



Full wwPDB EM Validation Report ⓘ

Mar 13, 2026 – 11:45 AM UTC

PDB ID : 8AGB / pdb_00008agb
EMDB ID : EMD-15419
Title : Structure of yeast oligosaccharyltransferase complex with lipid-linked oligosaccharide 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 : 3.00 Å(reported)

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A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

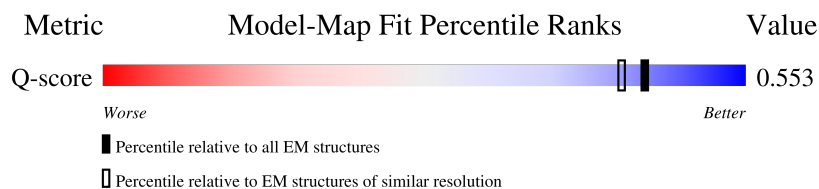
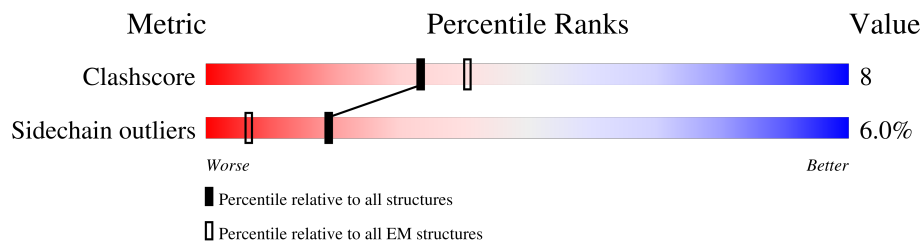
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

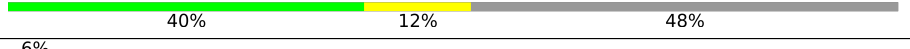
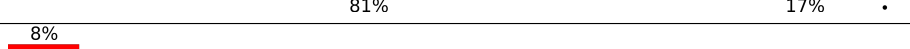
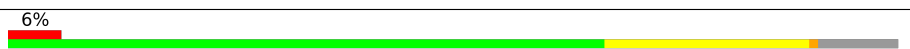
The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14081 (2.50 - 3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	718	
2	B	65	
3	C	86	
4	D	130	
5	E	476	

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Mol	Chain	Length	Quality of chain
6	F	285	21% 67% 20% 11%
7	G	430	69% 21% 8%
8	H	350	29% 5% 66%
9	I	7	29% 57% 14%
10	J	3	33% 100%
11	K	2	100%
12	L	11	50% 50%
			27% 27% 64% 9%

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 17202 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 glycosyltransferase subunit STT3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	642	Total	C	N	O	S	0	0
			5165	3422	824	896	23		

- Molecule 2 is a protein called Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit OST4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	34	Total	C	N	O	S	0	0
			258	166	38	50	4		

There are 29 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	37	ARG	-	expression tag	UNP Q99380
B	38	THR	-	expression tag	UNP Q99380
B	39	LEU	-	expression tag	UNP Q99380
B	40	GLN	-	expression tag	UNP Q99380
B	41	VAL	-	expression tag	UNP Q99380
B	42	ASP	-	expression tag	UNP Q99380
B	43	GLY	-	expression tag	UNP Q99380
B	44	GLY	-	expression tag	UNP Q99380
B	45	SER	-	expression tag	UNP Q99380
B	46	GLY	-	expression tag	UNP Q99380
B	47	GLY	-	expression tag	UNP Q99380
B	48	SER	-	expression tag	UNP Q99380
B	49	LEU	-	expression tag	UNP Q99380
B	50	GLU	-	expression tag	UNP Q99380
B	51	VAL	-	expression tag	UNP Q99380
B	52	LEU	-	expression tag	UNP Q99380
B	53	PHE	-	expression tag	UNP Q99380
B	54	GLN	-	expression tag	UNP Q99380
B	55	GLY	-	expression tag	UNP Q99380
B	56	PRO	-	expression tag	UNP Q99380

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Chain	Residue	Modelled	Actual	Comment	Reference
B	57	THR	-	expression tag	UNP Q99380
B	58	GLU	-	expression tag	UNP Q99380
B	59	THR	-	expression tag	UNP Q99380
B	60	SER	-	expression tag	UNP Q99380
B	61	GLN	-	expression tag	UNP Q99380
B	62	VAL	-	expression tag	UNP Q99380
B	63	ALA	-	expression tag	UNP Q99380
B	64	PRO	-	expression tag	UNP Q99380
B	65	ALA	-	expression tag	UNP Q99380

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	110	Total	C	N	O	S	0	0
			899	606	142	145	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	433	Total	C	N	O	S	0	0
			3499	2273	559	660	7		

- Molecule 6 is a protein called Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit SWP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	255	Total	C	N	O	S	0	0
			1914	1255	316	339	4		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	285	THR	-	expression tag	UNP Q02795

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Chain	Residue	Modelled	Actual	Comment	Reference
F	286	ILE	-	expression tag	UNP Q02795

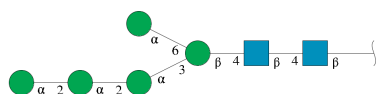
- Molecule 7 is a protein called Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit WBP1.

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

- Molecule 8 is a protein called Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit 3.

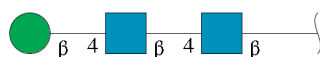
Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	120	Total	C	N	O	S	0	0
			973	662	147	159	5		

- Molecule 9 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
9	I	7	Total	C	N	O		0	0
			83	46	2	35			

- Molecule 10 is an oligosaccharide called 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
10	J	3	Total	C	N	O		0	0
			39	22	2	15			

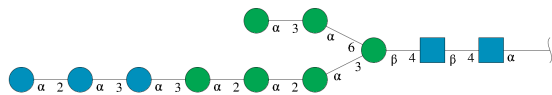
- Molecule 11 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-

acetamido-2-deoxy-beta-D-glucopyranose.



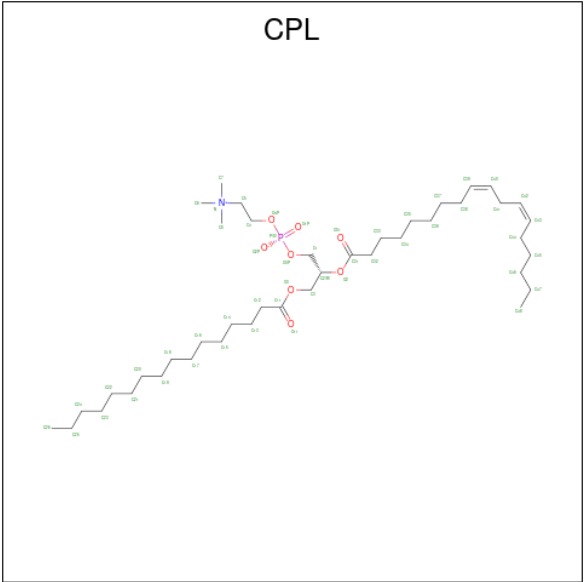
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
11	K	2	28	16	2	10	0	0

- 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-mannopyranos e-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-ace tamido-2-deoxy-alpha-D-glucopyranose.



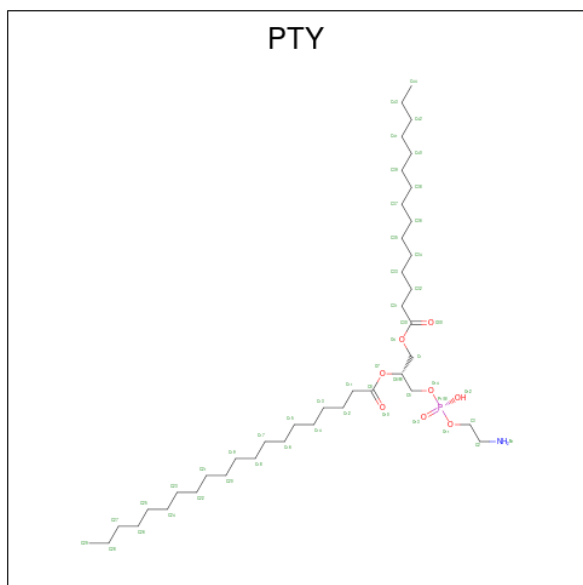
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
12	L	11	127	70	2	55	0	0

- Molecule 13 is 1-PALMITOYL-2-LINOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: CPL) (formula: C₄₂H₈₀NO₈P).



Mol	Chain	Residues	Atoms					AltConf
13	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
13	B	1	Total	C	N	O	P	0
			52	42	1	8	1	
13	E	1	Total	C	N	O	P	0
			52	42	1	8	1	
13	G	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 14 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula: $C_{40}H_{80}NO_8P$).

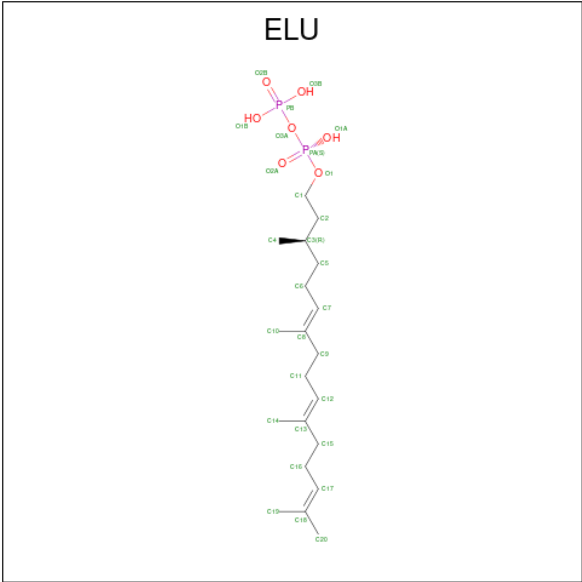


Mol	Chain	Residues	Atoms					AltConf
14	A	1	Total	C	N	O	P	0
			42	32	1	8	1	
14	F	1	Total	C	N	O	P	0
			42	32	1	8	1	

- Molecule 15 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

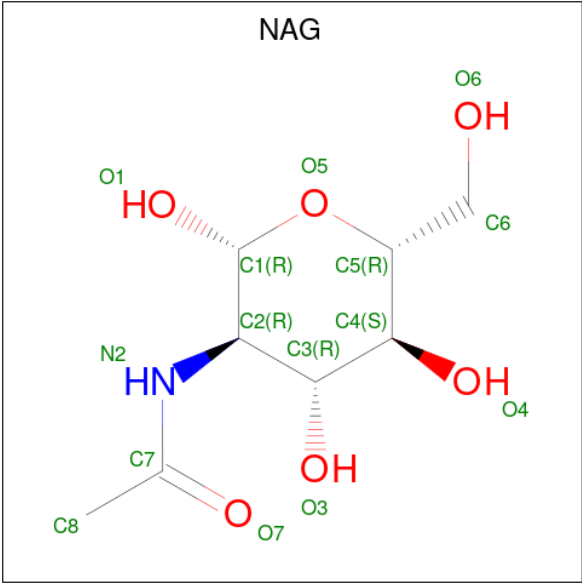
Mol	Chain	Residues	Atoms		AltConf
15	A	1	Total	Mn	0
			1	1	

- Molecule 16 is phosphono [(3 {R},6 {E},10 {E})-3,7,11,15-tetramethylhexadeca-6,10,14-trienyl] hydrogen phosphate (CCD ID: ELU) (formula: $C_{20}H_{38}O_7P_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 17 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).

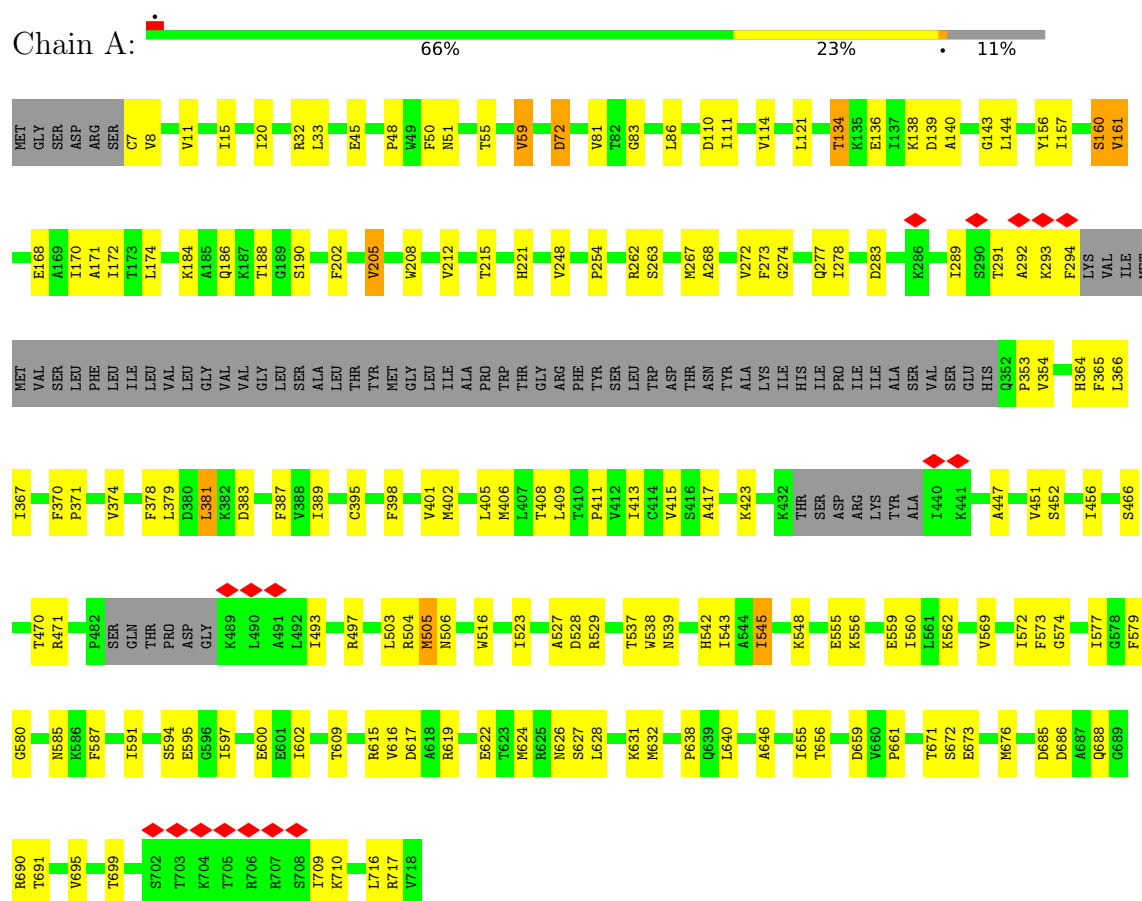


Mol	Chain	Residues	Atoms				AltConf
17	G	1	Total	C	N	O	0
			14	8	1	5	
17	G	1	Total	C	N	O	0
			14	8	1	5	

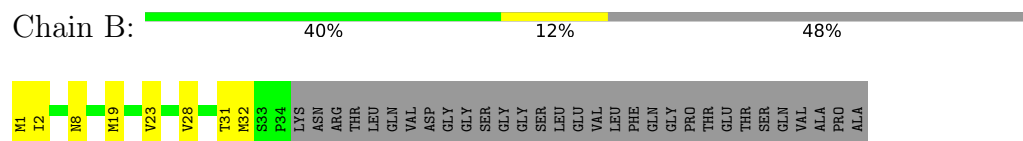
3 Residue-property plots

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

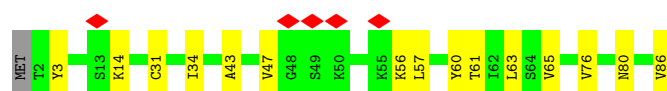
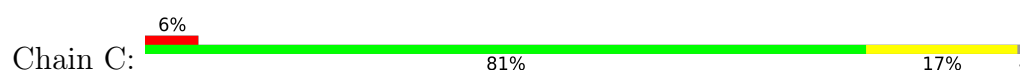
- Molecule 1: Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit STT3



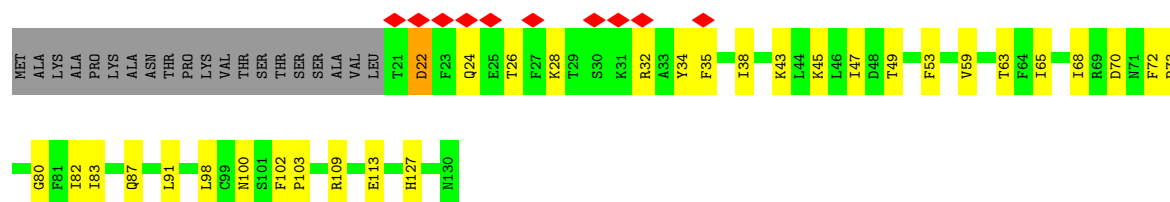
- Molecule 2: Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit OST4



