



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 05:18 AM UTC

PDB ID : 7DSN / pdb_00007dsn
EMDB ID : EMD-30839
Title : Overall structure of the LAT1-4F2hc bound with JX-119
Authors : Yan, R.H.; Li, Y.N.; Zhang, Y.Y.; Zhong, X.Y.; Zhou, Q.
Deposited on : 2020-12-31
Resolution : 3.10 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

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:

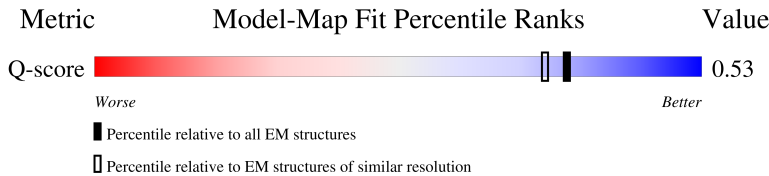
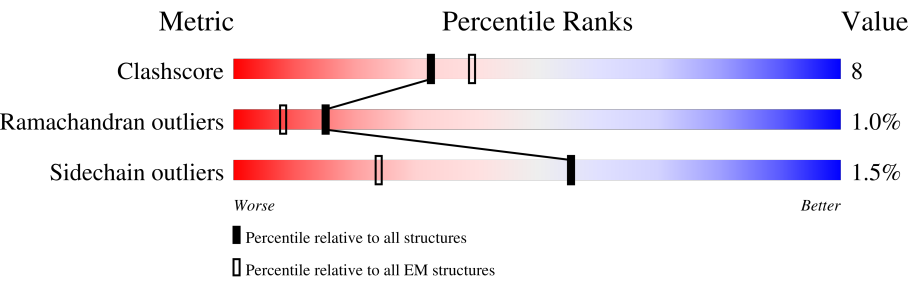
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.10 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14724 (2.60 - 3.60)

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	647	64% 8% 27%
2	B	527	11% 72% 13% 12%
3	C	2	50% 100%
3	D	2	50% 100%

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Mol	Chain	Length	Quality of chain
3	E	2	100% 50% 50%
3	F	2	100% 50% 50%

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
5	HO9	B	601	-	-	X	-
6	Y01	B	602	X	-	-	-
6	Y01	B	603	X	-	-	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7534 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 4F2 cell-surface antigen heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	471	Total	C	N	O	S	0	0
			3670	2348	629	686	7		

There are 17 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	initiating methionine	UNP J3KPF3
A	-12	ALA	-	expression tag	UNP J3KPF3
A	-11	HIS	-	expression tag	UNP J3KPF3
A	-10	HIS	-	expression tag	UNP J3KPF3
A	-9	HIS	-	expression tag	UNP J3KPF3
A	-8	HIS	-	expression tag	UNP J3KPF3
A	-7	HIS	-	expression tag	UNP J3KPF3
A	-6	HIS	-	expression tag	UNP J3KPF3
A	-5	HIS	-	expression tag	UNP J3KPF3
A	-4	HIS	-	expression tag	UNP J3KPF3
A	-3	HIS	-	expression tag	UNP J3KPF3
A	-2	HIS	-	expression tag	UNP J3KPF3
A	-1	SER	-	expression tag	UNP J3KPF3
A	0	GLY	-	expression tag	UNP J3KPF3
A	1	ARG	-	expression tag	UNP J3KPF3
A	632	LEU	-	expression tag	UNP J3KPF3
A	633	GLU	-	expression tag	UNP J3KPF3

- Molecule 2 is a protein called Large neutral amino acids transporter small subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	464	Total	C	N	O	S	0	0
			3586	2401	553	612	20		

There are 21 discrepancies between the modelled and reference sequences:

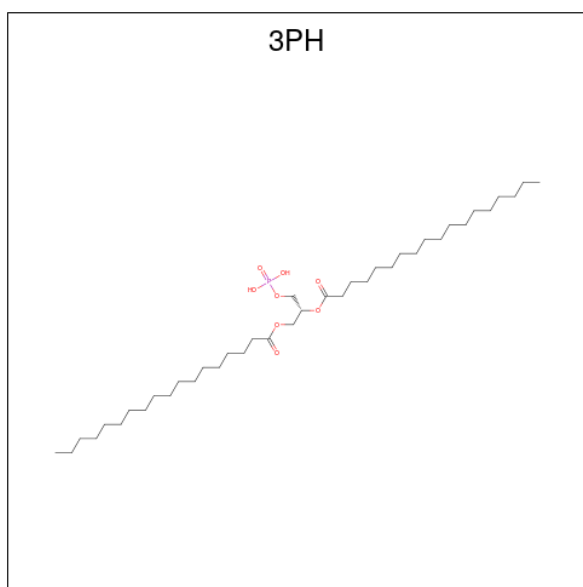
Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	MET	-	initiating methionine	UNP Q01650
B	-18	ALA	-	expression tag	UNP Q01650
B	-17	ASP	-	expression tag	UNP Q01650
B	-16	TYR	-	expression tag	UNP Q01650
B	-15	LYS	-	expression tag	UNP Q01650
B	-14	ASP	-	expression tag	UNP Q01650
B	-13	ASP	-	expression tag	UNP Q01650
B	-12	ASP	-	expression tag	UNP Q01650
B	-11	ASP	-	expression tag	UNP Q01650
B	-10	LYS	-	expression tag	UNP Q01650
B	-9	SER	-	expression tag	UNP Q01650
B	-8	GLY	-	expression tag	UNP Q01650
B	-7	PRO	-	expression tag	UNP Q01650
B	-6	ASP	-	expression tag	UNP Q01650
B	-5	GLU	-	expression tag	UNP Q01650
B	-4	VAL	-	expression tag	UNP Q01650
B	-3	ASP	-	expression tag	UNP Q01650
B	-2	ALA	-	expression tag	UNP Q01650
B	-1	SER	-	expression tag	UNP Q01650
B	0	GLY	-	expression tag	UNP Q01650
B	1	ARG	-	expression tag	UNP Q01650

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



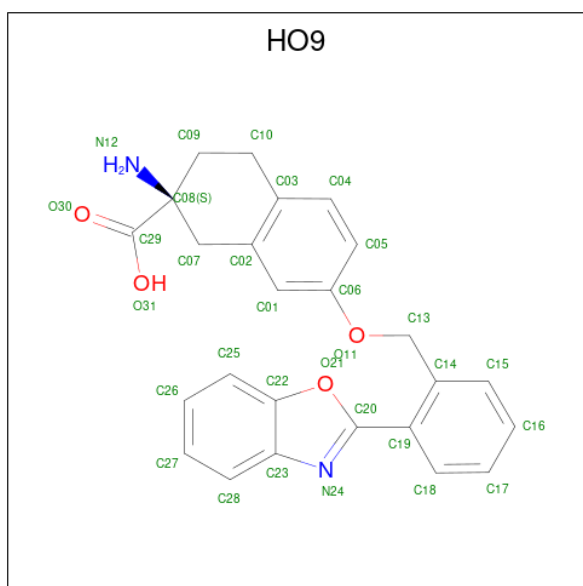
Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	2	Total	C	N	O	0	0
			28	16	2	10		
3	D	2	Total	C	N	O	0	0
			28	16	2	10		
3	E	2	Total	C	N	O	0	0
			28	16	2	10		
3	F	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (CCD ID: 3PH) (formula: C₃₉H₇₇O₈P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	O	P	0
			48	39	8	1	

- Molecule 5 is (2 {S})-2-azanyl-7-[[2-(1,3-benzoxazol-2-yl)phenyl]methoxy]-3,4-dihydro-1 {H}-naphthalene-2-carboxylic acid (CCD ID: HO9) (formula: $C_{25}H_{22}N_2O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
5	B	1	Total	C	N	O	0
			31	25	2	4	

- Molecule 6 is CHOLESTEROL HEMISUCCINATE (CCD ID: Y01) (formula: $C_{31}H_{50}O_4$).



Mol	Chain	Residues	Atoms			AltConf
6	B	1	Total 35	C 31	O 4	0
6	B	1	Total 35	C 31	O 4	0

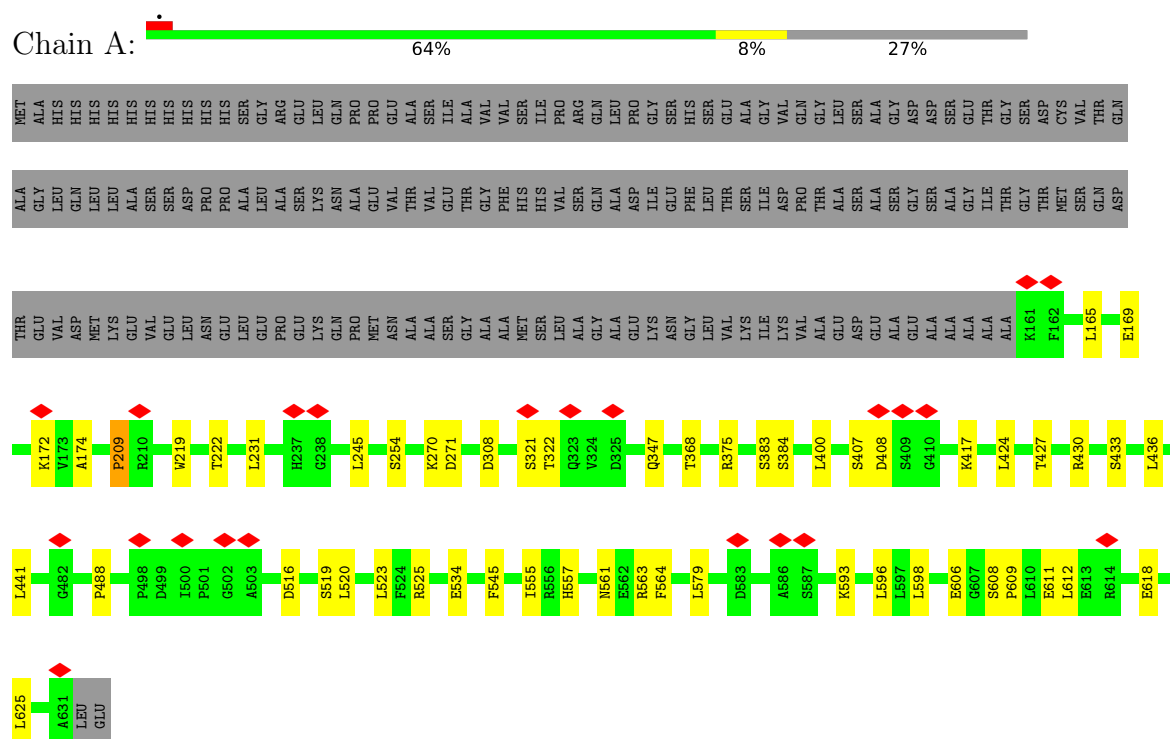
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	AltConf
7	B	17	Total O 17 17	0

