



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 11:24 AM UTC

PDB ID : 8PN9 / pdb_00008pn9
EMDB ID : EMD-17779
Title : Structure of human oligosaccharyltransferase OST-A complex bound to NGI-1
Authors : Ramirez, A.S.; Kowal, J.; Locher, K.P.
Deposited on : 2023-06-30
Resolution : 3.61 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:

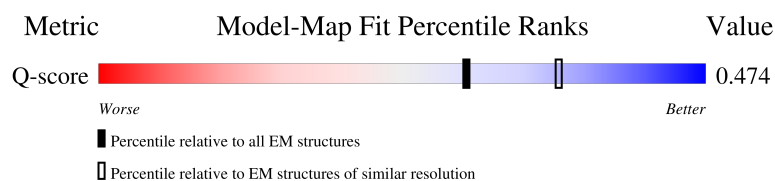
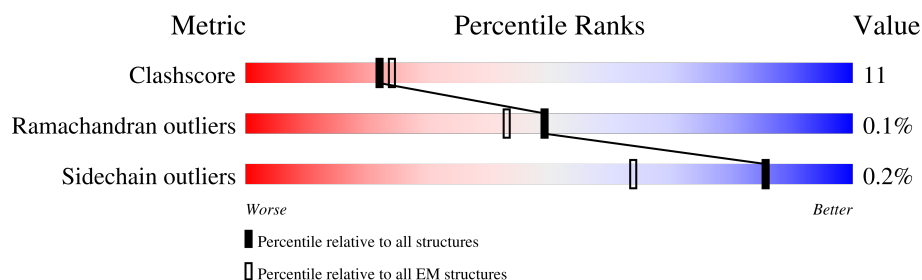
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.61 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	11801 (3.11 - 4.10)

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	705	
2	B	37	
3	C	79	
4	D	113	

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Mol	Chain	Length	Quality of chain
5	E	607	24% 71% 21% 8%
6	F	631	27% 11% 62%
7	H	149	59% 16% 25%
8	G	452	64% 27% 9%
9	I	2	50% 100%
10	J	8	12% 25% 75%
11	K	7	29% 29% 71%
12	N	11	27% 64% 9%

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 17885 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 STT3A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	655	Total	C	N	O	S	0	0
			5302	3478	852	936	36		

- Molecule 2 is a protein called Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	33	Total	C	N	O	S	0	0
			258	174	39	43	2		

- Molecule 3 is a protein called Transmembrane protein 258.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	78	Total	C	N	O	S	0	0
			634	435	91	105	3		

- Molecule 4 is a protein called Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit DAD1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	110	Total	C	N	O	S	0	0
			862	573	135	150	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	559	Total	C	N	O	S	0	0
			4180	2671	712	790	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	241	Total	C	N	O	S	0	0
			1919	1257	316	342	4		

- Molecule 7 is a protein called Oligosaccharyltransferase complex subunit OSTC.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	112	Total	C	N	O	S	0	0
			869	586	134	142	7		

- Molecule 8 is a protein called Dolichyl-diphosphooligosaccharide--protein glycosyltransferase 48 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	411	Total	C	N	O	S	0	0
			3238	2088	534	611	5		

There is a discrepancy between the modelled and reference sequences:

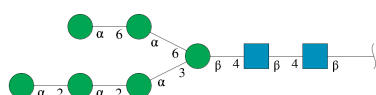
Chain	Residue	Modelled	Actual	Comment	Reference
G	8	GLY	ARG	variant	UNP P39656

- Molecule 9 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



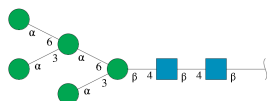
Mol	Chain	Residues	Atoms				AltConf	Trace
9	I	2	Total	C	N	O	0	0
			28	16	2	10		

- 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)-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.



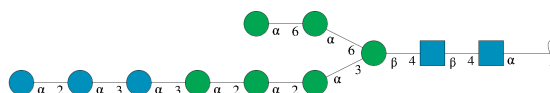
Mol	Chain	Residues	Atoms				AltConf	Trace
10	J	8	Total	C	N	O	0	0
			94	52	2	40		

- Molecule 11 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



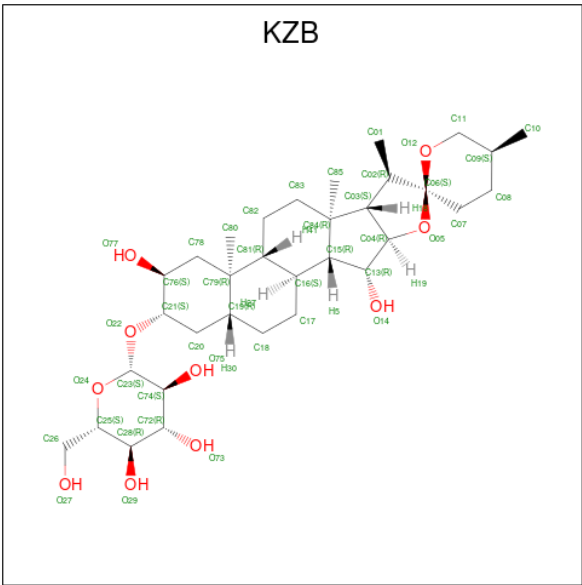
Mol	Chain	Residues	Atoms				AltConf	Trace
11	K	7	Total	C	N	O	0	0
			83	46	2	35		

- Molecule 12 is an oligosaccharide called 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-(1-6)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose.



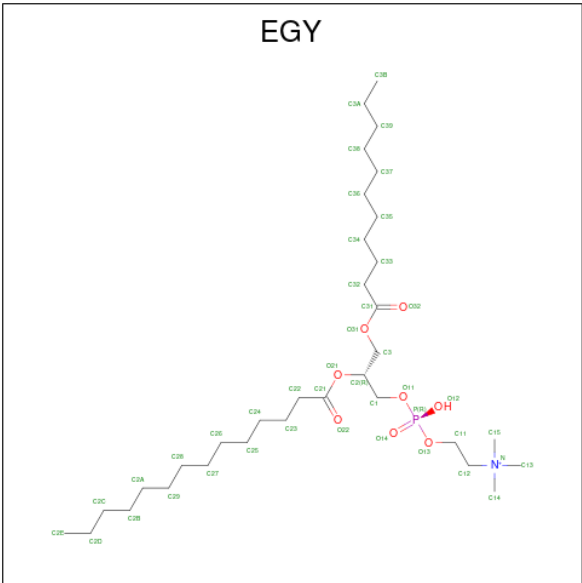
Mol	Chain	Residues	Atoms				AltConf	Trace
12	N	11	Total	C	N	O	0	0
			127	70	2	55		

- Molecule 13 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
13	A	1	Total	C	O	0
			32	27	5	
13	A	1	Total	C	O	0
			32	27	5	
13	F	1	Total	C	O	0
			32	27	5	
13	G	1	Total	C	O	0
			32	27	5	

- Molecule 14 is (4R,7R)-4-hydroxy-N,N,N-trimethyl-4,9-dioxo-7-[(undecanoyloxy)methyl]-3,5,8-trioxa-4lambda 5 -phosphadocosan-1-aminium (CCD ID: EGY) (formula: C₃₃H₆₇NO₈P).

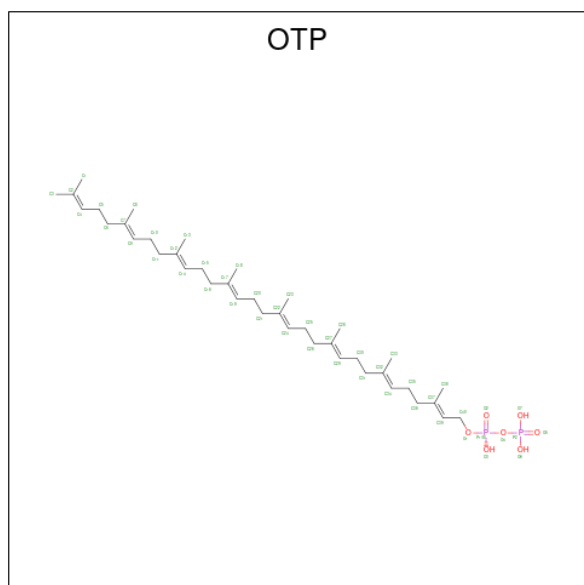


Mol	Chain	Residues	Atoms					AltConf
14	A	1	Total	C	N	O	P	0
			43	33	1	8	1	
14	F	1	Total	C	N	O	P	0
			43	33	1	8	1	

- 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 (2E,6E,10E,14E,18E,22E,26E)-3,7,11,15,19,23,27,31-OCTAMETHYLDOT RIACONTA-2,6,10,14,18,22,26,30-OCTAENYL TRIHYDROGEN DIPHOSPHATE (CCD ID: OTP) (formula: C₄₀H₆₈O₇P₂).



Mol	Chain	Residues	Atoms				AltConf
16	A	1	Total	C	O	P	0
			49	40	7	2	

- Molecule 17 is 5-(dimethylsulfamoyl)- {N}-(5-methyl-1,3-thiazol-2-yl)-2-pyrrolidin-1-yl -benzamide (CCD ID: ZXT) (formula: C₁₇H₂₂N₄O₃S₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
17	A	1	Total 26	C 17	N 4	O 3	S 2	0

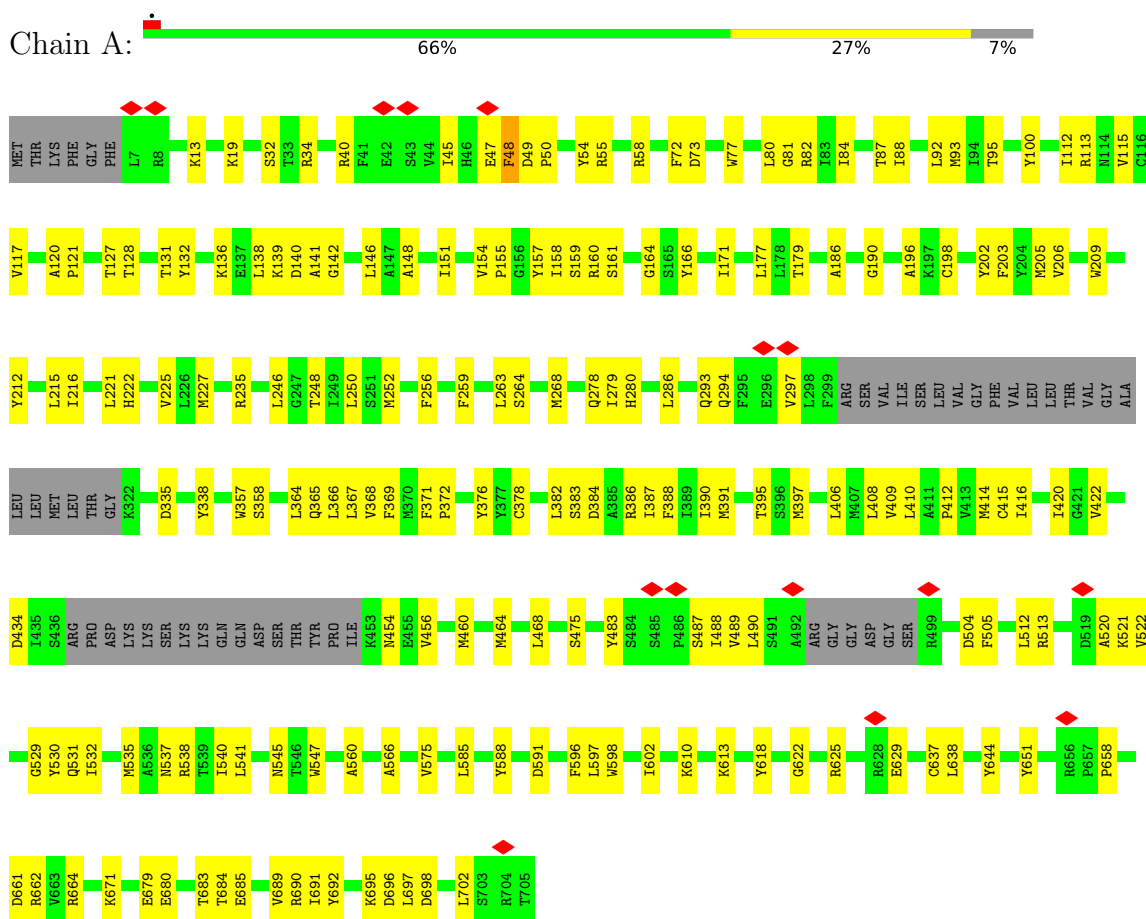
- Molecule 18 is water.

Mol	Chain	Residues	Atoms	AltConf
18	A	1	Total O 1 1	0

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.

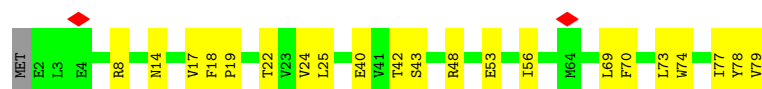
- Molecule 1: Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit STT3A



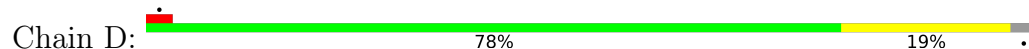
- Molecule 2: Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit 4



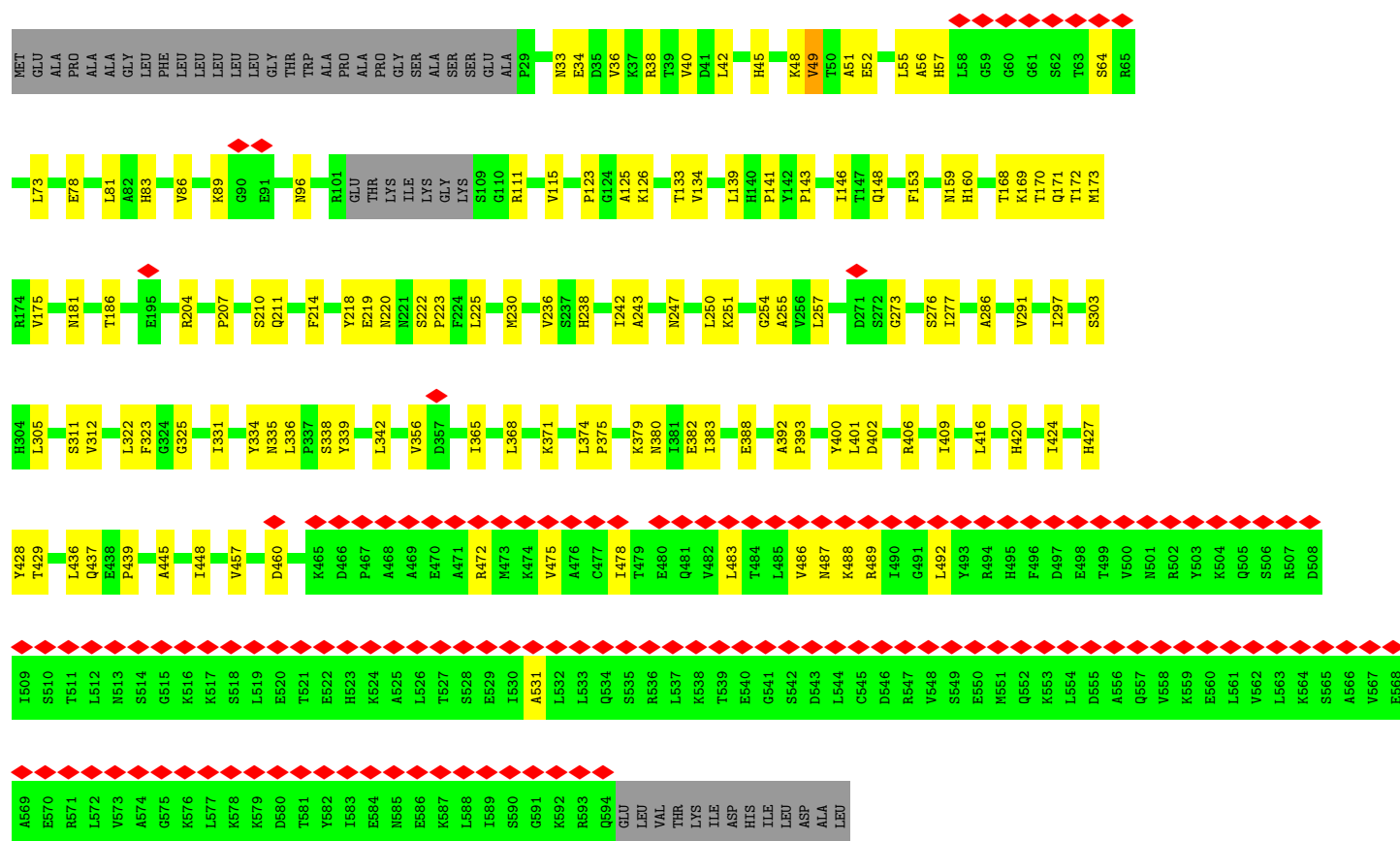
- Molecule 3: Transmembrane protein 258



- Molecule 4: Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit DAD1

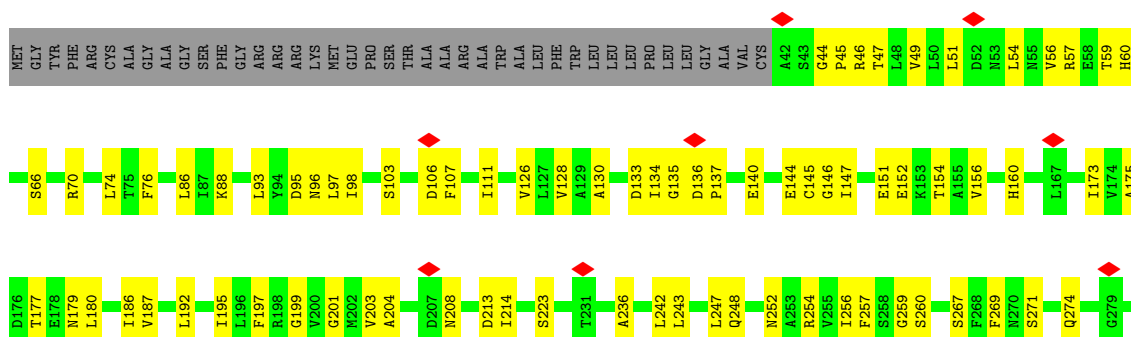


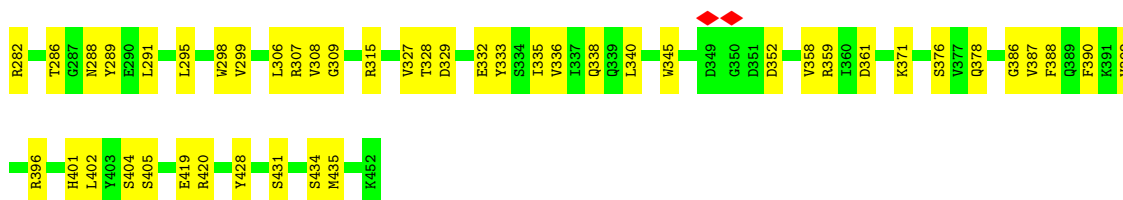
- Molecule 5: Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit 1



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







- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



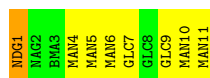
- Molecule 10: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 11: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	101699	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 ($e^-/\text{\AA}^2$)	54.2	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	0.516	Depositor
Minimum map value	-0.334	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.0735	Depositor
Map size ($\text{\AA}$)	331.776, 331.776, 331.776	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.648, 0.648, 0.648	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: NAG, OTP, MAN, NDG, BMA, ZXT, MN, GLC, KZB, EGY

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	0.22	0/5450	0.52	1/7402 (0.0%)
2	B	0.15	0/263	0.35	0/360
3	C	0.20	0/654	0.46	0/893
4	D	0.20	0/882	0.53	0/1197
5	E	0.16	0/4269	0.44	0/5827
6	F	0.17	0/1963	0.47	0/2668
7	H	0.18	0/891	0.43	0/1207
8	G	0.17	0/3320	0.44	0/4509
All	All	0.19	0/17692	0.47	1/24063 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	48	PHE	N-CA-C	5.18	119.31	112.89

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	5302	0	5241	151	0
2	B	258	0	272	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	634	0	647	15	0
4	D	862	0	880	21	0
5	E	4180	0	3884	89	0
6	F	1919	0	1962	46	0
7	H	869	0	903	17	0
8	G	3238	0	3179	88	0
9	I	28	0	25	0	0
10	J	94	0	79	1	0
11	K	83	0	70	2	0
12	N	127	0	105	1	0
13	A	64	0	0	0	0
13	F	32	0	0	0	0
13	G	32	0	0	0	0
14	A	43	0	0	1	0
14	F	43	0	0	3	0
15	A	1	0	0	0	0
16	A	49	0	65	4	0
17	A	26	0	0	1	0
18	A	1	0	0	0	0
All	All	17885	0	17312	404	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 11.

