



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 09:11 AM UTC

PDB ID : 9GXE / pdb_00009gxe
EMDB ID : EMD-51659
Title : Structure of the SARS-CoV spike glycoprotein in complex with a homotrimeric Bicycle molecule
Authors : Drulyte, I.; Pellegrino, S.; Harman, M.; Bezerra, G.A.
Deposited on : 2024-09-30
Resolution : 2.30 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:

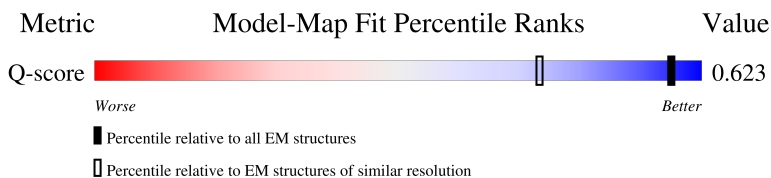
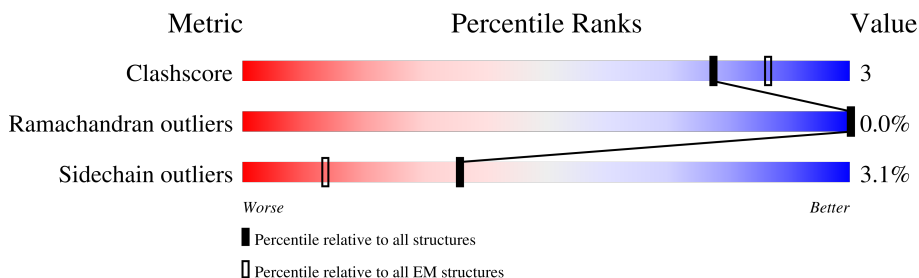
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

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

The reported resolution of this entry is 2.30 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	4254 (1.80 - 2.80)

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	1133	
1	B	1133	
1	C	1133	
2	D	16	

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Mol	Chain	Length	Quality of chain
2	E	16	
2	F	16	
3	AA	2	
3	AB	2	
3	AC	2	
3	BA	2	
3	BB	2	
3	BC	2	
3	CA	2	
3	CB	2	
3	CC	2	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 26514 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 Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1092	Total	C	N	O	S	0	0
			8542	5450	1426	1626	40		
1	B	1085	Total	C	N	O	S	0	0
			8491	5418	1419	1614	40		
1	C	1075	Total	C	N	O	S	0	0
			8406	5365	1401	1600	40		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	817	PRO	PHE	engineered mutation	UNP P0DTC2
A	892	PRO	ALA	engineered mutation	UNP P0DTC2
A	899	PRO	ALA	engineered mutation	UNP P0DTC2
A	942	PRO	ALA	engineered mutation	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	817	PRO	PHE	engineered mutation	UNP P0DTC2
B	892	PRO	ALA	engineered mutation	UNP P0DTC2
B	899	PRO	ALA	engineered mutation	UNP P0DTC2
B	942	PRO	ALA	engineered mutation	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
C	817	PRO	PHE	engineered mutation	UNP P0DTC2
C	892	PRO	ALA	engineered mutation	UNP P0DTC2
C	899	PRO	ALA	engineered mutation	UNP P0DTC2
C	942	PRO	ALA	engineered mutation	UNP P0DTC2
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	UNP P0DTC2

- Molecule 2 is a protein called Homotrimeric bicycle molecule.

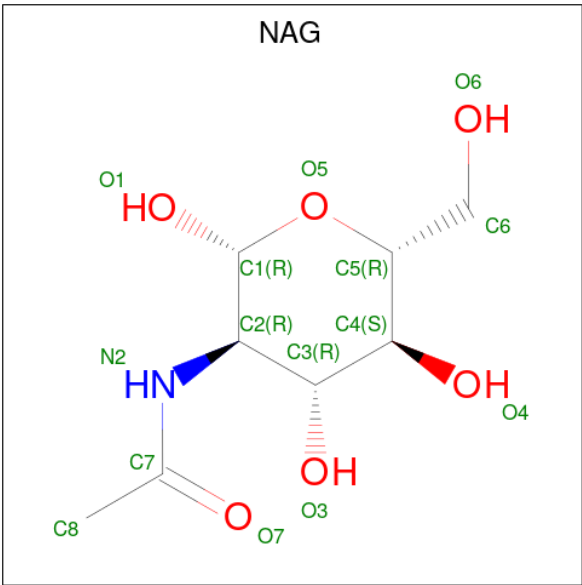
Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	16	Total	C	N	O	S	0	1
			101	63	18	17	3		
2	E	16	Total	C	N	O	S	0	1
			101	63	18	17	3		
2	F	16	Total	C	N	O	S	0	1
			101	63	18	17	3		

- 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	AA	2	Total	C	N	O		0	0
			28	16	2	10			
3	AB	2	Total	C	N	O		0	0
			28	16	2	10			
3	AC	2	Total	C	N	O		0	0
			28	16	2	10			
3	BA	2	Total	C	N	O		0	0
			28	16	2	10			
3	BB	2	Total	C	N	O		0	0
			28	16	2	10			
3	BC	2	Total	C	N	O		0	0
			28	16	2	10			
3	CA	2	Total	C	N	O		0	0
			28	16	2	10			
3	CB	2	Total	C	N	O		0	0
			28	16	2	10			
3	CC	2	Total	C	N	O		0	0
			28	16	2	10			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



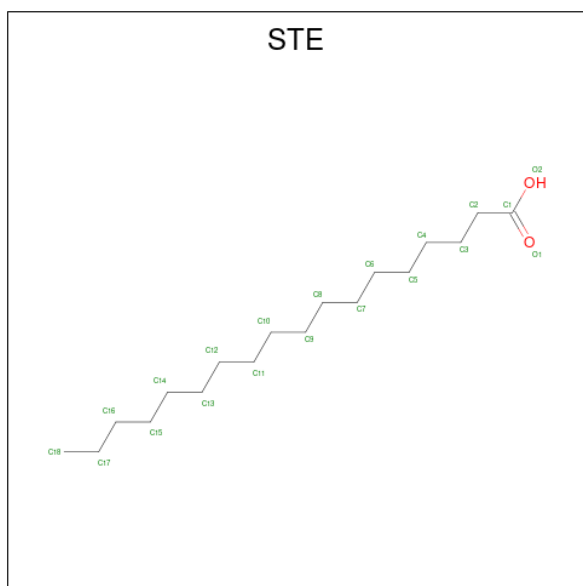
Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	

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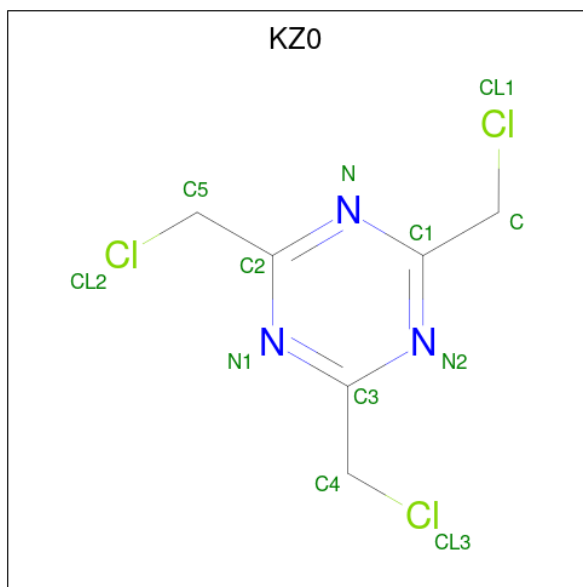
Mol	Chain	Residues	Atoms				AltConf
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 5 is STEARIC ACID (CCD ID: STE) (formula: $C_{18}H_{36}O_2$).



Mol	Chain	Residues	Atoms			AltConf
5	A	1	Total	C	O	0
			20	18	2	
5	B	1	Total	C	O	0
			20	18	2	
5	C	1	Total	C	O	0
			20	18	2	

- Molecule 6 is 2,4,6-tris(chloromethyl)-1,3,5-triazine (CCD ID: KZ0) (formula: $C_6H_6Cl_3N_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
6	D	1	Total	C	N	0
			9	6	3	
6	E	1	Total	C	N	0
			9	6	3	
6	F	1	Total	C	N	0
			9	6	3	

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		AltConf
7	A	45	Total	O	0
			45	45	
7	B	47	Total	O	0
			47	47	
7	C	47	Total	O	0
			47	47	

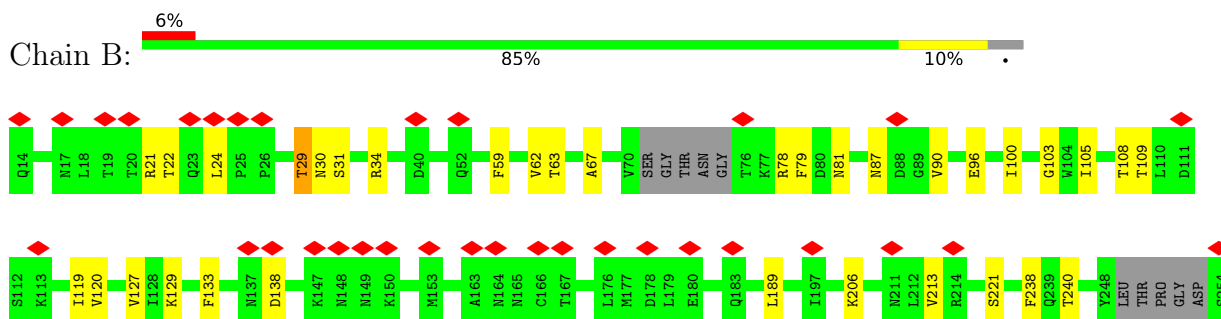
3 Residue-property plots

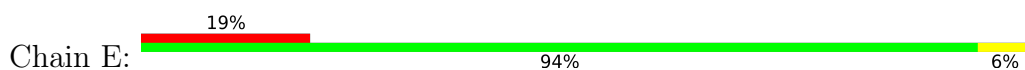
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

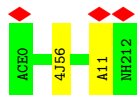
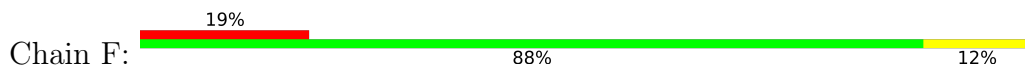


• Molecule 1: Spike glycoprotein





- Molecule 2: Homotrimeric bicycle molecule



- 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



- 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



- 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	429402	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.799	Depositor
Minimum map value	-0.345	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	321.189, 321.189, 321.189	wwPDB
Map dimensions	330, 330, 330	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.9733, 0.9733, 0.9733	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: KZ0, NH2, ACE, STE, OJY, NAG, DAL, 4J5

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	0.19	0/8743	0.42	1/11901 (0.0%)
1	B	0.19	0/8689	0.42	0/11825
1	C	0.19	0/8599	0.42	0/11700
2	D	0.68	0/73	0.64	0/97
2	E	0.68	0/73	0.69	0/97
2	F	0.68	0/73	0.65	0/97
All	All	0.20	0/26250	0.42	1/35717 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
All	All	0	3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	153	MET	CB-CG-SD	5.35	128.76	112.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1142	GLN	Peptide
1	B	1142	GLN	Peptide
1	C	1142	GLN	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8542	0	8323	48	0
1	B	8491	0	8274	58	0
1	C	8406	0	8197	54	0
2	D	101	0	85	0	0
2	E	101	0	85	0	0
2	F	101	0	85	0	0
3	AA	28	0	25	0	0
3	AB	28	0	25	0	0
3	AC	28	0	25	0	0
3	BA	28	0	25	0	0
3	BB	28	0	25	1	0
3	BC	28	0	25	0	0
3	CA	28	0	25	0	0
3	CB	28	0	25	0	0
3	CC	28	0	25	1	0
4	A	98	0	91	0	0
4	B	112	0	104	1	0
4	C	84	0	78	0	0
5	A	20	0	35	2	0
5	B	20	0	35	0	0
5	C	20	0	35	0	0
6	D	9	0	0	0	0
6	E	9	0	0	0	0
6	F	9	0	0	0	0
7	A	45	0	0	0	0
7	B	47	0	0	1	0
7	C	47	0	0	0	0
All	All	26514	0	25652	150	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 3.