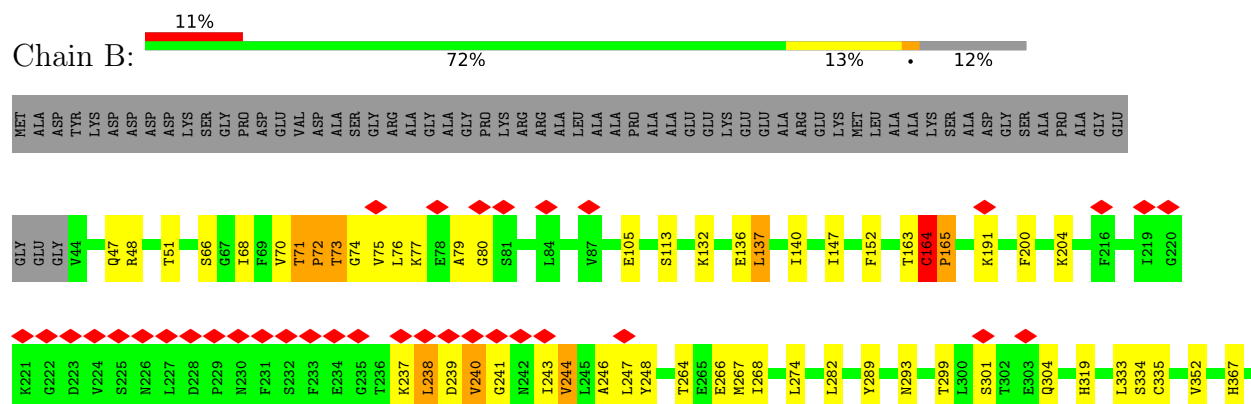
3 Residue-property plots

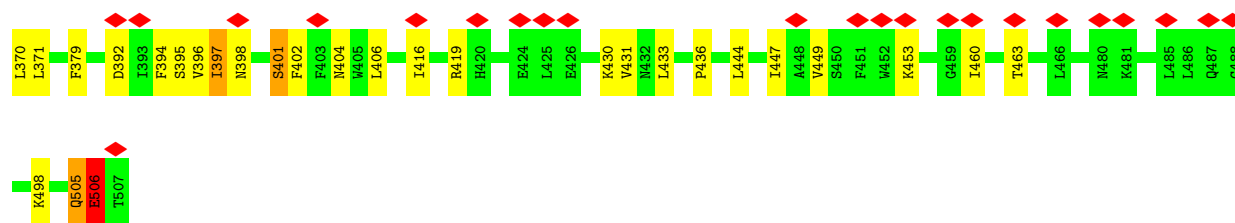
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: 4F2 cell-surface antigen heavy chain



- Molecule 2: Large neutral amino acids transporter small subunit 1





- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	641590	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.241	Depositor
Minimum map value	-0.142	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	278.272, 278.272, 278.272	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.087, 1.087, 1.087	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: HO9, 3PH, NAG, Y01

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	0.27	0/3755	0.57	2/5095 (0.0%)
2	B	0.30	0/3682	0.65	2/5033 (0.0%)
All	All	0.28	0/7437	0.61	4/10128 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	396	VAL	N-CA-C	-6.64	106.26	112.83
1	A	209	PRO	CA-C-N	5.43	131.91	121.54
1	A	209	PRO	C-N-CA	5.43	131.91	121.54
2	B	68	ILE	N-CA-C	-5.37	107.51	112.83

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	3670	0	3659	30	0
2	B	3586	0	3726	95	0
3	C	28	0	25	0	0
3	D	28	0	25	0	0
3	E	28	0	25	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	28	0	25	0	0
4	A	48	0	75	2	0
5	B	31	0	0	19	0
6	B	70	0	98	2	0
7	B	17	0	0	1	0
All	All	7534	0	7658	129	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (129) 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)
2:B:147:ILE:HG21	5:B:601:HO9:C27	1.37	1.51
2:B:147:ILE:HD13	5:B:601:HO9:C26	1.56	1.33
2:B:397:ILE:HD12	2:B:398:ASN:H	1.13	1.13
2:B:147:ILE:CG2	5:B:601:HO9:C27	2.27	1.12
2:B:248:TYR:OH	2:B:401:SER:HB3	1.53	1.08
2:B:397:ILE:HG22	5:B:601:HO9:O21	1.64	0.97
2:B:397:ILE:CD1	2:B:398:ASN:H	1.78	0.96
2:B:397:ILE:HD12	2:B:398:ASN:N	1.85	0.91
2:B:397:ILE:CD1	2:B:398:ASN:N	2.33	0.91
2:B:71:THR:H	2:B:72:PRO:HD2	1.35	0.88
2:B:397:ILE:CG2	5:B:601:HO9:O21	2.25	0.83
2:B:394:PHE:O	2:B:397:ILE:HG13	1.80	0.81
2:B:147:ILE:CD1	5:B:601:HO9:C26	2.51	0.79
2:B:147:ILE:HG21	5:B:601:HO9:C26	2.13	0.79
2:B:137:LEU:HD21	2:B:379:PHE:CZ	2.17	0.79
2:B:137:LEU:HD22	2:B:137:LEU:O	1.83	0.78
2:B:137:LEU:HD21	2:B:379:PHE:CE2	2.19	0.77
2:B:147:ILE:HD13	5:B:601:HO9:C27	2.15	0.77
2:B:71:THR:H	2:B:72:PRO:CD	1.97	0.76
2:B:397:ILE:CG2	5:B:601:HO9:C22	2.65	0.74
2:B:137:LEU:C	2:B:137:LEU:HD13	2.14	0.71
2:B:397:ILE:HD13	2:B:398:ASN:N	2.05	0.70
2:B:137:LEU:CD2	2:B:379:PHE:CE2	2.75	0.69
2:B:244:VAL:HG11	2:B:449:VAL:HG11	1.74	0.68
2:B:240:VAL:HA	2:B:243:ILE:HG12	1.74	0.68
2:B:70:VAL:O	2:B:71:THR:OG1	2.13	0.66
2:B:397:ILE:HG23	5:B:601:HO9:C25	2.27	0.65
2:B:75:VAL:O	2:B:79:ALA:HB3	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:601:HO9:C15	7:B:704:HOH:O	2.48	0.61
2:B:70:VAL:O	2:B:70:VAL:HG23	2.01	0.60
2:B:147:ILE:HD13	5:B:601:HO9:C25	2.29	0.60
2:B:397:ILE:CG2	5:B:601:HO9:C25	2.80	0.60
2:B:416:ILE:HD11	2:B:436:PRO:HB2	1.83	0.59
2:B:243:ILE:O	2:B:246:ALA:N	2.35	0.59
2:B:505:GLN:O	2:B:506:GLU:HB2	2.01	0.59
1:A:516:ASP:HB3	1:A:519:SER:HB2	1.84	0.59
2:B:113:SER:HB2	2:B:352:VAL:HG21	1.84	0.59
1:A:534:GLU:HG2	1:A:564:PHE:HE1	1.68	0.59
2:B:241:GLY:O	2:B:453:LYS:NZ	2.31	0.58
2:B:71:THR:C	2:B:73:THR:H	2.11	0.58
1:A:407:SER:OG	1:A:436:LEU:O	2.22	0.58
2:B:137:LEU:CD2	2:B:379:PHE:HE2	2.15	0.58
2:B:289:TYR:O	2:B:293:ASN:ND2	2.34	0.58
2:B:140:ILE:HD12	5:B:601:HO9:C17	2.34	0.57
2:B:243:ILE:O	2:B:246:ALA:HB3	2.04	0.57
2:B:137:LEU:HD23	2:B:379:PHE:HE2	1.69	0.57
2:B:47:GLN:HG3	2:B:371:LEU:HD13	1.87	0.57
1:A:427:THR:O	1:A:430:ARG:NH1	2.38	0.56
2:B:204:LYS:HZ2	2:B:334:SER:HA	1.71	0.56
2:B:404:ASN:OD1	5:B:601:HO9:C16	2.53	0.55
2:B:239:ASP:C	2:B:241:GLY:H	2.13	0.55
2:B:397:ILE:HG23	5:B:601:HO9:C22	2.36	0.54
2:B:243:ILE:HG22	2:B:247:LEU:CD2	2.38	0.54
2:B:240:VAL:HA	2:B:243:ILE:CG1	2.37	0.54
2:B:397:ILE:HD12	2:B:397:ILE:N	2.23	0.54
2:B:397:ILE:HD13	2:B:398:ASN:CG	2.33	0.53
1:A:368:THR:HG22	1:A:375:ARG:HB3	1.90	0.53
2:B:48:ARG:NH2	2:B:267:MET:O	2.42	0.52
1:A:174:ALA:HB2	2:B:498:LYS:HG2	1.91	0.52
1:A:383:SER:HA	3:E:1:NAG:H82	1.91	0.52
1:A:561:ASN:O	1:A:563:ARG:NH1	2.43	0.52
1:A:417:LYS:NZ	1:A:545:PHE:O	2.42	0.51
2:B:163:THR:C	2:B:164:CYS:SG	2.93	0.50
2:B:147:ILE:CD1	5:B:601:HO9:C27	2.86	0.49
2:B:404:ASN:CG	5:B:601:HO9:C16	2.85	0.49
1:A:545:PHE:HE1	1:A:579:LEU:HD22	1.77	0.49
2:B:301:SER:H	2:B:304:GLN:HE21	1.60	0.48
2:B:113:SER:OG	2:B:264:THR:O	2.27	0.48
2:B:132:LYS:NZ	2:B:136:GLU:OE2	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:75:VAL:O	2:B:79:ALA:CB	2.61	0.48
1:A:400:LEU:HD22	1:A:433:SER:HB2	1.96	0.48
2:B:239:ASP:C	2:B:240:VAL:HG23	2.37	0.47
2:B:267:MET:HE1	2:B:274:LEU:HD13	1.96	0.47
2:B:419:ARG:HD3	2:B:430:LYS:HZ1	1.79	0.47
2:B:191:LYS:NZ	6:B:603:Y01:OAG	2.41	0.47
1:A:231:LEU:HD11	1:A:245:LEU:HD22	1.96	0.47
1:A:169:GLU:HA	1:A:172:LYS:HE2	1.97	0.47
2:B:164:CYS:CB	2:B:165:PRO:CD	2.93	0.46
1:A:384:SER:OG	1:A:408:ASP:OD2	2.31	0.46
2:B:237:LYS:O	2:B:243:ILE:HD11	2.15	0.46
1:A:612:LEU:HD21	1:A:625:LEU:HD22	1.98	0.46
2:B:71:THR:C	2:B:73:THR:N	2.73	0.46
1:A:555:ILE:HG22	1:A:557:HIS:HD2	1.79	0.46
2:B:71:THR:O	2:B:71:THR:HG22	2.16	0.45
1:A:519:SER:OG	1:A:520:LEU:N	2.49	0.45
2:B:395:SER:O	2:B:395:SER:OG	2.31	0.45
1:A:308:ASP:OD2	1:A:347:GLN:NE2	2.50	0.45
2:B:406:LEU:HB2	2:B:447:ILE:HD12	1.98	0.45
2:B:243:ILE:HG22	2:B:247:LEU:HD23	1.98	0.45
5:B:601:HO9:C13	5:B:601:HO9:N24	2.80	0.45
1:A:441:LEU:HD11	1:A:488:PRO:HG3	1.98	0.44
2:B:73:THR:O	2:B:76:LEU:N	2.49	0.44
2:B:66:SER:O	2:B:70:VAL:HG22	2.17	0.44
2:B:164:CYS:HB2	2:B:165:PRO:CD	2.48	0.44
2:B:367:HIS:HD2	2:B:370:LEU:HB2	1.83	0.43
2:B:444:LEU:HA	2:B:447:ILE:HG22	1.99	0.43
2:B:237:LYS:HD2	2:B:237:LYS:N	2.34	0.43
4:A:701:3PH:H2C1	4:A:701:3PH:H2F2	1.83	0.43
1:A:254:SER:OG	1:A:525:ARG:NE	2.48	0.43
2:B:164:CYS:HB2	2:B:165:PRO:HD2	2.01	0.43
1:A:523:LEU:HD11	1:A:598:LEU:HD21	2.00	0.43
2:B:392:ASP:OD1	2:B:392:ASP:N	2.51	0.43
2:B:48:ARG:HG2	2:B:266:GLU:HA	2.00	0.43
2:B:51:THR:HG23	2:B:268:ILE:HD11	2.01	0.43
1:A:534:GLU:HG2	1:A:564:PHE:CE1	2.51	0.43
2:B:71:THR:O	2:B:73:THR:N	2.52	0.43
2:B:238:LEU:C	2:B:240:VAL:H	2.27	0.43
2:B:402:PHE:HB2	2:B:447:ILE:HG13	2.01	0.42
2:B:460:ILE:O	2:B:463:THR:OG1	2.37	0.42
2:B:397:ILE:CD1	2:B:398:ASN:OD1	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:105:GLU:HG2	2:B:431:VAL:HB	2.00	0.42
2:B:239:ASP:C	2:B:241:GLY:N	2.78	0.42
2:B:246:ALA:C	2:B:248:TYR:N	2.77	0.42
2:B:74:GLY:HA2	2:B:77:LYS:HE3	2.01	0.42
4:A:701:3PH:H281	4:A:701:3PH:H252	1.82	0.41
2:B:137:LEU:C	2:B:137:LEU:CD1	2.86	0.41
1:A:596:LEU:HD23	1:A:606:GLU:HA	2.01	0.41
2:B:152:PHE:HB2	2:B:335:CYS:HB2	2.03	0.41
2:B:200:PHE:HE2	2:B:333:LEU:HD22	1.85	0.41
1:A:270:LYS:HD3	1:A:270:LYS:HA	1.89	0.41
1:A:608:SER:HA	1:A:609:PRO:HD3	1.90	0.41
2:B:80:GLY:HA3	2:B:237:LYS:HD3	2.03	0.41
2:B:299:THR:OG1	2:B:319:HIS:NE2	2.42	0.41
1:A:593:LYS:HA	1:A:611:GLU:HA	2.02	0.40
6:B:603:Y01:HAC1	6:B:603:Y01:HAP1	1.95	0.40
1:A:270:LYS:HG3	1:A:271:ASP:H	1.85	0.40
1:A:424:LEU:HD23	1:A:424:LEU:HA	1.94	0.40
1:A:165:LEU:HD22	1:A:169:GLU:HG3	2.03	0.40
1:A:219:TRP:O	1:A:222:THR:OG1	2.35	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	A	469/647 (72%)	431 (92%)	35 (8%)	3 (1%)	21	52
2	B	462/527 (88%)	429 (93%)	27 (6%)	6 (1%)	9	35
All	All	931/1174 (79%)	860 (92%)	62 (7%)	9 (1%)	15	41

