAN	O2-C2-C3	-2.48	105.16	110.14
11	K	1	NAG	C3-C4-C5	2.48	114.67	110.24
12	L	10	MAN	O2-C2-C3	-2.37	105.39	110.14
12	L	7	GLC	C1-O5-C5	2.33	115.36	112.19
12	L	11	MAN	O2-C2-C3	-2.31	105.52	110.14
10	I	7	MAN	O2-C2-C3	-2.27	105.58	110.14
10	I	7	MAN	C1-O5-C5	2.24	115.23	112.19
10	I	4	MAN	C1-O5-C5	2.22	115.19	112.19
12	L	6	MAN	O2-C2-C3	-2.12	105.90	110.14
11	K	1	NAG	C1-O5-C5	2.12	115.06	112.19
12	L	3	BMA	O2-C2-C3	-2.11	105.91	110.14
10	I	3	BMA	O2-C2-C3	-2.09	105.95	110.14
12	L	1	NDG	C4-C3-C2	-2.06	108.00	111.02

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	I	2	NAG	O5-C5-C6-O6
12	L	1	NDG	O5-C5-C6-O6
11	K	1	NAG	O5-C5-C6-O6
11	K	2	NAG	O5-C5-C6-O6
10	I	1	NAG	O5-C5-C6-O6
12	L	6	MAN	O5-C5-C6-O6
10	I	1	NAG	C4-C5-C6-O6
10	I	1	NAG	C8-C7-N2-C2
10	I	1	NAG	O7-C7-N2-C2
11	K	1	NAG	C8-C7-N2-C2
11	K	1	NAG	O7-C7-N2-C2
10	I	2	NAG	C4-C5-C6-O6
12	L	1	NDG	C4-C5-C6-O6
12	L	6	MAN	C4-C5-C6-O6

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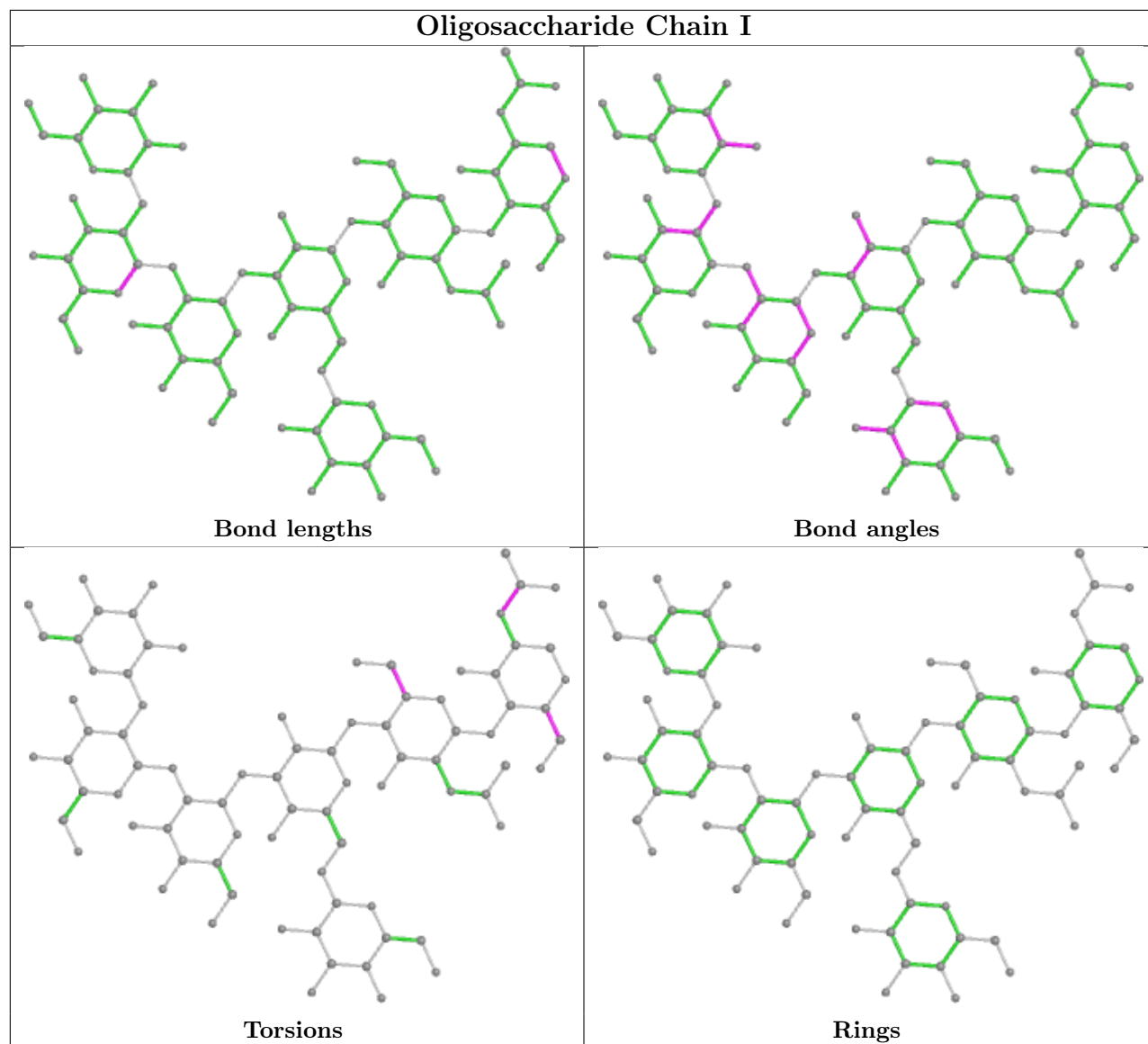
Mol	Chain	Res	Type	Atoms
11	J	2	NAG	O5-C5-C6-O6
11	J	2	NAG	C4-C5-C6-O6
11	K	2	NAG	C4-C5-C6-O6
12	L	4	MAN	O5-C5-C6-O6
12	L	7	GLC	C4-C5-C6-O6
11	K	1	NAG	C4-C5-C6-O6
12	L	11	MAN	C4-C5-C6-O6
12	L	11	MAN	O5-C5-C6-O6
12	L	7	GLC	O5-C5-C6-O6
11	K	2	NAG	C3-C2-N2-C7
12	L	9	GLC	O5-C5-C6-O6

There are no ring outliers.

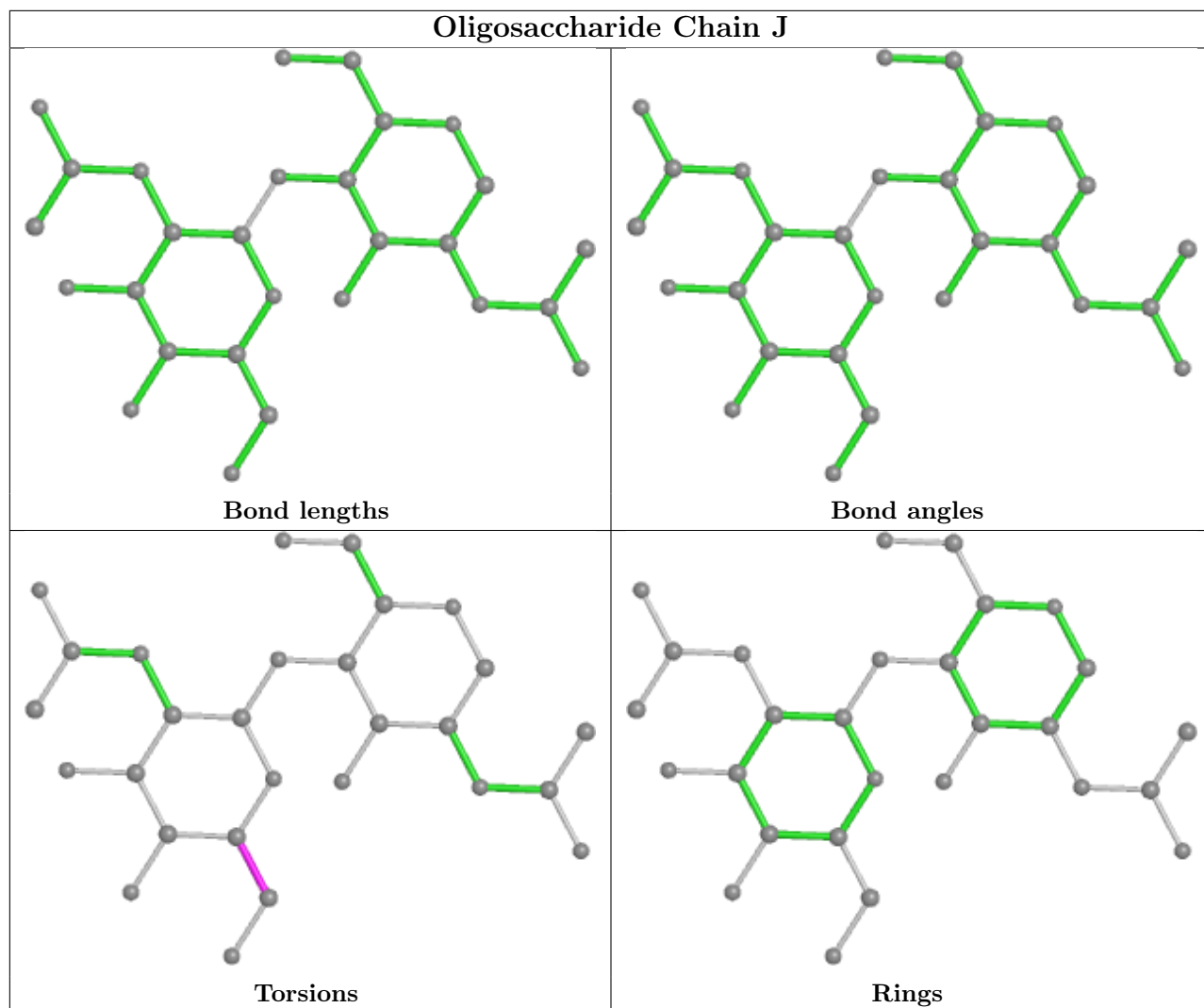
2 monomers are involved in 2 short contacts:

