



Full wwPDB EM Validation Report ⓘ

Mar 7, 2026 – 03:19 AM UTC

PDB ID : 8AGE / pdb_00008age
EMDB ID : EMD-15421
Title : Structure of yeast oligosaccharyltransferase complex with 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 : 2.80 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

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:

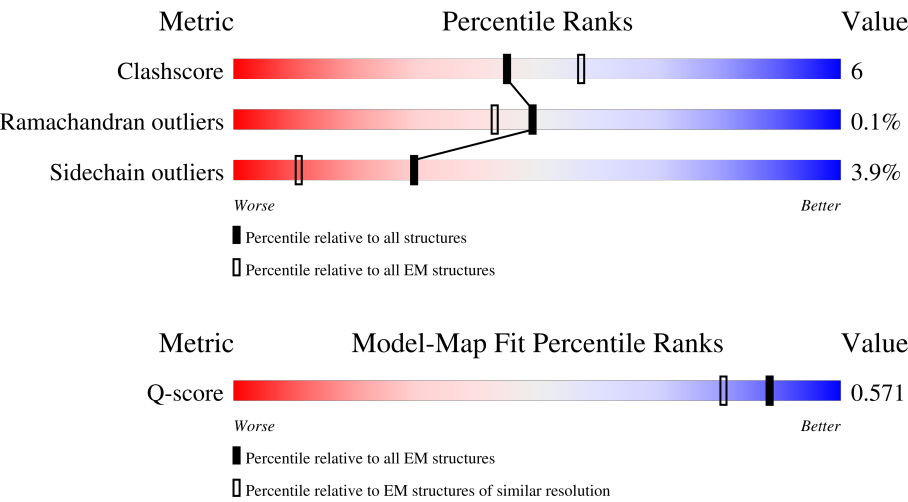
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.80 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	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11806 (2.30 - 3.30)

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	75%14%10%
2	B	65	42%8%49%
3	C	86	5%78%20%
4	D	130	7%70%14%16%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	E	476	
6	F	283	
7	G	430	
8	H	350	
9	P	7	
10	K	7	
11	I	2	
11	J	2	

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 17534 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	644	Total	C	N	O	S	0	0
			5191	3432	830	906	23		

- Molecule 2 is a protein called OST4 isoform 1.

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

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

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	57	THR	-	expression tag	UNP A0A8H8UM72
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
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	109	Total	C	N	O	S	0	0
			883	595	141	141	6		

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

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

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

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

- 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		

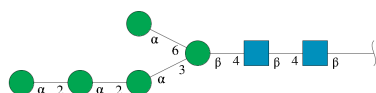
- Molecule 8 is a protein called OST3 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	133	Total	C	N	O	S	0	0
			1067	724	161	176	6		

- Molecule 9 is a protein called PEPTIDE.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	P	7	Total	C	N	O	0	1
			44	26	8	10		

- 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
10	K	7	Total	C	N	O	0	0
			83	46	2	35		

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



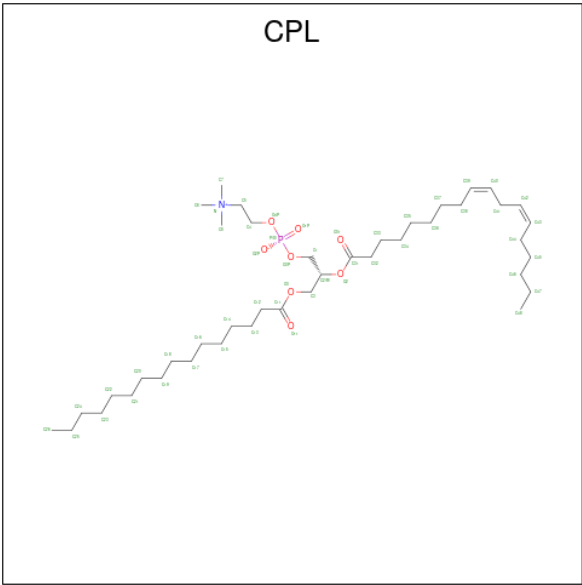
Mol	Chain	Residues	Atoms				AltConf	Trace
11	I	2	Total	C	N	O	0	0
			28	16	2	10		
11	J	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 12 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn) (labeled as "Ligand

of Interest" by depositor).

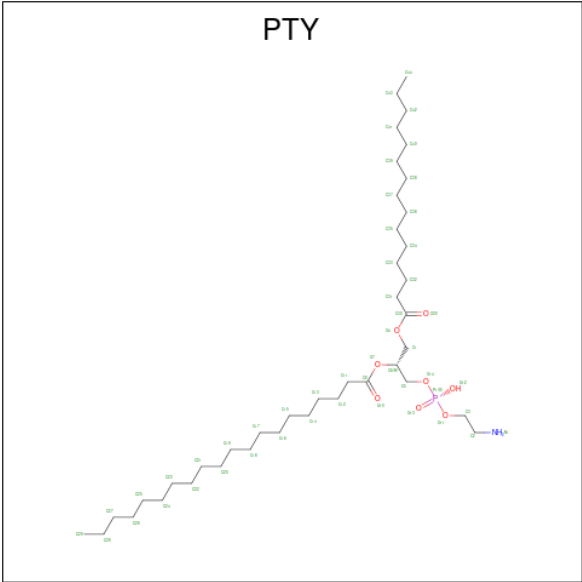
Mol	Chain	Residues	Atoms		AltConf
12	A	1	Total	Mn	0
			1	1	

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



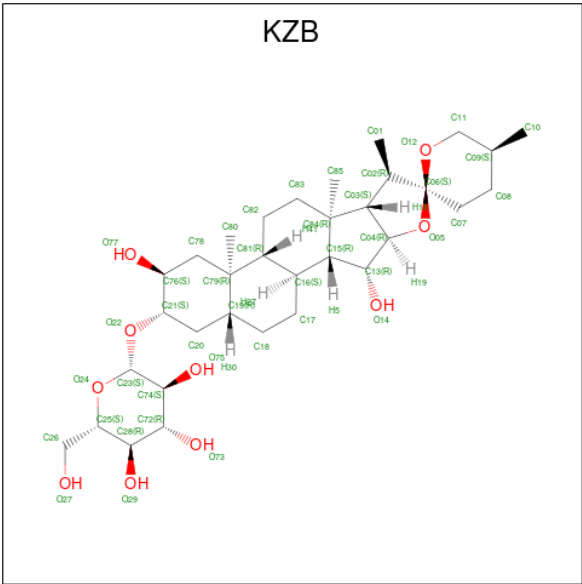
Mol	Chain	Residues	Atoms					AltConf
13	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
13	B	1	Total	C	N	O	P	0
			52	42	1	8	1	
13	E	1	Total	C	N	O	P	0
			52	42	1	8	1	
13	F	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 14 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula: C₄₀H₈₀NO₈P).



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

- Molecule 15 is (2 {S},3 {R},4 {R},5 {S},6 {S})-2-(hydroxymethyl)-6-[(1 {S},2 {R},3 {R},4 {R},5' {S},6 {S},7 {R},8 {S},9 {R},12 {R},13 {R},15 {S},16 {S},18 {R})-5',7,9,13-tetramethyl-3,15-bis(oxidanyl)spiro[5-oxapentacyclo[10.8.0.0^{2,9}.0^{4,8}.0^{13,18}]icosane-6,2'-oxane]-16-yl]oxy-oxane-3,4,5-triol (CCD ID: KZB) (formula: C₃₃H₅₄O₁₀).



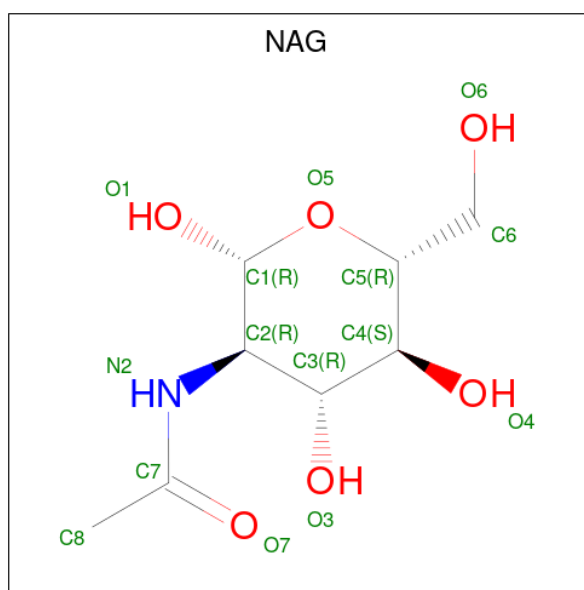
Mol	Chain	Residues	Atoms			AltConf
15	A	1	Total	C	O	0
			43	33	10	

Continued on next page...

Continued from previous page...

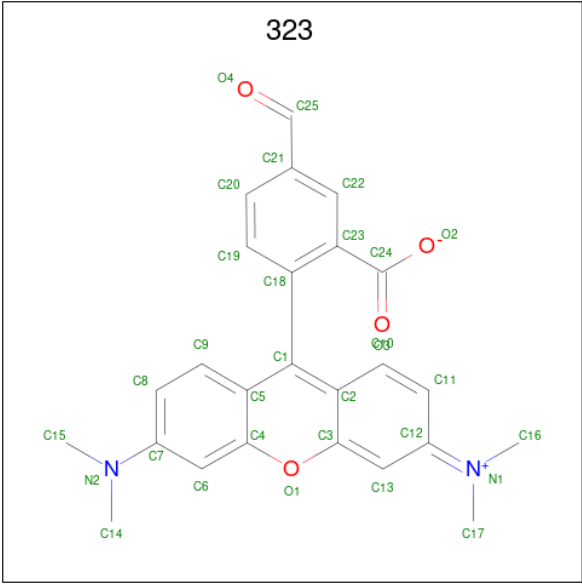
Mol	Chain	Residues	Atoms			AltConf
15	A	1	Total	C	O	0
			43	33	10	
15	A	1	Total	C	O	0
			43	33	10	
15	B	1	Total	C	O	0
			43	33	10	
15	B	1	Total	C	O	0
			43	33	10	
15	F	1	Total	C	O	0
			43	33	10	
15	F	1	Total	C	O	0
			43	33	10	
15	G	1	Total	C	O	0
			43	33	10	

- Molecule 16 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 17 is 2-[3,6-bis(dimethylamino)xanthen-9-yl]-5-methanoyl-benzoate (CCD ID: 323) (formula: $C_{25}H_{22}N_2O_4$).



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

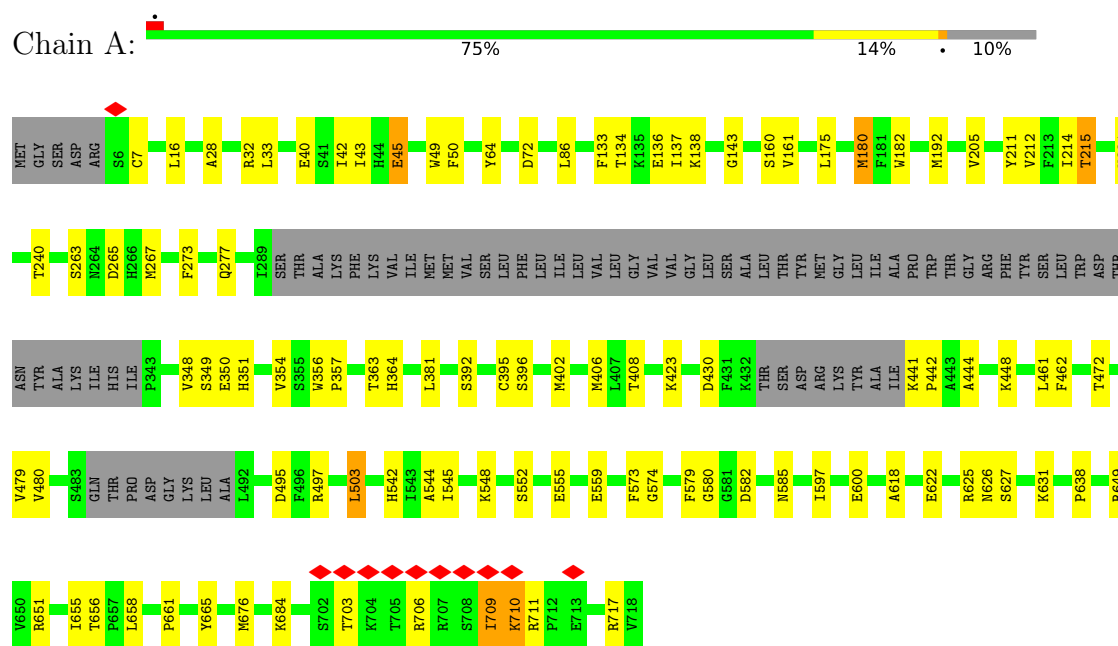
- Molecule 18 is water.

Mol	Chain	Residues	Atoms		AltConf
18	A	4	Total	O	0
			4	4	
18	C	1	Total	O	0
			1	1	
18	E	2	Total	O	0
			2	2	
18	G	2	Total	O	0
			2	2	

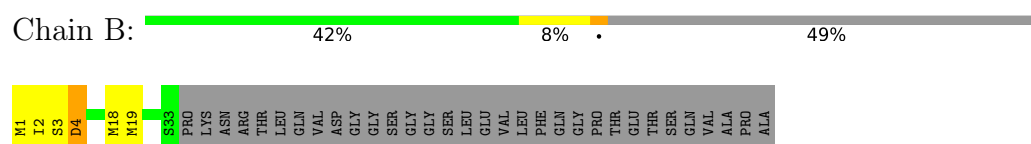
3 Residue-property plots

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.

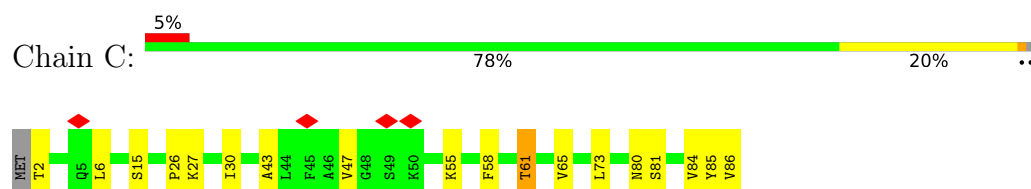
- Molecule 1: Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit STT3



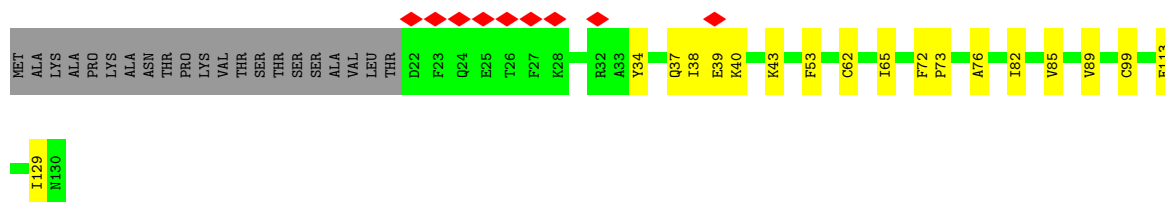
- Molecule 2: OST4 isoform 1



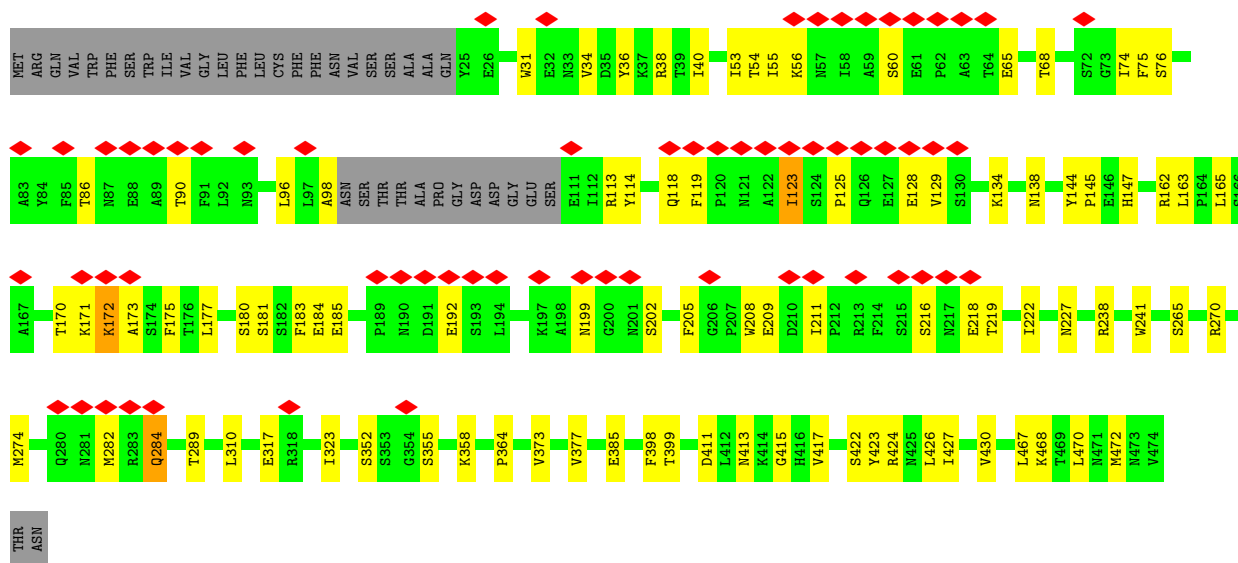
- Molecule 3: Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit OST5



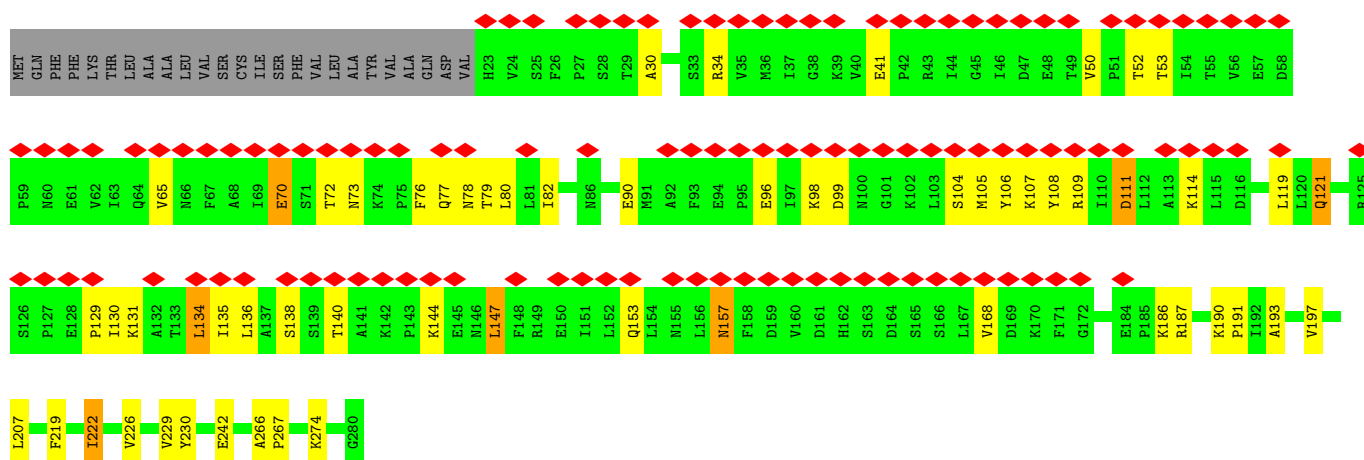
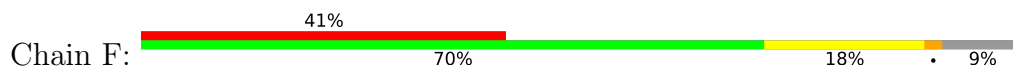
- Molecule 4: Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit OST2



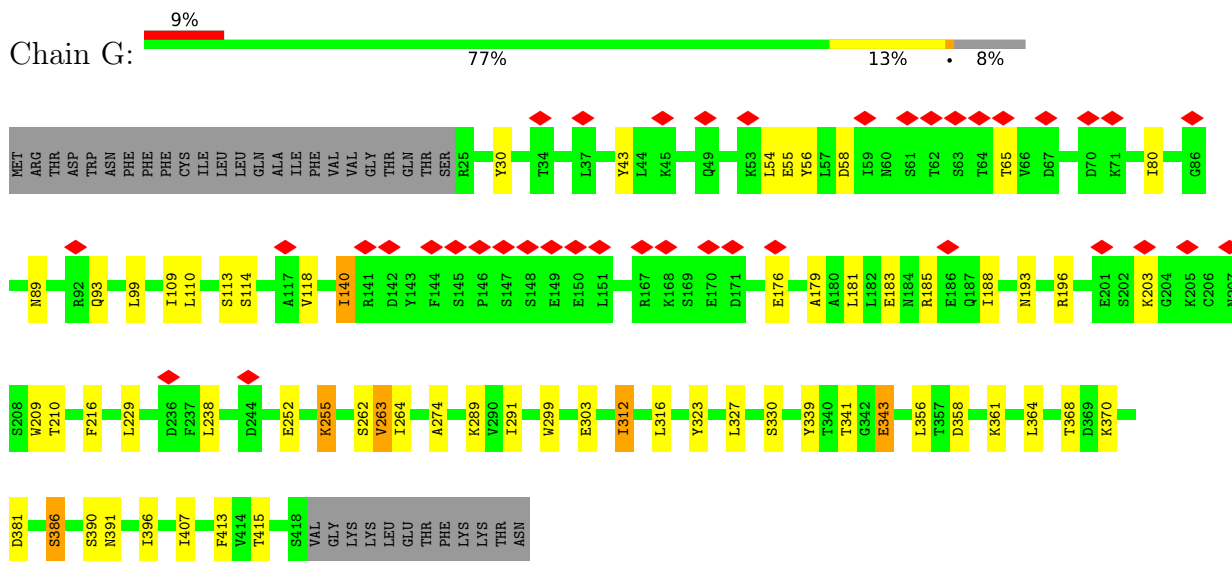
- Molecule 5: Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit 1