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	71	THR
2	B	240	VAL
2	B	506	GLU
1	A	209	PRO
1	A	321	SER
2	B	164	CYS
2	B	165	PRO
1	A	322	THR
2	B	72	PRO

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	394/529 (74%)	393 (100%)	1 (0%)	86	87
2	B	395/435 (91%)	384 (97%)	11 (3%)	38	66
All	All	789/964 (82%)	777 (98%)	12 (2%)	55	75

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	618	GLU
2	B	73	THR
2	B	137	LEU
2	B	164	CYS
2	B	238	LEU
2	B	244	VAL
2	B	282	LEU
2	B	397	ILE
2	B	401	SER
2	B	433	LEU
2	B	505	GLN
2	B	506	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	539	HIS
1	A	601	GLN
2	B	47	GLN
2	B	49	ASN
2	B	186	ASN
2	B	261	ASN
2	B	304	GLN
2	B	340	ASN

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 ⓘ

8 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
3	NAG	C	1	3,1	14,14,15	0.29	0	17,19,21	0.58	0
3	NAG	C	2	3	14,14,15	0.45	0	17,19,21	0.54	0
3	NAG	D	1	3,1	14,14,15	0.62	1 (7%)	17,19,21	0.93	0
3	NAG	D	2	3	14,14,15	0.34	0	17,19,21	0.74	1 (5%)
3	NAG	E	1	3,1	14,14,15	0.54	0	17,19,21	0.98	1 (5%)
3	NAG	E	2	3	14,14,15	0.28	0	17,19,21	0.60	1 (5%)
3	NAG	F	1	3,1	14,14,15	0.61	1 (7%)	17,19,21	0.95	1 (5%)
3	NAG	F	2	3	14,14,15	0.25	0	17,19,21	0.55	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	C	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	C	2	3	-	2/6/23/26	0/1/1/1
3	NAG	D	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1
3	NAG	E	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	0/6/23/26	0/1/1/1
3	NAG	F	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	F	2	3	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1	NAG	O5-C1	-2.10	1.40	1.43
3	F	1	NAG	O5-C1	-2.01	1.40	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1	NAG	C1-O5-C5	3.27	116.56	112.19
3	D	2	NAG	C1-O5-C5	2.31	115.28	112.19
3	F	1	NAG	C3-C4-C5	2.21	114.24	110.23
3	E	2	NAG	C1-O5-C5	2.04	114.93	112.19

There are no chirality outliers.

All (11) torsion outliers are listed below:

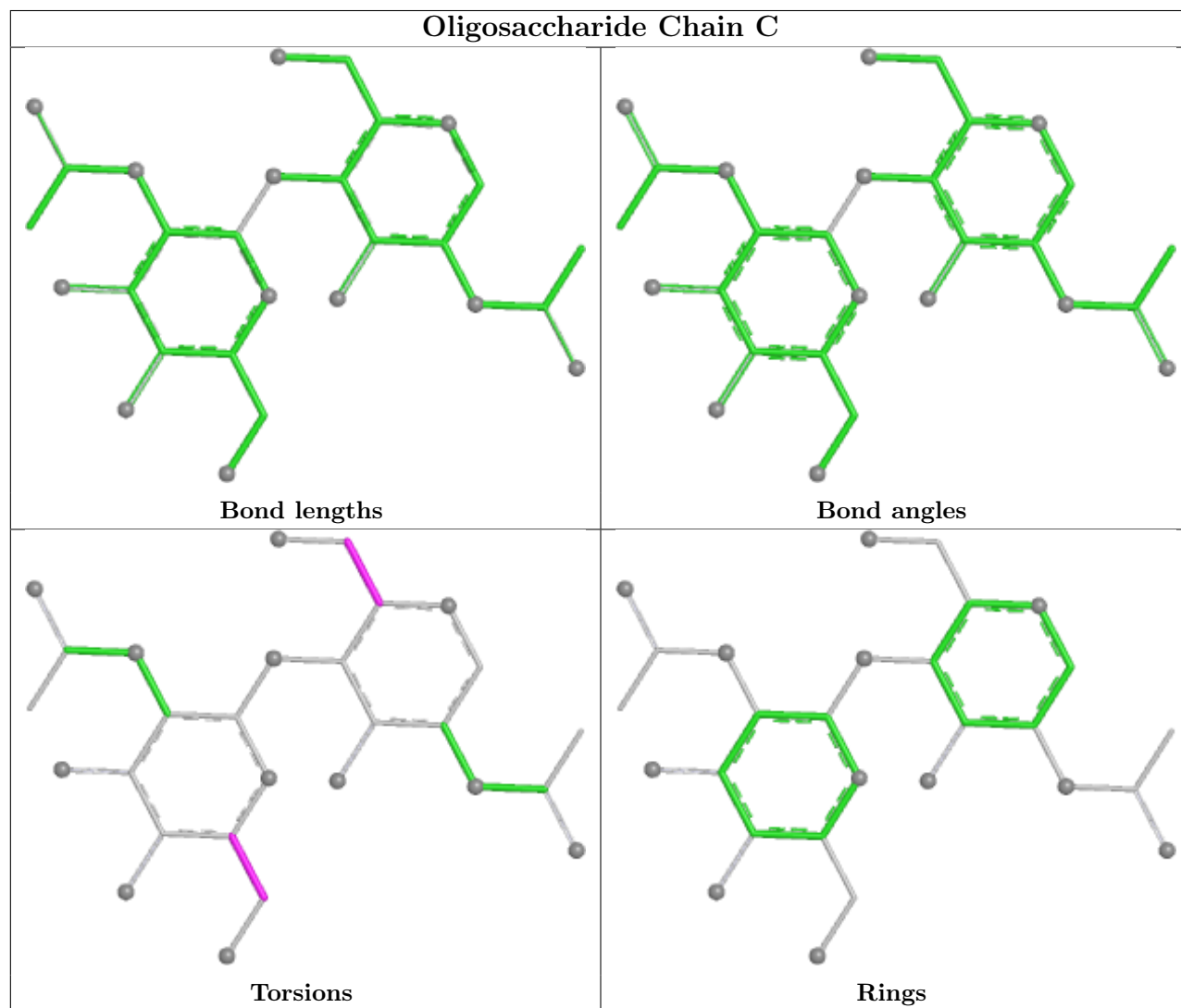
Mol	Chain	Res	Type	Atoms
3	F	1	NAG	O5-C5-C6-O6
3	F	1	NAG	C4-C5-C6-O6
3	D	1	NAG	O5-C5-C6-O6
3	C	2	NAG	O5-C5-C6-O6
3	D	2	NAG	C8-C7-N2-C2
3	D	2	NAG	O7-C7-N2-C2
3	C	2	NAG	C4-C5-C6-O6
3	D	1	NAG	C4-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6
3	C	1	NAG	O5-C5-C6-O6