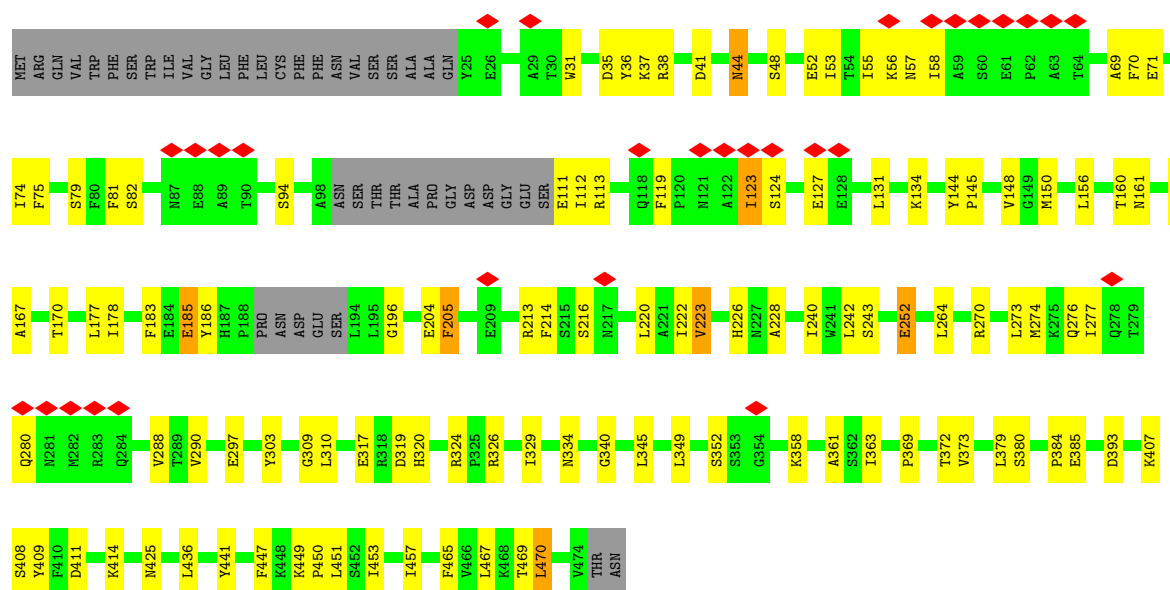
- Molecule 3: Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit OST5



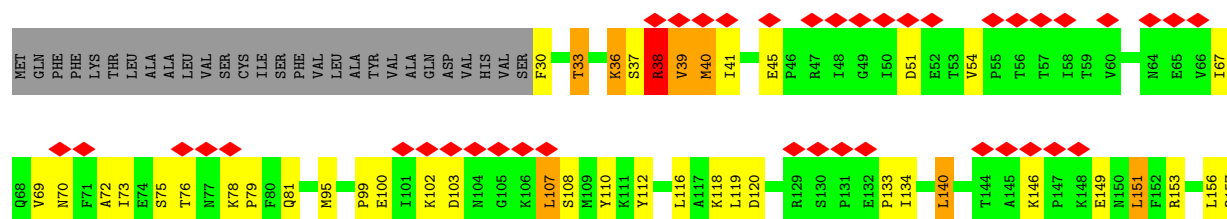
- Molecule 4: Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit OST2



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

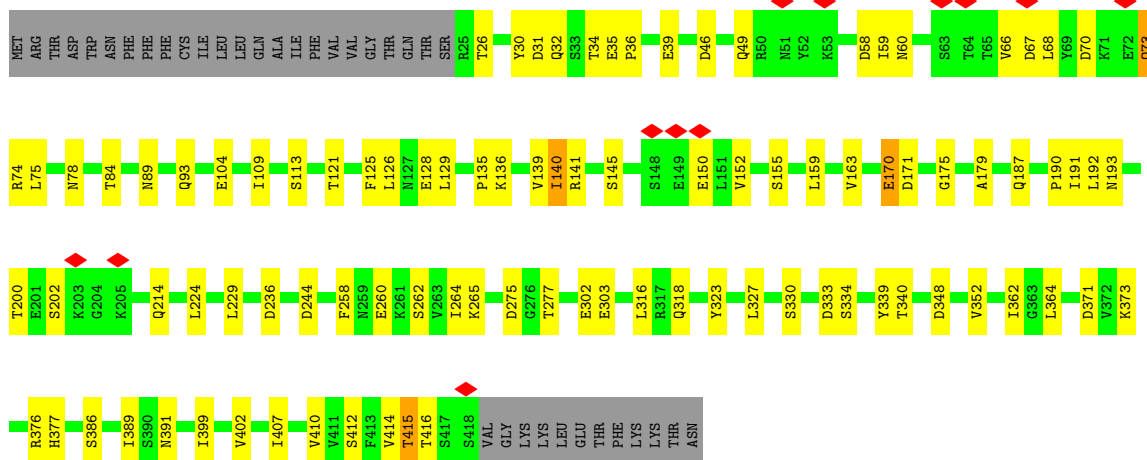


- Molecule 6: Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit SWP1

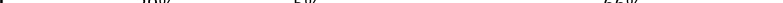


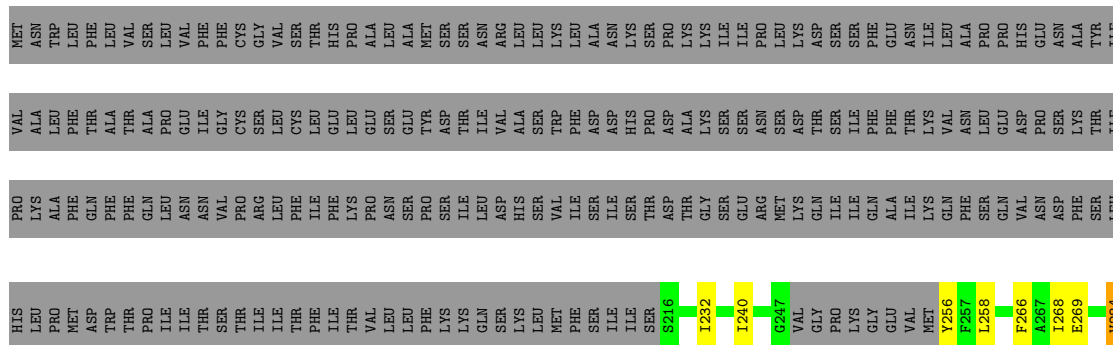
- Molecule 7: Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit WBP1

Chain G: 69% 21% 8%



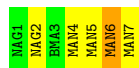
- Molecule 8: Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit 3

Chain H: 

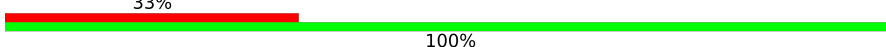


- Molecule 9: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I: 29% 57% 14%



- Molecule 10: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  33% 100%



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

Chain K:  100% 50% 50%



- 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

Chain L:  27% 27% 64% 9%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	89566	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	2.243	Depositor
Minimum map value	-1.111	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.061	Depositor
Recommended contour level	0.417	Depositor
Map size (Å)	326.40002, 326.40002, 326.40002	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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: MAN, GLC, MN, NAG, NDG, BMA, ELU, CPL, PTY

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	0.21	0/5316	0.43	0/7229
2	B	0.14	0/261	0.29	0/354
3	C	0.16	0/684	0.36	0/926
4	D	0.17	0/922	0.36	0/1243
5	E	0.16	0/3599	0.40	0/4897
6	F	0.18	0/1958	0.55	1/2666 (0.0%)
7	G	0.17	0/3283	0.40	0/4459
8	H	0.14	0/1001	0.33	0/1362
All	All	0.18	0/17024	0.42	1/23136 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	38	ARG	N-CA-C	-5.62	98.84	110.80

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	5165	0	5122	103	0
2	B	258	0	267	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	666	0	677	11	0
4	D	899	0	927	24	0
5	E	3499	0	3383	64	0
6	F	1914	0	1895	40	0
7	G	3201	0	3102	53	0
8	H	973	0	998	12	0
9	I	83	0	70	2	0
10	J	39	0	34	0	0
11	K	28	0	25	0	0
12	L	127	0	105	3	0
13	A	52	0	80	3	0
13	B	52	0	80	1	0
13	E	52	0	80	0	0
13	G	52	0	80	1	0
14	A	42	0	60	1	0
14	F	42	0	60	0	0
15	A	1	0	0	0	0
16	A	29	0	0	0	0
17	G	28	0	26	0	0
All	All	17202	0	17071	286	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 8.