All (150) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:67:ALA:O	1:C:262:ALA:HA	1.86	0.75
1:A:67:ALA:O	1:A:262:ALA:HA	1.96	0.65
1:C:19:THR:HA	1:C:21:ARG:HH21	1.66	0.61
1:C:180:GLU:HG2	1:C:182:LYS:HG2	1.85	0.59
1:B:825:LYS:NZ	1:B:941:THR:O	2.36	0.59
1:B:24:LEU:HD22	1:B:78:ARG:HD2	1.84	0.58
1:C:332:ILE:HD11	1:C:525:CYS:HB2	1.86	0.58
1:C:24:LEU:HD12	1:C:78:ARG:HH11	1.70	0.57
1:B:563:GLN:O	1:B:577:ARG:NH1	2.39	0.56
1:B:332:ILE:HD11	1:B:525:CYS:HB2	1.88	0.56
1:C:246:ARG:NH2	1:C:255:SER:O	2.38	0.56
1:B:34:ARG:HH12	1:B:189:LEU:HD21	1.69	0.56
1:A:24:LEU:HG	1:A:78:ARG:HD3	1.88	0.55
1:B:67:ALA:O	1:B:262:ALA:HA	2.06	0.55
1:A:319:ARG:HH22	1:B:739:THR:HB	1.72	0.55
1:B:138:ASP:N	1:B:138:ASP:OD1	2.38	0.55
1:C:1103:PHE:HZ	3:CC:1:NAG:H62	1.73	0.55
1:A:29:THR:OG1	1:A:30:ASN:N	2.40	0.54
5:A:1208:STE:H131	1:B:513:LEU:HD13	1.90	0.54
1:C:360:ASN:H	1:C:523:THR:HG22	1.72	0.54
1:A:804:GLN:OE1	1:A:935:GLN:NE2	2.39	0.54
1:C:409:GLN:HA	1:C:414:GLN:HG2	1.89	0.54
1:C:825:LYS:NZ	1:C:941:THR:O	2.41	0.54
1:B:22:THR:O	1:B:78:ARG:NH1	2.40	0.54
1:A:848:ASP:HB3	1:A:851:CYS:HB2	1.89	0.54
1:B:31:SER:O	1:B:59:PHE:HA	2.08	0.54
1:B:722:VAL:HG22	1:B:1065:VAL:HG22	1.90	0.54
1:A:189:LEU:HB2	1:A:210:ILE:HD13	1.89	0.53
1:A:310:LYS:HG3	1:A:600:PRO:HA	1.90	0.53
1:C:393:THR:HA	1:C:522:ALA:HA	1.89	0.53
1:B:724:THR:HG23	1:B:934:ILE:HD12	1.90	0.53
1:B:29:THR:OG1	1:B:30:ASN:N	2.41	0.52
1:C:1100:THR:OG1	1:C:1101:HIS:ND1	2.41	0.52
1:B:822:LEU:HD22	1:B:945:LEU:HD21	1.91	0.52
1:B:103:GLY:HA3	1:B:119:ILE:O	2.10	0.52
1:C:724:THR:HG23	1:C:934:ILE:HD12	1.91	0.52
1:C:848:ASP:HB3	1:C:851:CYS:HB2	1.91	0.52
1:C:362:VAL:HA	1:C:525:CYS:O	2.10	0.52
1:B:129:LYS:HG3	1:B:133:PHE:HZ	1.75	0.51
1:C:326:ILE:HD12	1:C:539:VAL:HG21	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:945:LEU:HD23	1:A:948:LEU:HD12	1.93	0.51
1:B:280:ASN:ND2	1:B:284:THR:O	2.43	0.51
1:B:1048:HIS:HA	1:B:1066:THR:HG22	1.93	0.51
1:C:131:CYS:HA	1:C:166:CYS:HB3	1.93	0.51
1:B:1100:THR:OG1	1:B:1101:HIS:ND1	2.44	0.50
1:C:1048:HIS:HA	1:C:1066:THR:HG22	1.94	0.50
1:B:1103:PHE:HZ	3:BB:1:NAG:H62	1.76	0.50
1:A:105:ILE:O	1:A:238:PHE:HA	2.11	0.50
1:A:1048:HIS:HA	1:A:1066:THR:HG22	1.92	0.50
1:A:722:VAL:HG22	1:A:1065:VAL:HG22	1.94	0.50
1:C:294:ASP:OD1	1:C:294:ASP:N	2.43	0.50
1:A:99:ASN:ND2	1:A:178:ASP:O	2.42	0.49
1:B:1086:LYS:HA	1:B:1125:ASN:HA	1.93	0.49
1:C:722:VAL:HG22	1:C:1065:VAL:HG22	1.92	0.49
1:B:1028:LYS:NZ	1:B:1042:PHE:O	2.41	0.49
1:A:337:PRO:HB2	1:A:340:GLU:HB2	1.94	0.49
1:B:29:THR:HG23	1:B:62:VAL:HG23	1.95	0.49
1:B:108:THR:HG23	1:B:109:THR:HG23	1.95	0.48
1:B:294:ASP:N	1:B:294:ASP:OD1	2.46	0.48
1:C:96:GLU:OE1	1:C:100:ILE:N	2.42	0.48
1:C:715:PRO:HA	1:C:1072:GLU:HA	1.95	0.48
1:C:280:ASN:ND2	1:C:284:THR:O	2.47	0.48
1:B:206:LYS:HA	1:B:206:LYS:HD2	1.67	0.47
1:C:337:PRO:HB2	1:C:340:GLU:HB2	1.96	0.47
1:B:393:THR:HA	1:B:522:ALA:HA	1.96	0.47
1:B:96:GLU:OE1	1:B:100:ILE:N	2.47	0.47
1:C:81:ASN:N	1:C:81:ASN:OD1	2.47	0.47
1:A:605:SER:OG	1:A:606:ASN:N	2.46	0.47
1:C:105:ILE:O	1:C:238:PHE:HA	2.15	0.47
1:A:280:ASN:ND2	1:A:284:THR:O	2.48	0.47
1:A:642:VAL:HG12	1:A:651:ILE:HG12	1.97	0.47
1:A:907:ASN:HD22	1:C:1107:ARG:HH22	1.62	0.47
1:A:724:THR:HG23	1:A:934:ILE:HD12	1.97	0.46
1:B:662:CYS:HB2	1:B:697:MET:HE3	1.98	0.46
1:C:822:LEU:HD22	1:C:945:LEU:HD21	1.97	0.46
1:A:457:ARG:NH2	4:B:1207:NAG:O7	2.47	0.46
1:B:903:ALA:HB2	1:B:916:LEU:HD22	1.97	0.46
1:C:156:GLU:OE1	1:C:158:ARG:NH1	2.47	0.46
1:A:1073:LYS:HE2	1:A:1073:LYS:HB3	1.71	0.46
1:B:715:PRO:HA	1:B:1072:GLU:HA	1.98	0.46
1:A:614:ASP:HA	1:B:834:ILE:HG23	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:ASN:OD1	1:B:81:ASN:N	2.48	0.46
1:B:733:LYS:NZ	1:B:775:ASP:OD2	2.43	0.46
1:C:743:CYS:HB3	1:C:749:CYS:HB3	1.74	0.46
1:C:97:LYS:NZ	1:C:182:LYS:O	2.48	0.46
1:A:743:CYS:HB3	1:A:749:CYS:HB3	1.71	0.46
1:C:376:THR:HB	1:C:435:ALA:HB3	1.98	0.46
1:B:614:ASP:HA	1:C:834:ILE:HG23	1.98	0.46
1:B:297:SER:HA	1:B:300:LYS:HD2	1.97	0.45
1:C:642:VAL:HG22	1:C:651:ILE:HG13	1.97	0.45
1:B:848:ASP:HB3	1:B:851:CYS:HB2	1.98	0.45
1:B:1073:LYS:HB3	1:B:1073:LYS:HE2	1.76	0.45
1:A:641:ASN:OD1	1:A:641:ASN:N	2.49	0.45
1:A:822:LEU:HD22	1:A:945:LEU:HD21	1.99	0.45
1:A:81:ASN:N	1:A:81:ASN:OD1	2.47	0.45
1:A:206:LYS:HA	1:A:206:LYS:HD2	1.78	0.45
1:B:376:THR:HB	1:B:435:ALA:HB3	1.98	0.45
1:A:1107:ARG:HH22	1:B:907:ASN:HD22	1.65	0.45
1:B:105:ILE:O	1:B:238:PHE:HA	2.17	0.45
1:C:406:GLU:OE1	1:C:495:TYR:OH	2.32	0.45
1:A:29:THR:HG23	1:A:62:VAL:HG23	1.98	0.45
1:C:903:ALA:HB2	1:C:916:LEU:HD12	1.99	0.44
1:A:376:THR:HB	1:A:435:ALA:HB3	1.98	0.44
1:B:1107:ARG:NH1	7:B:1307:HOH:O	2.43	0.44
1:B:786:LYS:HA	1:B:786:LYS:HD3	1.67	0.44
1:C:21:ARG:NH1	1:C:79:PHE:O	2.51	0.44
1:A:715:PRO:HA	1:A:1072:GLU:HA	1.99	0.43
1:A:841:LEU:HB2	1:C:588:THR:HG21	2.00	0.43
1:A:983:ARG:HD2	1:C:517:LEU:HD13	1.98	0.43
1:C:733:LYS:NZ	1:C:775:ASP:OD2	2.49	0.43
1:B:357:ARG:HH12	1:B:394:ASN:HB2	1.83	0.43
1:B:976:VAL:HB	1:B:979:ASP:HB3	2.01	0.43
1:C:18:LEU:HD22	1:C:258:TRP:CD1	2.54	0.43
1:C:206:LYS:HA	1:C:206:LYS:HD2	1.64	0.43
1:A:1097:SER:HB2	1:A:1102:TRP:CD2	2.54	0.43
1:C:605:SER:OG	1:C:606:ASN:N	2.52	0.43
1:A:852:ALA:O	1:A:856:ASN:ND2	2.51	0.42
1:C:880:GLY:O	1:C:884:SER:OG	2.34	0.42
1:A:722:VAL:HA	1:A:1064:HIS:O	2.19	0.42
1:C:676:THR:HA	1:C:690:GLN:HA	2.01	0.42
1:B:21:ARG:NH1	1:B:79:PHE:O	2.44	0.42
1:A:139:PRO:HA	1:A:158:ARG:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:TRP:HH2	1:A:214:ARG:HE	1.68	0.42
1:A:900:MET:HE2	1:A:900:MET:HB3	1.84	0.42
1:A:903:ALA:HB1	1:A:913:GLN:HB2	2.02	0.42
1:B:715:PRO:HD3	1:C:894:LEU:HD13	2.01	0.42
1:A:354:ASN:O	1:A:398:ASP:HA	2.20	0.41
1:B:722:VAL:HA	1:B:1064:HIS:O	2.19	0.41
1:A:78:ARG:NH2	1:A:80:ASP:OD2	2.54	0.41
1:A:280:ASN:HD21	1:A:284:THR:HB	1.86	0.41
1:A:120:VAL:HG12	1:A:127:VAL:HB	2.01	0.41
1:A:383:SER:OG	1:B:985:ASP:OD1	2.38	0.41
1:C:280:ASN:HD21	1:C:284:THR:HB	1.86	0.41
1:C:976:VAL:HB	1:C:979:ASP:HB3	2.01	0.41
1:B:319:ARG:H	1:B:319:ARG:HG2	1.76	0.41
1:B:777:ASN:OD1	1:B:1019:ARG:NH1	2.44	0.41
1:A:715:PRO:HD3	1:B:894:LEU:HD13	2.03	0.41
5:A:1208:STE:H91	1:B:387:LEU:HD13	2.03	0.41
1:B:642:VAL:HG22	1:B:651:ILE:HG13	2.02	0.41
1:B:605:SER:OG	1:B:606:ASN:N	2.54	0.41
1:C:81:ASN:O	1:C:239:GLN:NE2	2.46	0.40
1:C:258:TRP:HZ3	1:C:260:ALA:HB2	1.86	0.40
1:C:350:VAL:HG22	1:C:422:ASN:HB3	2.03	0.40
1:C:752:LEU:HD11	1:C:990:GLU:HG2	2.03	0.40
1:B:934:ILE:HD13	1:B:934:ILE:HA	1.96	0.40
1:C:203:ILE:HB	1:C:227:VAL:HG12	2.03	0.40
1:A:156:GLU:OE1	1:A:246:ARG:NE	2.45	0.40
1:A:393:THR:HG22	1:A:522:ALA:HB2	2.03	0.40
1:B:386:LYS:HD3	1:B:386:LYS:HA	1.96	0.40
1:C:1045:LYS:HE2	1:C:1045:LYS:HB2	1.70	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1080/1133 (95%)	1042 (96%)	38 (4%)	0	100	100
1	B	1071/1133 (94%)	1037 (97%)	34 (3%)	0	100	100
1	C	1057/1133 (93%)	1017 (96%)	40 (4%)	0	100	100
2	D	11/16 (69%)	10 (91%)	1 (9%)	0	100	100
2	E	11/16 (69%)	10 (91%)	1 (9%)	0	100	100
2	F	11/16 (69%)	10 (91%)	0	1 (9%)	0	0
All	All	3241/3447 (94%)	3126 (96%)	114 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	11	ALA

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	957/987 (97%)	923 (96%)	34 (4%)	31	47
1	B	951/987 (96%)	922 (97%)	29 (3%)	36	53
1	C	942/987 (95%)	916 (97%)	26 (3%)	38	56
2	D	8/9 (89%)	8 (100%)	0	100	100
2	E	8/9 (89%)	8 (100%)	0	100	100
2	F	8/9 (89%)	8 (100%)	0	100	100
All	All	2874/2988 (96%)	2785 (97%)	89 (3%)	36	52

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	THR
1	A	47	VAL
1	A	90	VAL
1	A	94	SER

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Mol	Chain	Res	Type
1	A	98	SER
1	A	120	VAL
1	A	161	SER
1	A	176	LEU
1	A	213	VAL
1	A	277	LEU
1	A	315	THR
1	A	494	SER
1	A	553	THR
1	A	558	LYS
1	A	596	SER
1	A	602	THR
1	A	604	THR
1	A	607	GLN
1	A	637	SER
1	A	641	ASN
1	A	645	THR
1	A	658	ASN
1	A	705	VAL
1	A	747	THR
1	A	827	THR
1	A	841	LEU
1	A	916	LEU
1	A	937	SER
1	A	964	LYS
1	A	1092	GLU
1	A	1094	VAL
1	A	1098	ASN
1	A	1136	THR
1	A	1142	GLN
1	B	29	THR
1	B	63	THR
1	B	87	ASN
1	B	90	VAL
1	B	120	VAL
1	B	127	VAL
1	B	213	VAL
1	B	221	SER
1	B	240	THR
1	B	259	THR
1	B	277	LEU
1	B	284	THR

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Mol	Chain	Res	Type
1	B	301	CYS
1	B	307	THR
1	B	315	THR
1	B	319	ARG
1	B	331	ASN
1	B	596	SER
1	B	604	THR
1	B	638	THR
1	B	640	SER
1	B	645	THR
1	B	875	SER
1	B	929	SER
1	B	937	SER
1	B	977	LEU
1	B	1100	THR
1	B	1141	LEU
1	B	1144	GLU
1	C	29	THR
1	C	90	VAL
1	C	94	SER
1	C	98	SER
1	C	112	SER
1	C	159	VAL
1	C	161	SER
1	C	179	LEU
1	C	213	VAL
1	C	277	LEU
1	C	307	THR
1	C	315	THR
1	C	319	ARG
1	C	345	THR
1	C	480	CYS
1	C	534	VAL
1	C	581	THR
1	C	590	CYS
1	C	596	SER
1	C	597	VAL
1	C	604	THR
1	C	827	THR
1	C	828	LEU
1	C	875	SER
1	C	937	SER

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Mol	Chain	Res	Type
1	C	1100	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	GLN
1	A	164	ASN
1	A	183	GLN
1	A	196	ASN
1	A	211	ASN
1	A	370	ASN
1	A	394	ASN
1	A	450	ASN
1	A	764	ASN
1	A	836	GLN
1	A	853	GLN
1	A	901	GLN
1	A	907	ASN
1	A	1002	GLN
1	A	1058	HIS
1	A	1074	ASN
1	A	1106	GLN
1	B	30	ASN
1	B	134	GLN
1	B	188	ASN
1	B	207	HIS
1	B	211	ASN
1	B	218	GLN
1	B	321	GLN
1	B	448	ASN
1	B	450	ASN
1	B	856	ASN
1	B	907	ASN
1	B	1058	HIS
1	B	1125	ASN
1	C	99	ASN
1	C	125	ASN
1	C	211	ASN
1	C	317	ASN
1	C	321	GLN
1	C	370	ASN
1	C	450	ASN

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Mol	Chain	Res	Type
1	C	764	ASN
1	C	856	ASN
1	C	907	ASN
1	C	1058	HIS
1	C	1106	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
2	4J5	E	6	2	8,9,10	2.47	2 (25%)	4,10,12	0.50	0
2	4J5	F	6	2	8,9,10	2.46	2 (25%)	4,10,12	0.50	0
2	DAL	F	7	2	3,4,5	1.04	0	2,4,6	0.80	0
2	4J5	D	6	2	8,9,10	2.47	2 (25%)	4,10,12	0.50	0
2	DAL	E	7	2	3,4,5	1.04	0	2,4,6	0.77	0
2	DAL	D	7	2	3,4,5	1.04	0	2,4,6	0.77	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
2	4J5	E	6	2	-	2/7/8/10	-
2	4J5	F	6	2	-	2/7/8/10	-
2	DAL	F	7	2	-	0/1/2/4	-
2	4J5	D	6	2	-	2/7/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DAL	E	7	2	-	1/1/2/4	-
2	DAL	D	7	2	-	0/1/2/4	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	6	4J5	CE-ND	4.58	1.42	1.33
2	E	6	4J5	CE-ND	4.57	1.42	1.33
2	F	6	4J5	CE-ND	4.54	1.42	1.33
2	D	6	4J5	CE-NH2	4.28	1.47	1.32
2	F	6	4J5	CE-NH2	4.25	1.47	1.32
2	E	6	4J5	CE-NH2	4.25	1.47	1.32

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	7	DAL	O-C-CA-CB
2	D	6	4J5	CA-CB-CG-ND
2	E	6	4J5	CA-CB-CG-ND
2	F	6	4J5	CA-CB-CG-ND
2	D	6	4J5	CB-CG-ND-CE
2	F	6	4J5	CB-CG-ND-CE
2	E	6	4J5	CB-CG-ND-CE

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

18 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	AA	1	3,1	14,14,15	0.82	1 (7%)	17,19,21	0.86	1 (5%)
3	NAG	AA	2	3	14,14,15	0.34	0	17,19,21	0.59	0
3	NAG	AB	1	3,1	14,14,15	0.21	0	17,19,21	0.54	0
3	NAG	AB	2	3	14,14,15	0.29	0	17,19,21	0.50	0
3	NAG	AC	1	3,1	14,14,15	0.27	0	17,19,21	0.59	0
3	NAG	AC	2	3	14,14,15	0.29	0	17,19,21	0.51	0
3	NAG	BA	1	3,1	14,14,15	0.24	0	17,19,21	0.56	0
3	NAG	BA	2	3	14,14,15	0.28	0	17,19,21	0.50	0
3	NAG	BB	1	3,1	14,14,15	0.36	0	17,19,21	0.53	0
3	NAG	BB	2	3	14,14,15	0.38	0	17,19,21	0.43	0
3	NAG	BC	1	3,1	14,14,15	0.28	0	17,19,21	0.56	0
3	NAG	BC	2	3	14,14,15	0.29	0	17,19,21	0.51	0
3	NAG	CA	1	3,1	14,14,15	0.25	0	17,19,21	0.55	0
3	NAG	CA	2	3	14,14,15	0.29	0	17,19,21	0.51	0
3	NAG	CB	1	3,1	14,14,15	0.28	0	17,19,21	0.58	0
3	NAG	CB	2	3	14,14,15	0.28	0	17,19,21	0.53	0
3	NAG	CC	1	3,1	14,14,15	0.36	0	17,19,21	0.56	0
3	NAG	CC	2	3	14,14,15	0.38	0	17,19,21	0.43	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	AA	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	AA	2	3	-	3/6/23/26	0/1/1/1
3	NAG	AB	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	AB	2	3	-	0/6/23/26	0/1/1/1
3	NAG	AC	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	AC	2	3	-	2/6/23/26	0/1/1/1
3	NAG	BA	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	BA	2	3	-	2/6/23/26	0/1/1/1
3	NAG	BB	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	BB	2	3	-	2/6/23/26	0/1/1/1
3	NAG	BC	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	BC	2	3	-	0/6/23/26	0/1/1/1
3	NAG	CA	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	CA	2	3	-	2/6/23/26	0/1/1/1
3	NAG	CB	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	CB	2	3	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	CC	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	CC	2	3	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	AA	1	NAG	C1-C2	2.61	1.55	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	AA	1	NAG	C1-O5-C5	3.08	116.31	112.19

There are no chirality outliers.