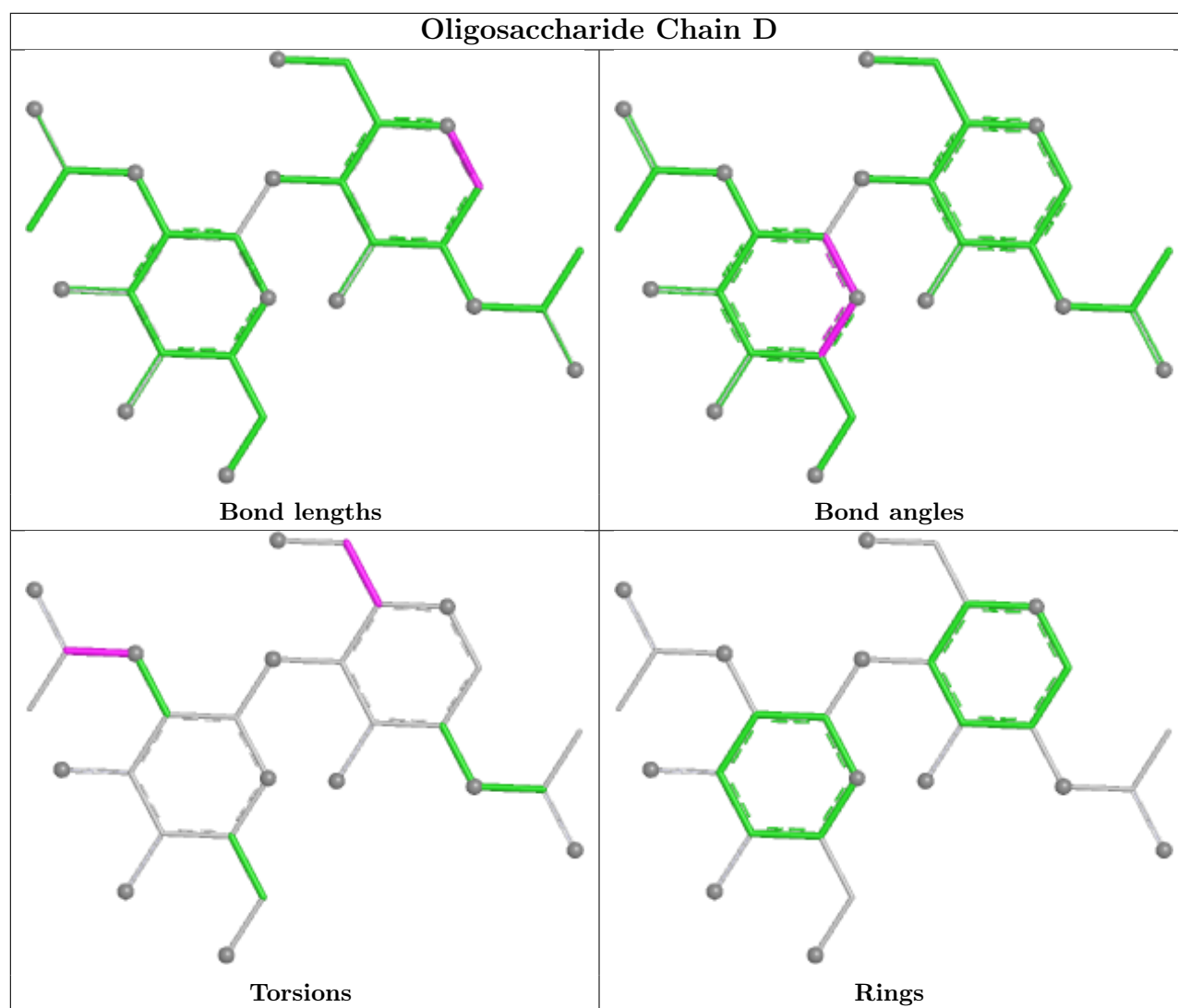
There are no ring outliers.

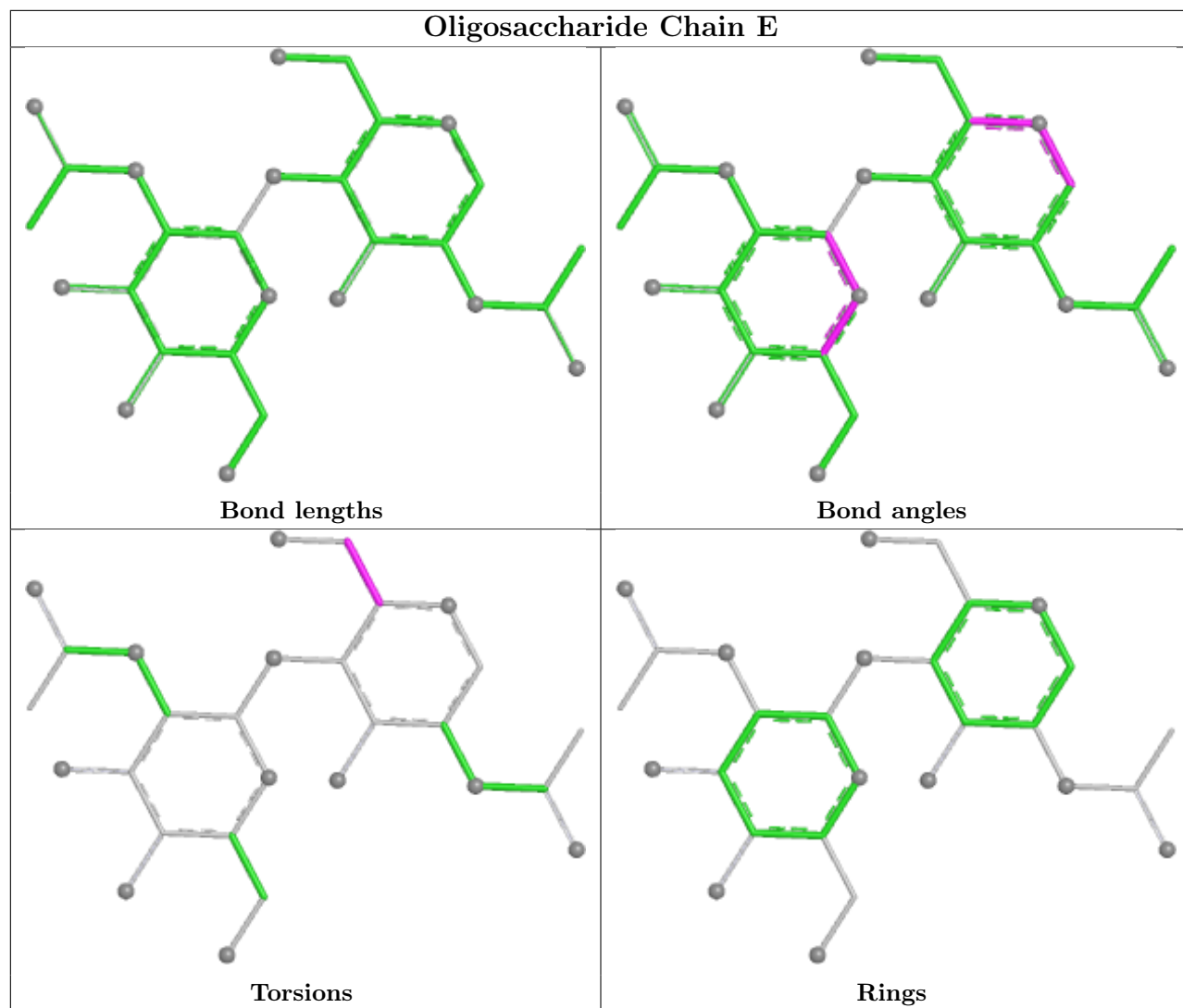
1 monomer is involved in 1 short contact:

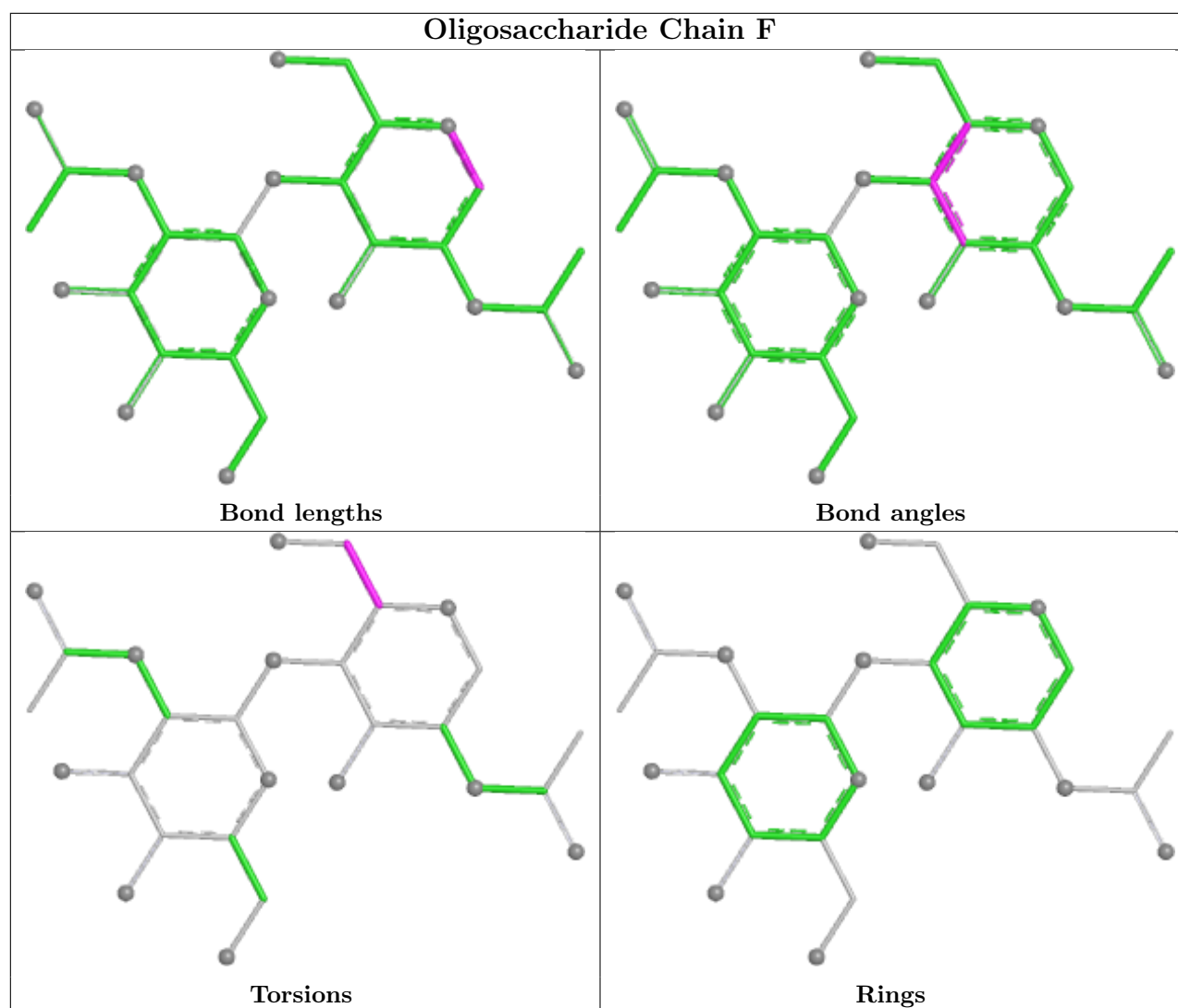
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	1	NAG	1	0

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](#)

4 ligands 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	$\# Z > 2$
5	HO9	B	601	-	33,35,35	6.12	26 (78%)	44,51,51	1.83	11 (25%)
6	Y01	B	603	-	38,38,38	3.42	15 (39%)	57,57,57	2.41	15 (26%)
6	Y01	B	602	-	38,38,38	3.46	15 (39%)	57,57,57	2.40	19 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	3PH	A	701	-	47,47,47	0.94	2 (4%)	50,52,52	1.08	3 (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
5	HO9	B	601	-	-	0/14/26/26	0/5/5/5
4	3PH	A	701	-	-	7/49/49/49	-
6	Y01	B	602	-	5/5/12/13	11/19/77/77	0/4/4/4
6	Y01	B	603	-	5/5/12/13	11/19/77/77	0/4/4/4

