



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 09:45 AM UTC

PDB ID : 7LZH / pdb_00007lzh
EMDB ID : EMD-23606
Title : Structure of the glutamate receptor-like channel AtGLR3.4
Authors : Gangwar, S.P.; Green, M.N.; Sobolevsky, A.I.
Deposited on : 2021-03-09
Resolution : 3.57 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:

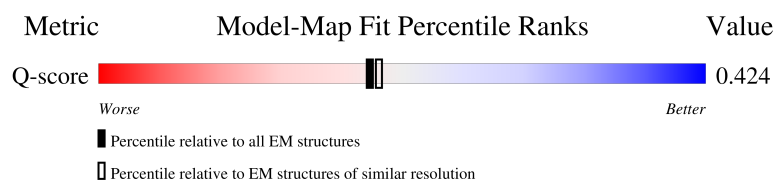
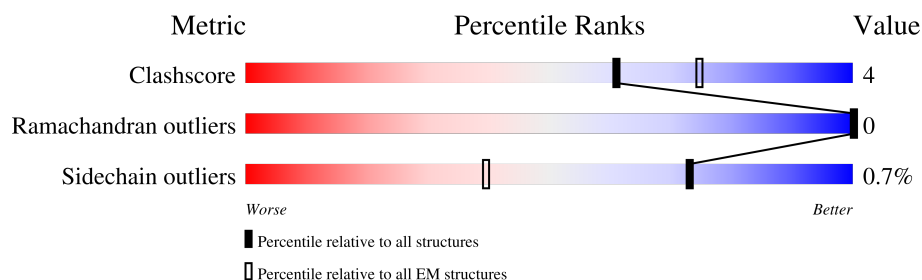
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.57 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.



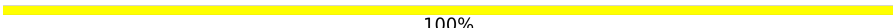
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12682 (3.07 - 4.07)

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	959	
1	B	959	
1	C	959	
1	D	959	

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Mol	Chain	Length	Quality of chain
2	E	2	 50% 50%
2	F	2	 50% 50%
2	G	2	 50% 50%
2	H	2	 50% 50%
2	I	2	 50% 50%
2	J	2	 100%
2	K	2	 50% 50%
2	L	2	 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
4	NAG	B	1002	X	-	-	-
4	NAG	C	1002	X	-	-	-
4	NAG	D	1002	X	-	-	-

2 Entry composition [i](#)

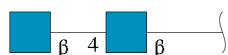
There are 5 unique types of molecules in this entry. The entry contains 25306 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Glutamate receptor 3.4.

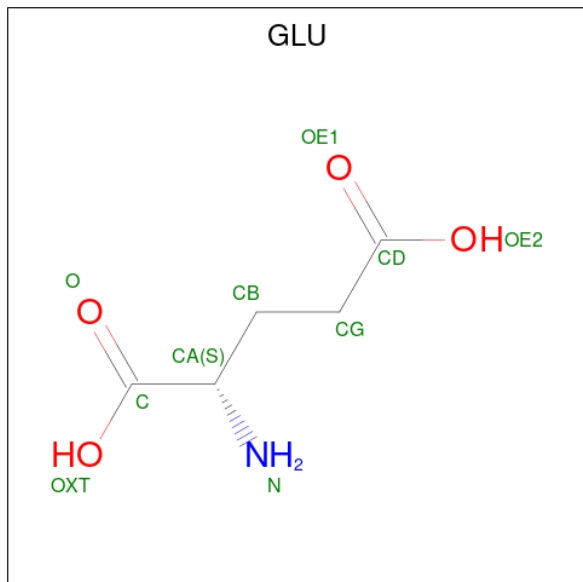
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	798	Total	C	N	O	S	0	0
			6251	4012	1055	1157	27		
1	B	788	Total	C	N	O	S	0	0
			6174	3969	1042	1137	26		
1	C	798	Total	C	N	O	S	0	0
			6251	4012	1055	1157	27		
1	D	788	Total	C	N	O	S	0	0
			6174	3969	1042	1137	26		