All (286) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:717:ARG:H	7:G:214:GLN:HE22	1.30	0.79
1:A:398:PHE:HB3	1:A:405:LEU:HD12	1.66	0.78
4:D:47:ILE:HG23	4:D:91:LEU:HD12	1.76	0.67
7:G:262:SER:HB3	7:G:364:LEU:HD23	1.77	0.67
1:A:110:ASP:OD1	1:A:111:ILE:N	2.27	0.66
1:A:466:SER:O	1:A:470:THR:HG23	1.94	0.66
1:A:134:THR:HB	1:A:143:GLY:HA2	1.79	0.64
6:F:156:LEU:HD21	6:F:158:LEU:HB3	1.81	0.63
4:D:102:PHE:HB3	4:D:103:PRO:HD2	1.81	0.62
1:A:136:GLU:OE2	1:A:184:LYS:NZ	2.32	0.62
1:A:688:GLN:HE22	7:G:104:GLU:HG2	1.64	0.62
2:B:31:THR:HG23	2:B:32:MET:HG2	1.80	0.62
6:F:253:TYR:HH	7:G:386:SER:HG	1.47	0.61
7:G:175:GLY:H	7:G:236:ASP:HB3	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:159:LEU:HD12	7:G:190:PRO:HB2	1.84	0.60
5:E:69:ALA:HB1	5:E:112:ILE:HD12	1.83	0.60
4:D:49:THR:OG1	6:F:215:TRP:NE1	2.35	0.59
6:F:199:ILE:O	6:F:203:ILE:HG12	2.03	0.59
6:F:51:ASP:O	6:F:153:ARG:NH2	2.36	0.59
5:E:411:ASP:OD1	5:E:449:LYS:NZ	2.35	0.58
6:F:30:PHE:N	6:F:108:SER:HG	2.01	0.58
5:E:177:LEU:HD12	5:E:222:ILE:HD13	1.85	0.58
6:F:75:SER:OG	6:F:76:THR:N	2.35	0.58
6:F:246:GLU:HG3	7:G:407:ILE:HD11	1.85	0.57
1:A:32:ARG:NE	1:A:160:SER:OG	2.37	0.57
1:A:186:GLN:HE22	1:A:383:ASP:HB3	1.70	0.56
7:G:303:GLU:N	7:G:303:GLU:OE1	2.38	0.56
7:G:333:ASP:CG	7:G:334:SER:H	2.13	0.56
5:E:290:VAL:HG23	5:E:324:ARG:HG2	1.86	0.56
5:E:41:ASP:HA	5:E:178:ILE:O	2.05	0.56
1:A:573:PHE:O	1:A:676:MET:HA	2.05	0.56
6:F:95:MET:HE1	6:F:120:ASP:H	1.71	0.56
5:E:226:HIS:CE1	5:E:228:ALA:HB3	2.41	0.55
7:G:126:LEU:O	7:G:129:LEU:N	2.38	0.55
1:A:574:GLY:HA3	1:A:579:PHE:HB3	1.88	0.55
5:E:252:GLU:OE1	5:E:303:TYR:OH	2.24	0.55
5:E:71:GLU:N	5:E:71:GLU:OE2	2.36	0.55
8:H:266:PHE:N	8:H:269:GLU:OE2	2.35	0.55
7:G:70:ASP:HB2	7:G:75:LEU:HD13	1.88	0.55
5:E:38:ARG:NH1	5:E:161:ASN:OD1	2.39	0.54
5:E:144:TYR:HB3	5:E:145:PRO:HD3	1.89	0.54
1:A:685:ASP:OD1	1:A:685:ASP:N	2.39	0.54
6:F:33:THR:HB	6:F:112:TYR:HB2	1.90	0.54
1:A:695:VAL:O	1:A:699:THR:HG23	2.07	0.54
1:A:254:PRO:HD3	13:G:503:CPL:H132	1.90	0.53
2:B:1:MET:HG2	2:B:2:ILE:H	1.73	0.53
7:G:376:ARG:HG2	7:G:377:HIS:H	1.73	0.53
7:G:192:LEU:HG	7:G:193:ASN:H	1.73	0.53
1:A:577:ILE:HD11	1:A:676:MET:HE3	1.91	0.53
5:E:81:PHE:CE2	5:E:94:SER:HB2	2.44	0.53
7:G:26:THR:HG23	7:G:78:ASN:HB2	1.91	0.53
6:F:253:TYR:OH	7:G:386:SER:OG	2.21	0.52
7:G:150:GLU:HG2	7:G:175:GLY:HA2	1.91	0.52
7:G:31:ASP:OD2	7:G:84:THR:HG23	2.09	0.52
1:A:8:VAL:O	1:A:11:VAL:HG12	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:LYS:HE3	1:A:423:LYS:HG2	1.91	0.52
6:F:30:PHE:N	6:F:108:SER:O	2.43	0.52
3:C:60:TYR:CE2	5:E:465:PHE:HB2	2.45	0.52
5:E:160:THR:OG1	5:E:161:ASN:N	2.42	0.52
6:F:146:LYS:HE3	6:F:149:GLU:HB2	1.92	0.52
3:C:61:THR:O	3:C:65:VAL:HG23	2.11	0.51
4:D:45:LYS:O	4:D:49:THR:HG23	2.11	0.51
5:E:185:GLU:HG3	5:E:186:TYR:N	2.24	0.51
7:G:302:GLU:OE1	7:G:302:GLU:N	2.42	0.51
4:D:24:GLN:OE1	4:D:24:GLN:N	2.42	0.51
5:E:150:MET:HE2	5:E:264:LEU:HD21	1.92	0.51
4:D:32:ARG:HA	4:D:35:PHE:CE2	2.45	0.51
5:E:317:GLU:O	5:E:320:HIS:HB2	2.10	0.51
1:A:212:VAL:HA	1:A:215:THR:HG22	1.91	0.51
7:G:187:GLN:HE21	7:G:224:LEU:HD21	1.75	0.51
3:C:31:CYS:O	3:C:34:ILE:HG12	2.10	0.51
4:D:80:GLY:O	4:D:83:ILE:HG22	2.11	0.51
4:D:34:TYR:O	4:D:38:ILE:HG23	2.11	0.51
7:G:152:VAL:HG13	7:G:171:ASP:HB3	1.91	0.50
3:C:57:LEU:O	3:C:61:THR:HG23	2.10	0.50
5:E:53:ILE:HG22	5:E:55:ILE:H	1.76	0.50
1:A:580:GLY:O	1:A:585:ASN:ND2	2.43	0.50
4:D:72:PHE:HE2	7:G:389:ILE:HD13	1.75	0.50
7:G:410:VAL:O	7:G:414:VAL:HG22	2.12	0.50
5:E:310:LEU:O	5:E:326:ARG:NH1	2.45	0.50
1:A:451:VAL:HG22	8:H:317:ALA:HB2	1.94	0.50
7:G:371:ASP:OD2	7:G:373:LYS:HE2	2.12	0.50
1:A:366:LEU:HD22	1:A:417:ALA:HB1	1.93	0.50
1:A:370:PHE:O	1:A:374:VAL:HG23	2.12	0.49
6:F:160:LEU:HB3	6:F:162:PHE:CD1	2.47	0.49
1:A:640:LEU:HD11	5:E:274:MET:HE2	1.95	0.49
1:A:528:ASP:O	1:A:529:ARG:HD3	2.13	0.49
5:E:349:LEU:HD12	5:E:361:ALA:HB2	1.94	0.49
1:A:51:ASN:O	1:A:55:THR:HG22	2.13	0.49
1:A:471:ARG:HH11	2:B:8:ASN:ND2	2.11	0.49
2:B:19:MET:O	2:B:23:VAL:HG23	2.13	0.49
8:H:256:TYR:HD2	8:H:268:ILE:HD13	1.78	0.49
1:A:221:HIS:CE1	1:A:387:PHE:HB2	2.48	0.49
1:A:600:GLU:OE1	1:A:600:GLU:N	2.34	0.49
5:E:276:GLN:HG3	5:E:280:GLN:CD	2.37	0.49
1:A:190:SER:OG	4:D:113:GLU:OE2	2.31	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:452:SER:O	1:A:456:ILE:HG13	2.13	0.49
7:G:89:ASN:O	7:G:93:GLN:HG2	2.12	0.49
7:G:30:TYR:CZ	7:G:58:ASP:HB2	2.48	0.48
6:F:38:ARG:HB2	6:F:116:LEU:HB3	1.94	0.48
5:E:196:GLY:HA2	5:E:205:PHE:HB3	1.94	0.48
7:G:109:ILE:HB	7:G:229:LEU:HD12	1.96	0.48
1:A:7:CYS:SG	1:A:8:VAL:N	2.86	0.48
1:A:263:SER:O	1:A:267:MET:HG2	2.13	0.48
6:F:67:ILE:HG13	6:F:69:VAL:HG22	1.95	0.48
1:A:171:ALA:HB2	1:A:208:TRP:HB2	1.94	0.48
1:A:293:LYS:NZ	4:D:22:ASP:HB3	2.28	0.48
6:F:36:LYS:O	6:F:37:SER:HB2	2.12	0.48
6:F:81:GLN:O	6:F:81:GLN:HG3	2.13	0.48
1:A:121:LEU:HD22	13:A:801:CPL:H263	1.95	0.48
1:A:545:ILE:HD11	9:I:2:NAG:H82	1.96	0.48
7:G:32:GLN:HE21	7:G:36:PRO:HB3	1.79	0.48
1:A:268:ALA:O	1:A:272:VAL:HG23	2.13	0.47
1:A:615:ARG:HH22	1:A:619:ARG:HH11	1.61	0.47
5:E:369:PRO:HD2	5:E:372:THR:HG21	1.96	0.47
7:G:32:GLN:NE2	7:G:36:PRO:HB3	2.29	0.47
1:A:504:ARG:O	1:A:529:ARG:NH1	2.47	0.47
5:E:449:LYS:HB3	5:E:450:PRO:HD3	1.96	0.47
1:A:378:PHE:HE1	14:A:802:PTY:H111	1.79	0.47
1:A:595:GLU:HG3	1:A:602:ILE:O	2.15	0.47
1:A:628:LEU:O	1:A:632:MET:HB2	2.14	0.47
4:D:68:ILE:HG13	4:D:70:ASP:H	1.80	0.47
4:D:72:PHE:CE2	7:G:389:ILE:HD13	2.49	0.47
5:E:31:TRP:CE3	5:E:55:ILE:HG12	2.50	0.47
6:F:226:ILE:HG12	7:G:415:THR:HG23	1.97	0.47
5:E:288:VAL:HB	5:E:329:ILE:HB	1.97	0.47
12:L:1:NDG:H6C1	12:L:2:NAG:HN2	1.79	0.47
8:H:294:LEU:O	8:H:298:LEU:HB2	2.14	0.47
5:E:384:PRO:HB2	5:E:441:TYR:CE1	2.50	0.47
5:E:408:SER:OG	5:E:409:TYR:N	2.48	0.47
8:H:284:VAL:O	8:H:288:VAL:HG23	2.15	0.46
7:G:412:SER:O	7:G:416:THR:HG23	2.15	0.46
1:A:202:PHE:HA	1:A:205:VAL:HG13	1.97	0.46
3:C:14:LYS:HE2	3:C:14:LYS:HB3	1.66	0.46
5:E:270:ARG:O	5:E:274:MET:HG3	2.15	0.46
6:F:202:LEU:O	6:F:206:ILE:HG12	2.15	0.46
5:E:240:ILE:HG21	5:E:363:ILE:HD13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:ASP:OD1	1:A:72:ASP:N	2.32	0.46
7:G:59:ILE:HB	7:G:89:ASN:HB3	1.98	0.46
1:A:516:TRP:CE3	1:A:516:TRP:HA	2.50	0.46
1:A:710:LYS:HA	1:A:710:LYS:HD3	1.80	0.46
5:E:447:PHE:O	5:E:451:LEU:HD13	2.15	0.46
6:F:200:PHE:O	6:F:204:ILE:HG13	2.16	0.46
1:A:289:ILE:HD12	1:A:293:LYS:HG3	1.97	0.46
1:A:409:LEU:O	1:A:413:ILE:HG13	2.16	0.46
7:G:258:PHE:O	7:G:260:GLU:HG2	2.15	0.46
6:F:45:GLU:N	6:F:157:GLN:O	2.35	0.46
5:E:119:PHE:HE1	5:E:131:LEU:HD21	1.81	0.45
5:E:213:ARG:HG3	5:E:214:PHE:HD2	1.81	0.45
1:A:171:ALA:O	1:A:174:LEU:N	2.50	0.45
6:F:40:MET:HE3	6:F:41:ILE:H	1.81	0.45
7:G:125:PHE:O	7:G:128:GLU:HB2	2.16	0.45
1:A:81:VAL:O	1:A:83:GLY:N	2.46	0.45
1:A:274:GLY:O	1:A:278:ILE:HG12	2.16	0.45
1:A:248:VAL:HB	4:D:82:ILE:HG21	1.99	0.45
1:A:493:ILE:HD13	1:A:577:ILE:HD12	1.98	0.45
5:E:79:SER:HG	5:E:425:ASN:C	2.25	0.45
1:A:505:MET:HE3	1:A:505:MET:HB3	1.67	0.45
1:A:556:LYS:O	1:A:560:ILE:HG13	2.16	0.45
6:F:39:VAL:HG23	6:F:162:PHE:CE2	2.51	0.45
7:G:163:VAL:HG11	7:G:191:ILE:HD13	1.96	0.45
1:A:156:TYR:CE1	1:A:172:ILE:HG21	2.51	0.45
4:D:53:PHE:CD2	6:F:211:LEU:HB2	2.52	0.45
5:E:44:ASN:ND2	5:E:44:ASN:H	2.13	0.45
5:E:303:TYR:CE2	5:E:340:GLY:HA3	2.51	0.45
1:A:291:THR:HG23	1:A:292:ALA:H	1.81	0.45
3:C:43:ALA:HB2	3:C:63:LEU:HB3	1.99	0.45
1:A:157:ILE:O	1:A:161:VAL:HG23	2.16	0.45
1:A:497:ARG:NH2	5:E:309:GLY:HA3	2.32	0.45
3:C:63:LEU:HD23	3:C:63:LEU:HA	1.84	0.45
5:E:56:LYS:HG2	5:E:57:ASN:N	2.31	0.45
5:E:297:GLU:OE2	5:E:297:GLU:N	2.50	0.45
6:F:45:GLU:O	6:F:157:GLN:HB3	2.17	0.45
7:G:327:LEU:HB3	7:G:339:TYR:HB3	1.98	0.45
1:A:401:VAL:HG12	1:A:402:MET:HG2	1.98	0.45
1:A:622:GLU:HG3	1:A:626:ASN:ND2	2.32	0.45
4:D:43:LYS:O	4:D:47:ILE:HG13	2.17	0.45
7:G:140:ILE:HD11	7:G:179:ALA:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:B:101:CPL:H412	13:B:101:CPL:H441	1.73	0.45
5:E:385:GLU:HG2	5:E:414:LYS:O	2.17	0.45
4:D:32:ARG:HA	4:D:35:PHE:CD2	2.52	0.44
6:F:107:LEU:HD22	6:F:107:LEU:HA	1.82	0.44
7:G:376:ARG:HD2	7:G:377:HIS:O	2.18	0.44
1:A:11:VAL:O	1:A:15:ILE:HG12	2.17	0.44
1:A:672:SER:OG	1:A:673:GLU:N	2.50	0.44
1:A:686:ASP:OD2	1:A:690:ARG:NE	2.50	0.44
7:G:46:ASP:HA	7:G:49:GLN:HG2	1.99	0.44
1:A:523:ILE:O	1:A:527:ALA:HB3	2.18	0.44
1:A:411:PRO:O	1:A:415:VAL:HG23	2.17	0.44
1:A:471:ARG:HH11	2:B:8:ASN:HD22	1.66	0.44
4:D:28:LYS:O	4:D:32:ARG:HG3	2.18	0.44
5:E:166:SER:OG	5:E:167:ALA:N	2.50	0.44
5:E:352:SER:HB2	5:E:358:LYS:HB3	2.00	0.44
1:A:548:LYS:HB2	1:A:594:SER:HB2	2.00	0.44
7:G:155:SER:HB2	7:G:170:GLU:O	2.17	0.44
1:A:656:THR:OG1	1:A:659:ASP:OD1	2.35	0.43
5:E:469:THR:O	5:E:469:THR:HG22	2.18	0.43
6:F:30:PHE:N	6:F:108:SER:OG	2.50	0.43
7:G:113:SER:O	7:G:113:SER:OG	2.35	0.43
5:E:242:LEU:HD23	5:E:345:LEU:HD11	2.00	0.43
1:A:273:PHE:O	1:A:277:GLN:HG2	2.19	0.43
1:A:506:ASN:ND2	5:E:334:ASN:H	2.15	0.43
3:C:76:VAL:HG13	3:C:86:VAL:HG21	2.00	0.43
5:E:123:ILE:HG23	5:E:127:GLU:HB2	2.00	0.43
6:F:221:ALA:HA	7:G:416:THR:HG21	1.99	0.43
7:G:34:THR:HG23	7:G:35:GLU:H	1.84	0.43
4:D:28:LYS:HB3	4:D:32:ARG:NH1	2.33	0.43
13:A:801:CPL:H441	13:A:801:CPL:H472	1.82	0.43
6:F:133:PRO:HB3	6:F:159:ASN:OD1	2.19	0.43
1:A:353:PRO:HB3	8:H:240:ILE:HD12	2.01	0.43
1:A:406:MET:HE3	1:A:406:MET:HB2	1.78	0.43
1:A:638:PRO:HA	1:A:646:ALA:HB2	1.99	0.43
5:E:124:SER:OG	5:E:127:GLU:HG2	2.19	0.43
5:E:273:LEU:O	5:E:277:ILE:HG12	2.19	0.43
7:G:316:LEU:HB3	7:G:323:TYR:HB2	2.00	0.43
1:A:277:GLN:HE21	1:A:277:GLN:HB3	1.65	0.43
5:E:35:ASP:OD1	5:E:36:TYR:N	2.51	0.43
1:A:631:LYS:HD2	1:A:661:PRO:HG2	2.01	0.43
1:A:59:VAL:HG21	1:A:111:ILE:HD13	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:ASP:OD1	1:A:140:ALA:N	2.50	0.43
1:A:378:PHE:CE2	1:A:389:ILE:HG21	2.54	0.43
5:E:41:ASP:HB3	5:E:48:SER:OG	2.18	0.43
7:G:264:ILE:HD11	7:G:364:LEU:HD13	2.00	0.43
1:A:353:PRO:HG3	8:H:240:ILE:HB	2.01	0.43
6:F:133:PRO:HB2	6:F:157:GLN:HG3	2.01	0.43
1:A:367:ILE:HG13	8:H:232:ILE:HD12	2.01	0.42
3:C:47:VAL:HA	3:C:56:LYS:HE3	2.01	0.42
4:D:109:ARG:O	4:D:113:GLU:HG3	2.19	0.42
1:A:186:GLN:HE22	1:A:383:ASP:CB	2.32	0.42
1:A:20:ILE:HG21	1:A:144:LEU:HD22	2.01	0.42
1:A:569:VAL:HG11	1:A:632:MET:HE1	2.02	0.42
1:A:717:ARG:H	7:G:214:GLN:NE2	2.06	0.42
3:C:80:ASN:HD21	3:C:86:VAL:H	1.67	0.42
5:E:205:PHE:CD1	5:E:205:PHE:N	2.88	0.42
6:F:140:LEU:HD12	6:F:151:LEU:HB3	2.00	0.42
7:G:275:ASP:OD1	7:G:277:THR:OG1	2.29	0.42
7:G:399:ILE:O	7:G:402:VAL:HG12	2.19	0.42
7:G:73:GLN:HE21	7:G:73:GLN:HB2	1.59	0.42
8:H:258:LEU:HD13	8:H:266:PHE:CZ	2.54	0.42
4:D:73:PRO:HA	12:L:8:GLC:O3	2.19	0.42
5:E:111:GLU:HG2	5:E:113:ARG:HH22	1.84	0.42
1:A:278:ILE:HG12	1:A:278:ILE:H	1.72	0.42
5:E:453:ILE:O	5:E:457:ILE:HG13	2.20	0.42
8:H:324:PHE:O	8:H:328:THR:HG23	2.19	0.42
1:A:562:LYS:HB3	1:A:562:LYS:HE2	1.70	0.42
5:E:37:LYS:HB2	5:E:52:GLU:HB3	2.01	0.42
6:F:159:ASN:O	6:F:160:LEU:HD23	2.20	0.42
6:F:227:PRO:HB2	6:F:231:THR:HG23	2.02	0.42
1:A:168:GLU:O	1:A:172:ILE:HG22	2.19	0.42
1:A:157:ILE:HG21	1:A:470:THR:HB	2.02	0.42
5:E:470:LEU:HD12	5:E:470:LEU:HA	1.83	0.42
4:D:127:HIS:HD2	6:F:252:TYR:OH	2.03	0.41
12:L:11:MAN:O4	12:L:11:MAN:O6	2.37	0.41
1:A:289:ILE:HG21	4:D:26:THR:HG22	2.03	0.41
1:A:447:ALA:HB2	8:H:310:ALA:HB1	2.01	0.41
5:E:183:PHE:HB3	5:E:222:ILE:HD11	2.02	0.41
1:A:157:ILE:HD12	1:A:470:THR:HG21	2.02	0.41
1:A:555:GLU:O	1:A:559:GLU:HG2	2.20	0.41
5:E:156:LEU:O	5:E:223:VAL:HA	2.20	0.41
1:A:33:LEU:HD13	13:A:801:CPL:H132	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:PHE:HE2	1:A:86:LEU:HD13	1.86	0.41
5:E:414:LYS:HB2	5:E:414:LYS:HE2	1.89	0.41
7:G:389:ILE:HG22	7:G:391:ASN:H	1.85	0.41
6:F:40:MET:HE3	6:F:40:MET:HB3	1.84	0.41
1:A:627:SER:O	1:A:631:LYS:HG2	2.20	0.41
3:C:3:TYR:HD1	5:E:393:ASP:HB3	1.85	0.41
5:E:134:LYS:HB3	5:E:134:LYS:HE3	1.80	0.41
6:F:99:PRO:HB2	6:F:110:TYR:HB3	2.02	0.41
7:G:39:GLU:H	7:G:39:GLU:HG2	1.70	0.41
8:H:339:PRO:O	8:H:341:PRO:HD3	2.21	0.41
1:A:364:HIS:C	1:A:366:LEU:H	2.29	0.41
5:E:70:PHE:HD2	5:E:75:PHE:HD2	1.70	0.41
7:G:330:SER:HB3	7:G:340:THR:HG22	2.02	0.41
1:A:587:PHE:O	1:A:591:ILE:HG13	2.21	0.40
1:A:709:ILE:HG21	7:G:135:PRO:HG3	2.03	0.40
5:E:361:ALA:O	5:E:436:LEU:HA	2.21	0.40
5:E:407:LYS:HB3	5:E:407:LYS:HE2	1.92	0.40
6:F:72:ALA:C	6:F:73:ILE:HD13	2.46	0.40
1:A:538:TRP:CZ3	1:A:539:ASN:HB2	2.55	0.40
1:A:110:ASP:O	1:A:114:VAL:HG23	2.20	0.40
1:A:381:LEU:HD12	1:A:381:LEU:HA	1.92	0.40
5:E:37:LYS:HB3	5:E:37:LYS:HE3	1.71	0.40
6:F:184:ILE:HD11	9:I:6:MAN:H3	2.04	0.40
1:A:616:VAL:HG12	1:A:624:MET:HE2	2.04	0.40
4:D:87:GLN:HE21	4:D:91:LEU:CD2	2.35	0.40
6:F:79:PRO:HG3	6:F:140:LEU:HB3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

5.3.2 Protein sidechains [i](#)

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	542/613 (88%)	508 (94%)	34 (6%)	16	48
2	B	31/55 (56%)	30 (97%)	1 (3%)	34	67
3	C	74/75 (99%)	74 (100%)	0	100	100
4	D	99/115 (86%)	93 (94%)	6 (6%)	17	49
5	E	389/426 (91%)	368 (95%)	21 (5%)	20	53
6	F	193/248 (78%)	173 (90%)	20 (10%)	7	28
7	G	359/392 (92%)	337 (94%)	22 (6%)	17	49
8	H	104/316 (33%)	100 (96%)	4 (4%)	29	63
All	All	1791/2240 (80%)	1683 (94%)	108 (6%)	19	50

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	GLU
1	A	48	PRO
1	A	59	VAL
1	A	72	ASP
1	A	134	THR
1	A	160	SER
1	A	161	VAL
1	A	170	ILE
1	A	188	THR
1	A	205	VAL
1	A	262	ARG
1	A	283	ASP
1	A	294	PHE
1	A	354	VAL
1	A	365	PHE
1	A	371	PRO
1	A	379	LEU
1	A	381	LEU
1	A	395	CYS
1	A	408	THR
1	A	503	LEU
1	A	505	MET
1	A	537	THR
1	A	542	HIS

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Mol	Chain	Res	Type
1	A	543	ILE
1	A	545	ILE
1	A	572	ILE
1	A	597	ILE
1	A	609	THR
1	A	617	ASP
1	A	655	ILE
1	A	671	THR
1	A	691	THR
1	A	716	LEU
2	B	28	VAL
4	D	22	ASP
4	D	59	VAL
4	D	63	THR
4	D	65	ILE
4	D	98	LEU
4	D	100	ASN
5	E	44	ASN
5	E	58	ILE
5	E	74	ILE
5	E	82	SER
5	E	123	ILE
5	E	148	VAL
5	E	170	THR
5	E	185	GLU
5	E	204	GLU
5	E	205	PHE
5	E	216	SER
5	E	220	LEU
5	E	223	VAL
5	E	243	SER
5	E	252	GLU
5	E	319	ASP
5	E	373	VAL
5	E	379	LEU
5	E	380	SER
5	E	467	LEU
5	E	470	LEU
6	F	33	THR
6	F	36	LYS
6	F	38	ARG
6	F	39	VAL

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Mol	Chain	Res	Type
6	F	40	MET
6	F	54	VAL
6	F	70	ASN
6	F	78	LYS
6	F	100	GLU
6	F	102	LYS
6	F	103	ASP
6	F	107	LEU
6	F	118	LYS
6	F	119	LEU
6	F	134	ILE
6	F	140	LEU
6	F	151	LEU
6	F	159	ASN
6	F	175	PHE
6	F	186	HIS
7	G	60	ASN
7	G	66	VAL
7	G	67	ASP
7	G	68	LEU
7	G	73	GLN
7	G	74	ARG
7	G	121	THR
7	G	136	LYS
7	G	139	VAL
7	G	140	ILE
7	G	141	ARG
7	G	145	SER
7	G	170	GLU
7	G	200	THR
7	G	202	SER
7	G	244	ASP
7	G	265	LYS
7	G	318	GLN
7	G	348	ASP
7	G	352	VAL
7	G	362	ILE
7	G	415	THR
8	H	284	VAL
8	H	286	VAL
8	H	291	ILE
8	H	312	LEU

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	186	GLN
1	A	193	HIS
1	A	266	HIS
1	A	277	GLN
1	A	506	ASN
1	A	535	ASN
1	A	542	HIS
1	A	653	GLN
1	A	688	GLN
2	B	6	GLN
2	B	8	ASN
3	C	21	HIS
3	C	25	GLN
3	C	80	ASN
4	D	87	GLN
4	D	108	ASN
4	D	122	HIS
4	D	127	HIS
5	E	44	ASN
5	E	118	GLN
5	E	217	ASN
5	E	226	HIS
5	E	235	ASN
5	E	334	ASN
5	E	367	ASN
5	E	416	HIS
6	F	90	ASN
6	F	92	ASN
6	F	104	ASN
6	F	125	GLN
6	F	157	GLN
6	F	166	HIS
6	F	182	HIS
6	F	217	ASN
6	F	224	ASN
6	F	225	ASN
7	G	49	GLN
7	G	108	ASN
7	G	157	HIS
7	G	214	GLN

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Mol	Chain	Res	Type
7	G	242	ASN
7	G	243	GLN
7	G	246	ASN
7	G	271	HIS
7	G	273	HIS
7	G	307	HIS
7	G	318	GLN
7	G	391	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