All (404) 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:560:ALA:HB2	1:A:596:PHE:CE2	2.04	0.92
1:A:488:ILE:HG22	1:A:488:ILE:O	1.73	0.86
8:G:51:LEU:HD23	8:G:56:VAL:HB	1.62	0.81
8:G:327:VAL:HG12	8:G:328:THR:HG23	1.65	0.79
6:F:599:MET:HG2	14:F:702:EGY:O32	1.83	0.78
6:F:415:ALA:HA	6:F:461:PHE:O	1.85	0.77
1:A:529:GLY:HA2	1:A:540:ILE:HD13	1.66	0.76
5:E:383:ILE:HD11	5:E:424:ILE:HD11	1.68	0.75
6:F:402:ALA:HB3	6:F:499:ALA:HB2	1.67	0.75
8:G:199:GLY:HA3	8:G:260:SER:HB2	1.69	0.75
5:E:247:ASN:HD22	5:E:331:ILE:HG12	1.51	0.74
8:G:49:VAL:HG22	8:G:98:ILE:HB	1.70	0.73
5:E:365:ILE:HB	5:E:416:LEU:HB2	1.72	0.72
4:D:41:GLN:NE2	8:G:431:SER:OG	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:530:TYR:OH	1:A:545:ASN:OD1	2.08	0.71
1:A:488:ILE:HD11	1:A:531:GLN:HE21	1.55	0.71
1:A:488:ILE:O	1:A:488:ILE:CG2	2.39	0.70
6:F:379:ASP:HB2	6:F:417:PHE:HB2	1.74	0.70
6:F:431:PRO:HG2	6:F:434:THR:HG22	1.73	0.69
1:A:560:ALA:HB2	1:A:596:PHE:HE2	1.58	0.69
6:F:589:LEU:HA	6:F:592:VAL:HG12	1.73	0.69
3:C:79:VAL:HG21	5:E:401:LEU:HB2	1.74	0.68
1:A:34:ARG:HH22	1:A:158:ILE:HA	1.59	0.68
1:A:535:MET:HG2	5:E:297:ILE:HD11	1.76	0.67
1:A:128:THR:HG23	1:A:148:ALA:HB1	1.77	0.66
8:G:286:THR:HG23	8:G:288:ASN:H	1.59	0.66
5:E:57:HIS:HB3	5:E:123:PRO:HA	1.77	0.66
8:G:130:ALA:HB1	8:G:134:ILE:HG22	1.78	0.65
8:G:197:PHE:HZ	8:G:259:GLY:HA3	1.62	0.65
8:G:306:LEU:HB2	8:G:402:LEU:HD11	1.78	0.65
1:A:47:GLU:HG2	1:A:487:SER:HB2	1.78	0.65
6:F:437:ARG:NH2	6:F:446:GLU:OE2	2.29	0.65
1:A:456:VAL:HG11	7:H:121:LEU:HD21	1.79	0.64
5:E:169:LYS:HG3	5:E:170:THR:H	1.62	0.64
8:G:333:TYR:O	8:G:376:SER:HA	1.98	0.64
1:A:371:PHE:HD2	1:A:414:MET:HG3	1.62	0.63
3:C:73:LEU:HD12	3:C:78:TYR:HA	1.80	0.63
1:A:54:TYR:OH	1:A:58:ARG:NH2	2.31	0.63
7:H:46:GLY:O	7:H:82:GLN:NE2	2.29	0.63
1:A:679:GLU:HB3	1:A:695:LYS:HE3	1.80	0.63
5:E:291:VAL:HG12	5:E:334:TYR:HB3	1.79	0.63
5:E:436:LEU:O	5:E:439:PRO:HD2	1.99	0.62
1:A:560:ALA:HA	1:A:637:CYS:HB2	1.81	0.62
1:A:221:LEU:HG	1:A:391:MET:HE2	1.82	0.62
1:A:154:VAL:HG13	1:A:157:TYR:HB3	1.81	0.62
1:A:489:VAL:HG12	1:A:489:VAL:O	2.00	0.62
1:A:488:ILE:HD11	1:A:531:GLN:NE2	2.15	0.61
1:A:136:LYS:HE2	1:A:141:ALA:HB2	1.81	0.61
1:A:48:PHE:O	1:A:530:TYR:HD2	1.83	0.61
5:E:478:ILE:HG21	5:E:531:ALA:HB2	1.81	0.61
1:A:34:ARG:HD2	1:A:121:PRO:HA	1.81	0.60
5:E:181:ASN:ND2	5:E:219:GLU:OE1	2.33	0.60
5:E:48:LYS:HB3	5:E:134:VAL:HG22	1.82	0.60
1:A:235:ARG:NH1	1:A:384:ASP:OD2	2.34	0.60
1:A:159:SER:HB3	1:A:483:TYR:CD2	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:625:ARG:HH12	1:A:629:GLU:HB2	1.66	0.60
8:G:256:ILE:HG21	8:G:299:VAL:HG21	1.84	0.60
1:A:683:THR:HG23	1:A:690:ARG:HG2	1.83	0.60
1:A:139:LYS:NZ	1:A:140:ASP:OD1	2.30	0.60
5:E:445:ALA:O	5:E:448:ILE:HG22	2.02	0.59
8:G:128:VAL:HG22	8:G:257:PHE:HA	1.83	0.59
1:A:248:THR:HG22	1:A:252:MET:HE2	1.85	0.59
1:A:532:ILE:HD12	1:A:540:ILE:HD12	1.85	0.59
1:A:488:ILE:HG23	1:A:505:PHE:HB2	1.85	0.58
4:D:34:ILE:HG12	8:G:435:MET:HE1	1.84	0.58
5:E:286:ALA:HB2	5:E:311:SER:HA	1.84	0.58
3:C:69:LEU:HD13	5:E:439:PRO:HG3	1.86	0.58
5:E:160:HIS:NE2	5:E:214:PHE:HB3	2.17	0.58
6:F:485:ILE:HD12	6:F:494:ILE:HD11	1.84	0.58
1:A:488:ILE:HG23	1:A:505:PHE:CB	2.34	0.58
4:D:91:GLU:OE1	4:D:91:GLU:N	2.37	0.58
6:F:493:PRO:HB2	8:G:160:HIS:CD2	2.39	0.58
5:E:338:SER:HB2	5:E:342:LEU:HD12	1.85	0.58
1:A:512:LEU:HD13	1:A:691:ILE:HD13	1.86	0.57
5:E:168:THR:OG1	5:E:171:GLN:NE2	2.37	0.57
8:G:103:SER:N	8:G:133:ASP:O	2.34	0.57
1:A:369:PHE:O	1:A:372:PRO:HD2	2.04	0.57
8:G:390:PHE:O	8:G:405:SER:HA	2.06	0.56
1:A:139:LYS:HD2	1:A:420:ILE:HG23	1.88	0.56
5:E:238:HIS:CE1	5:E:375:PRO:HG3	2.41	0.56
1:A:55:ARG:NH1	1:A:73:ASP:OD2	2.39	0.55
4:D:41:GLN:NE2	4:D:59:GLY:O	2.39	0.55
8:G:359:ARG:HB2	8:G:388:PHE:CE1	2.42	0.55
1:A:179:THR:HG21	1:A:215:LEU:HD13	1.89	0.55
1:A:504:ASP:HB3	1:A:684:THR:HG21	1.87	0.55
6:F:439:HIS:HB3	6:F:480:THR:HB	1.88	0.55
8:G:57:ARG:HD3	8:G:76:PHE:CG	2.42	0.54
5:E:207:PRO:HD2	5:E:210:SER:HB3	1.88	0.54
5:E:34:GLU:O	5:E:169:LYS:HB3	2.08	0.54
17:A:806:ZXT:S06	12:N:1:NDG:H6C2	2.48	0.54
8:G:156:VAL:HA	8:G:223:SER:HA	1.89	0.54
1:A:222:HIS:CE1	1:A:388:PHE:HB2	2.43	0.54
4:D:33:TYR:OH	8:G:434:SER:OG	2.24	0.54
1:A:92:LEU:HD13	1:A:171:ILE:HG21	1.90	0.53
1:A:82:ARG:NH2	1:A:84:ILE:HG12	2.24	0.53
3:C:14:ASN:O	3:C:17:VAL:HG22	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:16:TYR:OH	4:D:28:ASP:OD2	2.21	0.53
4:D:30:TYR:CZ	4:D:34:ILE:HD11	2.44	0.53
5:E:483:LEU:O	5:E:487:ASN:ND2	2.42	0.53
8:G:274:GLN:HB2	8:G:282:ARG:HG3	1.90	0.53
1:A:293:GLN:O	1:A:297:VAL:HG23	2.09	0.53
6:F:599:MET:CG	14:F:702:EGY:O32	2.55	0.53
7:H:77:TYR:CZ	7:H:144:PRO:HG2	2.44	0.53
5:E:33:ASN:HD22	5:E:168:THR:HG22	1.73	0.53
1:A:591:ASP:OD2	1:A:664:ARG:NH2	2.39	0.53
1:A:117:VAL:HG13	1:A:164:GLY:HA2	1.91	0.52
6:F:484:ILE:HG12	6:F:495:LEU:HD12	1.92	0.52
5:E:303:SER:O	11:K:2:NAG:H3	2.08	0.52
6:F:482:TYR:HA	6:F:497:ASN:HA	1.92	0.52
1:A:610:LYS:O	1:A:613:LYS:HG3	2.10	0.52
1:A:690:ARG:NH2	1:A:692:TYR:OH	2.35	0.52
4:D:31:LEU:HD11	4:D:71:VAL:HG22	1.92	0.52
8:G:47:THR:HG22	8:G:96:ASN:HB2	1.92	0.52
8:G:145:CYS:HB3	8:G:247:LEU:HD22	1.91	0.52
1:A:206:VAL:HG23	1:A:212:TYR:CG	2.45	0.52
1:A:416:ILE:O	1:A:420:ILE:HG13	2.10	0.52
8:G:203:VAL:HB	8:G:236:ALA:HB2	1.91	0.52
1:A:19:LYS:HD3	1:A:132:TYR:OH	2.10	0.51
1:A:45:ILE:HG22	1:A:50:PRO:HB2	1.92	0.51
1:A:159:SER:OG	1:A:160:ARG:HD2	2.10	0.51
1:A:378:CYS:HB3	1:A:390:ILE:HD11	1.91	0.51
5:E:488:LYS:O	5:E:492:LEU:HG	2.11	0.51
8:G:88:LYS:HB3	8:G:93:LEU:HD11	1.92	0.51
1:A:371:PHE:HB3	1:A:372:PRO:HD3	1.92	0.51
1:A:625:ARG:HH22	1:A:629:GLU:HB2	1.76	0.51
8:G:106:ASP:OD1	8:G:106:ASP:N	2.43	0.51
1:A:49:ASP:HB3	1:A:50:PRO:HD3	1.93	0.51
1:A:77:TRP:HA	1:A:541:LEU:O	2.10	0.51
5:E:251:LYS:HE2	5:E:325:GLY:HA2	1.93	0.51
4:D:62:SER:HB2	4:D:108:VAL:HG11	1.93	0.51
8:G:156:VAL:HG13	8:G:173:ILE:HG13	1.92	0.51
8:G:295:LEU:O	8:G:299:VAL:HG23	2.11	0.51
5:E:186:THR:HB	5:E:214:PHE:HB2	1.93	0.51
1:A:625:ARG:NH1	1:A:629:GLU:OE1	2.44	0.51
8:G:392:VAL:HG13	8:G:404:SER:HB3	1.92	0.51
8:G:180:LEU:HD21	8:G:187:VAL:HG21	1.91	0.51
8:G:252:ASN:HD21	8:G:401:HIS:H	1.59	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:38:ARG:O	5:E:173:MET:HA	2.11	0.51
8:G:54:LEU:HG	8:G:57:ARG:HH21	1.75	0.50
8:G:177:THR:HG21	8:G:192:LEU:O	2.11	0.50
8:G:195:ILE:O	8:G:195:ILE:HG13	2.11	0.50
5:E:483:LEU:O	5:E:486:VAL:HG12	2.11	0.50
6:F:487:ASP:HB3	6:F:490:LEU:HD13	1.94	0.50
1:A:87:THR:HA	1:A:256:PHE:HD1	1.76	0.50
1:A:294:GLN:HB3	4:D:8:VAL:HG21	1.94	0.50
5:E:243:ALA:HA	5:E:335:ASN:HA	1.94	0.50
8:G:201:GLY:HA2	8:G:243:LEU:HD23	1.94	0.50
1:A:205:MET:HE3	1:A:209:TRP:HE3	1.77	0.50
1:A:72:PHE:HZ	8:G:386:GLY:HA2	1.77	0.50
1:A:680:GLU:OE2	1:A:683:THR:OG1	2.25	0.50
3:C:43:SER:O	3:C:48:ARG:NH1	2.44	0.50
5:E:402:ASP:OD2	5:E:406:ARG:NE	2.40	0.50
1:A:490:LEU:CD1	1:A:588:TYR:CD1	2.95	0.49
5:E:159:ASN:HD21	5:E:211:GLN:HG3	1.77	0.49
5:E:305:LEU:HD22	11:K:2:NAG:H83	1.94	0.49
1:A:468:LEU:HB3	2:B:19:PHE:CD2	2.46	0.49
1:A:387:ILE:O	1:A:391:MET:HG2	2.12	0.49
5:E:42:LEU:HD23	5:E:139:LEU:HD21	1.95	0.49
5:E:83:HIS:HB2	5:E:420:HIS:CE1	2.47	0.49
8:G:371:LYS:HG3	8:G:371:LYS:O	2.11	0.49
1:A:151:ILE:O	1:A:154:VAL:HG12	2.13	0.49
8:G:315:ARG:NH1	8:G:329:ASP:OD2	2.45	0.49
5:E:49:VAL:HG22	5:E:133:THR:HG22	1.95	0.49
5:E:336:LEU:HD23	5:E:336:LEU:H	1.77	0.49
8:G:340:LEU:HD12	8:G:345:TRP:CZ2	2.48	0.49
7:H:126:VAL:O	7:H:130:LEU:HB2	2.11	0.49
1:A:80:LEU:HD21	10:J:1:NAG:H2	1.95	0.49
1:A:88:ILE:HD12	1:A:93:MET:HE3	1.94	0.49
5:E:38:ARG:HA	5:E:51:ALA:HA	1.95	0.49
5:E:52:GLU:OE1	5:E:52:GLU:N	2.46	0.49
5:E:371:LYS:HA	5:E:409:ILE:O	2.13	0.48
6:F:407:ILE:HG13	6:F:502:VAL:HB	1.94	0.48
8:G:254:ARG:NH2	8:G:298:TRP:O	2.46	0.48
8:G:307:ARG:NH1	8:G:338:GLN:OE1	2.44	0.48
8:G:147:ILE:HD12	8:G:257:PHE:CD2	2.49	0.48
1:A:34:ARG:NH2	1:A:161:SER:OG	2.46	0.48
1:A:382:LEU:HD22	14:A:803:EGY:C1	2.44	0.48
1:A:520:ALA:HB3	1:A:538:ARG:HD2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:TRP:O	1:A:81:GLY:N	2.44	0.48
5:E:141:PRO:HG3	5:E:254:GLY:HA2	1.94	0.48
5:E:230:MET:HE1	5:E:356:VAL:HG23	1.96	0.48
1:A:127:THR:HG23	1:A:177:LEU:HD12	1.95	0.48
1:A:368:VAL:HG13	7:H:41:TYR:OH	2.13	0.48
6:F:536:ARG:NH1	8:G:419:GLU:OE2	2.42	0.48
1:A:512:LEU:HD21	1:A:522:VAL:HG21	1.95	0.48
1:A:658:PRO:O	1:A:671:LYS:NZ	2.47	0.48
5:E:45:HIS:CD2	5:E:45:HIS:H	2.32	0.48
8:G:361:ASP:N	8:G:361:ASP:OD1	2.45	0.48
4:D:26:LEU:HG	6:F:560:TRP:NE1	2.28	0.48
8:G:97:LEU:HD23	8:G:126:VAL:HG13	1.95	0.48
8:G:248:GLN:NE2	8:G:252:ASN:HD22	2.12	0.48
5:E:146:ILE:HG12	5:E:255:ALA:HB1	1.95	0.47
4:D:106:LEU:HD23	14:F:702:EGY:C3B	2.45	0.47
6:F:449:PHE:CZ	6:F:471:GLU:HG2	2.49	0.47
8:G:134:ILE:HG13	8:G:135:GLY:H	1.79	0.47
6:F:418:PHE:O	6:F:458:VAL:HG13	2.13	0.47
6:F:468:ARG:HB3	6:F:471:GLU:HB3	1.97	0.47
7:H:60:GLY:HA3	7:H:72:VAL:H	1.78	0.47
8:G:103:SER:HB3	8:G:133:ASP:HB3	1.96	0.47
1:A:113:ARG:HD2	1:A:113:ARG:O	2.14	0.47
5:E:368:LEU:HD13	5:E:416:LEU:HG	1.96	0.47
5:E:460:ASP:OD1	5:E:460:ASP:N	2.46	0.47
6:F:376:THR:HB	6:F:419:GLN:HB3	1.96	0.47
6:F:498:VAL:HG23	6:F:499:ALA:H	1.79	0.47
5:E:257:LEU:HD13	5:E:323:PHE:HD2	1.80	0.47
1:A:100:TYR:HB2	1:A:115:VAL:HG11	1.96	0.47
1:A:598:TRP:O	1:A:602:ILE:HG13	2.15	0.47
8:G:267:SER:O	8:G:271:SER:HB3	2.15	0.47
1:A:92:LEU:HG	1:A:166:TYR:CZ	2.50	0.46
1:A:120:ALA:HB3	1:A:121:PRO:HD3	1.95	0.46
5:E:148:GLN:HG3	5:E:323:PHE:HE2	1.80	0.46
8:G:352:ASP:OD2	8:G:396:ARG:NH2	2.48	0.46
1:A:383:SER:O	1:A:387:ILE:HG13	2.15	0.46
5:E:382:GLU:HG2	5:E:427:HIS:HB2	1.97	0.46
1:A:490:LEU:HD12	1:A:588:TYR:CD1	2.50	0.46
5:E:96:ASN:OD1	5:E:96:ASN:N	2.48	0.46
5:E:472:ARG:O	5:E:475:VAL:HG12	2.16	0.46
8:G:107:PHE:HB3	8:G:111:ILE:HB	1.97	0.46
1:A:225:VAL:C	1:A:227:MET:H	2.23	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:513:ARG:NH1	1:A:535:MET:O	2.47	0.46
6:F:418:PHE:HB2	6:F:459:TYR:HB2	1.97	0.46
3:C:19:PRO:HB3	3:C:74:TRP:CE2	2.50	0.46
6:F:438:LEU:HB2	6:F:447:VAL:HG22	1.96	0.46
1:A:80:LEU:HD23	1:A:547:TRP:CH2	2.51	0.46
1:A:464:MET:HE1	7:H:101:PHE:HE2	1.80	0.46
5:E:55:LEU:O	5:E:126:LYS:HA	2.16	0.46
6:F:594:TRP:O	8:G:420:ARG:NH2	2.49	0.46
5:E:169:LYS:HG3	5:E:170:THR:HG23	1.97	0.46
5:E:222:SER:OG	5:E:223:PRO:HD2	2.16	0.46
1:A:47:GLU:HG2	1:A:487:SER:CB	2.45	0.46
1:A:48:PHE:O	1:A:530:TYR:CD2	2.67	0.46
1:A:155:PRO:HG3	1:A:475:SER:HA	1.98	0.46
5:E:273:GLY:O	5:E:276:SER:OG	2.34	0.46
1:A:434:ASP:HB2	1:A:454:ASN:HD21	1.81	0.45
4:D:16:TYR:O	4:D:16:TYR:CG	2.69	0.45
8:G:66:SER:OG	8:G:70:ARG:NH1	2.48	0.45
8:G:197:PHE:CZ	8:G:259:GLY:HA3	2.46	0.45
1:A:376:TYR:HB2	7:H:34:TYR:CZ	2.52	0.45
3:C:22:THR:OG1	3:C:70:PHE:HB3	2.16	0.45
6:F:593:TYR:HA	6:F:597:LEU:HB2	1.97	0.45
8:G:204:ALA:HB2	8:G:242:LEU:HD11	1.98	0.45
1:A:537:ASN:O	1:A:538:ARG:NH1	2.49	0.45
3:C:77:ILE:HD13	5:E:400:TYR:CE2	2.52	0.45
6:F:593:TYR:CD1	6:F:602:THR:HG21	2.51	0.45
8:G:59:THR:HG23	8:G:60:HIS:ND1	2.31	0.45
8:G:130:ALA:O	8:G:260:SER:HA	2.16	0.45
8:G:187:VAL:HG23	8:G:291:LEU:HD13	1.98	0.45
5:E:143:PRO:HD2	5:E:153:PHE:O	2.17	0.45
8:G:340:LEU:HD12	8:G:345:TRP:CH2	2.51	0.45
3:C:24:VAL:HG13	3:C:25:LEU:HD12	1.99	0.45
6:F:560:TRP:C	6:F:562:ARG:N	2.74	0.45
8:G:358:VAL:HG23	8:G:361:ASP:C	2.42	0.45
3:C:40:GLU:OE2	5:E:457:VAL:HG21	2.17	0.45
6:F:573:ALA:HB3	6:F:576:THR:HG22	1.99	0.45
8:G:44:GLY:N	8:G:95:ASP:OD2	2.27	0.45
8:G:56:VAL:HA	8:G:59:THR:HG22	1.98	0.45
16:A:805:OTP:H52	16:A:805:OTP:H81	1.64	0.45
5:E:236:VAL:HA	5:E:242:ILE:HG22	1.98	0.45
1:A:364:LEU:HD23	1:A:367:LEU:HD12	1.99	0.45
1:A:395:THR:HG21	16:A:805:OTP:H233	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:SER:O	1:A:268:MET:HG2	2.17	0.45
1:A:397:MET:HA	1:A:410:LEU:HD13	1.99	0.45
16:A:805:OTP:H302	16:A:805:OTP:H331	1.65	0.45
1:A:335:ASP:OD1	1:A:338:TYR:N	2.50	0.44
5:E:40:VAL:HG23	5:E:49:VAL:HG12	1.98	0.44
1:A:142:GLY:O	2:B:26:HIS:NE2	2.50	0.44
1:A:684:THR:HG22	1:A:685:GLU:H	1.82	0.44
1:A:206:VAL:HG23	1:A:212:TYR:CD2	2.53	0.44
5:E:170:THR:HG22	5:E:204:ARG:HG2	1.99	0.44
5:E:401:LEU:HD23	5:E:401:LEU:HA	1.83	0.44
5:E:36:VAL:HB	5:E:171:GLN:HB3	1.98	0.44
5:E:218:TYR:CE2	5:E:220:ASN:HB2	2.53	0.44
5:E:374:LEU:HB3	5:E:375:PRO:HD2	2.00	0.44
8:G:86:LEU:HB2	8:G:111:ILE:HD13	2.00	0.44
8:G:186:ILE:HG12	8:G:298:TRP:CE2	2.53	0.44
5:E:380:ASN:O	5:E:428:TYR:HA	2.18	0.44
1:A:205:MET:SD	1:A:215:LEU:HD11	2.57	0.44
1:A:364:LEU:HD22	1:A:414:MET:SD	2.58	0.44
1:A:644:TYR:OH	1:A:661:ASP:OD2	2.21	0.44
1:A:698:ASP:OD2	1:A:702:LEU:HB2	2.18	0.44
4:D:41:GLN:HE21	8:G:431:SER:CB	2.29	0.44
4:D:48:VAL:HG11	6:F:537:PRO:HG3	1.99	0.44
6:F:489:THR:C	6:F:490:LEU:HD12	2.43	0.44
8:G:214:ILE:HG21	8:G:295:LEU:HD21	1.99	0.44
1:A:139:LYS:HB2	1:A:139:LYS:HE2	1.81	0.43
1:A:278:GLN:C	1:A:280:HIS:H	2.26	0.43
5:E:277:ILE:HD11	5:E:322:LEU:HD22	2.00	0.43
5:E:335:ASN:OD1	5:E:335:ASN:N	2.51	0.43
6:F:416:LEU:HD11	6:F:418:PHE:CZ	2.52	0.43
7:H:124:GLY:O	7:H:128:VAL:HG23	2.17	0.43
5:E:40:VAL:O	5:E:175:VAL:HA	2.17	0.43
8:G:47:THR:OG1	8:G:74:LEU:HD23	2.18	0.43
1:A:128:THR:CG2	1:A:148:ALA:HB1	2.47	0.43
1:A:221:LEU:HG	1:A:391:MET:CE	2.47	0.43
1:A:365:GLN:O	1:A:366:LEU:HB3	2.18	0.43
1:A:696:ASP:OD1	1:A:697:LEU:N	2.51	0.43
5:E:277:ILE:HG13	5:E:277:ILE:O	2.18	0.43
4:D:26:LEU:HG	6:F:560:TRP:CE2	2.54	0.43
8:G:136:ASP:N	8:G:137:PRO:HD2	2.33	0.43
8:G:269:PHE:CE1	8:G:289:TYR:HA	2.54	0.43
1:A:585:LEU:O	1:A:662:ARG:NH2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:33:ASN:ND2	5:E:168:THR:HG22	2.33	0.43
5:E:388:GLU:O	5:E:388:GLU:HG3	2.18	0.43
6:F:421:VAL:HA	6:F:428:GLU:HA	2.01	0.43
1:A:358:SER:OG	7:H:79:VAL:O	2.30	0.43
6:F:476:SER:HB3	6:F:479:TYR:CE2	2.52	0.43
6:F:620:MET:HE2	6:F:620:MET:HB3	1.94	0.43
1:A:131:THR:HG21	1:A:151:ILE:HG13	1.99	0.43
1:A:246:LEU:O	1:A:250:LEU:HD23	2.19	0.43
1:A:684:THR:HG22	1:A:685:GLU:N	2.34	0.43
4:D:56:PHE:HB2	8:G:428:TYR:CZ	2.53	0.43
5:E:486:VAL:HG23	5:E:489:ARG:HH21	1.83	0.43
1:A:618:TYR:HB3	1:A:622:GLY:HA2	2.01	0.43
1:A:151:ILE:HD11	1:A:412:PRO:HA	2.00	0.43
1:A:357:TRP:CZ2	7:H:142:LYS:HD2	2.54	0.43
8:G:308:VAL:HG13	8:G:335:ILE:HD11	2.00	0.43
8:G:401:HIS:C	8:G:402:LEU:HD12	2.44	0.43
5:E:48:LYS:HA	5:E:134:VAL:HA	2.01	0.42
6:F:560:TRP:C	6:F:562:ARG:H	2.27	0.42
1:A:488:ILE:HG23	1:A:505:PHE:HB3	2.01	0.42
1:A:597:LEU:HD23	1:A:597:LEU:HA	1.85	0.42
8:G:213:ASP:HB3	8:G:242:LEU:HD13	2.01	0.42
1:A:160:ARG:HG2	1:A:408:LEU:HD21	2.00	0.42
8:G:51:LEU:HD11	8:G:76:PHE:HD2	1.85	0.42
1:A:202:TYR:CZ	1:A:216:ILE:HD11	2.54	0.42
1:A:460:MET:HE3	7:H:104:LEU:HD21	2.01	0.42
1:A:512:LEU:HD21	1:A:522:VAL:HG11	2.02	0.42
1:A:521:LYS:O	1:A:575:VAL:HG23	2.20	0.42
5:E:89:LYS:HD2	5:E:89:LYS:HA	1.94	0.42
8:G:45:PRO:O	8:G:47:THR:HG23	2.20	0.42
1:A:146:LEU:HD13	2:B:22:VAL:HG11	2.02	0.42
1:A:460:MET:HE3	7:H:104:LEU:CD2	2.49	0.42
5:E:379:LYS:HB2	5:E:429:THR:HG23	2.01	0.42
8:G:332:GLU:HG3	8:G:378:GLN:HG2	2.02	0.42
3:C:18:PHE:N	3:C:19:PRO:HD2	2.35	0.42
6:F:438:LEU:HB2	6:F:447:VAL:CG2	2.50	0.42
7:H:75:LEU:HD12	7:H:75:LEU:HA	1.83	0.42
8:G:256:ILE:CG2	8:G:299:VAL:HG21	2.49	0.42
1:A:146:LEU:HD21	1:A:422:VAL:HG12	2.02	0.42
1:A:250:LEU:CD2	4:D:107:VAL:HG21	2.50	0.42
1:A:406:LEU:C	1:A:408:LEU:H	2.28	0.42
4:D:46:LEU:HD23	4:D:46:LEU:HA	1.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:160:HIS:CD2	5:E:160:HIS:H	2.37	0.42
8:G:134:ILE:HG12	8:G:152:GLU:HA	2.00	0.42
1:A:151:ILE:HG12	1:A:415:CYS:SG	2.60	0.42
1:A:203:PHE:HA	1:A:206:VAL:HG12	2.02	0.42
5:E:392:ALA:HB1	5:E:393:PRO:HD2	2.01	0.42
1:A:32:SER:O	1:A:32:SER:OG	2.33	0.42
1:A:40:ARG:NE	2:B:4:ASP:OD2	2.44	0.42
6:F:381:SER:HB2	6:F:393:THR:HG22	2.02	0.42
1:A:259:PHE:O	1:A:263:LEU:HG	2.20	0.41
5:E:73:LEU:HD11	5:E:81:LEU:HD22	2.01	0.41
7:H:31:MET:C	7:H:33:VAL:N	2.78	0.41
6:F:589:LEU:HD11	6:F:605:TYR:HB3	2.01	0.41
6:F:619:ARG:O	6:F:623:GLN:HG2	2.20	0.41
8:G:140:GLU:O	8:G:144:GLU:HG2	2.21	0.41
5:E:40:VAL:HG13	5:E:175:VAL:HG22	2.02	0.41
5:E:225:LEU:HD21	5:E:250:LEU:HD12	2.02	0.41
6:F:423:VAL:C	6:F:425:THR:H	2.29	0.41
8:G:269:PHE:HE1	8:G:289:TYR:HA	1.85	0.41
1:A:138:LEU:O	1:A:386:ARG:NH2	2.53	0.41
16:A:805:OTP:H382	16:A:805:OTP:H402	1.78	0.41
2:B:1:MET:HB3	2:B:2:ILE:H	1.64	0.41
4:D:45:CYS:O	4:D:49:GLY:N	2.51	0.41
5:E:64:SER:HA	5:E:123:PRO:HD3	2.03	0.41
5:E:56:ALA:HA	5:E:125:ALA:O	2.20	0.41
6:F:503:ILE:HG13	6:F:505:PHE:HD1	1.86	0.41
1:A:92:LEU:HA	1:A:95:THR:HG22	2.03	0.41
1:A:196:ALA:C	1:A:198:CYS:H	2.28	0.41
4:D:17:LEU:HD23	4:D:17:LEU:HA	1.83	0.41
5:E:172:THR:O	5:E:172:THR:OG1	2.37	0.41
6:F:498:VAL:HG23	6:F:499:ALA:N	2.36	0.41
1:A:406:LEU:O	1:A:409:VAL:HG22	2.21	0.41
1:A:490:LEU:HD11	1:A:588:TYR:CD1	2.55	0.41
2:B:14:LEU:HD12	2:B:14:LEU:HA	1.89	0.41
5:E:141:PRO:HG3	5:E:255:ALA:H	1.86	0.41
8:G:309:GLY:HA3	8:G:336:VAL:HG13	2.03	0.41
1:A:58:ARG:HG3	1:A:112:ILE:HG21	2.02	0.40
1:A:366:LEU:HA	1:A:369:PHE:HD1	1.85	0.40
5:E:78:GLU:O	5:E:111:ARG:NH2	2.47	0.40
5:E:86:VAL:HG21	5:E:115:VAL:HG21	2.03	0.40
1:A:286:LEU:HA	1:A:286:LEU:HD23	1.84	0.40
1:A:406:LEU:C	1:A:408:LEU:N	2.79	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:70:ARG:HA	7:H:71:PRO:HD3	1.96	0.40
8:G:151:GLU:HB3	8:G:154:THR:HG23	2.04	0.40
8:G:175:ALA:HB3	8:G:195:ILE:HG13	2.02	0.40
8:G:179:ASN:OD1	8:G:179:ASN:N	2.54	0.40
1:A:278:GLN:C	1:A:280:HIS:N	2.78	0.40
1:A:651:TYR:CE2	1:A:658:PRO:HB3	2.56	0.40
6:F:545:PHE:O	6:F:549:ILE:HG12	2.21	0.40
8:G:146:GLY:HA3	8:G:208:ASN:ND2	2.37	0.40
1:A:13:LYS:NZ	3:C:42:THR:OG1	2.38	0.40
1:A:186:ALA:O	1:A:190:GLY:N	2.52	0.40
3:C:19:PRO:HB3	3:C:74:TRP:CZ2	2.56	0.40
3:C:53:GLU:O	3:C:56:ILE:HG22	2.21	0.40
5:E:286:ALA:HA	5:E:312:VAL:HG23	2.04	0.40
8:G:46:ARG:H	8:G:46:ARG:HG2	1.65	0.40
1:A:386:ARG:C	1:A:388:PHE:N	2.77	0.40
1:A:566:ALA:HB1	1:A:638:LEU:HD22	2.02	0.40
3:C:8:ARG:HD2	5:E:339:TYR:O	2.22	0.40
6:F:373:VAL:HG12	6:F:492:ASN:HB3	2.03	0.40
7:H:29:SER:HB2	7:H:32:THR:OG1	2.21	0.40
8:G:54:LEU:HD12	8:G:54:LEU:HA	1.88	0.40
8:G:107:PHE:HE2	8:G:137:PRO:HB2	1.86	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	647/705 (92%)	572 (88%)	74 (11%)	1 (0%)	43	71
2	B	31/37 (84%)	31 (100%)	0	0	100	100
3	C	76/79 (96%)	74 (97%)	2 (3%)	0	100	100
4	D	108/113 (96%)	103 (95%)	5 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	555/607 (91%)	511 (92%)	43 (8%)	1 (0%)	43	71
6	F	233/631 (37%)	207 (89%)	25 (11%)	1 (0%)	30	59
7	H	108/149 (72%)	95 (88%)	13 (12%)	0	100	100
8	G	409/452 (90%)	381 (93%)	28 (7%)	0	100	100
All	All	2167/2773 (78%)	1974 (91%)	190 (9%)	3 (0%)	49	78