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



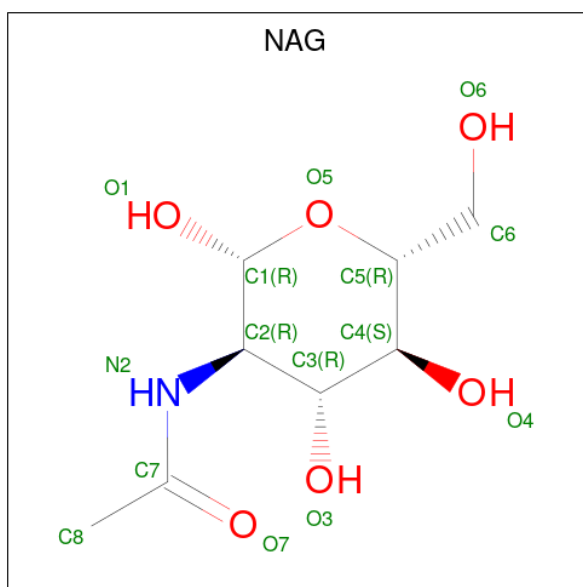
Mol	Chain	Residues	Atoms				AltConf	Trace
2	E	2	Total	C	N	O	0	0
			28	16	2	10		
2	F	2	Total	C	N	O	0	0
			28	16	2	10		
2	G	2	Total	C	N	O	0	0
			28	16	2	10		
2	H	2	Total	C	N	O	0	0
			28	16	2	10		
2	I	2	Total	C	N	O	0	0
			28	16	2	10		
2	J	2	Total	C	N	O	0	0
			28	16	2	10		
2	K	2	Total	C	N	O	0	0
			28	16	2	10		
2	L	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 3 is GLUTAMIC ACID (CCD ID: GLU) (formula: $C_5H_9NO_4$) (labeled as "Ligand of Interest" by depositor).



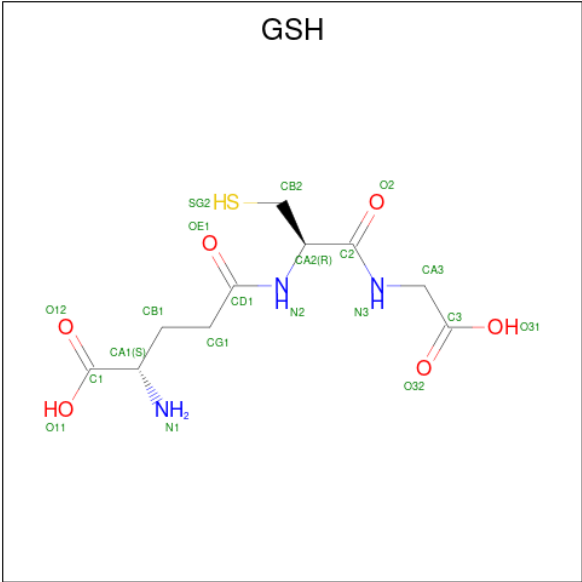
Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			10	5	1	4	
3	B	1	Total	C	N	O	0
			10	5	1	4	
3	C	1	Total	C	N	O	0
			10	5	1	4	
3	D	1	Total	C	N	O	0
			10	5	1	4	

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).