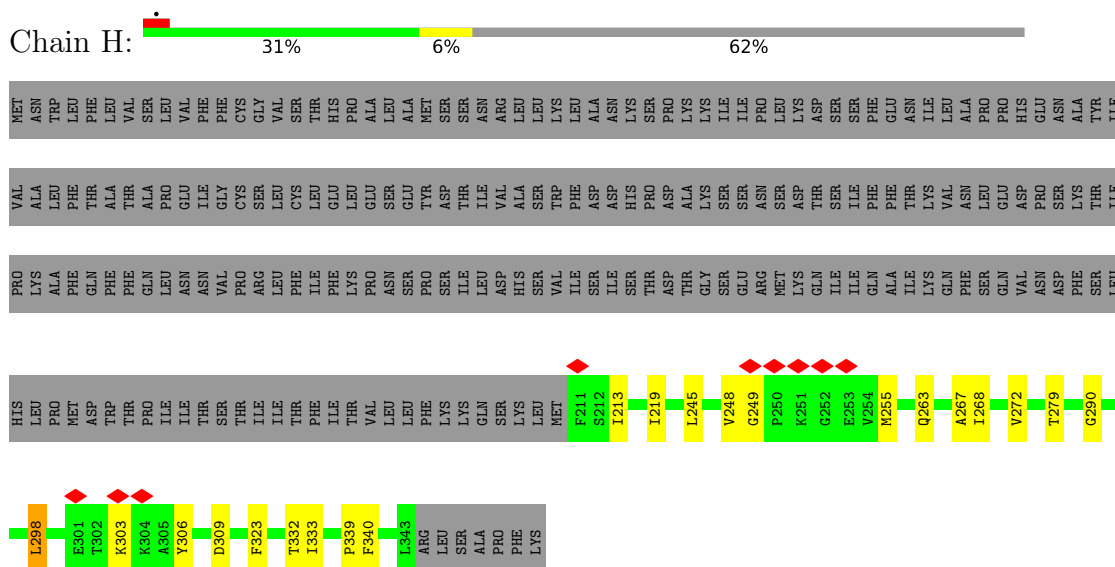
- Molecule 6: Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit 2



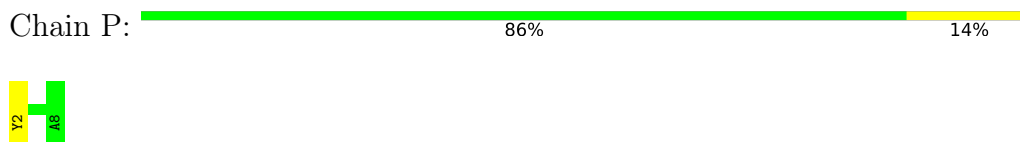
- Molecule 7: Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit WBP1



- 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

Chain I:  100%

MAG1
MAG2

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

Chain J:  100%
50% 50%

MAG1
MAG2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	72993	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 ($e^-/\text{\AA}^2$)	48.4	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.865	Depositor
Minimum map value	-0.884	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.050	Depositor
Recommended contour level	0.312	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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, 323, NAG, CPL, BMA, MN, PTY, KZB

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	0.18	0/5343	0.43	2/7265 (0.0%)
2	B	0.13	0/253	0.30	0/342
3	C	0.18	0/684	0.40	0/926
4	D	0.18	0/905	0.45	0/1220
5	E	0.14	0/3639	0.38	0/4954
6	F	0.21	0/1934	0.43	1/2637 (0.0%)
7	G	0.14	0/3283	0.36	0/4459
8	H	0.14	0/1098	0.33	0/1494
9	P	0.23	0/44	0.21	0/60
All	All	0.17	0/17183	0.40	3/23357 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	709	ILE	CA-C-N	6.22	133.43	121.54
1	A	709	ILE	C-N-CA	6.22	133.43	121.54
6	F	34	ARG	N-CA-C	-5.46	106.99	113.97

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5191	0	5158	65	0
2	B	251	0	260	4	0
3	C	666	0	677	11	0
4	D	883	0	911	13	0
5	E	3537	0	3412	41	0
6	F	1892	0	1831	38	0
7	G	3201	0	3101	42	0
8	H	1067	0	1099	12	0
9	P	44	0	36	1	0
10	K	83	0	70	1	0
11	I	28	0	25	0	0
11	J	28	0	25	0	0
12	A	1	0	0	0	0
13	A	52	0	80	1	0
13	B	52	0	80	4	0
13	E	52	0	80	4	0
13	F	52	0	80	1	0
14	A	42	0	60	0	0
15	A	129	0	0	0	0
15	B	86	0	0	0	0
15	F	86	0	0	0	0
15	G	43	0	0	0	0
16	G	28	0	26	0	0
17	P	31	0	21	0	0
18	A	4	0	0	0	0
18	C	1	0	0	0	0
18	E	2	0	0	0	0
18	G	2	0	0	0	0
All	All	17534	0	17032	217	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 6.

All (217) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:98:LYS:HB3	6:F:105:MET:HB3	1.55	0.88
7:G:140:ILE:HD11	7:G:179:ALA:HB2	1.68	0.76
1:A:32:ARG:NH1	1:A:160:SER:OG	2.20	0.74
1:A:656:THR:HG22	1:A:658:LEU:H	1.55	0.71
6:F:129:PRO:HB2	6:F:153:GLN:HB3	1.71	0.70
1:A:582:ASP:OD2	1:A:651:ARG:NH2	2.25	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:199:ASN:HB3	5:E:202:SER:HB2	1.73	0.70
5:E:238:ARG:NH1	5:E:364:PRO:O	2.25	0.69
7:G:264:ILE:HD11	7:G:364:LEU:HD22	1.74	0.69
6:F:41:GLU:O	6:F:153:GLN:NE2	2.26	0.69
1:A:134:THR:HB	1:A:143:GLY:HA2	1.75	0.69
1:A:548:LYS:O	1:A:552:SER:OG	2.14	0.65
6:F:50:VAL:HB	6:F:147:LEU:HD13	1.78	0.65
7:G:193:ASN:HA	7:G:216:PHE:HA	1.81	0.63
5:E:34:VAL:HA	5:E:171:LYS:HE2	1.80	0.63
2:B:18:MET:HE3	2:B:19:MET:HE3	1.81	0.63
1:A:638:PRO:HG3	1:A:655:ILE:HG22	1.79	0.62
1:A:430:ASP:O	1:A:448:LYS:NZ	2.31	0.62
6:F:136:LEU:HD23	6:F:147:LEU:HD23	1.82	0.62
1:A:351:HIS:HD2	1:A:402:MET:HE3	1.65	0.61
5:E:427:ILE:HB	5:E:430:VAL:HG22	1.84	0.60
6:F:53:THR:H	6:F:70:GLU:HG3	1.67	0.60
13:F:301:CPL:H141	13:F:301:CPL:H322	1.83	0.60
7:G:252:GLU:HA	7:G:255:LYS:HB2	1.83	0.60
5:E:144:TYR:HB3	5:E:145:PRO:HD3	1.84	0.59
1:A:138:LYS:HE3	1:A:423:LYS:HG2	1.84	0.59
5:E:227:ASN:ND2	5:E:284:GLN:O	2.36	0.59
6:F:78:ASN:HD22	6:F:106:TYR:HE2	1.50	0.59
4:D:76:ALA:HA	4:D:129:ILE:HG13	1.84	0.59
1:A:212:VAL:O	1:A:215:THR:HG22	2.03	0.58
3:C:47:VAL:HG11	5:E:468:LYS:HE3	1.85	0.58
5:E:138:ASN:O	5:E:138:ASN:ND2	2.36	0.58
1:A:703:THR:HG23	1:A:706:ARG:HA	1.84	0.58
1:A:175:LEU:HD12	1:A:214:ILE:HD11	1.85	0.58
7:G:262:SER:HB3	7:G:364:LEU:HD23	1.86	0.58
4:D:82:ILE:HA	4:D:85:VAL:HG22	1.86	0.58
6:F:76:PHE:HB3	6:F:138:SER:HB2	1.86	0.57
1:A:580:GLY:O	1:A:585:ASN:ND2	2.36	0.57
5:E:470:LEU:HD12	5:E:472:MET:HE2	1.85	0.57
1:A:28:ALA:O	1:A:32:ARG:HG2	2.04	0.57
8:H:249:GLY:HA2	8:H:255:MET:HE3	1.85	0.57
1:A:192:MET:HB2	4:D:113:GLU:HG2	1.87	0.57
1:A:182:TRP:HE1	1:A:221:HIS:HD2	1.52	0.56
6:F:226:VAL:O	6:F:229:VAL:HG12	2.07	0.55
6:F:266:ALA:HB3	6:F:267:PRO:HD3	1.88	0.55
1:A:72:ASP:OD1	1:A:72:ASP:N	2.33	0.54
1:A:240:THR:HG21	4:D:89:VAL:HB	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:LEU:HD13	13:A:802:CPL:H142	1.88	0.54
5:E:163:LEU:N	5:E:218:GLU:OE2	2.35	0.54
7:G:312:ILE:HB	7:G:327:LEU:HD12	1.89	0.54
1:A:544:ALA:CB	1:A:597:ILE:HG13	2.38	0.53
5:E:98:ALA:HA	5:E:113:ARG:HH12	1.73	0.53
6:F:52:THR:HA	6:F:70:GLU:HG3	1.91	0.53
6:F:193:ALA:O	6:F:197:VAL:HG23	2.08	0.53
8:H:294:LEU:O	8:H:298:LEU:HB2	2.09	0.53
5:E:183:PHE:HB3	5:E:222:ILE:HD11	1.89	0.53
6:F:30:ALA:HB2	6:F:107:LYS:HE2	1.91	0.52
5:E:98:ALA:HA	5:E:113:ARG:NH1	2.23	0.52
8:H:263:GLN:NE2	9:P:2:TYR:OH	2.42	0.52
6:F:96:GLU:CB	6:F:107:LYS:O	2.58	0.52
3:C:43:ALA:O	3:C:47:VAL:HG23	2.09	0.52
1:A:265:ASP:OD1	1:A:265:ASP:N	2.42	0.52
5:E:65:GLU:OE2	5:E:118:GLN:HG2	2.10	0.52
6:F:222:ILE:HD12	6:F:222:ILE:H	1.75	0.52
1:A:392:SER:O	1:A:396:SER:OG	2.19	0.51
5:E:175:PHE:HB3	5:E:205:PHE:HB2	1.92	0.51
1:A:495:ASP:HB2	1:A:676:MET:HE3	1.93	0.51
7:G:316:LEU:HB3	7:G:323:TYR:HB2	1.93	0.51
6:F:30:ALA:HA	6:F:65:VAL:HG23	1.91	0.51
4:D:72:PHE:HB3	4:D:73:PRO:HD3	1.93	0.51
6:F:219:PHE:HA	7:G:415:THR:HG22	1.93	0.50
1:A:354:VAL:HG11	1:A:406:MET:HE1	1.92	0.50
1:A:711:ARG:HD2	7:G:209:TRP:HA	1.93	0.50
5:E:60:SER:HA	5:E:125:PRO:HB3	1.93	0.50
1:A:717:ARG:NH1	7:G:183:GLU:O	2.44	0.50
7:G:415:THR:HG22	7:G:415:THR:O	2.12	0.50
1:A:618:ALA:HA	1:A:625:ARG:HH21	1.76	0.50
7:G:327:LEU:HB3	7:G:339:TYR:HB3	1.93	0.49
6:F:72:THR:OG1	6:F:73:ASN:N	2.46	0.49
6:F:105:MET:HE3	6:F:106:TYR:N	2.27	0.49
5:E:172:LYS:HD3	5:E:173:ALA:N	2.28	0.49
5:E:147:HIS:HB3	5:E:265:SER:HB3	1.95	0.48
1:A:711:ARG:HE	7:G:181:LEU:HD11	1.79	0.48
1:A:351:HIS:CD2	1:A:402:MET:HE3	2.49	0.48
1:A:631:LYS:HD3	1:A:661:PRO:HG2	1.95	0.48
1:A:555:GLU:O	1:A:559:GLU:HG2	2.12	0.47
5:E:352:SER:HB3	5:E:358:LYS:HB2	1.96	0.47
7:G:330:SER:O	7:G:330:SER:OG	2.32	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3:SER:OG	2:B:4:ASP:N	2.48	0.47
3:C:84:VAL:HG21	13:E:501:CPL:H121	1.95	0.47
5:E:76:SER:O	5:E:424:ARG:NH1	2.47	0.47
6:F:111:ASP:OD1	6:F:114:LYS:HB2	2.14	0.47
5:E:241:TRP:CD1	13:E:501:CPL:HC81	2.50	0.47
1:A:42:ILE:HG13	1:A:43:ILE:N	2.29	0.47
5:E:162:ARG:NH2	5:E:185:GLU:OE1	2.48	0.47
8:H:290:GLY:O	8:H:294:LEU:HG	2.15	0.47
6:F:78:ASN:N	6:F:78:ASN:OD1	2.48	0.47
5:E:208:TRP:HB2	5:E:211:ILE:HD11	1.97	0.47
7:G:114:SER:O	7:G:118:VAL:HG23	2.15	0.47
8:H:245:LEU:HA	8:H:267:ALA:HB3	1.97	0.47
2:B:1:MET:HA	13:B:103:CPL:HC11	1.98	0.46
4:D:34:TYR:CZ	4:D:38:ILE:HG21	2.50	0.46
3:C:26:PRO:HG3	3:C:81:SER:HB2	1.97	0.46
6:F:121:GLN:HE21	6:F:121:GLN:HB2	1.54	0.46
7:G:386:SER:HB2	7:G:396:ILE:HD11	1.97	0.46
1:A:574:GLY:HA3	1:A:579:PHE:HB3	1.95	0.46
1:A:263:SER:OG	1:A:265:ASP:OD1	2.31	0.46
1:A:240:THR:CG2	4:D:89:VAL:HB	2.45	0.45
5:E:40:ILE:HB	5:E:177:LEU:HD23	1.97	0.45
6:F:242:GLU:HG3	7:G:407:ILE:HD11	1.98	0.45
7:G:263:VAL:HG22	7:G:299:TRP:HB3	1.97	0.45
5:E:282:MET:SD	5:E:282:MET:N	2.87	0.45
1:A:627:SER:O	1:A:631:LYS:HG3	2.17	0.45
3:C:27:LYS:O	3:C:30:ILE:HG12	2.16	0.45
3:C:80:ASN:HD22	3:C:85:TYR:HA	1.82	0.45
6:F:96:GLU:HB2	6:F:107:LYS:O	2.17	0.45
1:A:64:TYR:OH	7:G:381:ASP:OD1	2.30	0.45
1:A:573:PHE:O	1:A:676:MET:HA	2.17	0.45
5:E:36:TYR:HE1	5:E:38:ARG:HB2	1.82	0.45
7:G:274:ALA:HA	7:G:291:ILE:HG13	1.98	0.45
7:G:289:LYS:NZ	7:G:343:GLU:OE1	2.40	0.45
1:A:381:LEU:HD23	1:A:381:LEU:HA	1.82	0.45
1:A:441:LYS:HA	1:A:441:LYS:HD3	1.76	0.45
6:F:78:ASN:HA	6:F:135:ILE:O	2.16	0.45
6:F:190:LYS:N	6:F:191:PRO:HD2	2.32	0.45
7:G:54:LEU:HD22	7:G:56:TYR:CZ	2.52	0.45
7:G:209:TRP:HD1	7:G:210:THR:HG23	1.82	0.45
7:G:30:TYR:CE2	7:G:58:ASP:HB2	2.52	0.45
7:G:358:ASP:OD1	7:G:368:THR:HG23	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:545:ILE:HD11	10:K:2:NAG:H82	1.98	0.44
6:F:186:LYS:NZ	6:F:187:ARG:O	2.43	0.44
3:C:80:ASN:HD21	3:C:86:VAL:H	1.66	0.44
4:D:43:LYS:HD3	7:G:413:PHE:CE1	2.52	0.44
1:A:364:HIS:HB3	1:A:462:PHE:HD1	1.82	0.44
5:E:68:THR:O	5:E:114:TYR:HA	2.18	0.44
6:F:79:THR:HG22	6:F:135:ILE:HB	2.00	0.44
4:D:53:PHE:CD1	6:F:207:LEU:HD13	2.53	0.44
5:E:385:GLU:OE1	5:E:413:ASN:HB2	2.17	0.44
6:F:30:ALA:HB3	6:F:109:ARG:HG2	1.99	0.44
6:F:80:LEU:HD23	6:F:134:LEU:HG	2.00	0.43
7:G:327:LEU:HD23	7:G:341:THR:HG22	1.99	0.43
8:H:268:ILE:O	8:H:272:VAL:HG23	2.17	0.43
7:G:80:ILE:HG23	7:G:110:LEU:HD23	2.00	0.43
1:A:684:LYS:HE2	1:A:684:LYS:HB3	1.83	0.43
3:C:6:LEU:HD12	3:C:6:LEU:HA	1.74	0.43
4:D:37:GLN:NE2	4:D:99:CYS:SG	2.92	0.43
5:E:56:LYS:HB3	5:E:128:GLU:OE1	2.19	0.43
7:G:54:LEU:HD23	7:G:55:GLU:N	2.32	0.43
8:H:339:PRO:HG2	8:H:340:PHE:CE2	2.53	0.43
1:A:43:ILE:HB	1:A:49:TRP:CZ2	2.54	0.43
1:A:444:ALA:O	1:A:448:LYS:HG3	2.17	0.43
13:B:103:CPL:H382	13:B:103:CPL:H411	1.69	0.43
5:E:180:SER:OG	5:E:181:SER:N	2.51	0.43
6:F:230:TYR:CE1	6:F:274:LYS:HG2	2.54	0.43
1:A:356:TRP:CG	1:A:357:PRO:HD3	2.54	0.43
7:G:185:ARG:HB2	7:G:188:ILE:HG13	2.00	0.43
1:A:263:SER:O	1:A:267:MET:HG2	2.19	0.42
4:D:40:LYS:HB3	4:D:40:LYS:HE3	1.71	0.42
7:G:43:TYR:HE2	7:G:238:LEU:HA	1.85	0.42
7:G:89:ASN:O	7:G:93:GLN:HG2	2.19	0.42
7:G:203:LYS:HE3	7:G:203:LYS:HB3	1.89	0.42
6:F:157:ASN:OD1	6:F:157:ASN:N	2.52	0.42
1:A:133:PHE:O	1:A:137:ILE:HG12	2.19	0.42
1:A:240:THR:HG23	1:A:273:PHE:HE1	1.84	0.42
1:A:503:LEU:HD12	1:A:503:LEU:HA	1.88	0.42
1:A:555:GLU:HG2	1:A:665:TYR:CZ	2.53	0.42
6:F:77:GLN:O	6:F:136:LEU:HA	2.19	0.42
5:E:31:TRP:CH2	5:E:123:ILE:HG12	2.55	0.42
5:E:377:VAL:HG21	5:E:426:LEU:HD12	2.02	0.42
6:F:82:ILE:HD12	6:F:131:LYS:O	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:709:ILE:O	1:A:710:LYS:O	2.38	0.42
13:B:103:CPL:H221	13:E:501:CPL:H182	2.02	0.42
4:D:62:CYS:O	4:D:65:ILE:HG22	2.19	0.42
7:G:193:ASN:HB3	7:G:216:PHE:CD2	2.55	0.42
7:G:356:LEU:HD13	7:G:370:LYS:HG2	2.01	0.42
2:B:1:MET:HG2	2:B:2:ILE:H	1.85	0.42
6:F:99:ASP:OD1	6:F:99:ASP:N	2.47	0.42
13:B:103:CPL:H222	13:B:103:CPL:H191	1.70	0.41
13:E:501:CPL:H202	13:E:501:CPL:H172	1.89	0.41
8:H:279:THR:HG21	8:H:323:PHE:CZ	2.55	0.41
1:A:40:GLU:OE2	1:A:497:ARG:NH2	2.53	0.41
7:G:99:LEU:HD23	7:G:99:LEU:HA	1.79	0.41
1:A:277:GLN:HE21	1:A:277:GLN:HB3	1.68	0.41
7:G:113:SER:O	7:G:113:SER:OG	2.36	0.41
8:H:303:LYS:HD2	8:H:303:LYS:HA	1.81	0.41
1:A:441:LYS:HD2	8:H:306:TYR:CE2	2.55	0.41
1:A:479:VAL:HG23	1:A:480:VAL:HG23	2.03	0.41
5:E:165:LEU:HB2	5:E:216:SER:HB3	2.02	0.41
1:A:50:PHE:HE2	1:A:86:LEU:HD13	1.85	0.41
7:G:109:ILE:O	7:G:229:LEU:HA	2.20	0.41
1:A:441:LYS:HA	1:A:442:PRO:HD3	1.91	0.41
3:C:55:LYS:HA	3:C:55:LYS:HD3	1.79	0.41
3:C:58:PHE:O	3:C:61:THR:HG22	2.20	0.41
5:E:134:LYS:HE3	5:E:134:LYS:HB3	1.82	0.41
6:F:219:PHE:O	6:F:222:ILE:HD11	2.21	0.41
1:A:348:VAL:HG12	1:A:350:GLU:HG2	2.03	0.41
1:A:649:ARG:HE	1:A:649:ARG:HB3	1.59	0.41
4:D:72:PHE:CD1	4:D:72:PHE:C	2.99	0.41
5:E:119:PHE:CE1	5:E:129:VAL:HG11	2.55	0.41
5:E:270:ARG:HG3	5:E:274:MET:HE2	2.03	0.41
5:E:398:PHE:HB3	5:E:423:TYR:CE1	2.56	0.41
5:E:399:THR:N	5:E:422:SER:O	2.52	0.41
6:F:90:GLU:OE2	7:G:196:ARG:HD2	2.21	0.41
7:G:176:GLU:H	7:G:176:GLU:HG2	1.68	0.41
7:G:391:ASN:OD1	7:G:391:ASN:N	2.53	0.41
1:A:205:VAL:HG22	1:A:211:TYR:CD2	2.56	0.41
5:E:75:PHE:CD2	5:E:113:ARG:HD3	2.56	0.41
5:E:184:GLU:O	5:E:222:ILE:HD12	2.20	0.41
1:A:16:LEU:HD12	1:A:16:LEU:HA	1.85	0.40
1:A:180:MET:HE3	1:A:180:MET:HB3	1.92	0.40
5:E:411:ASP:HB3	5:E:415:GLY:HA2	2.04	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:109:ILE:HB	7:G:229:LEU:HD12	2.04	0.40
1:A:622:GLU:O	1:A:626:ASN:ND2	2.54	0.40
8:H:219:ILE:HD13	8:H:219:ILE:HA	1.91	0.40
1:A:364:HIS:CE1	1:A:461:LEU:HD23	2.57	0.40
3:C:61:THR:O	3:C:65:VAL:HG23	2.21	0.40
8:H:295:ARG:HG3	8:H:309:ASP:OD1	2.22	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	636/718 (89%)	609 (96%)	25 (4%)	2 (0%)	36	66
2	B	31/65 (48%)	31 (100%)	0	0	100	100
3	C	83/86 (96%)	82 (99%)	1 (1%)	0	100	100
4	D	107/130 (82%)	101 (94%)	6 (6%)	0	100	100
5	E	434/476 (91%)	414 (95%)	20 (5%)	0	100	100
6	F	256/283 (90%)	234 (91%)	21 (8%)	1 (0%)	30	60
7	G	392/430 (91%)	380 (97%)	12 (3%)	0	100	100
8	H	131/350 (37%)	126 (96%)	5 (4%)	0	100	100
9	P	5/7 (71%)	5 (100%)	0	0	100	100
All	All	2075/2545 (82%)	1982 (96%)	90 (4%)	3 (0%)	49	77