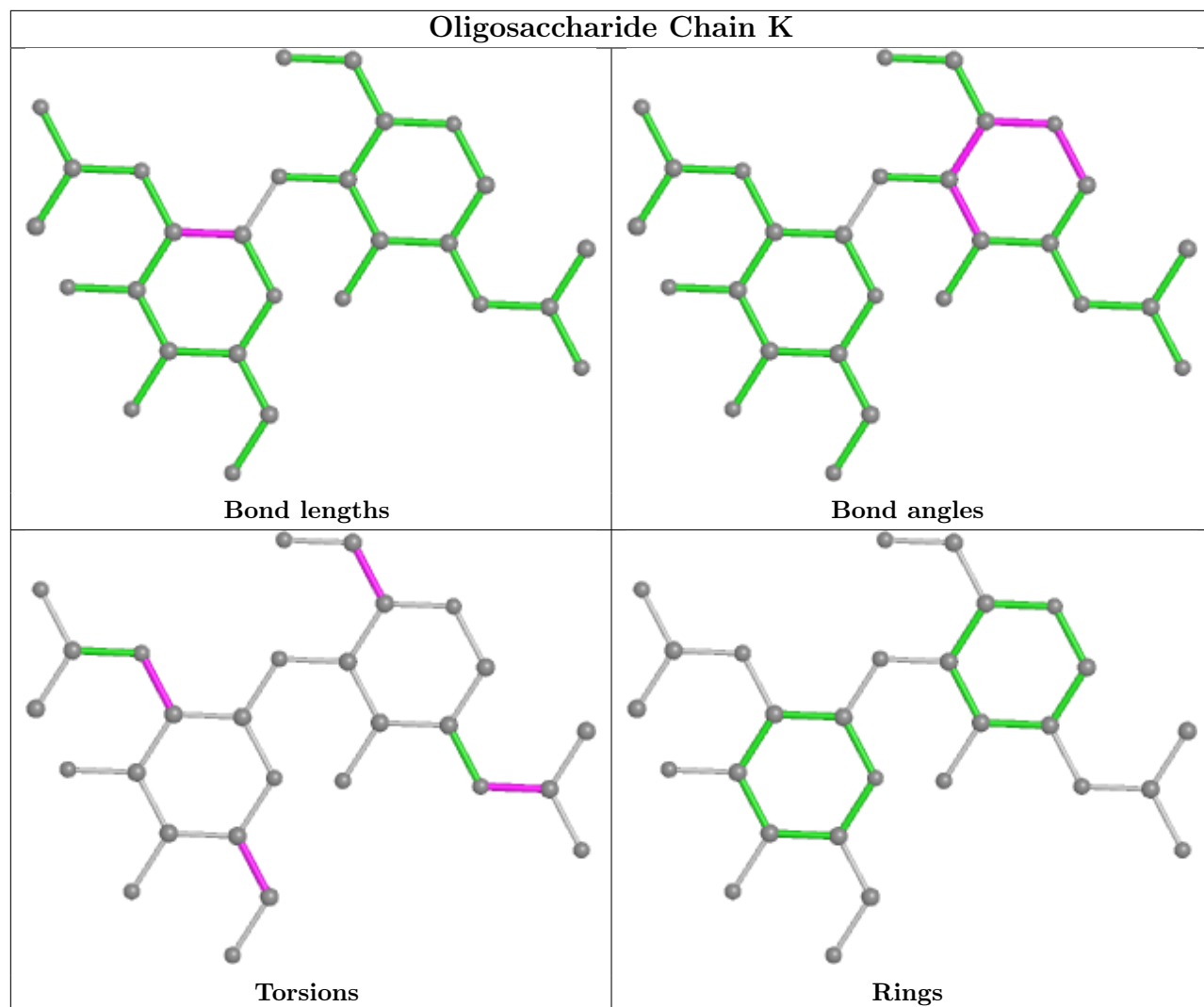
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	L	1	NDG	1	0
12	L	3	BMA	1	0

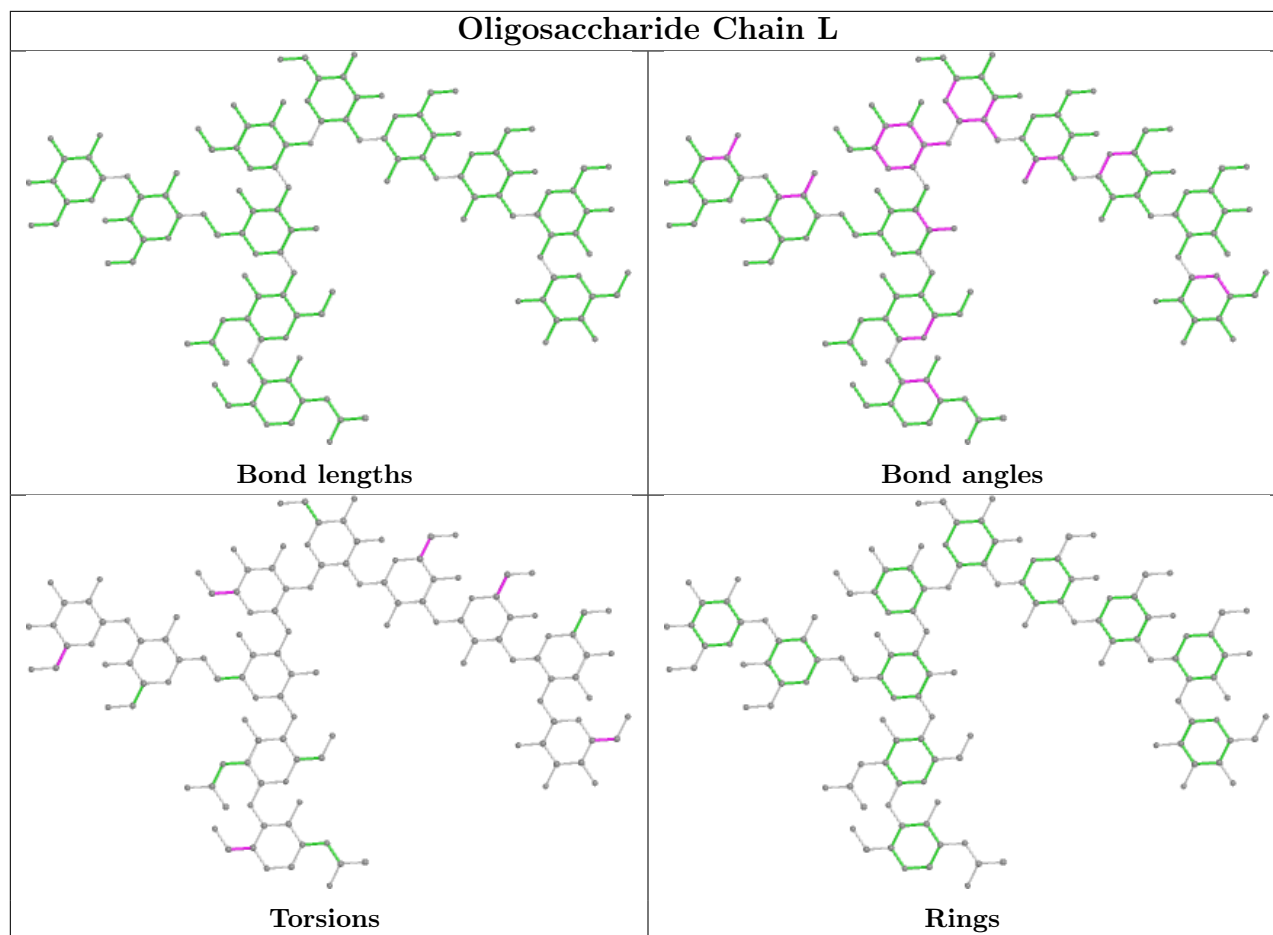
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











## 5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 1 is monoatomic - leaving 10 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$
14	CPL	F	301	-	51,51,51	0.37	0	57,59,59	0.40	0
15	PTY	H	901	-	41,41,49	0.94	3 (7%)	44,46,54	1.21	3 (6%)
17	NAG	G	502	7	14,14,15	1.08	2 (14%)	17,19,21	1.35	1 (5%)
14	CPL	C	101	-	51,51,51	1.25	5 (9%)	57,59,59	0.92	1 (1%)
18	323	P	101	9	34,34,34	2.34	9 (26%)	45,50,50	1.41	7 (15%)
17	NAG	G	501	7	14,14,15	0.46	0	17,19,21	0.72	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
13	ELU	A	1001	12,16	26,28,28	0.70	0	33,37,37	1.29	5 (15%)
14	CPL	E	501	-	51,51,51	1.26	5 (9%)	57,59,59	1.06	3 (5%)
14	CPL	A	1002	-	51,51,51	0.38	0	57,59,59	0.39	0
15	PTY	A	1003	-	41,41,49	0.92	2 (4%)	44,46,54	1.19	2 (4%)

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	CPL	F	301	-	-	32/55/55/55	-
15	PTY	H	901	-	-	27/45/45/53	-
17	NAG	G	502	7	-	2/6/23/26	0/1/1/1
14	CPL	C	101	-	-	32/55/55/55	-
18	323	P	101	9	-	6/16/69/69	0/4/4/4
17	NAG	G	501	7	-	0/6/23/26	0/1/1/1
13	ELU	A	1001	12,16	-	6/31/31/31	-
14	CPL	E	501	-	-	17/55/55/55	-
14	CPL	A	1002	-	-	29/55/55/55	-
15	PTY	A	1003	-	-	33/45/45/53	-

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	P	101	323	O1-C4	7.12	1.49	1.38
18	P	101	323	C7-N2	5.36	1.50	1.37
18	P	101	323	O1-C3	5.30	1.46	1.38
18	P	101	323	C23-C24	3.71	1.57	1.49
18	P	101	323	C18-C1	3.57	1.54	1.49
18	P	101	323	C17-N1	3.42	1.52	1.47
14	E	501	CPL	O3-C11	3.23	1.42	1.33
14	C	101	CPL	O3-C11	3.15	1.42	1.33
14	C	101	CPL	O2-C31	3.14	1.43	1.34
14	E	501	CPL	O2-C31	3.06	1.42	1.34
18	P	101	323	C21-C25	2.92	1.56	1.47
17	G	502	NAG	O5-C1	2.89	1.48	1.43
17	G	502	NAG	C1-C2	2.74	1.56	1.52
15	H	901	PTY	O7-C6	-2.63	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	E	501	CPL	O2-C2	-2.50	1.40	1.46
14	C	101	CPL	O2-C2	-2.47	1.40	1.46
15	A	1003	PTY	O7-C6	-2.45	1.40	1.46
15	A	1003	PTY	O4-C30	2.39	1.40	1.33
15	H	901	PTY	O4-C30	2.30	1.40	1.33
15	H	901	PTY	O4-C1	-2.28	1.39	1.45
14	C	101	CPL	P-O4P	2.25	1.68	1.59
18	P	101	323	C3-C2	-2.18	1.40	1.46
14	C	101	CPL	C32-C31	2.13	1.56	1.50
18	P	101	323	C1-C2	2.12	1.50	1.41
14	E	501	CPL	C32-C31	2.11	1.56	1.50
14	E	501	CPL	P-O4P	2.06	1.67	1.59

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	G	502	NAG	C1-O5-C5	5.18	119.21	112.19
15	H	901	PTY	O7-C8-C11	4.57	121.34	111.50
15	A	1003	PTY	O7-C8-C11	4.50	121.19	111.50
14	E	501	CPL	O2-C31-C32	3.81	119.71	111.50
18	P	101	323	O1-C3-C13	3.43	120.28	115.20
14	C	101	CPL	O2-C31-C32	3.32	118.65	111.50
18	P	101	323	O1-C4-C6	3.28	120.05	115.20
15	A	1003	PTY	O4-C30-C31	3.08	121.59	111.91
18	P	101	323	C23-C18-C1	-3.08	119.06	123.33
13	A	1001	ELU	PA-O3A-PB	-2.49	124.27	132.83
14	E	501	CPL	O3-C11-C12	2.37	119.36	111.91
13	A	1001	ELU	C10-C8-C9	2.37	119.26	115.27
18	P	101	323	C16-N1-C17	2.32	119.89	115.29
14	E	501	CPL	C2-O2-C31	-2.28	112.17	117.79
15	H	901	PTY	O4-C30-C31	2.27	119.02	111.91
13	A	1001	ELU	C14-C13-C12	-2.26	117.88	123.68
18	P	101	323	C10-C11-C12	-2.23	119.93	121.79
15	H	901	PTY	C6-O7-C8	-2.20	112.38	117.79
13	A	1001	ELU	C14-C13-C15	2.18	118.94	115.27
18	P	101	323	C5-C1-C18	2.18	120.75	117.16
13	A	1001	ELU	C11-C12-C13	-2.06	122.69	127.66
18	P	101	323	O1-C3-C2	-2.00	119.74	121.92

There are no chirality outliers.