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	603	Y01	CAI-CAZ	11.11	1.55	1.33
6	B	602	Y01	CAI-CAZ	11.06	1.55	1.33
5	B	601	HO9	C28-C23	10.81	1.57	1.40
5	B	601	HO9	C05-C04	9.53	1.54	1.38
5	B	601	HO9	C01-C06	9.13	1.54	1.39
6	B	602	Y01	CBI-CBG	-8.72	1.39	1.55
5	B	601	HO9	C19-C14	8.65	1.52	1.40
5	B	601	HO9	C05-C06	8.64	1.54	1.38
5	B	601	HO9	C18-C19	8.54	1.52	1.39
5	B	601	HO9	C25-C22	8.37	1.56	1.39
5	B	601	HO9	C16-C15	8.28	1.53	1.38
5	B	601	HO9	C17-C18	8.26	1.53	1.38
5	B	601	HO9	C04-C03	8.20	1.52	1.39
5	B	601	HO9	C15-C14	8.19	1.52	1.39
6	B	603	Y01	CBI-CBG	-7.91	1.40	1.55
5	B	601	HO9	C01-C02	7.91	1.51	1.39
5	B	601	HO9	C03-C02	7.46	1.54	1.40
5	B	601	HO9	C26-C25	7.10	1.51	1.38
5	B	601	HO9	C27-C28	6.94	1.50	1.38
5	B	601	HO9	C16-C17	6.80	1.53	1.38
6	B	603	Y01	CBD-CBG	6.45	1.65	1.53
6	B	603	Y01	CAK-CAI	6.43	1.63	1.50
6	B	602	Y01	CBH-CBF	6.42	1.66	1.56
6	B	602	Y01	CAK-CAI	6.35	1.63	1.50
6	B	602	Y01	CBD-CBG	6.16	1.65	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	603	Y01	CBH-CBF	6.06	1.65	1.56
6	B	603	Y01	CAU-CBI	5.03	1.62	1.54
6	B	602	Y01	CAU-CBI	4.90	1.62	1.54
5	B	601	HO9	C27-C26	4.76	1.48	1.38
5	B	601	HO9	C10-C03	4.67	1.59	1.51
4	A	701	3PH	O31-C31	4.21	1.45	1.33
6	B	602	Y01	CAQ-CBG	4.01	1.62	1.54
6	B	603	Y01	CAQ-CBG	3.92	1.62	1.54
4	A	701	3PH	O21-C21	3.83	1.45	1.34
6	B	602	Y01	CAV-CAZ	3.75	1.59	1.51
5	B	601	HO9	C07-C02	3.48	1.57	1.50
6	B	603	Y01	CAT-CBH	3.48	1.60	1.54
6	B	603	Y01	CAV-CAZ	3.43	1.58	1.51
6	B	602	Y01	CAP-CBE	-3.37	1.47	1.54
5	B	601	HO9	C07-C08	-3.30	1.50	1.54
6	B	603	Y01	CAP-CBE	-3.20	1.47	1.54
5	B	601	HO9	C23-N24	-3.16	1.33	1.39
6	B	603	Y01	OAW-CAY	3.08	1.43	1.34
6	B	602	Y01	CAT-CBH	3.07	1.59	1.54
6	B	603	Y01	CBI-CBE	3.06	1.60	1.55
6	B	602	Y01	OAW-CAY	3.03	1.42	1.34
6	B	602	Y01	OAW-CBC	-3.02	1.39	1.46
5	B	601	HO9	O21-C22	-2.97	1.33	1.38
6	B	603	Y01	OAW-CBC	-2.93	1.39	1.46
6	B	603	Y01	CAR-CBC	2.92	1.58	1.51
6	B	602	Y01	CAR-CBC	2.74	1.58	1.51
5	B	601	HO9	C09-C08	-2.72	1.51	1.54
6	B	602	Y01	CBI-CBE	2.66	1.59	1.55
6	B	603	Y01	CAS-CBF	-2.60	1.49	1.53
5	B	601	HO9	C20-N24	2.60	1.36	1.30
5	B	601	HO9	C19-C20	2.57	1.52	1.47
6	B	602	Y01	CAS-CBF	-2.42	1.49	1.53
5	B	601	HO9	C09-C10	-2.05	1.48	1.52

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	602	Y01	CAU-CBI-CBE	-7.41	105.69	116.60
6	B	603	Y01	CAU-CBI-CBE	-7.39	105.72	116.60
6	B	602	Y01	CAK-CAI-CAZ	-6.23	114.51	125.02
6	B	603	Y01	CAD-CBH-CBF	-5.99	104.94	111.66
6	B	602	Y01	CAV-CAZ-CAI	-5.60	112.98	120.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	601	HO9	O21-C20-N24	-5.56	108.40	115.10
6	B	603	Y01	CBF-CBD-CBG	5.31	116.02	109.09
6	B	603	Y01	CAK-CAI-CAZ	-5.02	116.55	125.02
6	B	602	Y01	CBI-CBE-CBB	-4.91	111.92	119.50
6	B	603	Y01	CBG-CBI-CBE	4.39	105.14	100.10
6	B	603	Y01	OAW-CAY-CAM	4.13	120.42	111.48
6	B	603	Y01	CAV-CAZ-CAI	-4.11	115.00	120.57
6	B	603	Y01	CBI-CBE-CBB	-4.07	113.22	119.50
6	B	602	Y01	CBH-CAZ-CAI	-4.06	117.01	122.93
6	B	602	Y01	OAW-CAY-CAM	4.05	120.23	111.48
6	B	603	Y01	CAT-CBH-CBF	3.82	113.80	108.74
6	B	603	Y01	CBF-CBH-CAZ	3.82	115.24	109.65
6	B	602	Y01	CBF-CBH-CAZ	3.80	115.22	109.65
4	A	701	3PH	O21-C21-C22	3.63	119.33	111.48
6	B	602	Y01	CAD-CBH-CAT	-3.53	104.06	109.43
5	B	601	HO9	C22-O21-C20	3.35	107.50	104.06
5	B	601	HO9	C23-N24-C20	3.32	108.14	104.53
5	B	601	HO9	O21-C20-C19	3.23	127.46	118.58
6	B	603	Y01	CAD-CBH-CAT	-3.17	104.60	109.43
6	B	602	Y01	CBF-CBD-CBG	3.14	113.19	109.09
5	B	601	HO9	C25-C22-C23	-3.07	119.89	123.62
5	B	601	HO9	C14-C19-C20	-2.92	117.72	122.88
6	B	602	Y01	CBG-CBI-CBE	2.92	103.45	100.10
5	B	601	HO9	C13-C14-C19	-2.88	117.86	122.06
6	B	602	Y01	CAD-CBH-CAZ	-2.86	104.02	108.38
5	B	601	HO9	C10-C03-C02	-2.86	114.67	120.77
6	B	602	Y01	CAD-CBH-CBF	-2.81	108.50	111.66
4	A	701	3PH	O31-C31-C32	2.69	120.05	111.83
6	B	602	Y01	CAT-CBH-CBF	2.67	112.27	108.74
5	B	601	HO9	O21-C22-C25	2.62	132.01	126.49
5	B	601	HO9	O31-C29-C08	2.59	120.61	113.69
6	B	602	Y01	CBI-CBG-CBD	-2.58	110.75	114.41
6	B	603	Y01	CAT-CAR-CBC	2.56	114.51	110.33
6	B	602	Y01	CAP-CBE-CBB	2.52	115.99	112.18
6	B	602	Y01	CAJ-CAO-CBB	-2.50	108.09	115.08
6	B	603	Y01	CAU-CBI-CBG	2.49	110.97	107.25
6	B	603	Y01	CBC-OAW-CAY	-2.43	111.98	117.80
6	B	602	Y01	CBD-CAK-CAI	-2.40	109.44	112.76
6	B	602	Y01	CAC-CBB-CAO	-2.26	106.84	110.34
4	A	701	3PH	C2-O21-C21	-2.14	112.66	117.80
5	B	601	HO9	C10-C03-C04	2.10	125.44	121.05
6	B	602	Y01	CBC-OAW-CAY	-2.09	112.80	117.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	603	Y01	CBH-CAZ-CAI	-2.08	119.89	122.93

All (10) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	B	602	Y01	CBF
6	B	602	Y01	CBI
6	B	602	Y01	CBD
6	B	602	Y01	CBB
6	B	602	Y01	CBH
6	B	603	Y01	CBF
6	B	603	Y01	CBI
6	B	603	Y01	CBD
6	B	603	Y01	CBB
6	B	603	Y01	CBH

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	602	Y01	CAO-CBB-CBE-CAP
6	B	602	Y01	CAO-CBB-CBE-CBI
6	B	602	Y01	CAC-CBB-CBE-CAP
6	B	602	Y01	CAM-CAY-OAW-CBC
6	B	603	Y01	CAO-CBB-CBE-CAP
6	B	603	Y01	CAC-CBB-CBE-CAP
6	B	603	Y01	CAM-CAY-OAW-CBC
6	B	603	Y01	CAX-CAL-CAM-CAY
6	B	602	Y01	CAC-CBB-CBE-CBI
6	B	603	Y01	OAG-CAY-OAW-CBC
6	B	602	Y01	OAG-CAY-OAW-CBC
6	B	603	Y01	CAO-CBB-CBE-CBI
6	B	603	Y01	CAC-CBB-CBE-CBI
6	B	603	Y01	CAN-CAJ-CAO-CBB
6	B	602	Y01	CAX-CAL-CAM-CAY
6	B	603	Y01	CAJ-CAN-CBA-CAA
6	B	603	Y01	CAJ-CAN-CBA-CAB
4	A	701	3PH	C3A-C3B-C3C-C3D
4	A	701	3PH	C3C-C3D-C3E-C3F
6	B	602	Y01	CAJ-CAN-CBA-CAA
6	B	602	Y01	CAJ-CAN-CBA-CAB
4	A	701	3PH	C3E-C3F-C3G-C3H
4	A	701	3PH	C2D-C2E-C2F-C2G

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Mol	Chain	Res	Type	Atoms
4	A	701	3PH	C39-C3A-C3B-C3C
6	B	603	Y01	CAO-CAJ-CAN-CBA
4	A	701	3PH	C1-O11-P-O13
4	A	701	3PH	C1-O11-P-O12
6	B	602	Y01	CAL-CAM-CAY-OAW
6	B	602	Y01	CAL-CAM-CAY-OAG

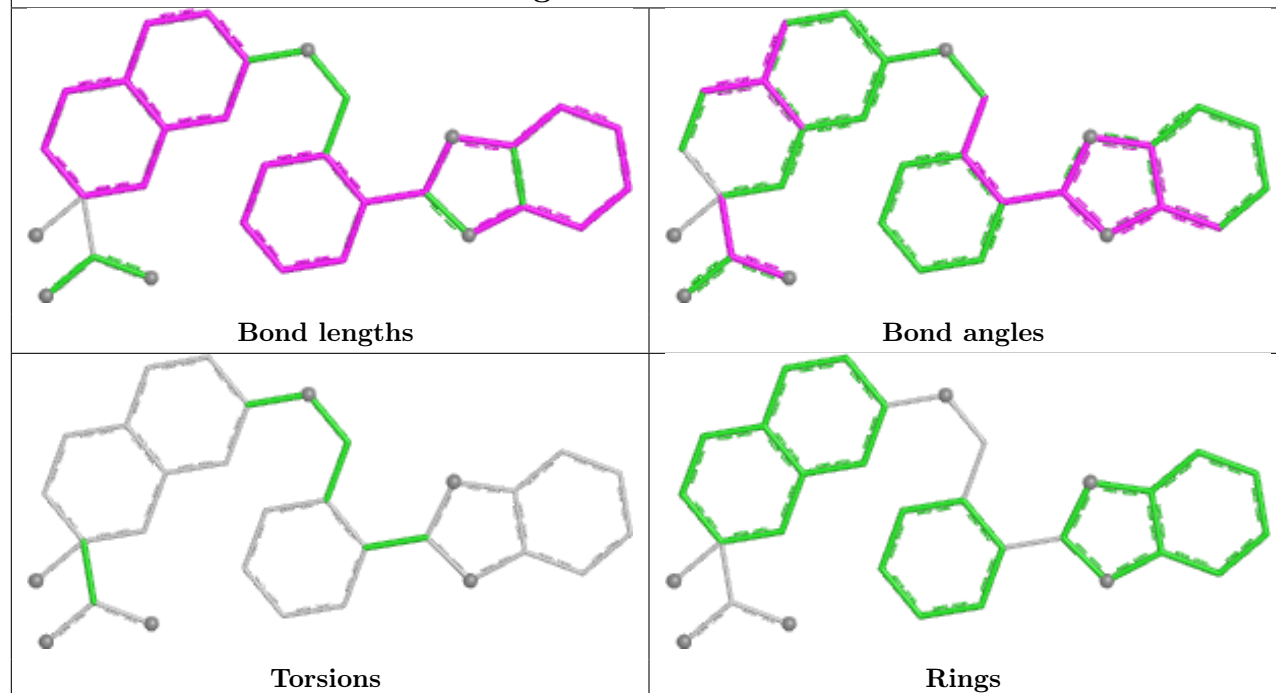
There are no ring outliers.