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	45	GLU
1	A	710	LYS
6	F	168	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	551/613 (90%)	537 (98%)	14 (2%)	42	76
2	B	30/55 (54%)	29 (97%)	1 (3%)	33	69
3	C	74/75 (99%)	70 (95%)	4 (5%)	20	51
4	D	96/115 (84%)	95 (99%)	1 (1%)	68	88
5	E	394/426 (92%)	372 (94%)	22 (6%)	19	50
6	F	181/246 (74%)	168 (93%)	13 (7%)	13	39
7	G	359/392 (92%)	349 (97%)	10 (3%)	38	73
8	H	115/316 (36%)	110 (96%)	5 (4%)	26	60
9	P	4/4 (100%)	4 (100%)	0	100	100
All	All	1804/2242 (80%)	1734 (96%)	70 (4%)	30	64

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	CYS
1	A	45	GLU
1	A	136	GLU
1	A	161	VAL
1	A	180	MET
1	A	215	THR
1	A	349	SER
1	A	363	THR
1	A	395	CYS
1	A	408	THR
1	A	472	THR
1	A	503	LEU
1	A	542	HIS
1	A	600	GLU
2	B	4	ASP
3	C	2	THR
3	C	15	SER
3	C	61	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	73	LEU
4	D	39	GLU
5	E	53	ILE
5	E	54	THR
5	E	55	ILE
5	E	74	ILE
5	E	86	THR
5	E	90	THR
5	E	96	LEU
5	E	123	ILE
5	E	170	THR
5	E	172	LYS
5	E	192	GLU
5	E	209	GLU
5	E	219	THR
5	E	284	GLN
5	E	289	THR
5	E	310	LEU
5	E	317	GLU
5	E	323	ILE
5	E	355	SER
5	E	373	VAL
5	E	417	VAL
5	E	467	LEU
6	F	70	GLU
6	F	104	SER
6	F	108	TYR
6	F	111	ASP
6	F	119	LEU
6	F	121	GLN
6	F	130	ILE
6	F	134	LEU
6	F	140	THR
6	F	144	LYS
6	F	147	LEU
6	F	157	ASN
6	F	222	ILE
7	G	65	THR
7	G	140	ILE
7	G	255	LYS
7	G	263	VAL
7	G	303	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	G	312	ILE
7	G	343	GLU
7	G	361	LYS
7	G	386	SER
7	G	390	SER
8	H	213	ILE
8	H	248	VAL
8	H	298	LEU
8	H	332	THR
8	H	333	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	HIS
1	A	60	ASN
1	A	193	HIS
1	A	221	HIS
1	A	277	GLN
1	A	351	HIS
1	A	352	GLN
1	A	642	ASN
1	A	652	GLN
1	A	653	GLN
2	B	26	HIS
3	C	11	HIS
3	C	80	ASN
4	D	97	GLN
5	E	126	GLN
5	E	147	HIS
5	E	154	GLN
5	E	201	ASN
5	E	226	HIS
5	E	227	ASN
5	E	232	GLN
5	E	276	GLN
5	E	406	GLN
5	E	413	ASN
5	E	416	HIS
5	E	429	GLN
6	F	121	GLN
6	F	179	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	G	93	GLN
7	G	105	ASN
7	G	108	ASN
7	G	138	HIS
7	G	214	GLN
7	G	226	ASN
7	G	242	ASN
7	G	271	HIS
7	G	273	HIS
7	G	318	GLN
8	H	238	ASN
8	H	263	GLN
8	H	265	GLN
8	H	292	GLN
8	H	297	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

11 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	$\# Z > 2$
11	NAG	I	1	11,5	14,14,15	0.31	0	17,19,21	0.41	0
11	NAG	I	2	11	14,14,15	0.22	0	17,19,21	0.53	0
11	NAG	J	1	11,5	14,14,15	0.41	0	17,19,21	1.30	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	NAG	J	2	11	14,14,15	0.24	0	17,19,21	0.54	0
10	NAG	K	1	10,1	14,14,15	0.39	0	17,19,21	0.51	0
10	NAG	K	2	10	14,14,15	0.26	0	17,19,21	0.56	0
10	BMA	K	3	10	11,11,12	0.60	0	15,15,17	0.85	0
10	MAN	K	4	10	11,11,12	0.72	0	15,15,17	1.16	2 (13%)
10	MAN	K	5	10	11,11,12	0.62	0	15,15,17	1.00	2 (13%)
10	MAN	K	6	10	11,11,12	0.61	0	15,15,17	0.94	2 (13%)
10	MAN	K	7	10	11,11,12	0.60	0	15,15,17	0.98	2 (13%)

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
11	NAG	I	1	11,5	-	0/6/23/26	0/1/1/1
11	NAG	I	2	11	-	1/6/23/26	0/1/1/1
11	NAG	J	1	11,5	-	4/6/23/26	0/1/1/1
11	NAG	J	2	11	-	4/6/23/26	0/1/1/1
10	NAG	K	1	10,1	-	2/6/23/26	0/1/1/1
10	NAG	K	2	10	-	0/6/23/26	0/1/1/1
10	BMA	K	3	10	-	0/2/19/22	0/1/1/1
10	MAN	K	4	10	-	2/2/19/22	0/1/1/1
10	MAN	K	5	10	-	0/2/19/22	0/1/1/1
10	MAN	K	6	10	-	0/2/19/22	0/1/1/1
10	MAN	K	7	10	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	J	1	NAG	C1-O5-C5	4.90	118.75	112.19
10	K	4	MAN	O2-C2-C3	-2.97	104.01	110.15
10	K	5	MAN	O2-C2-C3	-2.66	104.65	110.15
10	K	4	MAN	C1-O5-C5	2.53	115.57	112.19
10	K	7	MAN	C1-O5-C5	2.44	115.46	112.19
10	K	5	MAN	C1-O5-C5	2.25	115.20	112.19
10	K	6	MAN	C1-O5-C5	2.20	115.14	112.19
10	K	7	MAN	O2-C2-C3	-2.08	105.84	110.15
10	K	6	MAN	O2-C2-C3	-2.07	105.86	110.15

There are no chirality outliers.

All (13) torsion outliers are listed below:

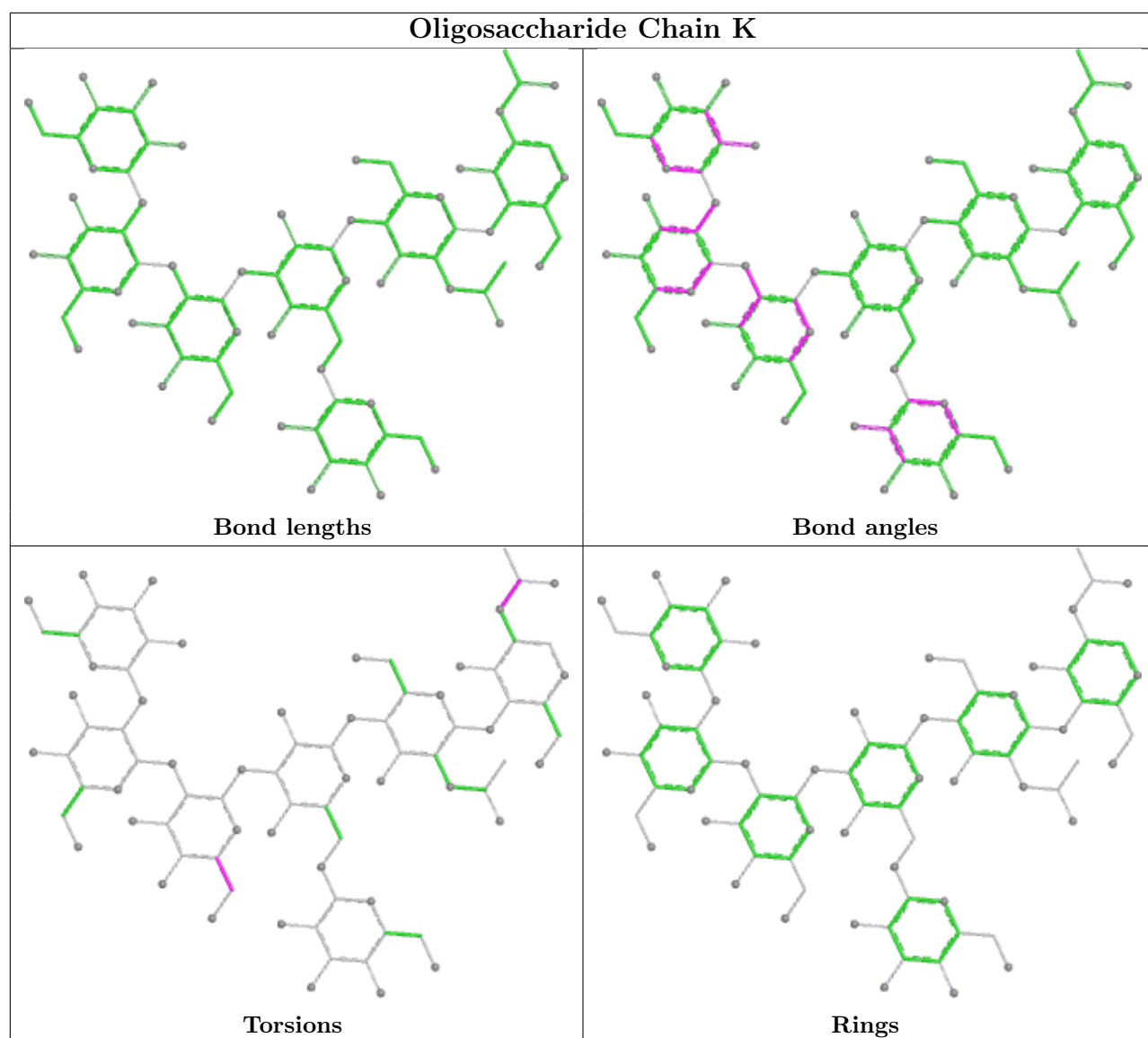
Mol	Chain	Res	Type	Atoms
11	J	2	NAG	C4-C5-C6-O6
10	K	4	MAN	O5-C5-C6-O6
11	J	1	NAG	O5-C5-C6-O6
10	K	4	MAN	C4-C5-C6-O6
11	J	2	NAG	O5-C5-C6-O6
11	J	1	NAG	C4-C5-C6-O6
10	K	1	NAG	C8-C7-N2-C2
10	K	1	NAG	O7-C7-N2-C2
11	J	1	NAG	C8-C7-N2-C2
11	J	1	NAG	O7-C7-N2-C2
11	J	2	NAG	C1-C2-N2-C7
11	J	2	NAG	C3-C2-N2-C7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

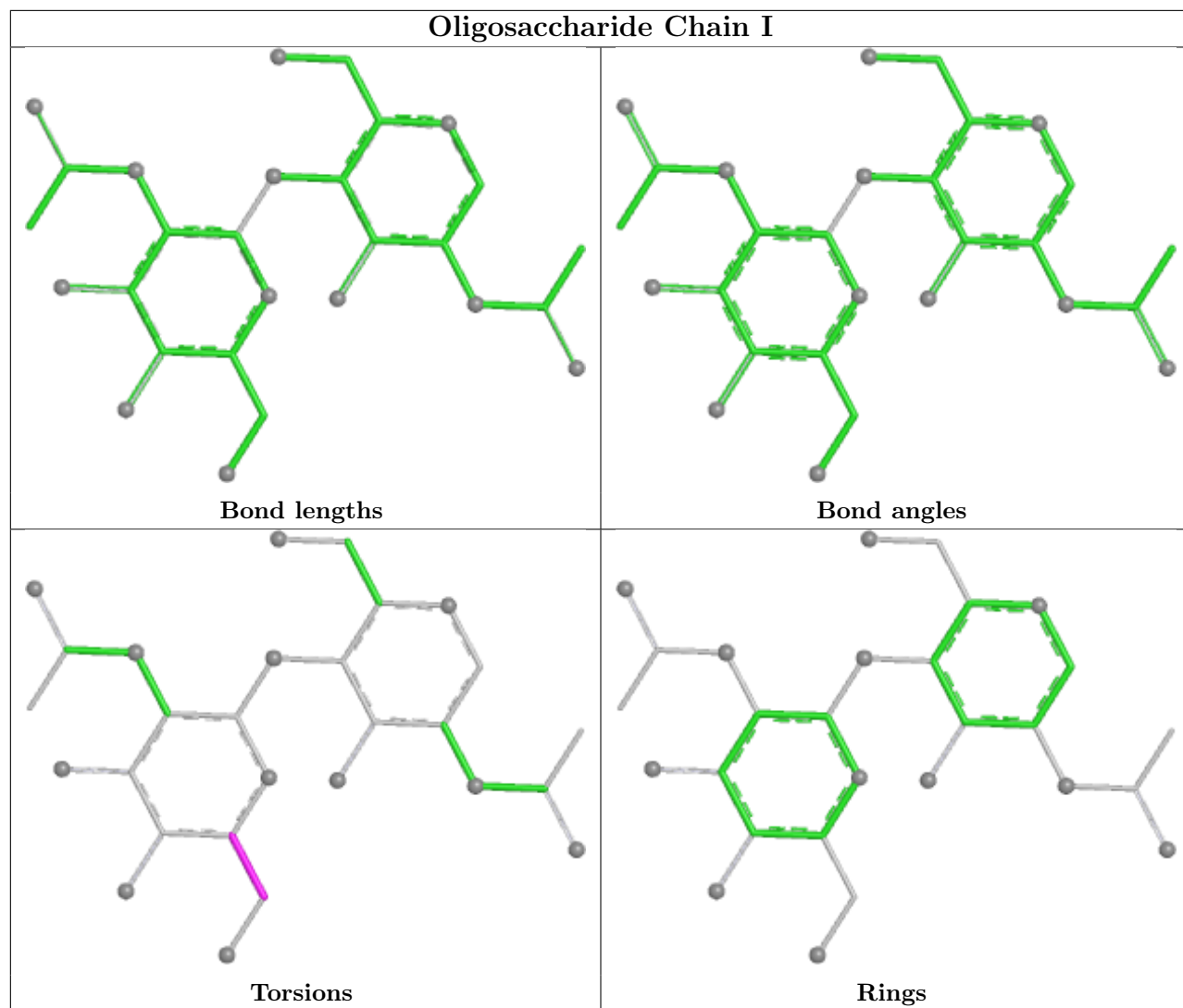
There are no ring outliers.

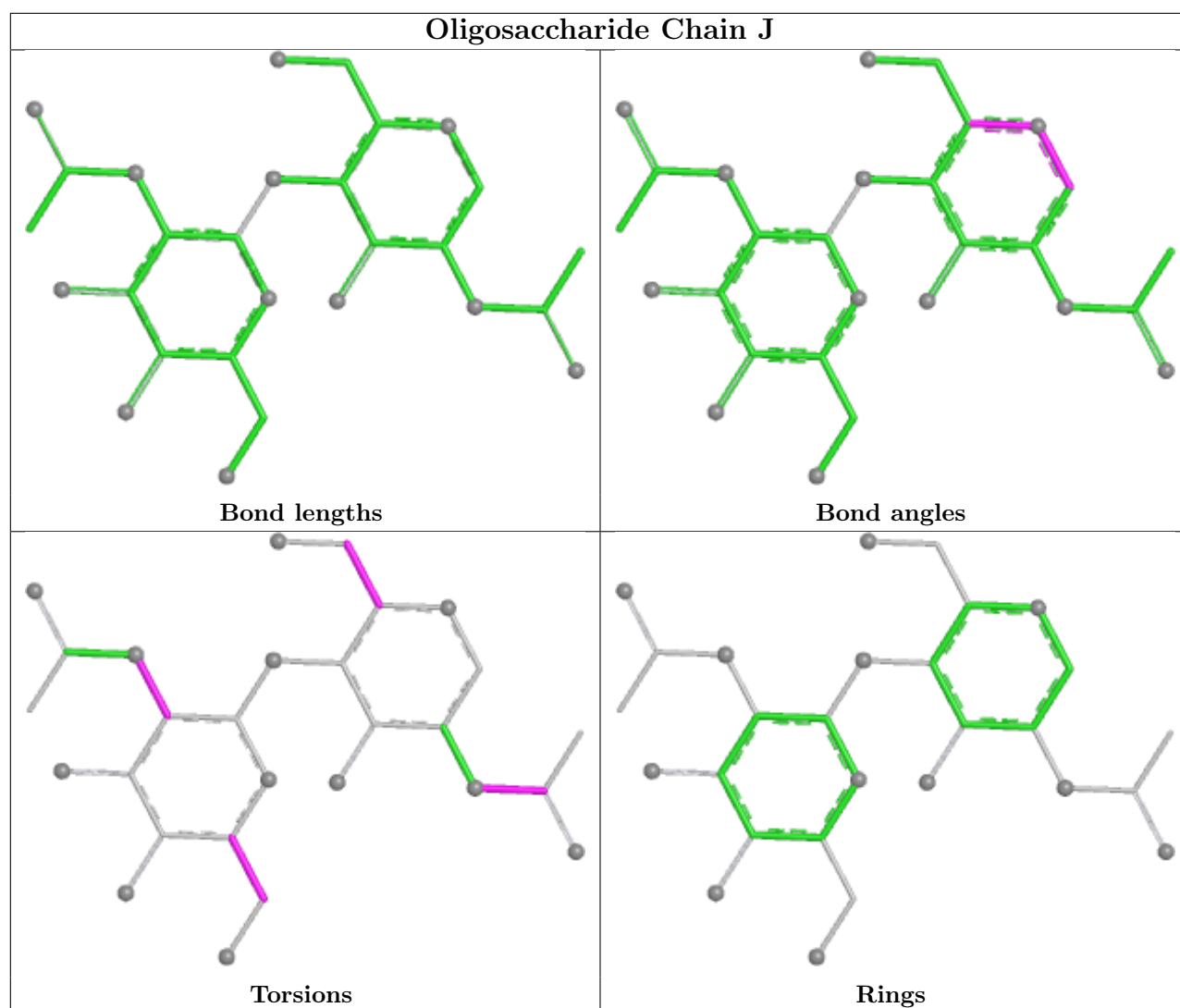
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	K	2	NAG	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 17 ligands modelled in this entry, 1 is monoatomic - leaving 16 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	$\# Z > 2$
15	KZB	F	303	-	49,49,49	0.63	0	75,80,80	1.68	11 (14%)
13	CPL	E	501	-	51,51,51	1.31	6 (11%)	57,59,59	1.02	2 (3%)
15	KZB	G	503	-	49,49,49	0.58	0	75,80,80	1.65	11 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	KZB	A	805	-	49,49,49	0.67	0	75,80,80	2.34	20 (26%)
17	323	P	101	9	34,34,34	2.46	10 (29%)	50,50,50	1.21	4 (8%)
13	CPL	B	103	-	51,51,51	1.31	6 (11%)	57,59,59	1.07	2 (3%)
15	KZB	B	102	-	49,49,49	0.67	0	75,80,80	1.78	15 (20%)
15	KZB	F	302	-	49,49,49	0.63	1 (2%)	75,80,80	1.95	16 (21%)
16	NAG	G	501	7	14,14,15	0.47	0	17,19,21	1.30	1 (5%)
13	CPL	F	301	-	51,51,51	1.32	5 (9%)	57,59,59	1.07	2 (3%)
13	CPL	A	802	-	51,51,51	1.30	5 (9%)	57,59,59	0.94	2 (3%)
15	KZB	B	101	-	49,49,49	0.71	1 (2%)	75,80,80	1.86	13 (17%)
16	NAG	G	502	7	14,14,15	1.06	2 (14%)	17,19,21	1.15	1 (5%)
15	KZB	A	806	-	49,49,49	0.64	0	75,80,80	1.58	13 (17%)
14	PTY	A	803	-	41,41,49	0.95	4 (9%)	44,46,54	1.09	2 (4%)
15	KZB	A	804	-	49,49,49	0.71	1 (2%)	75,80,80	1.93	17 (22%)