All (184) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	A	1001	ELU	C1-O1-PA-O3A
13	A	1001	ELU	O1-C1-C2-C3
14	A	1002	CPL	O2-C2-C3-O3
14	A	1002	CPL	C41-C42-C43-C44
14	C	101	CPL	C1-O3P-P-O1P
14	E	501	CPL	O4P-C4-C5-N
14	E	501	CPL	C32-C31-O2-C2
14	F	301	CPL	O2-C2-C3-O3
14	F	301	CPL	C38-C39-C40-C41
14	F	301	CPL	C1-O3P-P-O1P
14	F	301	CPL	C1-O3P-P-O2P
14	F	301	CPL	C1-O3P-P-O4P
15	A	1003	PTY	C11-C8-O7-C6
15	A	1003	PTY	C3-O11-P1-O12
15	A	1003	PTY	C3-O11-P1-O14
15	A	1003	PTY	C5-O14-P1-O11
15	A	1003	PTY	C5-O14-P1-O13
15	H	901	PTY	N1-C2-C3-O11
15	H	901	PTY	C3-O11-P1-O12
18	P	101	323	C18-C1-C5-C9
18	P	101	323	C2-C1-C5-C9
14	E	501	CPL	O31-C31-O2-C2
15	A	1003	PTY	O10-C8-O7-C6
14	A	1002	CPL	C36-C37-C38-C39
15	H	901	PTY	C31-C30-O4-C1
14	F	301	CPL	C35-C36-C37-C38
14	F	301	CPL	C19-C20-C21-C22
13	A	1001	ELU	C13-C15-C16-C17
14	A	1002	CPL	C19-C20-C21-C22
15	H	901	PTY	O30-C30-O4-C1
15	H	901	PTY	C38-C39-C40-C41
14	A	1002	CPL	C4-C5-N-C7
14	A	1002	CPL	C4-C5-N-C8
14	F	301	CPL	C4-C5-N-C8
14	A	1002	CPL	C11-C12-C13-C14
14	E	501	CPL	C12-C11-O3-C3
14	F	301	CPL	C4-C5-N-C6
14	F	301	CPL	C11-C12-C13-C14
14	F	301	CPL	C23-C24-C25-C26
14	C	101	CPL	C1-O3P-P-O4P
14	C	101	CPL	C4-O4P-P-O3P
14	F	301	CPL	C4-O4P-P-O3P
15	H	901	PTY	C3-O11-P1-O14

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Mol	Chain	Res	Type	Atoms
15	H	901	PTY	C5-O14-P1-O11
14	C	101	CPL	C12-C13-C14-C15
14	F	301	CPL	C32-C31-O2-C2
14	A	1002	CPL	C22-C23-C24-C25
14	A	1002	CPL	C32-C33-C34-C35
15	H	901	PTY	C15-C16-C17-C18
14	F	301	CPL	C17-C18-C19-C20
15	A	1003	PTY	C16-C17-C18-C19
15	H	901	PTY	C37-C38-C39-C40
14	F	301	CPL	O31-C31-O2-C2
15	A	1003	PTY	C30-C31-C32-C33
15	A	1003	PTY	C11-C12-C13-C14
14	C	101	CPL	C15-C16-C17-C18
15	H	901	PTY	C32-C33-C34-C35
14	A	1002	CPL	C44-C45-C46-C47
15	H	901	PTY	C16-C17-C18-C19
14	E	501	CPL	O11-C11-O3-C3
14	A	1002	CPL	C43-C44-C45-C46
14	C	101	CPL	C21-C22-C23-C24
14	C	101	CPL	C35-C36-C37-C38
14	F	301	CPL	C16-C17-C18-C19
14	A	1002	CPL	C4-C5-N-C6
14	F	301	CPL	C4-C5-N-C7
14	C	101	CPL	C14-C15-C16-C17
14	F	301	CPL	C15-C16-C17-C18
15	A	1003	PTY	C36-C37-C38-C39
15	H	901	PTY	C11-C12-C13-C14
15	A	1003	PTY	C40-C41-C42-C43
14	E	501	CPL	C35-C36-C37-C38
14	A	1002	CPL	C16-C17-C18-C19
14	A	1002	CPL	C12-C13-C14-C15
14	A	1002	CPL	C14-C15-C16-C17
14	A	1002	CPL	C34-C35-C36-C37
14	C	101	CPL	C16-C17-C18-C19
15	H	901	PTY	C34-C35-C36-C37
14	F	301	CPL	C44-C45-C46-C47
15	A	1003	PTY	C31-C32-C33-C34
14	A	1002	CPL	C33-C34-C35-C36
14	C	101	CPL	C11-C12-C13-C14
15	H	901	PTY	C17-C18-C19-C20
14	A	1002	CPL	C21-C22-C23-C24
14	C	101	CPL	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
15	H	901	PTY	O4-C1-C6-O7
14	C	101	CPL	C23-C24-C25-C26
14	C	101	CPL	C12-C11-O3-C3
14	E	501	CPL	C15-C16-C17-C18
15	A	1003	PTY	C33-C34-C35-C36
14	F	301	CPL	C1-C2-C3-O3
14	A	1002	CPL	C38-C39-C40-C41
14	F	301	CPL	C41-C42-C43-C44
14	A	1002	CPL	C23-C24-C25-C26
14	C	101	CPL	C45-C46-C47-C48
14	E	501	CPL	C16-C17-C18-C19
17	G	502	NAG	C4-C5-C6-O6
14	C	101	CPL	O3P-C1-C2-O2
14	A	1002	CPL	C31-C32-C33-C34
14	C	101	CPL	C43-C44-C45-C46
15	A	1003	PTY	C39-C40-C41-C42
15	H	901	PTY	O14-C5-C6-C1
14	A	1002	CPL	C17-C18-C19-C20
14	A	1002	CPL	C1-C2-C3-O3
15	H	901	PTY	O4-C1-C6-C5
15	A	1003	PTY	C34-C35-C36-C37
14	C	101	CPL	O11-C11-O3-C3
14	E	501	CPL	C39-C40-C41-C42
14	E	501	CPL	C40-C41-C42-C43
14	C	101	CPL	C44-C45-C46-C47
15	H	901	PTY	O14-C5-C6-O7
15	A	1003	PTY	C14-C15-C16-C17
14	E	501	CPL	O2-C2-C3-O3
15	H	901	PTY	C11-C8-O7-C6
14	C	101	CPL	C36-C37-C38-C39
14	C	101	CPL	C4-C5-N-C8
18	P	101	323	C22-C23-C24-O2
15	H	901	PTY	O10-C8-O7-C6
18	P	101	323	C22-C23-C24-O3
15	A	1003	PTY	O14-C5-C6-C1
13	A	1001	ELU	PA-O3A-PB-O2B
15	A	1003	PTY	O14-C5-C6-O7
14	C	101	CPL	C4-C5-N-C7
15	A	1003	PTY	C38-C39-C40-C41
15	A	1003	PTY	C17-C18-C19-C20
15	A	1003	PTY	C37-C38-C39-C40
13	A	1001	ELU	C1-O1-PA-O1A

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Mol	Chain	Res	Type	Atoms
14	C	101	CPL	C1-O3P-P-O2P
14	C	101	CPL	C4-O4P-P-O1P
14	F	301	CPL	C4-O4P-P-O1P
15	A	1003	PTY	C3-O11-P1-O13
15	H	901	PTY	C5-O14-P1-O12
14	A	1002	CPL	C12-C11-O3-C3
14	E	501	CPL	C12-C13-C14-C15
14	C	101	CPL	C33-C34-C35-C36
15	H	901	PTY	C2-C3-O11-P1
14	A	1002	CPL	O3-C11-C12-C13
15	A	1003	PTY	C32-C33-C34-C35
14	F	301	CPL	C31-C32-C33-C34
14	A	1002	CPL	C35-C36-C37-C38
14	E	501	CPL	C4-C5-N-C7
14	C	101	CPL	C34-C35-C36-C37
14	F	301	CPL	O4P-C4-C5-N
15	A	1003	PTY	C13-C14-C15-C16
18	P	101	323	C18-C23-C24-O2
14	A	1002	CPL	O11-C11-O3-C3
14	C	101	CPL	C4-C5-N-C6
15	A	1003	PTY	C5-C6-O7-C8
18	P	101	323	C18-C23-C24-O3
14	A	1002	CPL	C15-C16-C17-C18
14	E	501	CPL	C42-C43-C44-C45
14	C	101	CPL	O2-C2-C3-O3
15	A	1003	PTY	O4-C1-C6-O7
14	C	101	CPL	C1-C2-C3-O3
17	G	502	NAG	C3-C2-N2-C7
14	F	301	CPL	C42-C43-C44-C45
14	C	101	CPL	O3P-C1-C2-C3
15	A	1003	PTY	O30-C30-O4-C1
14	C	101	CPL	C31-C32-C33-C34
15	H	901	PTY	C41-C42-C43-C44
14	E	501	CPL	C1-C2-C3-O3
15	A	1003	PTY	C31-C30-O4-C1
14	A	1002	CPL	C37-C38-C39-C40
14	F	301	CPL	C40-C41-C42-C43
15	H	901	PTY	C13-C14-C15-C16
14	F	301	CPL	C21-C22-C23-C24
14	E	501	CPL	C4-C5-N-C6
14	E	501	CPL	C4-C5-N-C8
14	C	101	CPL	C42-C43-C44-C45

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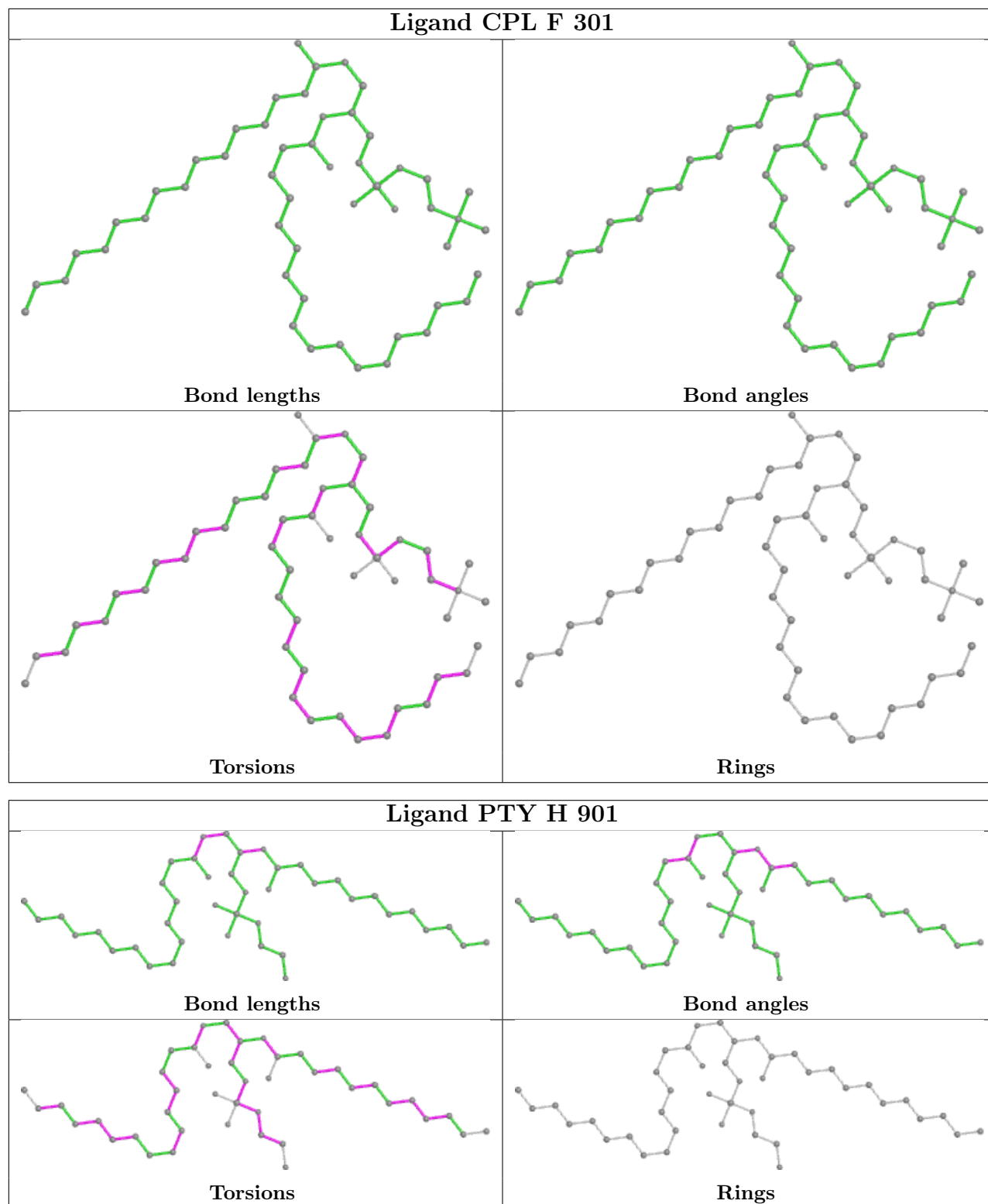
Mol	Chain	Res	Type	Atoms
15	A	1003	PTY	C35-C36-C37-C38
14	F	301	CPL	C37-C38-C39-C40
15	H	901	PTY	C39-C40-C41-C42
14	C	101	CPL	C37-C38-C39-C40
15	H	901	PTY	C31-C32-C33-C34
15	A	1003	PTY	C12-C11-C8-O7
14	F	301	CPL	C45-C46-C47-C48
15	A	1003	PTY	O4-C1-C6-C5
15	A	1003	PTY	C12-C11-C8-O10
14	F	301	CPL	C4-O4P-P-O2P
15	H	901	PTY	C5-O14-P1-O13
14	F	301	CPL	C12-C11-O3-C3
15	A	1003	PTY	C2-C3-O11-P1
14	F	301	CPL	O11-C11-O3-C3
13	A	1001	ELU	C4-C3-C5-C6

