



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 10:29 AM UTC

PDB ID : 9N2D / pdb_00009n2d
EMDB ID : EMD-48835
Title : Cryo-EM structure of an extended F. johnsoniae BAM complex, composite map
Authors : Deme, J.C.; Lea, S.M.
Deposited on : 2025-01-28
Resolution : 2.70 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:

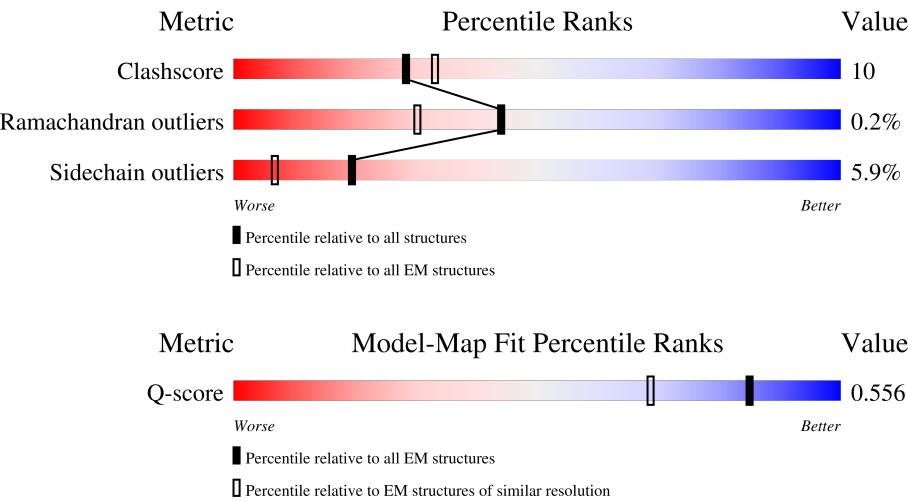
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.70 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	10327 (2.20 - 3.20)

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	F	264	5% 68% 22% • 8%
2	A	900	• 54% 14% • 31%
3	C	517	• 73% 23% •
4	B	409	75% 19% • 5%

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Mol	Chain	Length	Quality of chain
5	D	388	
6	E	249	
7	J	3	
8	G	2	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	GCU	J	2	X	-	-	-
7	MAN	J	3	X	-	-	-
8	GCU	G	2	X	-	-	-

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 18488 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 Bam D.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	F	244	Total	C	N	O	S	0	0
			1979	1276	317	381	5		

- Molecule 2 is a protein called Bam A.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	618	Total	C	N	O	S	1	0
			4936	3161	816	954	5		

- Molecule 3 is a protein called Bam H.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	517	Total	C	N	O	S	0	0
			4024	2537	660	820	7		

- Molecule 4 is a protein called Bam G.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	390	Total	C	N	O	S	0	0
			2995	1916	488	586	5		

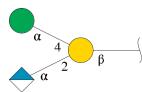
- Molecule 5 is a protein called Bam M.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	369	Total	C	N	O	S	0	0
			2947	1871	462	607	7		

- Molecule 6 is a protein called Bam P.

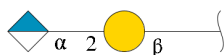
Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	146	Total	C	N	O	S	0	0
			1155	735	194	222	4		

- Molecule 7 is an oligosaccharide called alpha-D-glucopyranuronic acid-(1-2)-[alpha-D-mannopyranose-(1-4)]beta-D-galactopyranose.



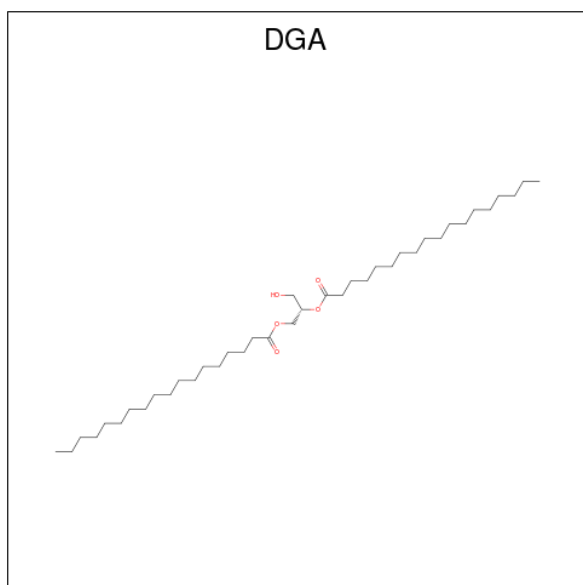
Mol	Chain	Residues	Atoms			AltConf	Trace
7	J	3	Total	C	O	0	0
			34	18	16		

- Molecule 8 is an oligosaccharide called alpha-D-glucopyranuronic acid-(1-2)-beta-D-galactopyranose.



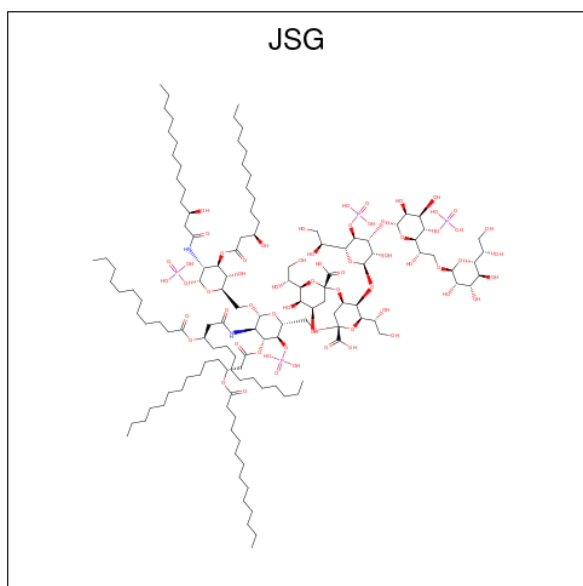
Mol	Chain	Residues	Atoms			AltConf	Trace
8	G	2	Total	C	O	0	0
			23	12	11		

- Molecule 9 is DIACYL GLYCEROL (CCD ID: DGA) (formula: C₃₉H₇₆O₅).



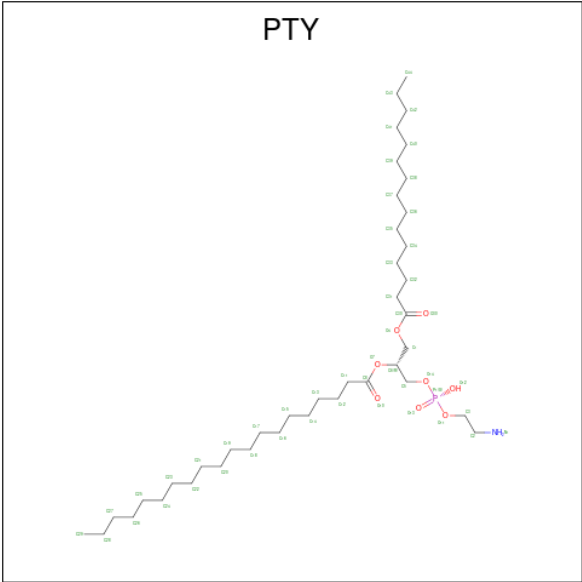
Mol	Chain	Residues	Atoms			AltConf
9	A	1	Total	C	O	0
			44	39	5	

- Molecule 10 is (2 {R},4 {R},5 {R},6 {R})-6-[(1 {R})-1,2-bis(oxidanyl)ethyl]-2-[(2 {R},4 {R},5 {R},6 {R})-6-[(1 {R})-1,2-bis(oxidanyl)ethyl]-5-[(2 {S},3 {S},4 {R},5 {R},6 {R})-6-[(1 {S})-1,2-bis(oxidanyl)ethyl]-4-[(2 {R},3 {S},4 {R},5 {S},6 {R})-6-[(1 {S})-2-[(2 {S},3 {S},4 {S},5 {S},6 {R})-6-[(1 {S})-1,2-bis(oxidanyl)ethyl]-3,4,5-tris(oxidanyl)oxan-2-yl]oxy-1-oxidanyl-ethyl]-3,4-bis(oxidanyl)-5-phosphonoxy-oxan-2-yl]oxy-3-oxidanyl-5-phosphonoxy-oxan-2-yl]oxy-2-carboxy-2-[(2 {R},3 {S},4 {R},5 {R},6 {R})-5-[(3 {R})-3-dodecanoyloxytetradecanoyl]amino]-6-[(2 {R},3 {S},4 {R},5 {R},6 {R})-3-oxidanyl-5-[(3 {R})-3-oxidanyltetradecanoyl]amino]-4-[(3 {R})-3-oxidanyltetradecanoyl]oxy-6-phosphonoxy-oxan-2-yl]methoxy]-3-phosphonoxy-4-[(3 {R})-3-tetradecanoyloxytetradecanoyl]oxy-oxan-2-yl]methoxy]oxan-4-yl]oxy-4,5-bis(oxidanyl)oxane-2-carboxylic acid (CCD ID: JSG) (formula: $C_{131}H_{240}N_2O_{63}P_4$).



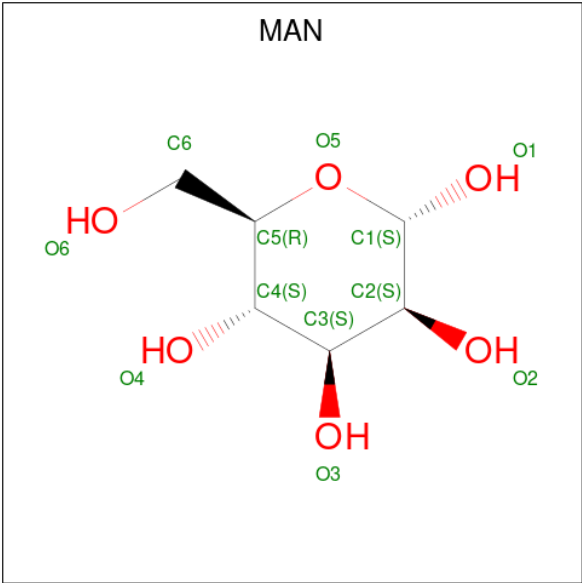
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
10	A	1	200	131	2	63	4	0

- Molecule 11 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula: $C_{40}H_{80}NO_8P$).



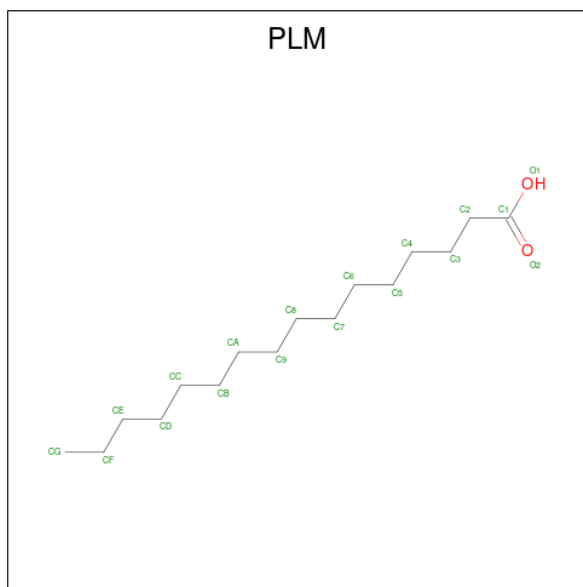
Mol	Chain	Residues	Atoms					AltConf
11	A	1	Total	C	N	O	P	0
			50	40	1	8	1	
11	A	1	Total	C	N	O	P	0
			50	40	1	8	1	

- Molecule 12 is alpha-D-mannopyranose (CCD ID: MAN) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			AltConf
12	C	1	Total	C	O	0
			11	6	5	

- Molecule 13 is PALMITIC ACID (CCD ID: PLM) (formula: C₁₆H₃₂O₂).



Mol	Chain	Residues	Atoms			AltConf
13	C	1	Total	C	O	0
			17	16	1	

- Molecule 14 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
14	D	7	Total	Ca	0
			7	7	

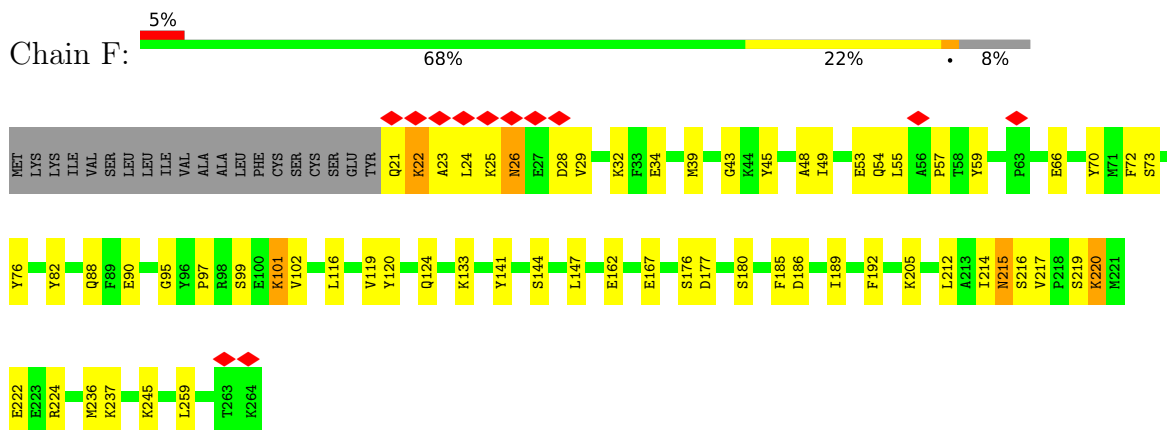
- Molecule 15 is water.