23 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	$\# Z > 2$
9	NAG	I	1	9,1	14,14,15	0.42	0	17,19,21	0.48	0
9	NAG	I	2	9	14,14,15	0.22	0	17,19,21	0.48	0
9	BMA	I	3	9	11,11,12	0.42	0	15,15,17	0.76	0
9	MAN	I	4	9	11,11,12	0.62	0	15,15,17	1.15	2 (13%)
9	MAN	I	5	9	11,11,12	0.65	0	15,15,17	0.97	1 (6%)
9	MAN	I	6	9	11,11,12	0.65	0	15,15,17	0.84	1 (6%)
9	MAN	I	7	9	11,11,12	0.66	0	15,15,17	0.87	1 (6%)
10	NAG	J	1	10,5	14,14,15	0.24	0	17,19,21	0.40	0
10	NAG	J	2	10	14,14,15	0.18	0	17,19,21	0.50	0
10	BMA	J	3	10	11,11,12	0.58	0	15,15,17	0.72	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	NAG	K	1	5,11	14,14,15	0.74	1 (7%)	17,19,21	1.03	1 (5%)
11	NAG	K	2	11	14,14,15	0.23	0	17,19,21	0.53	0
12	NDG	L	1	12,16	14,14,15	0.24	0	17,19,21	0.44	0
12	MAN	L	10	12	11,11,12	1.03	1 (9%)	15,15,17	1.21	2 (13%)
12	MAN	L	11	12	11,11,12	0.86	0	15,15,17	1.25	2 (13%)
12	NAG	L	2	12	14,14,15	0.26	0	17,19,21	0.53	0
12	BMA	L	3	12	11,11,12	0.50	0	15,15,17	0.64	0
12	MAN	L	4	12	11,11,12	0.66	0	15,15,17	1.25	2 (13%)
12	MAN	L	5	12	11,11,12	0.88	1 (9%)	15,15,17	0.98	1 (6%)
12	MAN	L	6	12	11,11,12	0.62	0	15,15,17	0.88	1 (6%)
12	GLC	L	7	12	11,11,12	0.60	0	15,15,17	0.73	0
12	GLC	L	8	12	11,11,12	0.59	0	15,15,17	0.66	0
12	GLC	L	9	12	11,11,12	0.62	0	15,15,17	0.68	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	NAG	I	1	9,1	-	2/6/23/26	0/1/1/1
9	NAG	I	2	9	-	2/6/23/26	0/1/1/1
9	BMA	I	3	9	-	2/2/19/22	0/1/1/1
9	MAN	I	4	9	-	2/2/19/22	0/1/1/1
9	MAN	I	5	9	-	0/2/19/22	0/1/1/1
9	MAN	I	6	9	-	0/2/19/22	0/1/1/1
9	MAN	I	7	9	-	0/2/19/22	0/1/1/1
10	NAG	J	1	10,5	-	2/6/23/26	0/1/1/1
10	NAG	J	2	10	-	2/6/23/26	0/1/1/1
10	BMA	J	3	10	-	2/2/19/22	0/1/1/1
11	NAG	K	1	5,11	-	4/6/23/26	0/1/1/1
11	NAG	K	2	11	-	4/6/23/26	0/1/1/1
12	NDG	L	1	12,16	-	2/6/23/26	0/1/1/1
12	MAN	L	10	12	-	2/2/19/22	0/1/1/1
12	MAN	L	11	12	-	1/2/19/22	1/1/1/1
12	NAG	L	2	12	-	1/6/23/26	0/1/1/1
12	BMA	L	3	12	-	0/2/19/22	0/1/1/1
12	MAN	L	4	12	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	MAN	L	5	12	-	0/2/19/22	0/1/1/1
12	MAN	L	6	12	-	0/2/19/22	0/1/1/1
12	GLC	L	7	12	-	0/2/19/22	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)
12	L	10	MAN	C1-C2	2.63	1.58	1.52
11	K	1	NAG	O5-C1	2.40	1.47	1.43
12	L	5	MAN	O5-C1	-2.01	1.40	1.43

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	K	1	NAG	C1-O5-C5	3.95	117.48	112.19
12	L	11	MAN	C1-O5-C5	3.41	116.76	112.19
12	L	4	MAN	O2-C2-C3	-3.10	103.73	110.15
9	I	4	MAN	O2-C2-C3	-3.10	103.73	110.15
12	L	5	MAN	O2-C2-C3	-3.03	103.88	110.15
12	L	4	MAN	C1-O5-C5	2.99	116.19	112.19
9	I	5	MAN	O2-C2-C3	-2.59	104.79	110.15
12	L	10	MAN	C1-C2-C3	2.59	113.41	109.64
9	I	4	MAN	C1-O5-C5	2.52	115.57	112.19
12	L	11	MAN	O2-C2-C3	-2.18	105.63	110.15
12	L	6	MAN	O2-C2-C3	-2.16	105.67	110.15
9	I	6	MAN	O2-C2-C3	-2.15	105.70	110.15
9	I	7	MAN	O2-C2-C3	-2.12	105.75	110.15
12	L	10	MAN	O2-C2-C3	-2.10	105.79	110.15

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	L	4	MAN	C4-C5-C6-O6
12	L	1	NDG	O5-C5-C6-O6
9	I	2	NAG	O5-C5-C6-O6
12	L	4	MAN	O5-C5-C6-O6
10	J	2	NAG	O5-C5-C6-O6
9	I	4	MAN	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
9	I	2	NAG	C4-C5-C6-O6
9	I	3	BMA	C4-C5-C6-O6
12	L	1	NDG	C4-C5-C6-O6
9	I	4	MAN	C4-C5-C6-O6
10	J	2	NAG	C4-C5-C6-O6
9	I	1	NAG	C8-C7-N2-C2
9	I	1	NAG	O7-C7-N2-C2
11	K	1	NAG	C8-C7-N2-C2
11	K	1	NAG	O7-C7-N2-C2
11	K	1	NAG	O5-C5-C6-O6
9	I	3	BMA	O5-C5-C6-O6
10	J	1	NAG	C4-C5-C6-O6
12	L	9	GLC	O5-C5-C6-O6
12	L	11	MAN	O5-C5-C6-O6
10	J	1	NAG	O5-C5-C6-O6
11	K	2	NAG	C4-C5-C6-O6
10	J	3	BMA	C4-C5-C6-O6
11	K	2	NAG	O5-C5-C6-O6
11	K	2	NAG	C3-C2-N2-C7
12	L	10	MAN	C4-C5-C6-O6
12	L	10	MAN	O5-C5-C6-O6
11	K	2	NAG	C1-C2-N2-C7
11	K	1	NAG	C4-C5-C6-O6
10	J	3	BMA	O5-C5-C6-O6
12	L	2	NAG	O5-C5-C6-O6

All (1) ring outliers are listed below:

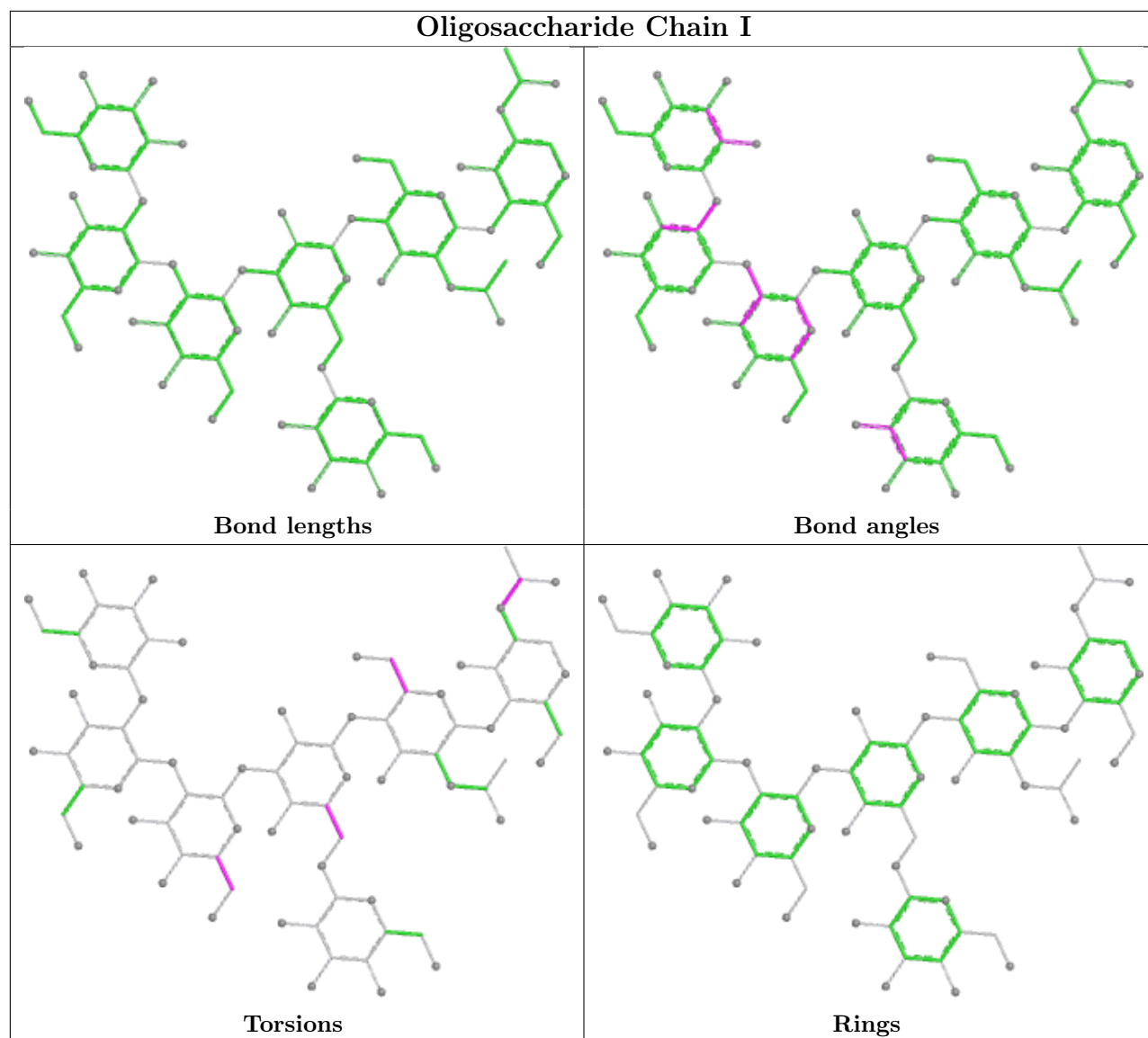
Mol	Chain	Res	Type	Atoms
12	L	11	MAN	C1-C2-C3-C4-C5-O5

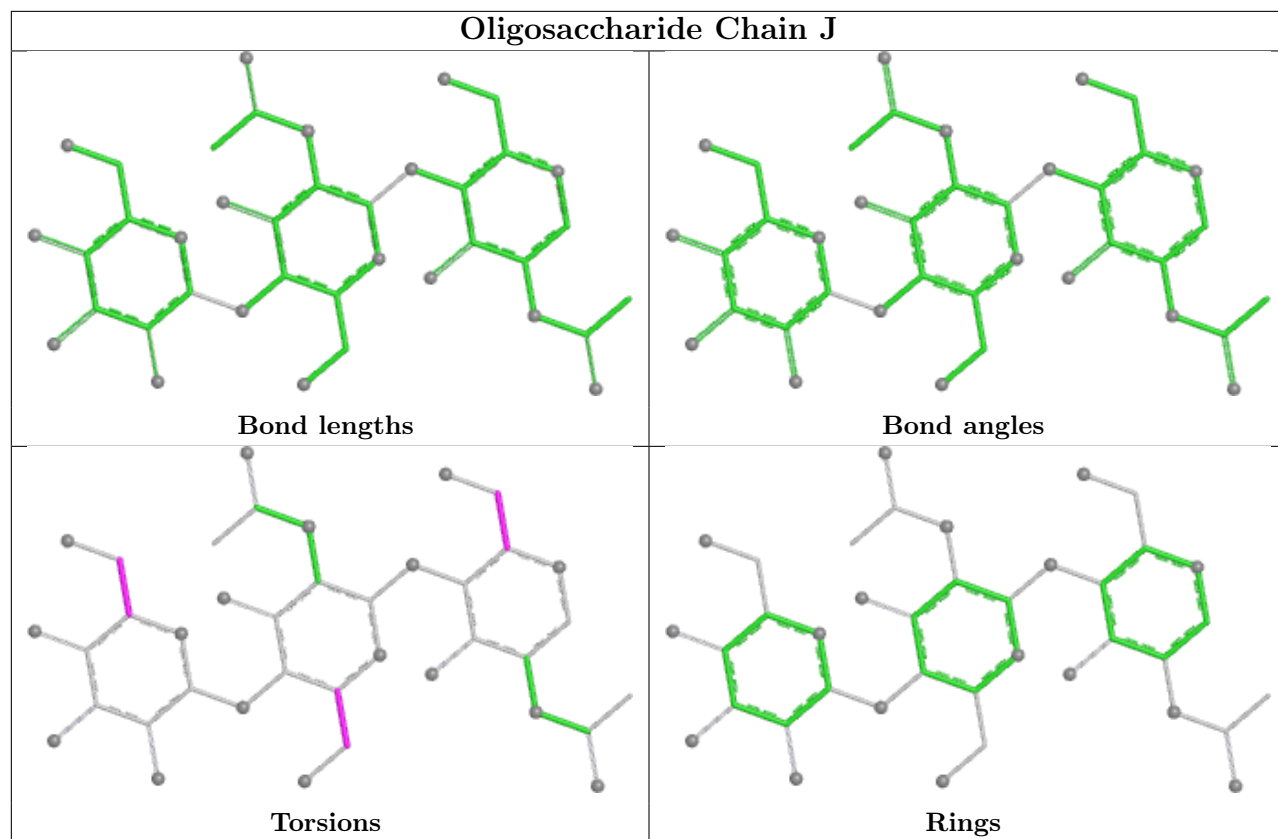
6 monomers are involved in 5 short contacts:

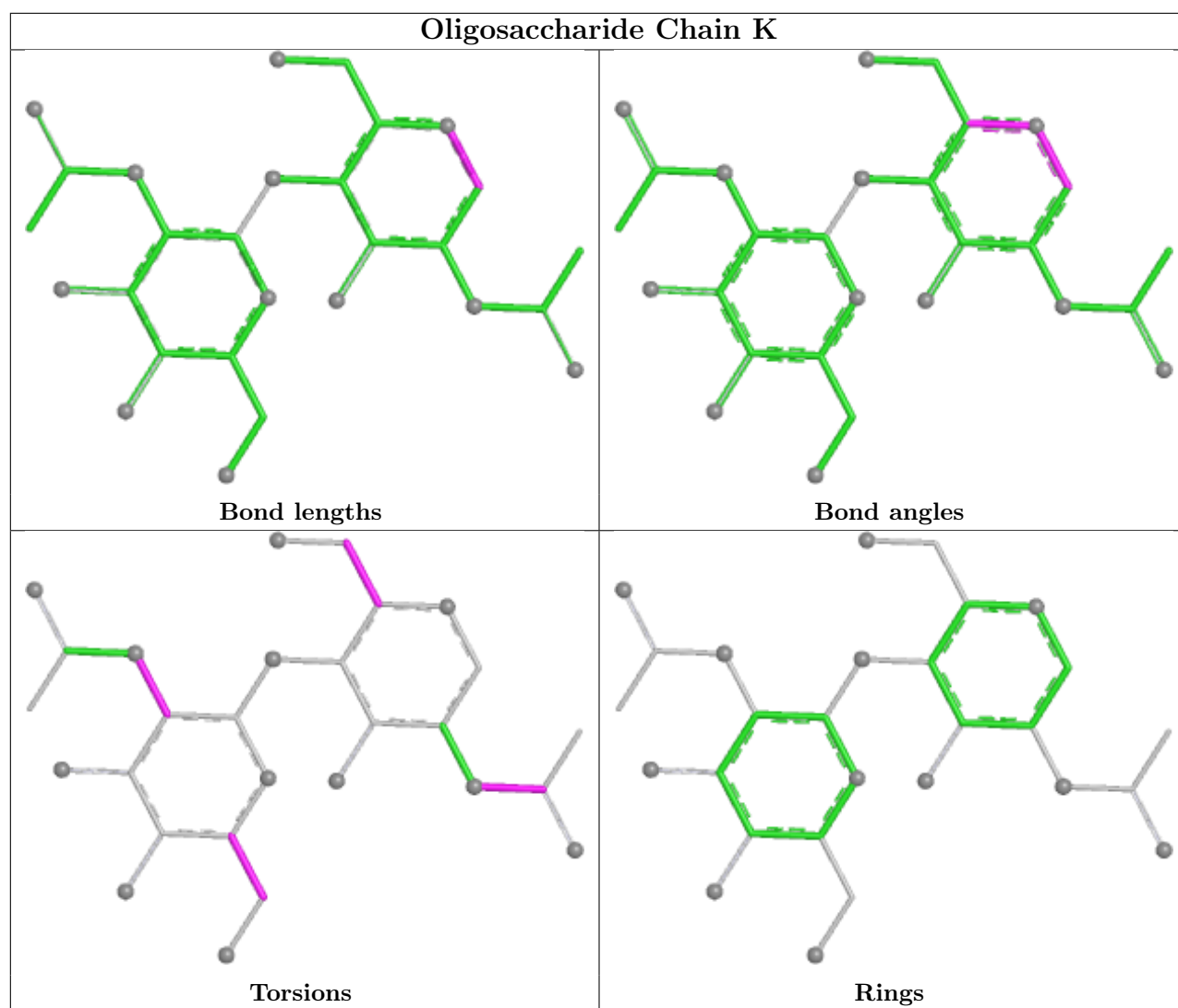
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	I	6	MAN	1	0
12	L	1	NDG	1	0
12	L	8	GLC	1	0
12	L	2	NAG	1	0
9	I	2	NAG	1	0
12	L	11	MAN	1	0