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
15	KZB	F	303	-	-	2/6/121/121	0/7/7/7
13	CPL	E	501	-	-	21/55/55/55	-
15	KZB	G	503	-	-	3/6/121/121	0/7/7/7
15	KZB	A	805	-	-	6/6/121/121	0/7/7/7
17	323	P	101	9	-	14/20/69/69	0/4/4/4
13	CPL	B	103	-	-	18/55/55/55	-
15	KZB	B	102	-	-	4/6/121/121	0/7/7/7
15	KZB	F	302	-	-	0/6/121/121	0/7/7/7
16	NAG	G	501	7	-	0/6/23/26	0/1/1/1
13	CPL	F	301	-	-	20/55/55/55	-
13	CPL	A	802	-	-	10/55/55/55	-
15	KZB	B	101	-	-	4/6/121/121	0/7/7/7
16	NAG	G	502	7	-	3/6/23/26	0/1/1/1
15	KZB	A	806	-	-	3/6/121/121	0/7/7/7
14	PTY	A	803	-	-	18/45/45/53	-
15	KZB	A	804	-	-	2/6/121/121	0/7/7/7

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	P	101	323	O1-C4	7.15	1.49	1.38
17	P	101	323	C7-N2	5.34	1.50	1.37
17	P	101	323	O1-C3	5.14	1.46	1.37
17	P	101	323	C18-C1	3.70	1.54	1.49
17	P	101	323	C23-C24	3.69	1.57	1.49
17	P	101	323	C17-N1	3.57	1.52	1.46
17	P	101	323	C2-C1	3.55	1.50	1.40
13	F	301	CPL	O2-C31	3.36	1.43	1.34
17	P	101	323	C12-N1	-3.29	1.30	1.34
13	B	103	CPL	O2-C31	3.29	1.43	1.34
13	F	301	CPL	O3-C11	3.29	1.42	1.33
13	A	802	CPL	O2-C31	3.29	1.43	1.34
13	E	501	CPL	O3-C11	3.28	1.42	1.33
13	B	103	CPL	O3-C11	3.28	1.42	1.33
13	E	501	CPL	O2-C31	3.26	1.43	1.34
13	A	802	CPL	O3-C11	3.17	1.42	1.33
16	G	502	NAG	O5-C1	3.10	1.48	1.43
17	P	101	323	C21-C25	2.88	1.56	1.47
14	A	803	PTY	O7-C6	-2.64	1.40	1.46
13	B	103	CPL	P-O4P	2.42	1.68	1.59
16	G	502	NAG	C1-C2	2.39	1.55	1.52
13	E	501	CPL	O2-C2	-2.37	1.41	1.46
13	F	301	CPL	P-O4P	2.37	1.68	1.59
13	B	103	CPL	O2-C2	-2.35	1.41	1.46
13	A	802	CPL	P-O4P	2.33	1.68	1.59
13	F	301	CPL	O2-C2	-2.32	1.41	1.46
13	A	802	CPL	O2-C2	-2.30	1.41	1.46
14	A	803	PTY	O4-C30	2.30	1.40	1.33
13	E	501	CPL	P-O4P	2.27	1.68	1.59
13	E	501	CPL	C32-C31	2.25	1.57	1.50
14	A	803	PTY	O4-C1	-2.24	1.40	1.45
13	B	103	CPL	C32-C31	2.24	1.57	1.50
13	F	301	CPL	C32-C31	2.24	1.57	1.50
13	A	802	CPL	C32-C31	2.23	1.57	1.50
15	F	302	KZB	C84-C03	-2.14	1.52	1.56
15	A	804	KZB	C84-C03	-2.12	1.52	1.56
15	B	101	KZB	C84-C03	-2.11	1.52	1.56
14	A	803	PTY	O7-C8	2.06	1.40	1.34
13	E	501	CPL	P-O3P	2.05	1.67	1.59
13	B	103	CPL	P-O3P	2.02	1.67	1.59
17	P	101	323	C15-N2	2.02	1.50	1.45

All (132) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	F	302	KZB	O05-C04-C13	9.05	128.53	110.20
15	B	101	KZB	O05-C04-C13	8.86	128.14	110.20
15	A	804	KZB	O05-C04-C13	8.86	128.12	110.20
15	A	806	KZB	O05-C04-C13	8.61	127.63	110.20
15	A	805	KZB	O05-C04-C13	8.57	127.55	110.20
15	F	303	KZB	O05-C04-C13	8.47	127.35	110.20
15	G	503	KZB	O05-C04-C13	8.33	127.05	110.20
15	B	102	KZB	O05-C04-C13	8.31	127.02	110.20
15	A	805	KZB	C79-C81-C16	-6.64	105.69	112.43
15	A	805	KZB	C78-C76-C21	5.40	117.69	110.46
15	B	101	KZB	C02-C03-C04	-5.07	96.13	104.28
16	G	501	NAG	C1-O5-C5	4.98	118.87	112.19
15	A	805	KZB	C17-C16-C81	-4.86	104.69	110.52
15	A	804	KZB	C15-C16-C81	-4.85	100.61	109.17
15	A	805	KZB	C78-C79-C19	4.80	111.82	107.23
15	A	804	KZB	C17-C16-C81	-4.69	104.89	110.52
15	F	302	KZB	C78-C79-C19	4.69	111.71	107.23
15	A	805	KZB	C03-C84-C15	-4.68	93.10	100.16
15	A	804	KZB	C84-C15-C16	-4.58	107.51	113.90
15	B	102	KZB	C79-C81-C16	-4.55	107.81	112.43
15	A	805	KZB	C84-C03-C02	4.52	133.86	120.50
15	F	303	KZB	C02-C03-C04	-4.44	97.15	104.28
15	A	805	KZB	C20-C19-C79	-4.32	108.06	112.66
16	G	502	NAG	C1-O5-C5	4.30	117.95	112.19
13	F	301	CPL	O2-C31-C32	4.30	120.78	111.48
15	G	503	KZB	C84-C03-C02	4.21	132.95	120.50
13	B	103	CPL	O2-C31-C32	4.12	120.38	111.48
15	A	805	KZB	C83-C84-C03	4.05	121.13	115.36
15	A	804	KZB	C02-C03-C04	-4.04	97.78	104.28
13	E	501	CPL	O2-C31-C32	3.93	119.97	111.48
14	A	803	PTY	O7-C8-C11	3.85	119.82	111.48
15	A	805	KZB	C82-C83-C84	-3.81	106.32	112.74
15	B	101	KZB	O12-C11-C09	-3.81	107.28	112.17
15	F	302	KZB	C17-C16-C81	-3.76	106.02	110.52
15	F	303	KZB	C79-C81-C16	-3.71	108.66	112.43
15	B	102	KZB	C17-C16-C81	-3.70	106.08	110.52
15	F	302	KZB	C79-C81-C16	-3.70	108.67	112.43
15	B	101	KZB	C17-C16-C81	-3.57	106.24	110.52
15	B	101	KZB	C82-C81-C79	-3.51	109.96	113.91
15	A	806	KZB	C84-C03-C02	3.49	130.81	120.50
15	B	102	KZB	C84-C03-C02	3.49	130.81	120.50
15	B	101	KZB	C84-C03-C02	3.45	130.68	120.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	804	KZB	C18-C17-C16	-3.44	106.68	112.16
15	A	804	KZB	C84-C03-C02	3.40	130.56	120.50
15	F	302	KZB	C07-C06-C02	-3.39	109.52	115.66
13	A	802	CPL	O2-C31-C32	3.36	118.76	111.48
15	B	101	KZB	C79-C81-C16	-3.34	109.04	112.43
15	B	101	KZB	C06-C02-C03	-3.33	98.46	103.37
15	F	302	KZB	O12-C06-C07	3.33	113.66	110.76
15	F	303	KZB	C84-C03-C02	3.30	130.24	120.50
15	A	805	KZB	C81-C79-C19	-3.26	103.99	108.51
15	F	302	KZB	O12-C11-C09	-3.22	108.04	112.17
15	A	805	KZB	C08-C07-C06	-3.20	106.92	111.93
15	F	303	KZB	C17-C16-C81	-3.12	106.78	110.52
15	A	806	KZB	C02-C03-C04	-3.11	99.28	104.28
15	B	102	KZB	C02-C03-C04	-3.10	99.30	104.28
15	F	302	KZB	C20-C21-C76	-3.07	107.86	111.07
15	F	302	KZB	C84-C03-C02	3.06	129.54	120.50
15	F	302	KZB	C23-O22-C21	-3.05	110.16	115.27
15	F	302	KZB	C19-C20-C21	-3.05	105.33	112.87
15	B	101	KZB	O12-C06-C07	3.00	113.37	110.76
15	A	804	KZB	C06-C02-C03	-2.94	99.03	103.37
15	A	805	KZB	C19-C20-C21	-2.93	105.64	112.87
15	F	302	KZB	C82-C83-C84	-2.92	107.81	112.74
15	F	303	KZB	C18-C17-C16	-2.91	107.53	112.16
15	G	503	KZB	C18-C17-C16	-2.87	107.58	112.16
15	G	503	KZB	C17-C18-C19	-2.84	106.34	111.84
15	B	102	KZB	C23-O24-C25	2.82	119.23	113.72
13	B	103	CPL	O3-C11-C12	2.81	120.42	111.83
15	B	102	KZB	O22-C21-C20	-2.78	104.23	109.64
15	F	302	KZB	C78-C76-C21	-2.77	106.75	110.46
15	G	503	KZB	C83-C84-C03	2.77	119.30	115.36
15	B	101	KZB	C20-C19-C79	-2.74	109.74	112.66
15	B	101	KZB	C84-C15-C16	-2.71	110.13	113.90
17	P	101	323	C23-C18-C1	-2.70	119.65	123.42
15	G	503	KZB	C20-C19-C79	-2.68	109.81	112.66
15	B	101	KZB	C18-C17-C16	-2.67	107.91	112.16
15	A	804	KZB	C83-C84-C03	2.66	119.14	115.36
13	F	301	CPL	O3-C11-C12	2.58	119.69	111.83
15	F	302	KZB	C81-C79-C19	-2.57	104.94	108.51
15	B	102	KZB	C18-C17-C16	-2.56	108.07	112.16
14	A	803	PTY	O4-C30-C31	2.55	119.60	111.83
17	P	101	323	C6-C7-N2	-2.54	118.53	121.33
13	E	501	CPL	O3-C11-C12	2.53	119.56	111.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	805	KZB	C20-C21-C76	2.53	113.72	111.07
15	G	503	KZB	C02-C03-C04	-2.47	100.31	104.28
15	A	805	KZB	C06-C02-C03	-2.42	99.81	103.37
15	A	806	KZB	C20-C19-C79	-2.42	110.09	112.66
15	F	303	KZB	C84-C15-C16	-2.40	110.55	113.90
15	A	806	KZB	C82-C81-C79	-2.39	111.22	113.91
17	P	101	323	C17-N1-C16	2.38	120.20	115.43
15	A	804	KZB	C79-C81-C16	-2.38	110.02	112.43
15	A	806	KZB	C84-C15-C16	-2.37	110.59	113.90
15	A	806	KZB	C18-C17-C16	-2.35	108.41	112.16
15	G	503	KZB	C19-C20-C21	-2.33	107.12	112.87
15	A	806	KZB	C78-C76-C21	2.31	113.54	110.46
15	A	805	KZB	C79-C78-C76	2.30	117.95	114.17
15	G	503	KZB	C01-C02-C06	-2.30	111.23	114.94
15	B	102	KZB	C83-C84-C03	2.29	118.62	115.36
15	F	303	KZB	C07-C06-C02	-2.28	111.53	115.66
15	B	102	KZB	C07-C06-C02	-2.28	111.54	115.66
15	F	303	KZB	C82-C81-C79	-2.27	111.35	113.91
15	B	102	KZB	O24-C25-C26	2.23	111.97	106.44
15	A	804	KZB	C78-C79-C19	2.23	109.36	107.23
15	A	806	KZB	C08-C07-C06	-2.21	108.47	111.93
15	A	804	KZB	C03-C84-C15	-2.20	96.84	100.16
15	A	806	KZB	O12-C11-C09	-2.18	109.38	112.17
15	F	303	KZB	C20-C19-C79	-2.17	110.35	112.66
15	A	804	KZB	O12-C11-C09	-2.16	109.39	112.17
15	B	102	KZB	C78-C76-C21	2.16	113.35	110.46
15	G	503	KZB	O12-C11-C09	-2.16	109.39	112.17
15	B	102	KZB	C23-C74-C72	2.15	114.54	110.01
15	A	805	KZB	C82-C81-C16	2.14	114.77	111.78
15	A	804	KZB	C81-C79-C19	-2.14	105.55	108.51
17	P	101	323	O1-C4-C6	2.13	118.86	115.83
15	A	805	KZB	C72-C28-C25	-2.13	106.36	110.23
15	A	805	KZB	C18-C17-C16	-2.13	108.77	112.16
15	A	805	KZB	C01-C02-C06	-2.12	111.52	114.94
15	B	102	KZB	O12-C11-C09	-2.12	109.45	112.17
15	F	302	KZB	C82-C81-C79	-2.10	111.54	113.91
15	A	804	KZB	C17-C16-C15	2.06	115.20	112.29
15	F	302	KZB	C79-C78-C76	-2.06	110.78	114.17
15	B	101	KZB	C79-C78-C76	-2.04	110.82	114.17
15	A	806	KZB	C17-C18-C19	-2.04	107.89	111.84
15	B	102	KZB	C79-C78-C76	-2.04	110.82	114.17
15	A	804	KZB	C07-C06-C02	-2.03	111.97	115.66

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	804	KZB	C79-C78-C76	-2.02	110.84	114.17
15	A	806	KZB	C07-C06-C02	-2.02	112.01	115.66
15	A	806	KZB	C17-C16-C81	-2.01	108.11	110.52
15	F	303	KZB	C79-C78-C76	-2.00	110.88	114.17
15	G	503	KZB	C78-C76-C21	2.00	113.14	110.46
13	A	802	CPL	O3-C11-C12	2.00	117.93	111.83

There are no chirality outliers.

All (128) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	E	501	CPL	O4P-C4-C5-N
13	F	301	CPL	O2-C2-C3-O3
13	F	301	CPL	O4P-C4-C5-N
14	A	803	PTY	O4-C1-C6-O7
14	A	803	PTY	C3-O11-P1-O13
14	A	803	PTY	C3-O11-P1-O14
15	A	805	KZB	C76-C21-O22-C23
17	P	101	323	C18-C1-C5-C9
17	P	101	323	C2-C1-C5-C9
17	P	101	323	C11-C12-N1-C16
17	P	101	323	C13-C12-N1-C16
17	P	101	323	C11-C12-N1-C17
17	P	101	323	C13-C12-N1-C17
15	A	806	KZB	O24-C23-O22-C21
15	B	102	KZB	O24-C23-O22-C21
15	B	101	KZB	C74-C23-O22-C21
15	B	102	KZB	C74-C23-O22-C21
13	E	501	CPL	C12-C11-O3-C3
15	A	804	KZB	O24-C25-C26-O27
15	A	805	KZB	O24-C25-C26-O27
15	B	101	KZB	O24-C25-C26-O27
15	A	804	KZB	C28-C25-C26-O27
14	A	803	PTY	C11-C8-O7-C6
15	B	101	KZB	O24-C23-O22-C21
13	E	501	CPL	O11-C11-O3-C3
15	F	303	KZB	O24-C25-C26-O27
13	B	103	CPL	C12-C13-C14-C15
15	A	805	KZB	C74-C23-O22-C21
15	A	806	KZB	O24-C25-C26-O27
15	F	303	KZB	C28-C25-C26-O27
15	A	805	KZB	O24-C23-O22-C21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	B	101	KZB	C28-C25-C26-O27
14	A	803	PTY	O10-C8-O7-C6
15	A	805	KZB	C28-C25-C26-O27
15	A	805	KZB	C20-C21-O22-C23
13	F	301	CPL	C31-C32-C33-C34
13	B	103	CPL	C12-C11-O3-C3
13	E	501	CPL	C31-C32-C33-C34
13	B	103	CPL	C21-C22-C23-C24
13	E	501	CPL	C21-C22-C23-C24
14	A	803	PTY	C15-C16-C17-C18
13	B	103	CPL	C33-C34-C35-C36
14	A	803	PTY	C30-C31-C32-C33
13	F	301	CPL	C15-C16-C17-C18
13	F	301	CPL	C16-C17-C18-C19
17	P	101	323	C6-C7-N2-C14
17	P	101	323	C8-C7-N2-C15
13	E	501	CPL	C12-C13-C14-C15
13	E	501	CPL	C35-C36-C37-C38
13	B	103	CPL	O11-C11-O3-C3
13	B	103	CPL	C16-C17-C18-C19
13	F	301	CPL	C34-C35-C36-C37
13	E	501	CPL	C32-C31-O2-C2
14	A	803	PTY	C16-C17-C18-C19
13	A	802	CPL	C22-C23-C24-C25
13	F	301	CPL	C32-C31-O2-C2
13	F	301	CPL	O31-C31-O2-C2
13	E	501	CPL	C33-C34-C35-C36
13	F	301	CPL	C14-C15-C16-C17
17	P	101	323	C8-C7-N2-C14
13	E	501	CPL	C15-C16-C17-C18
15	B	102	KZB	O24-C25-C26-O27
17	P	101	323	C6-C7-N2-C15
14	A	803	PTY	C36-C37-C38-C39
13	F	301	CPL	C21-C22-C23-C24
13	F	301	CPL	O3P-C1-C2-C3
14	A	803	PTY	O14-C5-C6-C1
13	E	501	CPL	O31-C31-O2-C2
13	F	301	CPL	C11-C12-C13-C14
14	A	803	PTY	C32-C33-C34-C35
13	A	802	CPL	C1-C2-C3-O3
13	F	301	CPL	C1-C2-C3-O3
13	E	501	CPL	C36-C37-C38-C39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	E	501	CPL	C34-C35-C36-C37
16	G	502	NAG	O5-C5-C6-O6
13	F	301	CPL	C12-C13-C14-C15
13	E	501	CPL	C16-C17-C18-C19
13	B	103	CPL	C19-C20-C21-C22
13	F	301	CPL	C17-C18-C19-C20
13	A	802	CPL	O2-C2-C3-O3
13	A	802	CPL	C31-C32-C33-C34
13	E	501	CPL	C11-C12-C13-C14
14	A	803	PTY	O4-C1-C6-C5
14	A	803	PTY	O14-C5-C6-O7
13	A	802	CPL	C39-C40-C41-C42
16	G	502	NAG	C1-C2-N2-C7
14	A	803	PTY	C5-C6-O7-C8
13	E	501	CPL	C1-C2-C3-O3
17	P	101	323	C22-C23-C24-O3
13	B	103	CPL	C14-C15-C16-C17
13	E	501	CPL	O2-C2-C3-O3
17	P	101	323	C22-C23-C24-O2
13	A	802	CPL	C32-C33-C34-C35
15	B	102	KZB	C20-C21-O22-C23
13	B	103	CPL	C4-C5-N-C8
13	F	301	CPL	C44-C45-C46-C47
13	E	501	CPL	C42-C43-C44-C45
13	A	802	CPL	C19-C20-C21-C22
14	A	803	PTY	C37-C38-C39-C40
13	B	103	CPL	C1-O3P-P-O1P
13	E	501	CPL	C1-O3P-P-O2P
13	E	501	CPL	C44-C45-C46-C47
13	B	103	CPL	C18-C19-C20-C21
17	P	101	323	C18-C23-C24-O3
13	F	301	CPL	C13-C14-C15-C16
13	B	103	CPL	C23-C24-C25-C26
13	B	103	CPL	C4-C5-N-C7
13	F	301	CPL	O3P-C1-C2-O2
17	P	101	323	C18-C23-C24-O2
14	A	803	PTY	O4-C30-C31-C32
13	A	802	CPL	C33-C34-C35-C36
14	A	803	PTY	C31-C32-C33-C34
15	A	806	KZB	C28-C25-C26-O27
13	B	103	CPL	C4-C5-N-C6
13	A	802	CPL	C37-C38-C39-C40

Continued on next page...

Continued from previous page...