All (17) torsion outliers are listed below:

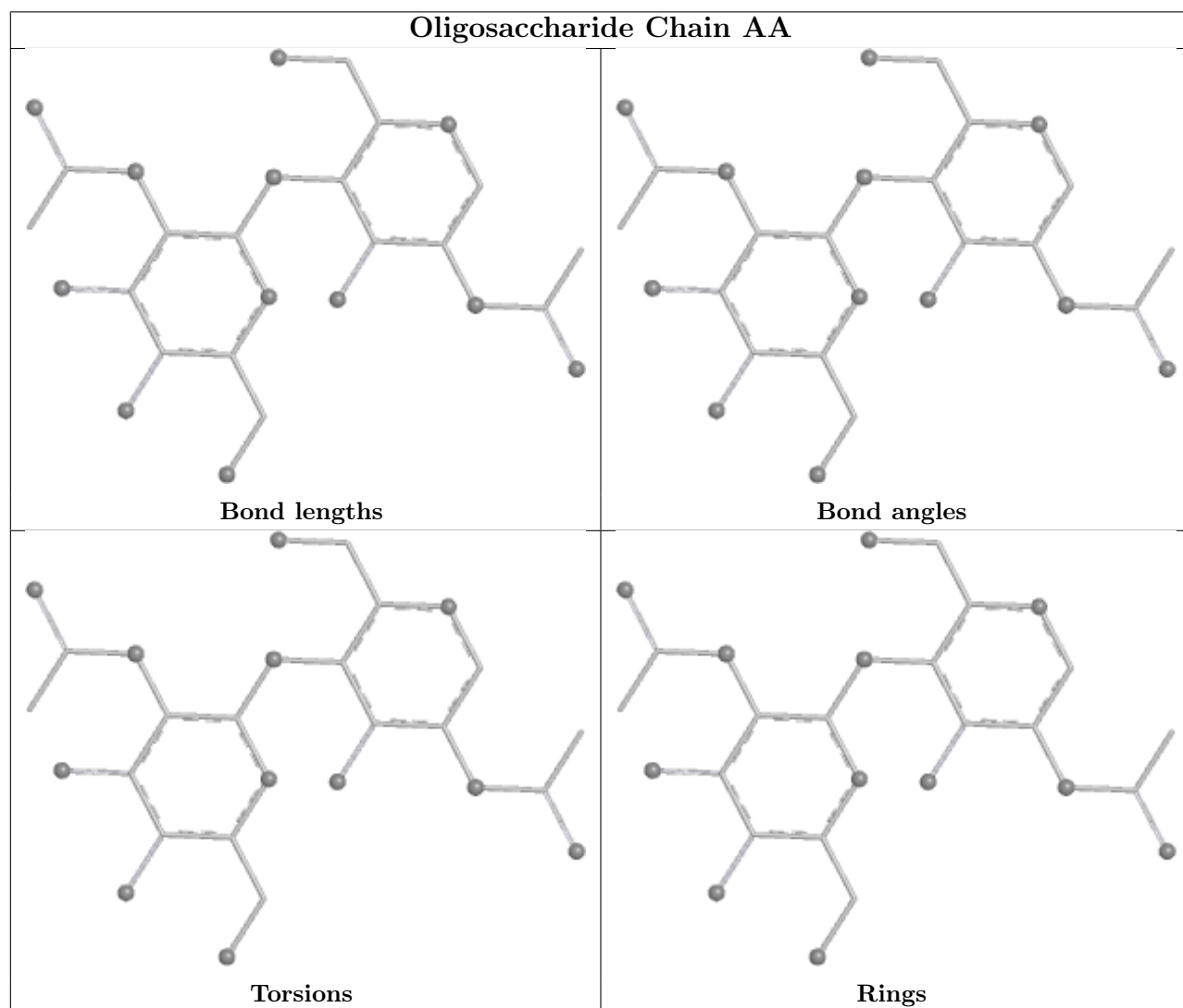
Mol	Chain	Res	Type	Atoms
3	CC	2	NAG	O5-C5-C6-O6
3	BB	2	NAG	O5-C5-C6-O6
3	BB	2	NAG	C4-C5-C6-O6
3	BA	2	NAG	O5-C5-C6-O6
3	CC	2	NAG	C4-C5-C6-O6
3	AA	2	NAG	C8-C7-N2-C2
3	AA	2	NAG	O7-C7-N2-C2
3	BA	2	NAG	C4-C5-C6-O6
3	CA	2	NAG	O5-C5-C6-O6
3	CA	2	NAG	C4-C5-C6-O6
3	AA	2	NAG	O5-C5-C6-O6
3	CA	1	NAG	C4-C5-C6-O6
3	CB	2	NAG	C4-C5-C6-O6
3	CA	1	NAG	O5-C5-C6-O6
3	AC	2	NAG	C4-C5-C6-O6
3	CB	2	NAG	O5-C5-C6-O6
3	AC	2	NAG	O5-C5-C6-O6

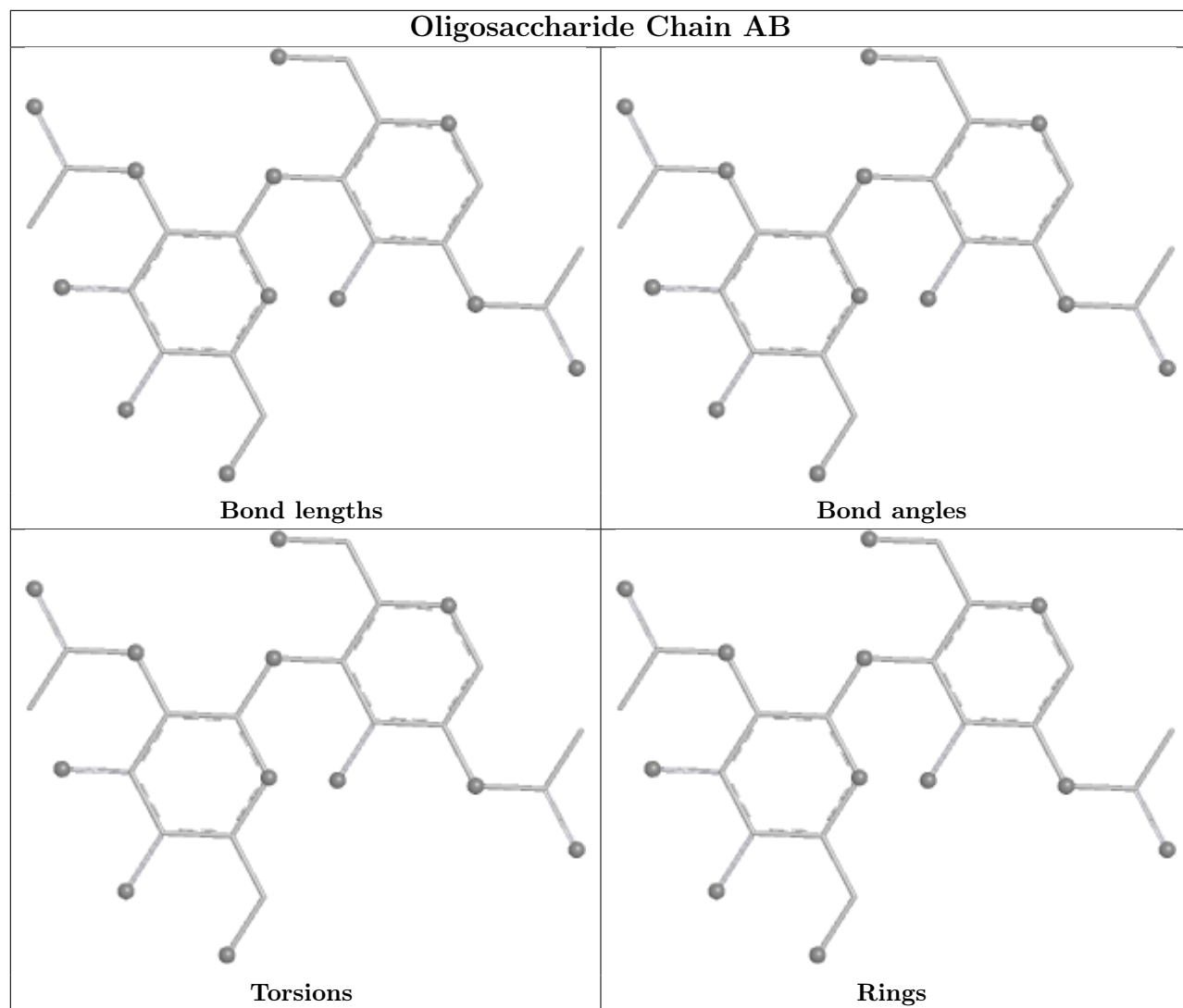
There are no ring outliers.

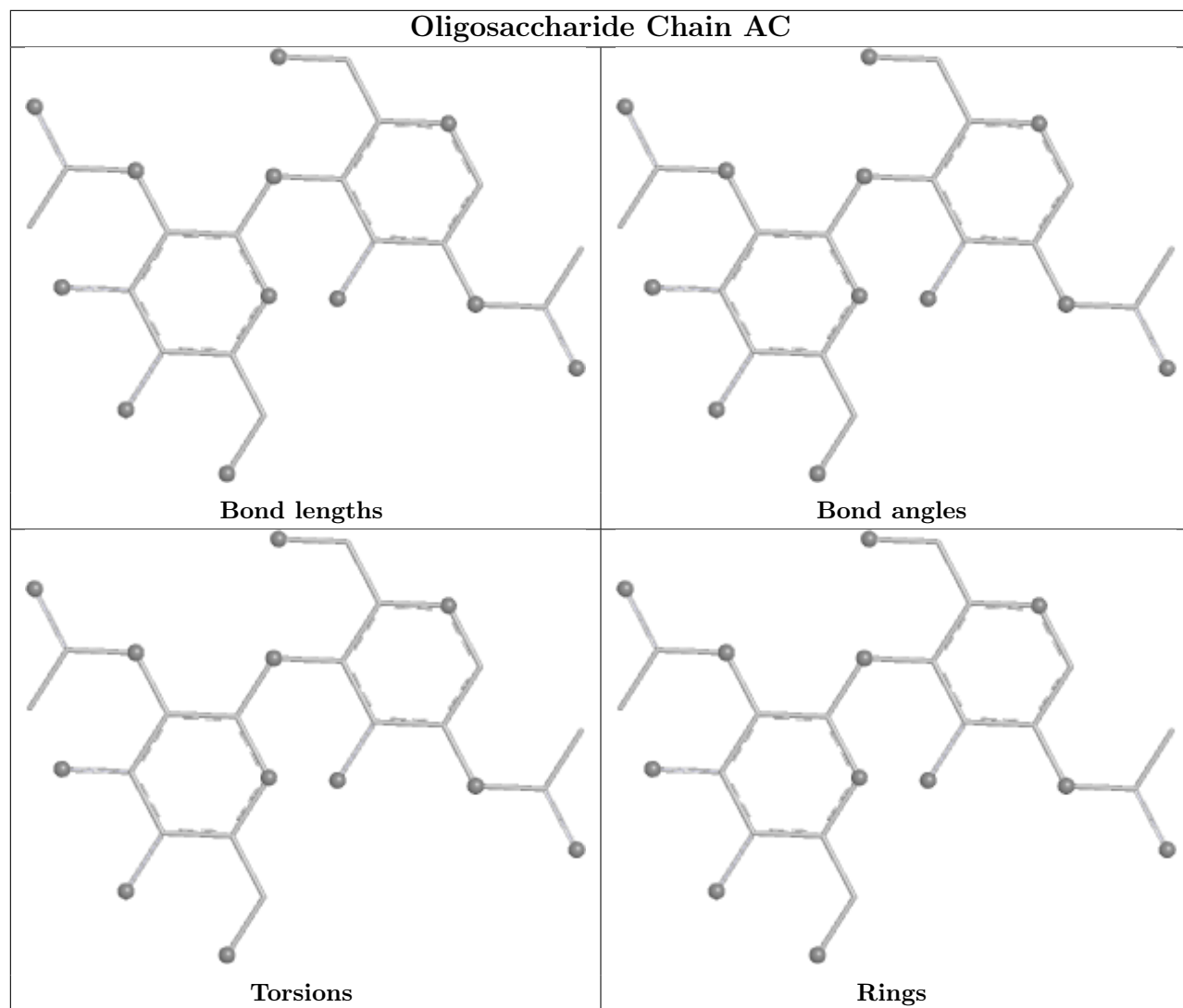
2 monomers are involved in 2 short contacts:

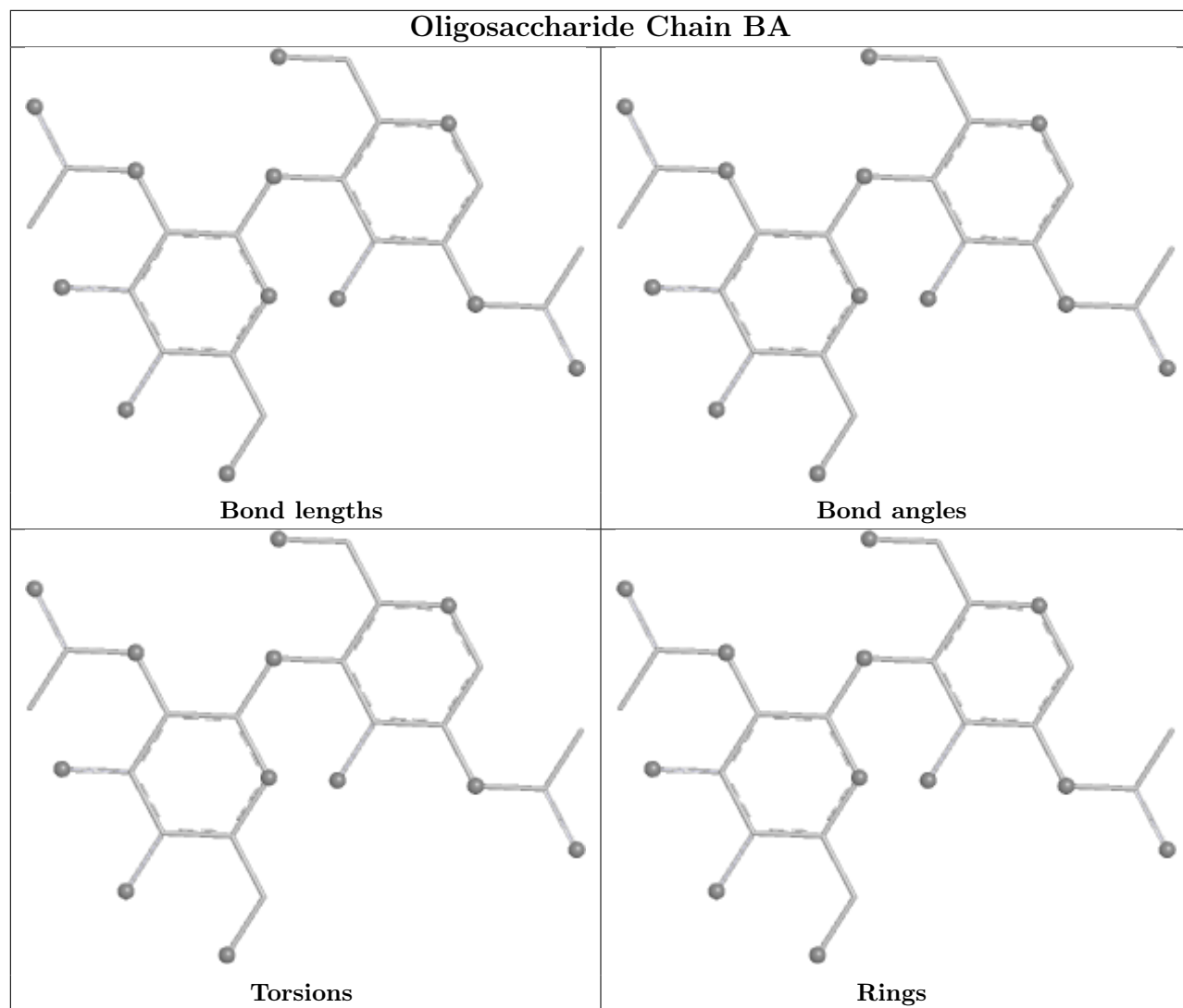
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	BB	1	NAG	1	0
3	CC	1	NAG	1	0