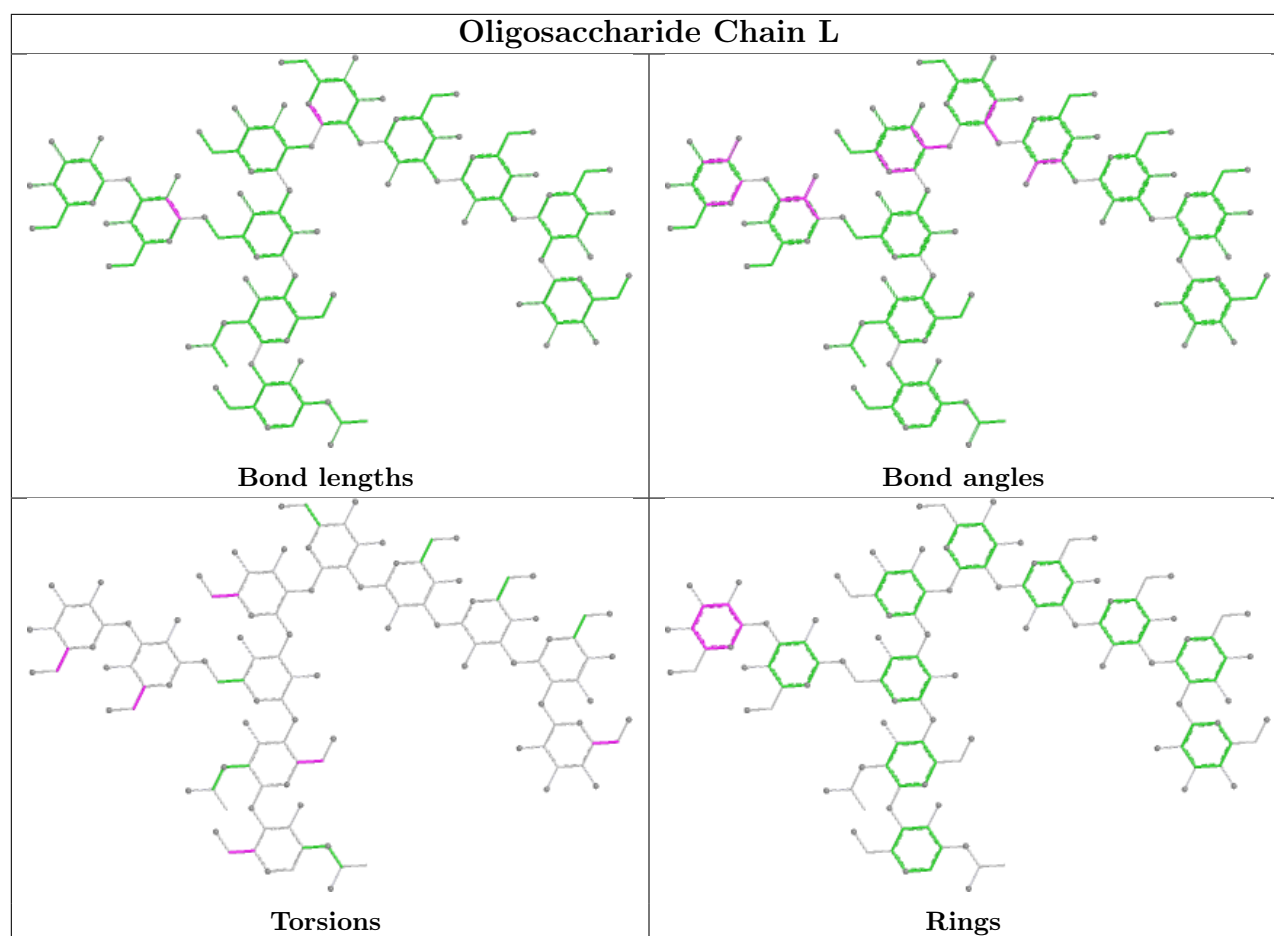
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for oligosaccharide.









5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 1 is monoatomic - leaving 9 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	$\# Z > 2$
13	CPL	E	501	-	51,51,51	0.38	0	57,59,59	0.34	0
17	NAG	G	502	7	14,14,15	1.12	1 (7%)	17,19,21	1.08	2 (11%)
16	ELU	A	804	15,12	27,28,28	1.30	1 (3%)	33,37,37	1.35	6 (18%)
17	NAG	G	501	7	14,14,15	0.70	1 (7%)	17,19,21	1.02	1 (5%)
13	CPL	B	101	-	51,51,51	1.31	6 (11%)	57,59,59	1.03	2 (3%)
14	PTY	F	301	-	41,41,49	0.96	4 (9%)	44,46,54	1.08	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CPL	G	503	-	51,51,51	1.31	6 (11%)	57,59,59	1.07	3 (5%)
14	PTY	A	802	-	41,41,49	0.95	4 (9%)	44,46,54	1.08	2 (4%)
13	CPL	A	801	-	51,51,51	1.30	5 (9%)	57,59,59	0.89	1 (1%)

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
13	CPL	E	501	-	-	27/55/55/55	-
17	NAG	G	502	7	-	1/6/23/26	0/1/1/1
16	ELU	A	804	15,12	-	15/31/31/31	-
17	NAG	G	501	7	-	2/6/23/26	0/1/1/1
13	CPL	B	101	-	-	15/55/55/55	-
14	PTY	F	301	-	-	22/45/45/53	-
13	CPL	G	503	-	-	22/55/55/55	-
14	PTY	A	802	-	-	24/45/45/53	-
13	CPL	A	801	-	-	15/55/55/55	-

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	A	804	ELU	PA-O3A	5.55	1.65	1.59
17	G	502	NAG	O5-C1	-4.04	1.36	1.43
13	B	101	CPL	O2-C31	3.39	1.43	1.34
13	B	101	CPL	O3-C11	3.34	1.43	1.33
13	G	503	CPL	O2-C31	3.29	1.43	1.34
13	A	801	CPL	O3-C11	3.25	1.42	1.33
13	G	503	CPL	O3-C11	3.25	1.42	1.33
13	A	801	CPL	O2-C31	3.21	1.43	1.34
14	F	301	PTY	O7-C6	-2.81	1.40	1.46
14	A	802	PTY	O7-C6	-2.59	1.40	1.46
13	A	801	CPL	O2-C2	-2.51	1.40	1.46
13	G	503	CPL	P-O4P	2.45	1.69	1.59
13	B	101	CPL	P-O4P	2.39	1.68	1.59
14	F	301	PTY	O4-C30	2.35	1.40	1.33
14	A	802	PTY	O4-C30	2.32	1.40	1.33
13	G	503	CPL	O2-C2	-2.31	1.41	1.46
13	A	801	CPL	P-O4P	2.30	1.68	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	101	CPL	C32-C31	2.29	1.57	1.50
13	G	503	CPL	C32-C31	2.25	1.57	1.50
13	B	101	CPL	O2-C2	-2.22	1.41	1.46
14	A	802	PTY	O4-C1	-2.20	1.40	1.45
13	A	801	CPL	C32-C31	2.19	1.57	1.50
14	F	301	PTY	O4-C1	-2.16	1.40	1.45
14	A	802	PTY	O7-C8	2.10	1.40	1.34
13	G	503	CPL	P-O3P	2.08	1.67	1.59
13	B	101	CPL	P-O3P	2.07	1.67	1.59
14	F	301	PTY	O7-C8	2.01	1.40	1.34
17	G	501	NAG	O5-C1	2.01	1.47	1.43

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	G	503	CPL	O2-C31-C32	4.06	120.27	111.48
14	A	802	PTY	O7-C8-C11	3.89	119.89	111.48
17	G	501	NAG	C1-O5-C5	3.87	117.38	112.19
13	B	101	CPL	O2-C31-C32	3.87	119.86	111.48
14	F	301	PTY	O7-C8-C11	3.66	119.41	111.48
17	G	502	NAG	C3-C4-C5	3.35	116.31	110.23
16	A	804	ELU	C6-C7-C8	-3.34	119.97	127.62
13	A	801	CPL	O2-C31-C32	3.27	118.55	111.48
16	A	804	ELU	C10-C8-C9	2.93	120.31	115.23
14	F	301	PTY	O4-C30-C31	2.77	120.27	111.83
13	B	101	CPL	O3-C11-C12	2.75	120.21	111.83
14	A	802	PTY	O4-C30-C31	2.56	119.63	111.83
16	A	804	ELU	C14-C13-C15	2.55	119.66	115.23
17	G	502	NAG	C4-C3-C2	2.45	114.61	111.02
13	G	503	CPL	O3-C11-C12	2.44	119.28	111.83
13	G	503	CPL	C4-C5-N	-2.44	108.00	115.82
16	A	804	ELU	C16-C17-C18	-2.38	119.71	127.64
16	A	804	ELU	C11-C12-C13	-2.21	122.57	127.62
16	A	804	ELU	C19-C18-C20	2.09	119.39	114.59

There are no chirality outliers.

All (143) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	B	101	CPL	O4P-C4-C5-N
13	E	501	CPL	O4P-C4-C5-N
13	E	501	CPL	C32-C31-O2-C2

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Mol	Chain	Res	Type	Atoms
13	E	501	CPL	O31-C31-O2-C2
13	E	501	CPL	C1-O3P-P-O2P
13	E	501	CPL	C1-O3P-P-O4P
13	G	503	CPL	C32-C31-O2-C2
14	A	802	PTY	C3-O11-P1-O13
14	A	802	PTY	C3-O11-P1-O14
14	F	301	PTY	O4-C1-C6-O7
14	F	301	PTY	N1-C2-C3-O11
14	F	301	PTY	C3-O11-P1-O12
14	F	301	PTY	C3-O11-P1-O14
16	A	804	ELU	C1-O1-PA-O2A
16	A	804	ELU	C1-O1-PA-O1A
16	A	804	ELU	C1-O1-PA-O3A
16	A	804	ELU	O1-C1-C2-C3
16	A	804	ELU	C1-C2-C3-C4
16	A	804	ELU	C1-C2-C3-C5
13	G	503	CPL	O31-C31-O2-C2
16	A	804	ELU	C14-C13-C15-C16
16	A	804	ELU	C12-C13-C15-C16
13	G	503	CPL	O11-C11-O3-C3
13	G	503	CPL	C12-C11-O3-C3
16	A	804	ELU	C10-C8-C9-C11
16	A	804	ELU	C7-C8-C9-C11
13	E	501	CPL	C41-C42-C43-C44
17	G	501	NAG	O5-C5-C6-O6
13	B	101	CPL	C12-C11-O3-C3
17	G	501	NAG	C4-C5-C6-O6
16	A	804	ELU	C4-C3-C5-C6
13	E	501	CPL	C12-C11-O3-C3
13	G	503	CPL	C31-C32-C33-C34
16	A	804	ELU	C12-C11-C9-C8
13	B	101	CPL	O11-C11-O3-C3
14	F	301	PTY	C31-C32-C33-C34
13	G	503	CPL	C11-C12-C13-C14
13	E	501	CPL	O11-C11-O3-C3
13	E	501	CPL	C32-C33-C34-C35
13	B	101	CPL	C12-C13-C14-C15
13	G	503	CPL	C16-C17-C18-C19
13	E	501	CPL	C15-C16-C17-C18
13	E	501	CPL	C11-C12-C13-C14
13	E	501	CPL	C16-C17-C18-C19
13	G	503	CPL	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
13	E	501	CPL	C12-C13-C14-C15
14	F	301	PTY	C32-C33-C34-C35
14	A	802	PTY	C30-C31-C32-C33
13	B	101	CPL	C21-C22-C23-C24
13	G	503	CPL	C12-C13-C14-C15
13	B	101	CPL	C13-C14-C15-C16
14	A	802	PTY	C11-C8-O7-C6
14	A	802	PTY	C32-C33-C34-C35
13	A	801	CPL	C4-C5-N-C8
14	F	301	PTY	C8-C11-C12-C13
14	A	802	PTY	O10-C8-O7-C6
13	A	801	CPL	C34-C35-C36-C37
14	A	802	PTY	C16-C17-C18-C19
14	A	802	PTY	C39-C40-C41-C42
14	F	301	PTY	C36-C37-C38-C39
14	A	802	PTY	O4-C1-C6-O7
14	A	802	PTY	C17-C18-C19-C20
13	A	801	CPL	C16-C17-C18-C19
13	B	101	CPL	C23-C24-C25-C26
16	A	804	ELU	C13-C15-C16-C17
13	A	801	CPL	C4-C5-N-C6
14	F	301	PTY	C30-C31-C32-C33
14	F	301	PTY	C35-C36-C37-C38
13	B	101	CPL	C35-C36-C37-C38
13	E	501	CPL	C23-C24-C25-C26
14	F	301	PTY	C37-C38-C39-C40
14	A	802	PTY	O14-C5-C6-C1
16	A	804	ELU	C2-C3-C5-C6
13	G	503	CPL	C23-C24-C25-C26
13	A	801	CPL	C4-C5-N-C7
13	E	501	CPL	C1-C2-C3-O3
13	G	503	CPL	C1-C2-C3-O3
14	A	802	PTY	O4-C1-C6-C5
14	F	301	PTY	O4-C1-C6-C5
13	G	503	CPL	O3P-C1-C2-O2
14	A	802	PTY	O14-C5-C6-O7
13	E	501	CPL	C42-C43-C44-C45
17	G	502	NAG	C4-C5-C6-O6
13	E	501	CPL	C38-C39-C40-C41
13	E	501	CPL	C18-C19-C20-C21
13	A	801	CPL	C39-C40-C41-C42
13	E	501	CPL	C39-C40-C41-C42

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Mol	Chain	Res	Type	Atoms
13	G	503	CPL	C40-C41-C42-C43
13	G	503	CPL	C13-C14-C15-C16
16	A	804	ELU	PB-O3A-PA-O1
13	B	101	CPL	C15-C16-C17-C18
13	E	501	CPL	C33-C34-C35-C36
13	E	501	CPL	O3P-C1-C2-C3
13	E	501	CPL	C34-C35-C36-C37
13	A	801	CPL	C43-C44-C45-C46
13	E	501	CPL	O3P-C1-C2-O2
13	A	801	CPL	C14-C15-C16-C17
13	G	503	CPL	O2-C2-C3-O3
13	G	503	CPL	C35-C36-C37-C38
14	A	802	PTY	C11-C12-C13-C14
13	G	503	CPL	O4P-C4-C5-N
13	G	503	CPL	C19-C20-C21-C22
14	F	301	PTY	O14-C5-C6-C1
13	G	503	CPL	C34-C35-C36-C37
13	B	101	CPL	C18-C19-C20-C21
14	F	301	PTY	O14-C5-C6-O7
14	F	301	PTY	C11-C12-C13-C14
13	E	501	CPL	O2-C2-C3-O3
13	A	801	CPL	C1-C2-C3-O3
13	B	101	CPL	C16-C17-C18-C19
13	A	801	CPL	C1-O3P-P-O1P
13	B	101	CPL	C4-O4P-P-O1P
14	A	802	PTY	N1-C2-C3-O11
14	F	301	PTY	C3-O11-P1-O13
14	A	802	PTY	C5-C6-O7-C8
13	A	801	CPL	C15-C16-C17-C18
14	A	802	PTY	O4-C30-C31-C32
14	F	301	PTY	O4-C30-C31-C32
13	E	501	CPL	C13-C14-C15-C16
13	G	503	CPL	C42-C43-C44-C45
13	A	801	CPL	O2-C2-C3-O3
13	B	101	CPL	C36-C37-C38-C39
13	A	801	CPL	O11-C11-O3-C3
13	A	801	CPL	C12-C11-O3-C3
13	A	801	CPL	C32-C33-C34-C35
14	F	301	PTY	C12-C11-C8-O7
14	A	802	PTY	C15-C16-C17-C18
14	A	802	PTY	C6-C5-O14-P1
14	A	802	PTY	C12-C11-C8-O7