3 monomers are involved in 23 short contacts:

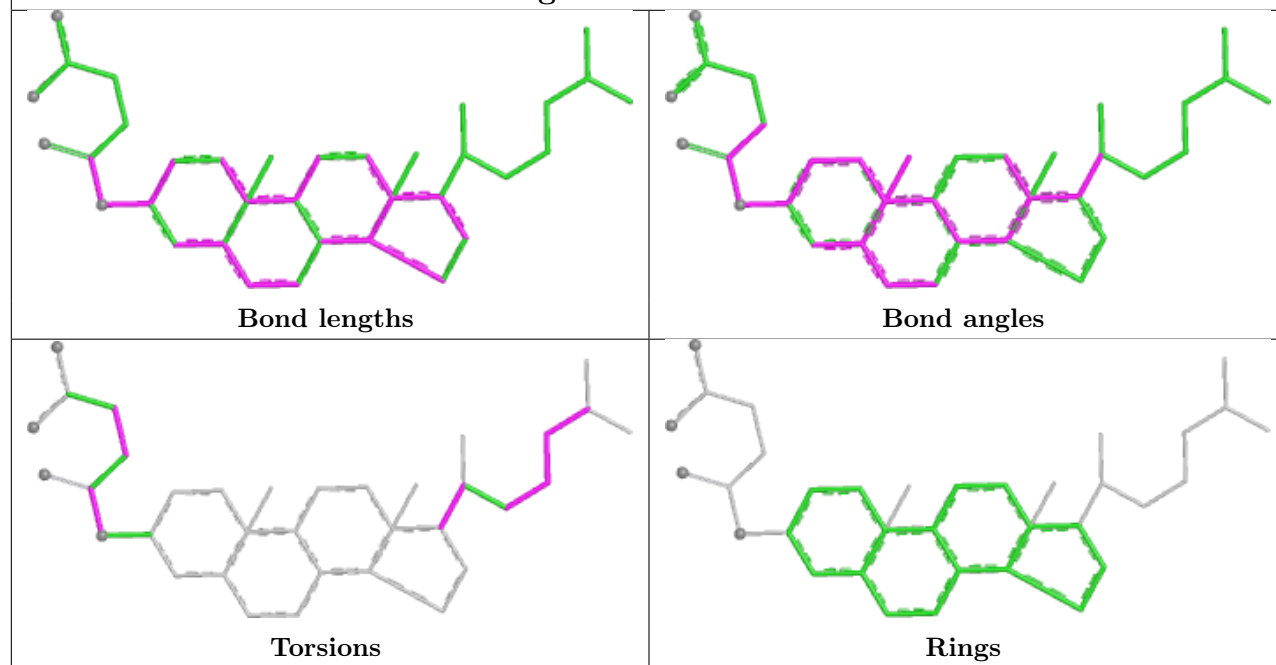
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	601	HO9	19	0
6	B	603	Y01	2	0
4	A	701	3PH	2	0

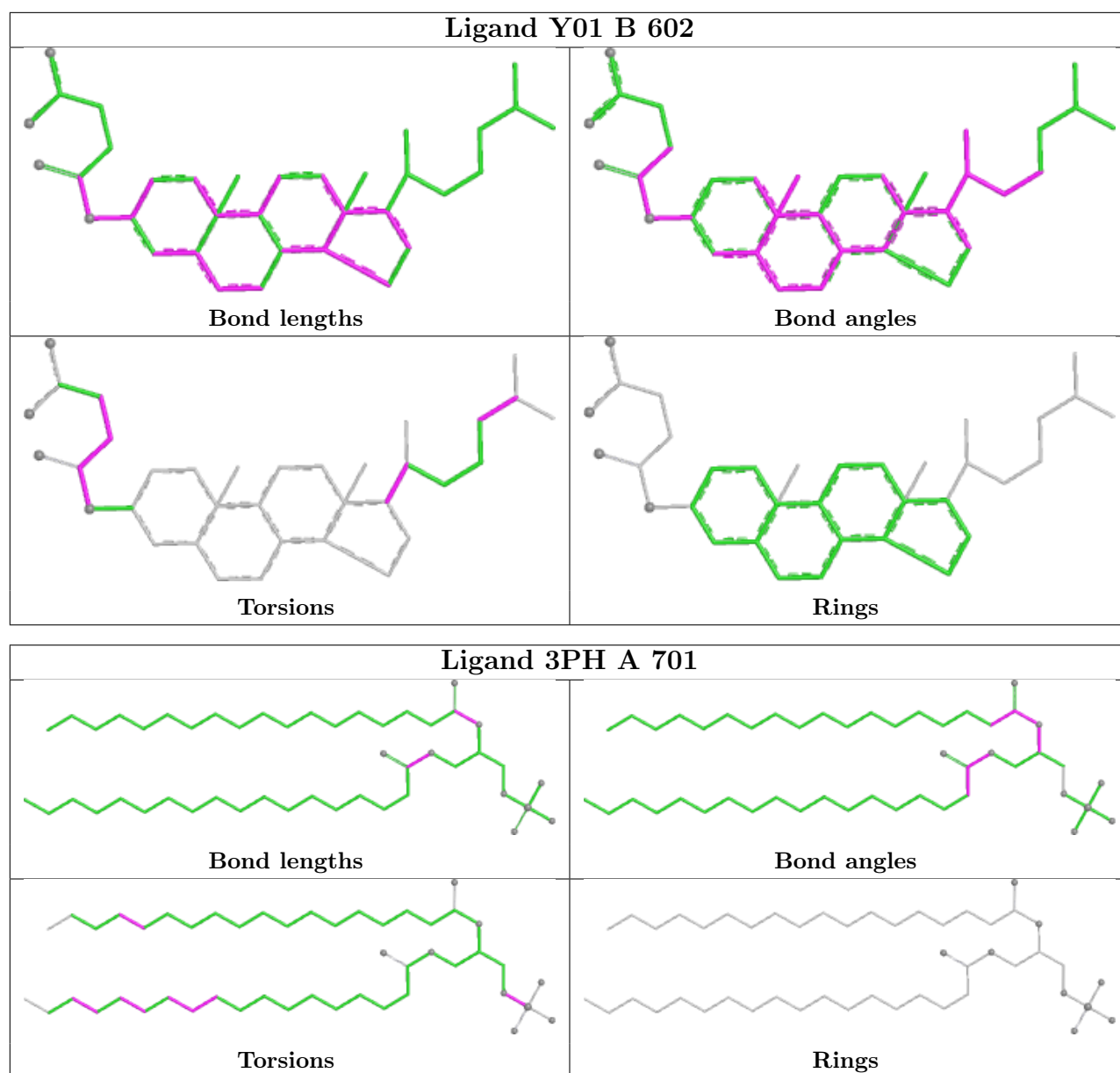
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 HO9 B 601



Ligand Y01 B 603





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.

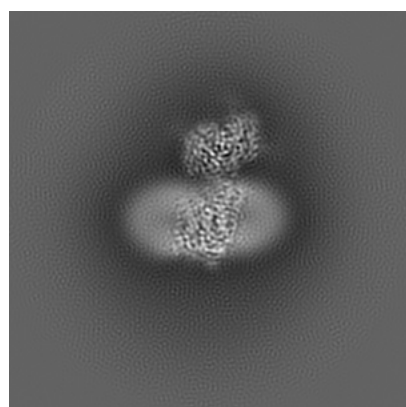
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30839. These allow visual inspection of the internal detail of the map and identification of artifacts.

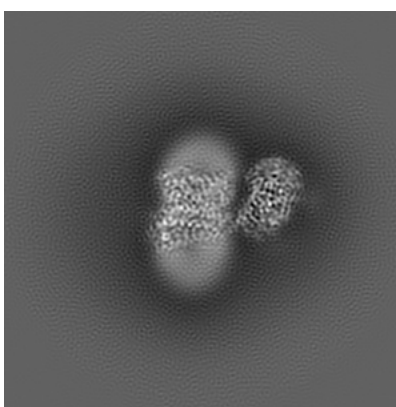
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

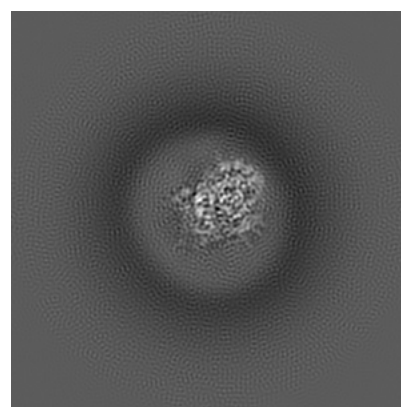
6.1.1 Primary map



X



Y

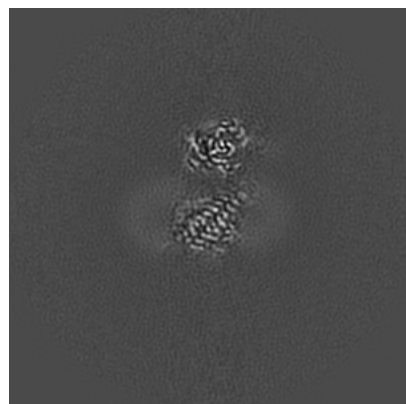


Z

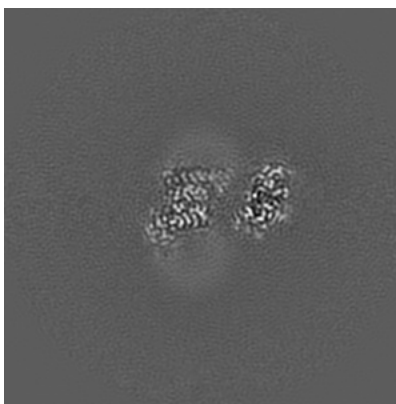
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