Mol	Chain	Residues	Atoms		AltConf
15	A	6	Total	O	0
			6	6	
15	C	8	Total	O	0
			8	8	
15	B	1	Total	O	0
			1	1	
15	D	1	Total	O	0
			1	1	

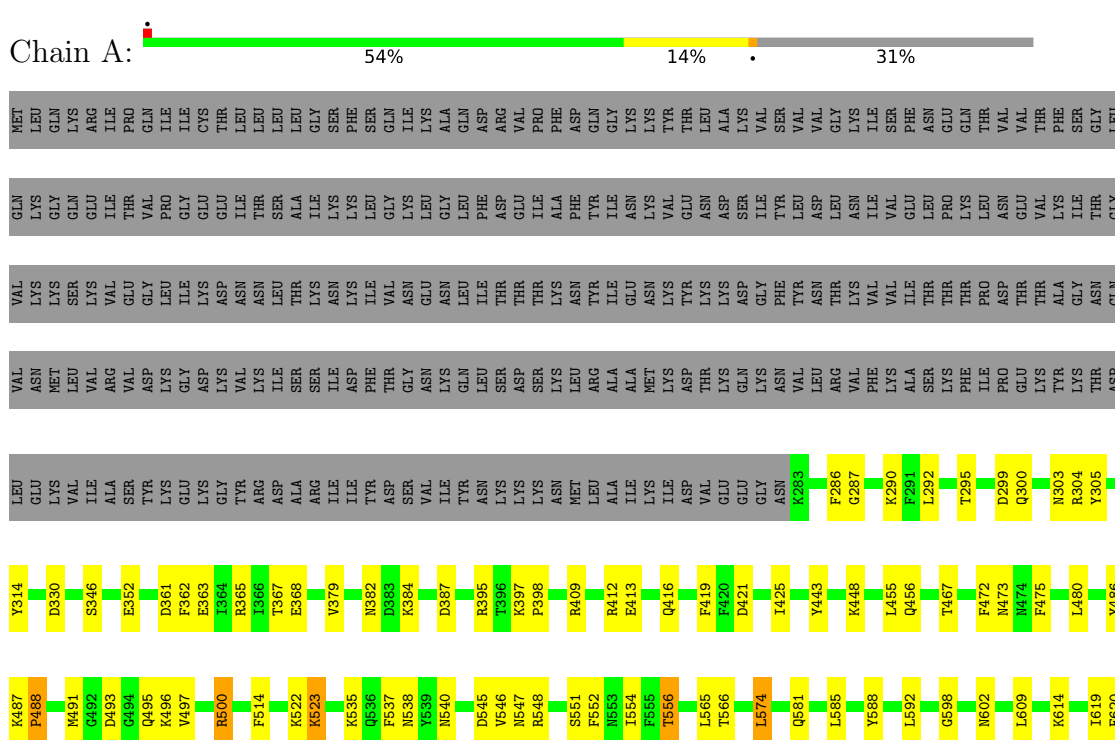
3 Residue-property plots

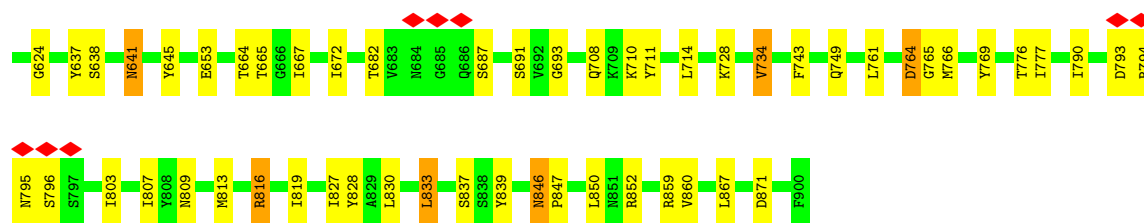
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Bam D

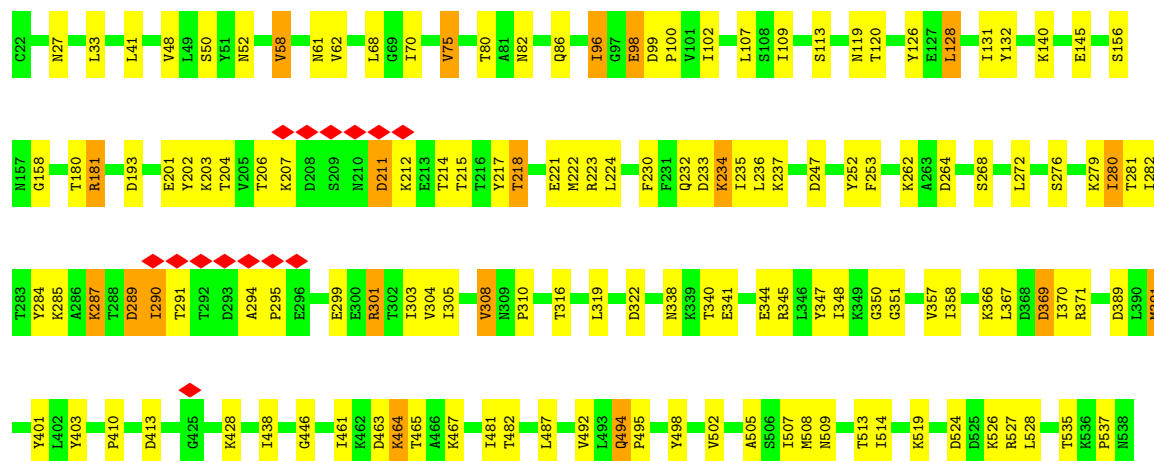


• Molecule 2: Bam A

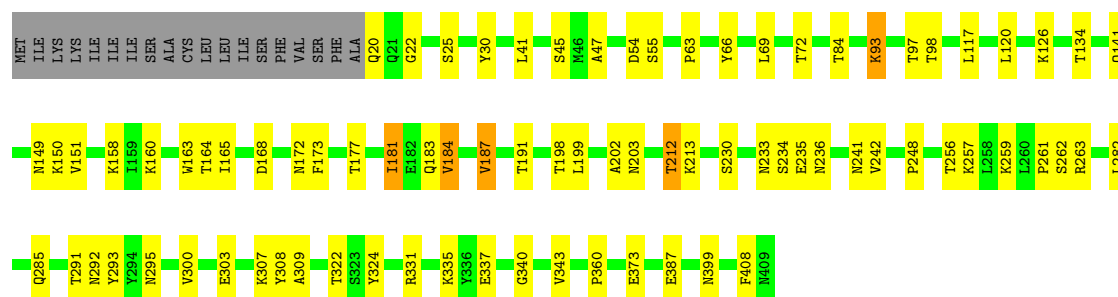
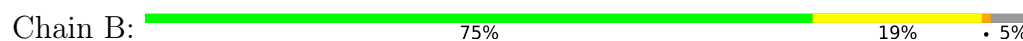




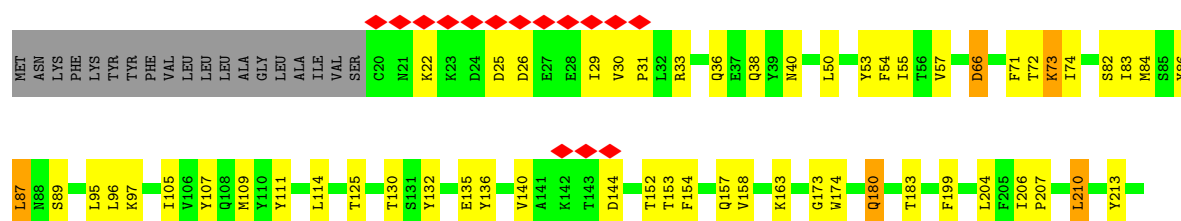
• Molecule 3: Bam H

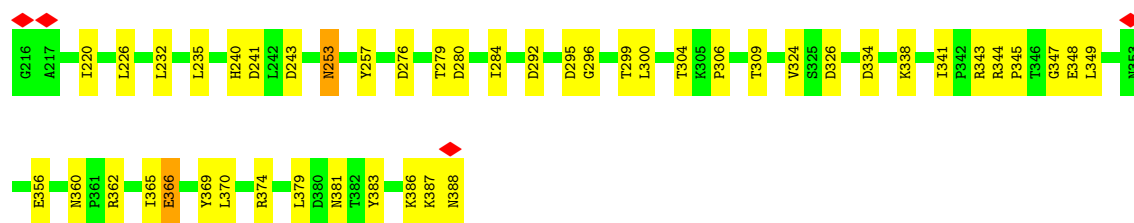


• Molecule 4: Bam G

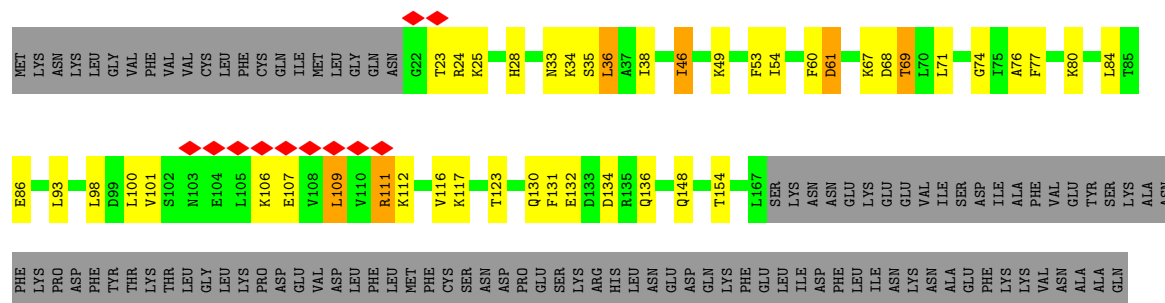


• Molecule 5: Bam M

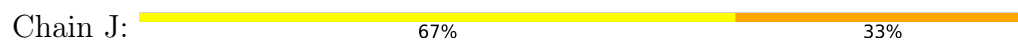




• Molecule 6: Bam P



• Molecule 7: alpha-D-glucopyranuronic acid-(1-2)-[alpha-D-mannopyranose-(1-4)]beta-D-galactopyranose



• Molecule 8: alpha-D-glucopyranuronic acid-(1-2)-beta-D-galactopyranose



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	55796	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60.3	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	16.665	Depositor
Minimum map value	-1.207	Depositor
Average map value	0.114	Depositor
Map value standard deviation	0.382	Depositor
Recommended contour level	2.75	Depositor
Map size (Å)	374.784, 374.784, 374.784	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.732, 0.732, 0.732	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, GCU, PTY, JSG, PLM, CA, GAL, DGA

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	F	0.11	0/2024	0.28	0/2725
2	A	0.14	0/5062	0.39	0/6849
3	C	0.15	0/4101	0.39	0/5565
4	B	0.14	0/3062	0.40	0/4148
5	D	0.15	0/3028	0.40	0/4127
6	E	0.12	0/1169	0.33	0/1569
All	All	0.14	0/18446	0.38	0/24983

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	F	1979	0	1945	40	0
2	A	4936	0	4765	97	0
3	C	4024	0	3931	80	0
4	B	2995	0	2937	48	0
5	D	2947	0	2753	66	0
6	E	1155	0	1198	26	0
7	J	34	0	25	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	G	23	0	15	3	0
9	A	44	0	75	3	0
10	A	200	0	0	2	0
11	A	100	0	158	1	0
12	C	11	0	10	3	0
13	C	17	0	31	4	0
14	D	7	0	0	0	0
15	A	6	0	0	2	0
15	B	1	0	0	0	0
15	C	8	0	0	1	0
15	D	1	0	0	0	0
All	All	18488	0	17843	345	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 10.