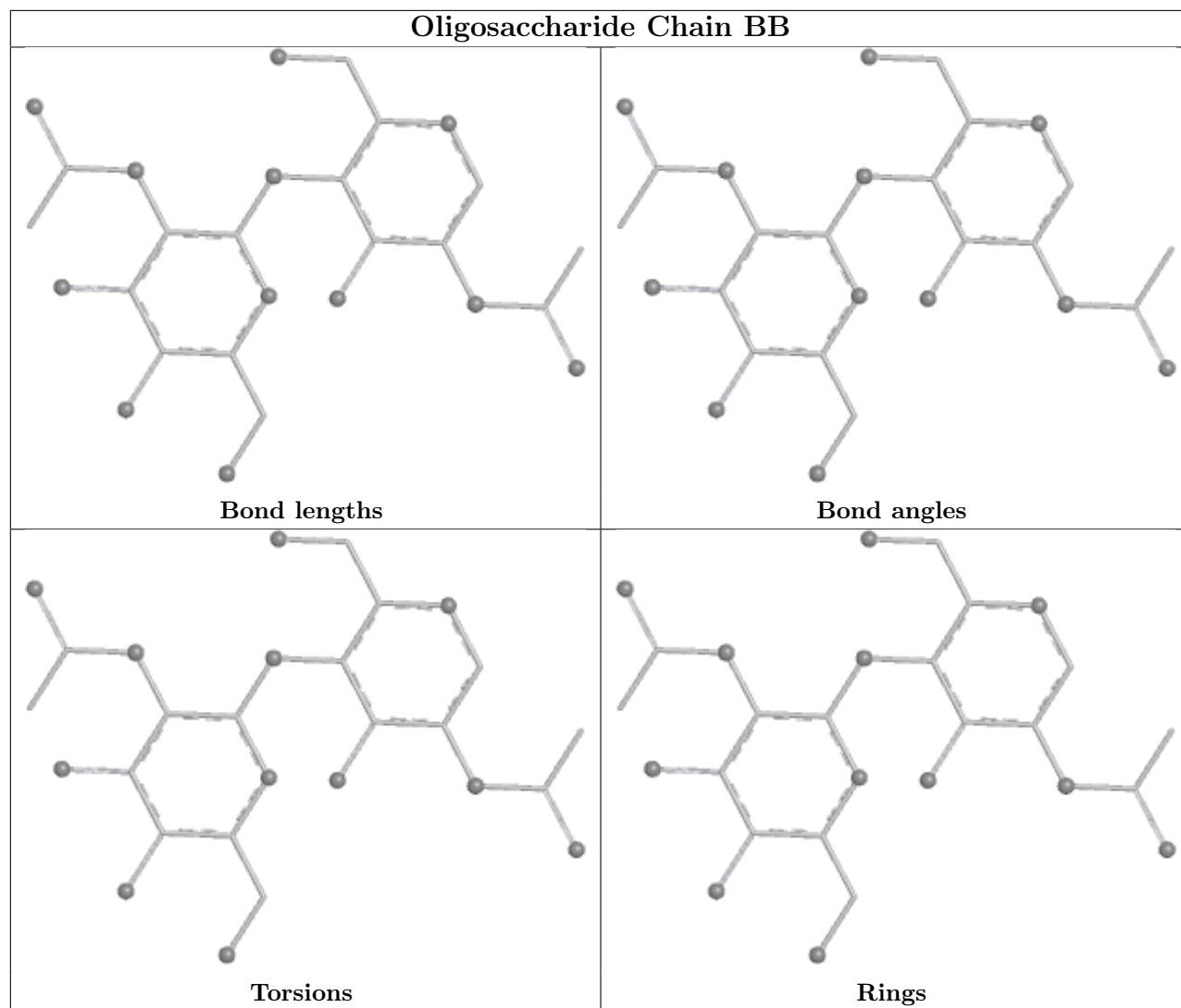
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