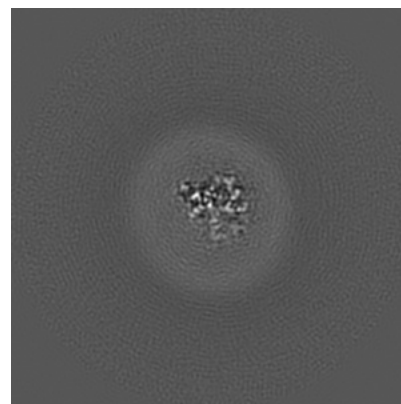
6.2.1 Primary map



X Index: 128



Y Index: 128

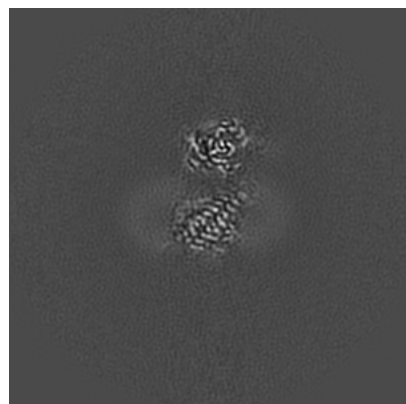


Z Index: 128

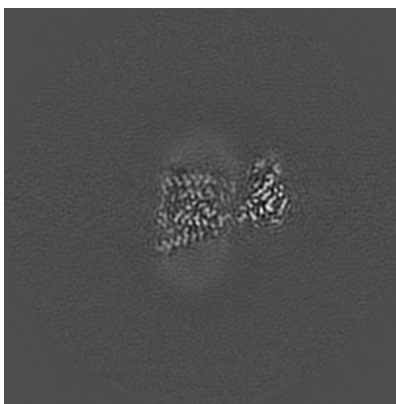
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

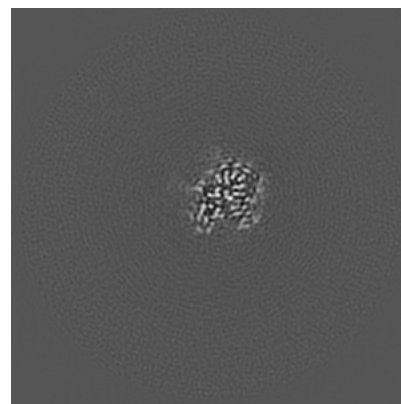
6.3.1 Primary map



X Index: 128



Y Index: 136

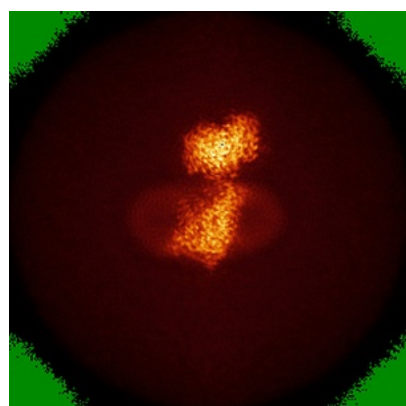


Z Index: 170

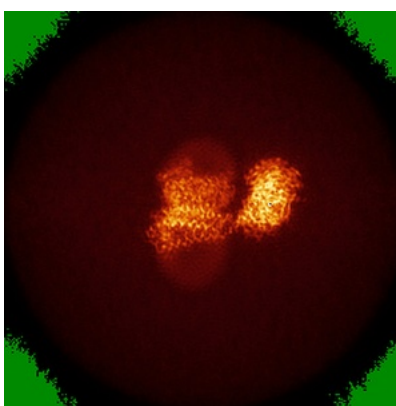
The images above show the largest variance slices of the map in three orthogonal directions.

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

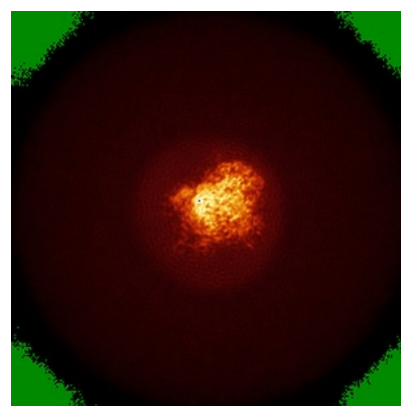
6.4.1 Primary map



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.

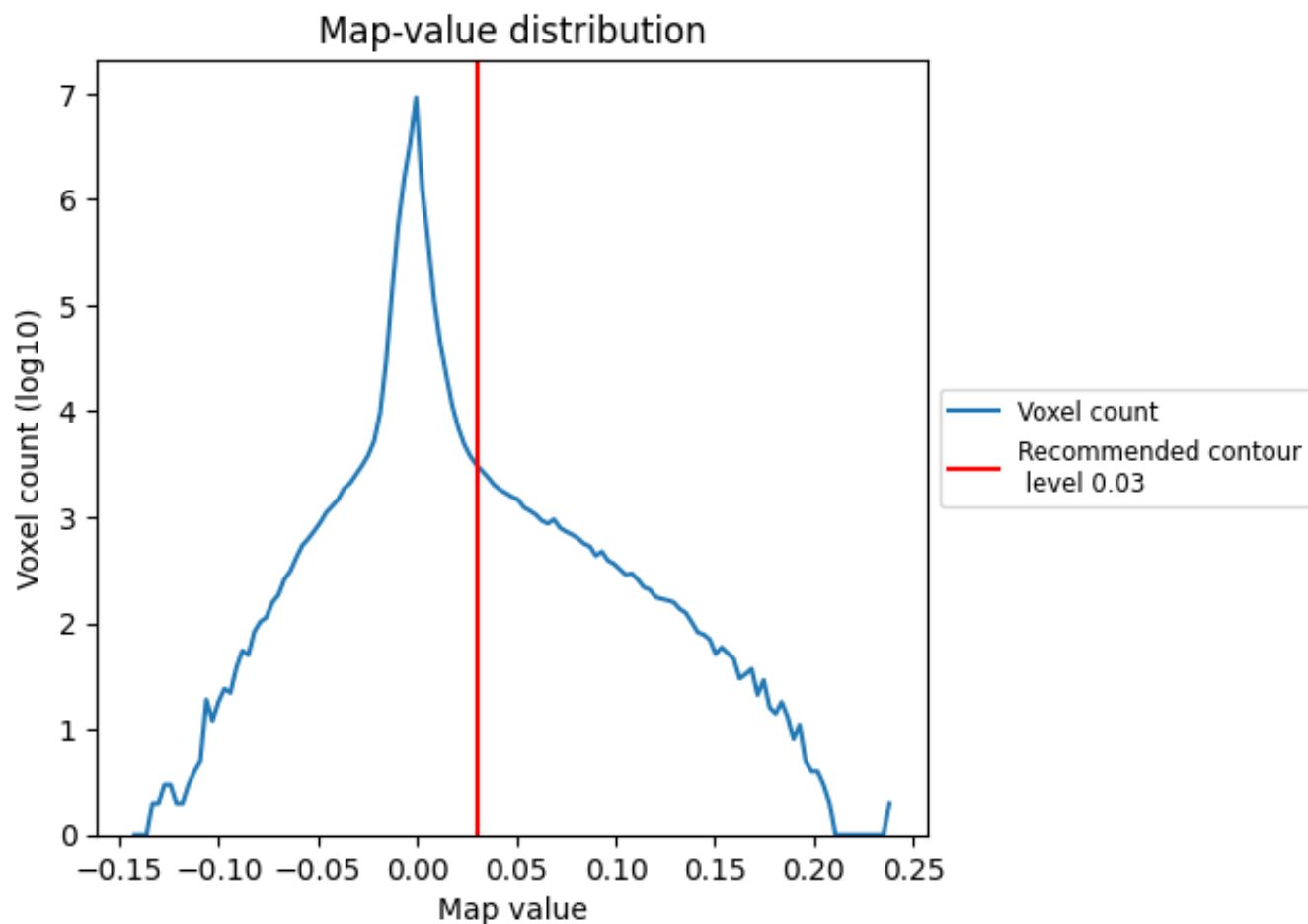
6.6 Mask visualisation

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

7 Map analysis [i](#)

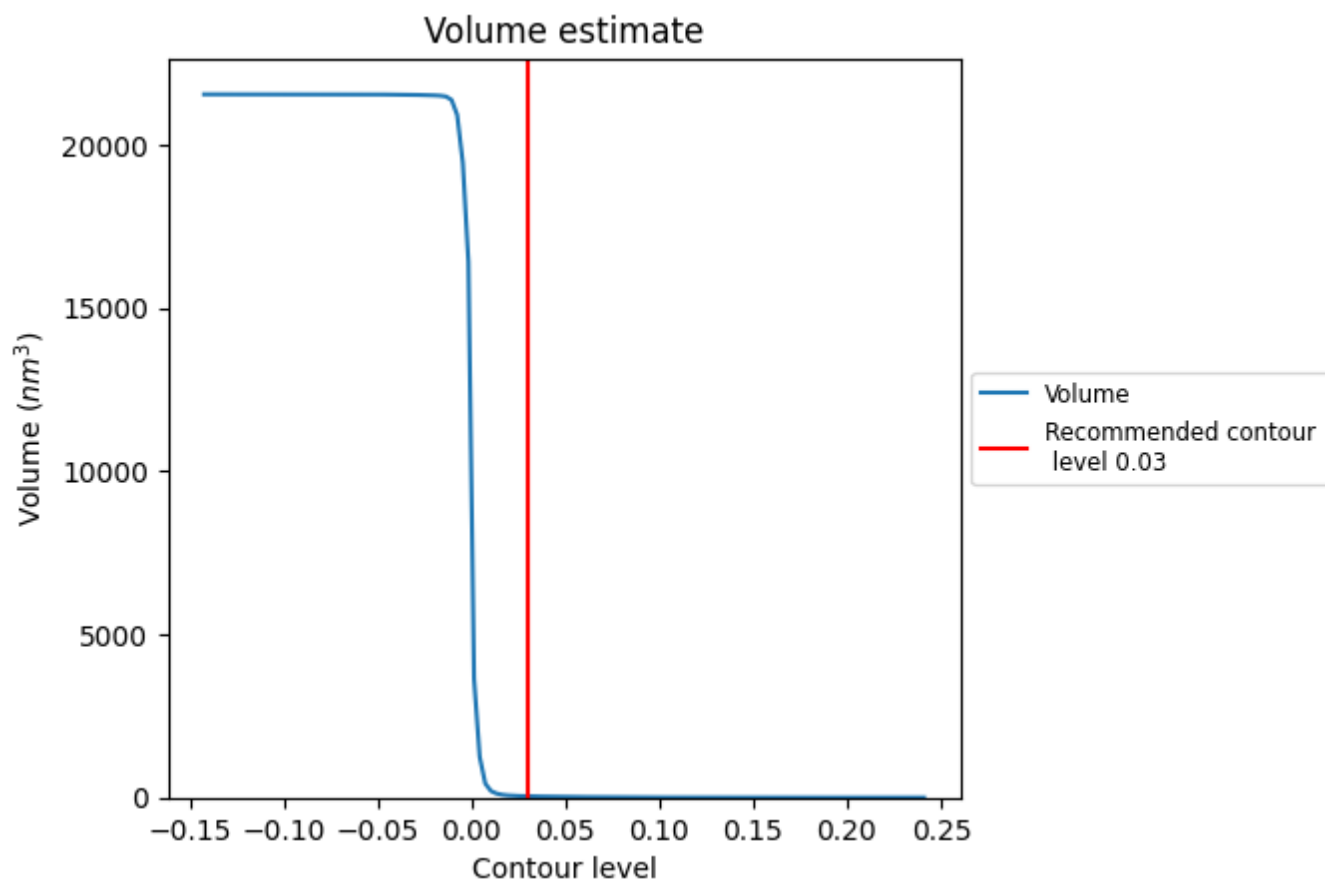
This section contains the results of statistical analysis of the map.

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.