All (345) 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)
12:C:601:MAN:C1	8:G:1:GAL:O4	1.65	1.43
12:C:601:MAN:O5	8:G:1:GAL:O4	1.75	1.03
3:C:206:THR:HG1	3:C:214:THR:HG1	1.23	0.81
1:F:212:LEU:HG	1:F:224:ARG:HD3	1.63	0.81
4:B:261:PRO:O	4:B:263:ARG:NH1	2.17	0.77
1:F:21:GLN:HE22	1:F:25:LYS:HE3	1.50	0.77
2:A:592:LEU:HD22	2:A:803:ILE:HG13	1.70	0.73
3:C:344:GLU:HG3	3:C:519:LYS:HD3	1.73	0.70
5:D:87:LEU:O	5:D:89:SER:N	2.26	0.69
3:C:280:ILE:HG23	3:C:305:ILE:HB	1.74	0.68
5:D:341:ILE:O	5:D:374:ARG:NH1	2.26	0.68
1:F:26:ASN:HD21	1:F:28:ASP:HB3	1.57	0.68
1:F:119:VAL:O	1:F:124:GLN:NE2	2.25	0.68
3:C:369:ASP:N	3:C:369:ASP:OD1	2.27	0.68
5:D:33:ARG:O	5:D:213:TYR:OH	2.10	0.67
3:C:98:GLU:HG3	3:C:287:LYS:HB2	1.76	0.67
2:A:556:THR:HB	2:A:581:GLN:HG2	1.77	0.67
3:C:289:ASP:N	3:C:289:ASP:OD1	2.28	0.66
2:A:638:SER:HA	2:A:641:ASN:HD21	1.60	0.66
2:A:859:ARG:NH2	2:A:871:ASP:OD2	2.29	0.66
4:B:324:TYR:OH	4:B:360:PRO:O	2.14	0.66
5:D:154:PHE:HE1	5:D:157:GLN:HB2	1.59	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:307:LYS:HG3	4:B:337:GLU:HG2	1.76	0.65
2:A:813:MET:HE2	9:A:1001:DGA:HAV1	1.78	0.64
3:C:401:TYR:O	15:C:701:HOH:O	2.14	0.64
4:B:184:VAL:HG22	4:B:187:VAL:HG22	1.80	0.64
1:F:217:VAL:HG12	1:F:219:SER:H	1.62	0.64
2:A:472[A]:PHE:HZ	2:A:491:MET:HG2	1.63	0.64
3:C:82:ASN:HB2	3:C:319:LEU:HB2	1.78	0.63
3:C:481:ILE:HD13	3:C:508:MET:HE1	1.79	0.63
4:B:141:GLN:HB3	4:B:181:ILE:HG23	1.81	0.63
3:C:282:ILE:HB	3:C:303:ILE:HG13	1.81	0.63
2:A:487:LYS:H	2:A:487:LYS:HD2	1.63	0.63
5:D:356:GLU:OE1	5:D:362:ARG:NH1	2.31	0.63
2:A:830:LEU:HD21	2:A:859:ARG:HH21	1.63	0.62
2:A:382:ASN:ND2	2:A:387:ASP:OD1	2.33	0.62
5:D:326:ASP:OD1	5:D:334:ASP:HA	2.00	0.61
2:A:300:GLN:HG2	2:A:304:ARG:HE	1.65	0.61
2:A:637:TYR:O	2:A:641:ASN:ND2	2.34	0.61
4:B:234:SER:HB3	4:B:256:THR:HG23	1.82	0.60
4:B:160:LYS:HB2	4:B:163:TRP:HB3	1.82	0.60
2:A:346:SER:HA	2:A:367:THR:O	2.02	0.59
2:A:552:PHE:HB3	2:A:585:LEU:HD13	1.85	0.59
4:B:181:ILE:HD11	4:B:183:GLN:HE21	1.67	0.59
1:F:222:GLU:N	1:F:222:GLU:OE1	2.33	0.59
2:A:833:LEU:HD13	9:A:1001:DGA:HAF1	1.86	0.58
10:A:1002:JSG:ODJ	10:A:1002:JSG:OBL	2.21	0.58
4:B:120:LEU:HB2	4:B:150:LYS:HG3	1.84	0.58
6:E:54:ILE:HD13	6:E:60:PHE:HB3	1.85	0.58
3:C:140:LYS:HG3	3:C:193:ASP:HA	1.85	0.58
5:D:365:ILE:HG13	5:D:366:GLU:H	1.68	0.58
3:C:128:LEU:HB3	3:C:131:ILE:HD13	1.86	0.58
4:B:303:GLU:HG2	4:B:340:GLY:HA2	1.84	0.58
1:F:212:LEU:O	1:F:216:SER:HB2	2.03	0.58
5:D:109:MET:HE2	5:D:204:LEU:HB2	1.85	0.58
3:C:107:LEU:HD23	3:C:224:LEU:HD12	1.84	0.58
3:C:234:LYS:HB3	3:C:235:ILE:HD12	1.86	0.58
2:A:379:VAL:HG12	2:A:443:TYR:HB2	1.86	0.57
3:C:33:LEU:O	4:B:30:TYR:OH	2.22	0.57
2:A:522:LYS:O	2:A:523:LYS:NZ	2.37	0.57
3:C:524:ASP:OD1	3:C:527:ARG:NH2	2.38	0.57
1:F:32:LYS:HE3	1:F:55:LEU:HD21	1.87	0.57
5:D:345:PRO:HB2	5:D:362:ARG:HB3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:743:PHE:HD1	2:A:807:ILE:HD12	1.70	0.57
4:B:63:PRO:HG3	4:B:168:ASP:OD2	2.05	0.57
2:A:641:ASN:ND2	2:A:641:ASN:O	2.38	0.56
2:A:419:PHE:HE1	2:A:473:ASN:HB2	1.70	0.56
3:C:70:ILE:HG12	3:C:80:THR:HG23	1.87	0.56
2:A:397:LYS:NZ	6:E:136:GLN:OE1	2.37	0.56
6:E:80:LYS:HD3	6:E:98:LEU:HD13	1.86	0.56
1:F:22:LYS:H	1:F:22:LYS:HD3	1.71	0.56
2:A:672:ILE:HG12	2:A:691:SER:HB2	1.88	0.55
5:D:280:ASP:OD1	5:D:280:ASP:N	2.36	0.55
4:B:300:VAL:HG22	4:B:343:VAL:HG13	1.89	0.55
5:D:135:GLU:HG2	5:D:154:PHE:HA	1.89	0.55
4:B:120:LEU:HD13	4:B:150:LYS:HD2	1.89	0.54
5:D:30:VAL:N	5:D:31:PRO:HD2	2.22	0.54
2:A:556:THR:HB	2:A:581:GLN:HE21	1.71	0.54
2:A:852:ARG:HD2	13:C:602:PLM:H41	1.89	0.54
5:D:105:ILE:HD11	5:D:107:TYR:CZ	2.42	0.54
13:C:602:PLM:H62	4:B:97:THR:HG21	1.89	0.54
3:C:52:ASN:HD21	3:C:347:TYR:H	1.55	0.54
5:D:349:LEU:HD21	5:D:356:GLU:HG3	1.89	0.54
3:C:494:GLN:HG3	3:C:495:PRO:HD2	1.90	0.54
2:A:540:ASN:HB3	2:A:545:ASP:OD1	2.09	0.53
2:A:425:ILE:O	6:E:123:THR:HG21	2.08	0.53
5:D:386:LYS:NZ	5:D:388:ASN:O	2.31	0.53
6:E:46:ILE:O	6:E:49:LYS:NZ	2.29	0.53
1:F:29:VAL:HG13	1:F:55:LEU:HD22	1.89	0.53
2:A:809:ASN:HD21	2:A:850:LEU:HD21	1.72	0.53
3:C:366:LYS:O	3:C:370:ILE:HG12	2.08	0.53
2:A:500:ARG:HG3	6:E:148:GLN:HB2	1.91	0.53
2:A:645:TYR:O	2:A:710:LYS:NZ	2.40	0.53
4:B:25:SER:OG	4:B:387:GLU:OE2	2.25	0.53
4:B:236:ASN:HB3	4:B:293:TYR:CZ	2.44	0.53
3:C:294:ALA:N	3:C:295:PRO:HD3	2.24	0.52
2:A:352:GLU:HG2	2:A:362:PHE:CE2	2.44	0.52
2:A:592:LEU:HD23	2:A:592:LEU:H	1.74	0.52
3:C:202:TYR:HB2	3:C:218:THR:HG23	1.92	0.52
5:D:136:TYR:CZ	5:D:153:THR:HB	2.45	0.52
1:F:90:GLU:OE2	1:F:133:LYS:NZ	2.42	0.52
5:D:86:TYR:O	5:D:95:LEU:HB3	2.10	0.52
2:A:475:PHE:HZ	2:A:480:LEU:HD23	1.74	0.51
2:A:585:LEU:HD12	2:A:588:TYR:HB3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:711:TYR:HA	15:A:1104:HOH:O	2.10	0.51
5:D:66:ASP:OD1	5:D:66:ASP:N	2.41	0.51
5:D:57:VAL:HG21	5:D:114:LEU:HD22	1.93	0.51
6:E:33:ASN:ND2	6:E:100:LEU:HB2	2.25	0.51
5:D:180:GLN:OE1	5:D:257:TYR:OH	2.29	0.51
5:D:343:ARG:HB3	5:D:374:ARG:HB2	1.93	0.51
1:F:180:SER:OG	2:A:397:LYS:HB3	2.10	0.51
3:C:276:SER:HB2	3:C:310:PRO:HD2	1.93	0.51
4:B:84:THR:HG22	4:B:93:LYS:HG3	1.92	0.51
2:A:839:TYR:OH	2:A:846:ASN:O	2.26	0.51
5:D:36:GLN:OE1	5:D:40:ASN:ND2	2.43	0.51
1:F:23:ALA:HB1	1:F:32:LYS:HA	1.92	0.51
3:C:96:ILE:HD13	3:C:96:ILE:H	1.76	0.51
1:F:32:LYS:HB3	1:F:55:LEU:HD11	1.92	0.51
6:E:28:HIS:ND1	6:E:61:ASP:OD2	2.44	0.51
2:A:664:THR:HG23	2:A:672:ILE:HB	1.91	0.50
3:C:109:ILE:HD12	3:C:222:MET:HE2	1.92	0.50
4:B:66:TYR:HA	4:B:69:LEU:HD23	1.93	0.50
4:B:151:VAL:HG23	4:B:173:PHE:HE1	1.76	0.50
3:C:221:GLU:HG3	3:C:223:ARG:HG3	1.93	0.50
3:C:102:ILE:HB	3:C:236:LEU:HD22	1.93	0.50
1:F:120:TYR:CE2	1:F:167:GLU:HG3	2.46	0.50
1:F:236:MET:HE1	1:F:245:LYS:HG3	1.93	0.50
2:A:764:ASP:N	2:A:764:ASP:OD1	2.43	0.50
5:D:279:THR:OG1	5:D:292:ASP:O	2.30	0.50
2:A:693:GLY:HA3	5:D:388:ASN:HD21	1.76	0.50
5:D:206:ILE:HD11	5:D:210:LEU:HD23	1.93	0.50
3:C:113:SER:OG	3:C:126:TYR:HB3	2.12	0.50
2:A:852:ARG:HB3	13:C:602:PLM:H82	1.93	0.49
3:C:350:GLY:HA3	3:C:509:ASN:O	2.12	0.49
1:F:53:GLU:OE2	1:F:76:TYR:OH	2.26	0.49
2:A:614:LYS:HA	2:A:624:GLY:HA3	1.94	0.49
4:B:47:ALA:HB1	4:B:309:ALA:HB1	1.94	0.49
6:E:134:ASP:N	6:E:134:ASP:OD1	2.45	0.49
1:F:24:LEU:HA	1:F:32:LYS:HD3	1.94	0.49
2:A:665:THR:OG1	5:D:296:GLY:O	2.23	0.49
1:F:185:PHE:O	1:F:189:ILE:HG13	2.13	0.49
2:A:545:ASP:OD1	2:A:545:ASP:N	2.46	0.49
3:C:230:PHE:O	3:C:234:LYS:HB2	2.13	0.49
2:A:295:THR:OG1	2:A:368:GLU:OE1	2.31	0.49
5:D:183:THR:HG21	5:D:235:LEU:HD22	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:367:LEU:HD11	3:C:461:ILE:HG22	1.93	0.48
3:C:505:ALA:HA	3:C:508:MET:HE3	1.95	0.48
6:E:23:THR:HB	6:E:25:LYS:HG2	1.95	0.48
2:A:299:ASP:O	2:A:303:ASN:ND2	2.34	0.48
5:D:206:ILE:HD12	5:D:207:PRO:HD2	1.96	0.48
3:C:284:TYR:HE1	3:C:303:ILE:HG23	1.77	0.48
1:F:99:SER:HB3	1:F:102:VAL:HG23	1.94	0.48
3:C:27:ASN:ND2	4:B:126:LYS:O	2.46	0.48
1:F:180:SER:HB3	2:A:398:PRO:HD2	1.95	0.48
3:C:119:ASN:ND2	3:C:120:THR:O	2.46	0.48
6:E:68:ASP:HB3	6:E:84:LEU:HD12	1.95	0.48
4:B:282:LEU:HD12	4:B:308:TYR:HD1	1.78	0.48
5:D:344:ARG:HH11	5:D:383:TYR:HA	1.79	0.48
2:A:287:GLY:O	2:A:361:ASP:HA	2.13	0.48
2:A:412:ARG:O	2:A:416:GLN:HG2	2.14	0.48
2:A:766:MET:HE2	2:A:769:TYR:HD2	1.79	0.48
4:B:22:GLY:HA2	4:B:98:THR:HG21	1.96	0.48
4:B:335:LYS:HD2	4:B:337:GLU:OE2	2.14	0.48
5:D:300:LEU:O	5:D:304:THR:OG1	2.24	0.48
1:F:49:ILE:O	1:F:53:GLU:HG3	2.14	0.48
1:F:73:SER:HB3	1:F:88:GLN:HB3	1.96	0.48
4:B:303:GLU:N	4:B:340:GLY:O	2.38	0.48
2:A:330:ASP:OD1	2:A:330:ASP:N	2.43	0.48
2:A:837:SER:OG	2:A:850:LEU:HA	2.13	0.48
3:C:463:ASP:OD1	3:C:465:THR:HG22	2.13	0.48
2:A:409:ARG:NH1	6:E:131:PHE:HB3	2.29	0.47
2:A:809:ASN:ND2	2:A:850:LEU:HD21	2.29	0.47
4:B:199:LEU:HA	4:B:233:ASN:O	2.13	0.47
5:D:173:GLY:HA3	5:D:206:ILE:HG12	1.96	0.47
5:D:387:LYS:HG2	5:D:388:ASN:ND2	2.30	0.47
2:A:497:VAL:HG12	2:A:514:PHE:HD1	1.80	0.47
3:C:290:ILE:O	3:C:291:THR:OG1	2.29	0.47
5:D:295:ASP:HB3	5:D:381:ASN:HA	1.96	0.47
2:A:286:PHE:CE2	2:A:314:TYR:HA	2.50	0.47
9:A:1001:DGA:HB22	13:C:602:PLM:H22	1.96	0.47
3:C:180:THR:HG22	3:C:181:ARG:H	1.80	0.47
1:F:39:MET:HB2	1:F:48:ALA:HB2	1.96	0.47
5:D:125:THR:O	5:D:240:HIS:HE1	1.98	0.47
2:A:852:ARG:NH2	4:B:20:GLN:HA	2.30	0.47
4:B:45:SER:OG	4:B:331:ARG:HD2	2.15	0.47
6:E:106:LYS:HG3	6:E:107:GLU:OE1	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:552:PHE:HE2	2:A:554:ILE:HD11	1.80	0.46
3:C:391:MET:SD	3:C:513:THR:HA	2.55	0.46
5:D:53:TYR:O	5:D:83:ILE:HG13	2.16	0.46
5:D:220:ILE:HG21	5:D:226:LEU:HD21	1.98	0.46
3:C:492:VAL:HG22	3:C:498:TYR:CE1	2.51	0.46
4:B:212:THR:HG22	4:B:213:LYS:H	1.79	0.46
5:D:154:PHE:CE1	5:D:157:GLN:HB2	2.44	0.46
3:C:61:ASN:HA	3:C:316:THR:O	2.15	0.46
2:A:537:PHE:CD1	2:A:551:SER:HB2	2.51	0.46
1:F:21:GLN:NE2	1:F:25:LYS:HE3	2.25	0.46
4:B:292:ASN:N	4:B:295:ASN:OD1	2.45	0.46
1:F:141:TYR:O	1:F:144:SER:OG	2.29	0.46
3:C:207:LYS:HE3	3:C:211:ASP:O	2.16	0.46
2:A:734:VAL:HG22	2:A:816:ARG:HG3	1.98	0.46
3:C:75:VAL:HG21	3:C:514:ILE:HD11	1.98	0.46
4:B:55:SER:H	7:J:1:GAL:H5	1.81	0.46
5:D:365:ILE:O	5:D:366:GLU:HB2	2.16	0.46
6:E:35:SER:C	6:E:109:LEU:HB2	2.41	0.46
2:A:487:LYS:O	2:A:488:PRO:C	2.58	0.45
2:A:602:ASN:HB2	2:A:714:LEU:HD22	1.98	0.45
5:D:130:THR:HB	5:D:232:LEU:HA	1.98	0.45
2:A:598:GLY:HA3	2:A:708:GLN:OE1	2.17	0.45
3:C:58:VAL:HG13	3:C:487:LEU:HD23	1.97	0.45
3:C:262:LYS:HG2	3:C:268:SER:OG	2.16	0.45
3:C:264:ASP:N	3:C:264:ASP:OD1	2.49	0.45
4:B:241:ASN:OD1	4:B:248:PRO:HB3	2.16	0.45
5:D:87:LEU:HD23	5:D:87:LEU:HA	1.81	0.45
2:A:766:MET:HE2	2:A:769:TYR:CD2	2.52	0.45
3:C:247:ASP:N	3:C:247:ASP:OD1	2.49	0.45
5:D:38:GLN:HG2	5:D:213:TYR:HE1	1.81	0.45
1:F:53:GLU:HG2	1:F:72:PHE:HZ	1.82	0.45
3:C:371:ARG:NH2	3:C:464:LYS:HA	2.32	0.45
4:B:160:LYS:HD3	4:B:163:TRP:HE3	1.82	0.45
5:D:132:TYR:CD2	5:D:174:TRP:HH2	2.35	0.45
3:C:234:LYS:HD3	3:C:252:TYR:CE2	2.52	0.45
3:C:236:LEU:HD21	3:C:284:TYR:HB3	1.98	0.45
4:B:158:LYS:HG2	4:B:164:THR:HG22	1.98	0.45
2:A:473:ASN:HA	2:A:496:LYS:HG2	1.99	0.45
4:B:203:ASN:HB3	4:B:230:SER:HB2	1.98	0.45
5:D:54:PHE:HD1	5:D:74:ILE:HG12	1.82	0.45
5:D:96:LEU:HB2	5:D:111:TYR:CZ	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:761:LEU:HD12	2:A:777:ILE:HB	1.99	0.44
5:D:241:ASP:OD1	5:D:241:ASP:N	2.33	0.44
1:F:66:GLU:OE2	1:F:99:SER:OG	2.36	0.44
3:C:100:PRO:O	3:C:237:LYS:NZ	2.49	0.44
3:C:232:GLN:O	3:C:237:LYS:N	2.51	0.44
4:B:150:LYS:NZ	4:B:172:ASN:OD1	2.43	0.44
2:A:765:GLY:HA2	2:A:776:THR:HG22	1.99	0.44
3:C:132:TYR:HE2	3:C:272:LEU:HG	1.83	0.44
3:C:340:THR:OG1	3:C:341:GLU:OE1	2.36	0.44
3:C:100:PRO:HD2	3:C:237:LYS:HZ2	1.83	0.44
3:C:492:VAL:HG22	3:C:498:TYR:HE1	1.82	0.44
2:A:592:LEU:HD13	2:A:803:ILE:HD11	1.99	0.43
3:C:338:ASN:ND2	3:C:341:GLU:OE1	2.50	0.43
3:C:351:GLY:HA2	3:C:507:ILE:HA	1.99	0.43
3:C:367:LEU:CD1	3:C:461:ILE:HG22	2.48	0.43
5:D:199:PHE:HB2	5:D:232:LEU:O	2.18	0.43
3:C:410:PRO:HG3	3:C:482:THR:OG1	2.17	0.43
5:D:253:ASN:HD21	5:D:276:ASP:HB3	1.83	0.43
3:C:348:ILE:O	3:C:348:ILE:HG13	2.19	0.43
4:B:30:TYR:CZ	4:B:300:VAL:HG21	2.53	0.43
5:D:360:ASN:OD1	5:D:360:ASN:N	2.51	0.43
6:E:74:GLY:HA3	6:E:77:PHE:CZ	2.52	0.43
3:C:70:ILE:HB	3:C:268:SER:HB3	2.00	0.43
5:D:158:VAL:HG13	5:D:158:VAL:O	2.18	0.43
2:A:538:ASN:HD22	2:A:547:ASN:HD21	1.67	0.43
1:F:220:LYS:HD3	4:B:408:PHE:CZ	2.54	0.43
5:D:144:ASP:OD1	5:D:144:ASP:N	2.51	0.43
3:C:281:THR:HG22	3:C:304:VAL:HG12	2.01	0.43
5:D:25:ASP:OD1	5:D:25:ASP:N	2.51	0.43
2:A:292:LEU:HD23	2:A:292:LEU:HA	1.81	0.43
3:C:202:TYR:HB2	3:C:218:THR:CG2	2.49	0.43
2:A:682:THR:HA	2:A:687:SER:HA	2.01	0.42
3:C:156:SER:O	3:C:158:GLY:N	2.52	0.42
5:D:243:ASP:HB2	5:D:299:THR:HB	2.01	0.42
6:E:80:LYS:HD3	6:E:98:LEU:HA	2.00	0.42
3:C:102:ILE:HG22	3:C:232:GLN:OE1	2.19	0.42
4:B:198:THR:OG1	4:B:235:GLU:HB2	2.19	0.42
5:D:348:GLU:N	5:D:348:GLU:OE1	2.53	0.42
6:E:68:ASP:OD1	6:E:69:THR:N	2.52	0.42
2:A:395:ARG:CZ	2:A:413:GLU:HG3	2.49	0.42
2:A:395:ARG:HH21	6:E:134:ASP:CG	2.28	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:565:LEU:HD11	2:A:574:LEU:HB2	2.01	0.42
4:B:262:SER:O	4:B:285:GLN:HA	2.19	0.42
2:A:475:PHE:O	2:A:495:GLN:HB2	2.19	0.42
5:D:279:THR:HG21	5:D:379:LEU:HD22	2.02	0.42
1:F:53:GLU:HG2	1:F:72:PHE:CZ	2.54	0.42
2:A:300:GLN:CD	2:A:304:ARG:HH21	2.27	0.42
5:D:241:ASP:OD2	5:D:243:ASP:CG	2.63	0.42
3:C:401:TYR:CE2	3:C:403:TYR:HB3	2.55	0.42
5:D:132:TYR:CE2	5:D:174:TRP:HH2	2.38	0.42
2:A:828:TYR:OH	2:A:859:ARG:HD2	2.20	0.42
4:B:54:ASP:OD1	4:B:55:SER:N	2.53	0.42
5:D:347:GLY:HA2	5:D:365:ILE:HG23	2.02	0.42
1:F:43:GLY:HA2	1:F:45:TYR:CZ	2.55	0.42
2:A:292:LEU:HD12	2:A:363:GLU:OE2	2.20	0.42
5:D:55:ILE:HG22	5:D:71:PHE:CD1	2.55	0.42
5:D:306:PRO:HD2	5:D:309:THR:HG21	2.02	0.42
3:C:86:GLN:O	3:C:308:VAL:HB	2.20	0.41
3:C:99:ASP:HB3	3:C:287:LYS:HG2	2.00	0.41
3:C:535:THR:O	3:C:537:PRO:HD3	2.20	0.41
4:B:120:LEU:HB2	4:B:150:LYS:CG	2.49	0.41
1:F:95:GLY:O	1:F:97:PRO:HD3	2.20	0.41
2:A:314:TYR:HE1	2:A:362:PHE:CZ	2.38	0.41
12:C:601:MAN:C1	8:G:1:GAL:C4	2.85	0.41
5:D:38:GLN:HG2	5:D:213:TYR:CE1	2.55	0.41
6:E:111:ARG:HA	6:E:111:ARG:HH11	1.86	0.41
1:F:176:SER:O	1:F:177:ASP:C	2.62	0.41
1:F:214:ILE:HG13	1:F:215:ASN:CG	2.46	0.41
2:A:619:ILE:HD13	6:E:130:GLN:HG3	2.02	0.41
2:A:653:GLU:CD	2:A:653:GLU:H	2.27	0.41
2:A:794:ARG:HB3	2:A:794:ARG:NH1	2.35	0.41
3:C:230:PHE:CZ	3:C:234:LYS:HG3	2.56	0.41
3:C:285:LYS:HA	3:C:299:GLU:O	2.20	0.41
6:E:33:ASN:HB3	6:E:36:LEU:O	2.20	0.41
1:F:162:GLU:HG2	1:F:192:PHE:CD1	2.55	0.41
2:A:728:LYS:HG3	2:A:728:LYS:O	2.20	0.41
2:A:793:ASP:O	2:A:795:ASN:N	2.53	0.41
3:C:48:VAL:CG1	3:C:358:ILE:HG23	2.51	0.41
1:F:186:ASP:OD1	1:F:205:LYS:HD2	2.20	0.41
2:A:641:ASN:N	2:A:641:ASN:HD22	2.18	0.41
4:B:72:THR:O	4:B:399:ASN:HA	2.21	0.41
5:D:50:LEU:O	5:D:82:SER:OG	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:76:ALA:O	6:E:101:VAL:HG22	2.21	0.41
1:F:70:TYR:CZ	1:F:101:LYS:HD3	2.55	0.41
1:F:82:TYR:HB2	1:F:116:LEU:HD21	2.02	0.41
10:A:1002:JSG:OBO	10:A:1002:JSG:OBS	2.39	0.41
3:C:52:ASN:ND2	3:C:347:TYR:H	2.18	0.41
3:C:284:TYR:CZ	3:C:301:ARG:HB2	2.56	0.41
5:D:135:GLU:HB3	5:D:152:THR:OG1	2.20	0.41
5:D:369:TYR:O	5:D:370:LEU:HD13	2.21	0.41
3:C:289:ASP:O	3:C:291:THR:HG23	2.21	0.41
4:B:198:THR:O	4:B:234:SER:HA	2.20	0.41
6:E:71:LEU:HD12	6:E:80:LYS:O	2.21	0.41
1:F:259:LEU:HD23	1:F:259:LEU:HA	1.91	0.41
2:A:365:ARG:HB3	6:E:53:PHE:CZ	2.55	0.41
2:A:472[A]:PHE:CZ	2:A:491:MET:HG2	2.50	0.41
2:A:847:PRO:HD2	4:B:149:ASN:ND2	2.36	0.41
3:C:145:GLU:HG3	3:C:253:PHE:CE1	2.55	0.41
4:B:202:ALA:O	4:B:230:SER:OG	2.36	0.41
3:C:50:SER:HA	3:C:357:VAL:O	2.21	0.40
6:E:33:ASN:HD21	6:E:100:LEU:HB2	1.85	0.40
1:F:54:GLN:O	1:F:57:PRO:HD2	2.22	0.40
2:A:467:THR:OG1	15:A:1101:HOH:O	2.22	0.40
2:A:566:THR:HG21	11:A:1003:PTY:HN12	1.86	0.40
2:A:620:PHE:HE1	2:A:816:ARG:HB2	1.85	0.40
2:A:794:ARG:HB3	2:A:794:ARG:HH11	1.86	0.40
5:D:30:VAL:O	5:D:31:PRO:C	2.65	0.40
2:A:827:ILE:HG23	2:A:860:VAL:HG22	2.03	0.40
2:A:847:PRO:CB	4:B:117:LEU:HD21	2.52	0.40
3:C:203:LYS:HB2	3:C:217:TYR:CE1	2.56	0.40
3:C:438:ILE:HD11	3:C:446:GLY:HA3	2.03	0.40
2:A:421:ASP:HA	2:A:448:LYS:HD3	2.04	0.40
2:A:793:ASP:HB2	2:A:796:SER:HB3	2.03	0.40
5:D:338:LYS:O	5:D:370:LEU:HD11	2.22	0.40
2:A:456:GLN:HA	6:E:154:THR:O	2.21	0.40
2:A:548:ARG:HA	2:A:548:ARG:HD2	1.92	0.40
2:A:816:ARG:H	2:A:816:ARG:HG2	1.67	0.40
5:D:73:LYS:H	5:D:73:LYS:NZ	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	F	242/264 (92%)	230 (95%)	12 (5%)	0	100	100
2	A	617/900 (69%)	599 (97%)	17 (3%)	1 (0%)	43	68
3	C	515/517 (100%)	490 (95%)	23 (4%)	2 (0%)	30	54
4	B	388/409 (95%)	378 (97%)	10 (3%)	0	100	100
5	D	367/388 (95%)	345 (94%)	21 (6%)	1 (0%)	36	60
6	E	144/249 (58%)	135 (94%)	9 (6%)	0	100	100
All	All	2273/2727 (83%)	2177 (96%)	92 (4%)	4 (0%)	44	68