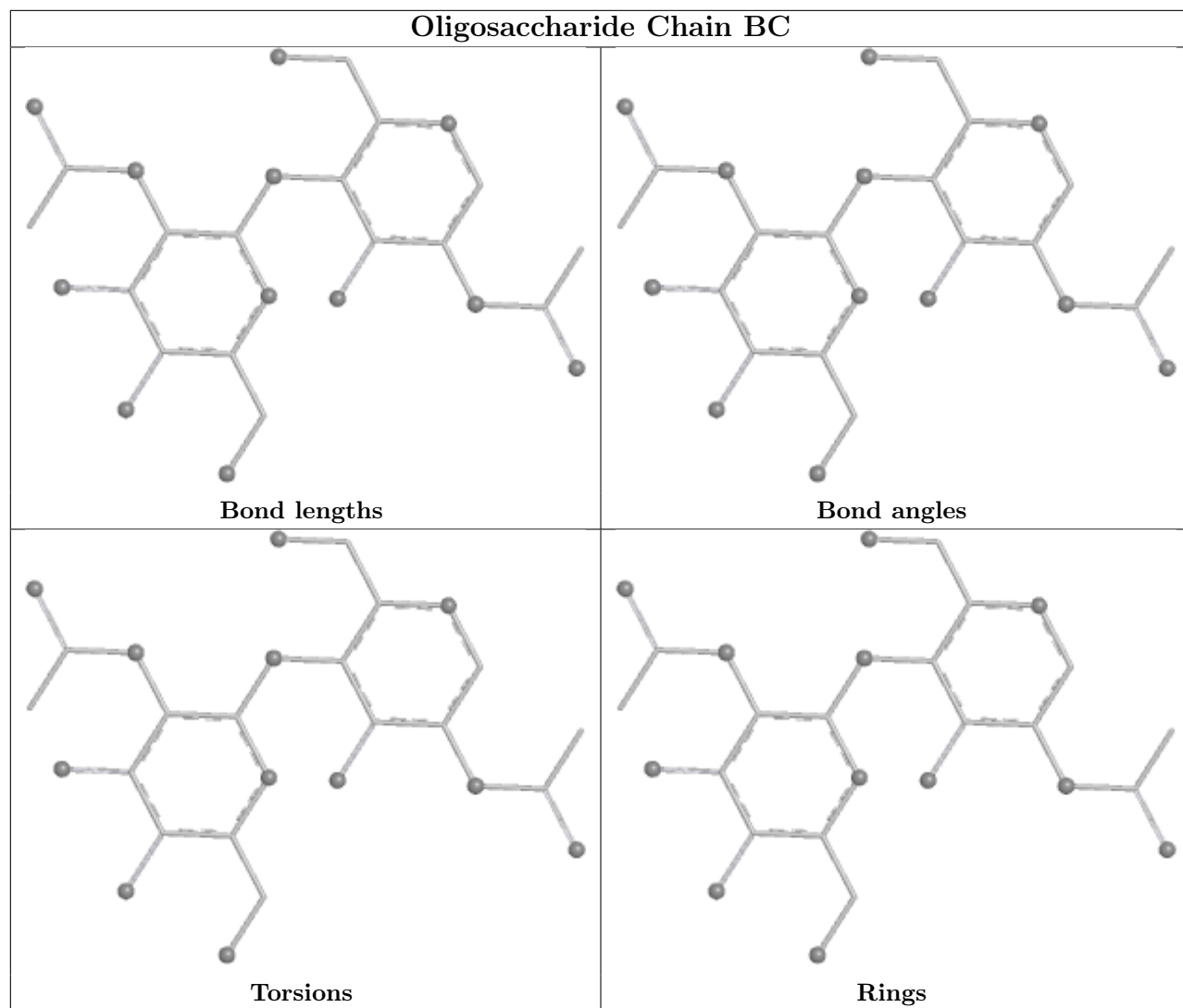


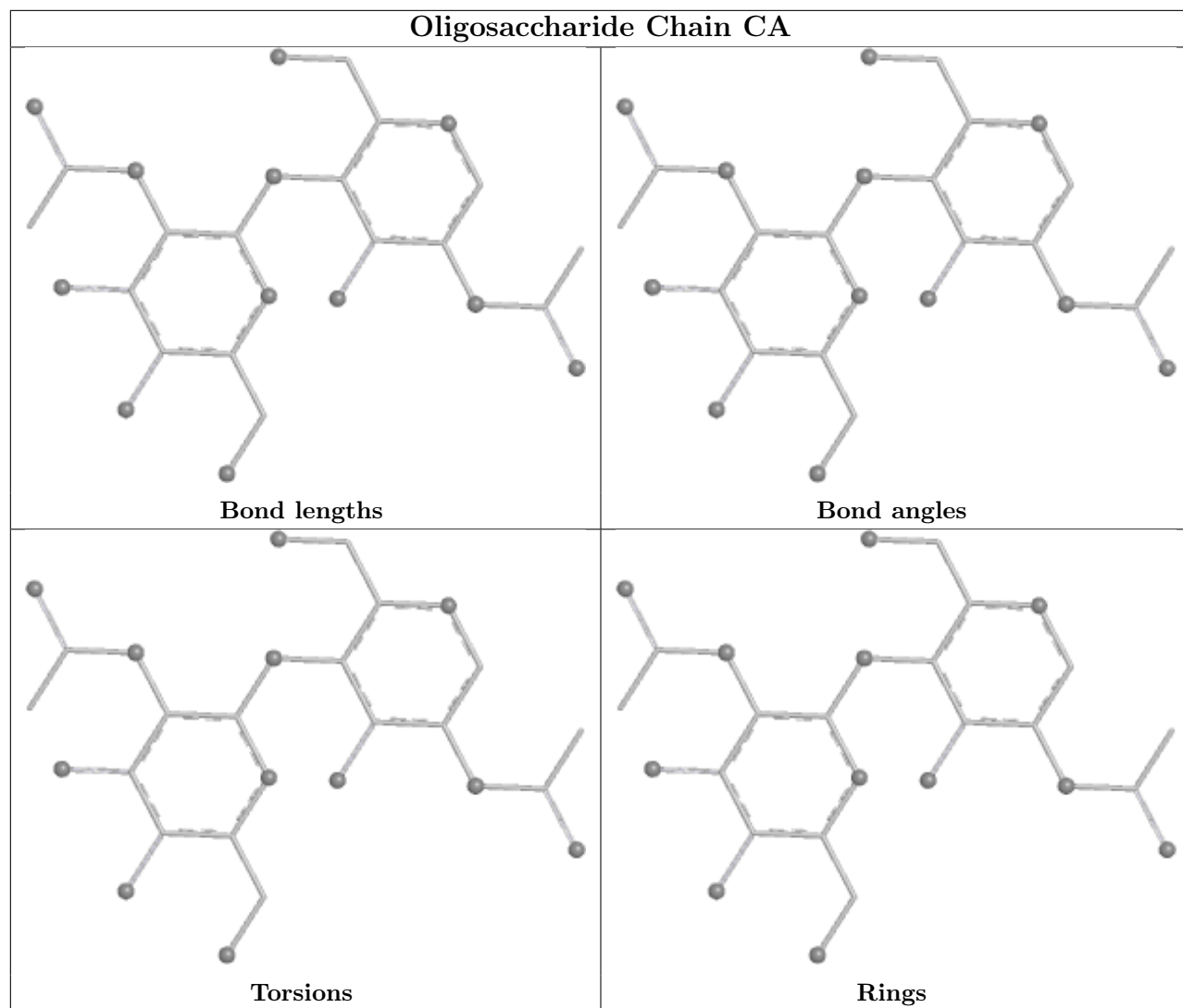


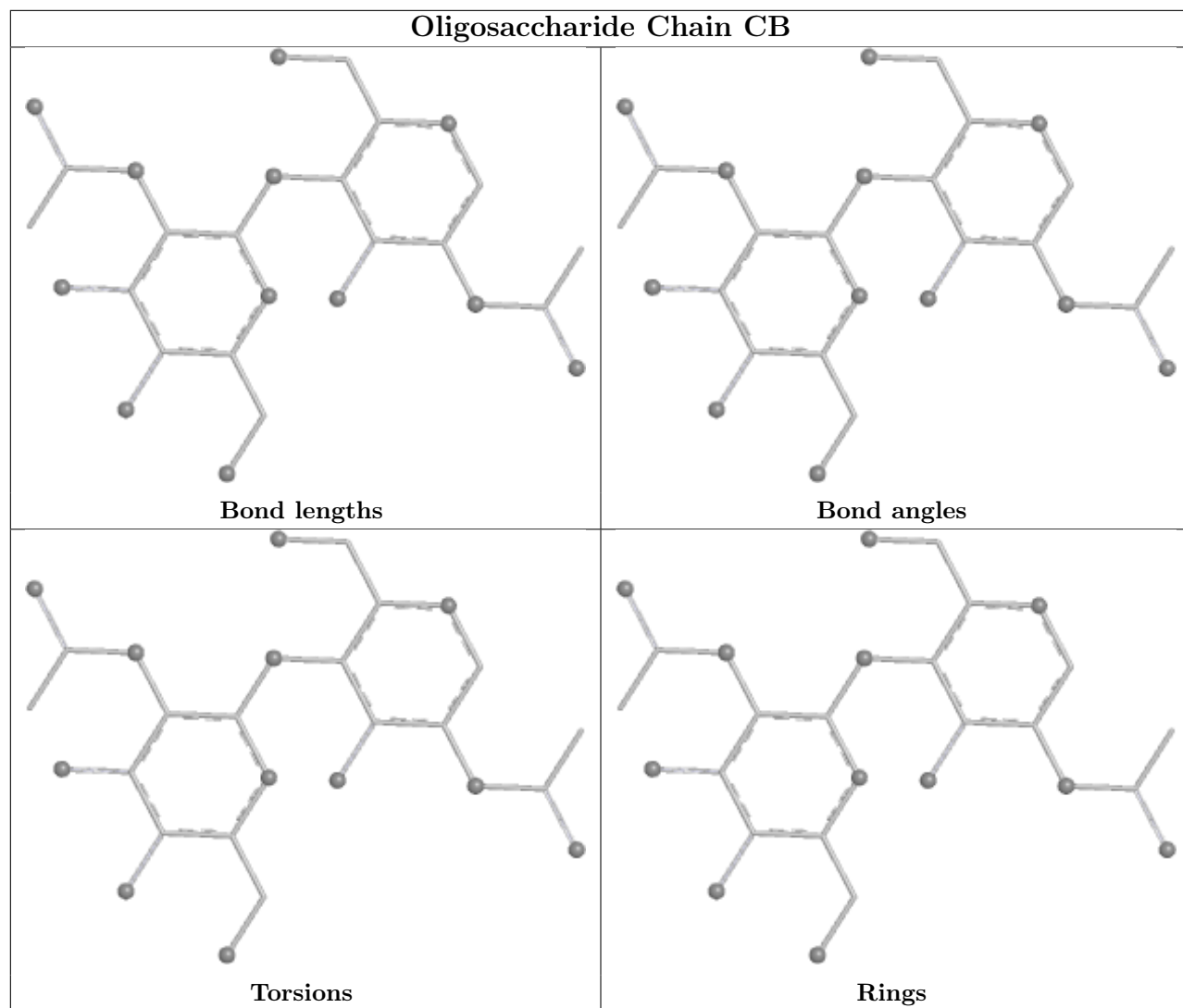


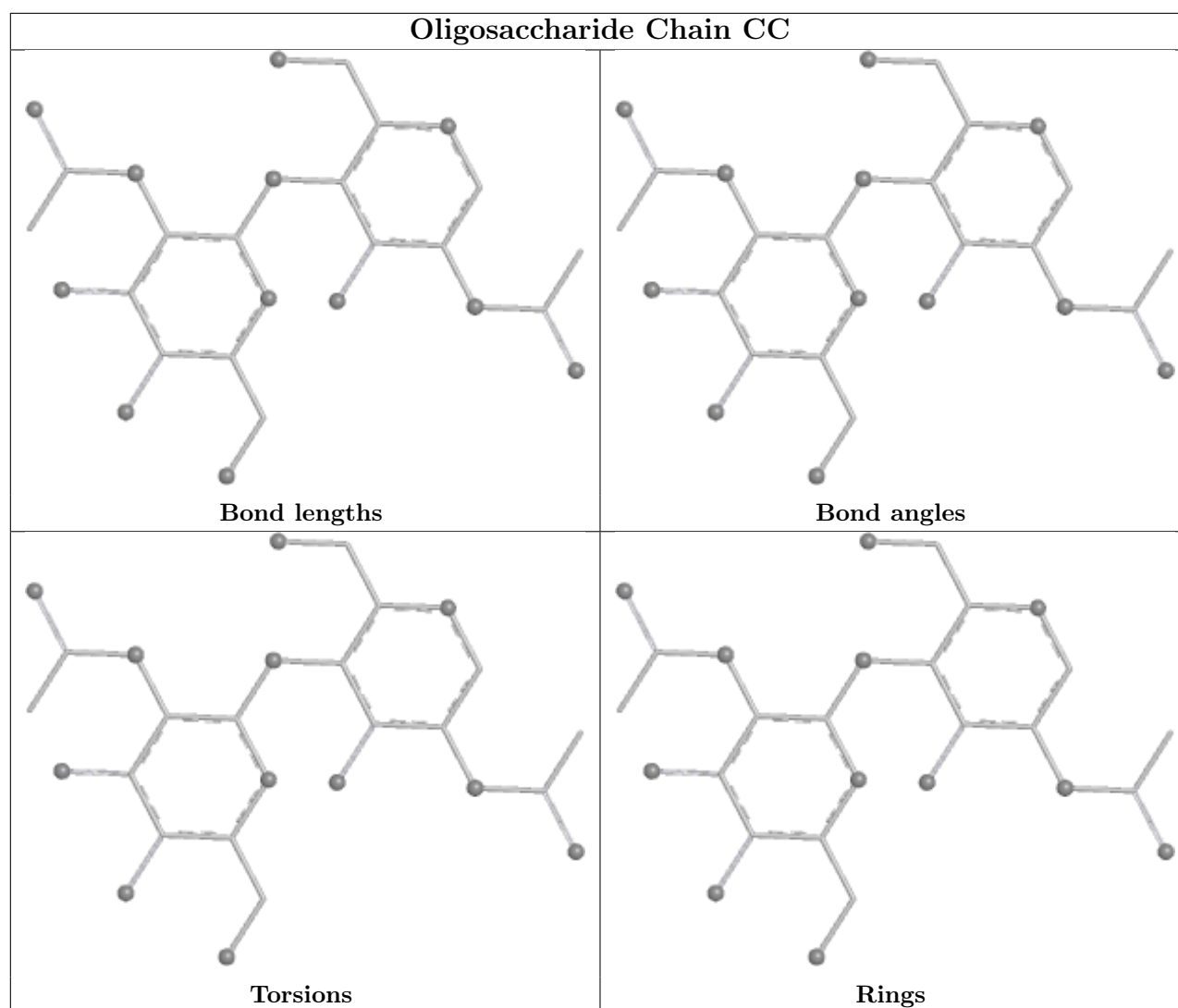












5.6 Ligand geometry [i](#)

27 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	$\# Z > 2$
4	NAG	A	1203	1	14,14,15	0.32	0	17,19,21	0.58	0
4	NAG	A	1205	1	14,14,15	0.33	0	17,19,21	0.60	1 (5%)
4	NAG	C	1201	1	14,14,15	0.26	0	17,19,21	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	KZ0	E	101	2	9,9,12	1.07	0	12,12,15	4.03	6 (50%)
4	NAG	A	1201	1	14,14,15	0.25	0	17,19,21	0.46	0
4	NAG	B	1204	1	14,14,15	0.34	0	17,19,21	0.60	1 (5%)
4	NAG	B	1208	1	14,14,15	0.41	0	17,19,21	0.56	0
6	KZ0	D	101	2	9,9,12	1.07	0	12,12,15	4.03	6 (50%)
4	NAG	A	1207	1	14,14,15	0.38	0	17,19,21	0.61	1 (5%)
4	NAG	C	1204	1	14,14,15	0.36	0	17,19,21	0.61	1 (5%)
4	NAG	A	1204	1	14,14,15	0.37	0	17,19,21	0.61	1 (5%)
4	NAG	B	1205	1	14,14,15	0.30	0	17,19,21	0.59	0
4	NAG	C	1206	1	14,14,15	0.41	0	17,19,21	0.61	1 (5%)
4	NAG	B	1207	1	14,14,15	0.41	0	17,19,21	0.57	0
5	STE	A	1208	-	19,19,19	0.58	0	19,19,19	0.53	0
4	NAG	B	1203	1	14,14,15	0.50	0	17,19,21	1.09	2 (11%)
4	NAG	A	1206	1	14,14,15	0.43	0	17,19,21	0.54	0
4	NAG	B	1202	1	14,14,15	0.31	0	17,19,21	0.58	0
6	KZ0	F	101	2	9,9,12	1.06	0	12,12,15	4.06	6 (50%)
4	NAG	C	1202	1	14,14,15	0.41	0	17,19,21	0.59	1 (5%)
4	NAG	C	1203	1	14,14,15	0.32	0	17,19,21	0.56	0
4	NAG	B	1206	1	14,14,15	0.38	0	17,19,21	0.53	0
4	NAG	C	1205	1	14,14,15	0.31	0	17,19,21	0.58	0
5	STE	C	1207	-	19,19,19	0.58	0	19,19,19	0.54	0
5	STE	B	1209	-	19,19,19	0.58	0	19,19,19	0.54	0
4	NAG	A	1202	1	14,14,15	0.39	0	17,19,21	0.56	0
4	NAG	B	1201	1	14,14,15	0.26	0	17,19,21	0.47	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
4	NAG	A	1203	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1205	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1201	1	-	0/6/23/26	0/1/1/1
6	KZ0	E	101	2	-	-	0/1/1/1
4	NAG	A	1201	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1204	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1208	1	-	2/6/23/26	0/1/1/1
6	KZ0	D	101	2	-	-	0/1/1/1
4	NAG	A	1207	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	1204	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1204	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1205	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1206	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1207	1	-	0/6/23/26	0/1/1/1
5	STE	A	1208	-	-	6/17/17/17	-
4	NAG	B	1203	1	-	4/6/23/26	0/1/1/1
4	NAG	A	1206	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1202	1	-	2/6/23/26	0/1/1/1
6	KZ0	F	101	2	-	-	0/1/1/1
4	NAG	C	1202	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1203	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1206	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1205	1	-	2/6/23/26	0/1/1/1
5	STE	C	1207	-	-	10/17/17/17	-
5	STE	B	1209	-	-	5/17/17/17	-
4	NAG	A	1202	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1201	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	101	KZ0	C3-N1-C2	6.94	119.99	115.18
6	F	101	KZ0	C3-N2-C1	6.93	119.98	115.18
6	F	101	KZ0	C2-N-C1	6.91	119.97	115.18
6	E	101	KZ0	C3-N2-C1	6.90	119.96	115.18
6	D	101	KZ0	C3-N1-C2	6.89	119.96	115.18
6	D	101	KZ0	C3-N2-C1	6.89	119.96	115.18
6	E	101	KZ0	C2-N-C1	6.86	119.94	115.18
6	D	101	KZ0	C2-N-C1	6.86	119.94	115.18
6	E	101	KZ0	C3-N1-C2	6.86	119.93	115.18
6	F	101	KZ0	N2-C3-N1	-3.28	119.98	125.77
6	F	101	KZ0	N2-C1-N	-3.27	120.00	125.77
4	B	1203	NAG	C2-N2-C7	3.26	127.27	122.90
6	E	101	KZ0	N2-C1-N	-3.26	120.02	125.77
6	D	101	KZ0	N-C2-N1	-3.25	120.03	125.77
6	E	101	KZ0	N2-C3-N1	-3.25	120.04	125.77
6	D	101	KZ0	N2-C1-N	-3.24	120.06	125.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	101	KZ0	N-C2-N1	-3.23	120.06	125.77
6	D	101	KZ0	N2-C3-N1	-3.23	120.06	125.77
6	E	101	KZ0	N-C2-N1	-3.21	120.11	125.77
4	C	1204	NAG	C1-O5-C5	2.10	115.00	112.19
4	A	1204	NAG	C1-O5-C5	2.10	115.00	112.19
4	C	1206	NAG	C1-O5-C5	2.08	114.98	112.19
4	A	1207	NAG	C1-O5-C5	2.08	114.97	112.19
4	B	1204	NAG	C1-O5-C5	2.05	114.94	112.19
4	C	1202	NAG	C1-O5-C5	2.04	114.93	112.19
4	B	1203	NAG	C1-O5-C5	2.02	114.90	112.19
4	A	1205	NAG	C1-O5-C5	2.00	114.87	112.19

There are no chirality outliers.

All (47) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1207	NAG	O5-C5-C6-O6
4	A	1206	NAG	C4-C5-C6-O6
4	B	1208	NAG	C4-C5-C6-O6
4	C	1202	NAG	O5-C5-C6-O6
4	B	1206	NAG	O5-C5-C6-O6
4	B	1204	NAG	O5-C5-C6-O6
4	A	1207	NAG	C4-C5-C6-O6
4	B	1206	NAG	C4-C5-C6-O6
4	A	1202	NAG	O5-C5-C6-O6
4	B	1204	NAG	C4-C5-C6-O6
4	C	1202	NAG	C4-C5-C6-O6
4	B	1208	NAG	O5-C5-C6-O6
4	A	1206	NAG	O5-C5-C6-O6
4	A	1202	NAG	C4-C5-C6-O6
4	B	1203	NAG	O5-C5-C6-O6
4	B	1203	NAG	C4-C5-C6-O6
5	C	1207	STE	C10-C11-C12-C13
4	B	1202	NAG	O5-C5-C6-O6
4	B	1202	NAG	C4-C5-C6-O6
5	B	1209	STE	C1-C2-C3-C4
5	C	1207	STE	C11-C12-C13-C14
5	A	1208	STE	C14-C15-C16-C17
5	B	1209	STE	C6-C7-C8-C9
5	B	1209	STE	C12-C13-C14-C15
5	C	1207	STE	C3-C4-C5-C6
5	C	1207	STE	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
5	C	1207	STE	C14-C15-C16-C17
5	A	1208	STE	C7-C8-C9-C10
4	C	1205	NAG	C4-C5-C6-O6
4	A	1204	NAG	C4-C5-C6-O6
4	C	1205	NAG	O5-C5-C6-O6
4	A	1204	NAG	O5-C5-C6-O6
5	B	1209	STE	C10-C11-C12-C13
5	C	1207	STE	C4-C5-C6-C7
4	C	1204	NAG	C4-C5-C6-O6
4	C	1204	NAG	O5-C5-C6-O6
5	C	1207	STE	O1-C1-C2-C3
5	C	1207	STE	C11-C10-C9-C8
5	A	1208	STE	O1-C1-C2-C3
5	C	1207	STE	C6-C7-C8-C9
4	B	1203	NAG	C1-C2-N2-C7
5	A	1208	STE	O2-C1-C2-C3
5	A	1208	STE	C4-C5-C6-C7
5	C	1207	STE	O2-C1-C2-C3
4	B	1203	NAG	C3-C2-N2-C7
5	A	1208	STE	C11-C10-C9-C8
5	B	1209	STE	C7-C8-C9-C10

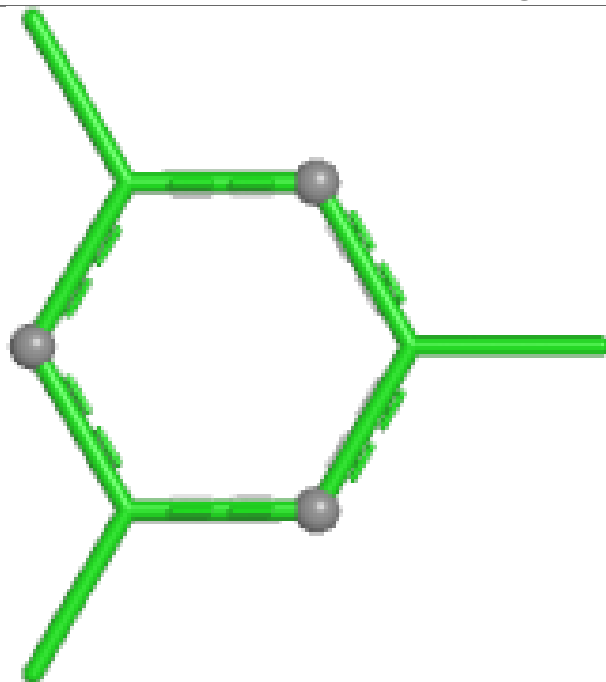
There are no ring outliers.

2 monomers are involved in 3 short contacts:

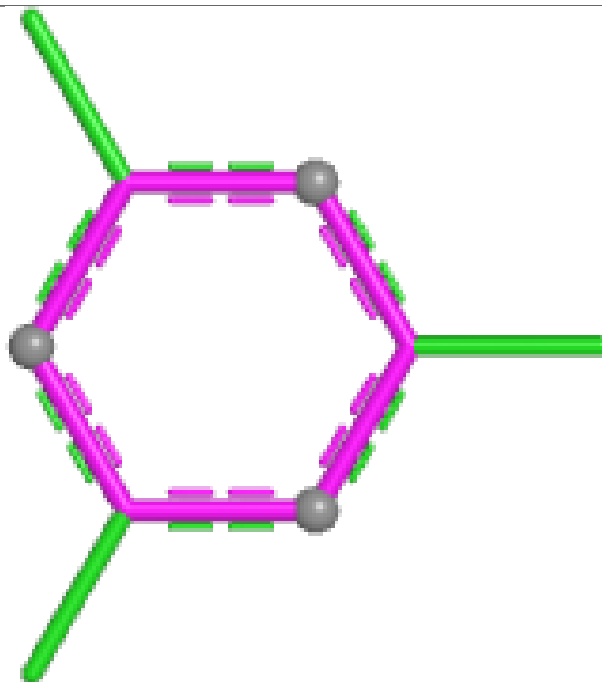
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1207	NAG	1	0
5	A	1208	STE	2	0

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.