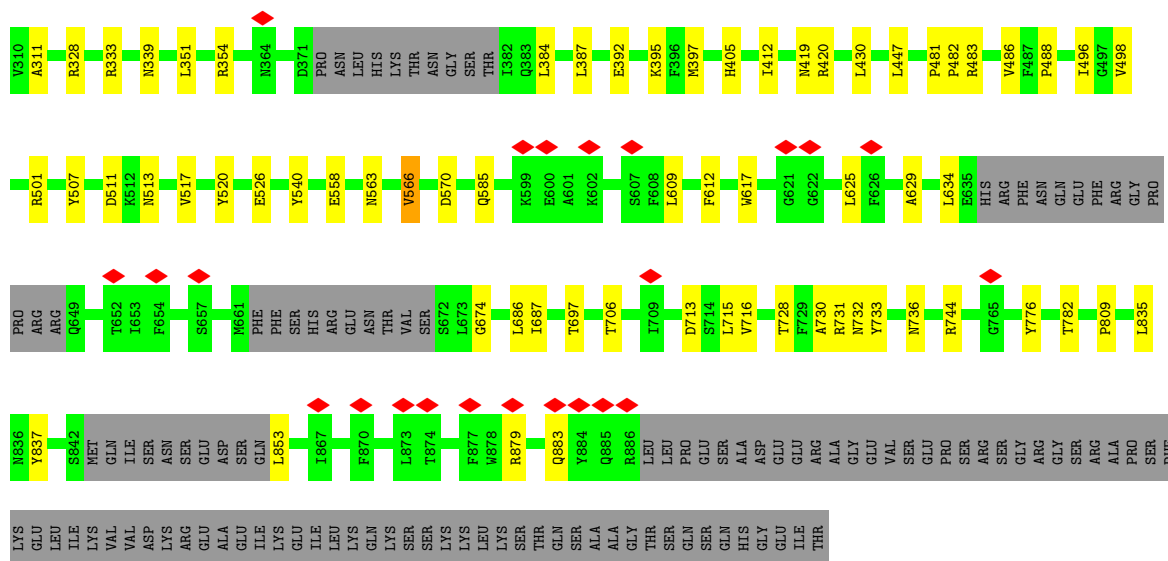


Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	D	1	Total	C	N	O	0
			14	8	1	5	
4	D	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 5 is GLUTATHIONE (CCD ID: GSH) (formula: $C_{10}H_{17}N_3O_6S$) (labeled as "Ligand of Interest" by depositor).

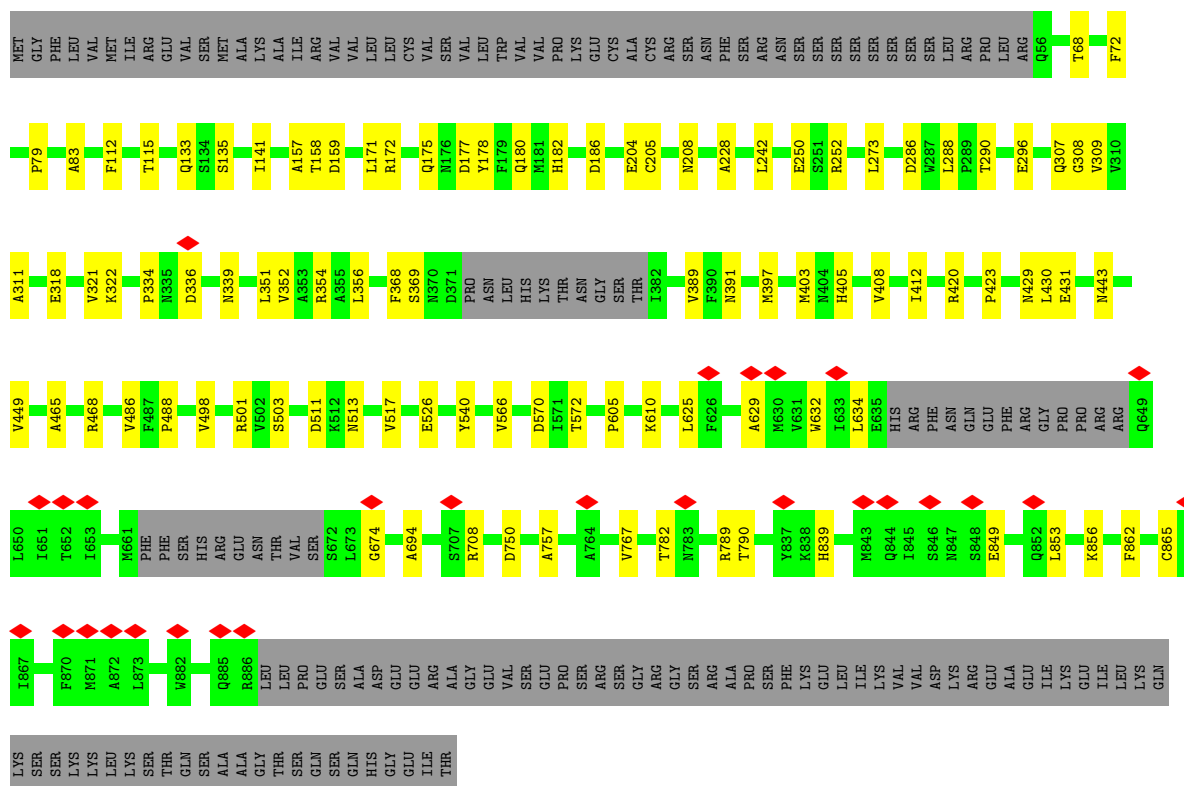


Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	S	0
			20	10	3	6	1	
5	B	1	Total	C	N	O	S	0
			20	10	3	6	1	
5	C	1	Total	C	N	O	S	0
			20	10	3	6	1	
5	D	1	Total	C	N	O	S	0
			20	10	3	6	1	