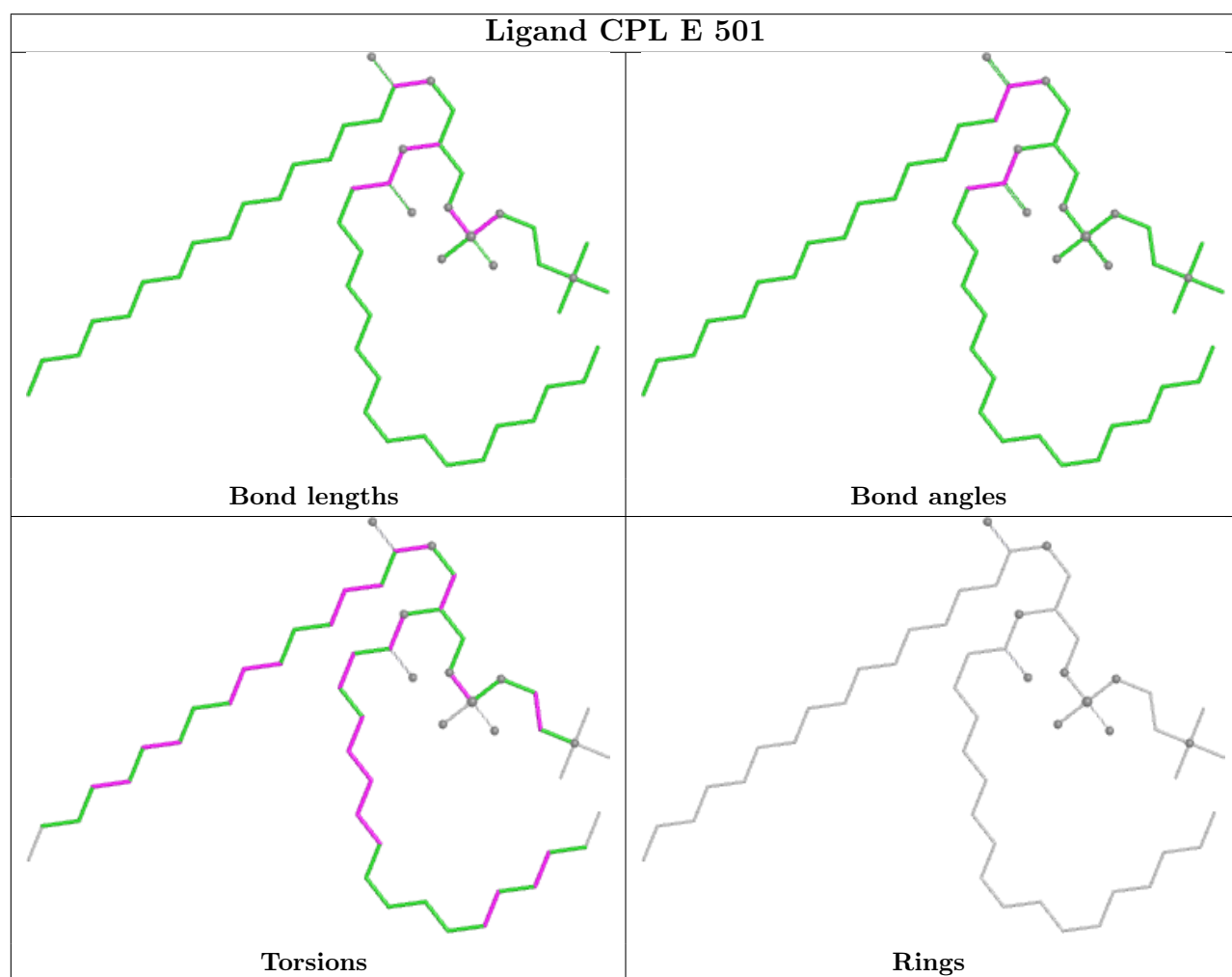
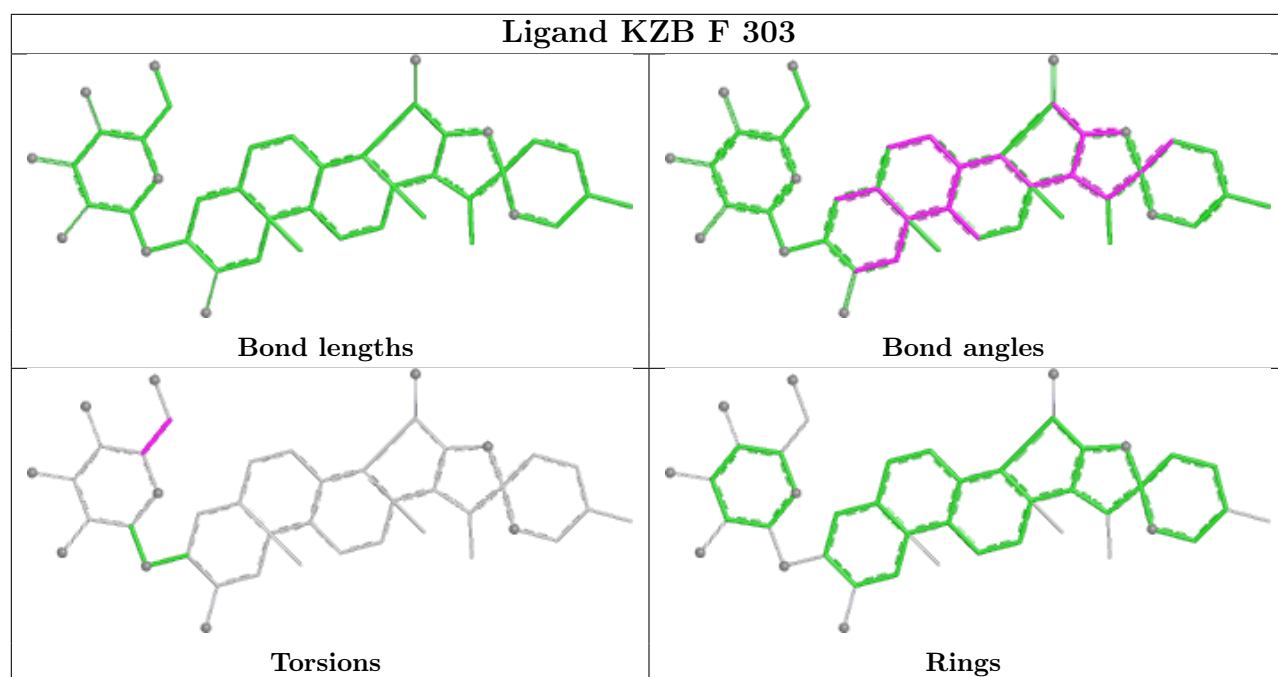
Mol	Chain	Res	Type	Atoms
13	A	802	CPL	C42-C43-C44-C45
13	F	301	CPL	C40-C41-C42-C43
15	G	503	KZB	O24-C23-O22-C21
16	G	502	NAG	C3-C2-N2-C7
14	A	803	PTY	C18-C19-C20-C21
13	F	301	CPL	C37-C38-C39-C40
13	B	103	CPL	C5-C4-O4P-P
13	B	103	CPL	C42-C43-C44-C45
13	E	501	CPL	C19-C20-C21-C22
15	G	503	KZB	C28-C25-C26-O27
13	B	103	CPL	C13-C14-C15-C16
13	B	103	CPL	C15-C16-C17-C18
15	G	503	KZB	C74-C23-O22-C21

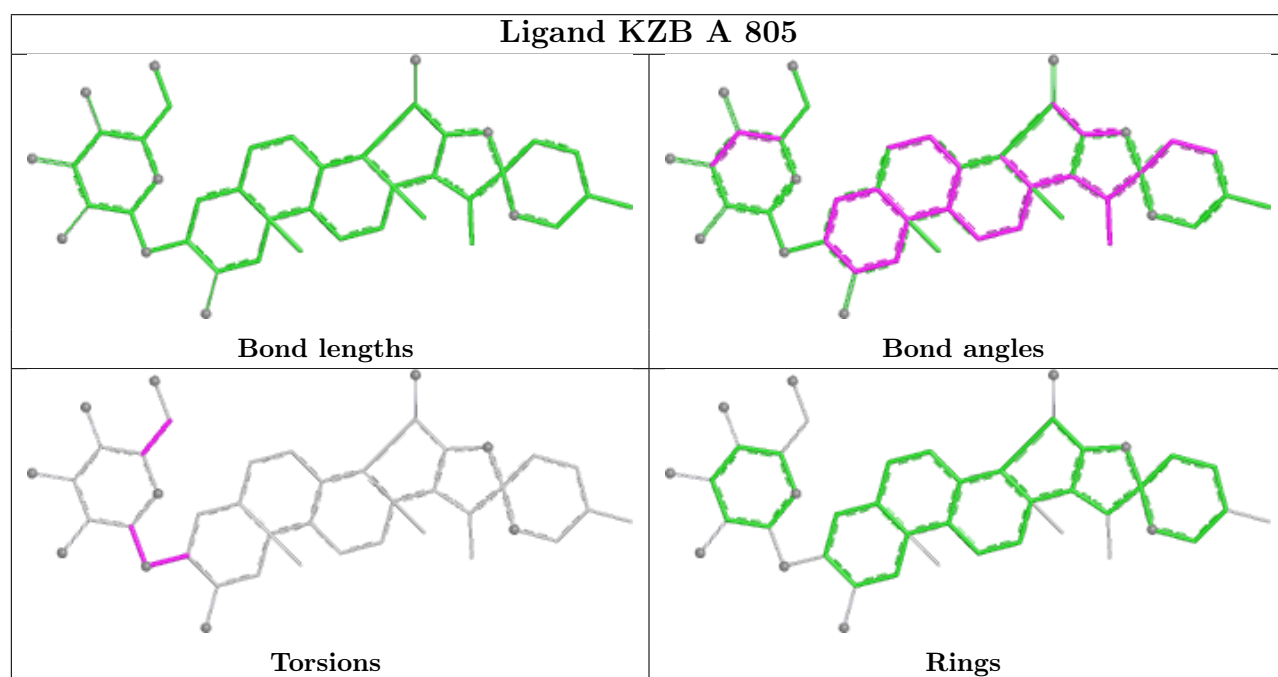
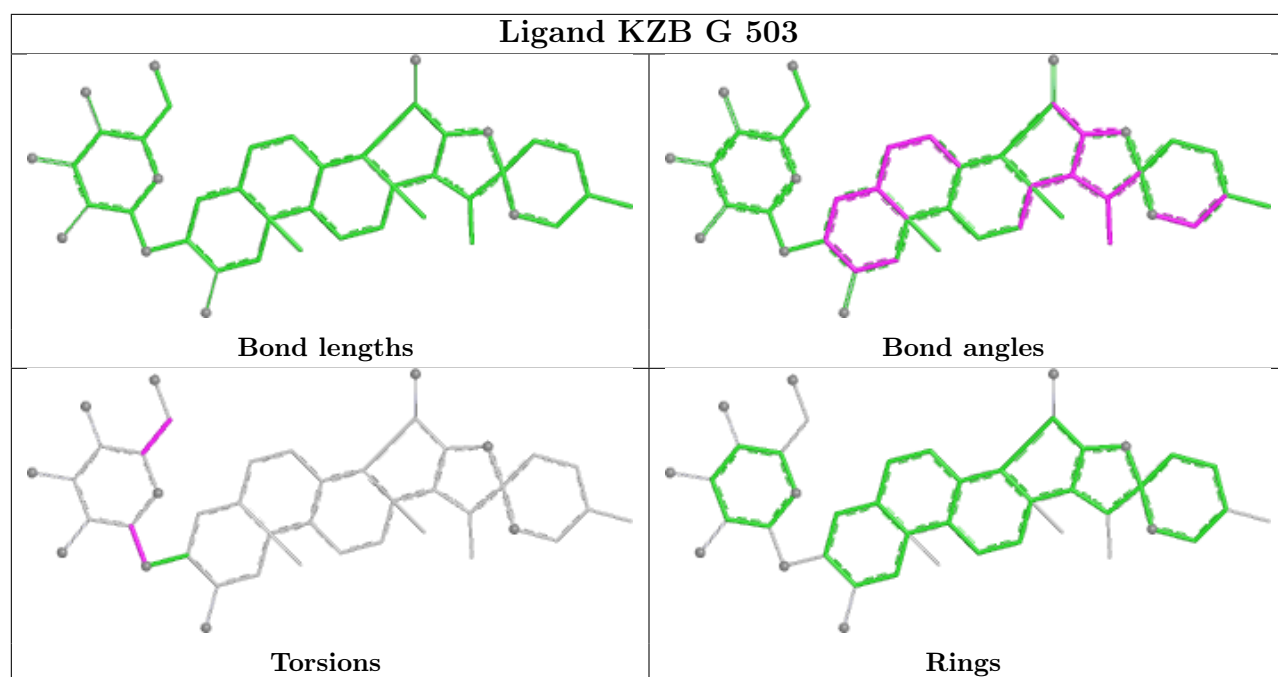
There are no ring outliers.

4 monomers are involved in 9 short contacts:

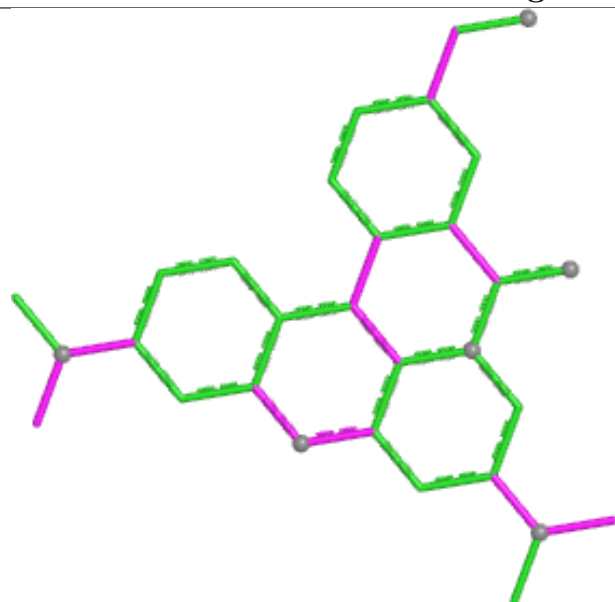
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	E	501	CPL	4	0
13	B	103	CPL	4	0
13	F	301	CPL	1	0
13	A	802	CPL	1	0

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.

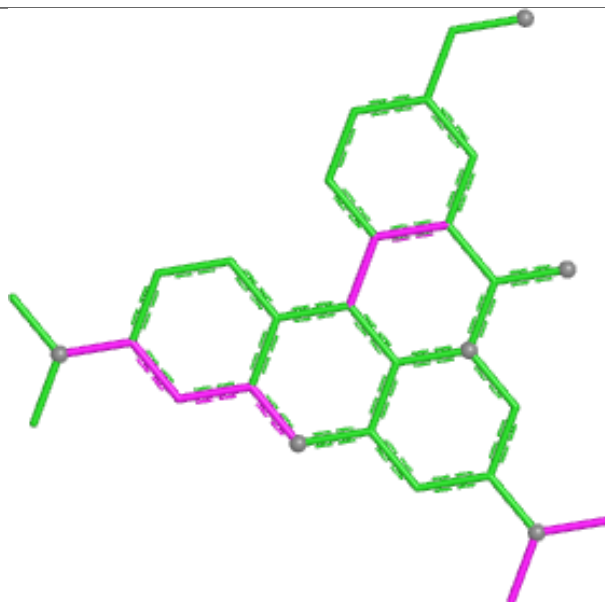




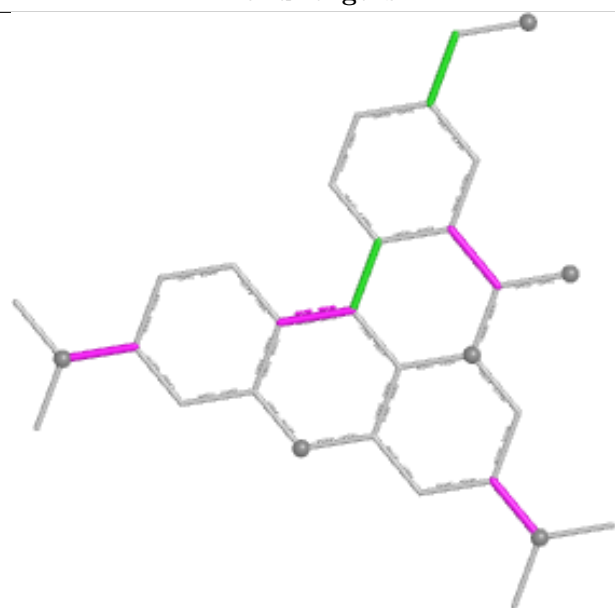
Ligand 323 P 101



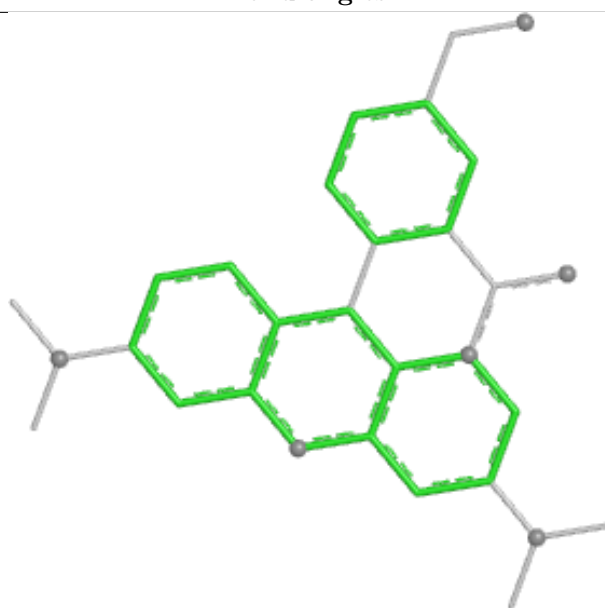
Bond lengths



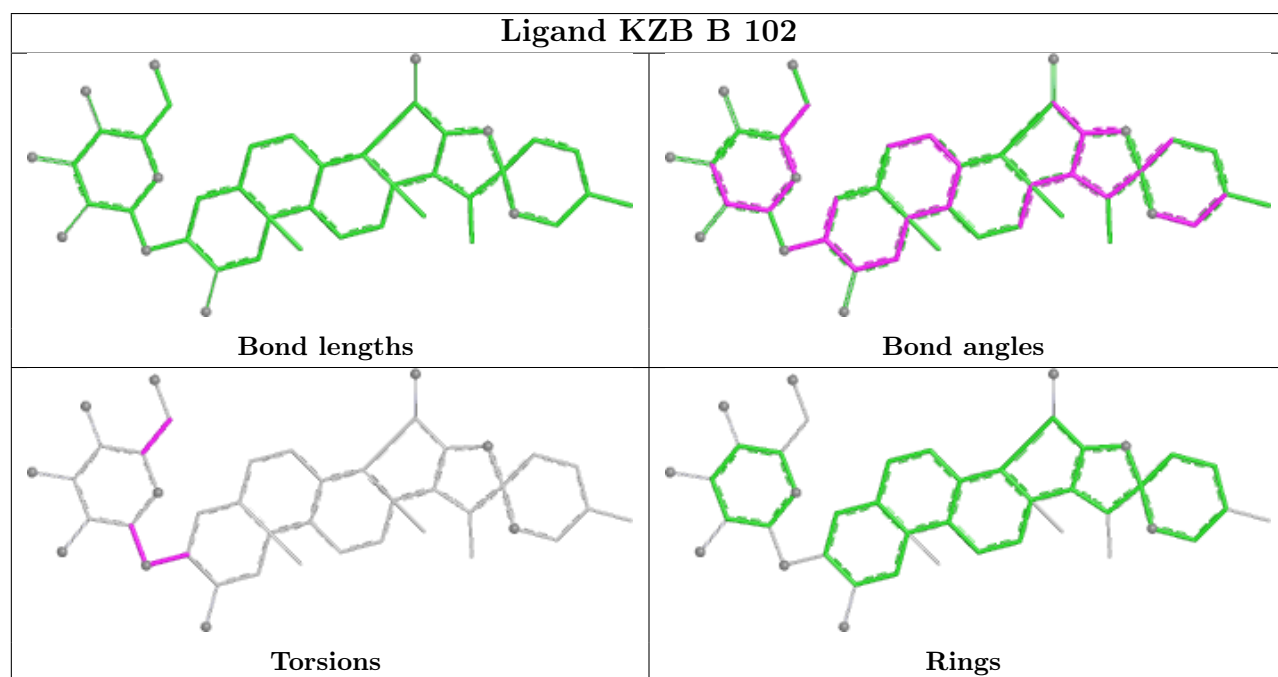
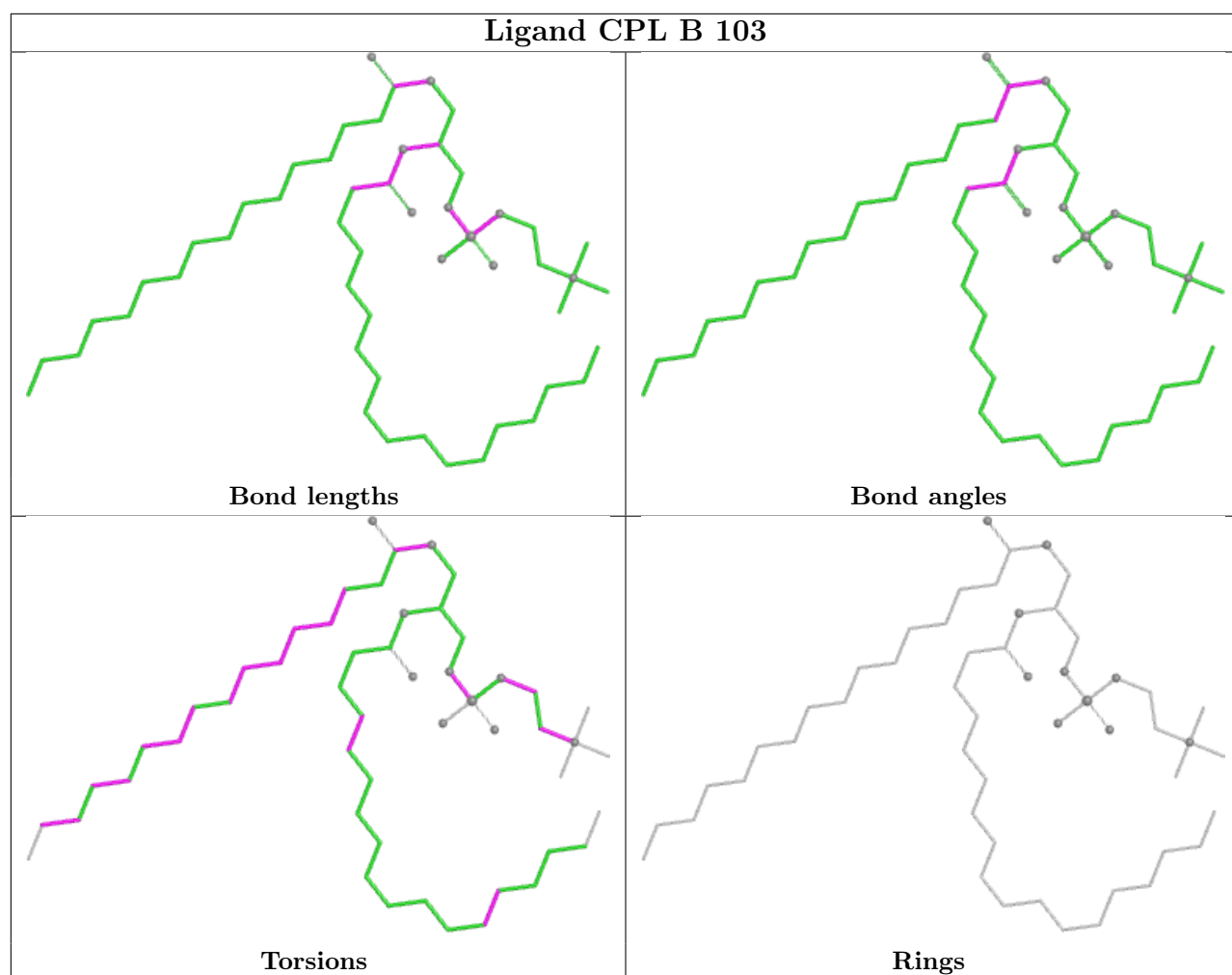
Bond angles