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	437	GLN
1	A	279	ILE
6	F	436	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	573/615 (93%)	572 (100%)	1 (0%)	87	84
2	B	29/33 (88%)	29 (100%)	0	100	100
3	C	69/70 (99%)	69 (100%)	0	100	100
4	D	96/98 (98%)	96 (100%)	0	100	100
5	E	409/537 (76%)	408 (100%)	1 (0%)	87	84
6	F	211/541 (39%)	211 (100%)	0	100	100
7	H	94/130 (72%)	94 (100%)	0	100	100
8	G	357/386 (92%)	356 (100%)	1 (0%)	86	81
All	All	1838/2410 (76%)	1835 (100%)	3 (0%)	85	84

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	689	VAL

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Mol	Chain	Res	Type
5	E	49	VAL
8	G	387	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	234	HIS
1	A	278	GLN
1	A	365	GLN
1	A	454	ASN
1	A	514	HIS
1	A	531	GLN
1	A	549	ASN
4	D	41	GLN
4	D	86	GLN
4	D	110	ASN
5	E	45	HIS
5	E	83	HIS
5	E	137	HIS
5	E	238	HIS
5	E	247	ASN
5	E	267	GLN
5	E	420	HIS
5	E	487	ASN
6	F	580	HIS
6	F	601	GLN
6	F	623	GLN
7	H	108	ASN
8	G	55	ASN
8	G	208	ASN
8	G	252	ASN
8	G	281	GLN
8	G	448	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 ⓘ