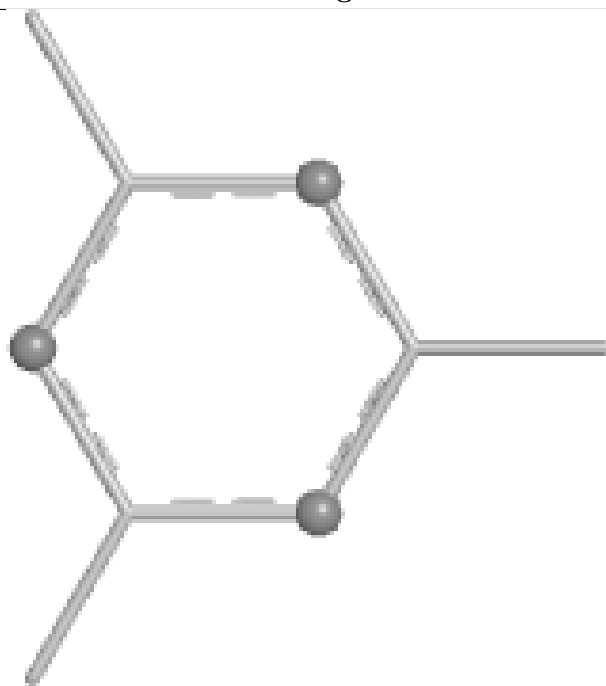
Ligand KZ0 E 101



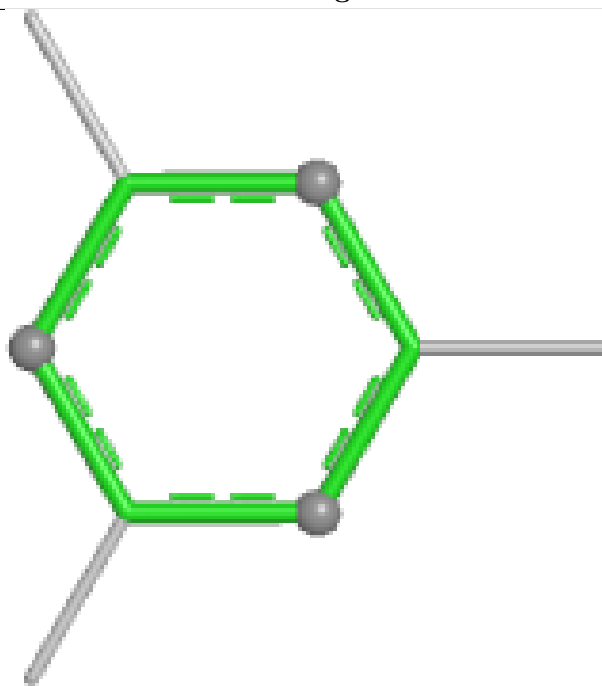
Bond lengths



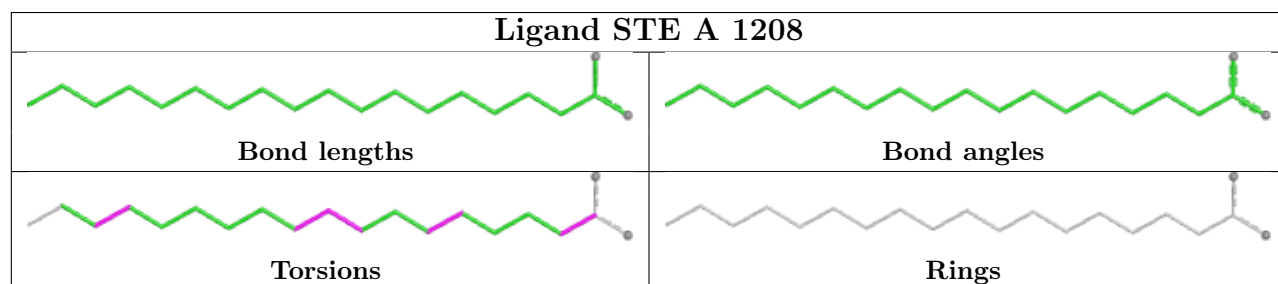
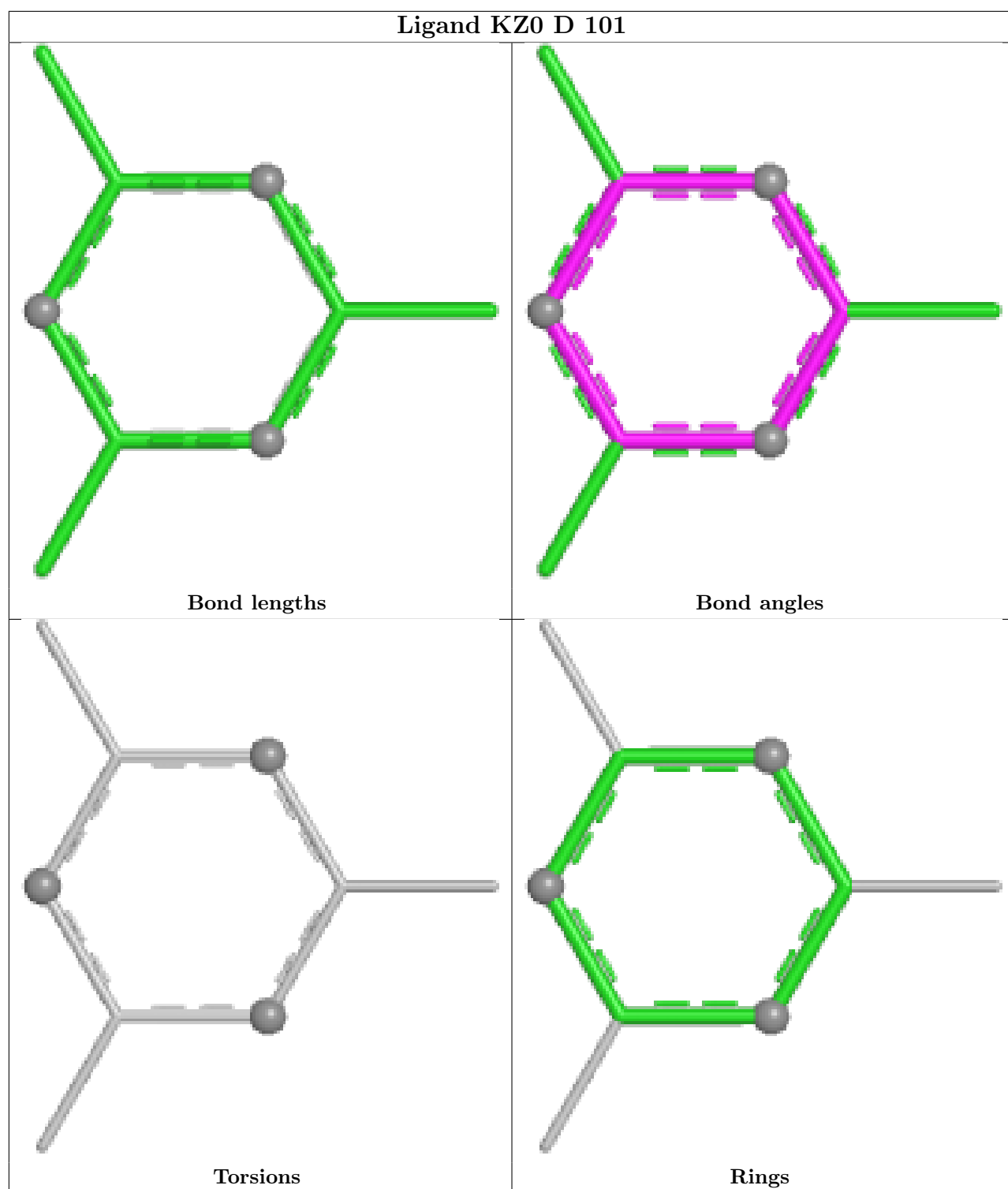
Bond angles

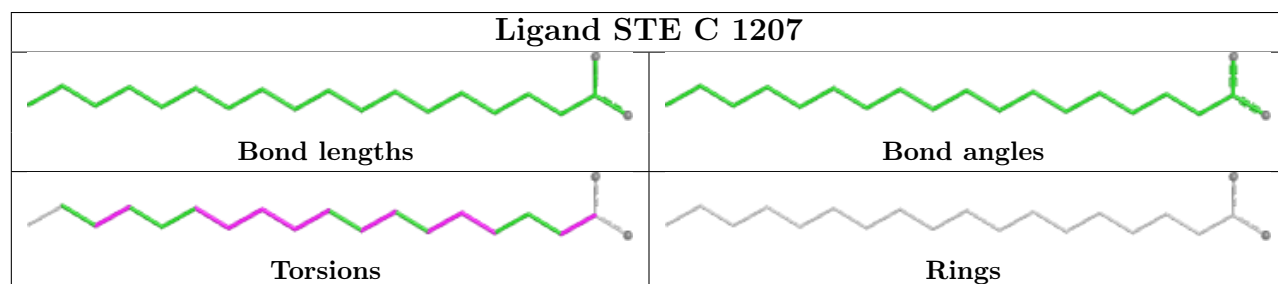
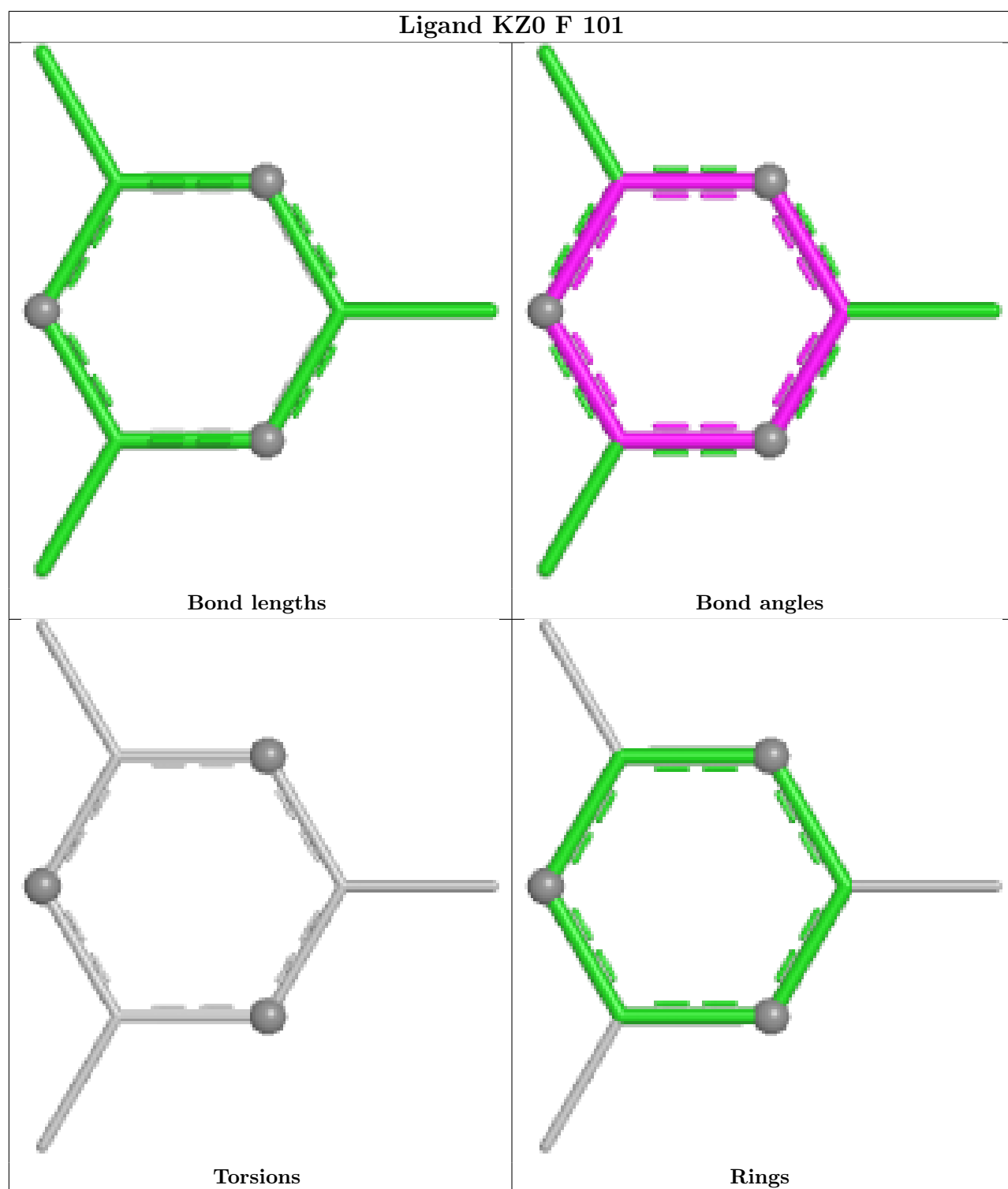


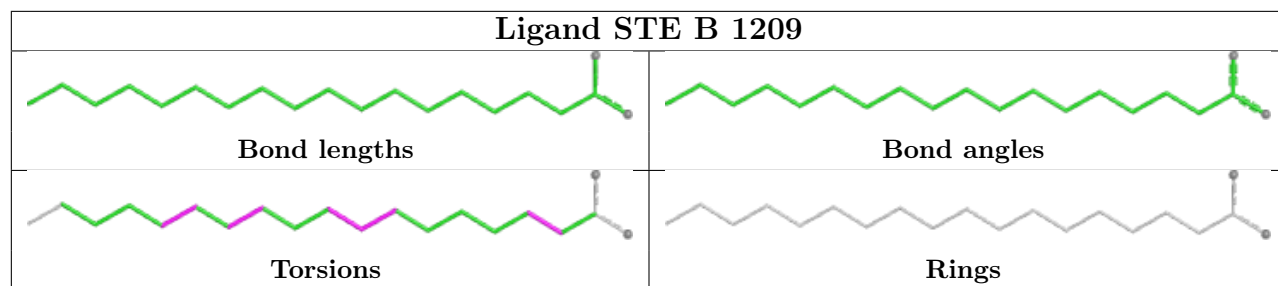
Torsions



Rings







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

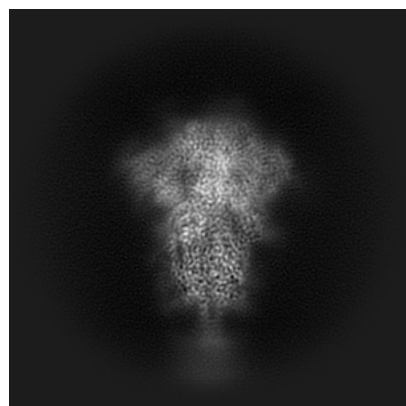
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51659. These allow visual inspection of the internal detail of the map and identification of artifacts.

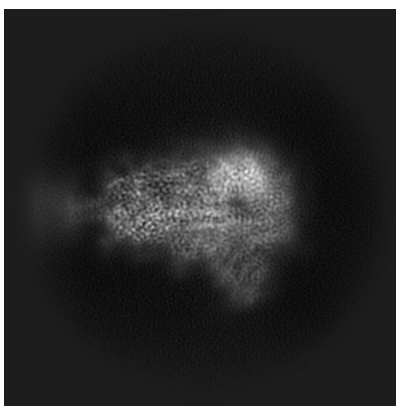
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

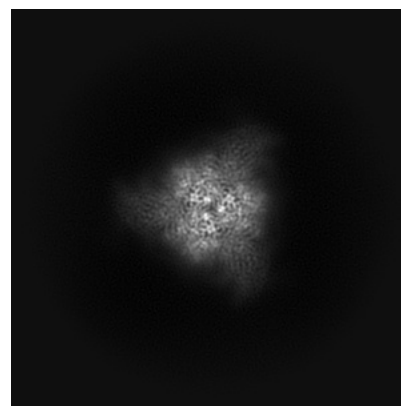
6.1.1 Primary map



X

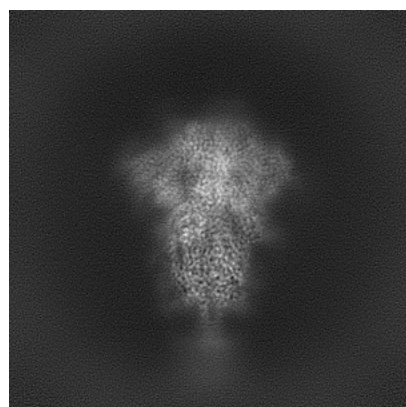


Y

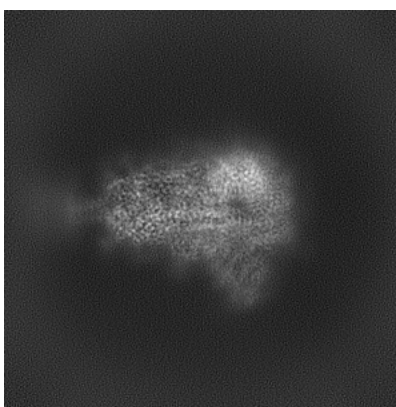


Z

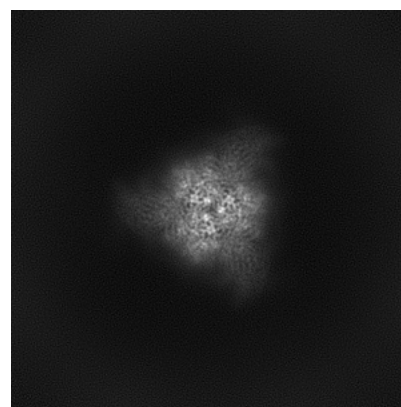
6.1.2 Raw map



X



Y

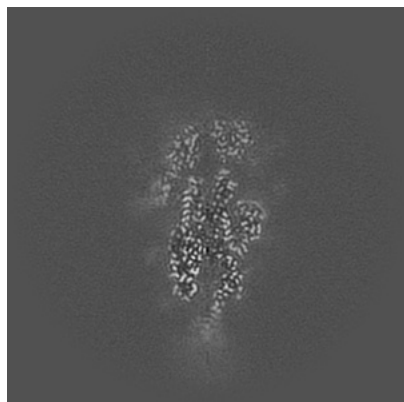


Z

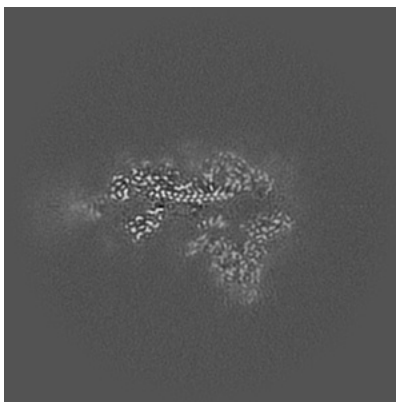
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

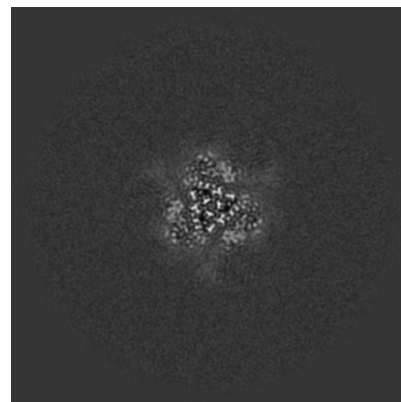
6.2.1 Primary map



X Index: 165

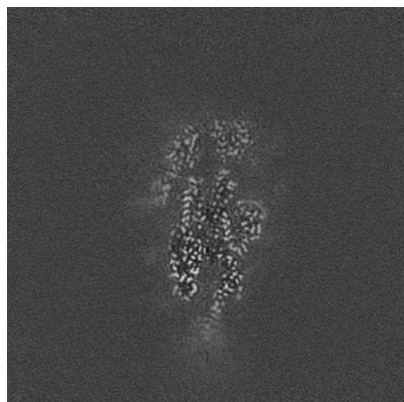


Y Index: 165

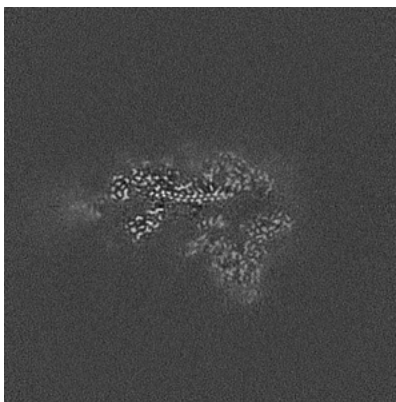


Z Index: 165

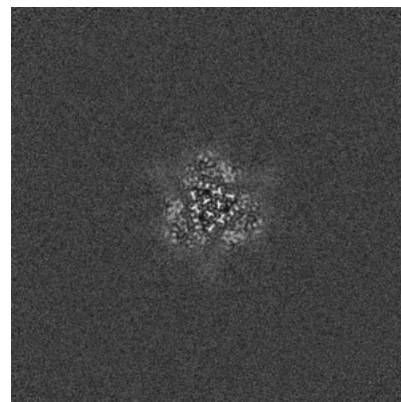
6.2.2 Raw map



X Index: 165



Y Index: 165

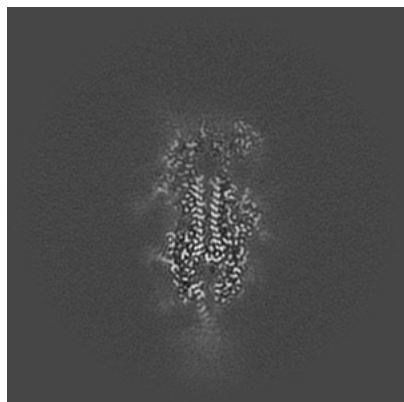


Z Index: 165

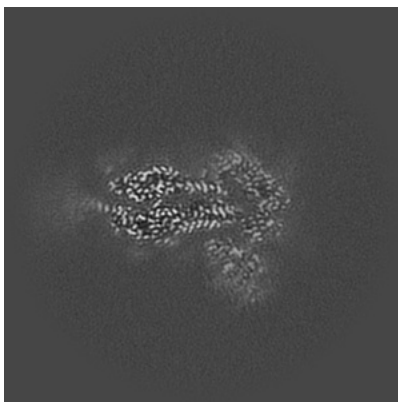
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