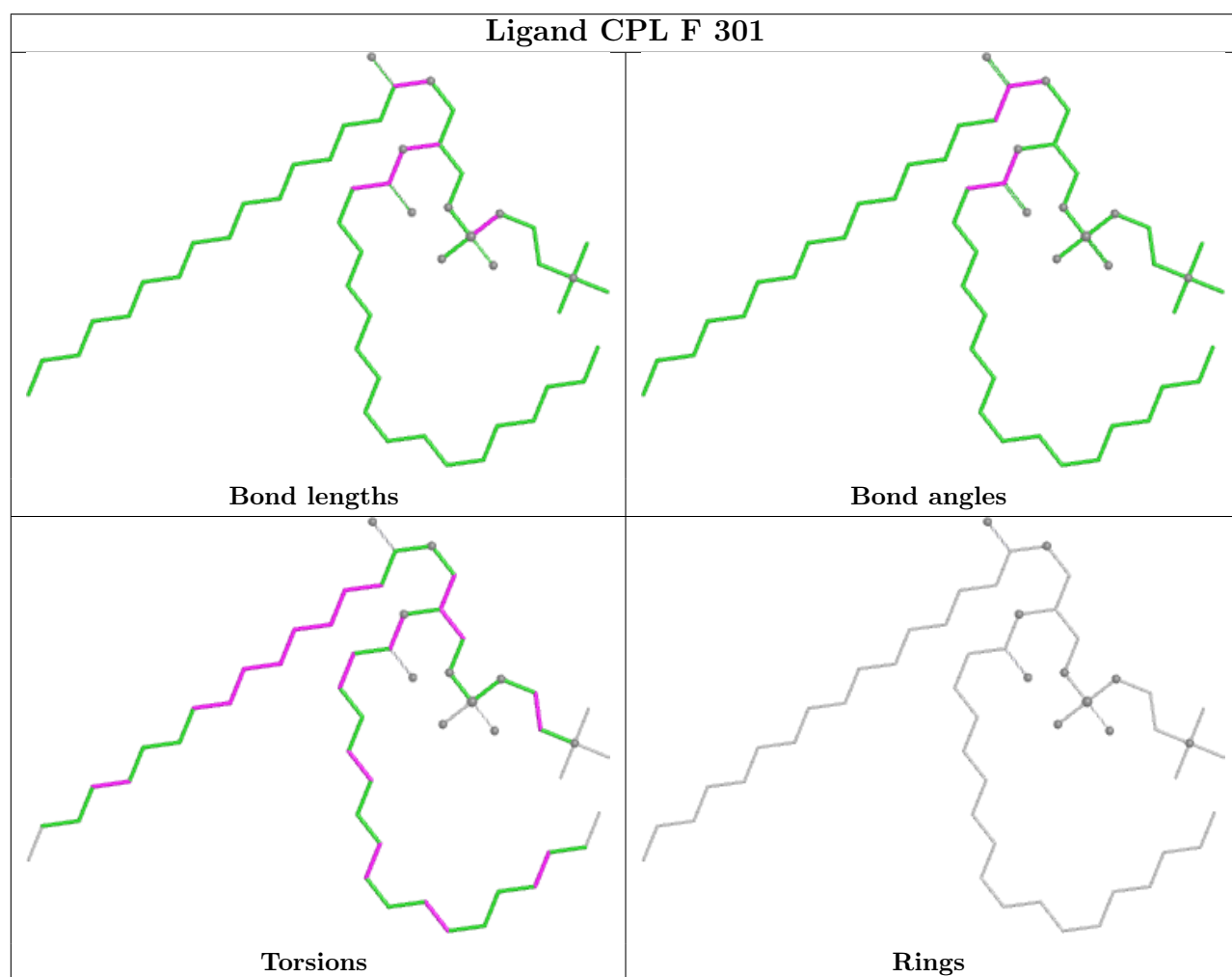
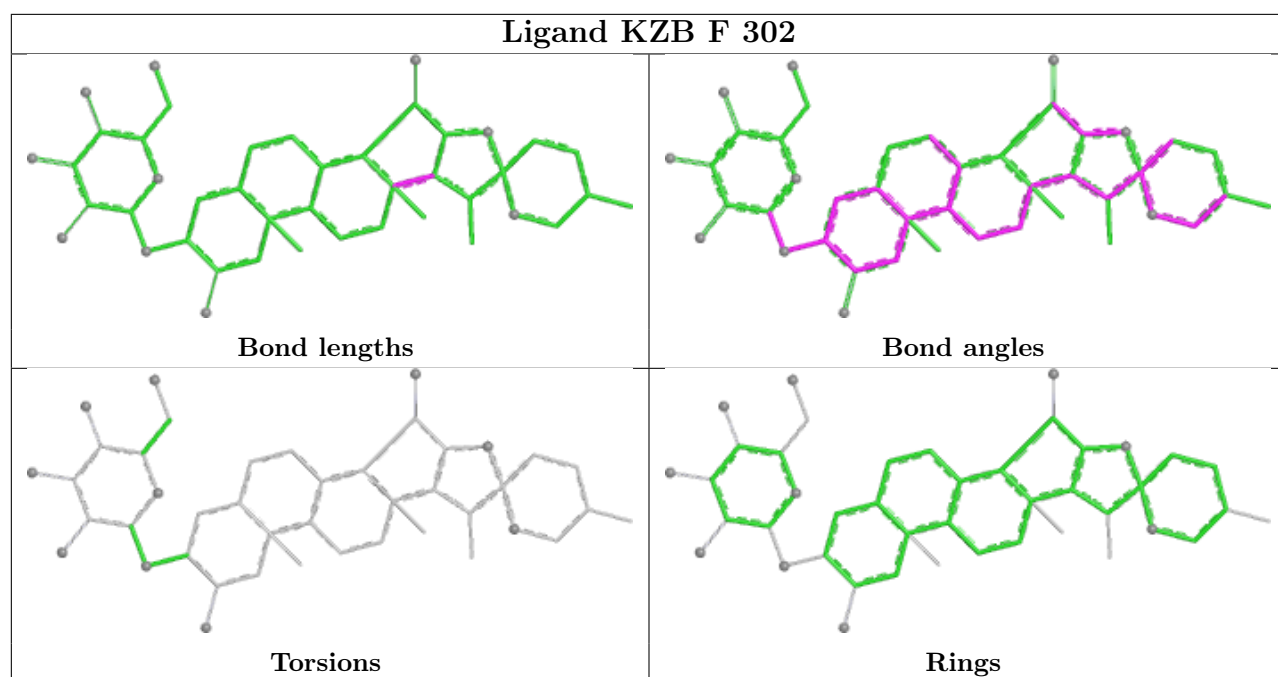


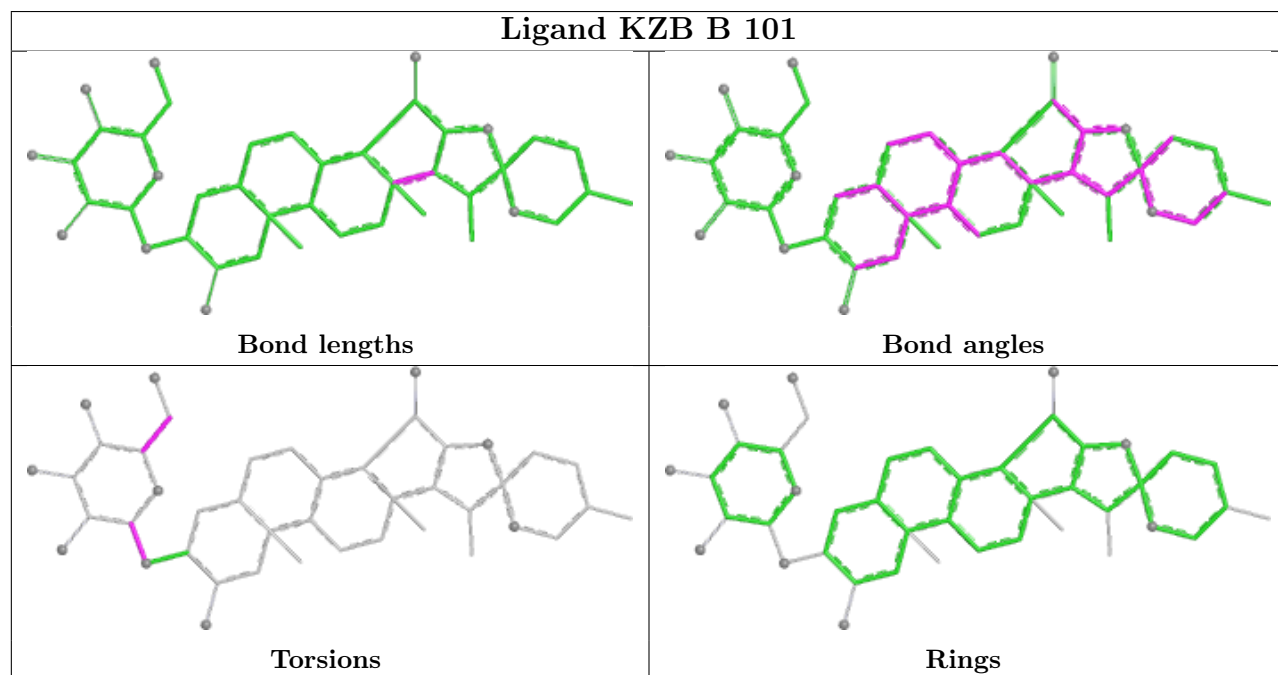
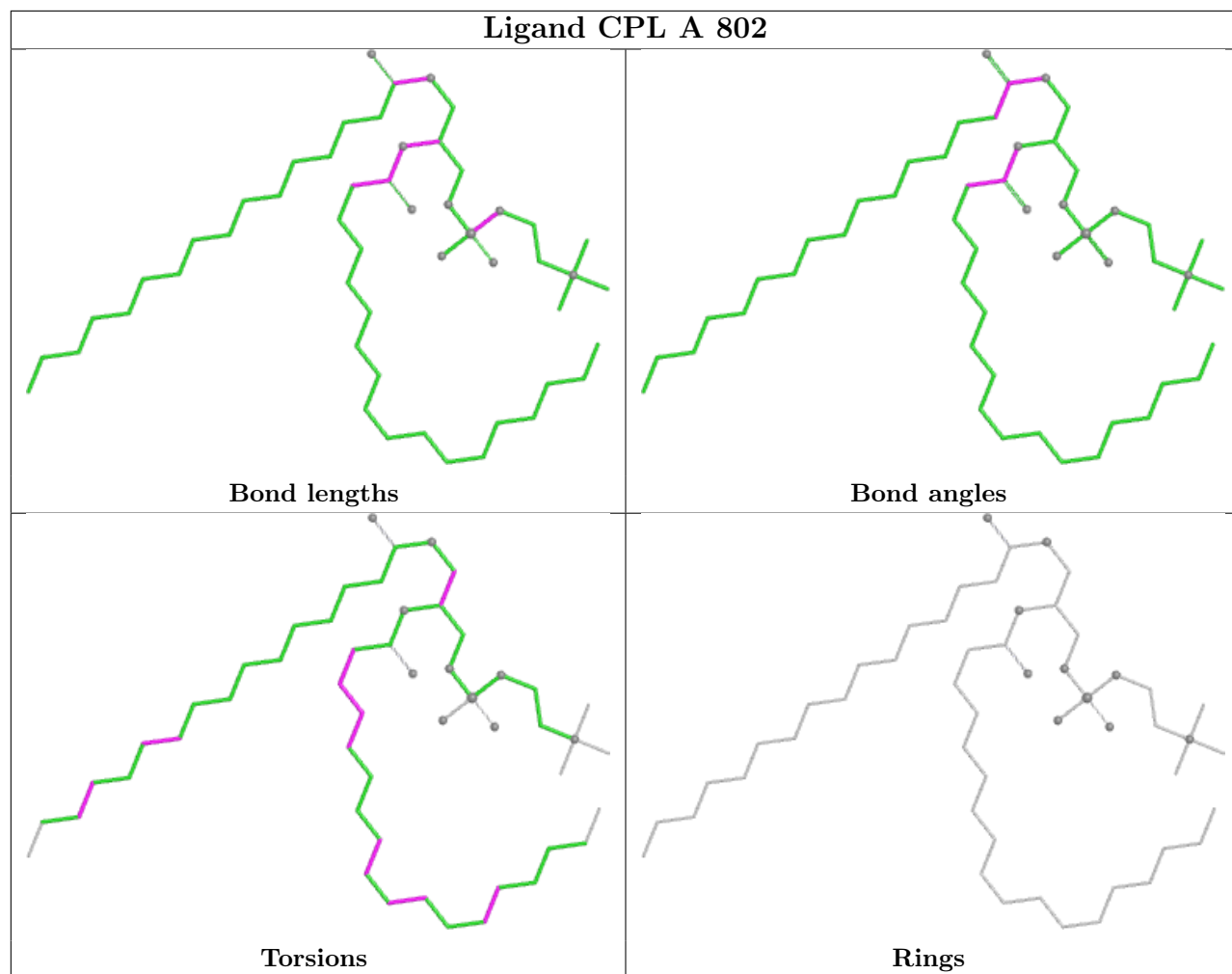
Torsions

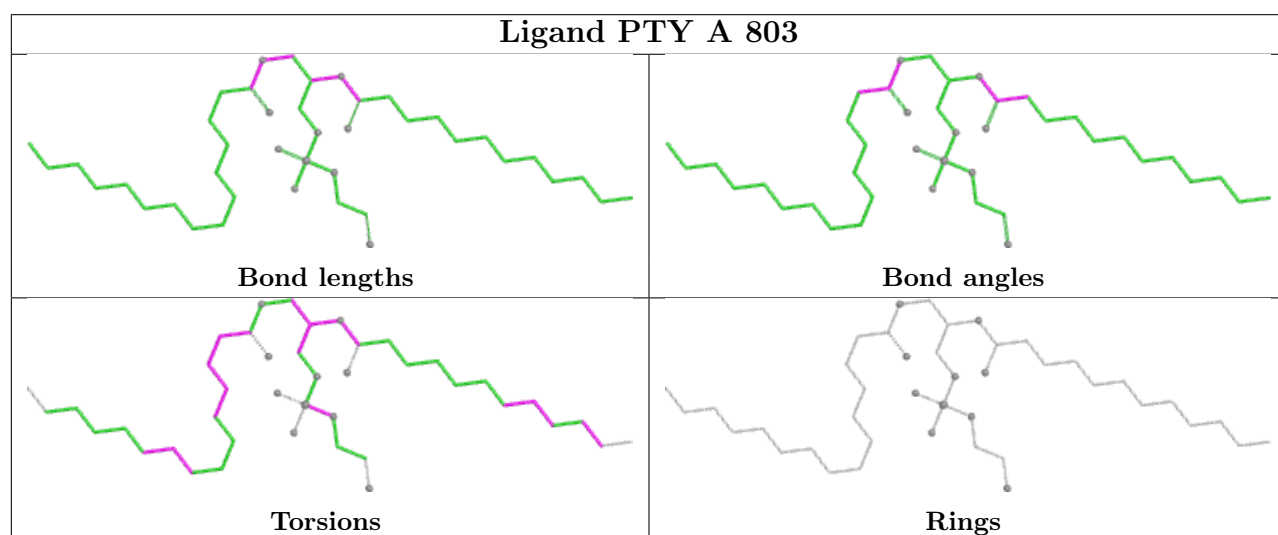
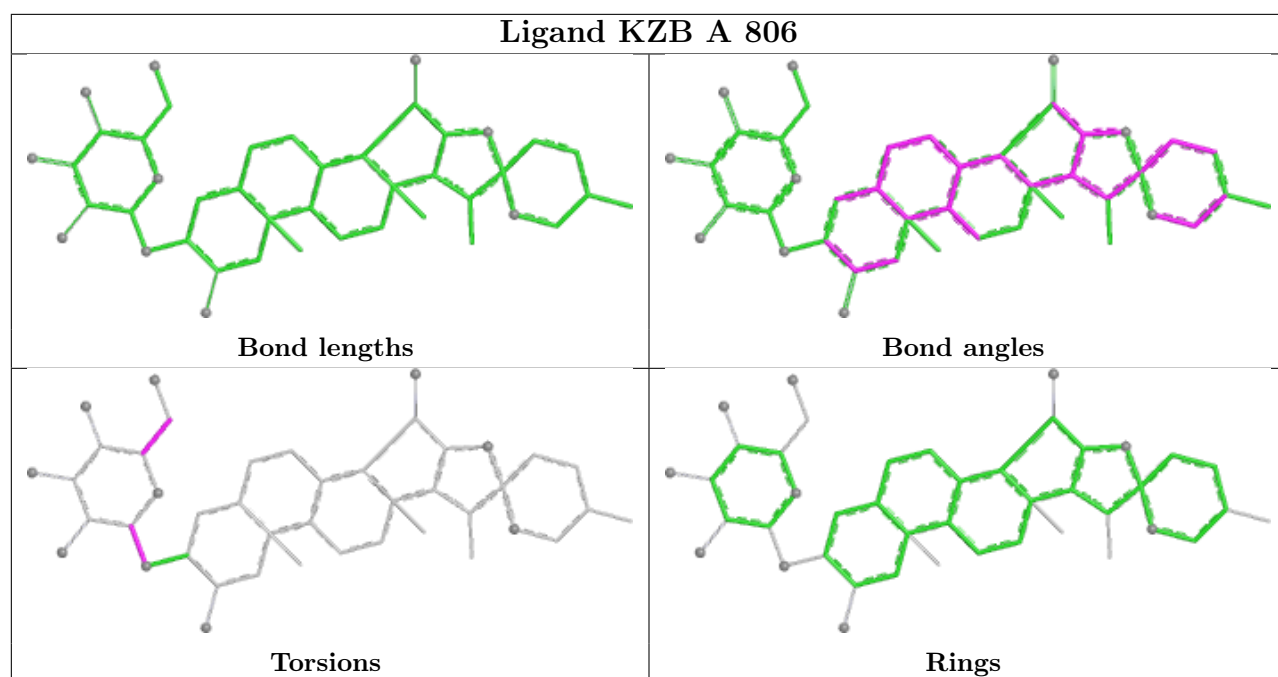


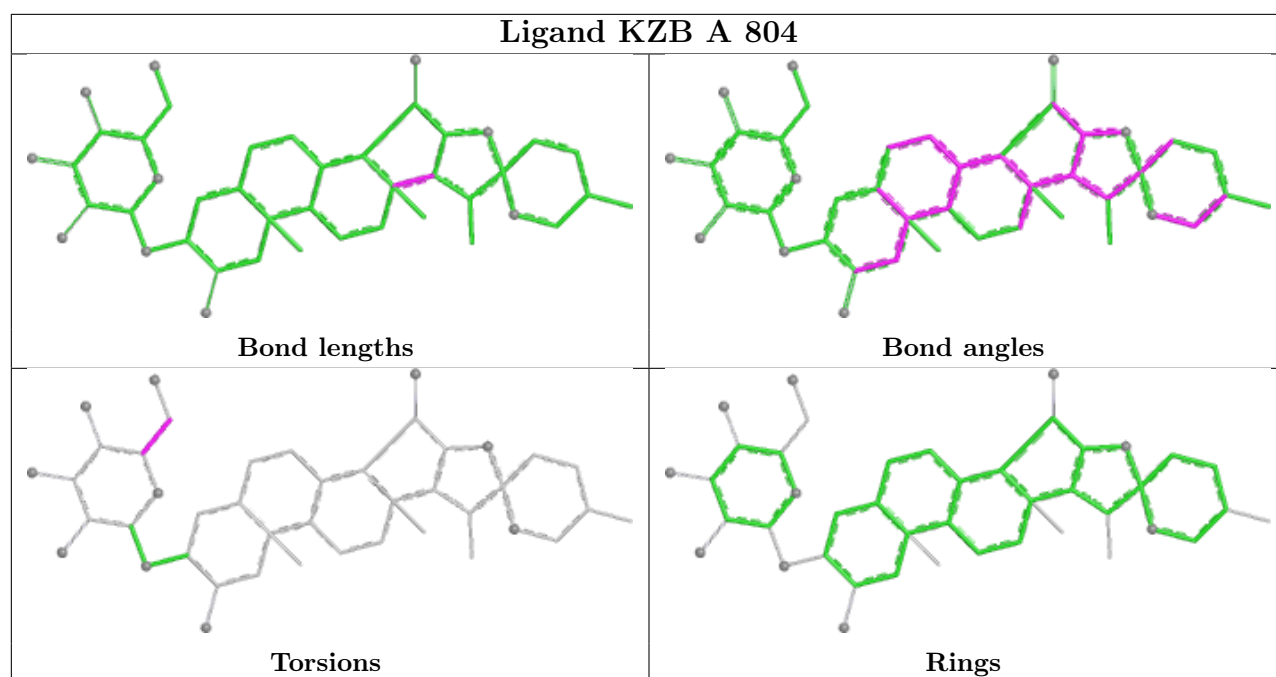
Rings











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

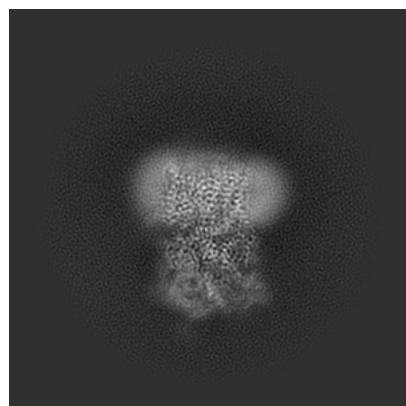
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15421. These allow visual inspection of the internal detail of the map and identification of artifacts.