28 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	1,9	14,14,15	0.25	0	17,19,21	0.44	0
9	NAG	I	2	9	14,14,15	0.25	0	17,19,21	0.46	0
10	NAG	J	1	1,10	14,14,15	0.45	0	17,19,21	0.57	0
10	NAG	J	2	10	14,14,15	0.27	0	17,19,21	0.65	0
10	BMA	J	3	10	11,11,12	0.67	0	15,15,17	0.72	0
10	MAN	J	4	10	11,11,12	0.63	0	15,15,17	1.20	2 (13%)
10	MAN	J	5	10	11,11,12	0.56	0	15,15,17	1.01	2 (13%)
10	MAN	J	6	10	11,11,12	0.66	0	15,15,17	0.84	1 (6%)
10	MAN	J	7	10	11,11,12	0.87	1 (9%)	15,15,17	1.23	2 (13%)
10	MAN	J	8	10	11,11,12	0.70	0	15,15,17	1.07	2 (13%)
11	NAG	K	1	5,11	14,14,15	0.31	0	17,19,21	0.41	0
11	NAG	K	2	11	14,14,15	0.30	0	17,19,21	0.41	0
11	BMA	K	3	11	11,11,12	0.45	0	15,15,17	0.82	0
11	MAN	K	4	11	11,11,12	0.56	0	15,15,17	1.01	2 (13%)
11	MAN	K	5	11	11,11,12	0.65	0	15,15,17	1.01	2 (13%)
11	MAN	K	6	11	11,11,12	0.62	0	15,15,17	0.90	1 (6%)
11	MAN	K	7	11	11,11,12	0.69	0	15,15,17	0.83	1 (6%)
12	NDG	N	1	12,16	14,14,15	0.60	0	17,19,21	1.22	3 (17%)
12	MAN	N	10	12	11,11,12	0.82	1 (9%)	15,15,17	1.10	2 (13%)
12	MAN	N	11	12	11,11,12	1.13	1 (9%)	15,15,17	1.67	3 (20%)
12	NAG	N	2	12	14,14,15	0.35	0	17,19,21	0.58	0
12	BMA	N	3	12	11,11,12	0.66	0	15,15,17	0.73	0
12	MAN	N	4	12	11,11,12	0.59	0	15,15,17	1.18	2 (13%)
12	MAN	N	5	12	11,11,12	0.57	0	15,15,17	1.08	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	MAN	N	6	12	11,11,12	0.58	0	15,15,17	0.99	2 (13%)
12	GLC	N	7	12	11,11,12	0.54	0	15,15,17	0.99	1 (6%)
12	GLC	N	8	12	11,11,12	0.58	0	15,15,17	0.85	0
12	GLC	N	9	12	11,11,12	0.57	0	15,15,17	0.83	1 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	I	1	1,9	-	4/6/23/26	0/1/1/1
9	NAG	I	2	9	-	2/6/23/26	0/1/1/1
10	NAG	J	1	1,10	-	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
10	MAN	J	4	10	-	2/2/19/22	0/1/1/1
10	MAN	J	5	10	-	0/2/19/22	0/1/1/1
10	MAN	J	6	10	-	0/2/19/22	0/1/1/1
10	MAN	J	7	10	-	0/2/19/22	1/1/1/1
10	MAN	J	8	10	-	2/2/19/22	1/1/1/1
11	NAG	K	1	5,11	-	0/6/23/26	0/1/1/1
11	NAG	K	2	11	-	2/6/23/26	0/1/1/1
11	BMA	K	3	11	-	0/2/19/22	0/1/1/1
11	MAN	K	4	11	-	2/2/19/22	0/1/1/1
11	MAN	K	5	11	-	1/2/19/22	0/1/1/1
11	MAN	K	6	11	-	0/2/19/22	0/1/1/1
11	MAN	K	7	11	-	0/2/19/22	0/1/1/1
12	NDG	N	1	12,16	-	2/6/23/26	0/1/1/1
12	MAN	N	10	12	-	0/2/19/22	0/1/1/1
12	MAN	N	11	12	-	2/2/19/22	0/1/1/1
12	NAG	N	2	12	-	2/6/23/26	0/1/1/1
12	BMA	N	3	12	-	0/2/19/22	0/1/1/1
12	MAN	N	4	12	-	2/2/19/22	0/1/1/1
12	MAN	N	5	12	-	2/2/19/22	0/1/1/1
12	MAN	N	6	12	-	2/2/19/22	0/1/1/1
12	GLC	N	7	12	-	2/2/19/22	0/1/1/1
12	GLC	N	8	12	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	GLC	N	9	12	-	0/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	N	11	MAN	C1-C2	3.02	1.59	1.52
12	N	10	MAN	C1-C2	2.28	1.57	1.52
10	J	7	MAN	C1-C2	2.23	1.57	1.52

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	N	11	MAN	C1-O5-C5	5.05	118.95	112.19
10	J	7	MAN	C1-O5-C5	3.34	116.67	112.19
10	J	8	MAN	C1-O5-C5	3.09	116.33	112.19
12	N	7	GLC	C1-O5-C5	3.06	116.29	112.19
12	N	5	MAN	O2-C2-C3	-2.95	104.03	110.15
12	N	4	MAN	O2-C2-C3	-2.92	104.10	110.15
10	J	4	MAN	O2-C2-C3	-2.89	104.16	110.15
10	J	4	MAN	C1-O5-C5	2.86	116.02	112.19
12	N	4	MAN	C1-O5-C5	2.82	115.97	112.19
10	J	5	MAN	O2-C2-C3	-2.71	104.53	110.15
10	J	7	MAN	O2-C2-C3	-2.70	104.56	110.15
11	K	4	MAN	C1-O5-C5	2.53	115.57	112.19
12	N	9	GLC	C1-O5-C5	2.51	115.55	112.19
12	N	1	NDG	C1-O5-C5	2.50	115.54	112.19
12	N	5	MAN	C1-O5-C5	2.40	115.40	112.19
11	K	5	MAN	C1-O5-C5	2.39	115.39	112.19
11	K	4	MAN	O2-C2-C3	-2.32	105.35	110.15
12	N	10	MAN	C1-O5-C5	2.27	115.23	112.19
12	N	6	MAN	O2-C2-C3	-2.26	105.46	110.15
11	K	6	MAN	O2-C2-C3	-2.24	105.52	110.15
12	N	6	MAN	C1-O5-C5	2.22	115.17	112.19
12	N	10	MAN	O2-C2-C3	-2.20	105.59	110.15
10	J	5	MAN	C1-O5-C5	2.19	115.12	112.19
12	N	1	NDG	C1-C2-N2	2.18	113.87	110.43
12	N	11	MAN	O2-C2-C3	-2.15	105.69	110.15
11	K	7	MAN	O2-C2-C3	-2.15	105.70	110.15
10	J	8	MAN	O2-C2-C3	-2.15	105.70	110.15
12	N	11	MAN	C1-C2-C3	2.14	112.75	109.64
10	J	6	MAN	O2-C2-C3	-2.10	105.79	110.15
11	K	5	MAN	O2-C2-C3	-2.09	105.82	110.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	N	1	NDG	O5-C5-C6	-2.03	103.71	107.66

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	K	2	NAG	O5-C5-C6-O6
12	N	2	NAG	O5-C5-C6-O6
12	N	1	NDG	O5-C5-C6-O6
10	J	2	NAG	O5-C5-C6-O6
10	J	4	MAN	O5-C5-C6-O6
11	K	2	NAG	C4-C5-C6-O6
12	N	2	NAG	C4-C5-C6-O6
10	J	8	MAN	O5-C5-C6-O6
10	J	4	MAN	C4-C5-C6-O6
9	I	2	NAG	O5-C5-C6-O6
12	N	5	MAN	O5-C5-C6-O6
9	I	2	NAG	C4-C5-C6-O6
12	N	1	NDG	C4-C5-C6-O6
12	N	4	MAN	O5-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
12	N	4	MAN	C4-C5-C6-O6
12	N	6	MAN	O5-C5-C6-O6
9	I	1	NAG	C4-C5-C6-O6
11	K	4	MAN	C4-C5-C6-O6
12	N	5	MAN	C4-C5-C6-O6
12	N	7	GLC	O5-C5-C6-O6
12	N	11	MAN	O5-C5-C6-O6
9	I	1	NAG	O5-C5-C6-O6
12	N	11	MAN	C4-C5-C6-O6
10	J	8	MAN	C4-C5-C6-O6
12	N	8	GLC	O5-C5-C6-O6
10	J	3	BMA	C4-C5-C6-O6
11	K	4	MAN	O5-C5-C6-O6
10	J	1	NAG	C4-C5-C6-O6
10	J	3	BMA	O5-C5-C6-O6
10	J	1	NAG	O5-C5-C6-O6
12	N	6	MAN	C4-C5-C6-O6
12	N	7	GLC	C4-C5-C6-O6
11	K	5	MAN	C4-C5-C6-O6

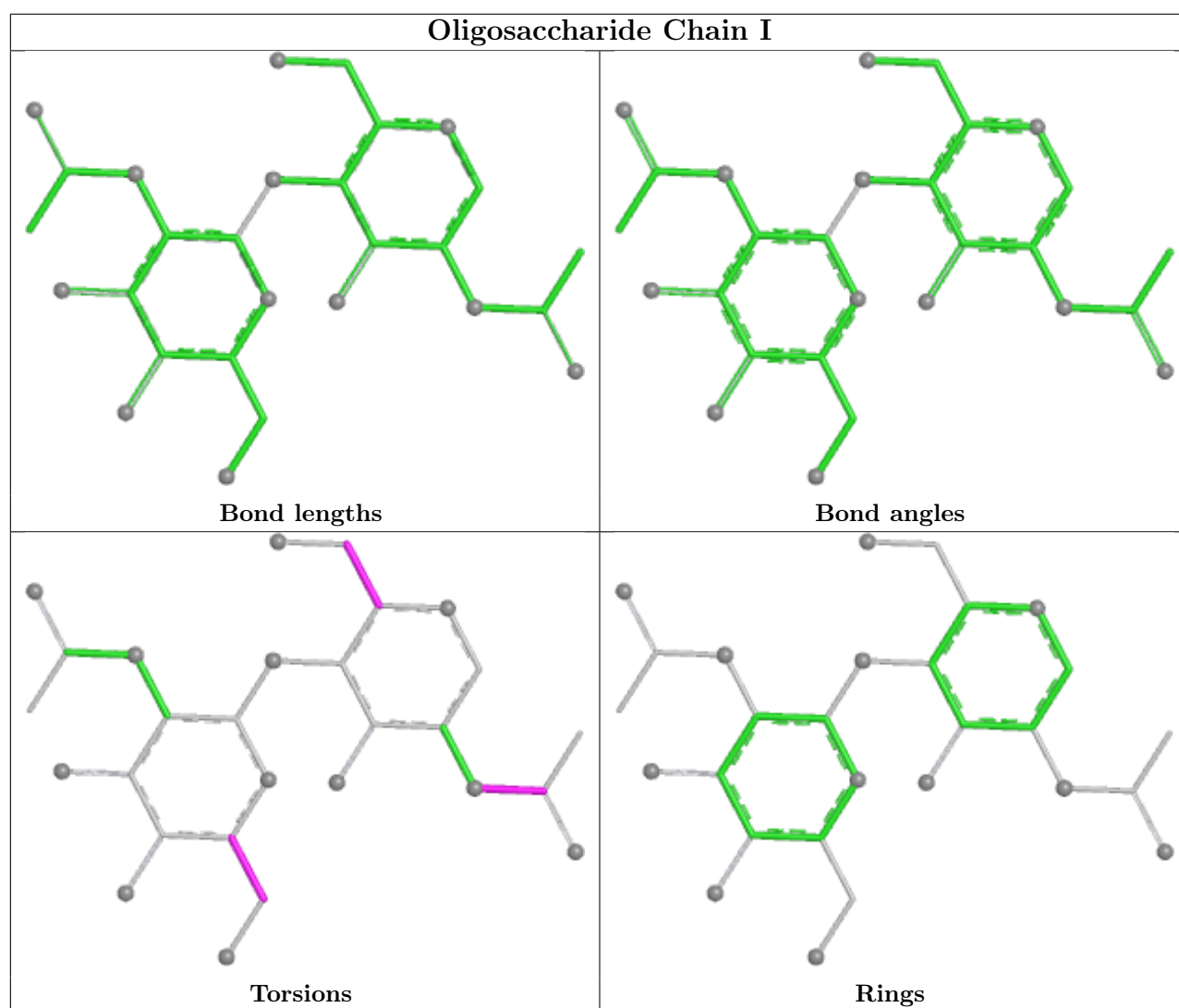
All (2) ring outliers are listed below:

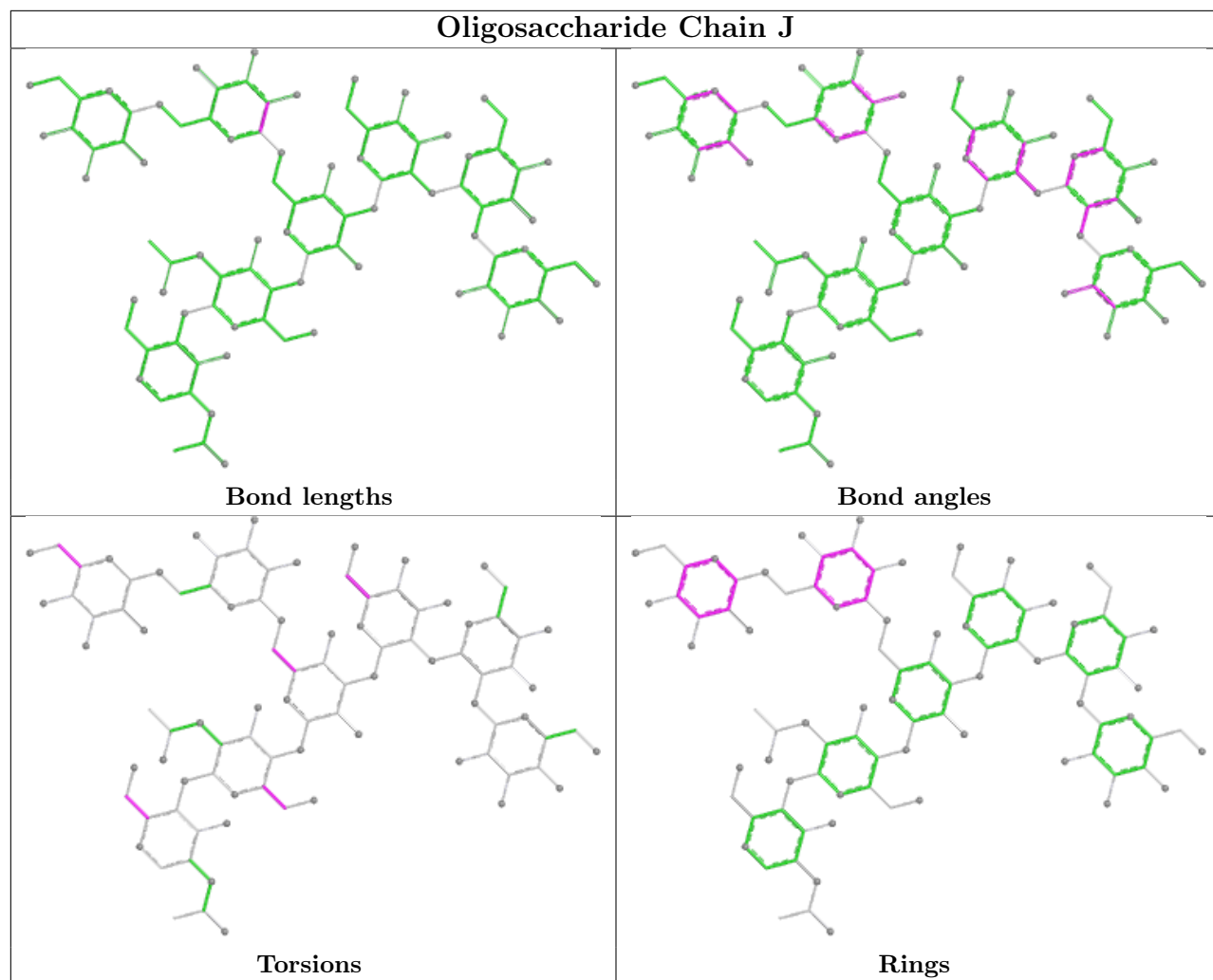
Mol	Chain	Res	Type	Atoms
10	J	8	MAN	C1-C2-C3-C4-C5-O5
10	J	7	MAN	C1-C2-C3-C4-C5-O5

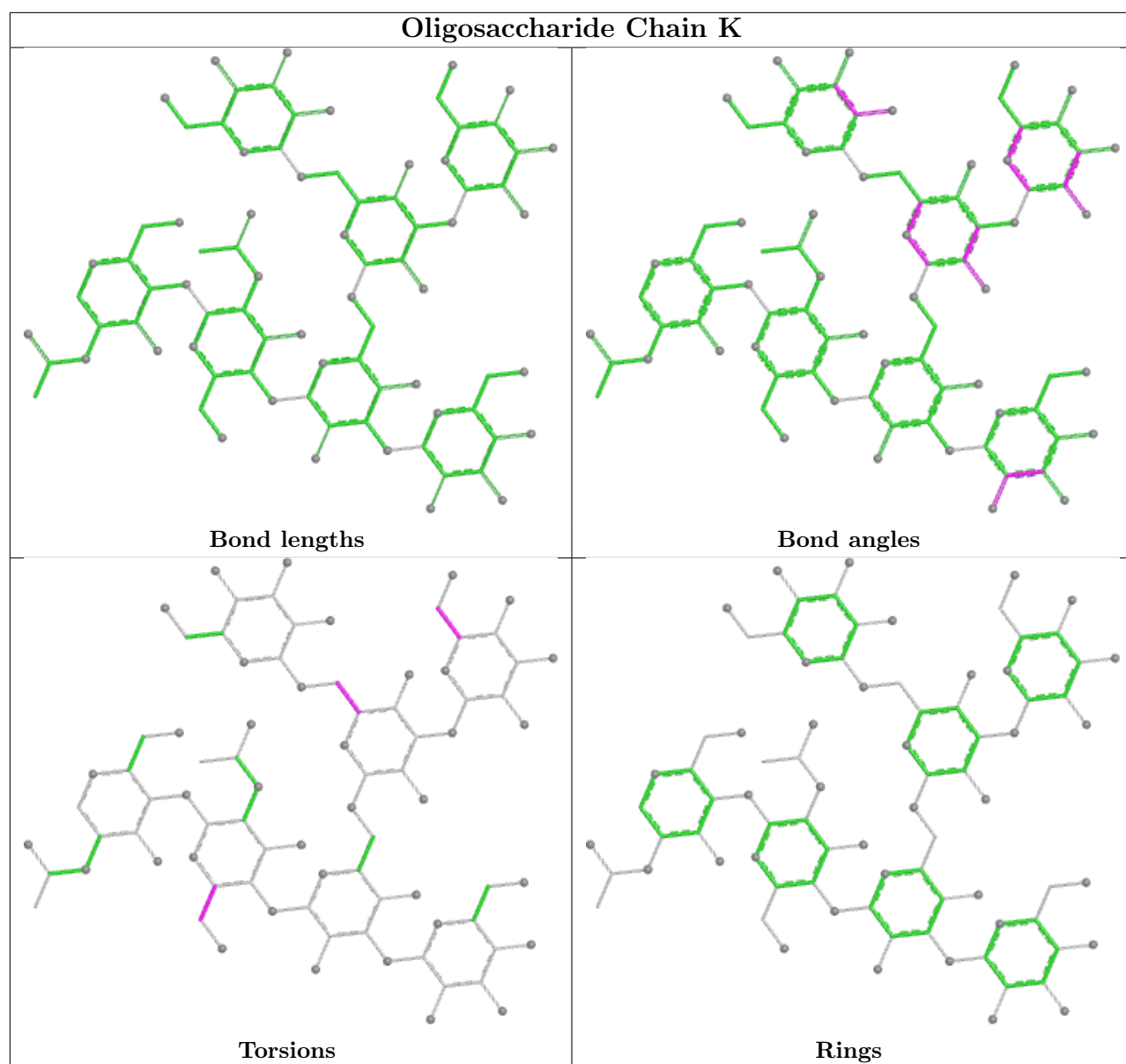
3 monomers are involved in 4 short contacts:

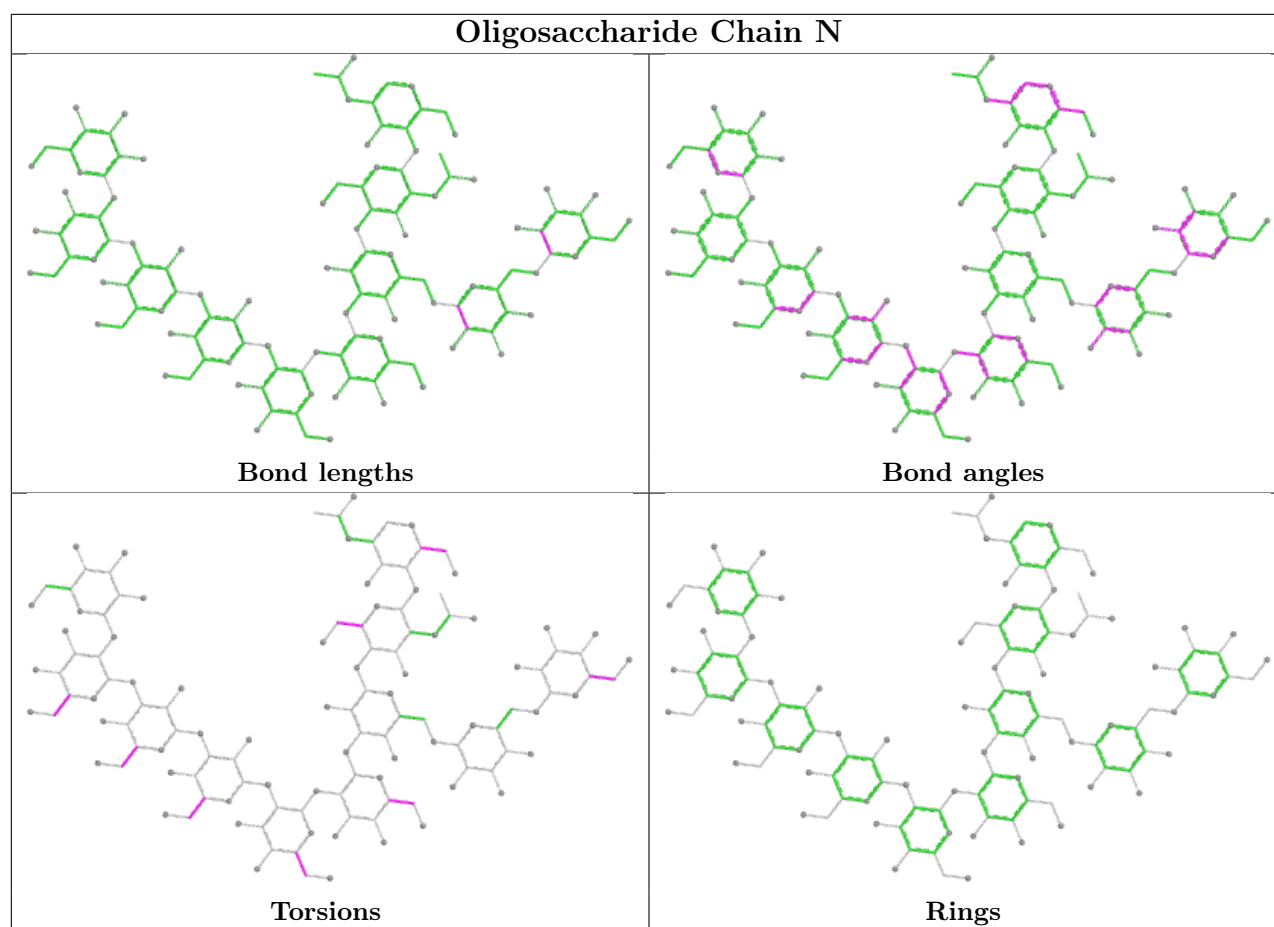
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	N	1	NDG	1	0
11	K	2	NAG	2	0
10	J	1	NAG	1	0

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 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 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	KZB	A	801	-	37,37,49	0.69	1 (2%)	58,62,80	2.04	15 (25%)
14	EGY	A	803	-	42,42,42	1.07	3 (7%)	48,50,50	1.14	2 (4%)
16	OTP	A	805	12	47,48,48	2.28	13 (27%)	57,61,61	2.39	20 (35%)
13	KZB	F	701	-	37,37,49	0.74	1 (2%)	58,62,80	1.92	11 (18%)
13	KZB	A	802	-	37,37,49	0.78	1 (2%)	58,62,80	2.02	12 (20%)
17	ZXT	A	806	-	28,28,28	3.57	15 (53%)	41,41,41	3.35	12 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	EGY	F	702	-	42,42,42	1.09	4 (9%)	48,50,50	1.19	2 (4%)
13	KZB	G	501	-	37,37,49	0.77	1 (2%)	58,62,80	1.92	14 (24%)

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	KZB	A	801	-	-	-	0/6/6/7
14	EGY	A	803	-	-	26/46/46/46	-
16	OTP	A	805	12	-	14/55/55/55	-
13	KZB	F	701	-	-	-	0/6/6/7
13	KZB	A	802	-	-	-	0/6/6/7
17	ZXT	A	806	-	-	9/24/31/31	0/3/3/3
14	EGY	F	702	-	-	22/46/46/46	-
13	KZB	G	501	-	-	-	0/6/6/7

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	A	805	OTP	C39-C37	9.16	1.54	1.33
17	A	806	ZXT	C05-S06	-8.53	1.59	1.73
17	A	806	ZXT	O18-S16	6.96	1.50	1.43
17	A	806	ZXT	C08-N07	6.70	1.49	1.37
16	A	805	OTP	P1-O4	6.08	1.66	1.59
17	A	806	ZXT	C05-N07	5.70	1.46	1.38
17	A	806	ZXT	C05-N04	5.22	1.39	1.31
17	A	806	ZXT	C03-N04	4.89	1.46	1.37
17	A	806	ZXT	C02-S06	-4.80	1.60	1.72
17	A	806	ZXT	S16-N19	4.20	1.75	1.62
17	A	806	ZXT	C03-C02	3.52	1.40	1.34
17	A	806	ZXT	C13-C14	3.29	1.44	1.38
16	A	805	OTP	P2-O7	3.03	1.66	1.54
17	A	806	ZXT	C10-C11	2.94	1.45	1.41
14	F	702	EGY	O21-C2	-2.91	1.39	1.46
17	A	806	ZXT	C14-S16	2.90	1.80	1.76
14	A	803	EGY	O21-C2	-2.76	1.40	1.46
14	A	803	EGY	O31-C3	-2.53	1.39	1.45
16	A	805	OTP	C11-C12	2.41	1.56	1.51
16	A	805	OTP	C26-C27	2.36	1.56	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	A	805	OTP	C21-C22	2.35	1.56	1.51
14	F	702	EGY	O31-C31	2.35	1.40	1.33
17	A	806	ZXT	C10-C08	2.22	1.54	1.50
16	A	805	OTP	C16-C17	2.22	1.55	1.51
16	A	805	OTP	P2-O6	-2.21	1.46	1.54
14	A	803	EGY	O31-C31	2.21	1.39	1.33
13	G	501	KZB	C84-C03	-2.20	1.51	1.56
17	A	806	ZXT	O17-S16	-2.19	1.41	1.43
13	A	802	KZB	C84-C03	-2.18	1.52	1.56
16	A	805	OTP	C29-C27	2.17	1.38	1.33
14	F	702	EGY	O31-C3	-2.16	1.40	1.45
17	A	806	ZXT	C20-N19	2.16	1.50	1.47
13	F	701	KZB	C84-C03	-2.15	1.52	1.56
16	A	805	OTP	P1-O3	-2.08	1.45	1.55
16	A	805	OTP	C35-C34	2.08	1.56	1.50
14	F	702	EGY	C12-N	-2.06	1.45	1.51
16	A	805	OTP	C24-C22	2.04	1.37	1.33
13	A	801	KZB	C84-C03	-2.02	1.52	1.56
16	A	805	OTP	P1-O1	2.01	1.67	1.59

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	806	ZXT	C02-S06-C05	13.54	99.29	89.32
13	A	802	KZB	O05-C04-C13	9.44	129.30	110.20
17	A	806	ZXT	C05-N07-C08	-9.31	108.25	123.67
16	A	805	OTP	C40-C39-C37	-9.04	111.39	126.20
13	F	701	KZB	O05-C04-C13	8.71	127.83	110.20
13	G	501	KZB	O05-C04-C13	8.62	127.64	110.20
13	A	801	KZB	O05-C04-C13	8.24	126.88	110.20
17	A	806	ZXT	C02-C03-N04	-6.84	110.06	117.12
16	A	805	OTP	C38-C37-C39	-5.64	109.13	123.63
16	A	805	OTP	C36-C37-C39	-5.14	109.62	121.17
13	A	801	KZB	C79-C81-C16	-5.06	107.30	112.43
17	A	806	ZXT	S06-C05-N04	-4.99	110.12	115.58
13	A	802	KZB	C19-C20-C21	-4.95	108.52	114.40
13	F	701	KZB	C19-C20-C21	-4.64	108.89	114.40
14	A	803	EGY	O21-C21-C22	4.49	121.20	111.48
13	A	801	KZB	C17-C16-C81	-4.48	105.15	110.52
14	F	702	EGY	O21-C21-C22	4.44	121.09	111.48
17	A	806	ZXT	C26-N22-C11	-4.17	109.32	121.51
13	A	801	KZB	C19-C20-C21	-3.94	109.72	114.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	805	OTP	C20-C19-C17	-3.88	118.74	127.62
16	A	805	OTP	C35-C34-C32	-3.79	118.94	127.62
17	A	806	ZXT	C23-N22-C11	-3.76	110.52	121.51
13	G	501	KZB	C82-C81-C79	-3.73	109.71	113.91
16	A	805	OTP	C25-C24-C22	-3.68	119.20	127.62
13	F	701	KZB	C17-C16-C81	-3.65	106.15	110.52
17	A	806	ZXT	C20-N19-S16	-3.63	108.47	116.53
16	A	805	OTP	C10-C9-C7	-3.58	119.44	127.62
17	A	806	ZXT	C01-C02-C03	-3.52	125.70	129.10
13	G	501	KZB	C19-C20-C21	-3.47	110.27	114.40
13	G	501	KZB	C17-C16-C81	-3.47	106.36	110.52
13	F	701	KZB	O12-C11-C09	-3.45	107.74	112.17
13	A	801	KZB	C84-C03-C02	3.41	130.57	120.50
17	A	806	ZXT	C21-N19-S16	-3.40	109.00	116.53
13	G	501	KZB	C84-C03-C02	3.40	130.53	120.50
13	A	802	KZB	C84-C03-C02	3.38	130.49	120.50
13	A	802	KZB	C20-C19-C79	-3.35	109.09	112.66
16	A	805	OTP	C38-C37-C36	-3.33	109.44	115.23
16	A	805	OTP	C30-C29-C27	-3.32	120.02	127.62
13	G	501	KZB	C02-C03-C04	-3.28	99.00	104.28
13	A	801	KZB	C82-C81-C79	-3.27	110.22	113.91
13	F	701	KZB	C84-C03-C02	3.23	130.04	120.50
13	A	802	KZB	C78-C79-C19	3.17	110.25	107.23
17	A	806	ZXT	C21-N19-C20	-3.14	108.52	114.75
13	A	801	KZB	C18-C17-C16	-3.11	107.19	112.16
14	F	702	EGY	O31-C31-C32	3.10	121.30	111.83
16	A	805	OTP	C18-C17-C16	3.06	120.54	115.23
16	A	805	OTP	C33-C32-C31	3.03	120.48	115.23
13	G	501	KZB	C06-C02-C03	-3.02	98.92	103.37
16	A	805	OTP	C8-C7-C6	2.96	120.37	115.23
13	A	801	KZB	C84-C15-C16	-2.94	109.80	113.90
13	F	701	KZB	C78-C79-C19	2.94	110.04	107.23
13	A	801	KZB	C02-C03-C04	-2.92	99.59	104.28
16	A	805	OTP	C15-C14-C12	-2.91	120.96	127.62
16	A	805	OTP	C23-C22-C21	2.89	120.25	115.23
13	A	802	KZB	C08-C07-C06	-2.85	107.47	111.93
13	G	501	KZB	C79-C81-C16	-2.84	109.54	112.43
13	F	701	KZB	C82-C83-C84	-2.83	107.97	112.74
13	A	802	KZB	C78-C76-C21	2.76	114.48	111.40
13	A	802	KZB	C82-C81-C79	-2.69	110.88	113.91
14	A	803	EGY	O31-C31-C32	2.67	119.98	111.83
16	A	805	OTP	O6-P2-O5	-2.62	100.63	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	805	OTP	C28-C27-C26	2.61	119.75	115.23
13	G	501	KZB	C79-C78-C76	-2.58	109.92	114.17
13	A	802	KZB	C07-C06-C02	-2.57	111.00	115.66
13	F	701	KZB	C82-C81-C79	-2.57	111.01	113.91
16	A	805	OTP	C13-C12-C11	2.56	119.67	115.23
13	G	501	KZB	C07-C06-C02	-2.56	111.03	115.66
13	A	802	KZB	C84-C15-C16	-2.55	110.35	113.90
13	A	802	KZB	C20-C21-C76	2.51	113.48	110.38
13	A	801	KZB	C20-C19-C79	-2.50	110.00	112.66
17	A	806	ZXT	N07-C05-N04	2.44	125.81	121.19
13	A	801	KZB	O12-C11-C09	-2.42	109.06	112.17
13	A	801	KZB	C79-C78-C76	-2.42	110.19	114.17
13	G	501	KZB	C20-C19-C79	-2.39	110.12	112.66
13	F	701	KZB	O12-C06-C07	2.38	112.83	110.76
16	A	805	OTP	O3-P1-O2	-2.37	101.43	112.44
16	A	805	OTP	C1-C2-C3	2.32	119.93	114.59
17	A	806	ZXT	C10-C08-N07	2.28	119.68	115.39
13	A	801	KZB	C06-C02-C03	-2.28	100.01	103.37
13	F	701	KZB	C07-C06-C02	-2.26	111.57	115.66
13	A	802	KZB	C17-C18-C19	-2.25	107.48	111.84
13	F	701	KZB	C79-C81-C16	-2.16	110.23	112.43
13	A	801	KZB	C08-C07-C06	-2.12	108.61	111.93
13	G	501	KZB	C18-C17-C16	-2.06	108.88	112.16
13	G	501	KZB	C84-C15-C16	-2.04	111.05	113.90
13	A	801	KZB	C83-C84-C03	2.02	118.23	115.36
13	G	501	KZB	C82-C83-C84	-2.00	109.36	112.74
16	A	805	OTP	O6-P2-O4	2.00	111.35	104.64

There are no chirality outliers.

All (71) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	803	EGY	C11-O13-P-O12
14	A	803	EGY	C11-O13-P-O14
14	A	803	EGY	C11-O13-P-O11
14	A	803	EGY	C1-O11-P-O14
14	A	803	EGY	C1-O11-P-O13
14	A	803	EGY	O13-C11-C12-N
14	F	702	EGY	C1-O11-P-O12
14	F	702	EGY	C1-O11-P-O14
14	F	702	EGY	C1-O11-P-O13
14	F	702	EGY	O13-C11-C12-N

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Mol	Chain	Res	Type	Atoms
16	A	805	OTP	C19-C20-C21-C22
17	A	806	ZXT	N04-C05-N07-C08
17	A	806	ZXT	S06-C05-N07-C08
16	A	805	OTP	C5-C6-C7-C8
16	A	805	OTP	C35-C36-C37-C39
14	F	702	EGY	C22-C21-O21-C2
16	A	805	OTP	C30-C31-C32-C33
16	A	805	OTP	C30-C31-C32-C34
16	A	805	OTP	C5-C6-C7-C9
16	A	805	OTP	C9-C10-C11-C12
16	A	805	OTP	C4-C5-C6-C7
14	A	803	EGY	C37-C38-C39-C3A
14	A	803	EGY	C35-C36-C37-C38
14	A	803	EGY	C32-C31-O31-C3
14	A	803	EGY	C21-C22-C23-C24
14	F	702	EGY	O22-C21-O21-C2
16	A	805	OTP	C29-C30-C31-C32
16	A	805	OTP	C24-C25-C26-C27
16	A	805	OTP	C15-C16-C17-C18
17	A	806	ZXT	C20-N19-S16-O17
14	A	803	EGY	O32-C31-O31-C3
17	A	806	ZXT	C12-C11-N22-C26
17	A	806	ZXT	C12-C11-N22-C23
14	F	702	EGY	C27-C28-C29-C2A
14	A	803	EGY	C25-C26-C27-C28
14	A	803	EGY	C27-C28-C29-C2A
14	F	702	EGY	C23-C24-C25-C26
16	A	805	OTP	C15-C16-C17-C19
14	A	803	EGY	C26-C27-C28-C29
16	A	805	OTP	C35-C36-C37-C38
14	A	803	EGY	C2A-C2B-C2C-C2D
14	F	702	EGY	C1-C2-C3-O31
17	A	806	ZXT	C10-C11-N22-C26
17	A	806	ZXT	C10-C11-N22-C23
14	A	803	EGY	O11-C1-C2-O21
14	F	702	EGY	C32-C31-O31-C3
14	A	803	EGY	C38-C39-C3A-C3B
14	F	702	EGY	C36-C37-C38-C39
14	A	803	EGY	C23-C24-C25-C26
16	A	805	OTP	C38-C37-C39-C40
14	F	702	EGY	C25-C26-C27-C28
14	F	702	EGY	C37-C38-C39-C3A

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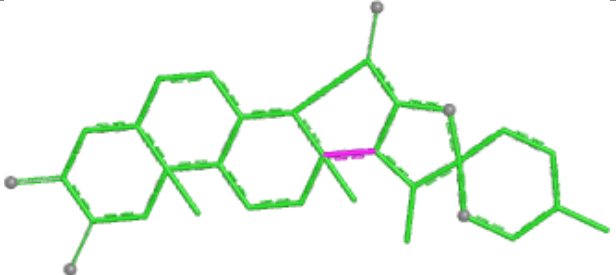
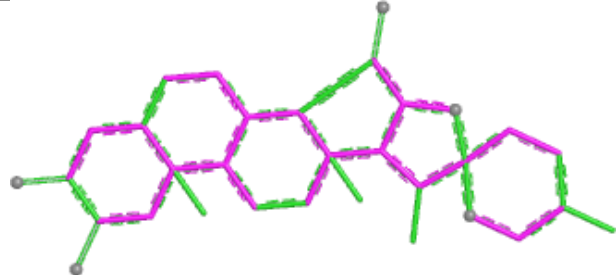
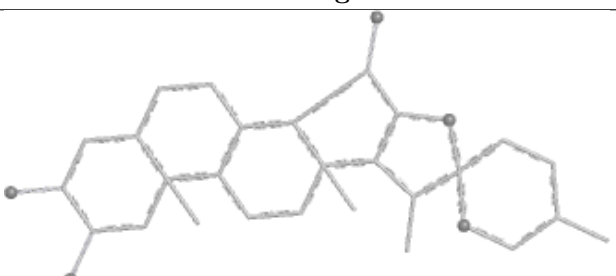
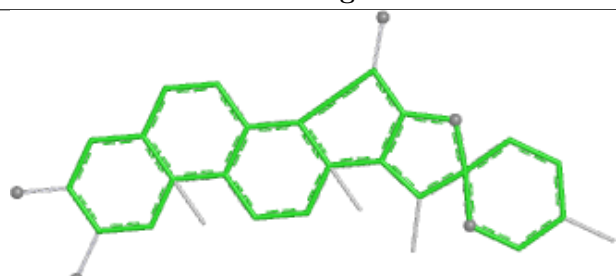
Mol	Chain	Res	Type	Atoms
14	F	702	EGY	O32-C31-O31-C3
14	A	803	EGY	C29-C2A-C2B-C2C
14	A	803	EGY	C22-C21-O21-C2
14	A	803	EGY	O11-C1-C2-C3
14	F	702	EGY	O11-C1-C2-C3
17	A	806	ZXT	C20-N19-S16-C14
14	A	803	EGY	O22-C21-O21-C2
14	F	702	EGY	O11-C1-C2-O21
14	F	702	EGY	O21-C2-C3-O31
14	F	702	EGY	C35-C36-C37-C38
14	F	702	EGY	C11-C12-N-C13
14	A	803	EGY	C28-C29-C2A-C2B
17	A	806	ZXT	C21-N19-S16-O18
14	F	702	EGY	C11-C12-N-C14
14	A	803	EGY	C33-C34-C35-C36
14	F	702	EGY	C11-C12-N-C15
14	A	803	EGY	C11-C12-N-C14
14	A	803	EGY	C11-C12-N-C13
14	F	702	EGY	C38-C39-C3A-C3B

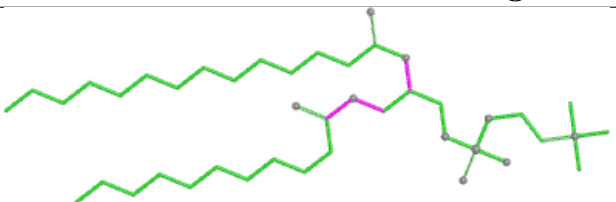
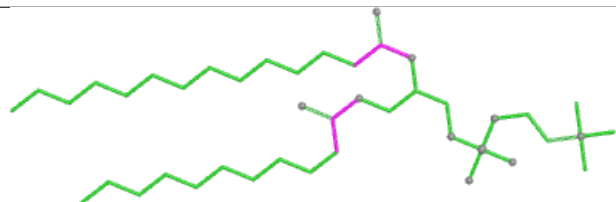
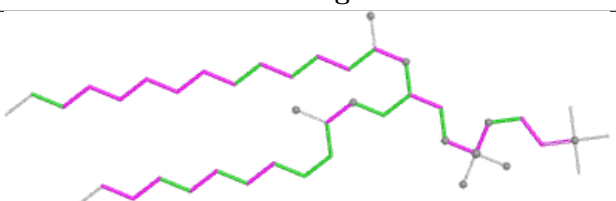
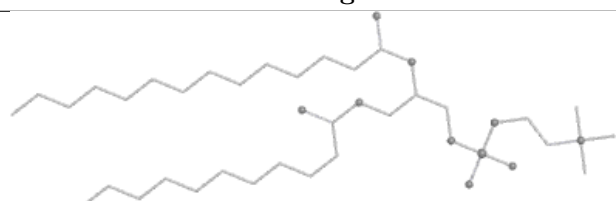
There are no ring outliers.