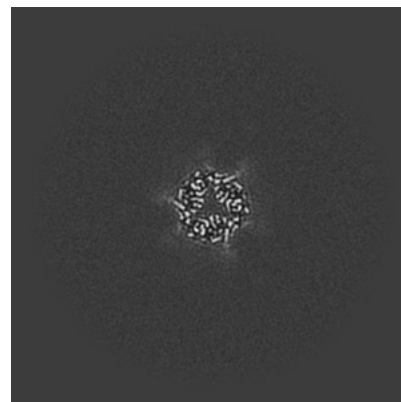
6.3.1 Primary map



X Index: 160

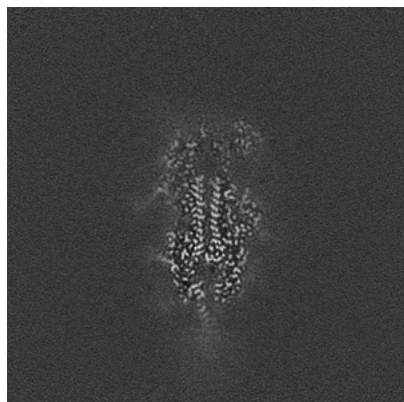


Y Index: 174

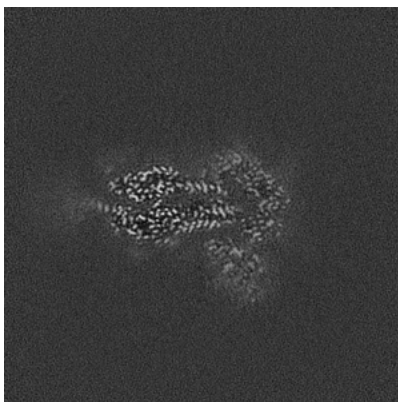


Z Index: 110

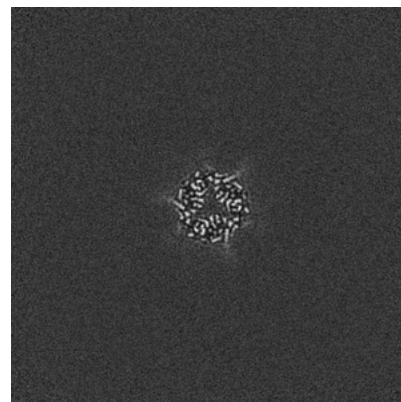
6.3.2 Raw map



X Index: 160



Y Index: 174

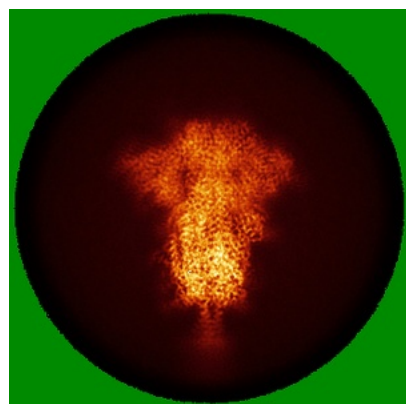


Z Index: 110

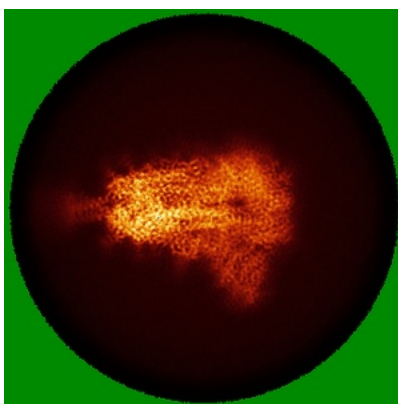
The images above show the largest variance slices of the map in three orthogonal directions.

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

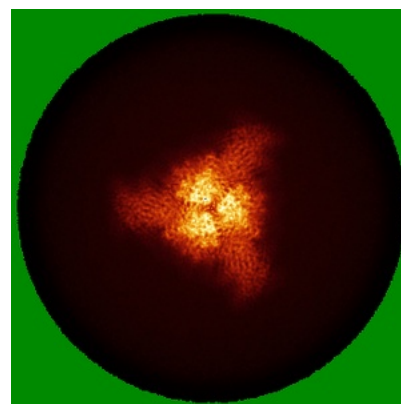
6.4.1 Primary map



X



Y

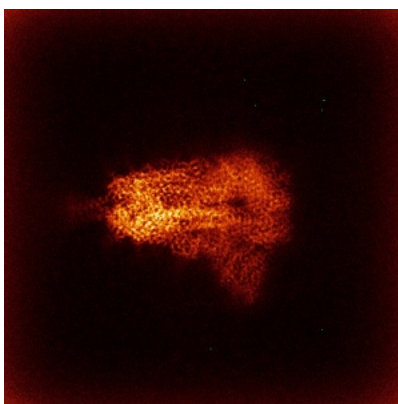


Z

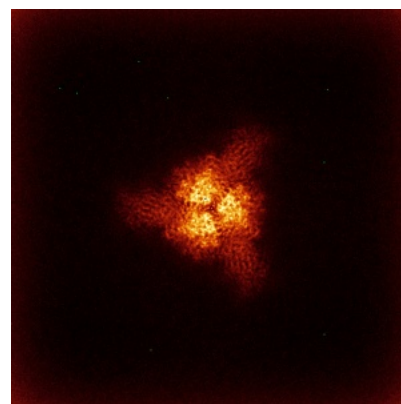
6.4.2 Raw map



X



Y

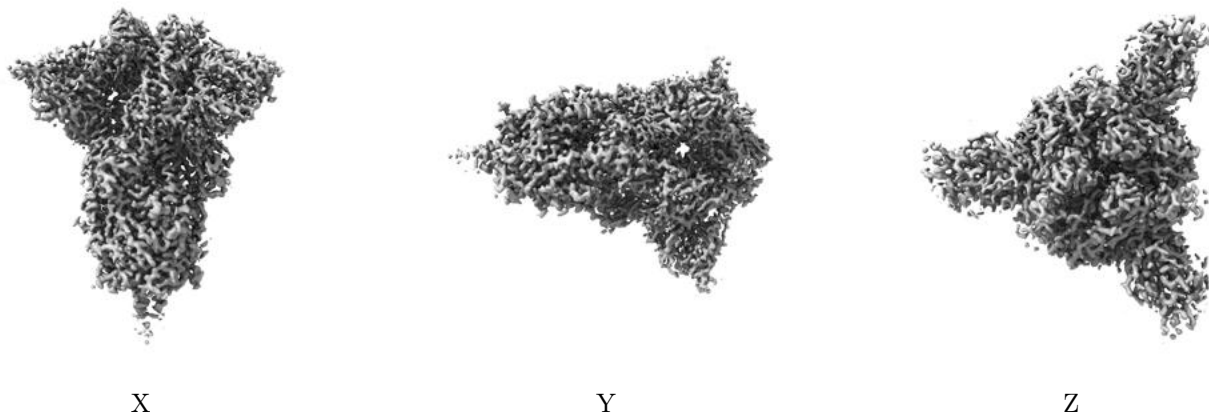


Z

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

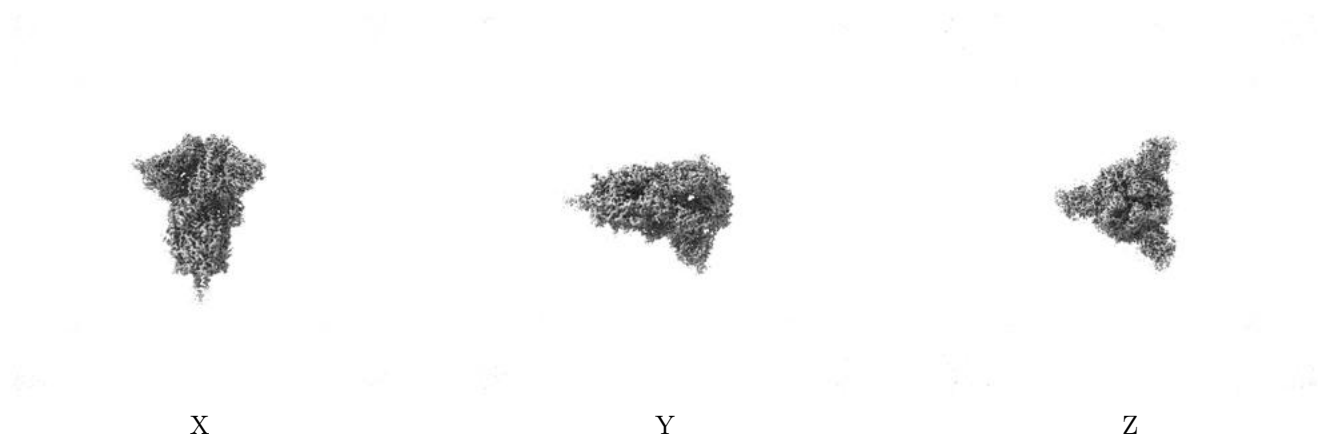
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

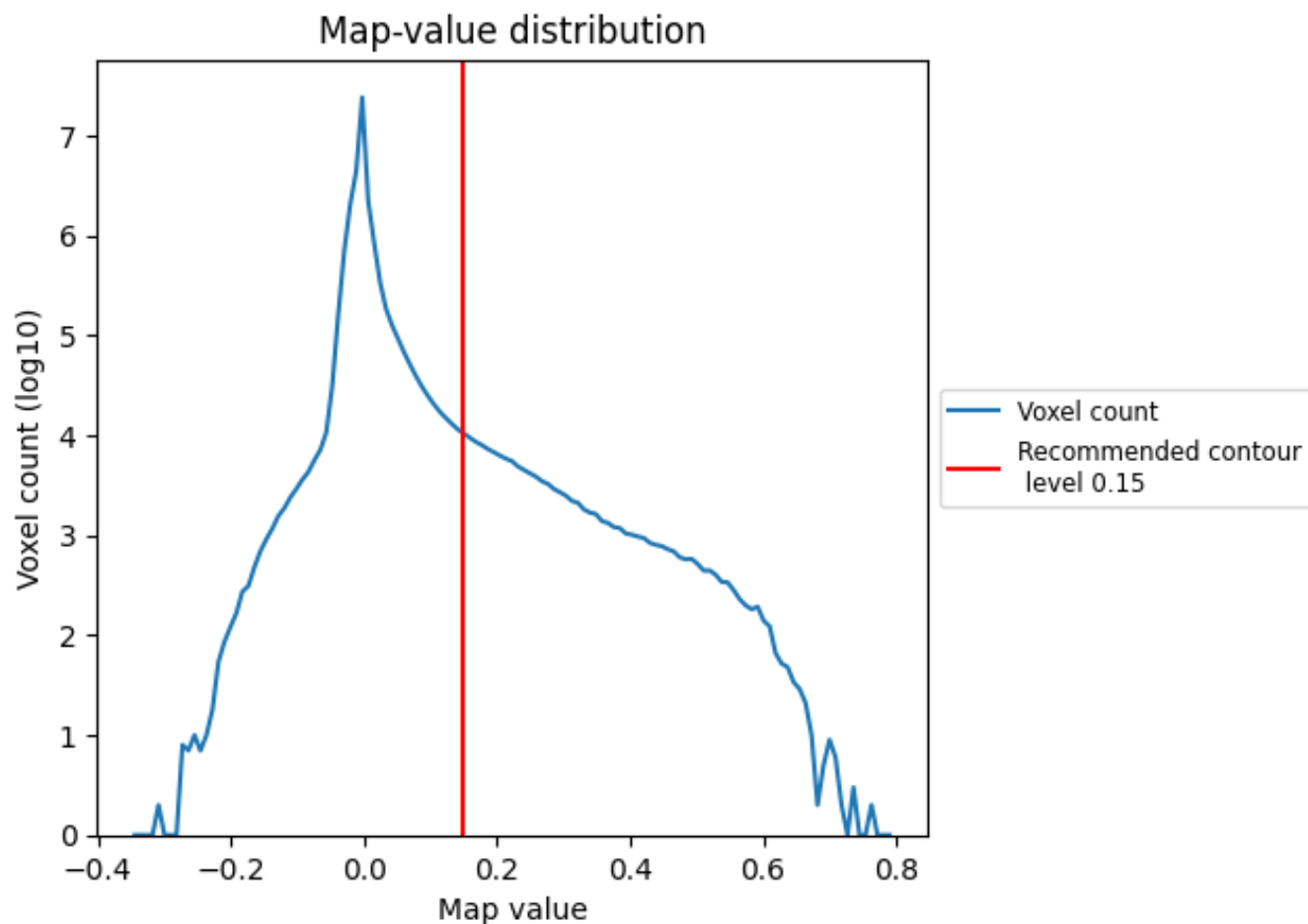
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

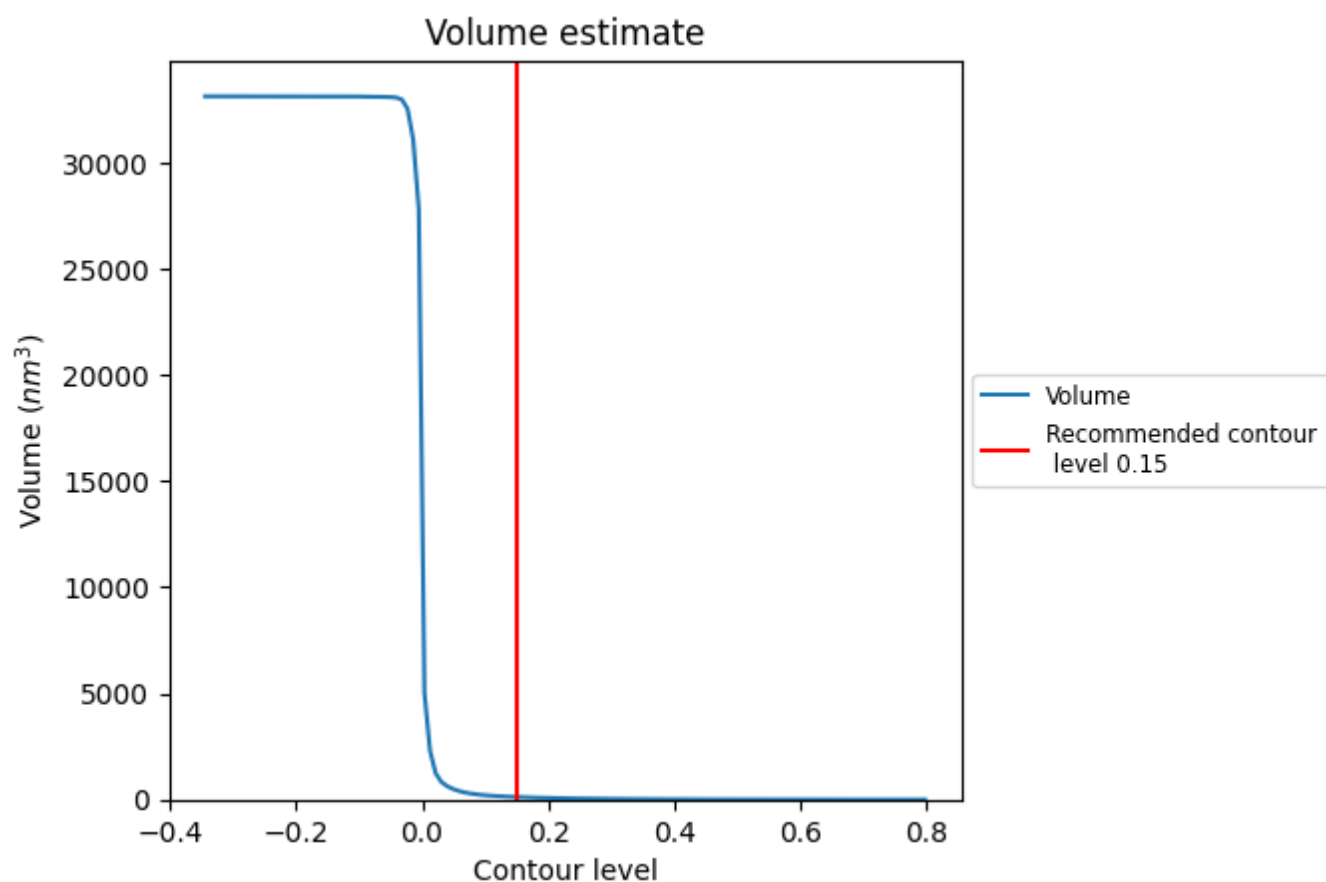
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