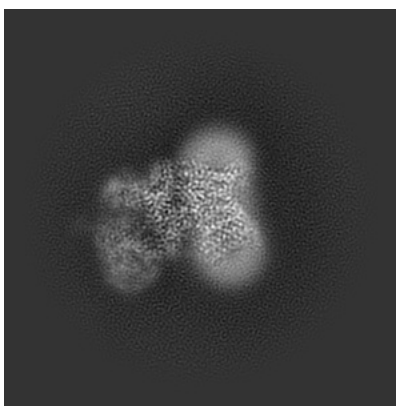
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

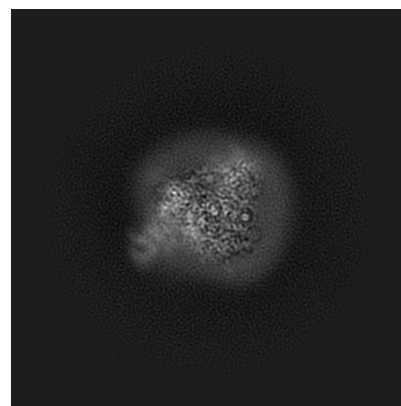
6.1.1 Primary map



X

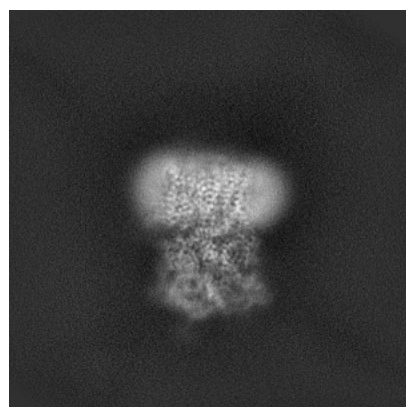


Y

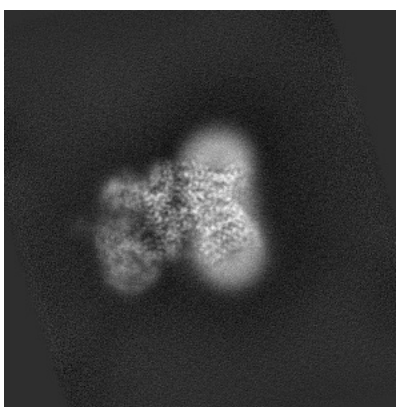


Z

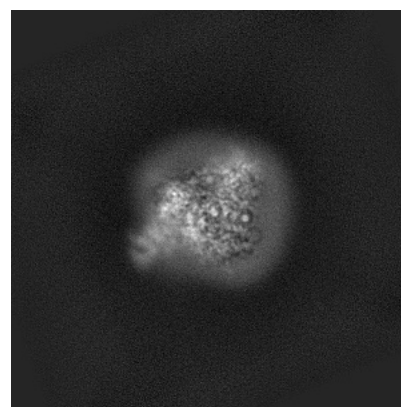
6.1.2 Raw map



X



Y

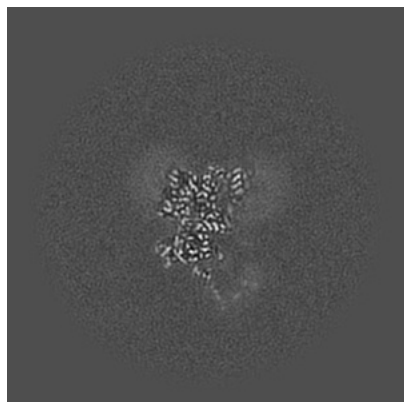


Z

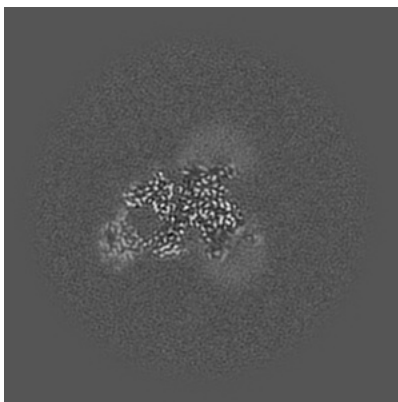
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

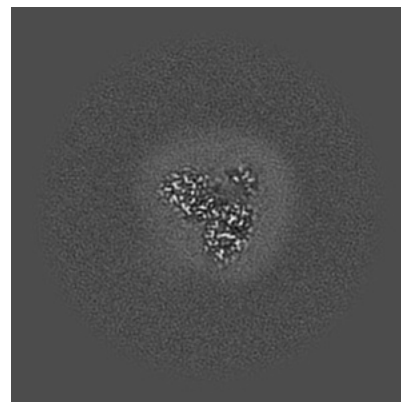
6.2.1 Primary map



X Index: 192

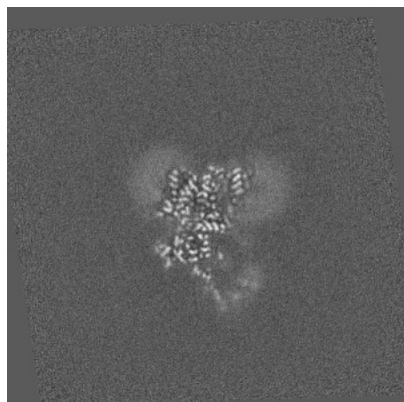


Y Index: 192

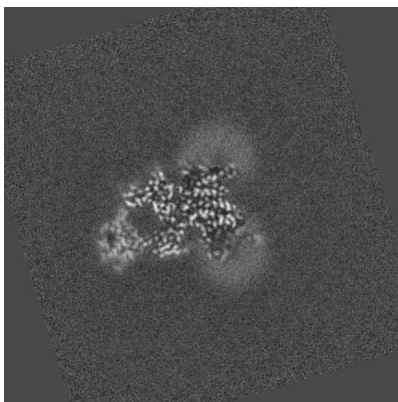


Z Index: 192

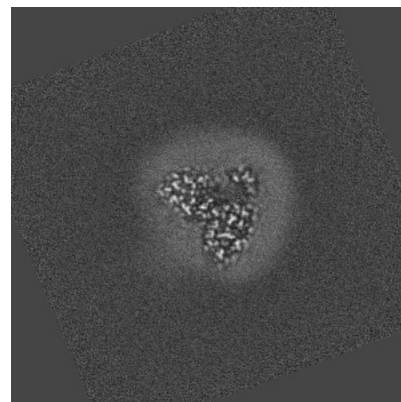
6.2.2 Raw map



X Index: 192



Y Index: 192

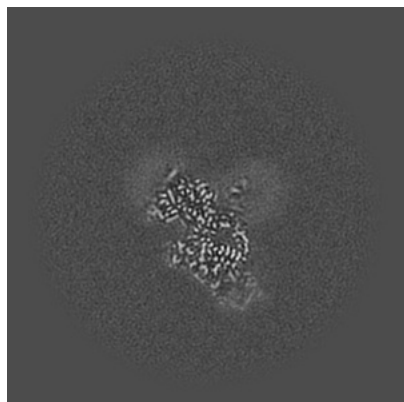


Z Index: 192

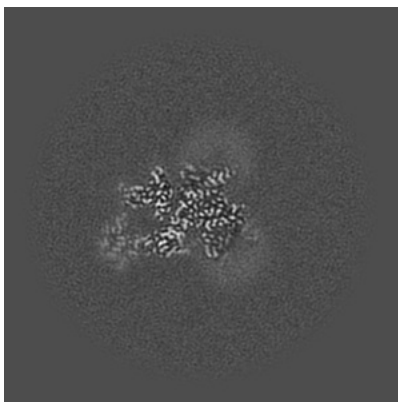
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

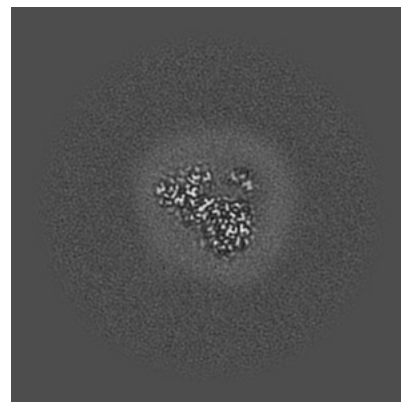
6.3.1 Primary map



X Index: 206

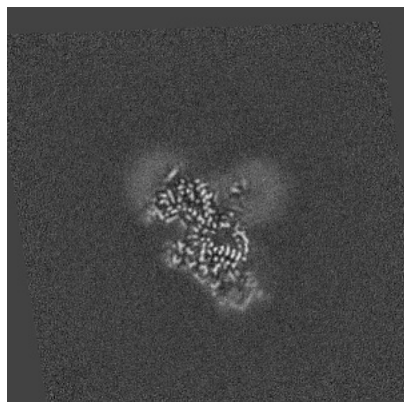


Y Index: 194

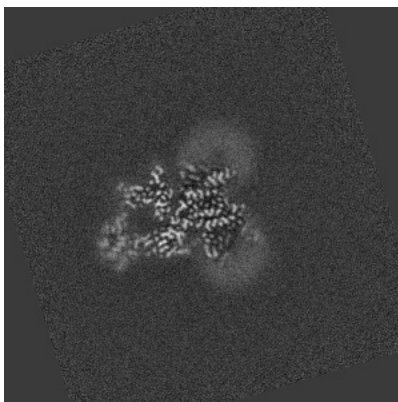


Z Index: 200

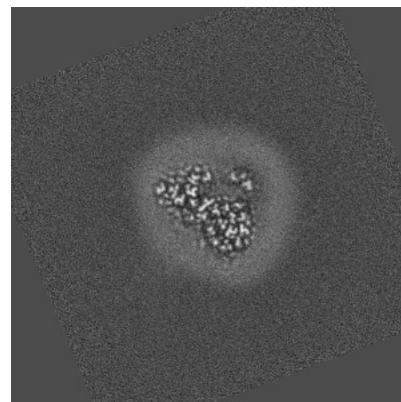
6.3.2 Raw map



X Index: 206



Y Index: 194

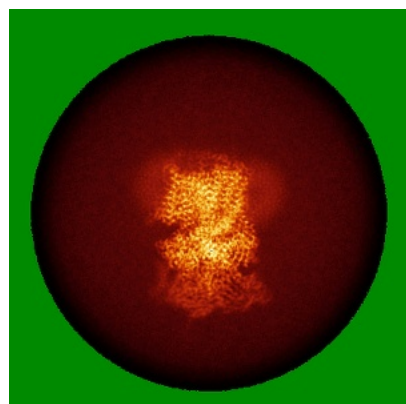


Z Index: 200

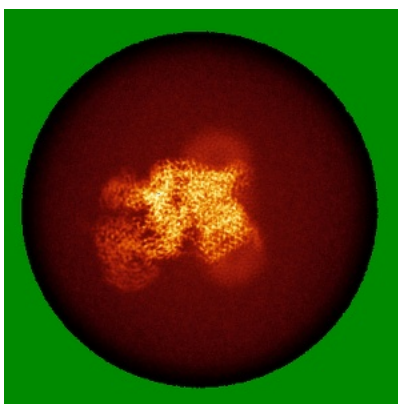
The images above show the largest variance slices of the map in three orthogonal directions.

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

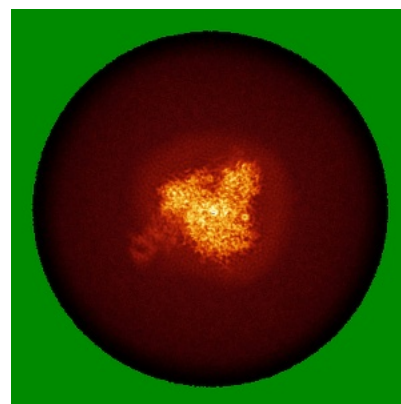
6.4.1 Primary map



X

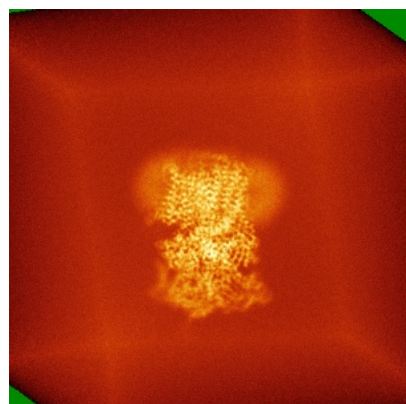


Y

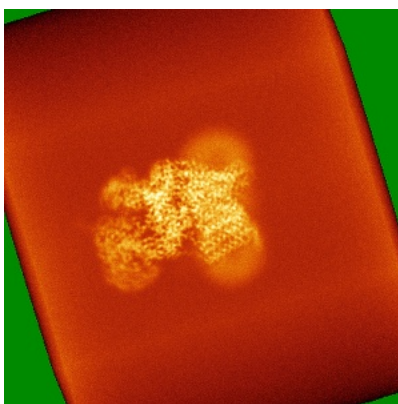


Z

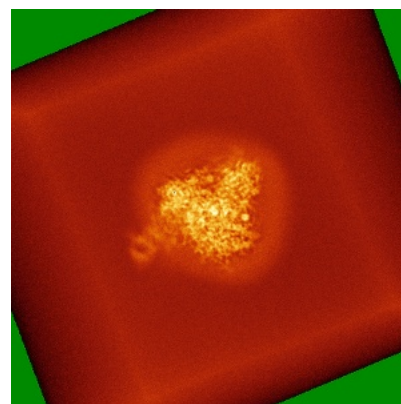
6.4.2 Raw map



X



Y

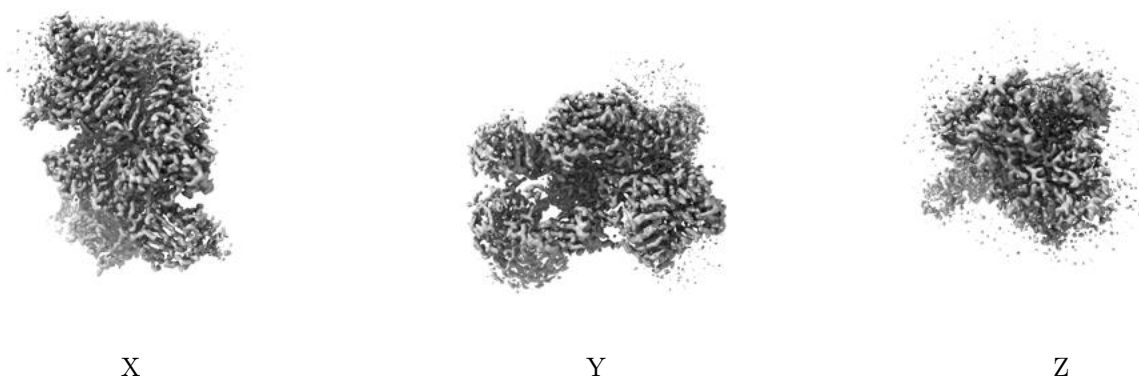


Z

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

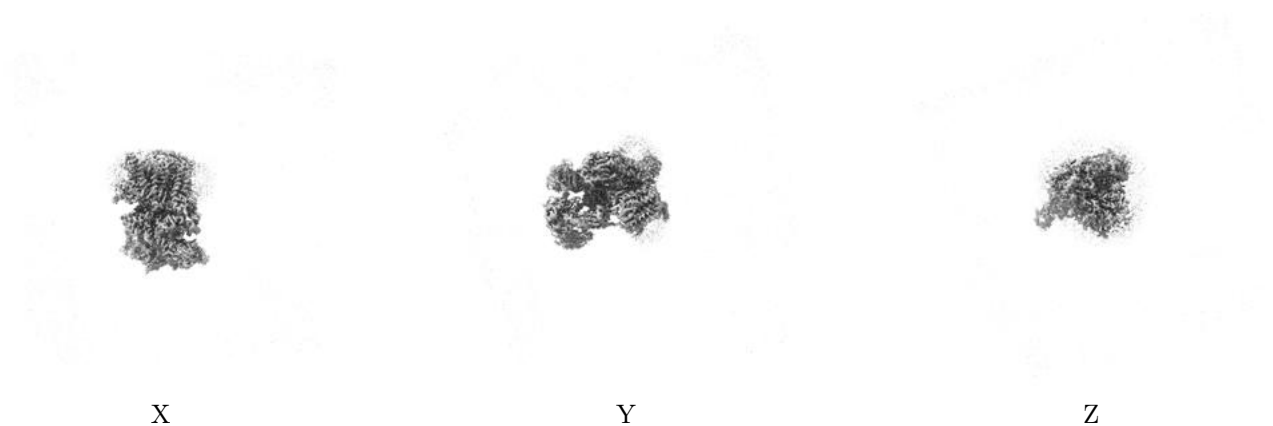
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.312. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

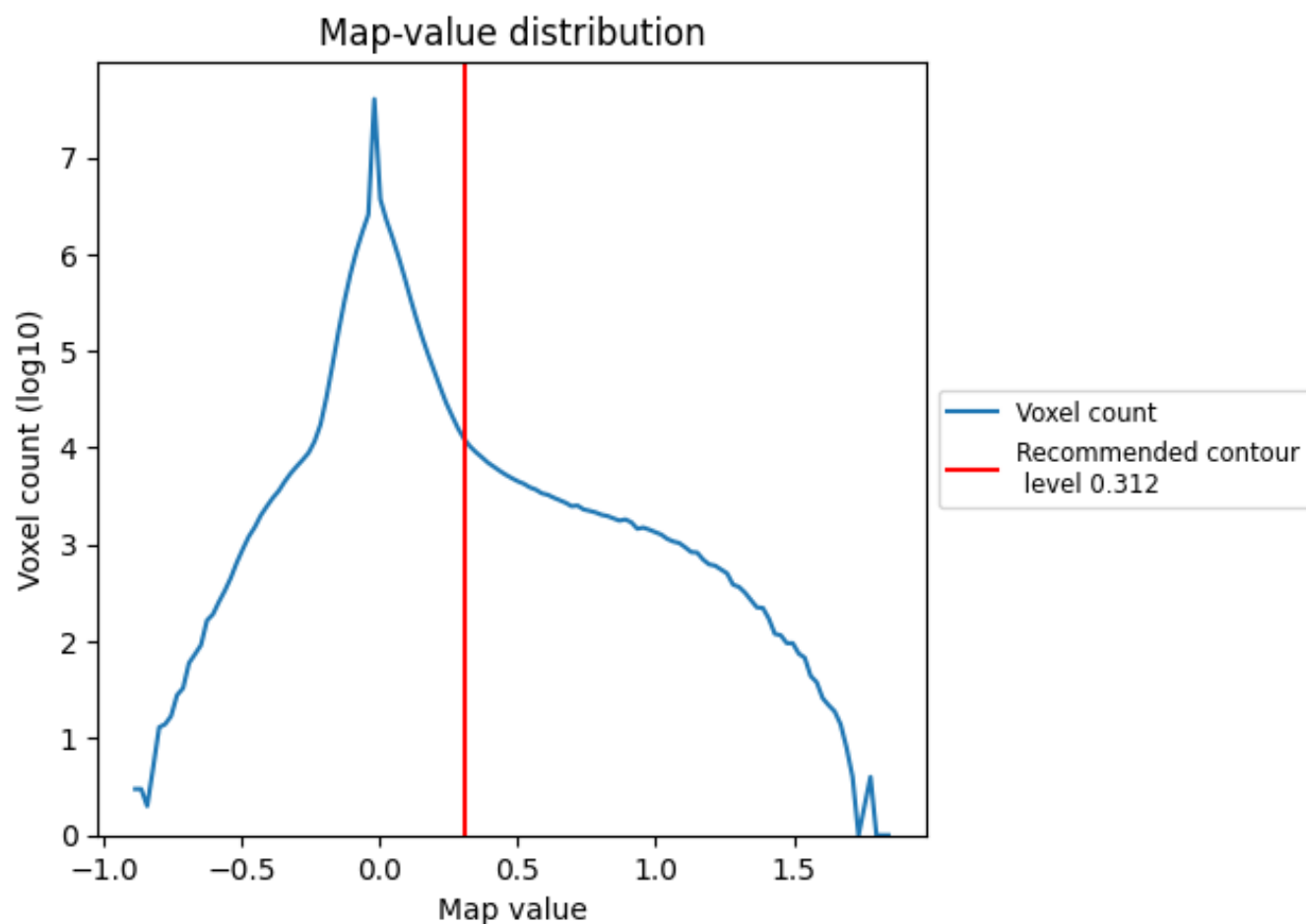
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