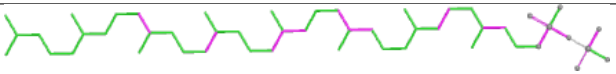
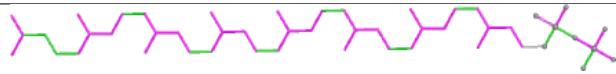
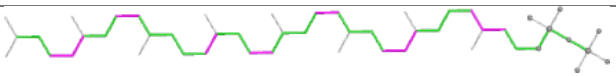
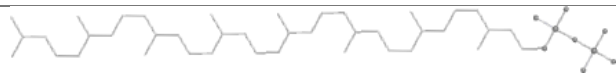
4 monomers are involved in 9 short contacts:

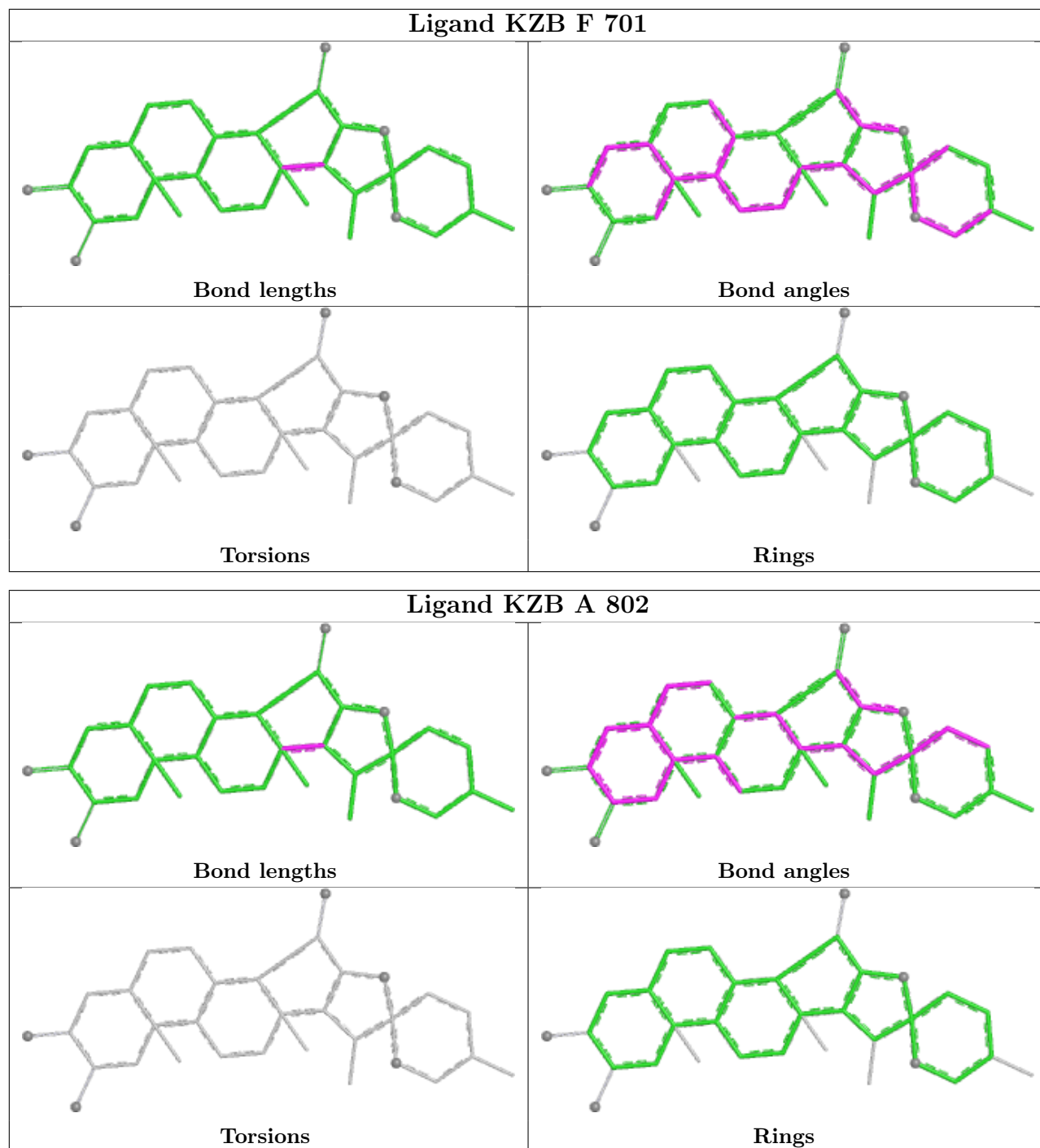
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	A	803	EGY	1	0
16	A	805	OTP	4	0
17	A	806	ZXT	1	0
14	F	702	EGY	3	0

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.

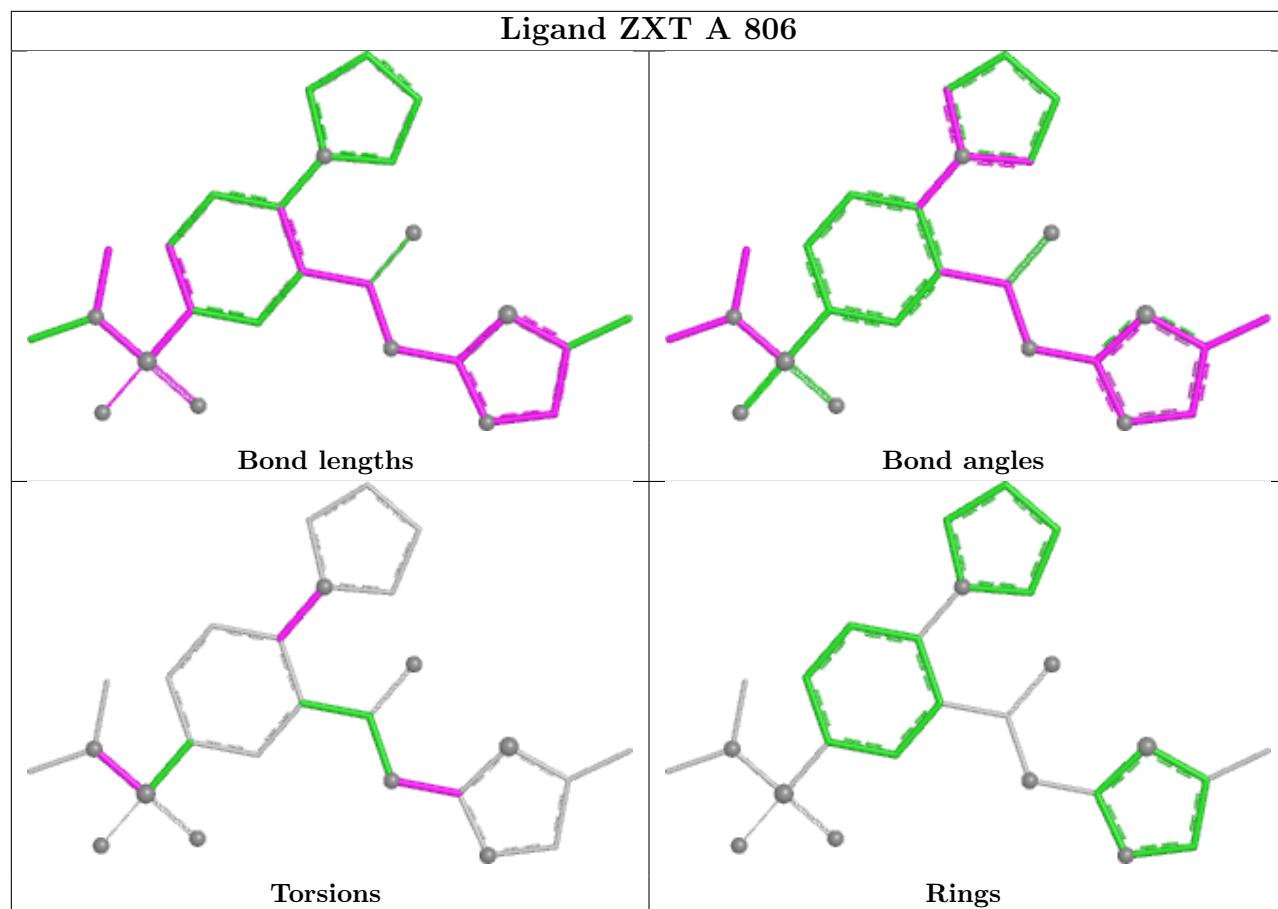
Ligand KZB A 801	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand EGY A 803	
	
Bond lengths	Bond angles
	
Torsions	Rings

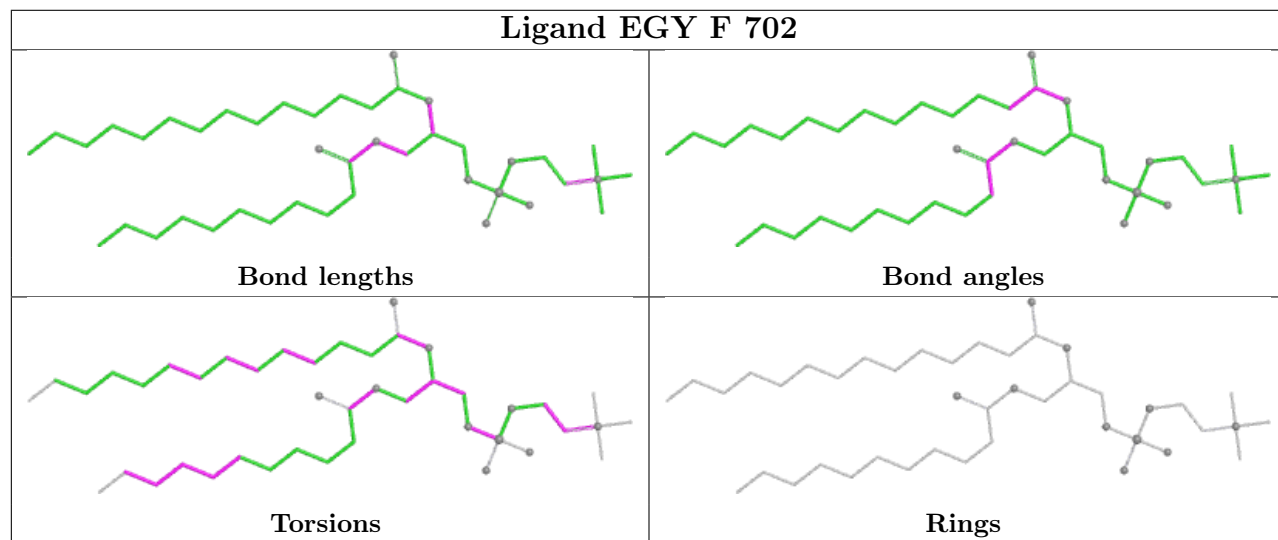
Ligand OTP A 805	
	
Bond lengths	Bond angles
	
Torsions	Rings

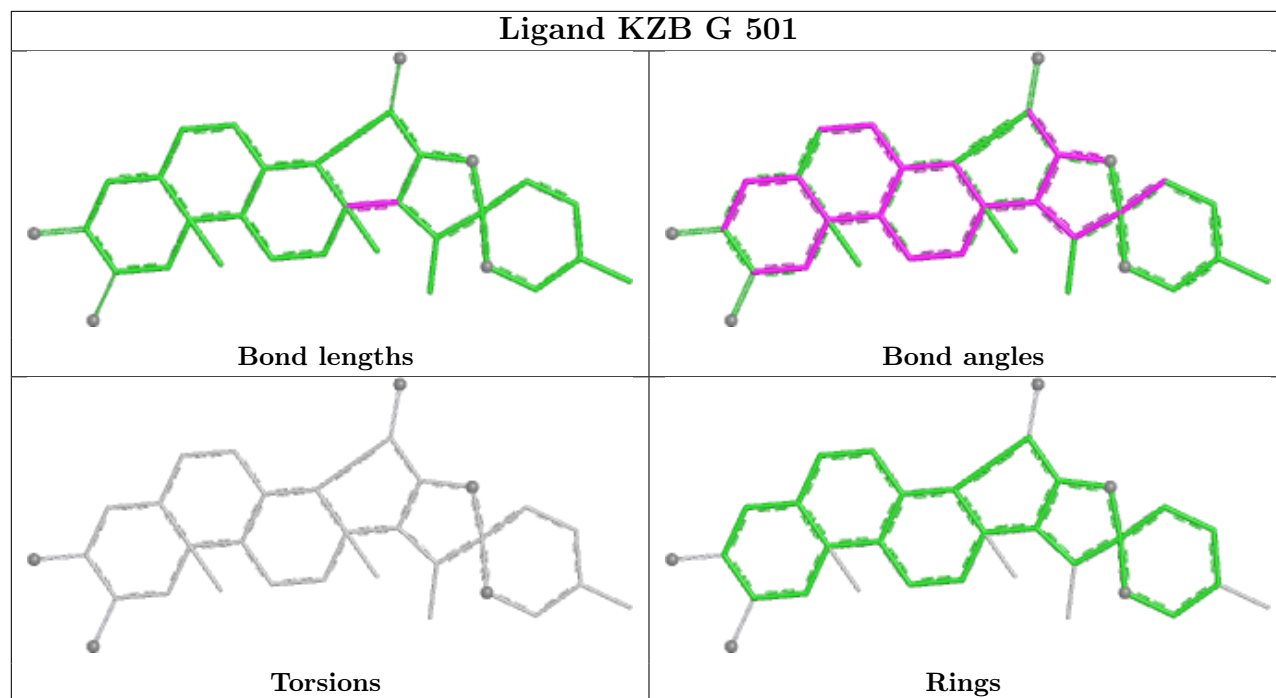


Ligand ZXT A 806



Ligand EGY F 702





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.

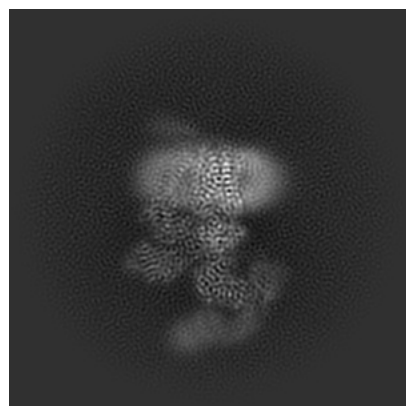
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17779. These allow visual inspection of the internal detail of the map and identification of artifacts.