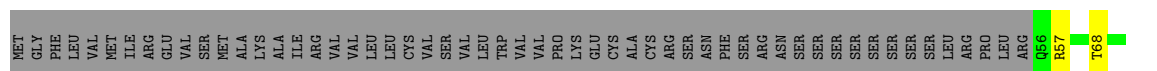
• Molecule 1: Glutamate receptor 3.4

Chain C: 73% 10% 17%



• Molecule 1: Glutamate receptor 3.4

Chain D: 72% 10% 18%

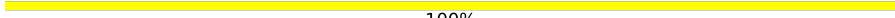


- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  50% 50%

MAG1
MAG2

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

Chain J:  100%

MAG1
MAG2

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

Chain K:  50% 50%

MAG1
MAG2

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

Chain L:  50% 50%

MAG1
MAG2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	110630	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	58	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.446	Depositor
Minimum map value	-1.539	Depositor
Average map value	0.014	Depositor
Map value standard deviation	0.065	Depositor
Recommended contour level	0.26	Depositor
Map size ($\text{\AA}$)	298.8, 298.8, 298.8	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.83, 0.83, 0.83	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, GSH

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	0.36	0/6401	0.62	2/8708 (0.0%)
1	B	0.39	0/6323	0.59	1/8602 (0.0%)
1	C	0.36	0/6401	0.60	1/8708 (0.0%)
1	D	0.39	0/6323	0.59	0/8602
All	All	0.37	0/25448	0.60	4/34620 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	108	ASN	CB-CA-C	-16.64	90.75	111.22
1	A	449	VAL	N-CA-C	-6.45	107.58	113.71
1	C	449	VAL	N-CA-C	-6.33	107.69	113.71
1	B	108	ASN	N-CA-C	-5.19	103.81	111.81

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6251	0	6137	60	0
1	B	6174	0	6069	59	0
1	C	6251	0	6137	57	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	6174	0	6069	52	0
2	E	28	0	25	1	0
2	F	28	0	25	0	0
2	G	28	0	25	0	0
2	H	28	0	25	0	0
2	I	28	0	25	0	0
2	J	28	0	25	0	0
2	K	28	0	25	0	0
2	L	28	0	25	0	0
3	A	10	0	5	1	0
3	B	10	0	5	1	0
3	C	10	0	5	1	0
3	D	10	0	5	1	0
4	A	28	0	26	0	0
4	B	28	0	26	0	0
4	C	28	0	26	0	0
4	D	28	0	26	0	0
5	A	20	0	15	3	0
5	B	20	0	15	1	0
5	C	20	0	15	3	0
5	D	20	0	15	1	0
All	All	25306	0	24796	219	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 4.