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	488	PRO
3	C	211	ASP
5	D	366	GLU
3	C	290	ILE

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	F	205/223 (92%)	196 (96%)	9 (4%)	25	53
2	A	529/783 (68%)	505 (96%)	24 (4%)	24	52
3	C	446/446 (100%)	411 (92%)	35 (8%)	11	29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	B	323/340 (95%)	307 (95%)	16 (5%)	22	48
5	D	324/340 (95%)	308 (95%)	16 (5%)	22	49
6	E	133/228 (58%)	117 (88%)	16 (12%)	5	12
All	All	1960/2360 (83%)	1844 (94%)	116 (6%)	19	42

All (116) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	22	LYS
1	F	26	ASN
1	F	34	GLU
1	F	59	TYR
1	F	101	LYS
1	F	147	LEU
1	F	215	ASN
1	F	220	LYS
1	F	237	LYS
2	A	290	LYS
2	A	305	TYR
2	A	384	LYS
2	A	455	LEU
2	A	486	TYR
2	A	493	ASP
2	A	500	ARG
2	A	523	LYS
2	A	535	LYS
2	A	546	VAL
2	A	556	THR
2	A	574	LEU
2	A	609	LEU
2	A	641	ASN
2	A	667	ILE
2	A	734	VAL
2	A	749	GLN
2	A	764	ASP
2	A	790	ILE
2	A	816	ARG
2	A	819	ILE
2	A	833	LEU
2	A	846	ASN
2	A	867	LEU

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Mol	Chain	Res	Type
3	C	41	LEU
3	C	58	VAL
3	C	62	VAL
3	C	68	LEU
3	C	75	VAL
3	C	96	ILE
3	C	98	GLU
3	C	128	LEU
3	C	181	ARG
3	C	201	GLU
3	C	204	THR
3	C	212	LYS
3	C	215	THR
3	C	218	THR
3	C	233	ASP
3	C	234	LYS
3	C	279	LYS
3	C	280	ILE
3	C	287	LYS
3	C	289	ASP
3	C	301	ARG
3	C	308	VAL
3	C	322	ASP
3	C	345	ARG
3	C	369	ASP
3	C	389	ASP
3	C	391	MET
3	C	413	ASP
3	C	428	LYS
3	C	464	LYS
3	C	467	LYS
3	C	494	GLN
3	C	502	VAL
3	C	526	LYS
3	C	528	LEU
4	B	41	LEU
4	B	93	LYS
4	B	134	THR
4	B	165	ILE
4	B	177	THR
4	B	181	ILE
4	B	184	VAL

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Mol	Chain	Res	Type
4	B	187	VAL
4	B	191	THR
4	B	212	THR
4	B	242	VAL
4	B	257	LYS
4	B	259	LYS
4	B	291	THR
4	B	322	THR
4	B	373	GLU
5	D	22	LYS
5	D	26	ASP
5	D	29	ILE
5	D	66	ASP
5	D	72	THR
5	D	73	LYS
5	D	84	MET
5	D	87	LEU
5	D	97	LYS
5	D	140	VAL
5	D	163	LYS
5	D	180	GLN
5	D	210	LEU
5	D	253	ASN
5	D	284	ILE
5	D	324	VAL
6	E	24	ARG
6	E	34	LYS
6	E	36	LEU
6	E	38	ILE
6	E	46	ILE
6	E	61	ASP
6	E	67	LYS
6	E	69	THR
6	E	86	GLU
6	E	93	LEU
6	E	109	LEU
6	E	111	ARG
6	E	112	LYS
6	E	116	VAL
6	E	117	LYS
6	E	132	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28)

such sidechains are listed below:

Mol	Chain	Res	Type
1	F	21	GLN
1	F	81	GLN
1	F	215	ASN
1	F	250	GLN
2	A	538	ASN
2	A	540	ASN
2	A	553	ASN
2	A	641	ASN
3	C	27	ASN
3	C	52	ASN
3	C	53	GLN
3	C	136	ASN
3	C	149	GLN
3	C	381	ASN
3	C	407	ASN
3	C	439	ASN
3	C	489	ASN
4	B	162	HIS
4	B	183	GLN
4	B	289	GLN
4	B	383	ASN
5	D	36	GLN
5	D	40	ASN
5	D	88	ASN
5	D	359	ASN
6	E	47	ASN
6	E	103	ASN
6	E	130	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

5 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	$\# Z > 2$
8	GAL	G	1	8	11,11,12	0.92	0	15,15,17	1.74	3 (20%)
8	GCU	G	2	8	12,12,13	1.13	2 (16%)	14,17,19	1.39	1 (7%)
7	GAL	J	1	7	11,11,12	0.78	0	15,15,17	1.10	1 (6%)
7	GCU	J	2	7	12,12,13	1.11	1 (8%)	14,17,19	0.96	0
7	MAN	J	3	7	11,11,12	0.84	1 (9%)	15,15,17	1.05	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
8	GAL	G	1	8	-	2/2/19/22	0/1/1/1
8	GCU	G	2	8	1/1/5/6	1/4/21/24	0/1/1/1
7	GAL	J	1	7	-	2/2/19/22	0/1/1/1
7	GCU	J	2	7	1/1/5/6	2/4/21/24	0/1/1/1
7	MAN	J	3	7	1/1/4/5	2/2/19/22	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	J	2	GCU	O6B-C6	-2.25	1.23	1.30
8	G	2	GCU	O6B-C6	-2.22	1.23	1.30
7	J	3	MAN	O5-C1	-2.10	1.40	1.43
8	G	2	GCU	O5-C1	-2.01	1.40	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	G	1	GAL	O4-C4-C5	4.25	119.80	109.32
8	G	2	GCU	C1-C2-C3	3.30	114.45	109.64
8	G	1	GAL	C1-C2-C3	-2.78	105.60	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	G	1	GAL	O5-C1-C2	-2.72	104.31	110.79
7	J	1	GAL	C1-C2-C3	-2.26	106.35	109.64
7	J	3	MAN	C1-O5-C5	2.17	115.09	112.19

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	J	2	GCU	C1
7	J	3	MAN	C1
8	G	2	GCU	C1

All (9) torsion outliers are listed below:

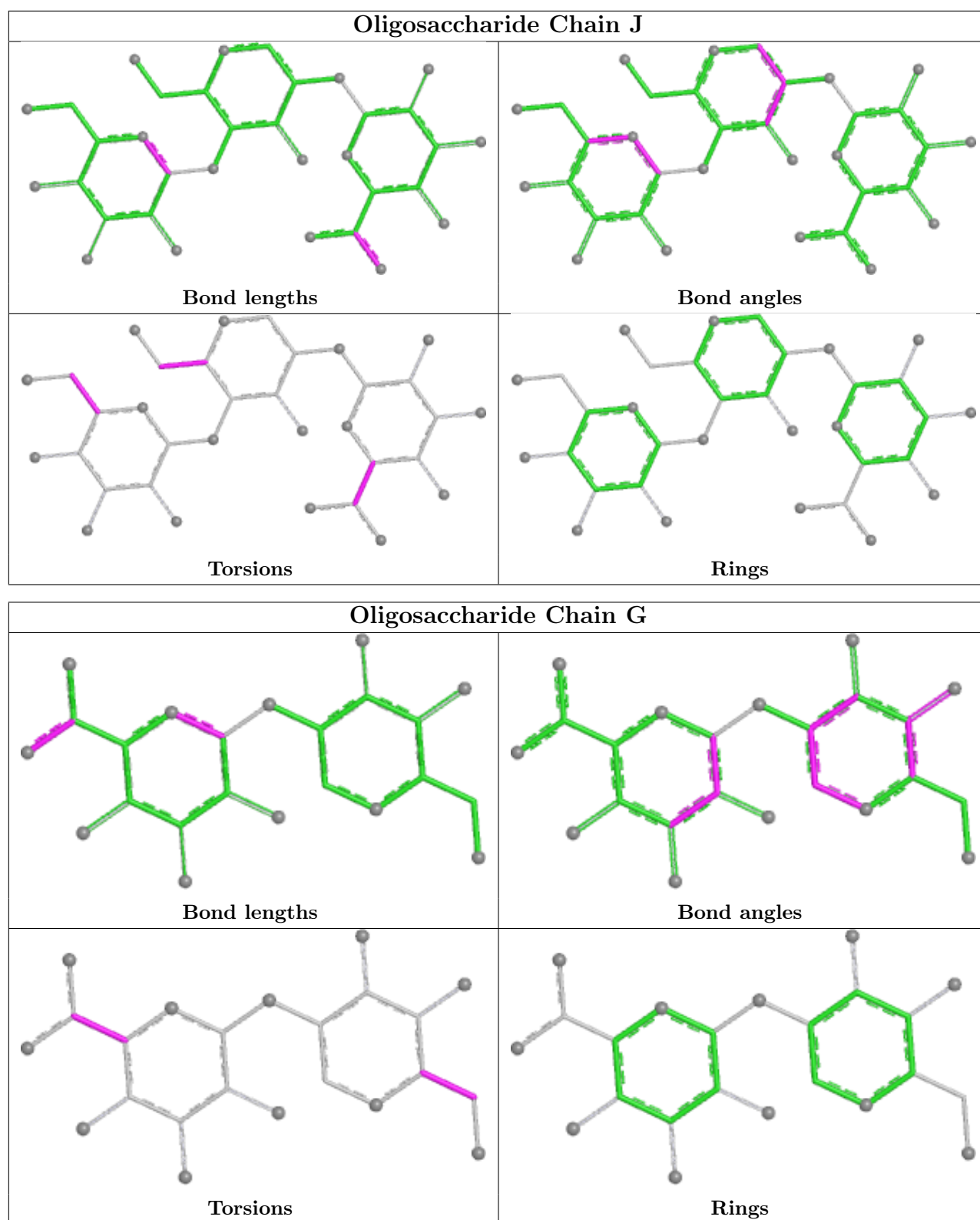
Mol	Chain	Res	Type	Atoms
7	J	2	GCU	C4-C5-C6-O6A
7	J	2	GCU	C4-C5-C6-O6B
7	J	1	GAL	O5-C5-C6-O6
7	J	1	GAL	C4-C5-C6-O6
8	G	1	GAL	C4-C5-C6-O6
7	J	3	MAN	O5-C5-C6-O6
7	J	3	MAN	C4-C5-C6-O6
8	G	2	GCU	C4-C5-C6-O6A
8	G	1	GAL	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	J	1	GAL	1	0
8	G	1	GAL	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 oligosaccharide.



5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 7 are monoatomic - leaving 6 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$
10	JSG	A	1002	-	204,206,206	0.71	2 (0%)	264,278,278	1.67	40 (15%)
11	PTY	A	1004	-	49,49,49	0.46	0	52,54,54	0.39	0
9	DGA	A	1001	3	43,43,43	0.34	0	45,45,45	0.40	0
11	PTY	A	1003	-	49,49,49	0.46	0	52,54,54	0.45	0
13	PLM	C	602	3	15,16,17	0.31	0	14,15,17	0.37	0
12	MAN	C	601	-	11,11,12	1.02	1 (9%)	15,15,17	0.96	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	JSG	A	1002	-	-	65/195/333/333	0/7/7/7
11	PTY	A	1004	-	-	25/53/53/53	-
9	DGA	A	1001	3	-	18/45/45/45	-
11	PTY	A	1003	-	-	21/53/53/53	-
13	PLM	C	602	3	-	5/14/14/15	-
12	MAN	C	601	-	-	2/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	C	601	MAN	O5-C1	-2.67	1.39	1.43
10	A	1002	JSG	ODA-CDB	2.49	1.44	1.40
10	A	1002	JSG	CAN-NAO	2.02	1.49	1.45

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	1002	JSG	CDP-CDO-NAO	7.39	126.35	116.25
10	A	1002	JSG	CAN-NAO-CDO	7.14	133.41	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	1002	JSG	CCB-OCL-CCF	7.08	124.41	113.07
10	A	1002	JSG	OFJ-CGB-CGC	5.22	122.77	111.48
10	A	1002	JSG	O3-CFK-CFL	4.98	120.35	111.43
10	A	1002	JSG	OAQ-CEE-CEF	4.88	120.18	111.43
10	A	1002	JSG	OAU-CAL-CAN	-4.83	101.46	110.59
10	A	1002	JSG	CCT-CCS-CCR	-4.38	107.06	114.41
10	A	1002	JSG	CDB-ODL-CDF	4.30	119.96	113.07
10	A	1002	JSG	OFZ-CGN-CGP	4.25	120.67	111.48
10	A	1002	JSG	OCY-CCS-CCR	4.22	117.06	108.23
10	A	1002	JSG	OEC-CDO-NAO	-4.08	116.05	122.95
10	A	1002	JSG	CAV-CAT-CAR	3.92	120.30	112.07
10	A	1002	JSG	CAL-CAN-NAO	3.44	116.69	110.92
10	A	1002	JSG	CAP-CAN-NAO	3.41	116.34	110.91
10	A	1002	JSG	ODL-CDB-CDC	3.31	117.17	110.37
10	A	1002	JSG	CCO-OCY-CCS	3.29	118.34	113.07
10	A	1002	JSG	C1-C2-C3	-3.26	104.01	109.92
10	A	1002	JSG	OCL-CCF-CCE	3.16	114.84	108.23
10	A	1002	JSG	CDD-CDE-CDF	-2.90	103.09	109.68
10	A	1002	JSG	OCL-CCB-CCC	2.84	116.20	110.37
10	A	1002	JSG	PHG-OAM-CAL	2.83	131.13	123.54
10	A	1002	JSG	OEC-CDO-CDP	-2.69	117.60	121.54
10	A	1002	JSG	OFY-CFK-CFL	-2.61	118.59	124.65
10	A	1002	JSG	CBB-CBC-CBE	-2.53	106.16	110.87
10	A	1002	JSG	CDS-CDR-CDQ	-2.45	107.93	114.68
10	A	1002	JSG	CCQ-CCR-CCS	2.42	117.16	111.72
10	A	1002	JSG	OFJ-CGB-OGA	-2.41	118.07	123.70
10	A	1002	JSG	C1-O5-C5	-2.33	109.17	113.72
10	A	1002	JSG	CAL-CAN-CAP	-2.32	105.72	109.92
10	A	1002	JSG	OAQ-CAP-CAN	2.31	112.19	107.92
10	A	1002	JSG	CDB-CDC-CDD	2.30	114.84	110.01
10	A	1002	JSG	C6-C5-C4	-2.26	107.89	113.35
10	A	1002	JSG	OFZ-CFM-CFL	2.24	111.51	106.72
12	C	601	MAN	C1-O5-C5	2.21	115.15	112.19
10	A	1002	JSG	C8-C7-N2	2.16	119.20	116.25
10	A	1002	JSG	OES-CEE-CEF	-2.14	119.68	124.65
10	A	1002	JSG	OFJ-CEW-C8	2.10	111.22	106.72
10	A	1002	JSG	CCG-CCF-CCE	-2.09	110.91	114.41
10	A	1002	JSG	O1-CAV-CAT	-2.08	104.73	109.42
10	A	1002	JSG	CBQ-CBR-CBT	2.04	112.82	110.84

There are no chirality outliers.

All (136) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	1001	DGA	OG2-CG2-CG3-OXT
10	A	1002	JSG	C5-C4-O4-PHC
10	A	1002	JSG	C2-C1-O1-CAV
10	A	1002	JSG	OAU-CAL-OAM-PHG
10	A	1002	JSG	CAL-CAN-NAO-CDO
10	A	1002	JSG	OAY-CAX-CBA-CBB
10	A	1002	JSG	OAY-CAX-CBA-O6
10	A	1002	JSG	OAY-CAX-CBA-OBH
10	A	1002	JSG	OAZ-CAX-CBA-CBB
10	A	1002	JSG	OBN-CBM-CBP-OBW
10	A	1002	JSG	CBQ-CBP-OBD-CBC
10	A	1002	JSG	OBW-CBP-OBD-CBC
10	A	1002	JSG	CCF-CCG-CCH-OCN
10	A	1002	JSG	OCM-CCG-CCH-OCN
10	A	1002	JSG	CCS-CCT-CCU-ODA
10	A	1002	JSG	OCZ-CCT-CCU-ODA
10	A	1002	JSG	CEF-CEE-OAQ-CAP
10	A	1002	JSG	OET-CEG-CEH-CEI
10	A	1002	JSG	CGP-CGN-OFZ-CFM
10	A	1002	JSG	OGO-CGN-OFZ-CFM
11	A	1003	PTY	O4-C1-C6-O7
11	A	1003	PTY	N1-C2-C3-O11
11	A	1004	PTY	O4-C1-C6-O7
11	A	1004	PTY	N1-C2-C3-O11
11	A	1004	PTY	O10-C8-O7-C6
11	A	1004	PTY	C11-C8-O7-C6
9	A	1001	DGA	CA2-CA1-OG1-CG1
9	A	1001	DGA	OA1-CA1-OG1-CG1
10	A	1002	JSG	OES-CEE-OAQ-CAP
12	C	601	MAN	O5-C5-C6-O6
10	A	1002	JSG	CDP-CDO-NAO-CAN
11	A	1003	PTY	C31-C30-O4-C1
11	A	1003	PTY	O30-C30-O4-C1
10	A	1002	JSG	OEC-CDO-NAO-CAN
12	C	601	MAN	C4-C5-C6-O6
10	A	1002	JSG	C4-C5-C6-O6
10	A	1002	JSG	O5-C5-C6-O6
10	A	1002	JSG	CEF-CEG-CEH-CEI
11	A	1004	PTY	C8-C11-C12-C13
11	A	1004	PTY	C30-C31-C32-C33
11	A	1003	PTY	O10-C8-O7-C6
11	A	1003	PTY	C11-C8-O7-C6
10	A	1002	JSG	CDC-CDB-ODA-CCU