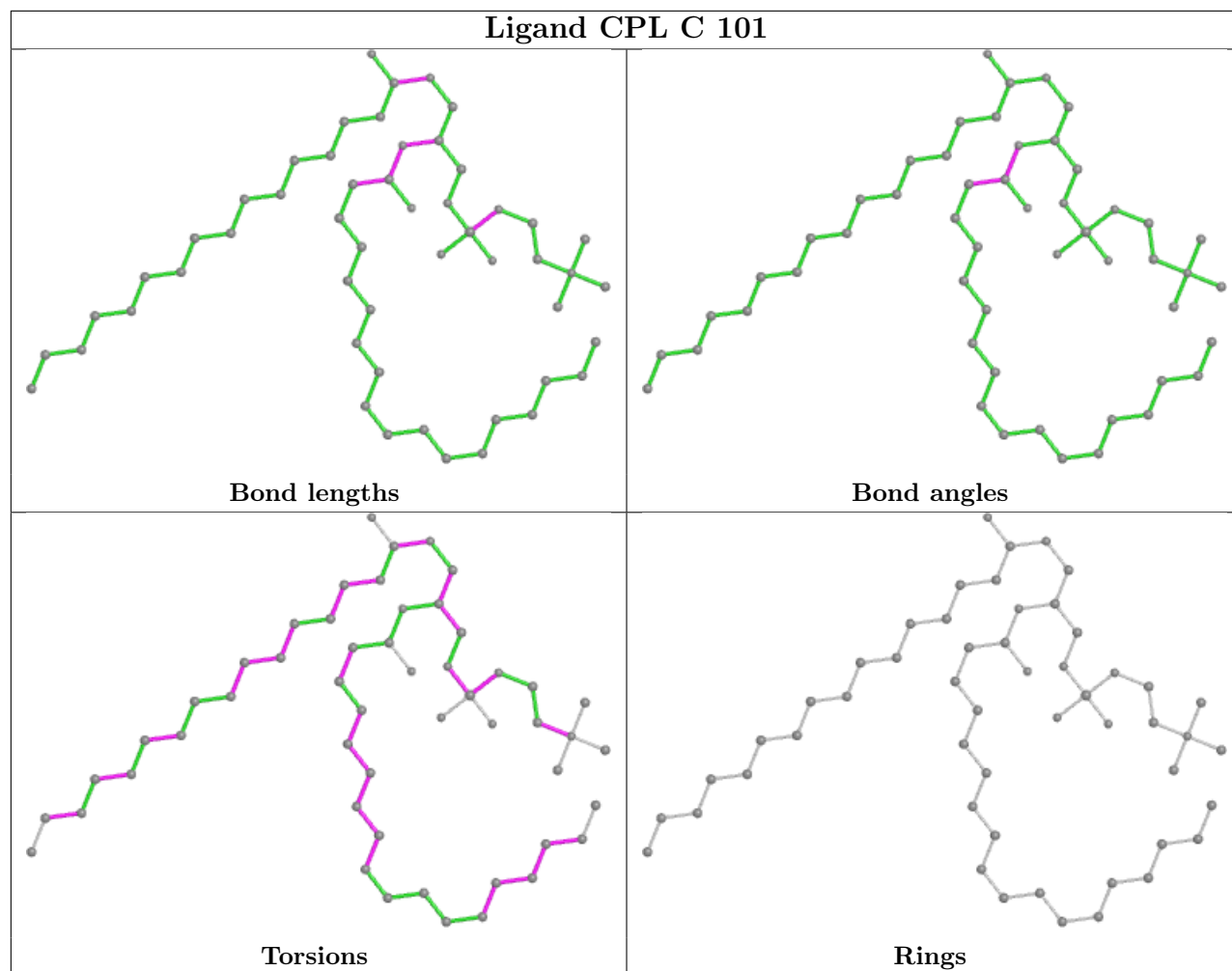
There are no ring outliers.

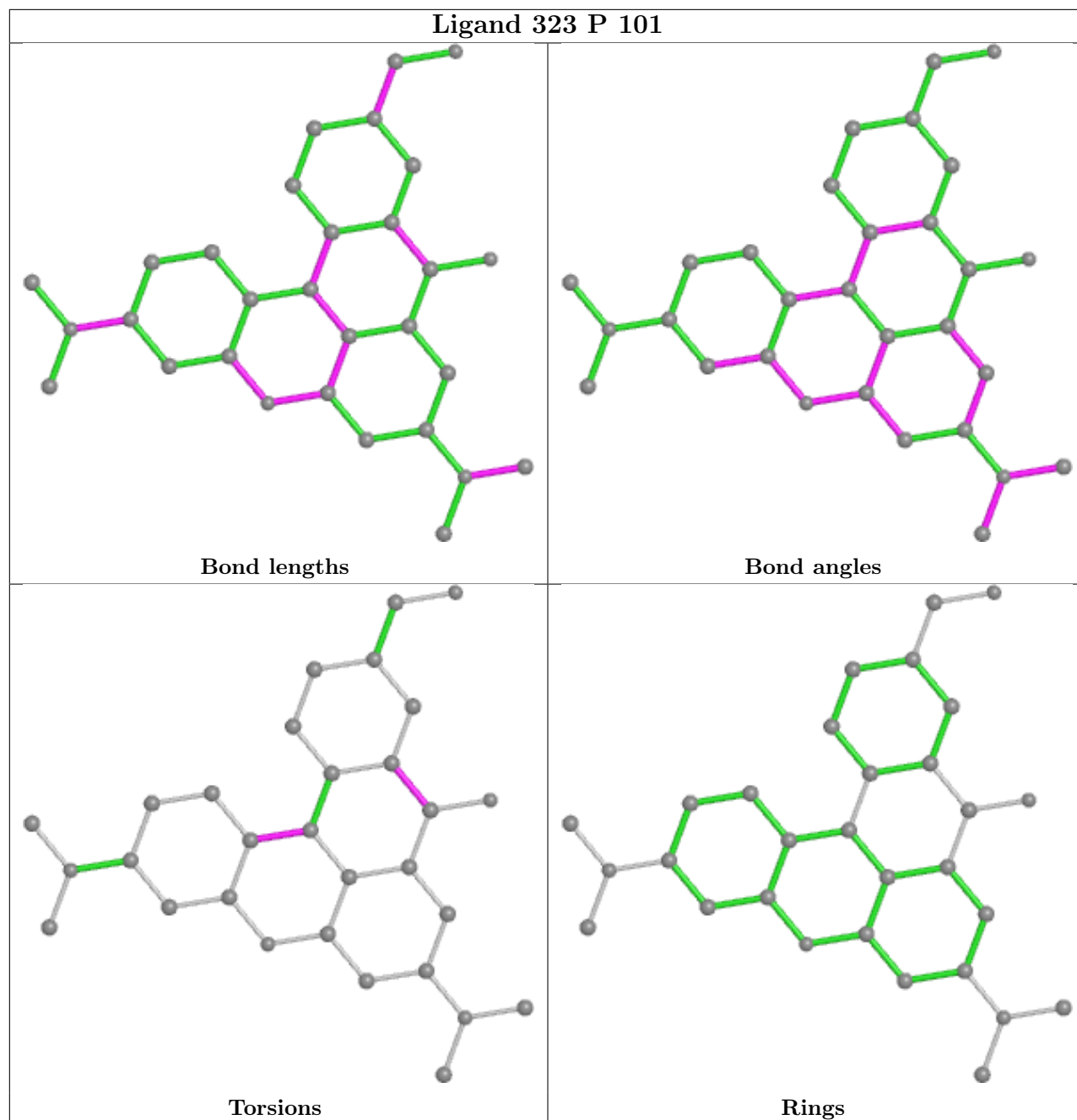
7 monomers are involved in 9 short contacts:

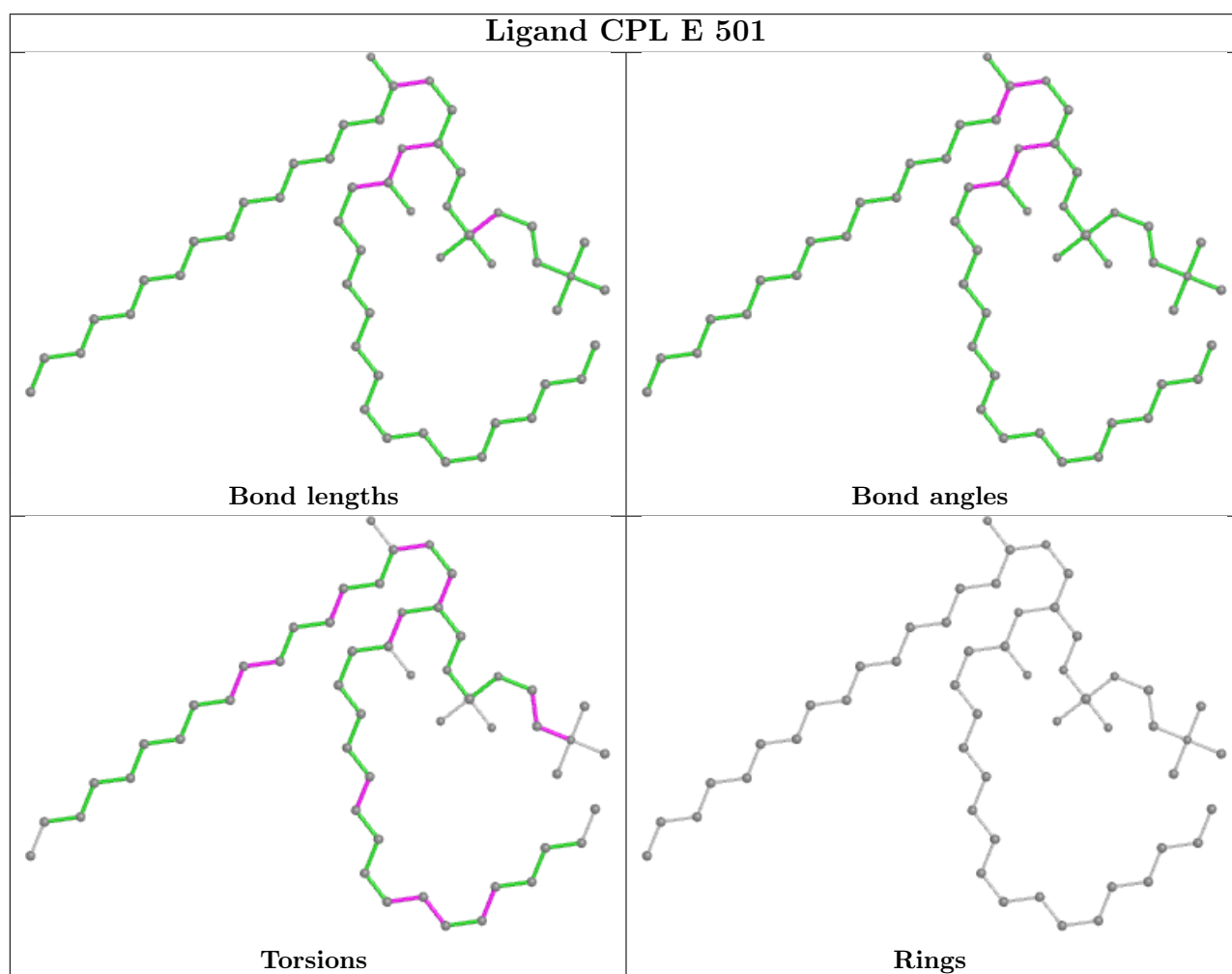
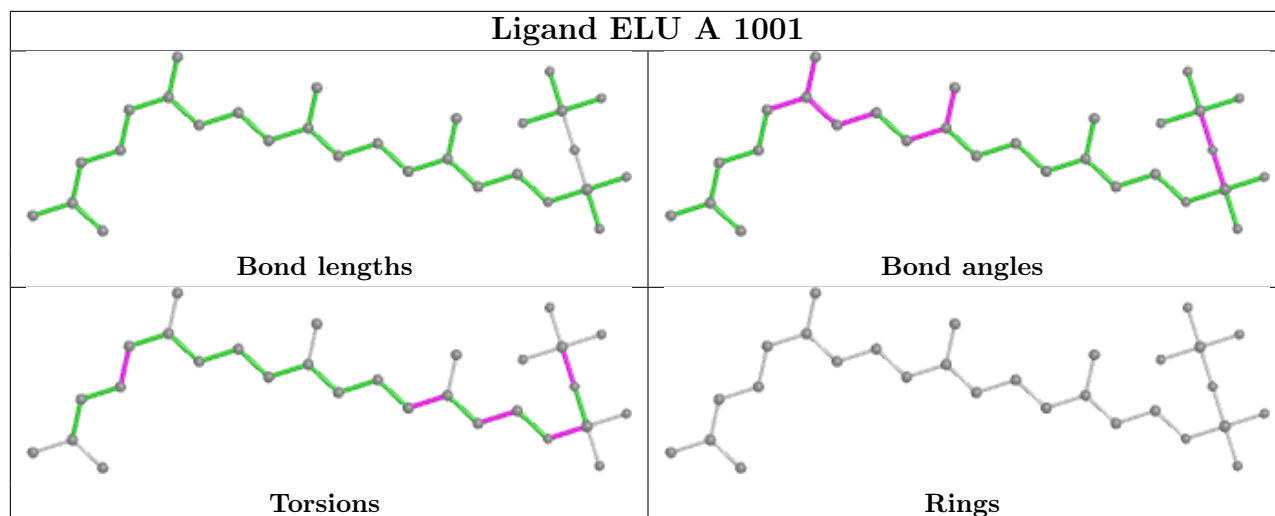
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	F	301	CPL	3	0
14	C	101	CPL	1	0
18	P	101	323	1	0
17	G	501	NAG	1	0
14	E	501	CPL	1	0
14	A	1002	CPL	2	0
15	A	1003	PTY	1	0

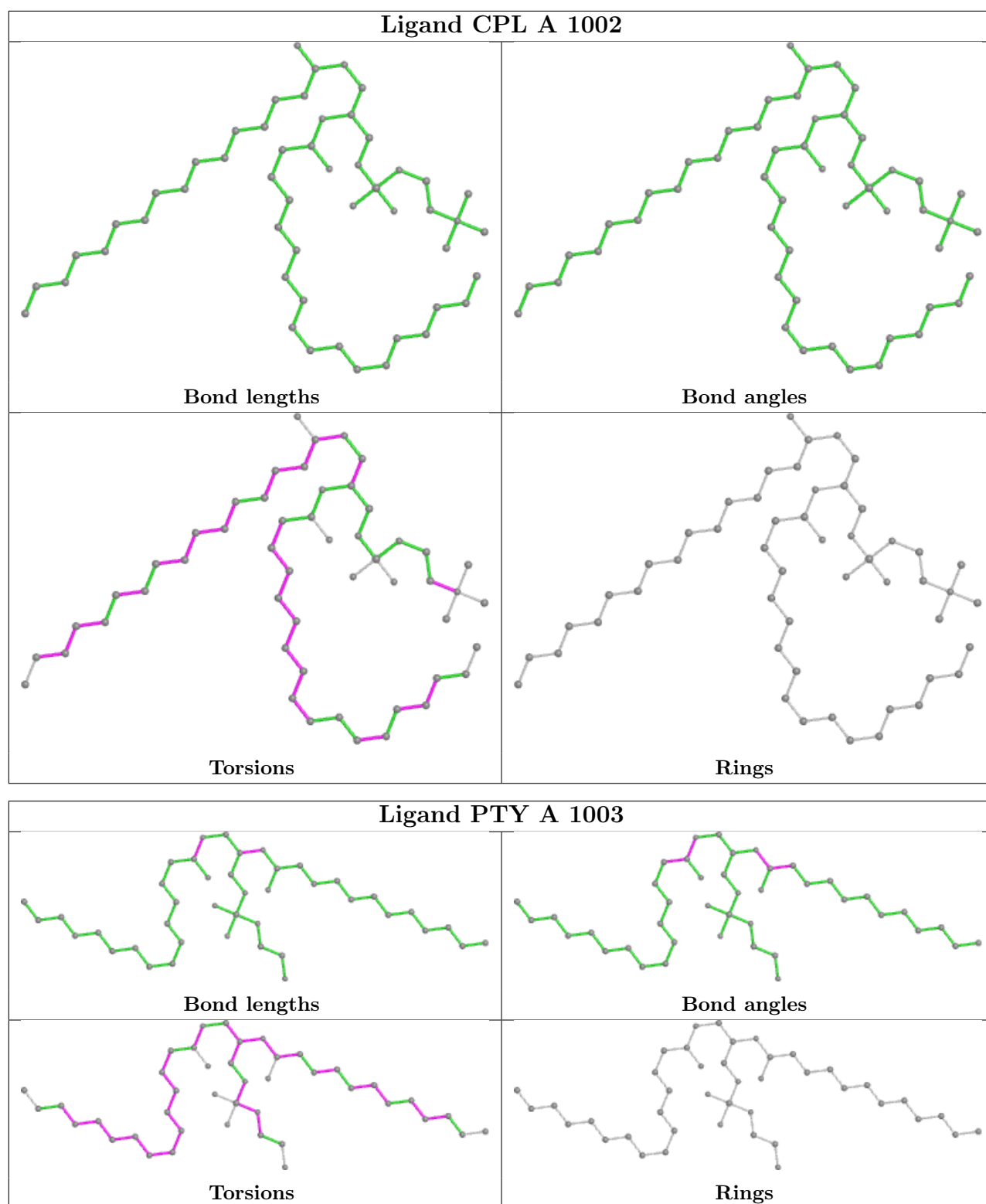
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.



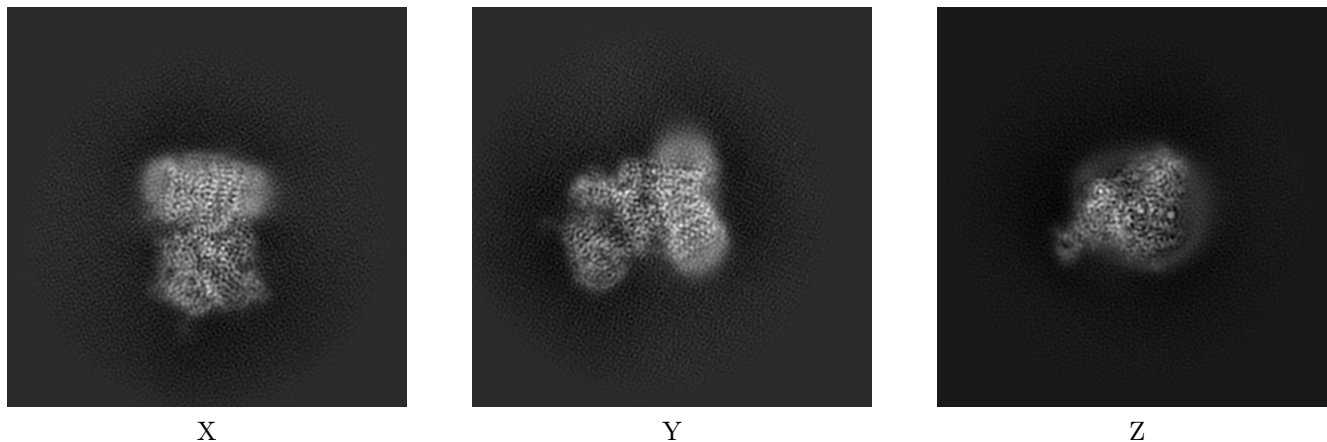
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15420. These allow visual inspection of the internal detail of the map and identification of artifacts.

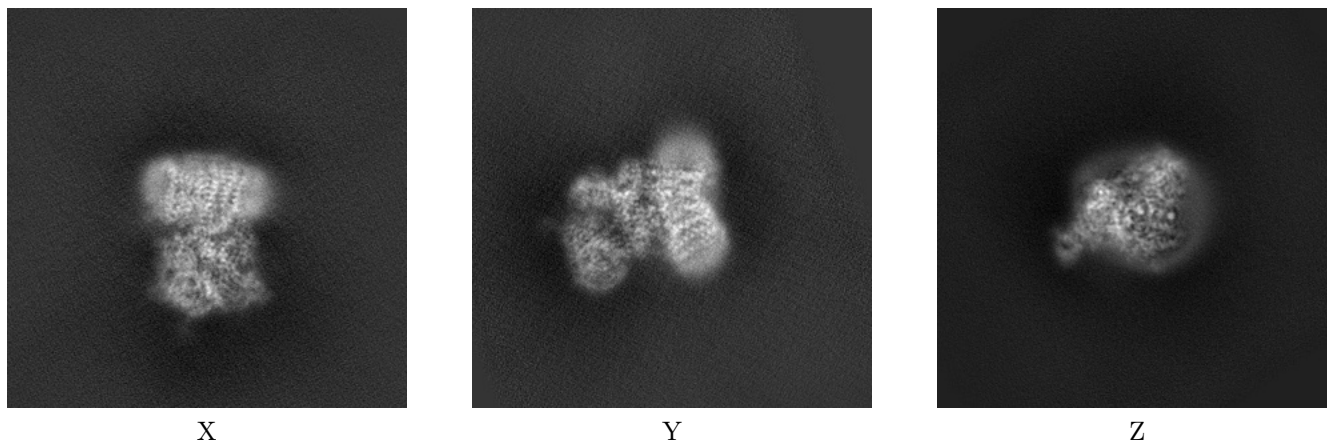
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

#### 6.1.1 Primary map



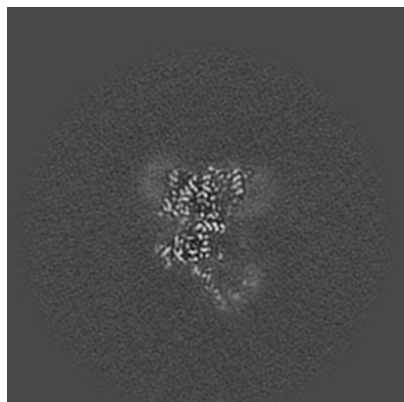
#### 6.1.2 Raw map



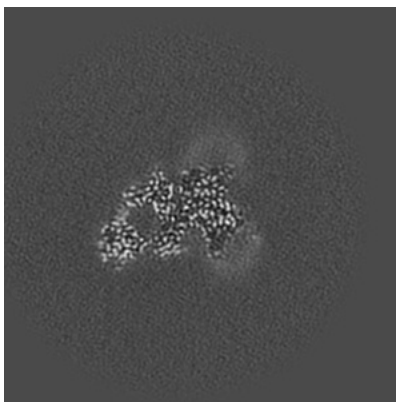
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