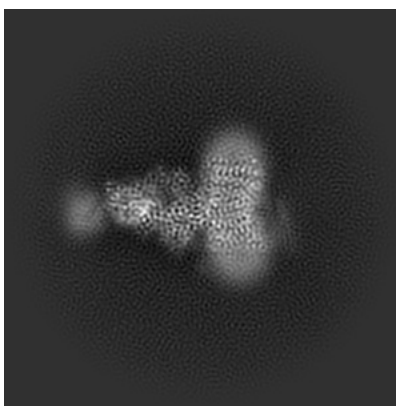
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

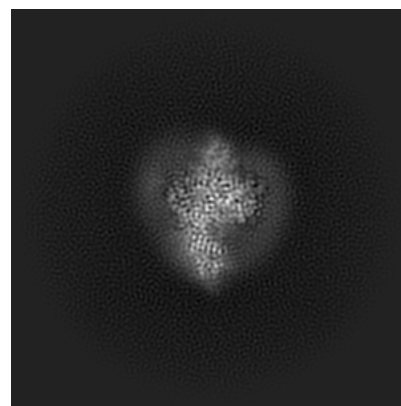
6.1.1 Primary map



X

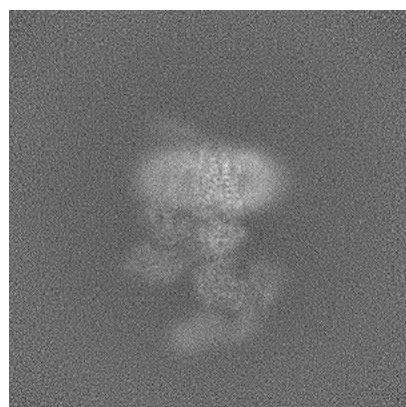


Y

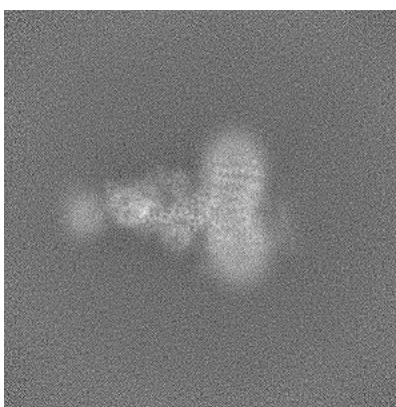


Z

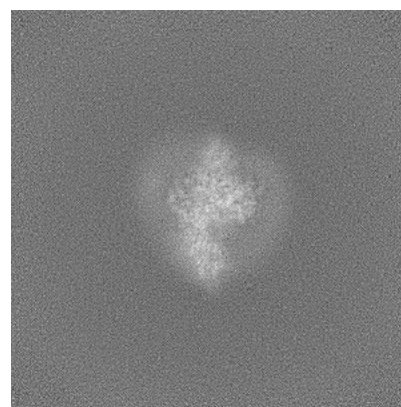
6.1.2 Raw map



X



Y

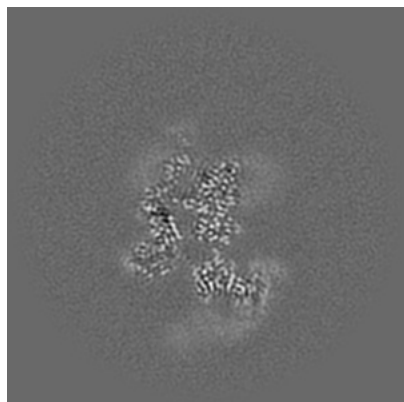


Z

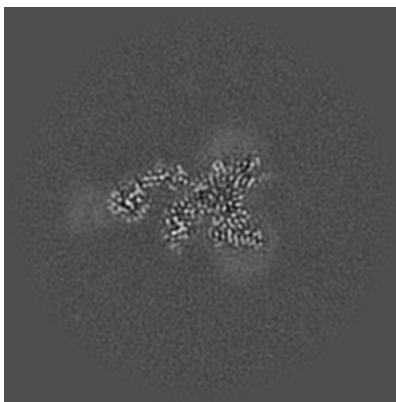
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

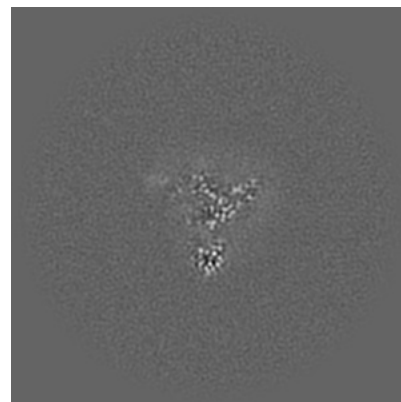
6.2.1 Primary map



X Index: 256

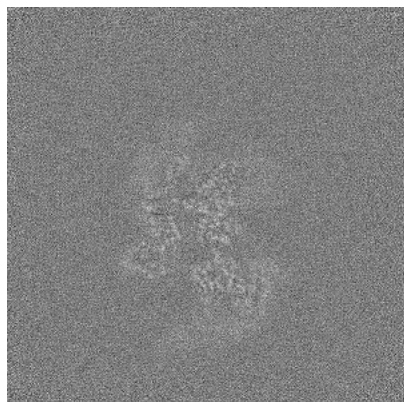


Y Index: 256

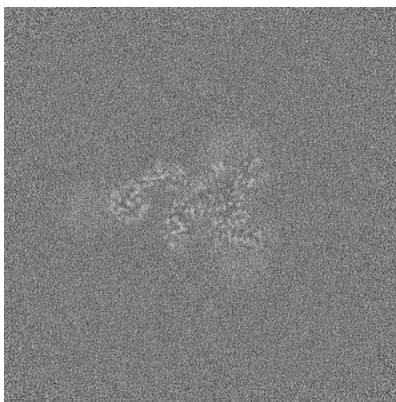


Z Index: 256

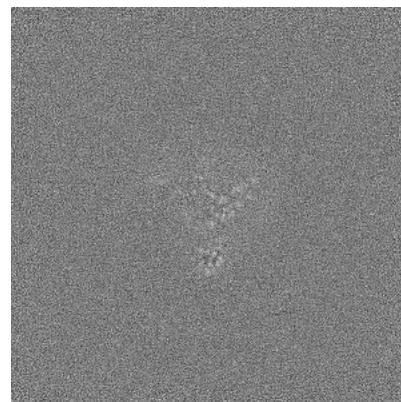
6.2.2 Raw map



X Index: 256



Y Index: 256

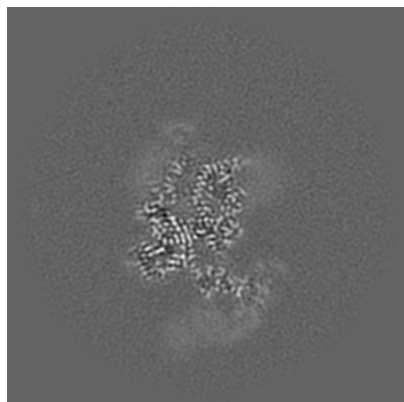


Z Index: 256

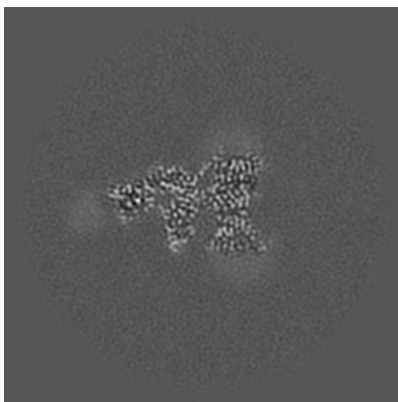
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

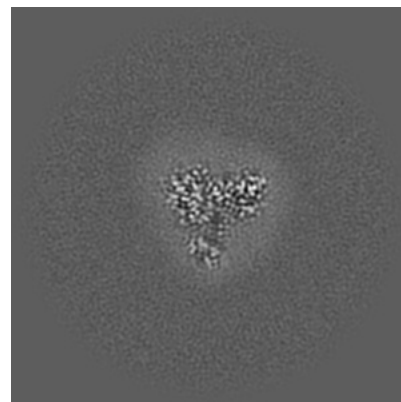
6.3.1 Primary map



X Index: 248

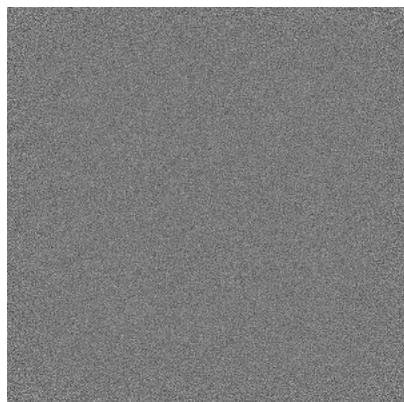


Y Index: 266

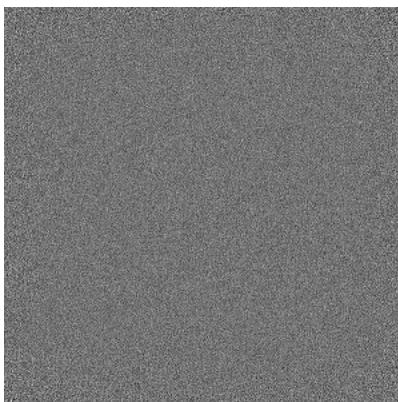


Z Index: 275

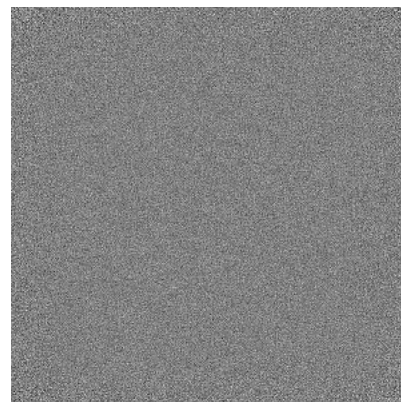
6.3.2 Raw map



X Index: 0



Y Index: 0

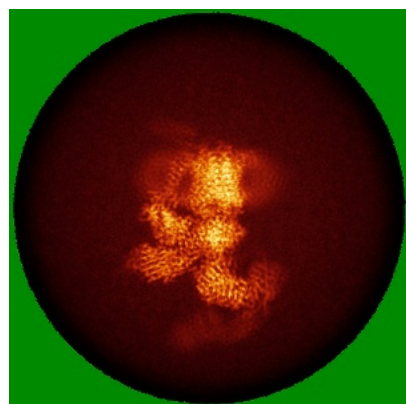


Z Index: 0

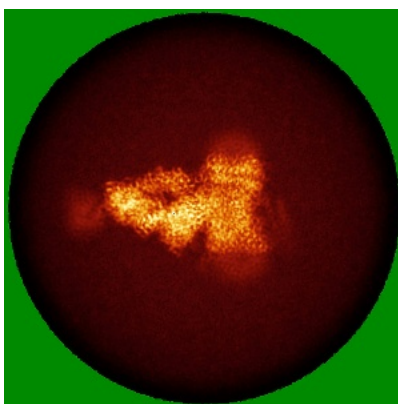
The images above show the largest variance slices of the map in three orthogonal directions.

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

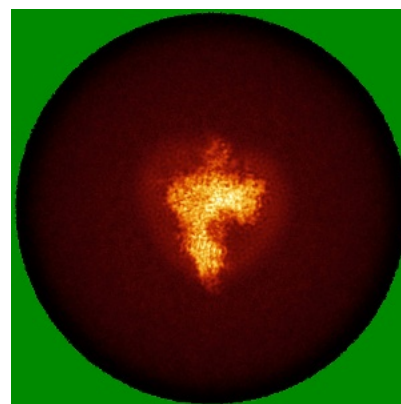
6.4.1 Primary map



X

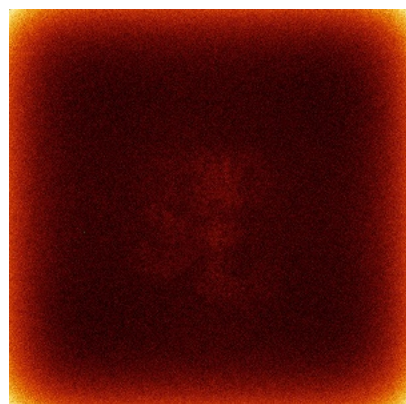


Y

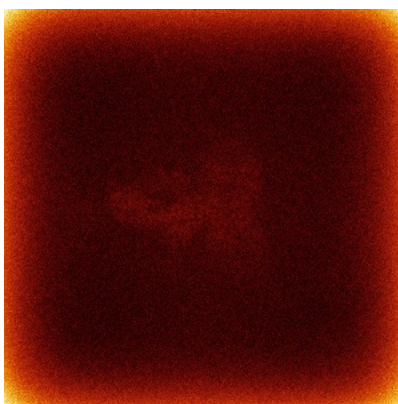


Z

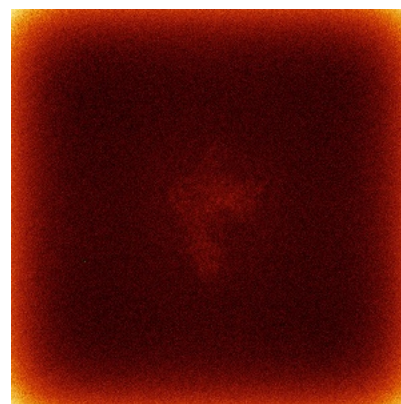
6.4.2 Raw map



X



Y

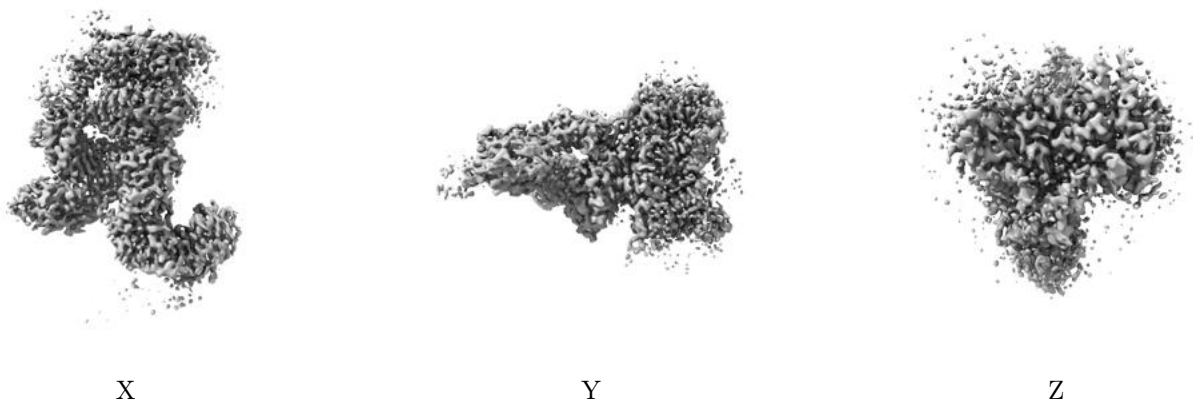


Z

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.

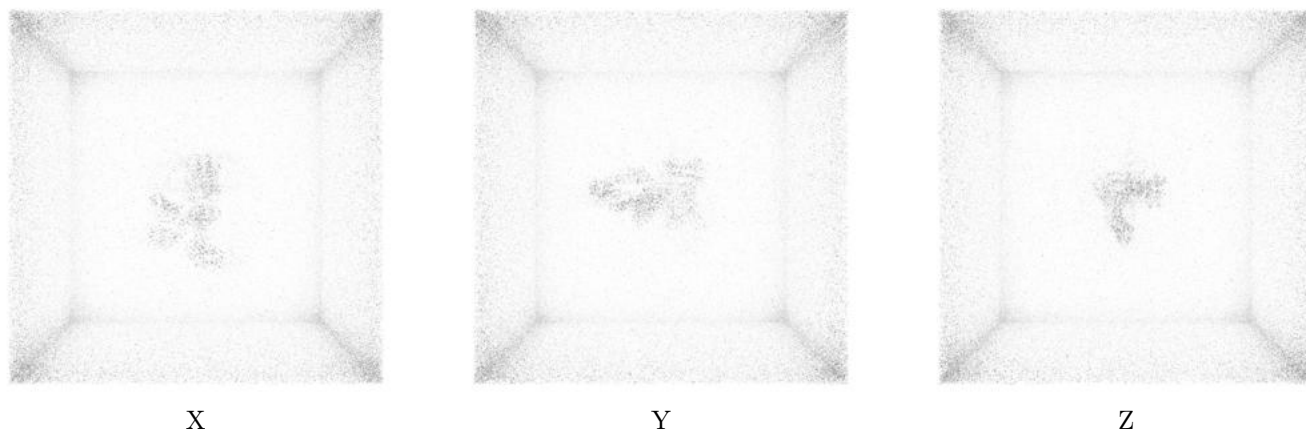
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0735. 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.

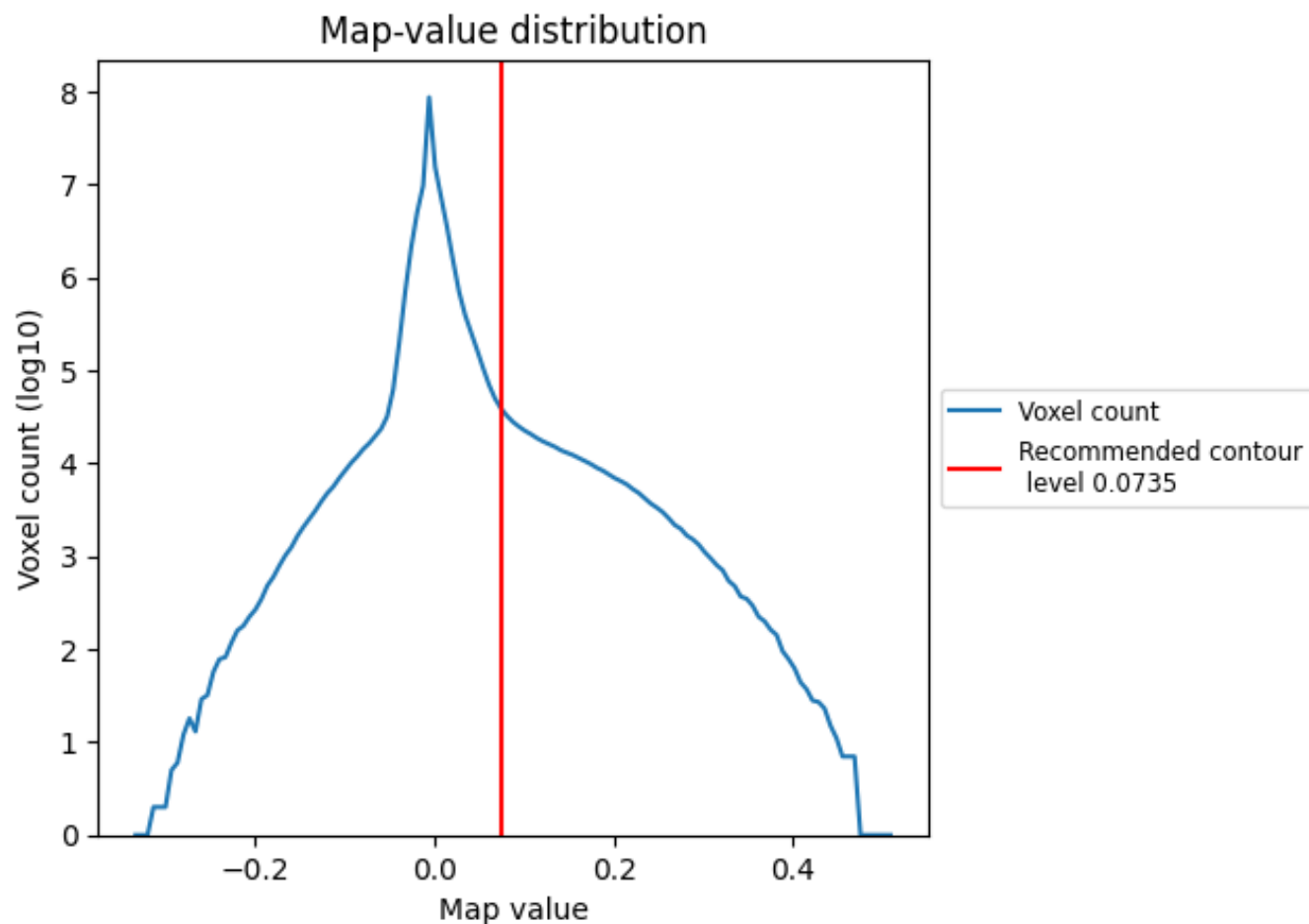
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

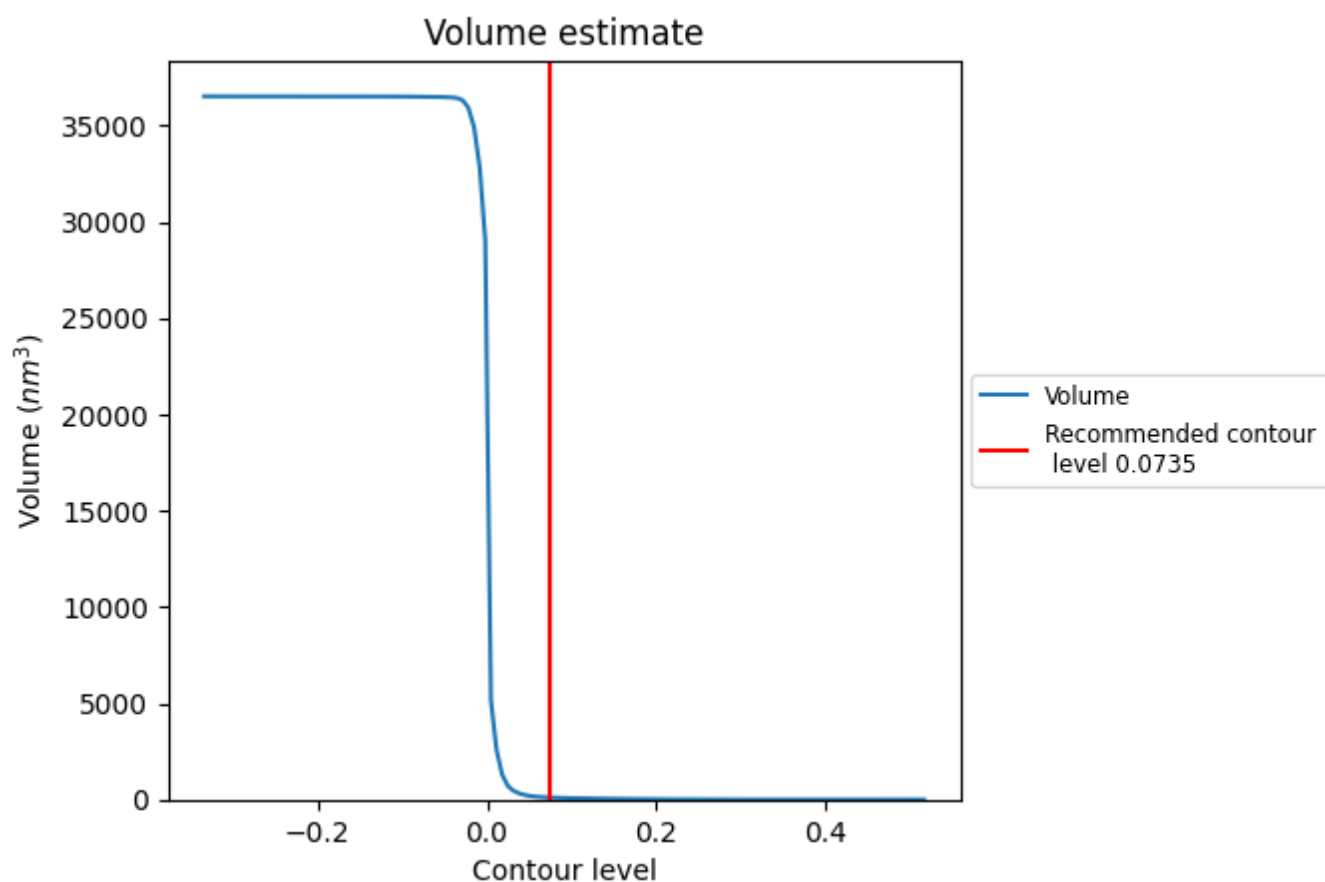
This section contains the results of statistical analysis of the map.