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Mol	Chain	Res	Type	Atoms
13	C	602	PLM	CD-CE-CF-CG
9	A	1001	DGA	CA1-CA2-CA3-CA4
10	A	1002	JSG	CDX-CDY-CDZ-CEA
10	A	1002	JSG	CGV-CGW-CGX-CGY
10	A	1002	JSG	CFB-CFC-CFD-CFE
10	A	1002	JSG	CFC-CFD-CFE-CFF
11	A	1003	PTY	C24-C25-C26-C27
10	A	1002	JSG	CGT-CGU-CGV-CGW
10	A	1002	JSG	CGX-CGY-CGZ-CHA
11	A	1004	PTY	C37-C38-C39-C40
11	A	1003	PTY	C18-C19-C20-C21
10	A	1002	JSG	CGQ-CGR-CGS-CGT
11	A	1003	PTY	C34-C35-C36-C37
11	A	1004	PTY	C38-C39-C40-C41
9	A	1001	DGA	CAB-CBB-CCB-CDB
11	A	1004	PTY	C16-C17-C18-C19
10	A	1002	JSG	CGC-CGD-CGE-CGF
9	A	1001	DGA	CBB-CCB-CDB-CEB
11	A	1003	PTY	C33-C34-C35-C36
13	C	602	PLM	C2-C3-C4-C5
11	A	1003	PTY	C13-C14-C15-C16
9	A	1001	DGA	CA7-CA8-CA9-CAA
11	A	1004	PTY	C11-C12-C13-C14
11	A	1004	PTY	C13-C14-C15-C16
11	A	1004	PTY	C40-C41-C42-C43
11	A	1003	PTY	C12-C13-C14-C15
11	A	1003	PTY	O4-C1-C6-C5
11	A	1003	PTY	C11-C12-C13-C14
11	A	1004	PTY	C21-C22-C23-C24
10	A	1002	JSG	CEL-CEM-CEN-CEO
10	A	1002	JSG	CEO-CEP-CEQ-CER
10	A	1002	JSG	CFA-CFB-CFC-CFD
11	A	1003	PTY	C19-C20-C21-C22
11	A	1004	PTY	C41-C42-C43-C44
9	A	1001	DGA	CFA-CGA-CHA-CIA
10	A	1002	JSG	C3-C4-O4-PHC
10	A	1002	JSG	CEJ-CEK-CEL-CEM
9	A	1001	DGA	CBB-CAB-CB9-CB8
9	A	1001	DGA	CFB-CGB-CHB-CIB
11	A	1004	PTY	C17-C18-C19-C20
13	C	602	PLM	C5-C6-C7-C8
11	A	1004	PTY	O14-C5-C6-C1

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Mol	Chain	Res	Type	Atoms
11	A	1004	PTY	O4-C1-C6-C5
9	A	1001	DGA	CG1-CG2-CG3-OXT
9	A	1001	DGA	CAA-CBA-CCA-CDA
11	A	1003	PTY	C17-C18-C19-C20
10	A	1002	JSG	CGU-CGV-CGW-CGX
10	A	1002	JSG	OAZ-CAX-CBA-OBH
10	A	1002	JSG	OBO-CBM-CBP-OBW
10	A	1002	JSG	CEK-CEL-CEM-CEN
10	A	1002	JSG	CDO-CDP-CDQ-CDR
9	A	1001	DGA	CCB-CDB-CEB-CFB
11	A	1004	PTY	C12-C13-C14-C15
10	A	1002	JSG	CGC-CGB-OFJ-CEW
13	C	602	PLM	C7-C8-C9-CA
10	A	1002	JSG	CDE-CDF-CDG-CDH
11	A	1003	PTY	C5-C6-O7-C8
10	A	1002	JSG	CBG-CBE-OBF-CCB
10	A	1002	JSG	CGD-CGE-CGF-CGG
9	A	1001	DGA	CB6-CB7-CB8-CB9
9	A	1001	DGA	CA3-CA4-CA5-CA6
10	A	1002	JSG	CFL-CFK-O3-C3
10	A	1002	JSG	OGA-CGB-OFJ-CEW
10	A	1002	JSG	C4-O4-PHC-OHE
11	A	1004	PTY	O14-C5-C6-O7
11	A	1003	PTY	C37-C38-C39-C40
11	A	1004	PTY	C33-C34-C35-C36
10	A	1002	JSG	OFY-CFK-O3-C3
11	A	1003	PTY	C5-O14-P1-O13
11	A	1004	PTY	C26-C27-C28-C29
13	C	602	PLM	C4-C5-C6-C7
10	A	1002	JSG	CEH-CEI-CEJ-CEK
10	A	1002	JSG	CBC-CBE-OBF-CCB
10	A	1002	JSG	CCE-OCK-PHO-OHR
10	A	1002	JSG	CDQ-CDR-CDS-CDT
10	A	1002	JSG	OES-CEE-CEF-CEG
10	A	1002	JSG	CFD-CFE-CFF-CFG
9	A	1001	DGA	CB7-CB8-CB9-CAB
10	A	1002	JSG	CCQ-CCR-OCX-PHK
10	A	1002	JSG	CGP-CGQ-CGR-CGS
10	A	1002	JSG	OAZ-CAX-CBA-O6
10	A	1002	JSG	OBN-CBM-CBP-OBW
11	A	1004	PTY	C18-C19-C20-C21
11	A	1004	PTY	C31-C32-C33-C34

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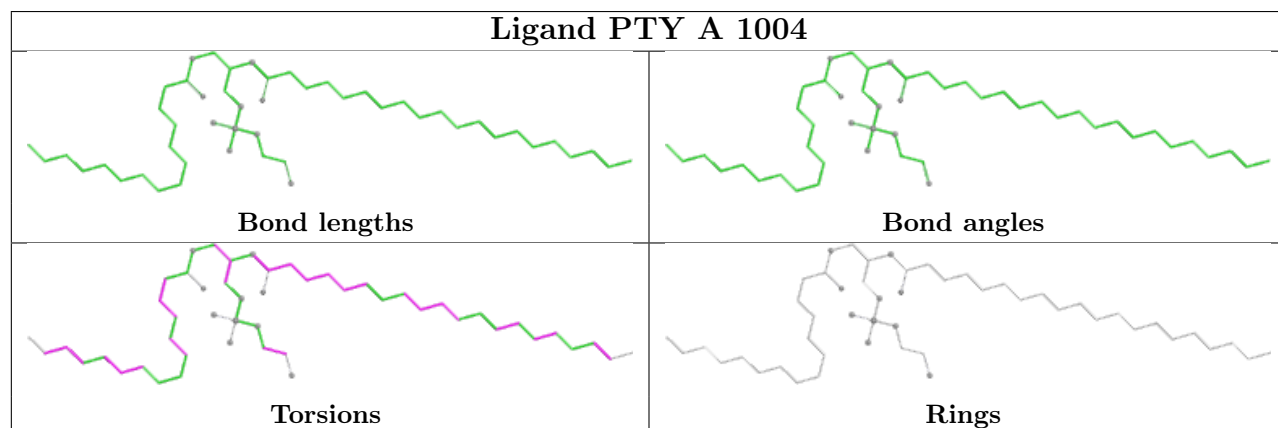
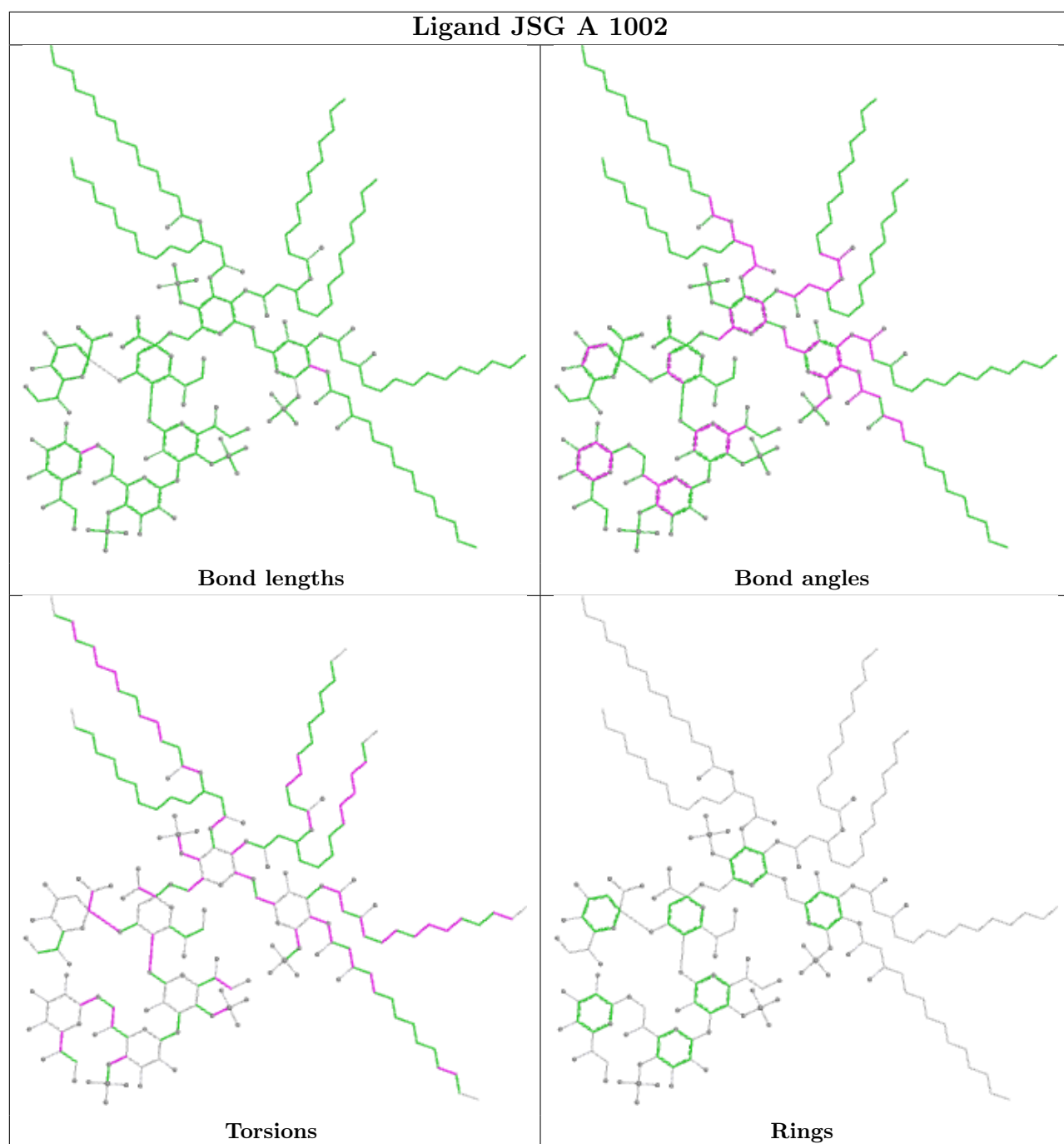
Mol	Chain	Res	Type	Atoms
10	A	1002	JSG	C1-C2-N2-C7
10	A	1002	JSG	OAQ-CEE-CEF-CEG
10	A	1002	JSG	OAU-CAT-CAV-O1
11	A	1003	PTY	O14-C5-C6-C1
11	A	1004	PTY	C23-C24-C25-C26
9	A	1001	DGA	OG1-CG1-CG2-CG3
9	A	1001	DGA	OG1-CA1-CA2-CA3
11	A	1004	PTY	C12-C11-C8-O7
11	A	1003	PTY	C21-C22-C23-C24

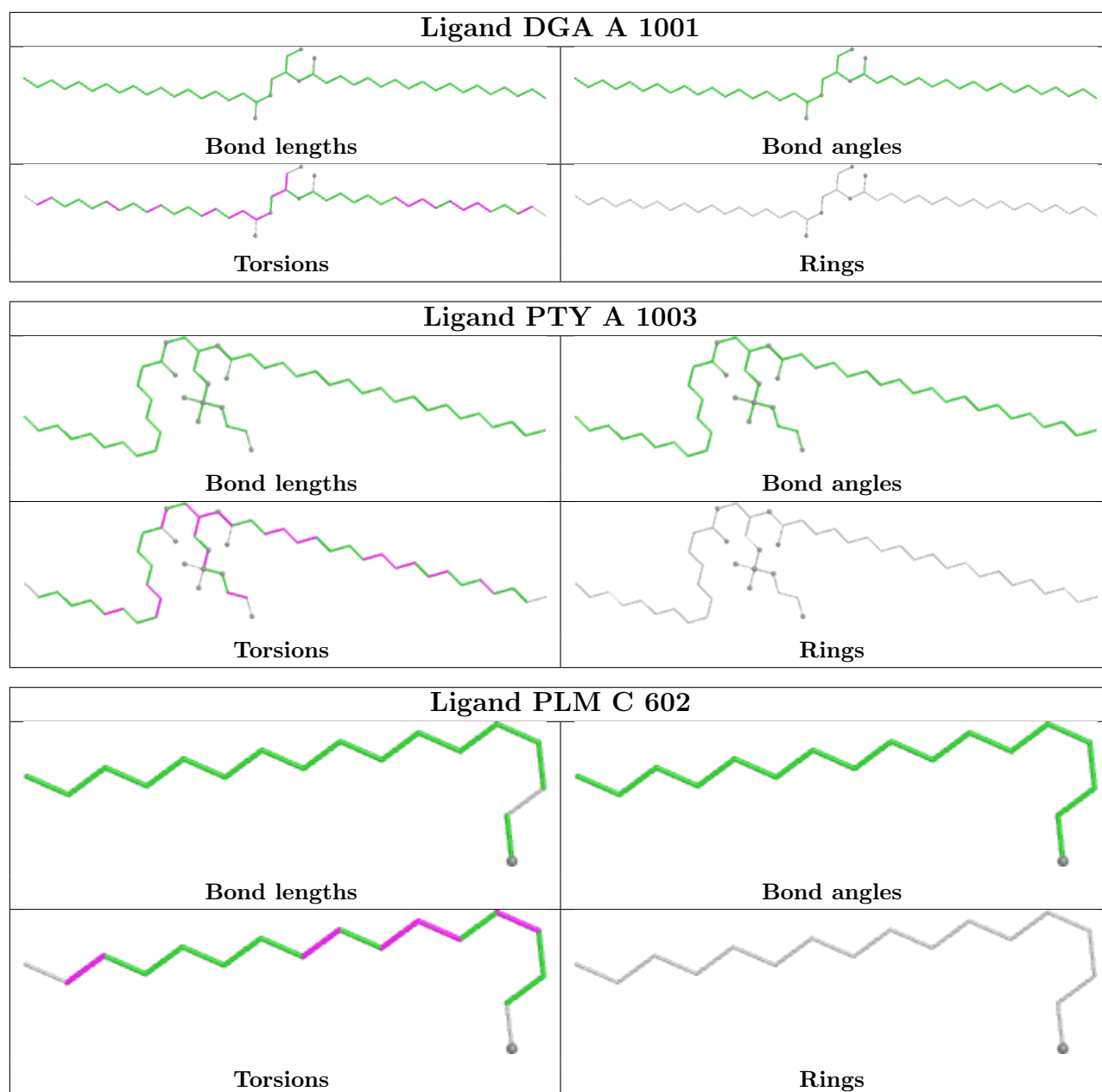
There are no ring outliers.