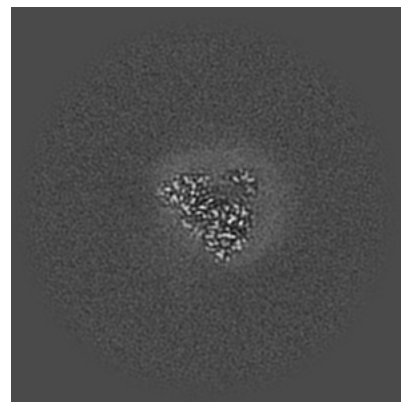
### 6.2.1 Primary map



X Index: 192

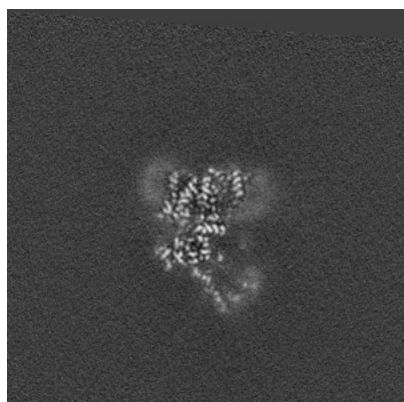


Y Index: 192

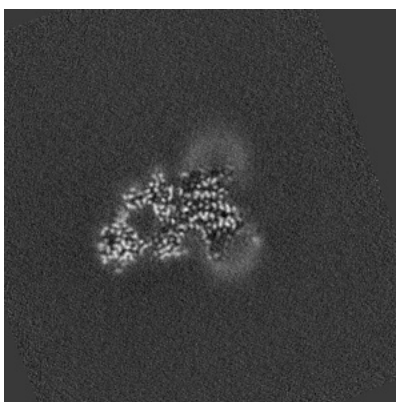


Z Index: 192

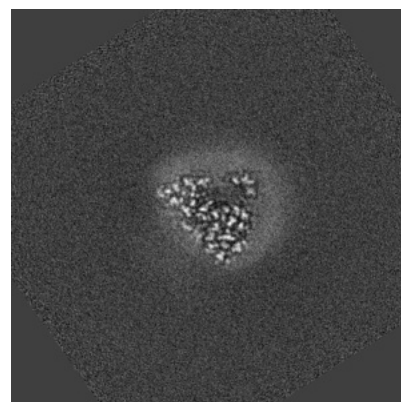
### 6.2.2 Raw map



X Index: 192



Y Index: 192

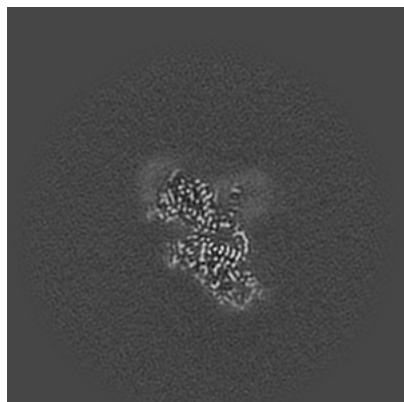


Z Index: 192

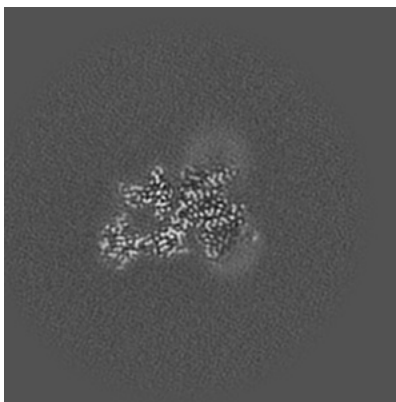
The images above show central slices of the map in three orthogonal directions.

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

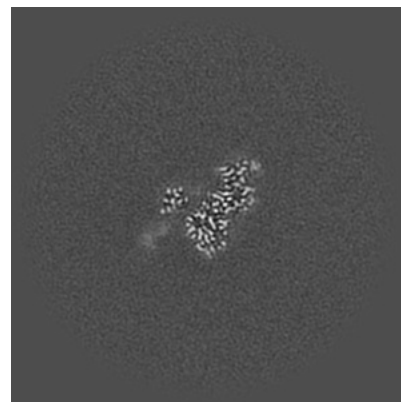
### 6.3.1 Primary map



X Index: 206

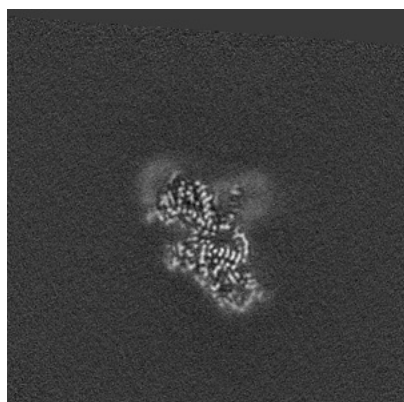


Y Index: 194

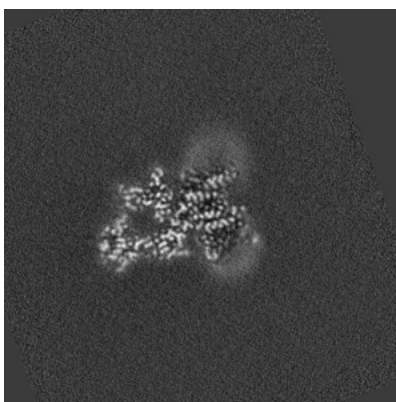


Z Index: 148

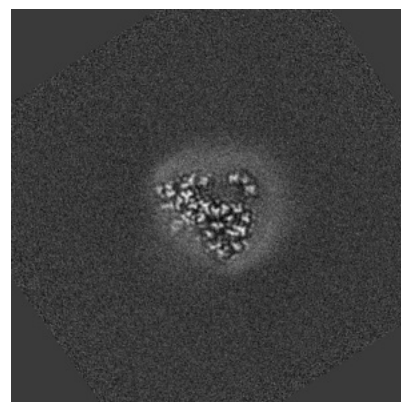
### 6.3.2 Raw map



X Index: 206



Y Index: 194

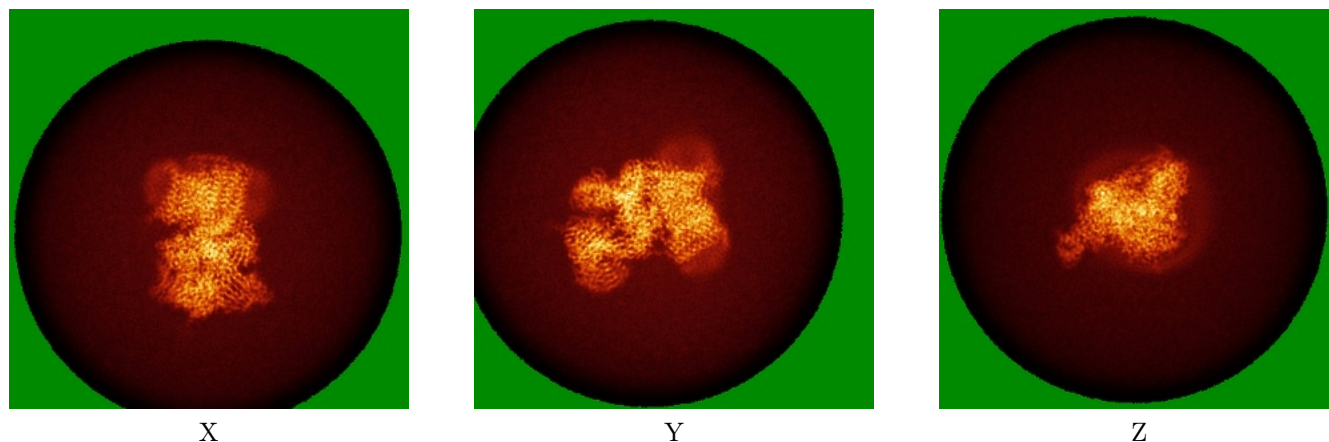


Z Index: 195

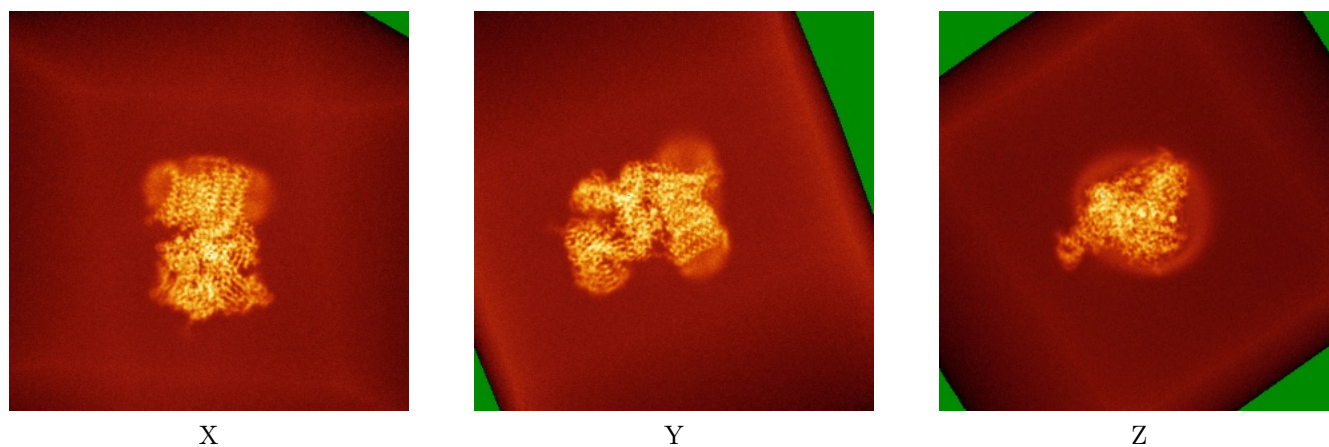
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



### 6.4.2 Raw map



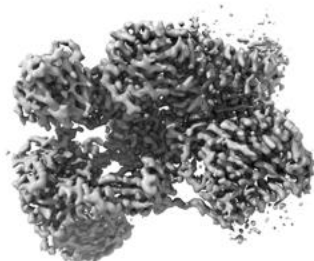
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 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 0.386. 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.