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.

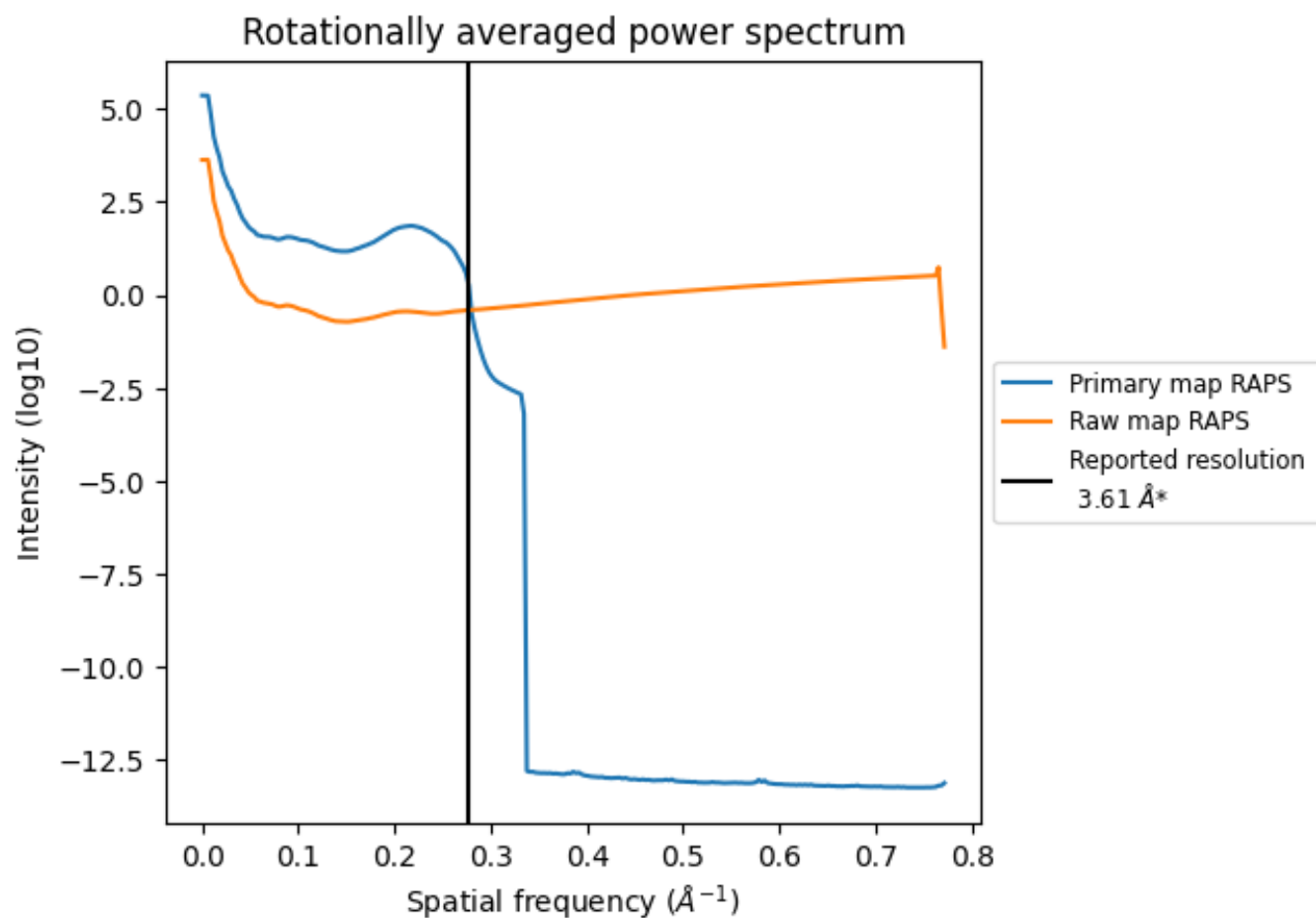
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 108 nm³; this corresponds to an approximate mass of 97 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 ⓘ

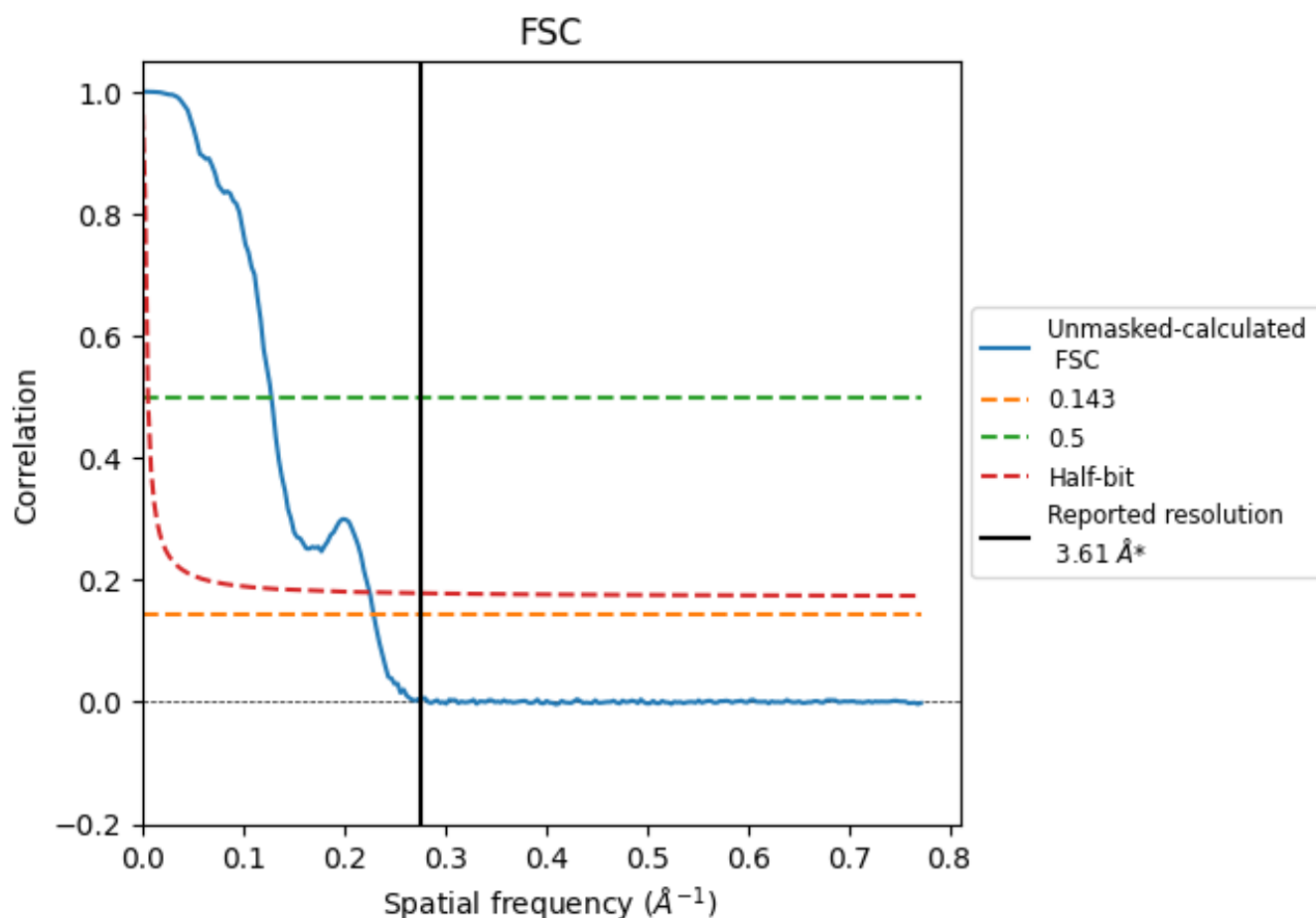


*Reported resolution corresponds to spatial frequency of 0.277 $\text{\AA}^{-1}$

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 $0.277 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

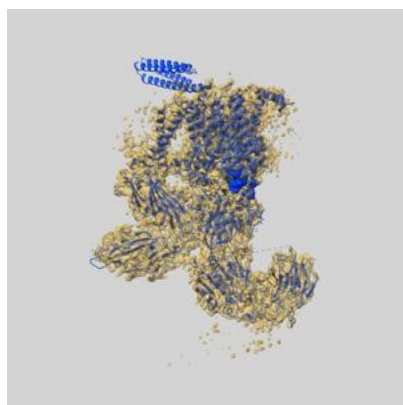
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.61	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.36	7.81	4.43

*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 4.36 differs from the reported value 3.61 by more than 10 %

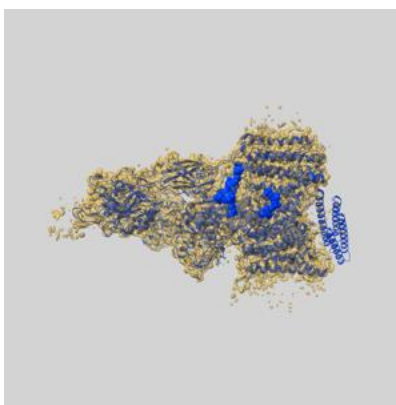
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-17779 and PDB model 8PN9. Per-residue inclusion information can be found in section [3](#) on page [10](#).

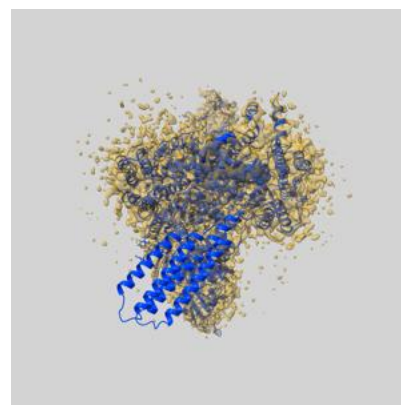
9.1 Map-model overlay [i](#)



X



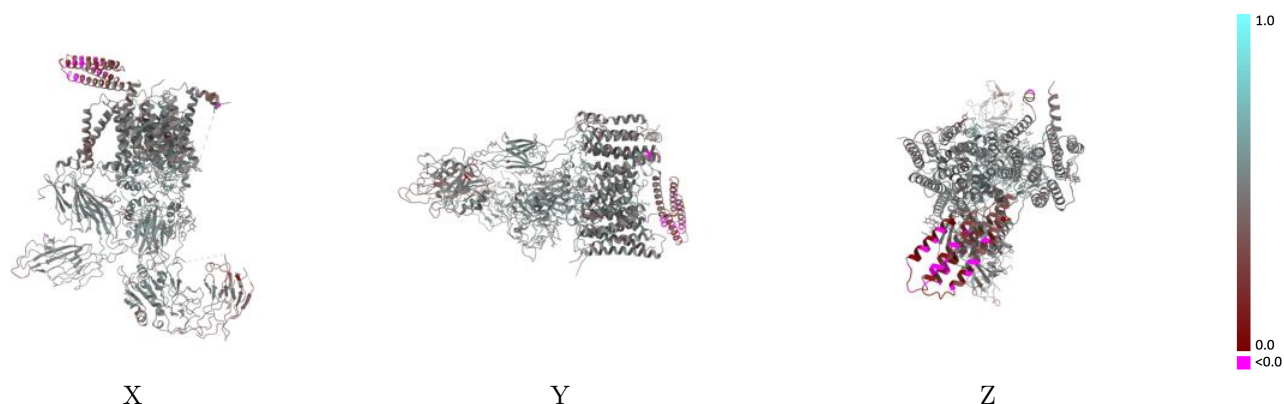
Y



Z

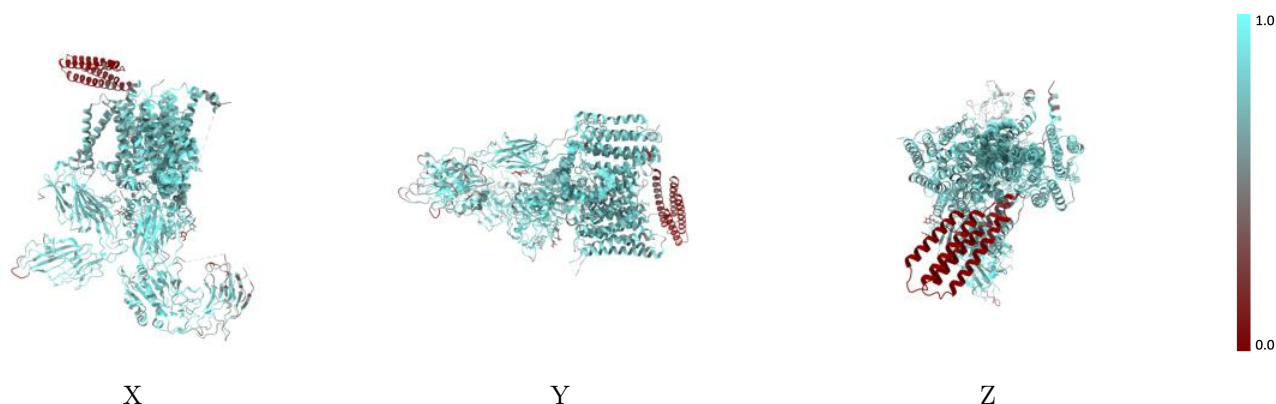
The images above show the 3D surface view of the map at the recommended contour level 0.0735 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



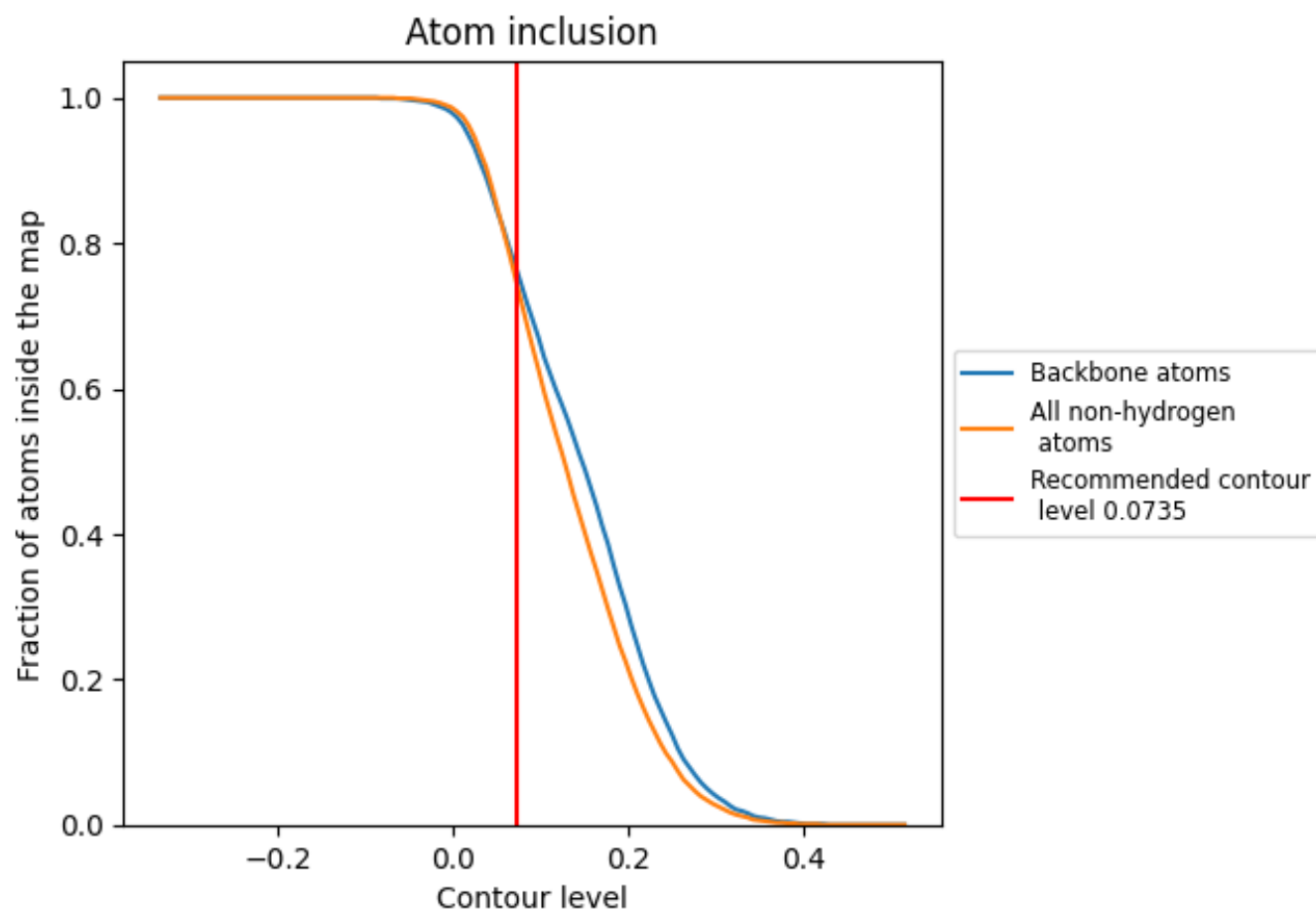
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0735).

9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 74% 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 (0.0735) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7410	0.4740
A	0.7980	0.5010
B	0.7620	0.4840
C	0.7290	0.4660
D	0.7870	0.4670
E	0.6640	0.4410
F	0.6820	0.4420
G	0.8000	0.4910
H	0.7400	0.4670
I	0.4290	0.3910
J	0.6060	0.4940
K	0.6260	0.4890
N	0.8030	0.5190

1.0

0.0

<0.0