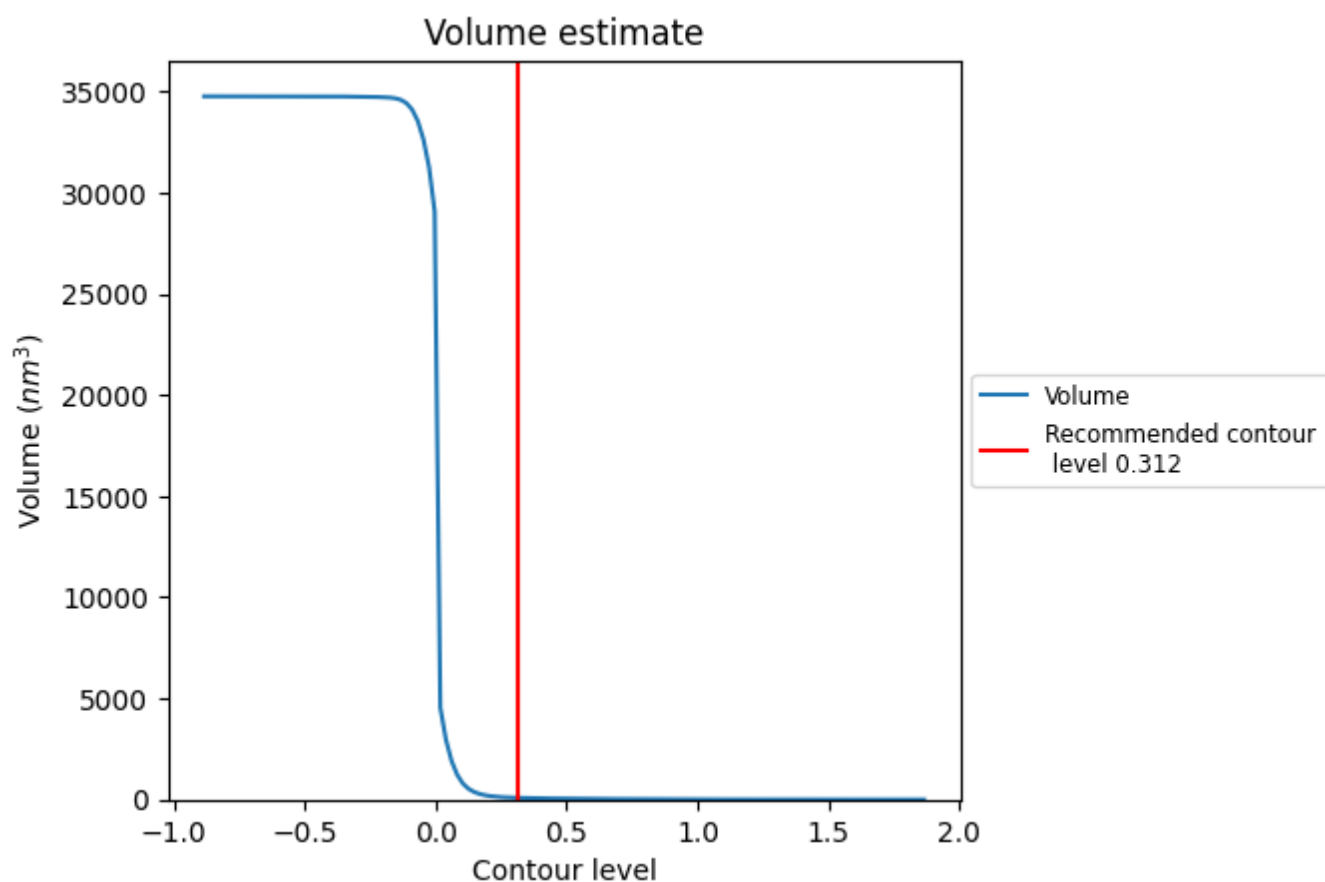
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

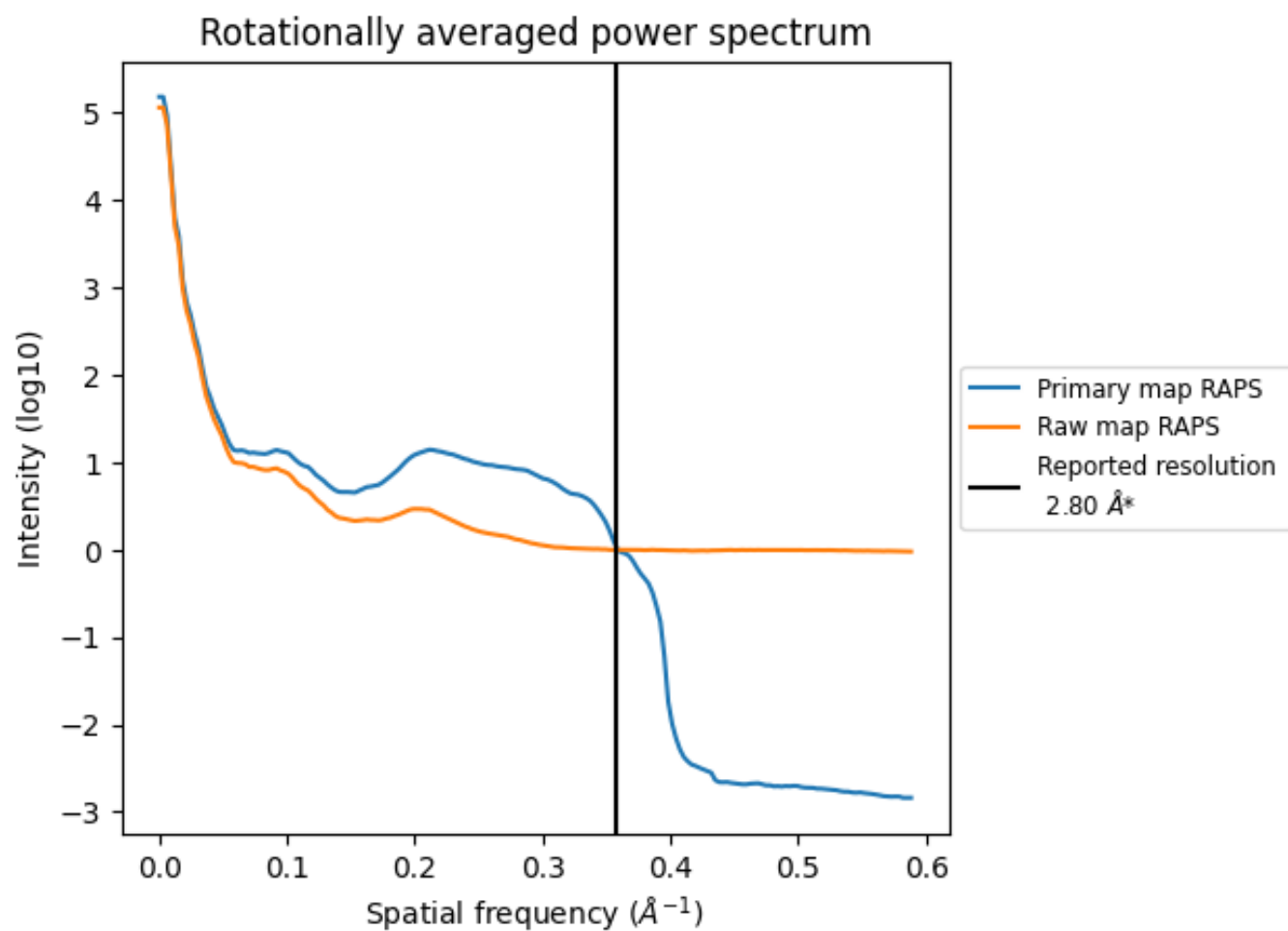
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 85 nm³; this corresponds to an approximate mass of 77 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 ⓘ

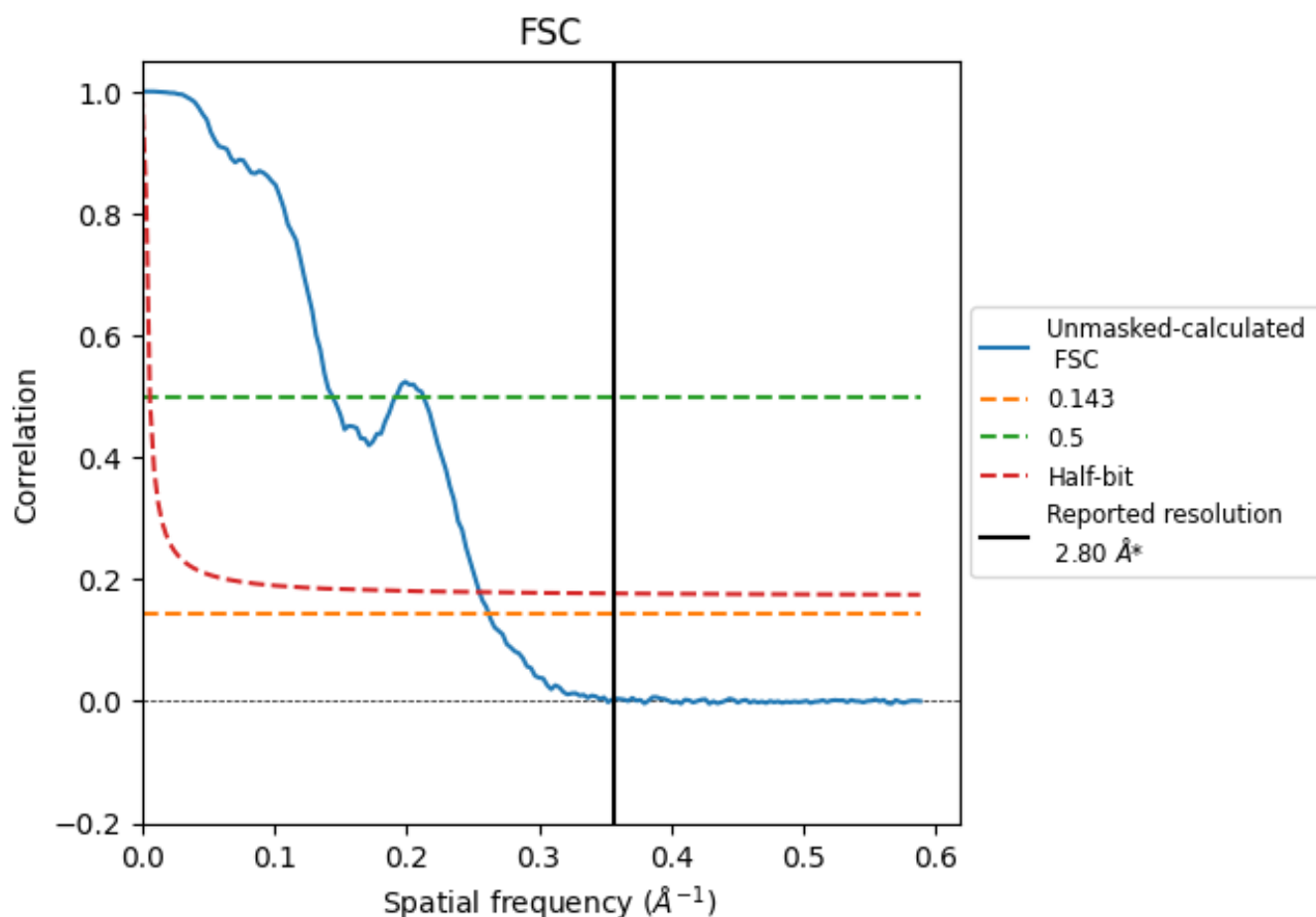


*Reported resolution corresponds to spatial frequency of 0.357 $\text{\AA}^{-1}$

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 0.357 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

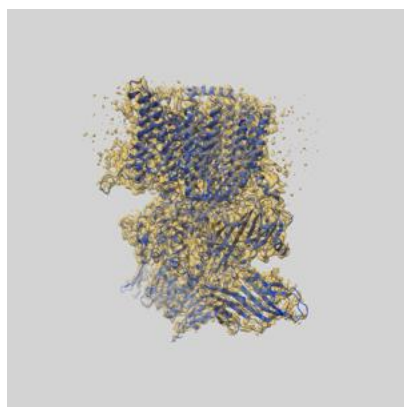
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.81	6.94	3.92

*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 3.81 differs from the reported value 2.8 by more than 10 %

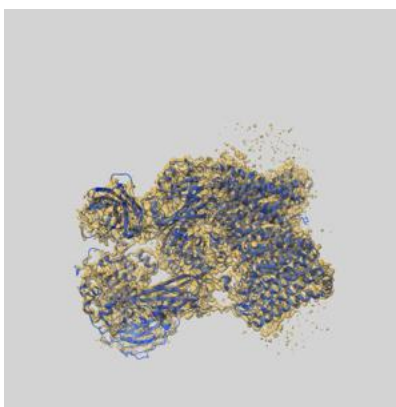
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-15421 and PDB model 8AGE. Per-residue inclusion information can be found in section 3 on page 11.

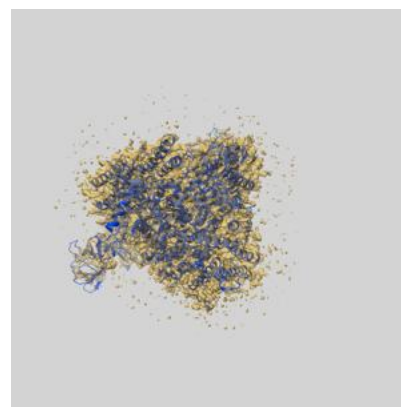
9.1 Map-model overlay [i](#)



X



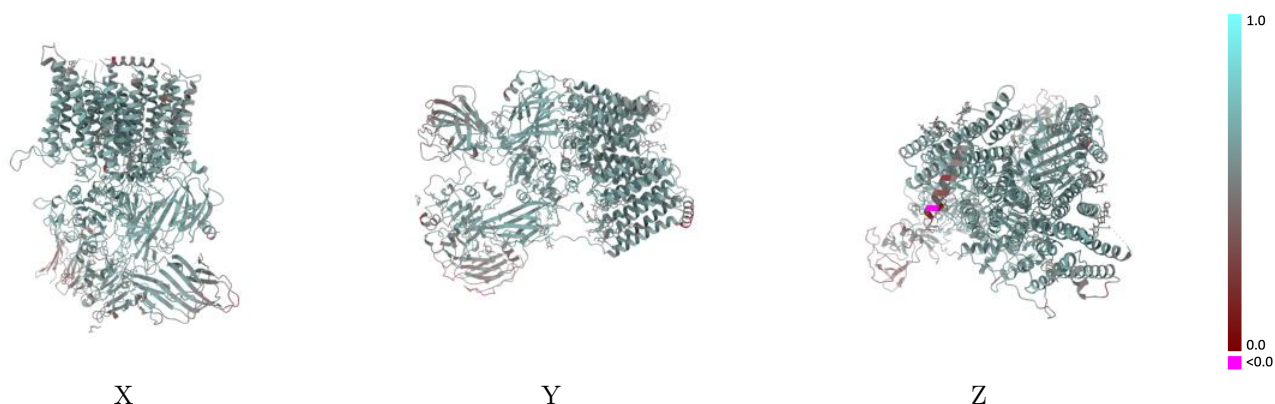
Y



Z

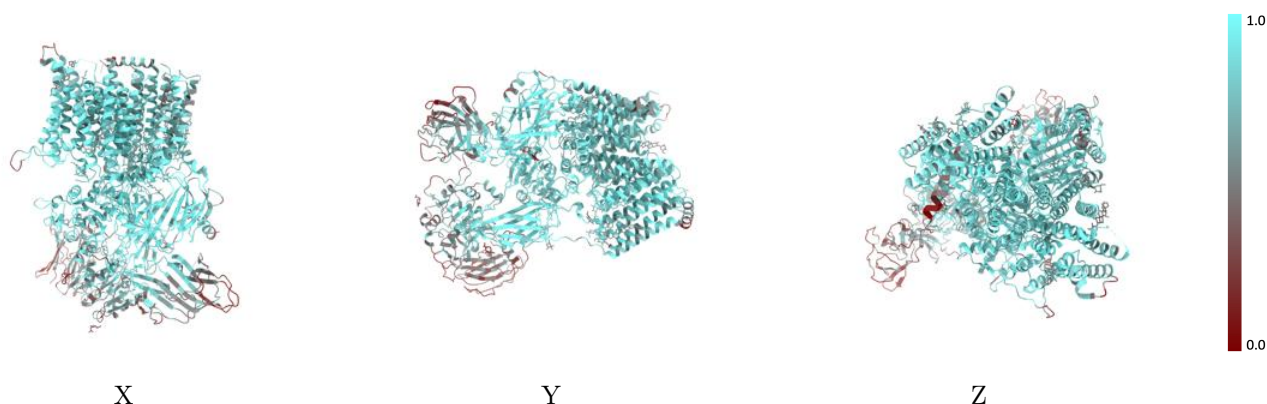
The images above show the 3D surface view of the map at the recommended contour level 0.312 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



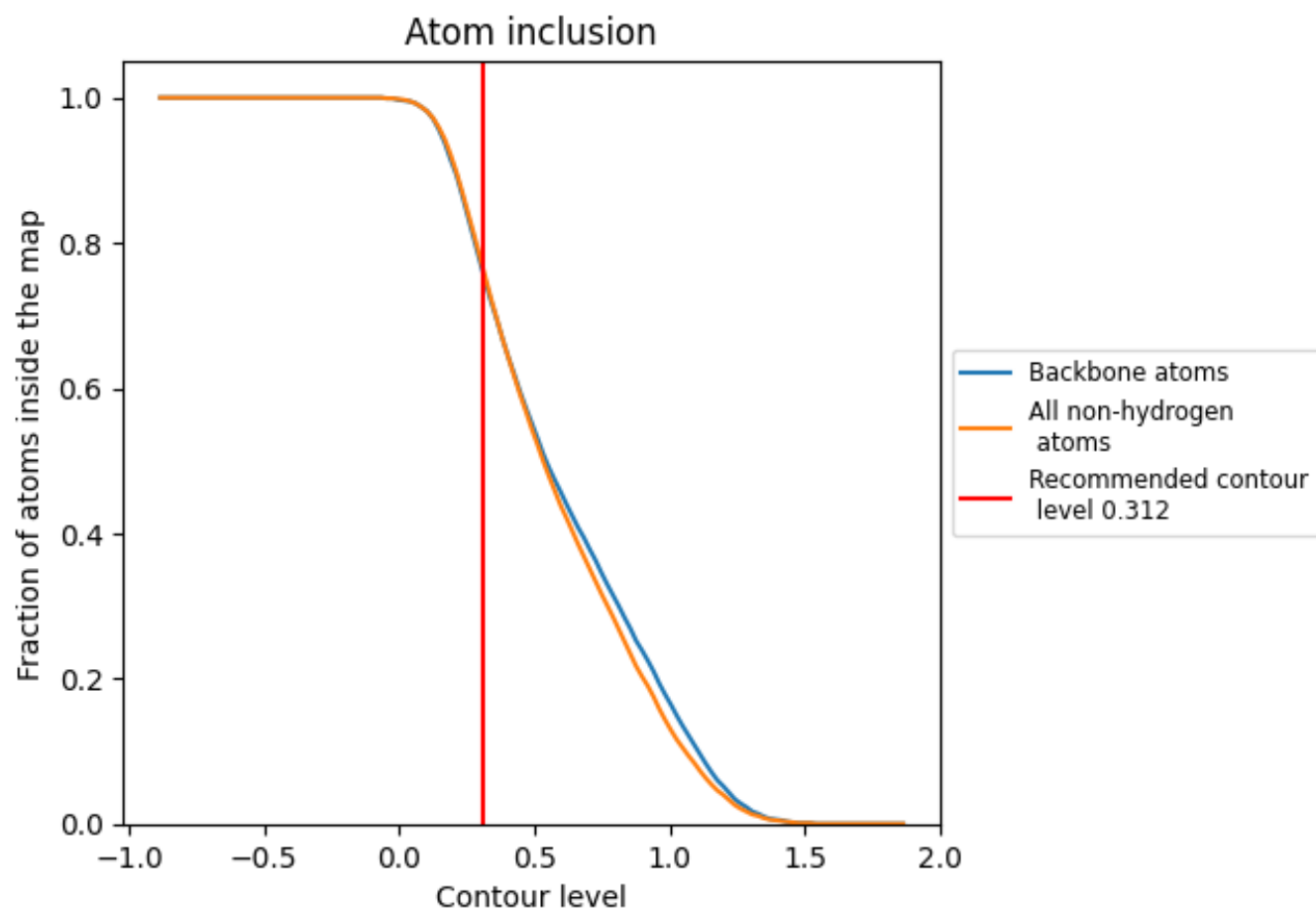
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.312).

9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 76% 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 (0.312) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7610	0.5710
A	0.8830	0.6100
B	0.7910	0.5650
C	0.7430	0.5580
D	0.8110	0.5630
E	0.7390	0.5700
F	0.5160	0.4820
G	0.7210	0.5680
H	0.8130	0.5770
I	0.9290	0.6130
J	0.1430	0.4020
K	0.8680	0.5880
P	0.7840	0.6040