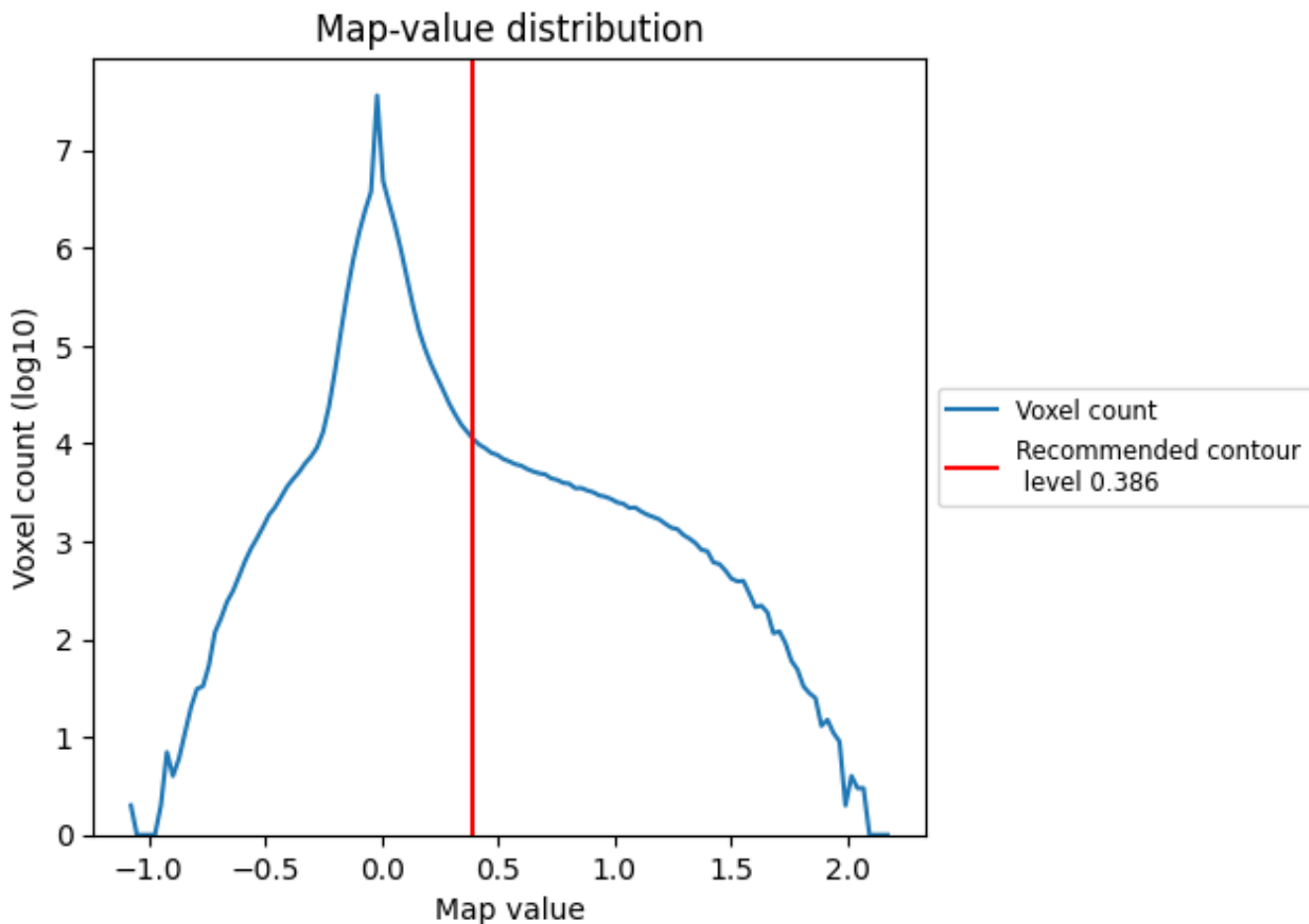
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

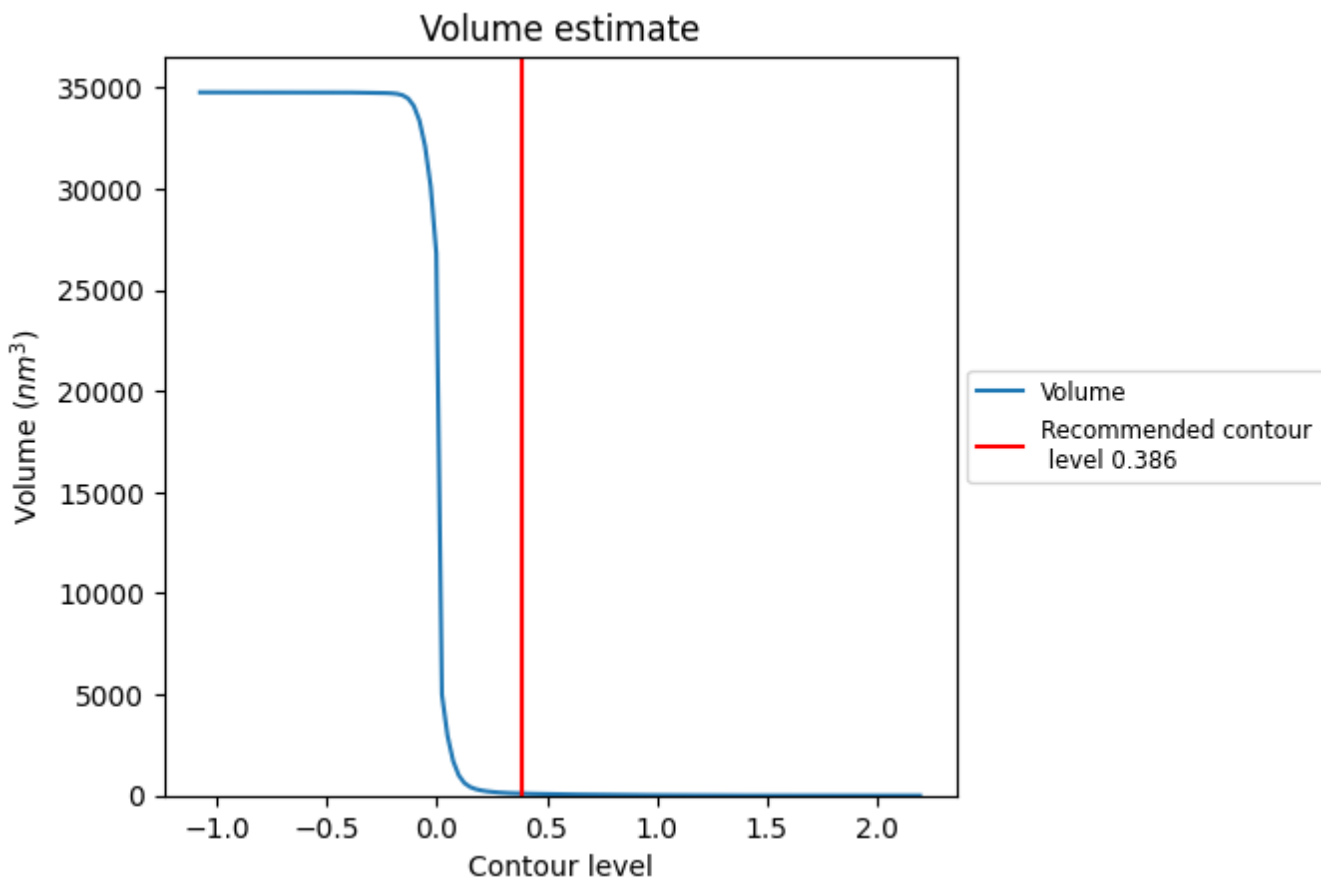
This section contains the results of statistical analysis of the map.

### 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.

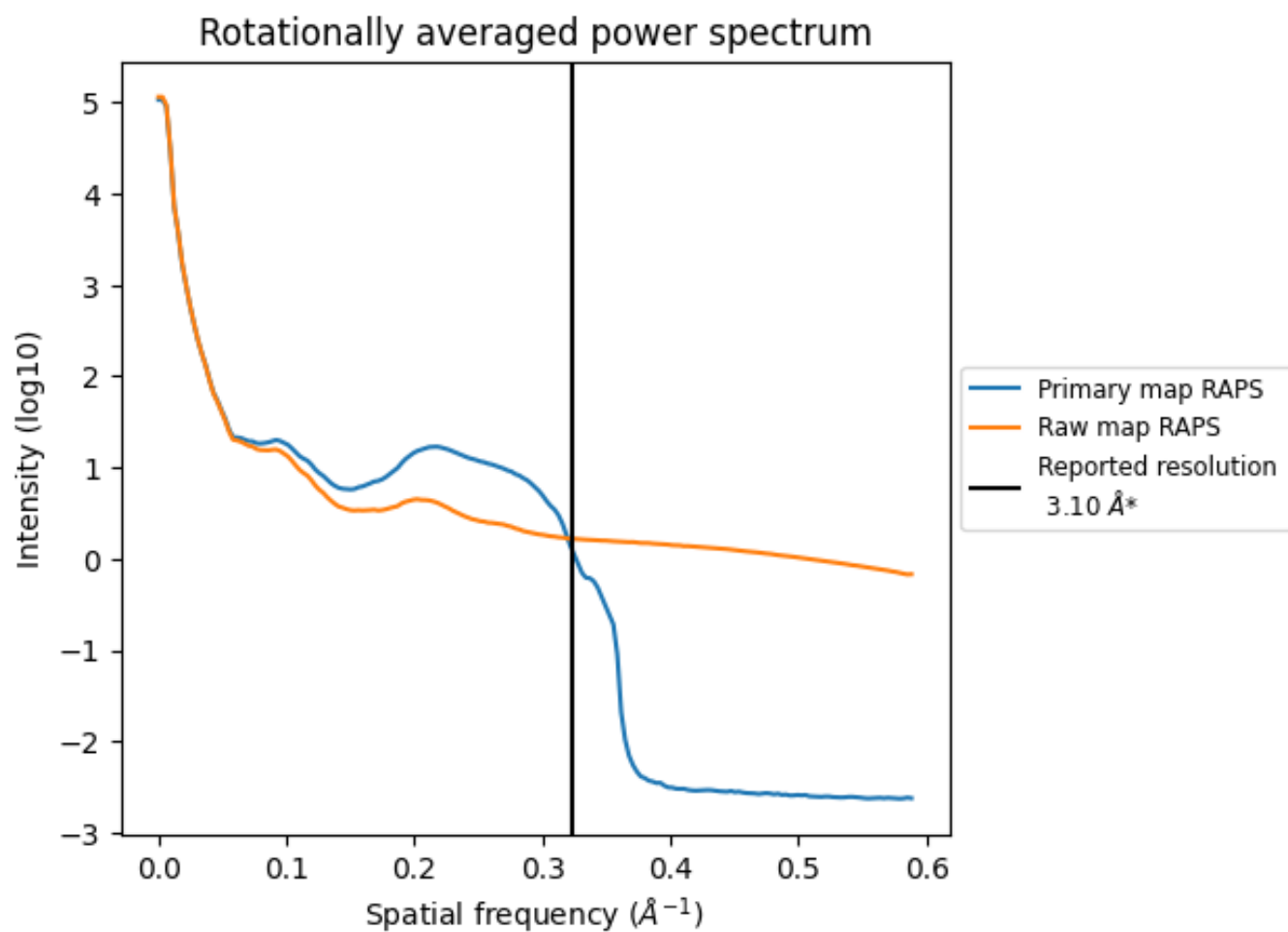
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 100 nm<sup>3</sup>; this corresponds to an approximate mass of 91 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



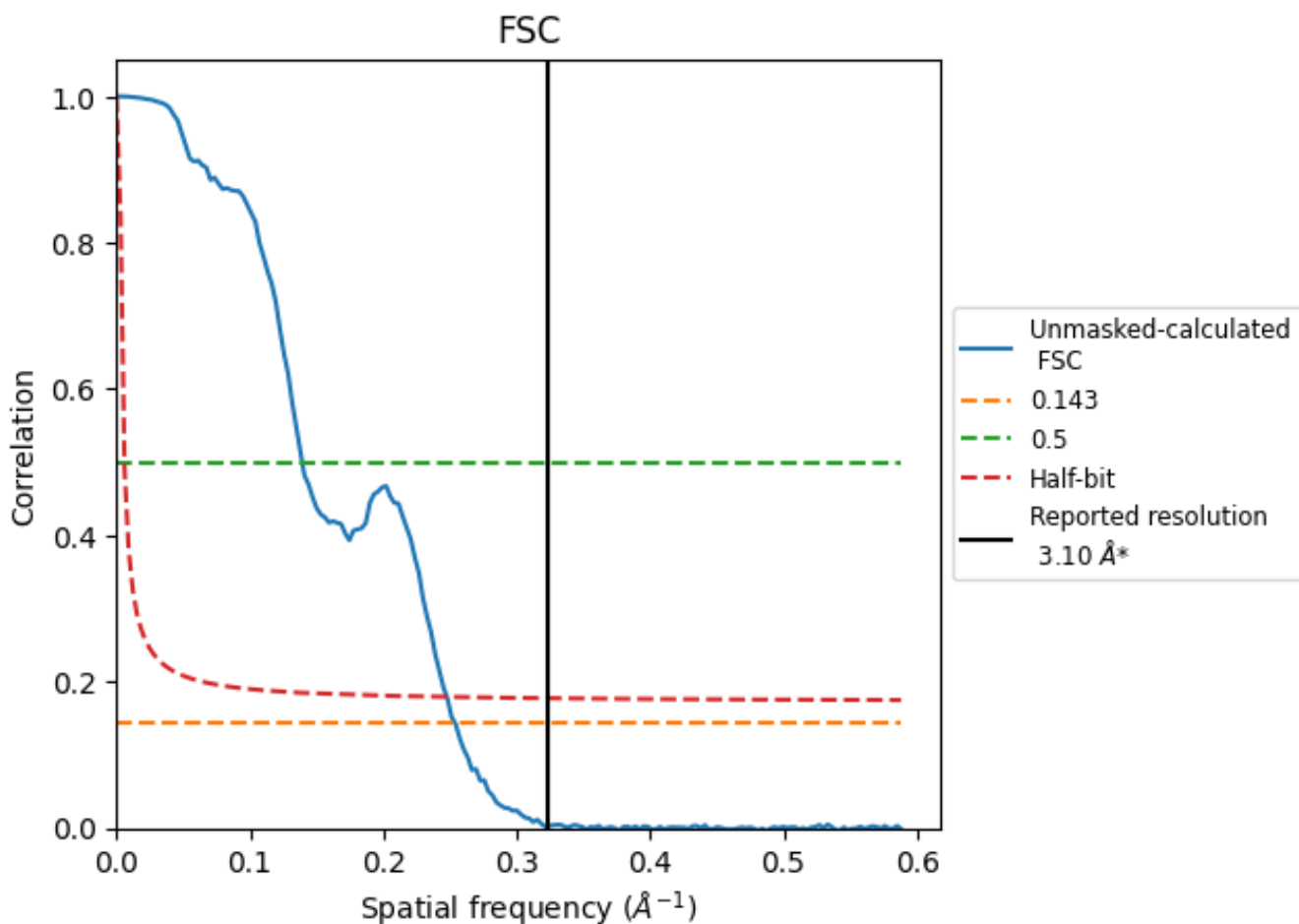
\*Reported resolution corresponds to spatial frequency of  $0.323 \text{ \AA}^{-1}$



## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.323 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

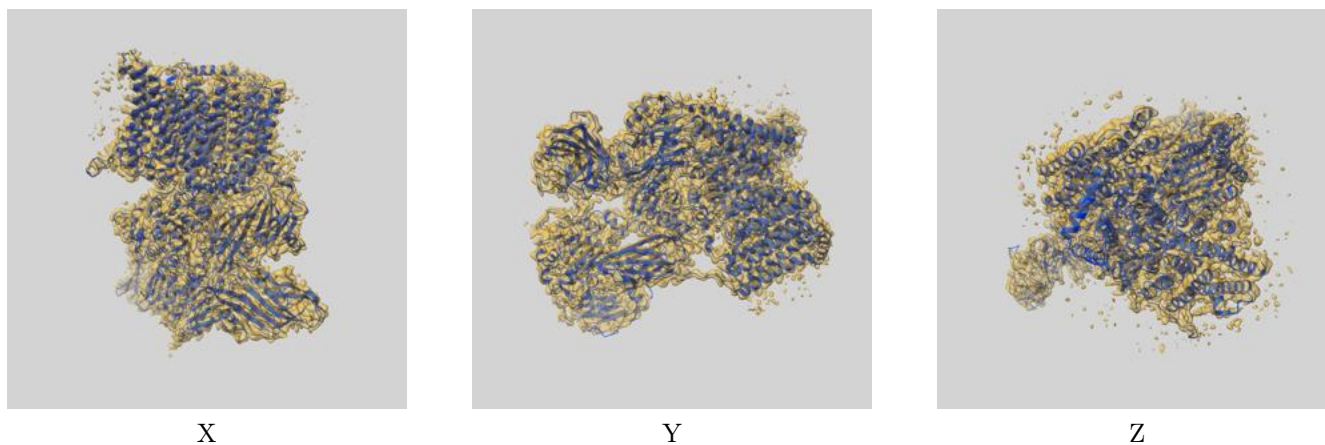
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.94	7.18	4.04

\*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 3.94 differs from the reported value 3.1 by more than 10 %

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

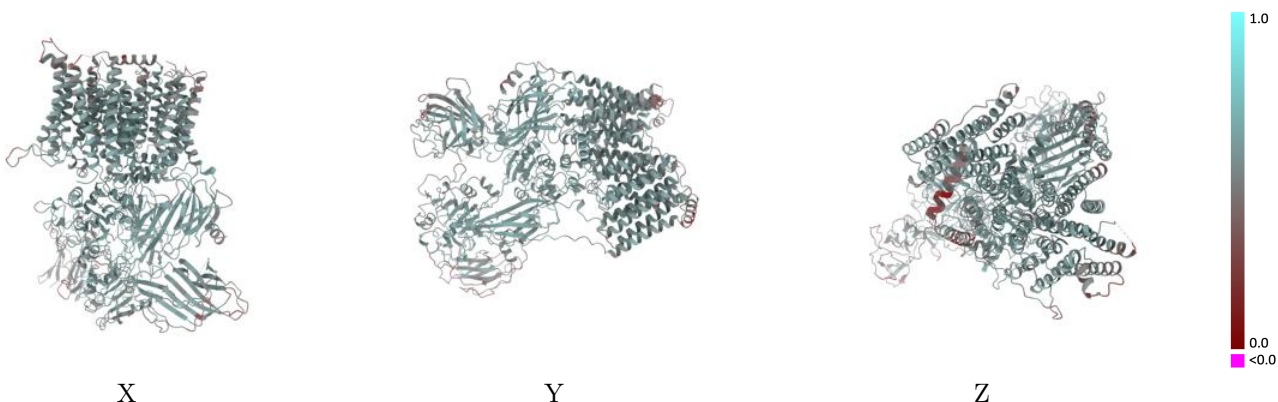
This section contains information regarding the fit between EMDB map EMD-15420 and PDB model 8AGC. Per-residue inclusion information can be found in section 3 on page 11.

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



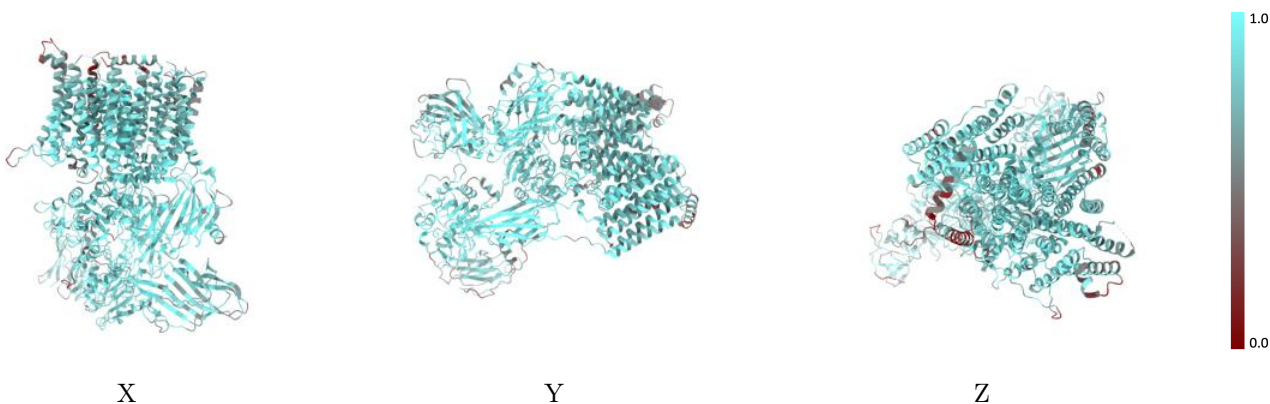
The images above show the 3D surface view of the map at the recommended contour level 0.386 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



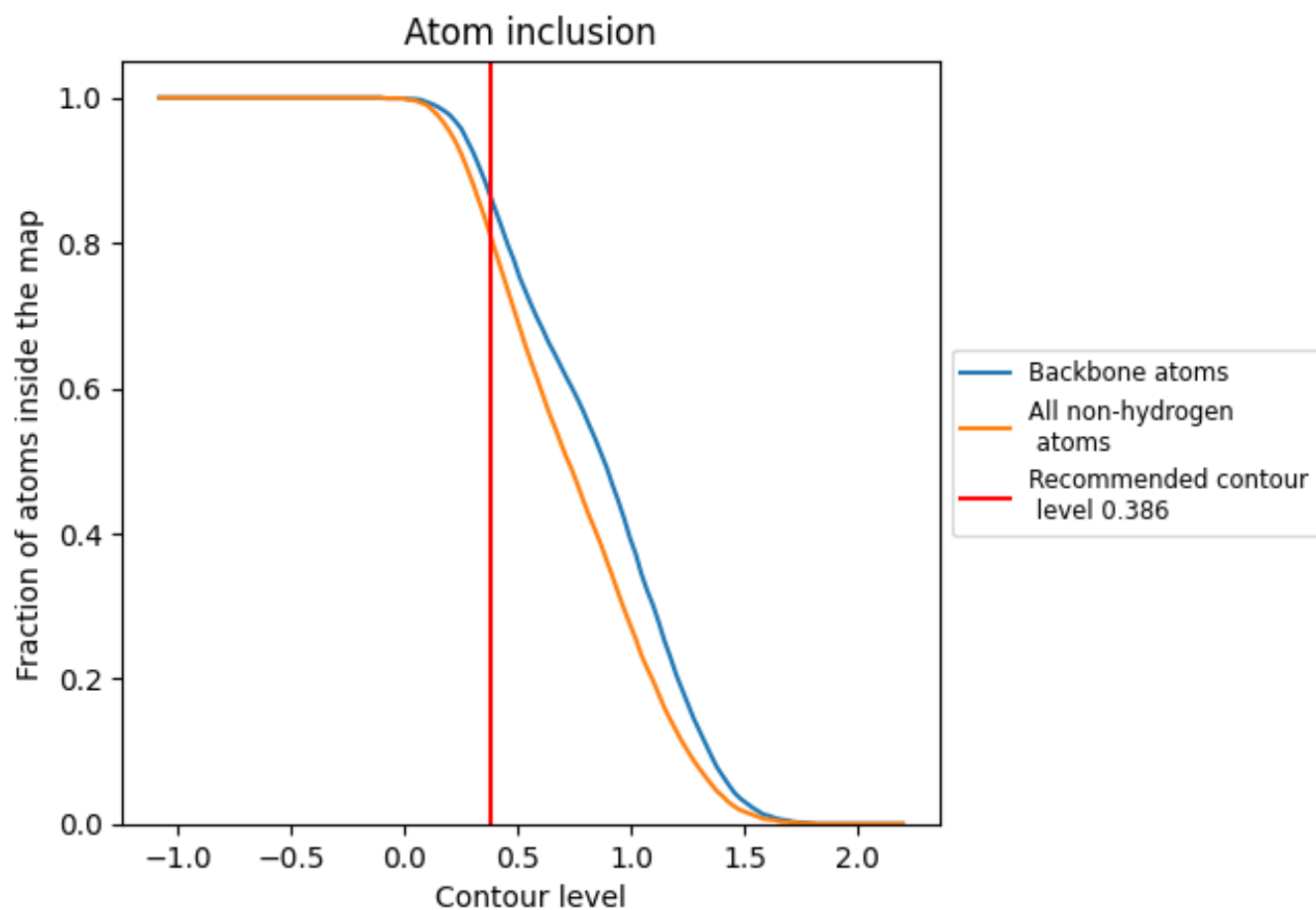
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.386).





























## 9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 80% 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 (0.386) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8050	 0.5480
A	 0.8340	 0.5680
B	 0.8120	 0.5600
C	 0.7410	 0.5360
D	 0.8050	 0.5370
E	 0.8230	 0.5530
F	 0.7070	 0.4930
G	 0.8620	 0.5590
H	 0.7410	 0.5210
I	 0.8920	 0.5780
J	 0.9640	 0.5800
K	 0.2500	 0.2970
L	 0.2440	 0.4830
P	 0.5070	 0.5580