5 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	1002	JSG	2	0
9	A	1001	DGA	3	0
11	A	1003	PTY	1	0
13	C	602	PLM	4	0
12	C	601	MAN	3	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

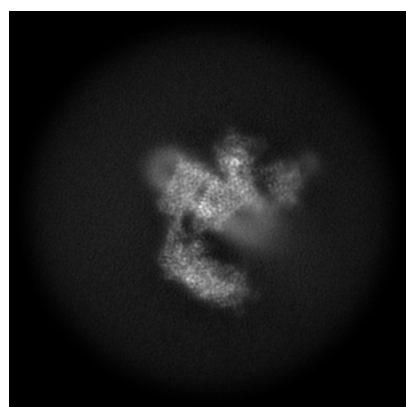
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-48835. These allow visual inspection of the internal detail of the map and identification of artifacts.

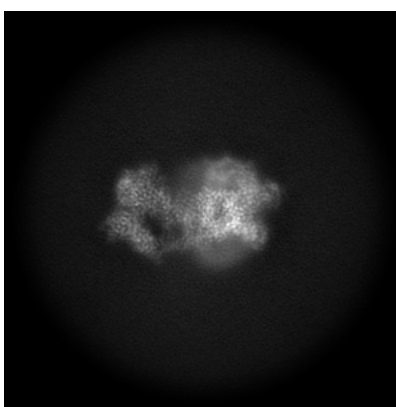
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

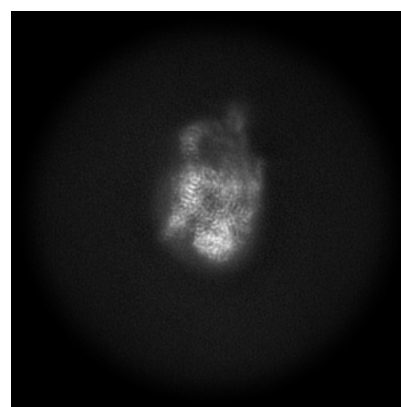
6.1.1 Primary map



X



Y

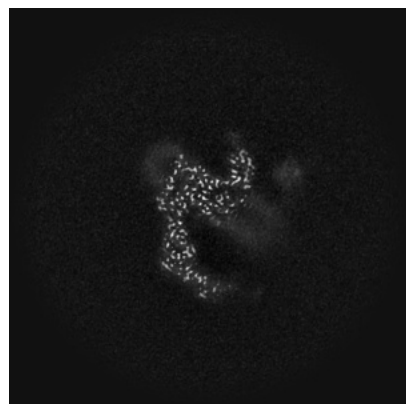


Z

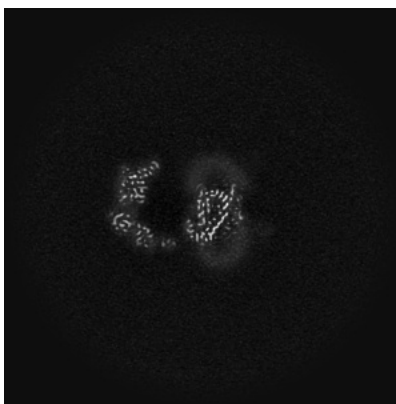
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

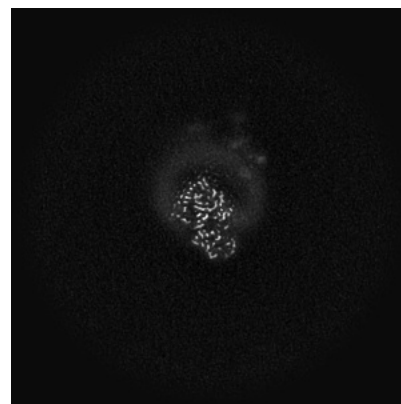
6.2.1 Primary map



X Index: 256



Y Index: 256

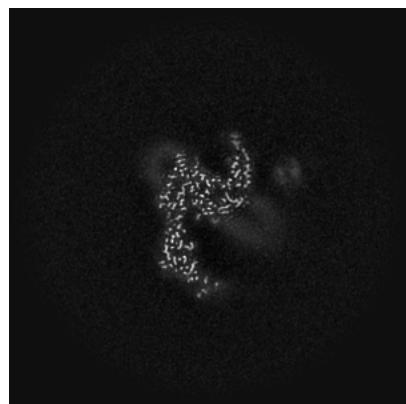


Z Index: 256

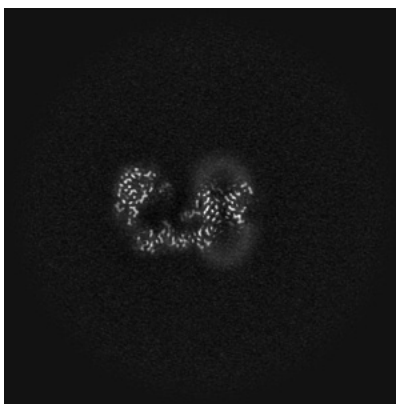
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

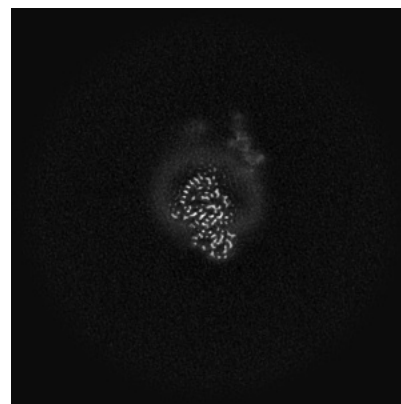
6.3.1 Primary map



X Index: 259



Y Index: 244

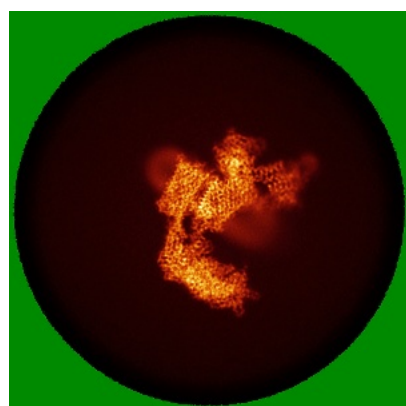


Z Index: 261

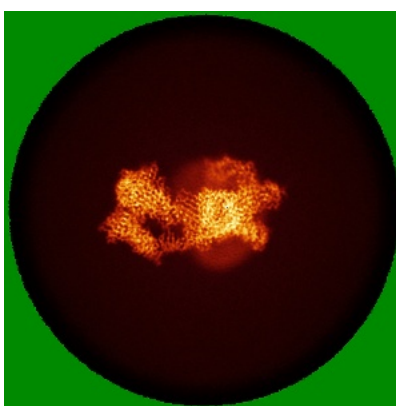
The images above show the largest variance slices of the map in three orthogonal directions.

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

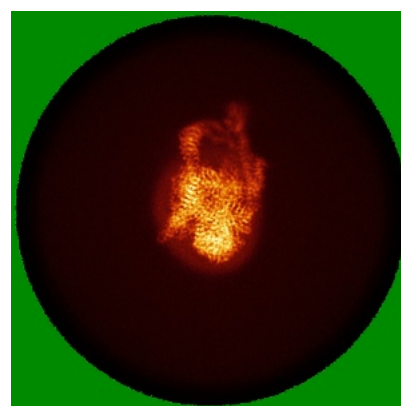
6.4.1 Primary map



X



Y



Z

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

This section was not generated.

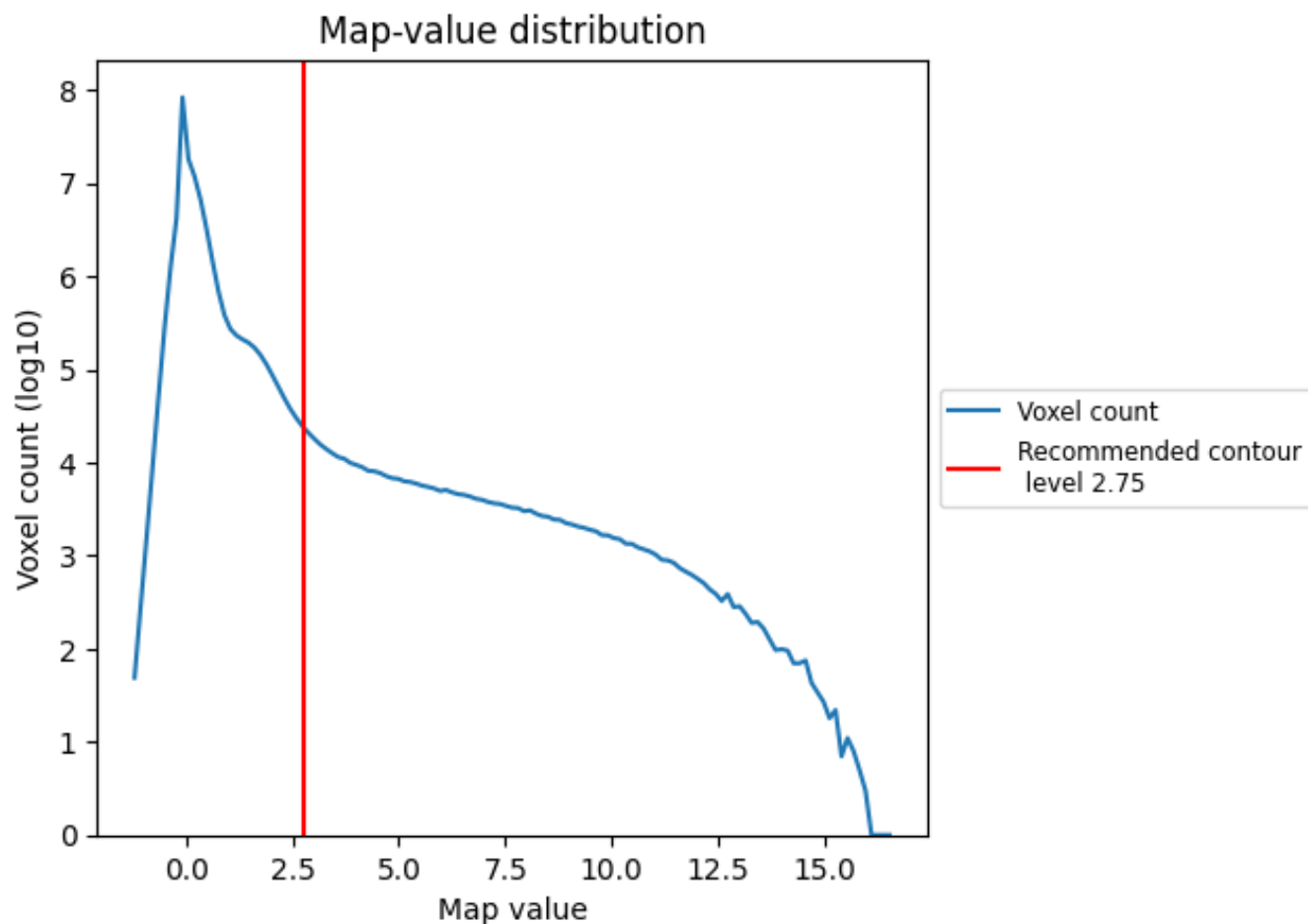
6.6 Mask visualisation

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

7 Map analysis [i](#)

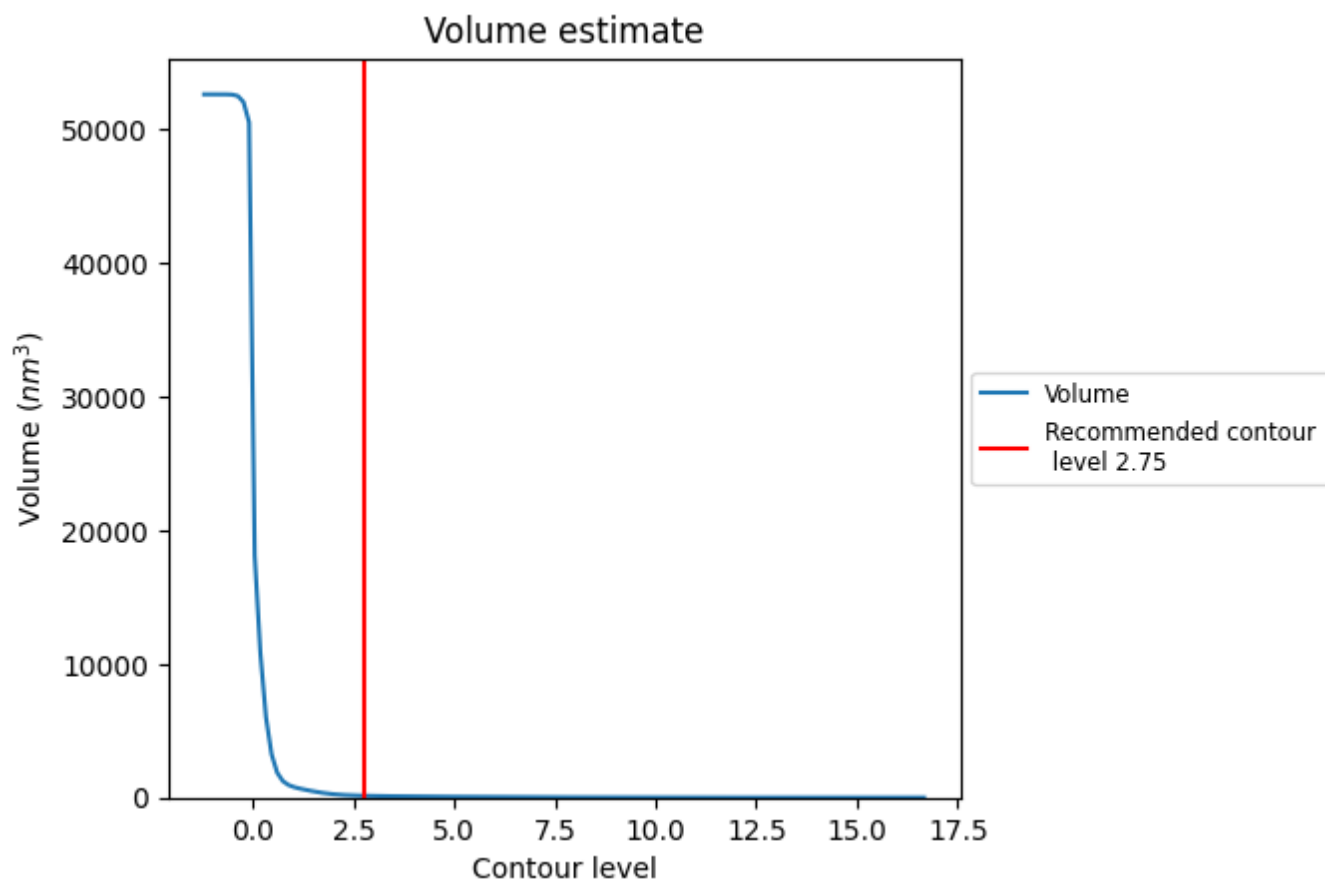
This section contains the results of statistical analysis of the map.