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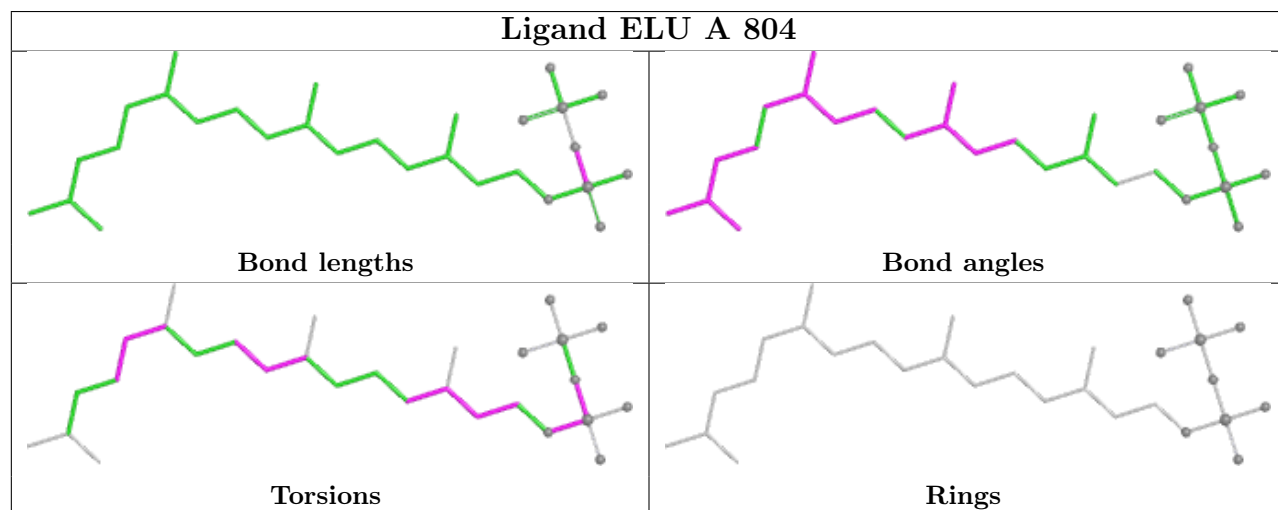
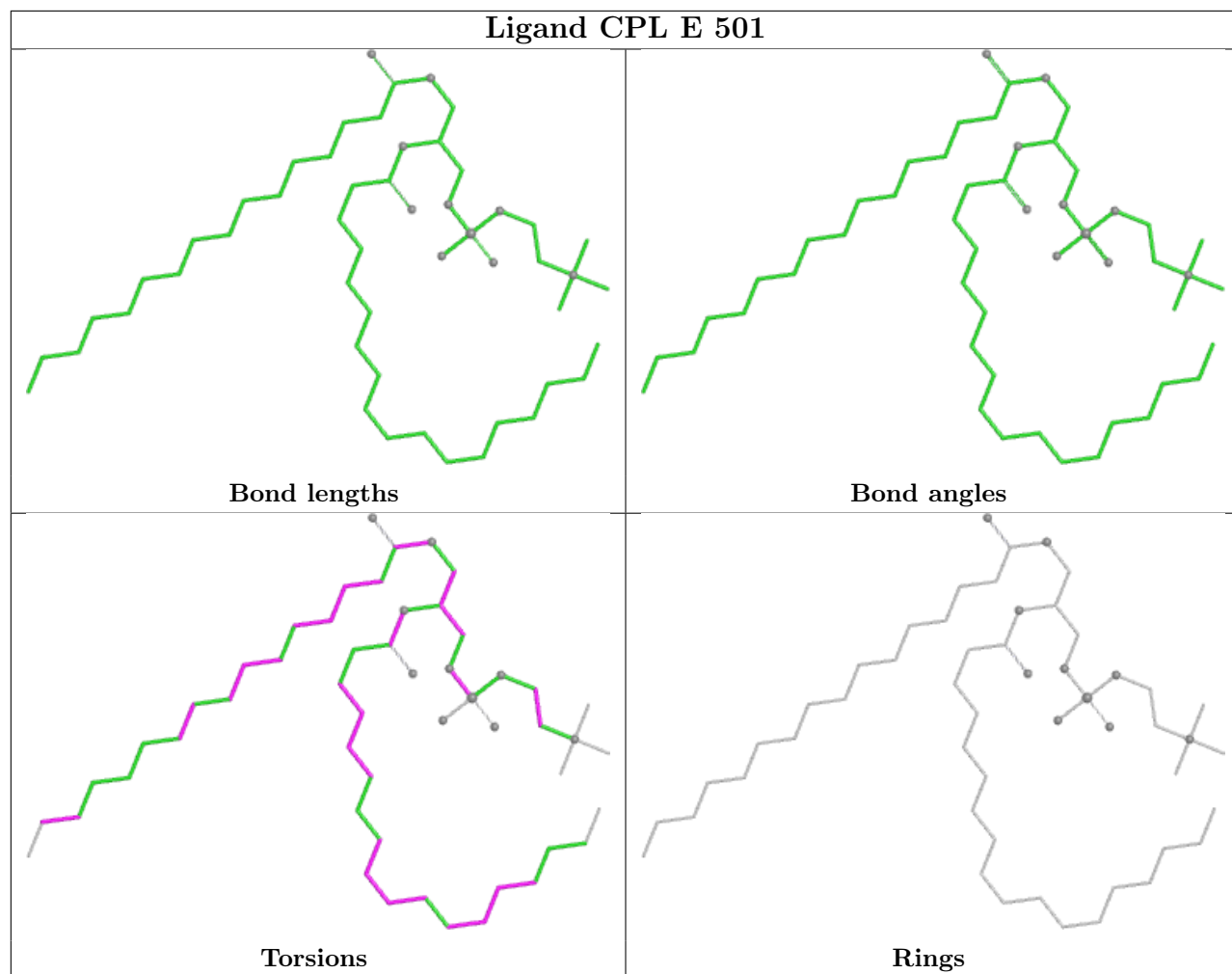
Mol	Chain	Res	Type	Atoms
13	E	501	CPL	C43-C44-C45-C46
13	G	503	CPL	O3P-C1-C2-C3
13	B	101	CPL	C37-C38-C39-C40
14	A	802	PTY	C37-C38-C39-C40
14	F	301	PTY	C16-C17-C18-C19
14	A	802	PTY	C31-C32-C33-C34
13	G	503	CPL	C37-C38-C39-C40
14	F	301	PTY	C34-C35-C36-C37
14	F	301	PTY	C40-C41-C42-C43
13	B	101	CPL	C32-C33-C34-C35
14	A	802	PTY	C38-C39-C40-C41
14	F	301	PTY	C15-C16-C17-C18
13	E	501	CPL	C37-C38-C39-C40
14	A	802	PTY	C18-C19-C20-C21

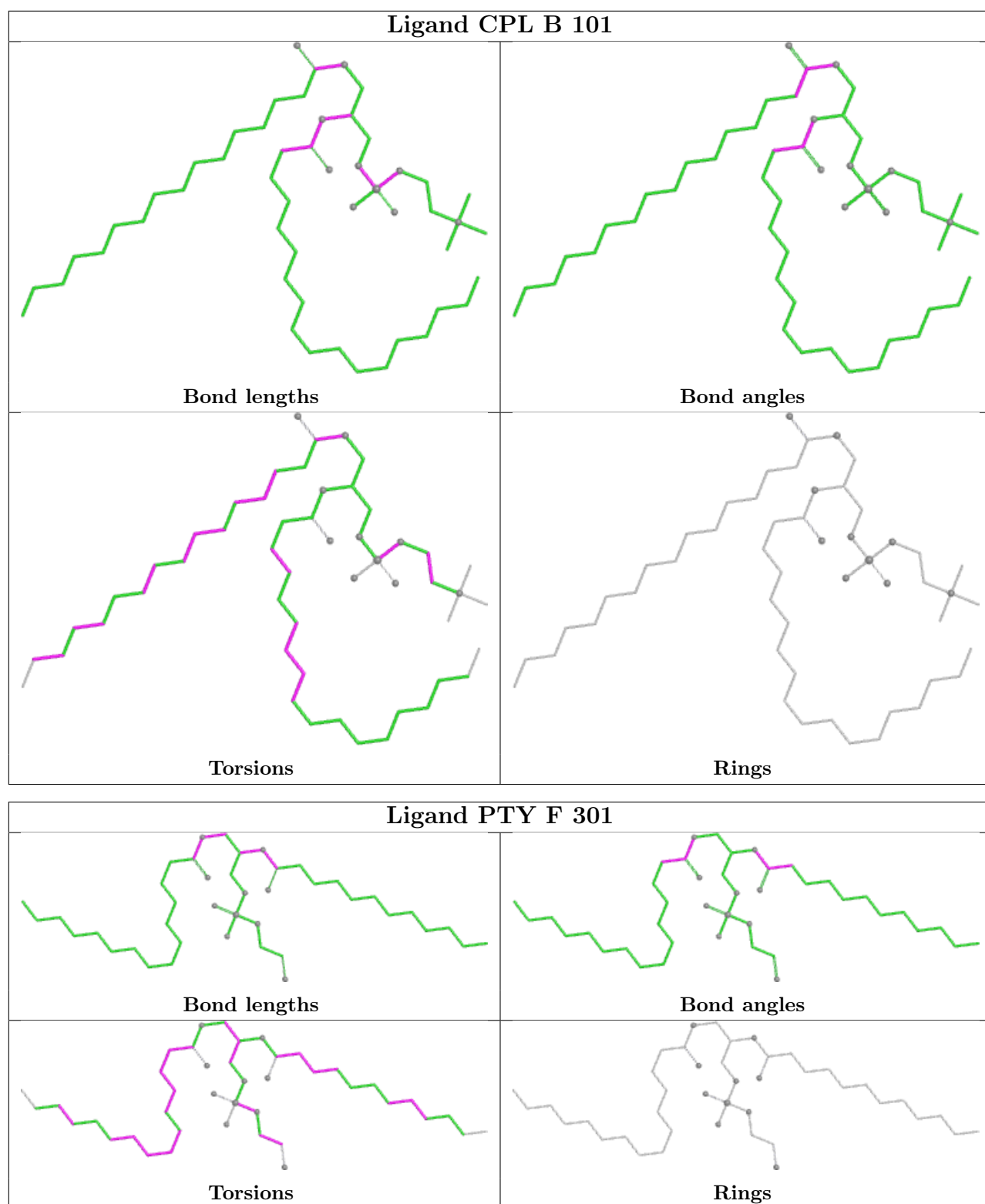
There are no ring outliers.

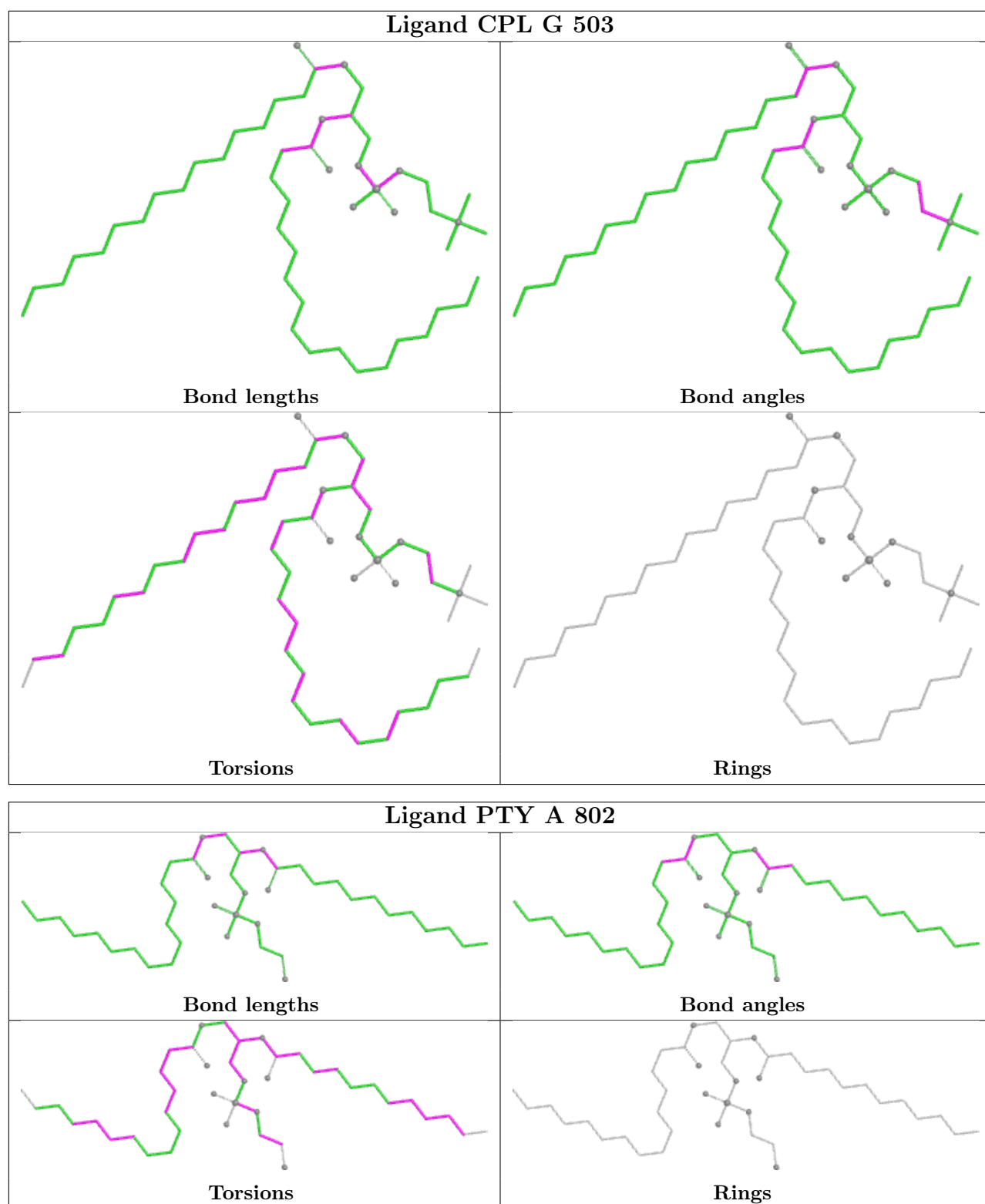
4 monomers are involved in 6 short contacts:

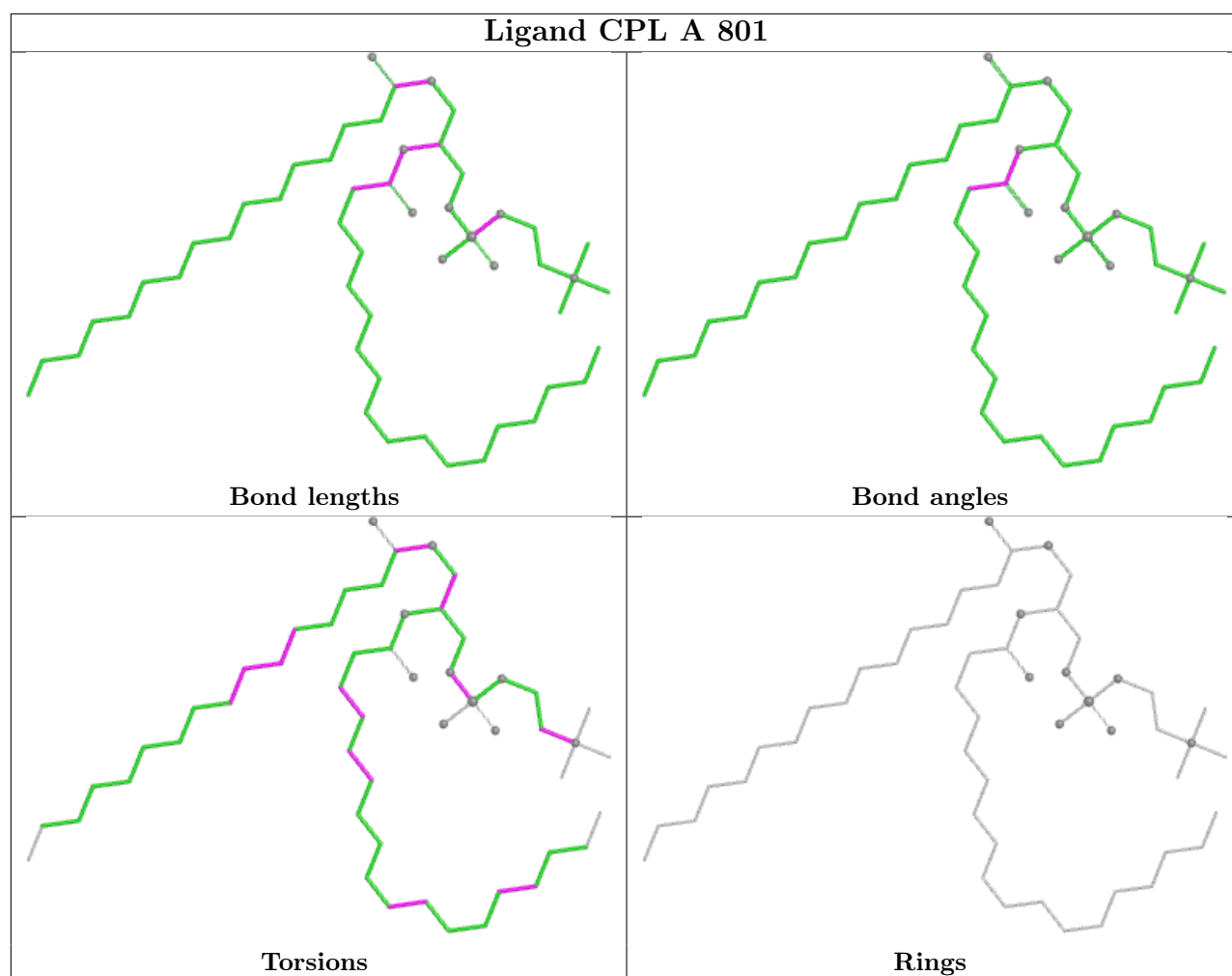
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	B	101	CPL	1	0
13	G	503	CPL	1	0
14	A	802	PTY	1	0
13	A	801	CPL	3	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

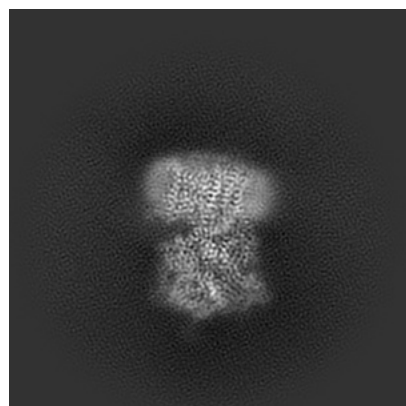
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15419. These allow visual inspection of the internal detail of the map and identification of artifacts.