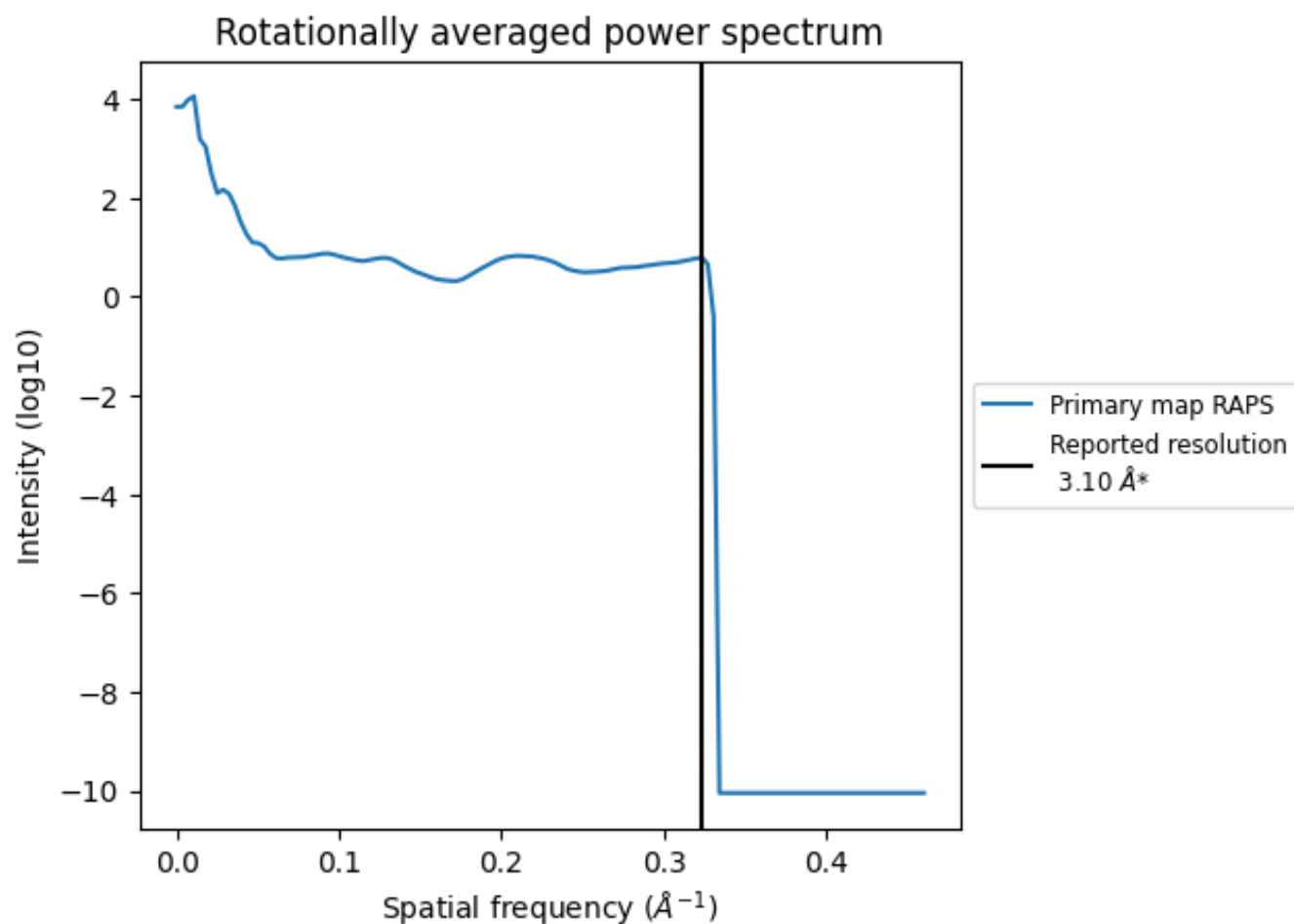
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 41 nm^3 ; this corresponds to an approximate mass of 37 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 0.323 $\text{\AA}^{-1}$

8 Fourier-Shell correlation

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

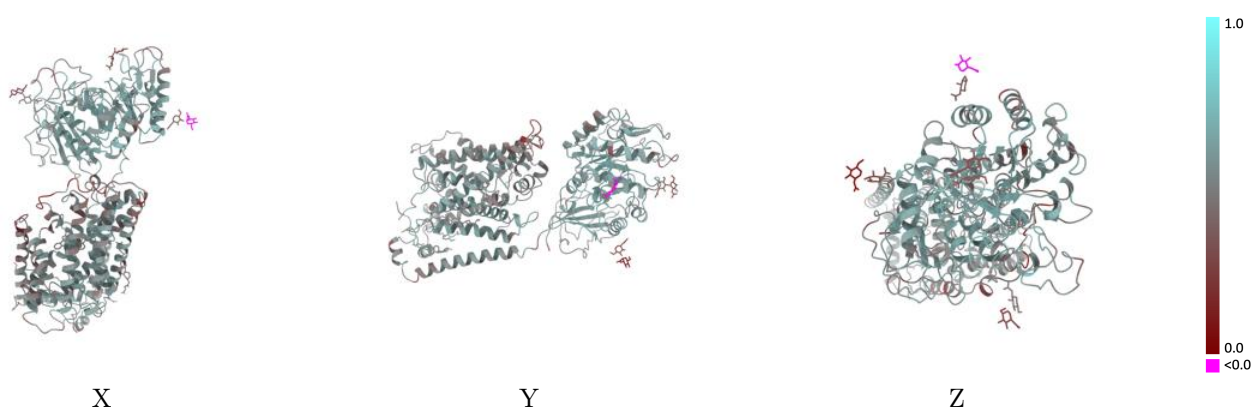
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-30839 and PDB model 7DSN. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)

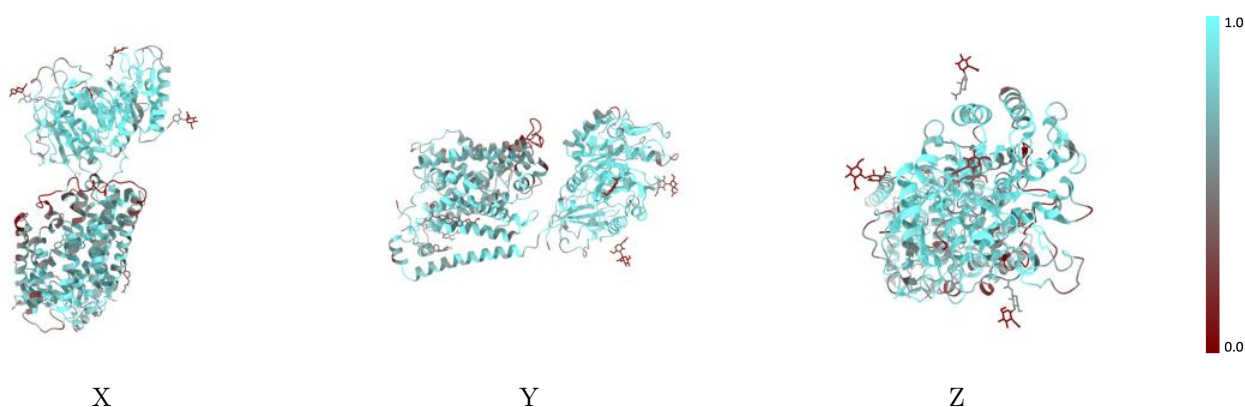
This section was not generated.

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



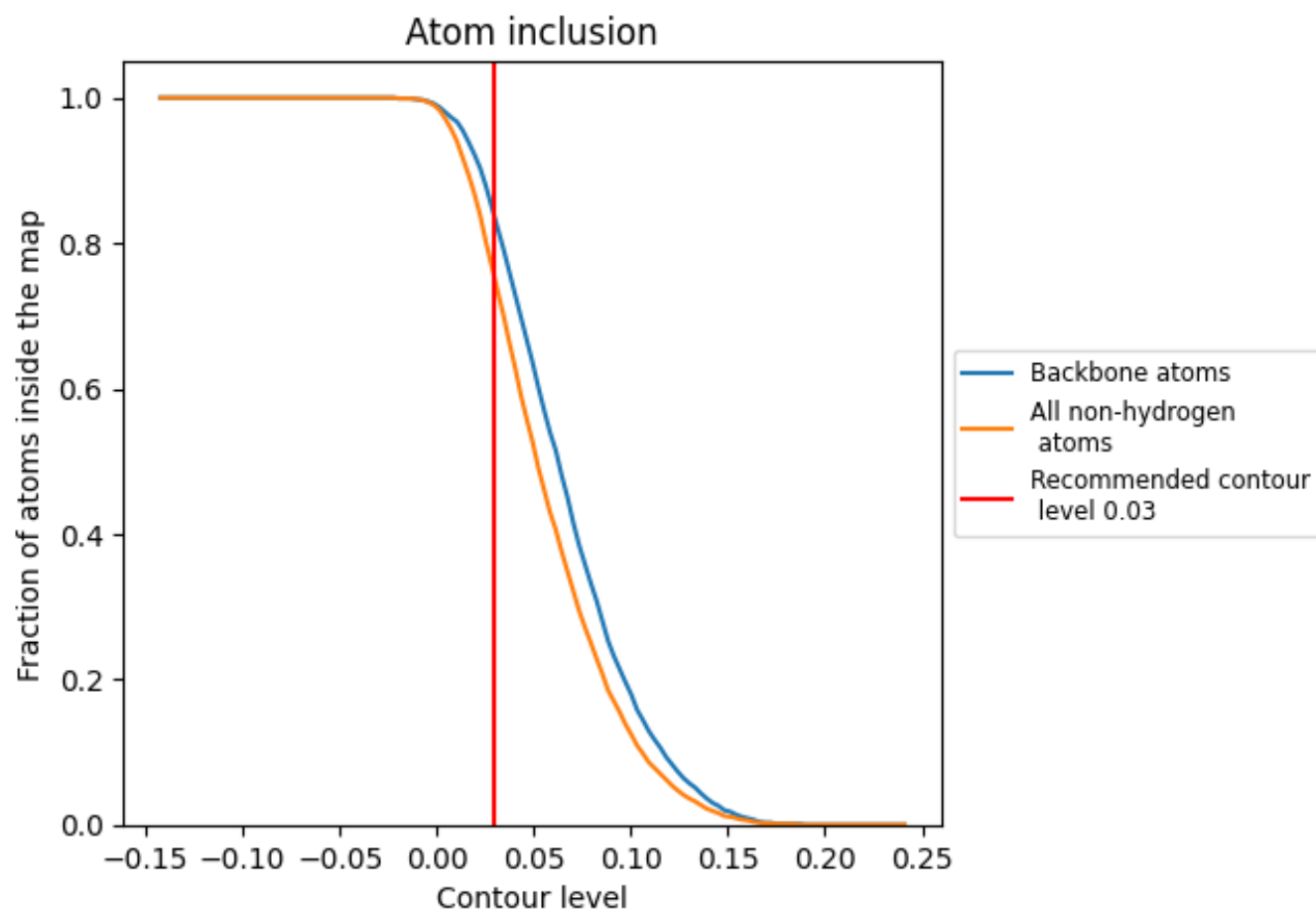
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).

9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 75% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7490	0.5300
A	0.8180	0.5600
B	0.6970	0.5090
C	0.2500	0.3430
D	0.2500	0.1300
E	0.2500	0.3020
F	0.0710	0.1620

1.0

0.0

<0.0