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.

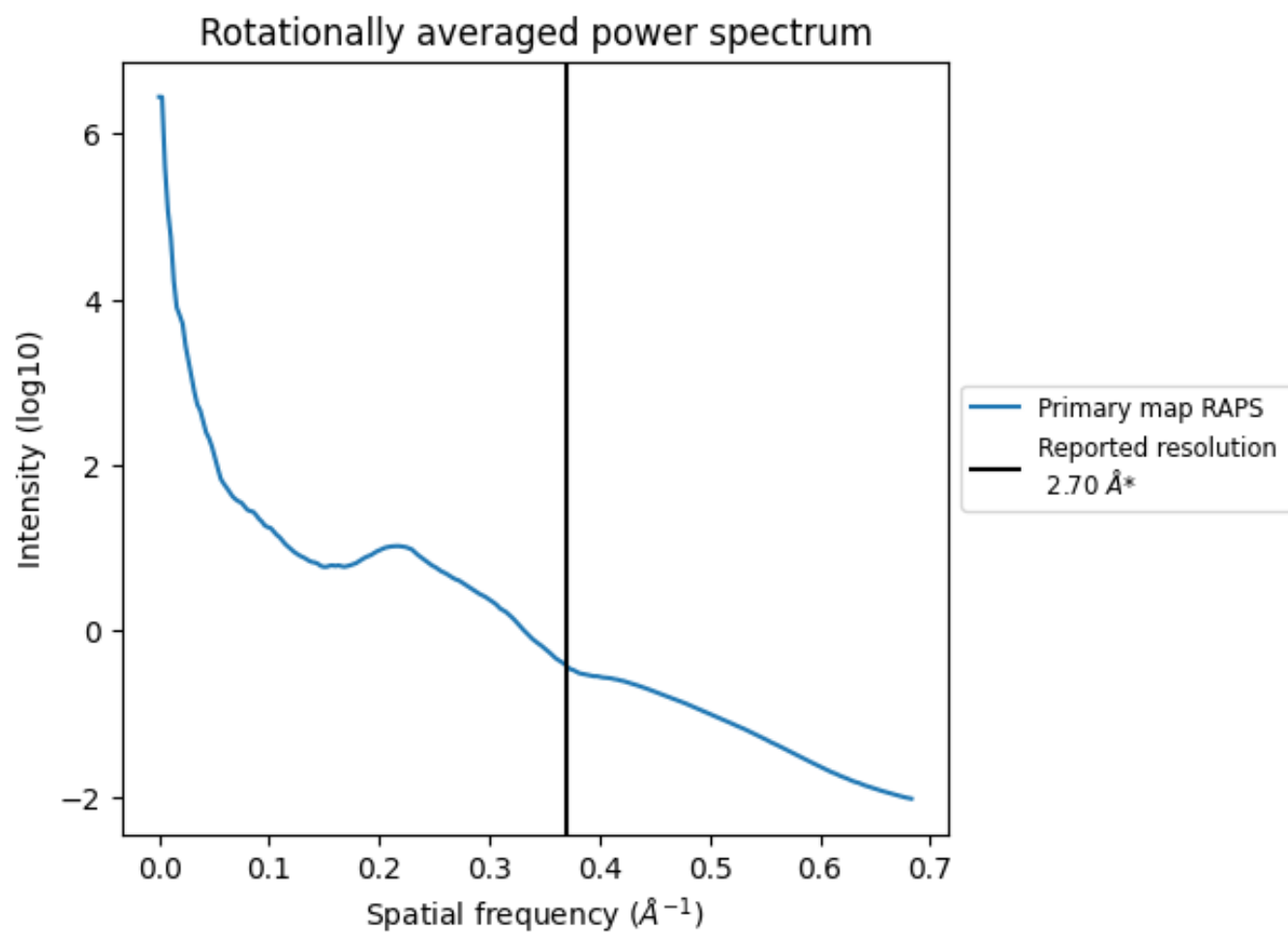
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 135 nm³; this corresponds to an approximate mass of 122 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 0.370 Å⁻¹

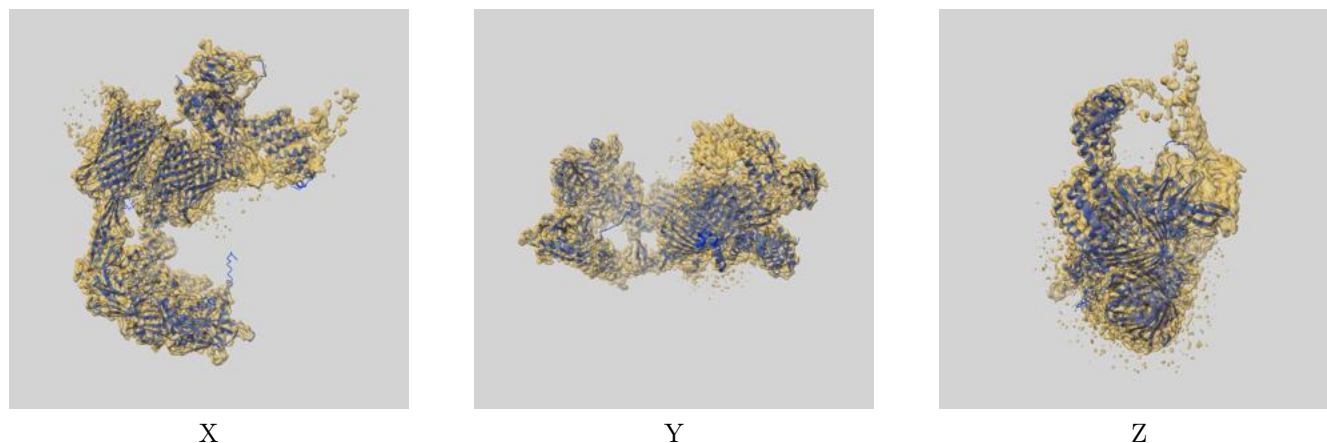
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

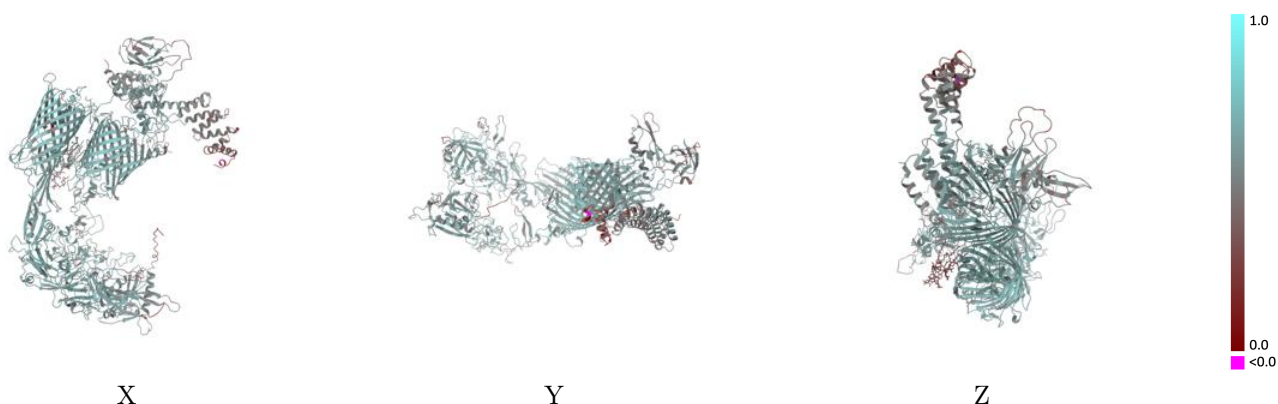
This section contains information regarding the fit between EMDB map EMD-48835 and PDB model 9N2D. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



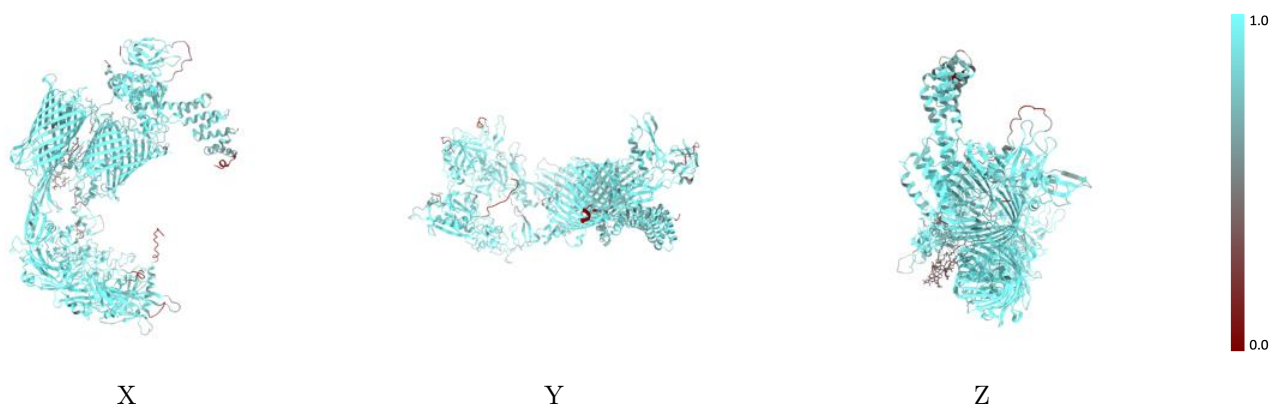
The images above show the 3D surface view of the map at the recommended contour level 2.75 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



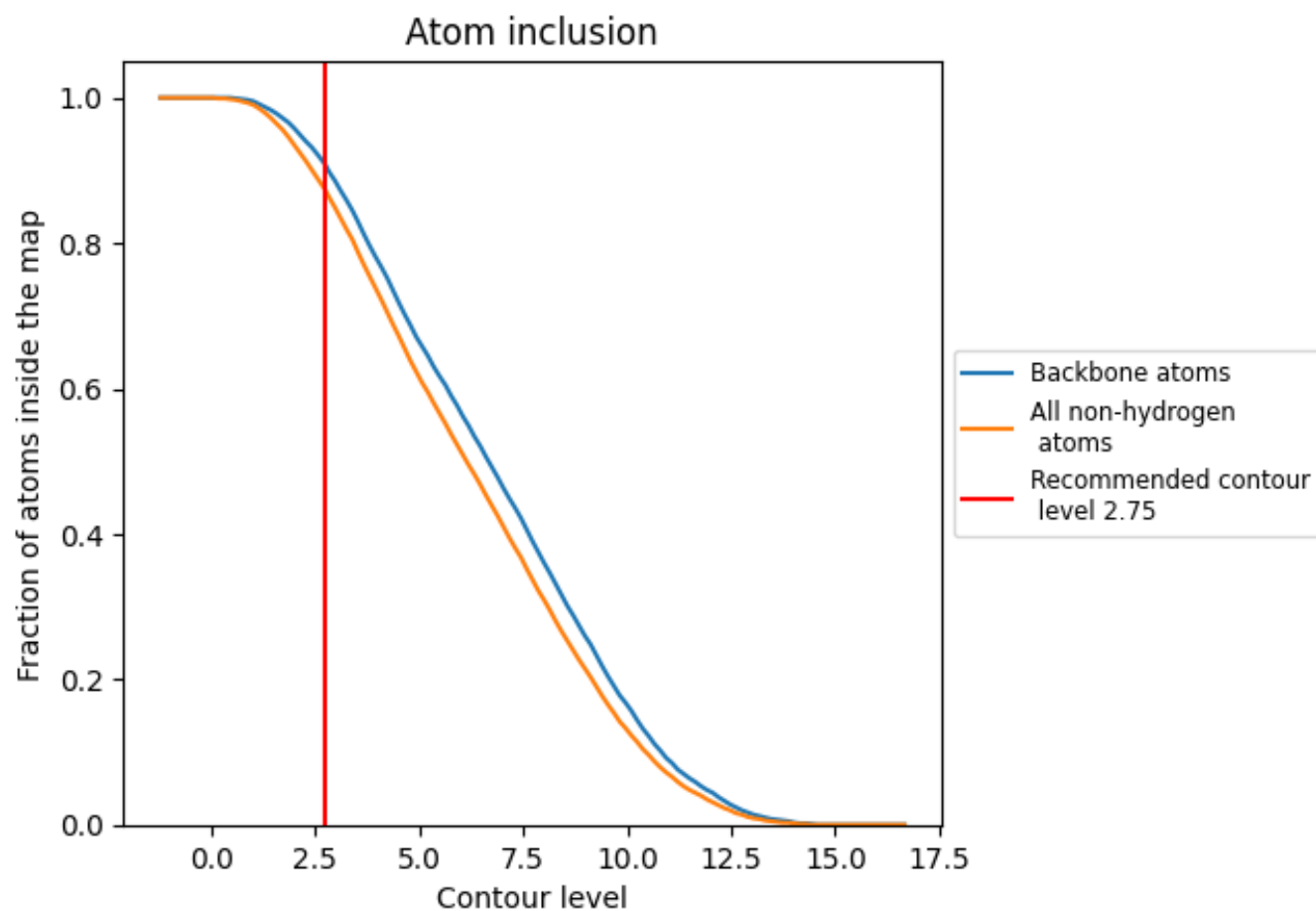
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (2.75).

9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 87% 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 (2.75) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8730	0.5560
A	0.8780	0.5680
B	0.9330	0.5990
C	0.9060	0.5770
D	0.8360	0.5460
E	0.7960	0.5070
F	0.8070	0.4600
G	0.7830	0.5080
J	0.9710	0.5880

1.0

0.0

<0.0