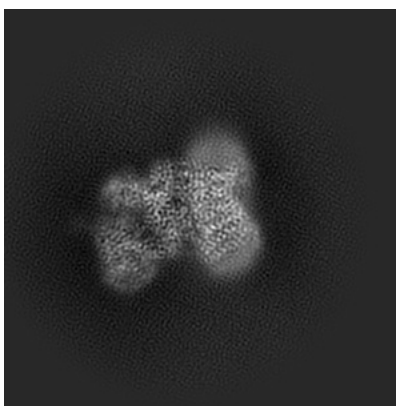
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

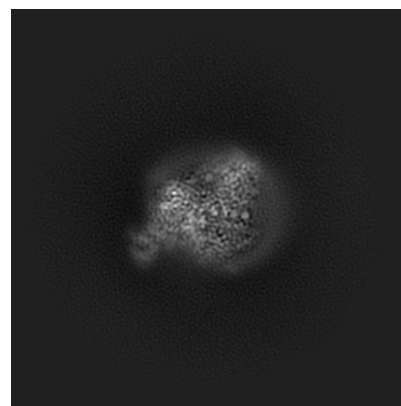
6.1.1 Primary map



X

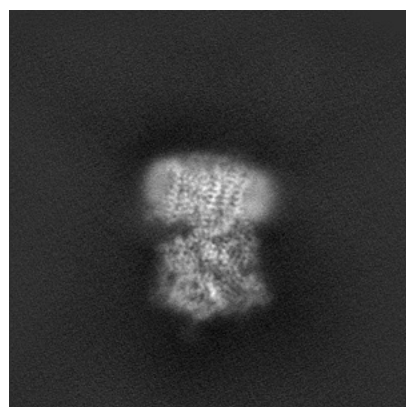


Y

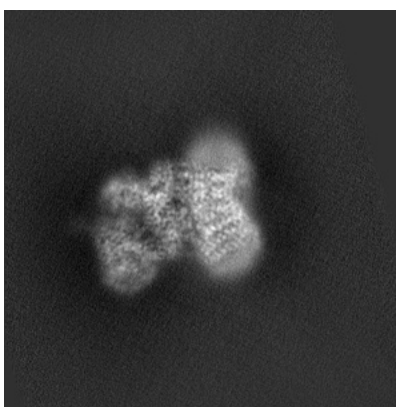


Z

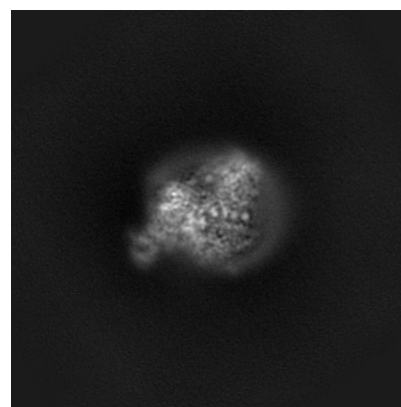
6.1.2 Raw map



X



Y

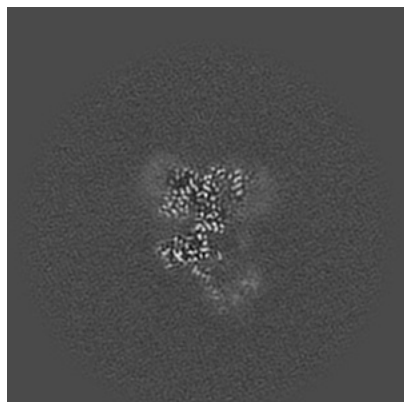


Z

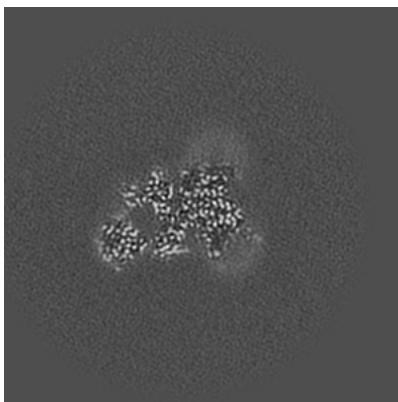
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

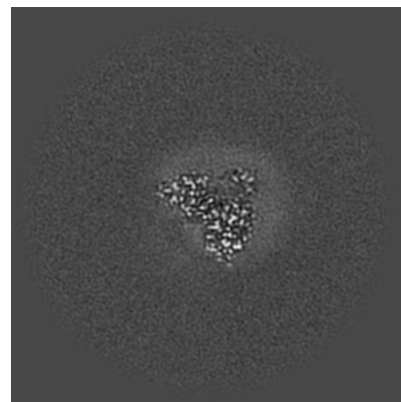
6.2.1 Primary map



X Index: 192

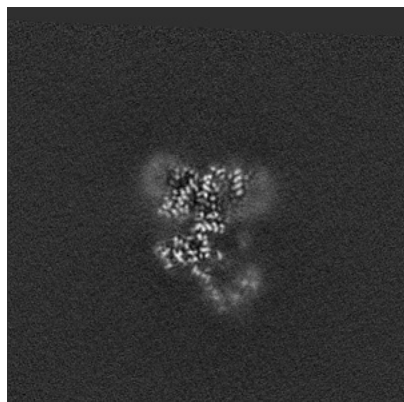


Y Index: 192

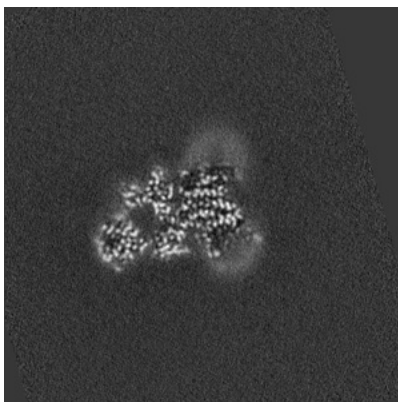


Z Index: 192

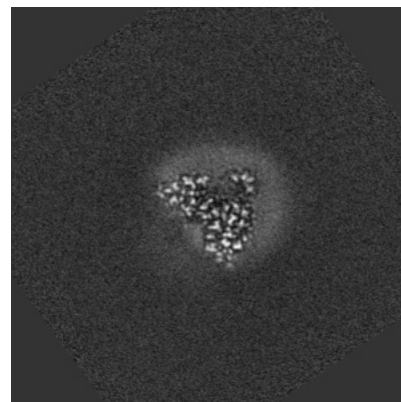
6.2.2 Raw map



X Index: 192



Y Index: 192

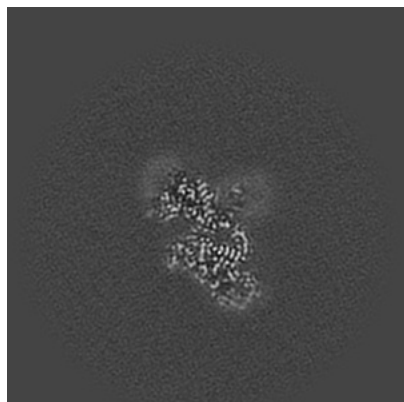


Z Index: 192

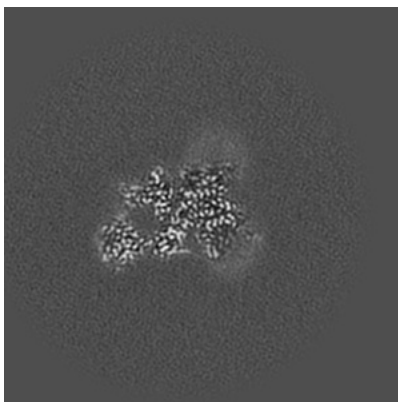
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

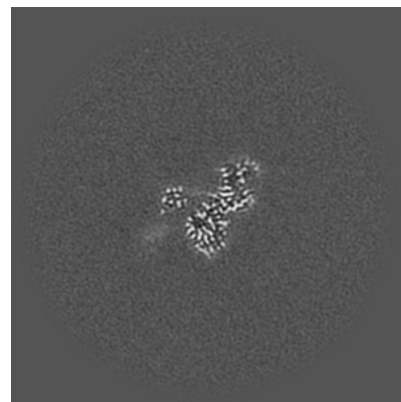
6.3.1 Primary map



X Index: 206

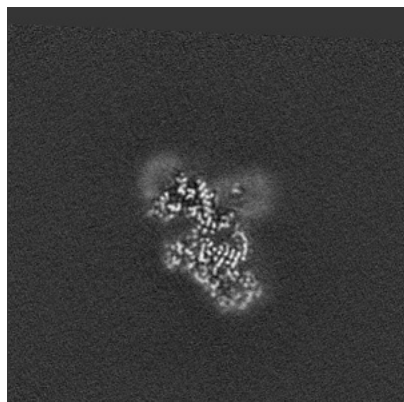


Y Index: 193

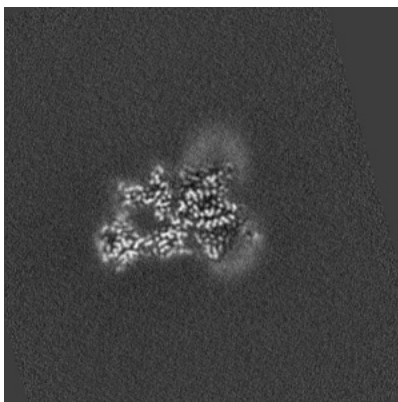


Z Index: 147

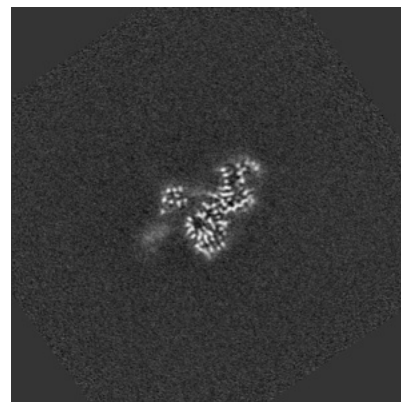
6.3.2 Raw map



X Index: 205



Y Index: 194

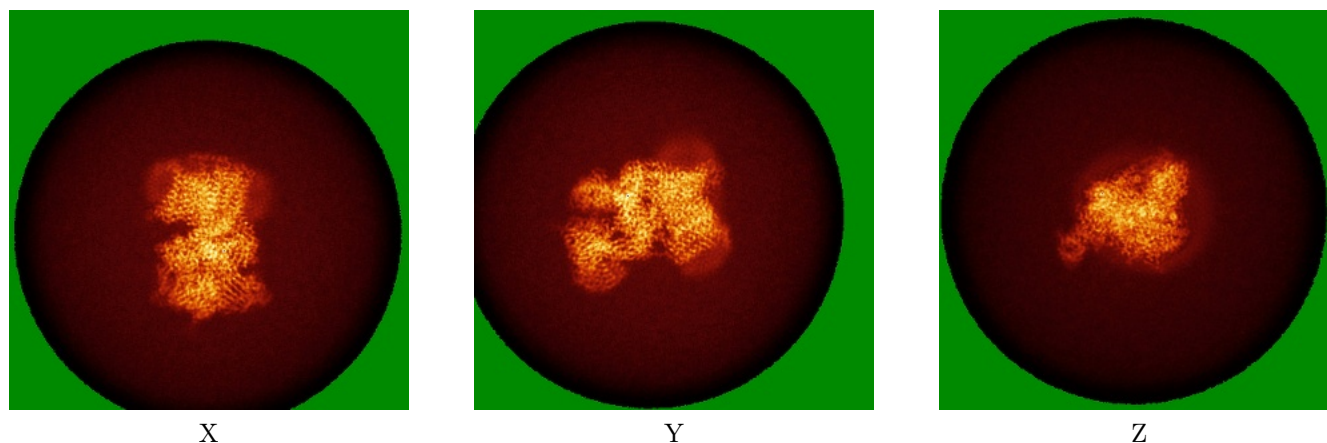


Z Index: 147

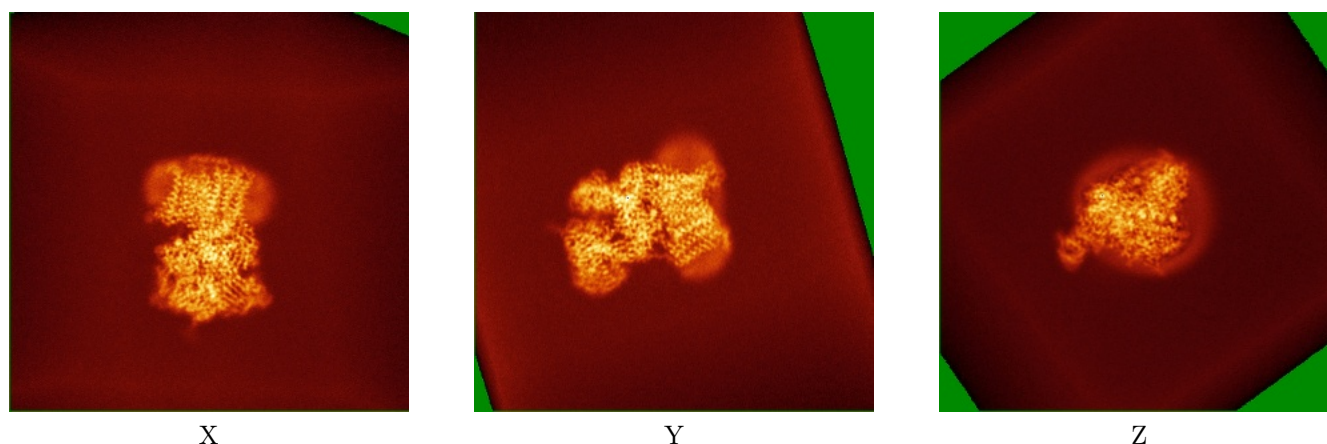
The images above show the largest variance slices of the map in three orthogonal directions.

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](#)

This section was not generated.

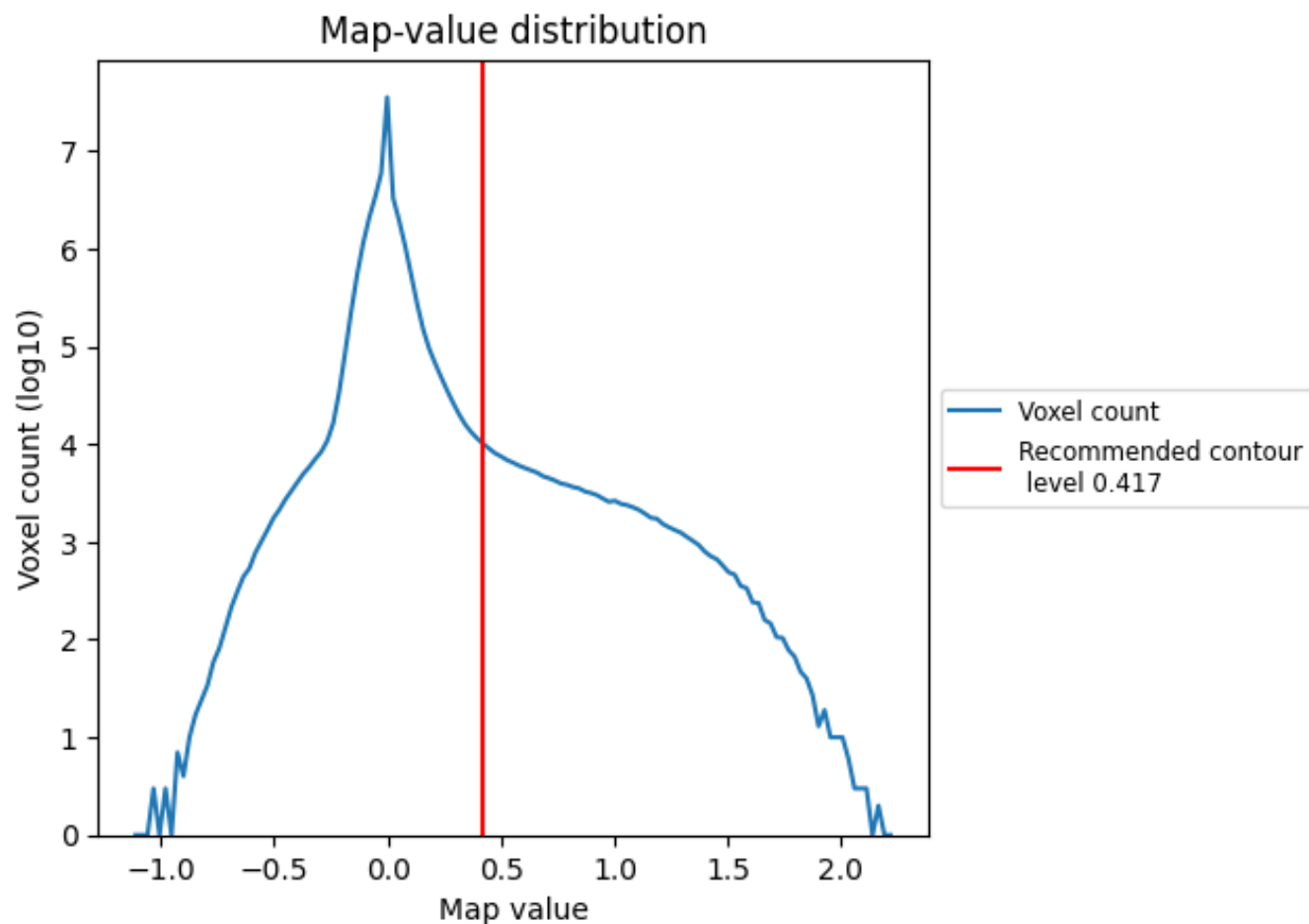
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

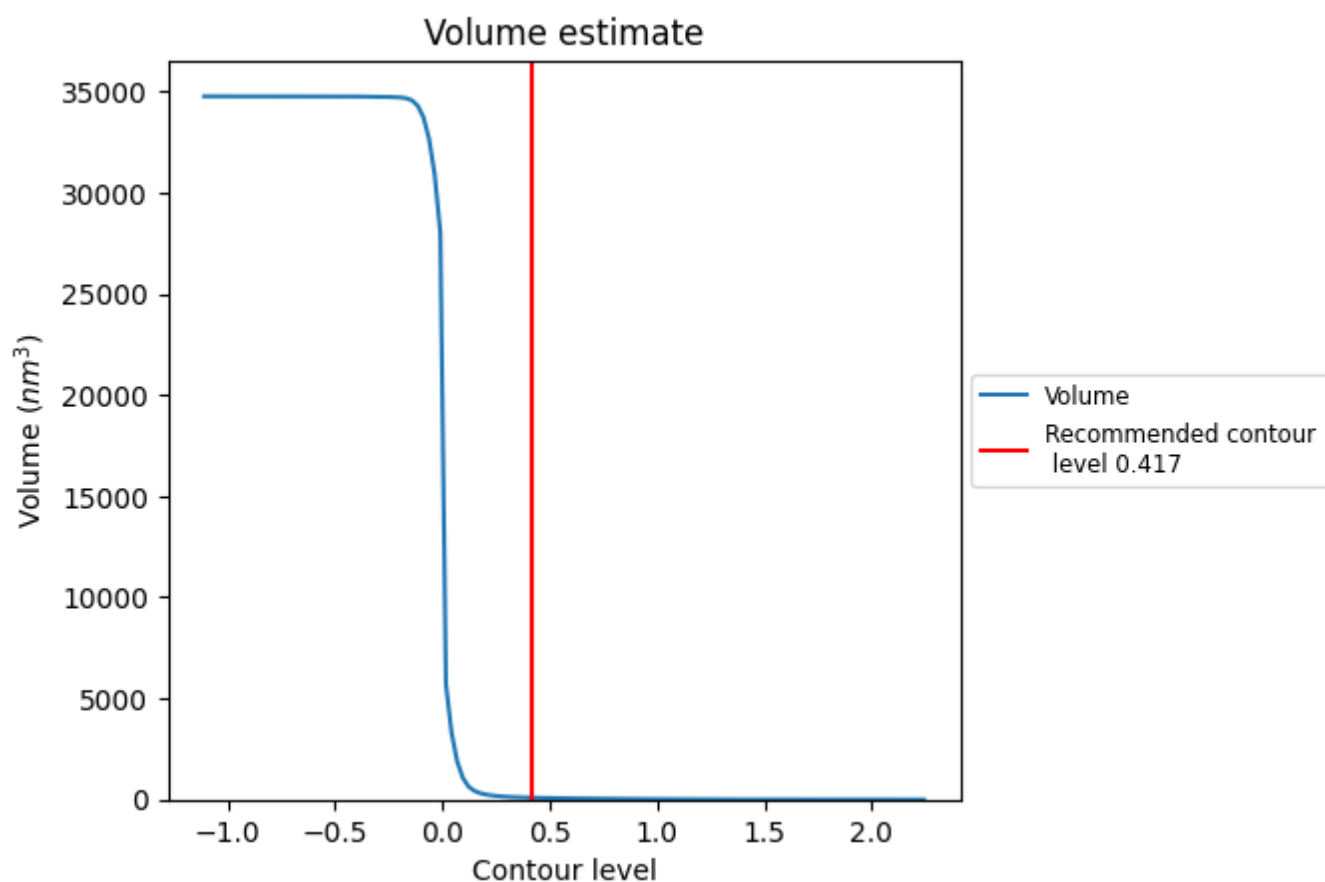
This section contains the results of statistical analysis of the map.