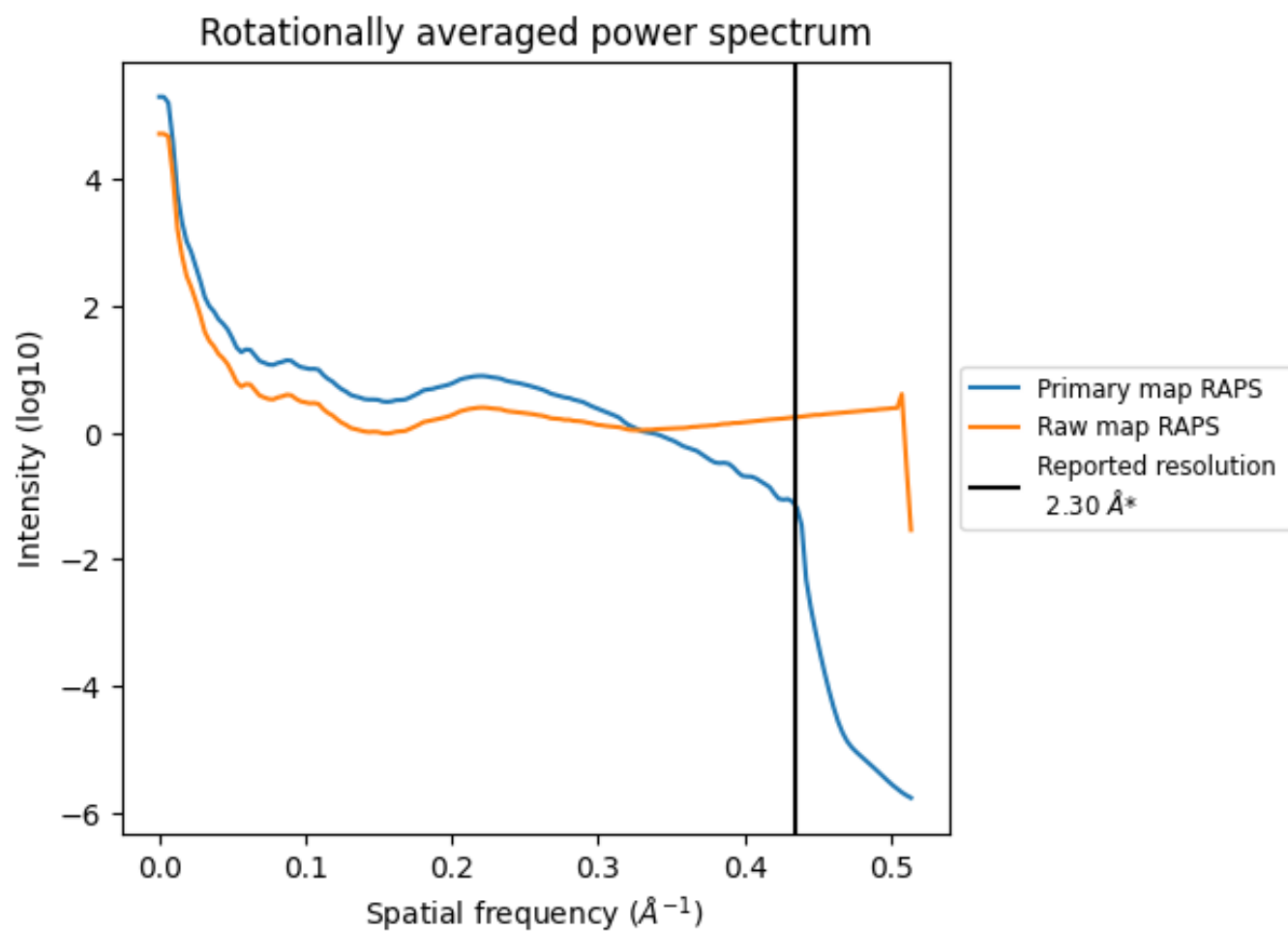
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 119 nm^3 ; this corresponds to an approximate mass of 108 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 ⓘ

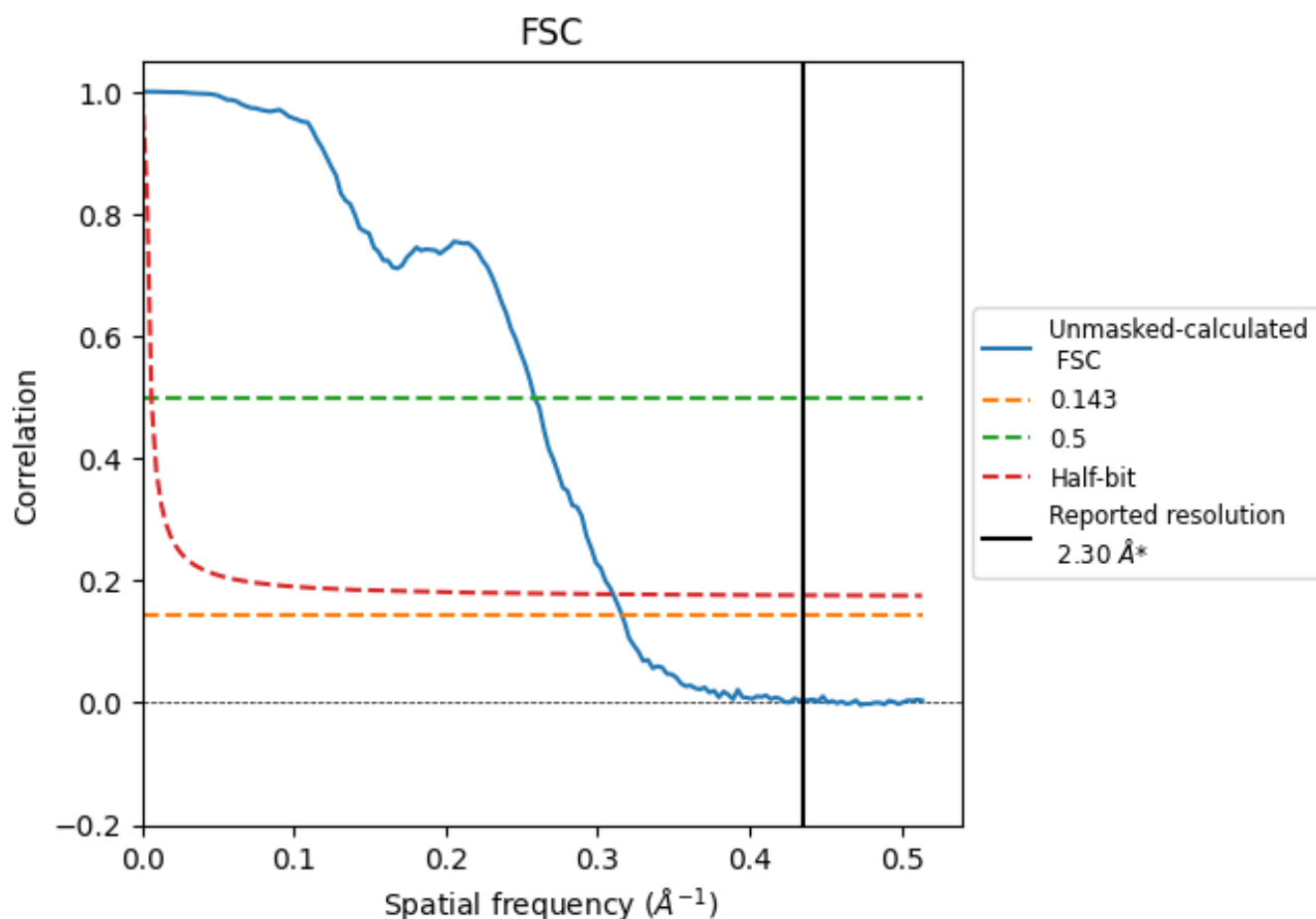


*Reported resolution corresponds to spatial frequency of 0.435 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.435 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

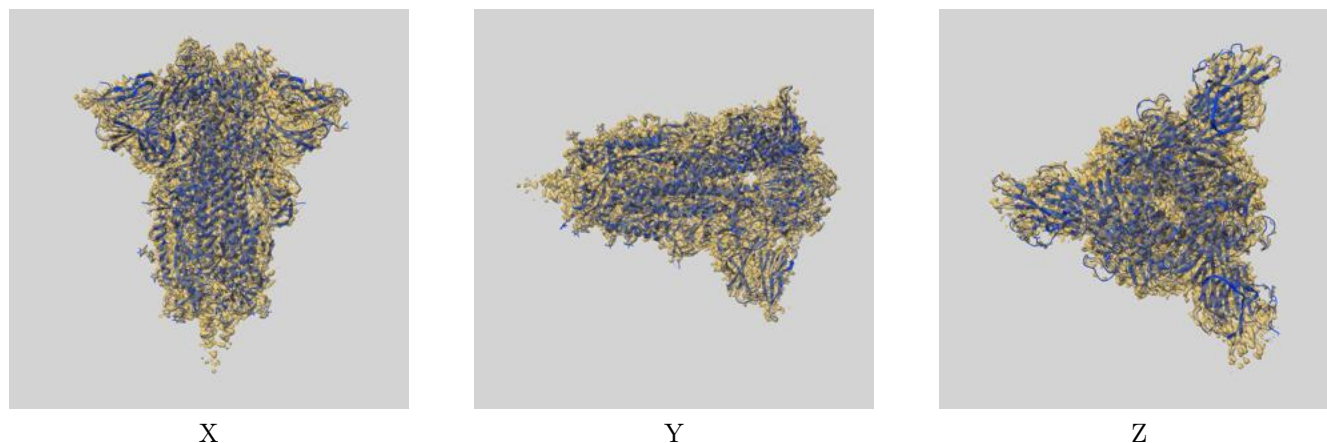
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.17	3.87	3.22

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.17 differs from the reported value 2.3 by more than 10 %

9 Map-model fit [i](#)

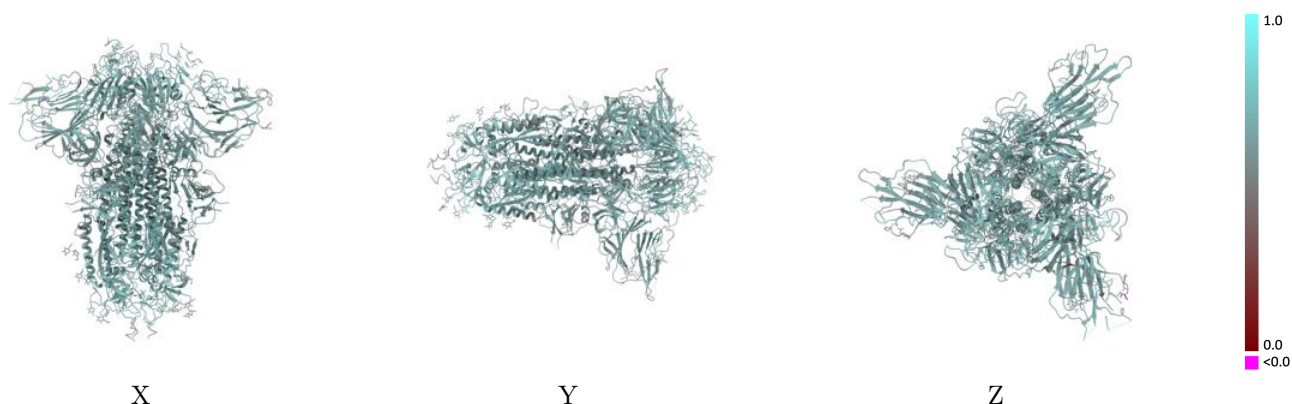
This section contains information regarding the fit between EMDB map EMD-51659 and PDB model 9GXE. Per-residue inclusion information can be found in [section 3](#) on [page 9](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



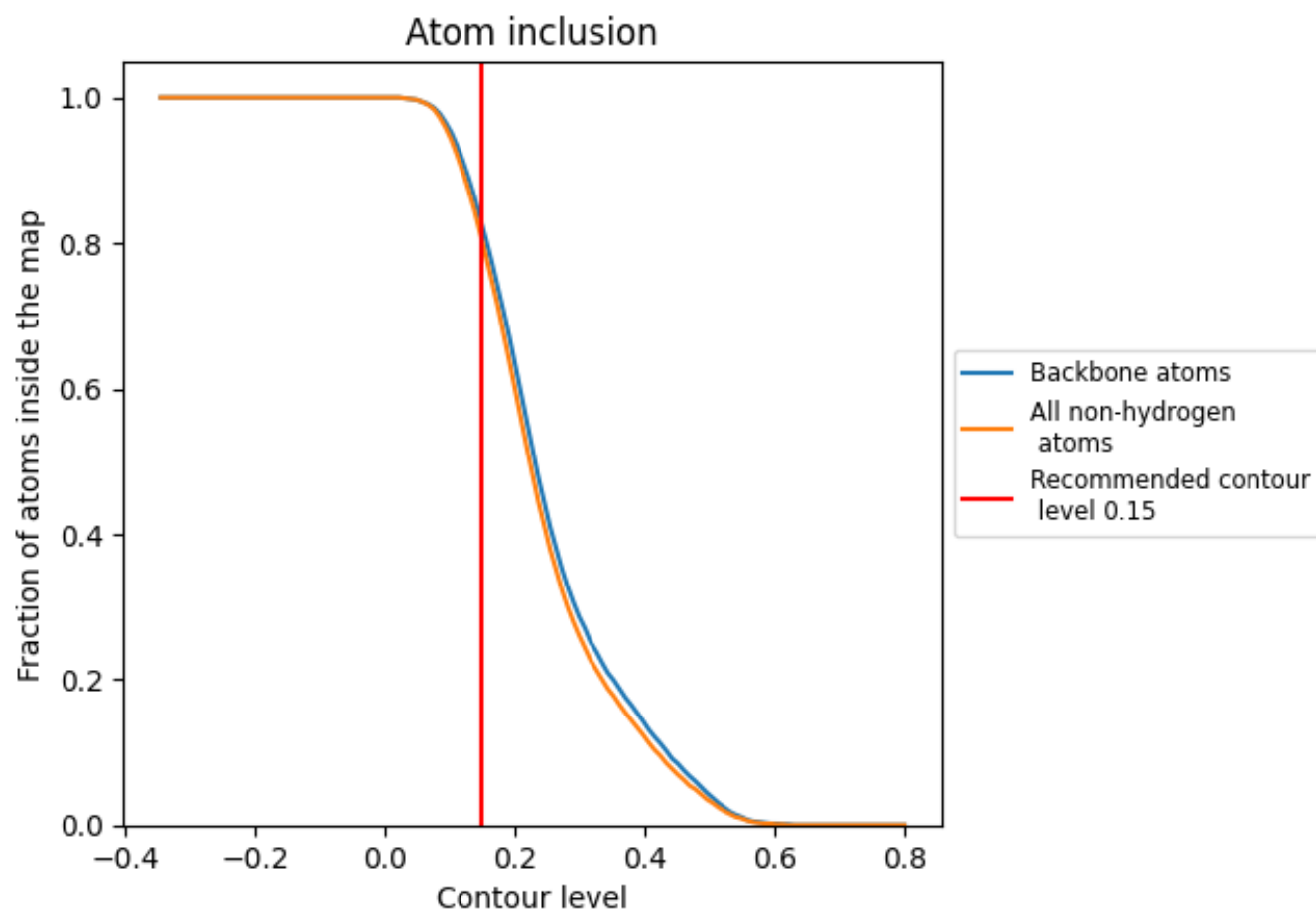
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.15).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 80% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8030	 0.6230
A	 0.8090	 0.6250
AA	 0.5710	 0.5140
AB	 0.4290	 0.5160
AC	 0.6790	 0.5750
B	 0.8090	 0.6230
BA	 0.6430	 0.5110
BB	 0.6070	 0.5670
BC	 0.7140	 0.5640
C	 0.8120	 0.6240
CA	 0.6430	 0.5120
CB	 0.7140	 0.5700
CC	 0.6070	 0.5590
D	 0.6410	 0.6120
E	 0.6230	 0.6270
F	 0.6230	 0.6110