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.

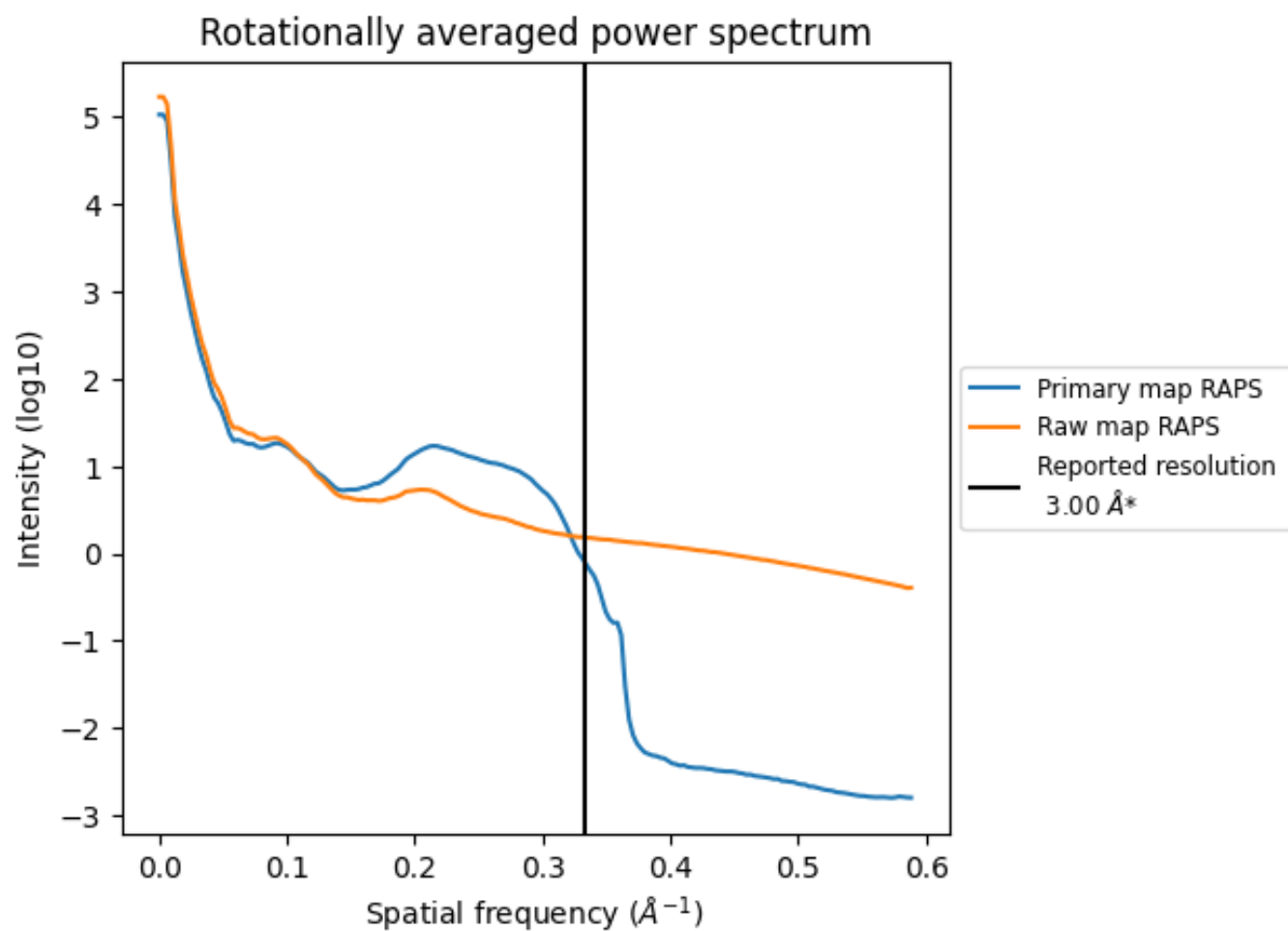
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 90 nm³; this corresponds to an approximate mass of 81 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 ⓘ

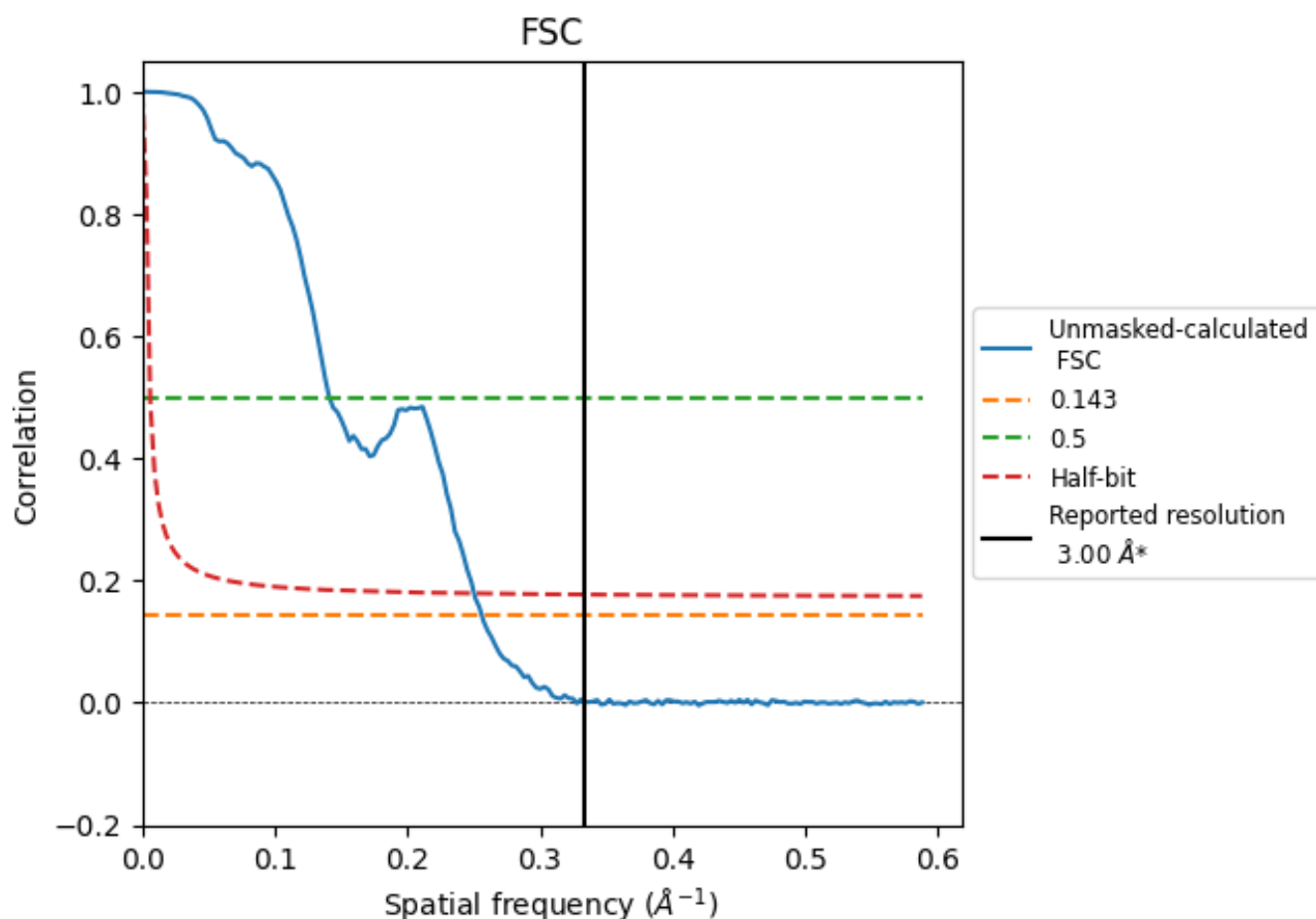


*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.333 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

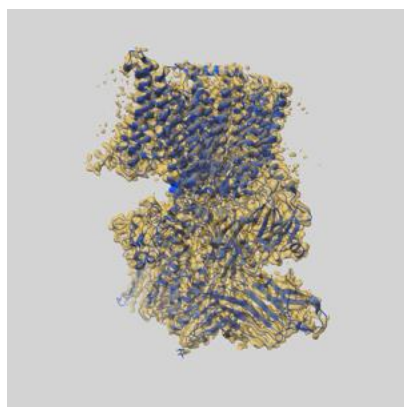
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.90	7.08	4.00

*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 3.90 differs from the reported value 3.0 by more than 10 %

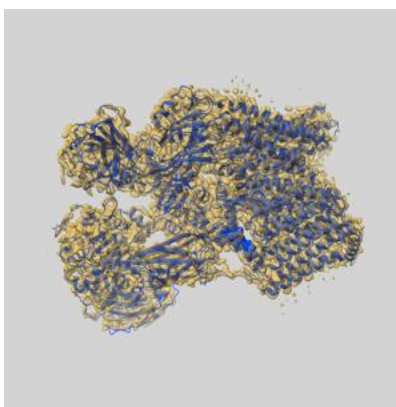
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-15419 and PDB model 8AGB. Per-residue inclusion information can be found in section [3](#) on page [10](#).

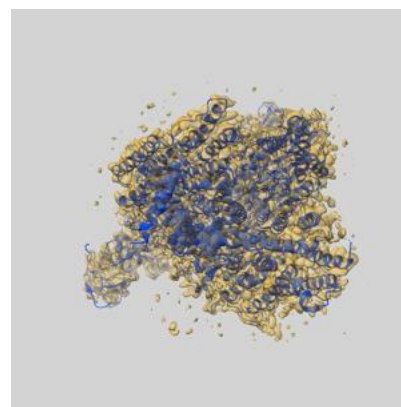
9.1 Map-model overlay [i](#)



X



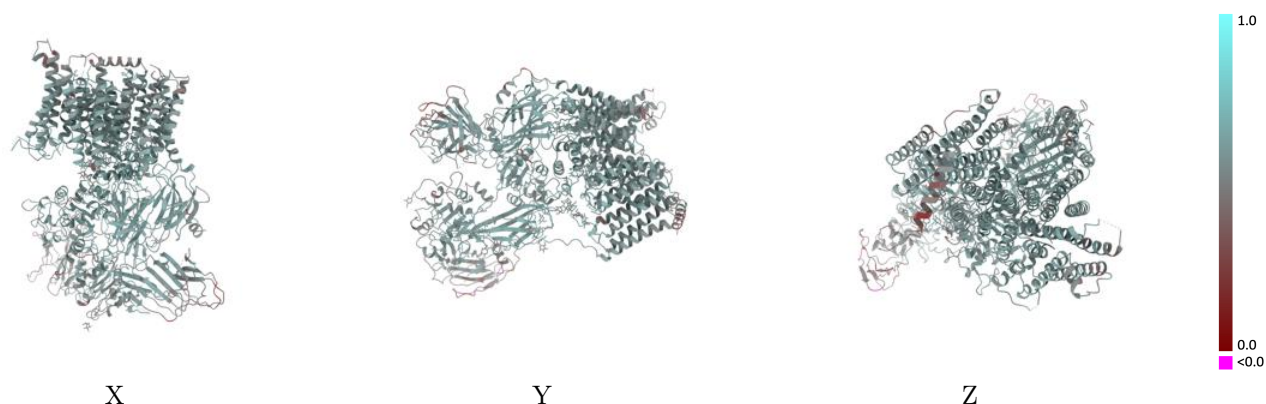
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.417 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](#)

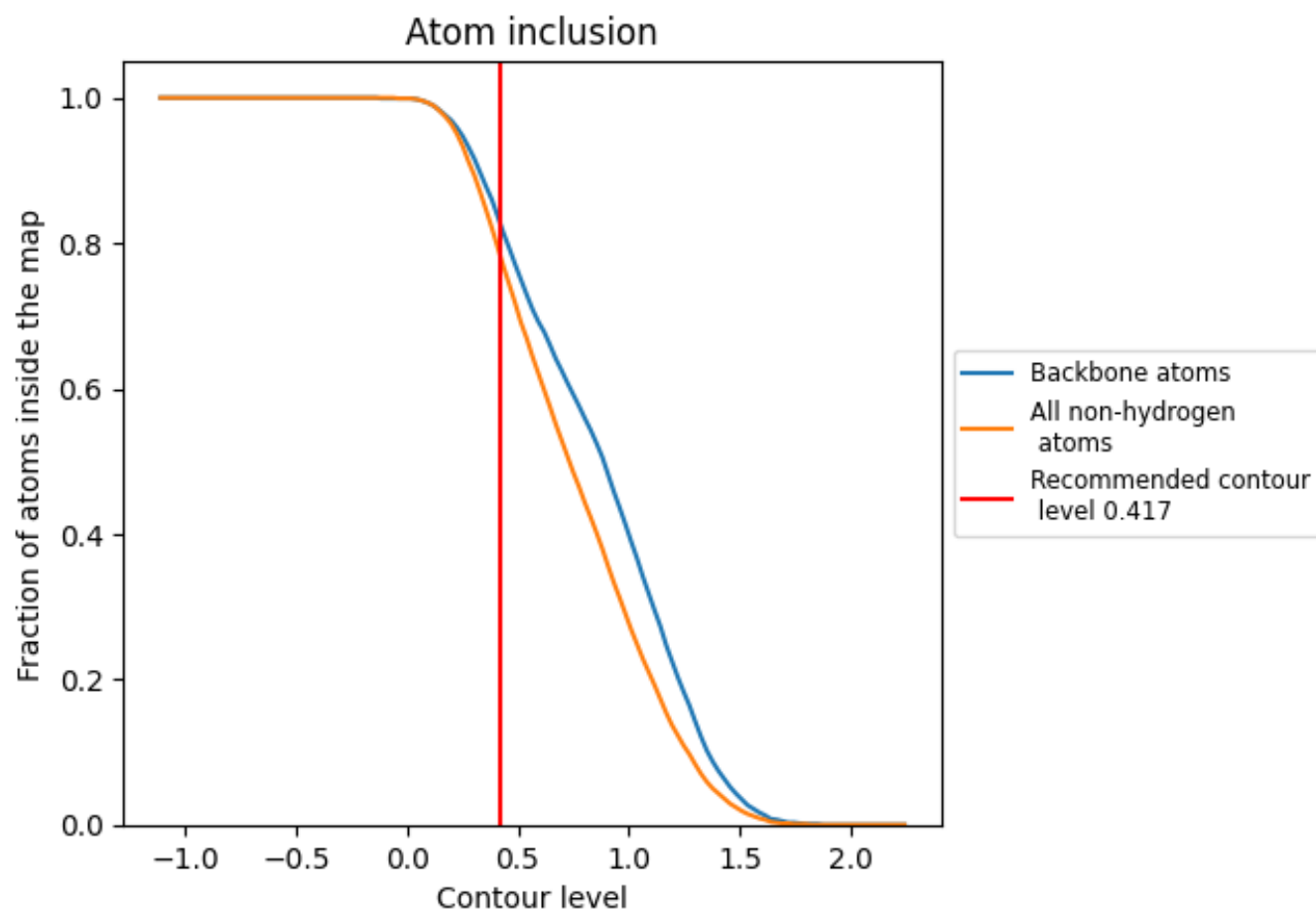


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 79% 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 (0.417) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7860	0.5530
A	0.8460	0.5810
B	0.7990	0.5680
C	0.7370	0.5350
D	0.7610	0.5340
E	0.7860	0.5530
F	0.6160	0.4740
G	0.8240	0.5590
H	0.7830	0.5570
I	0.8310	0.5620
J	0.6670	0.5690
K	0.1790	0.3840
L	0.5350	0.5350