All (219) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:CYS:SG	5:A:1004:GSH:SG2	2.36	1.23
1:C:205:CYS:SG	5:C:1004:GSH:SG2	2.36	1.22
1:D:205:CYS:SG	5:D:1004:GSH:SG2	2.36	1.22
1:B:205:CYS:SG	5:B:1004:GSH:SG2	2.36	1.15
1:A:108:ASN:HB2	1:A:113:ILE:HD11	1.59	0.84
1:C:205:CYS:CB	5:C:1004:GSH:SG2	2.80	0.69
1:B:501:ARG:NH1	1:B:570:ASP:OD2	2.29	0.66
1:D:501:ARG:NH1	1:D:570:ASP:OD2	2.29	0.66
1:C:171:LEU:HB2	1:C:397:MET:HE1	1.81	0.62
1:A:572:THR:HG1	3:A:1001:GLU:N	1.97	0.62
1:A:171:LEU:HB2	1:A:397:MET:HE1	1.81	0.62
1:B:57:ARG:HB3	1:B:98:ILE:HD11	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:605:PRO:HD3	1:C:856:LYS:HG2	1.81	0.62
1:C:572:THR:HG1	3:C:1001:GLU:N	1.98	0.62
1:D:57:ARG:HB3	1:D:98:ILE:HD11	1.81	0.61
1:A:605:PRO:HD3	1:A:856:LYS:HG2	1.81	0.61
1:B:172:ARG:NH2	1:B:176:ASN:OD1	2.34	0.61
1:B:351:LEU:HD12	1:B:412:ILE:HD12	1.82	0.61
1:D:172:ARG:NH2	1:D:176:ASN:OD1	2.34	0.60
1:D:351:LEU:HD12	1:D:412:ILE:HD12	1.82	0.60
1:B:412:ILE:HG22	1:B:420:ARG:HE	1.66	0.60
1:A:501:ARG:NH1	1:A:570:ASP:OD2	2.35	0.60
1:C:501:ARG:NH1	1:C:570:ASP:OD2	2.35	0.60
1:D:412:ILE:HG22	1:D:420:ARG:HE	1.66	0.60
1:A:205:CYS:CB	5:A:1004:GSH:SG2	2.90	0.59
1:D:511:ASP:OD2	1:D:513:ASN:ND2	2.37	0.58
1:C:180:GLN:HE22	1:C:286:ASP:HB2	1.69	0.57
1:D:303:MET:O	1:D:307:GLN:NE2	2.38	0.57
1:B:511:ASP:OD2	1:B:513:ASN:ND2	2.37	0.57
1:C:205:CYS:HB2	5:C:1004:GSH:SG2	2.45	0.57
1:C:72:PHE:O	1:C:339:ASN:ND2	2.38	0.57
1:B:72:PHE:O	1:B:339:ASN:ND2	2.38	0.56
1:C:175:GLN:HE21	1:C:420:ARG:HH11	1.53	0.56
1:D:72:PHE:O	1:D:339:ASN:ND2	2.38	0.56
1:B:303:MET:O	1:B:307:GLN:NE2	2.38	0.56
1:A:72:PHE:O	1:A:339:ASN:ND2	2.38	0.56
1:A:180:GLN:HE22	1:A:286:ASP:HB2	1.69	0.56
1:A:175:GLN:HE21	1:A:420:ARG:HH11	1.53	0.56
1:A:296:GLU:HG3	1:A:336:ASP:HB2	1.87	0.56
1:C:511:ASP:OD2	1:C:513:ASN:ND2	2.39	0.55
1:D:384:LEU:HD23	1:D:387:LEU:HD22	1.89	0.55
1:A:511:ASP:OD2	1:A:513:ASN:ND2	2.39	0.55
1:C:465:ALA:O	1:C:468:ARG:NH1	2.39	0.55
1:B:384:LEU:HD23	1:B:387:LEU:HD22	1.88	0.55
1:A:465:ALA:O	1:A:468:ARG:NH1	2.39	0.54
1:C:308:GLY:N	1:C:430:LEU:O	2.39	0.54
1:A:351:LEU:HD12	1:A:412:ILE:HD13	1.90	0.54
1:C:115:THR:HA	1:C:141:ILE:HD11	1.90	0.54
1:C:296:GLU:HG3	1:C:336:ASP:HB2	1.87	0.54
1:C:526:GLU:OE2	1:C:540:TYR:OH	2.25	0.54
1:A:115:THR:HA	1:A:141:ILE:HD11	1.90	0.54
1:B:558:GLU:OE1	1:B:563:ASN:ND2	2.36	0.53
1:B:715:LEU:O	1:B:744:ARG:NH2	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:159:ASP:O	1:C:172:ARG:NH1	2.38	0.53
1:C:351:LEU:HD12	1:C:412:ILE:HD13	1.89	0.53
1:A:308:GLY:N	1:A:430:LEU:O	2.39	0.53
1:A:307:GLN:NE2	1:A:431:GLU:O	2.42	0.52
1:C:429:ASN:HD22	1:C:430:LEU:H	1.57	0.52
1:C:288:LEU:HD23	1:C:311:ALA:HB2	1.91	0.52
1:C:307:GLN:NE2	1:C:431:GLU:O	2.42	0.52
1:D:558:GLU:OE1	1:D:563:ASN:ND2	2.36	0.52
1:C:250:GLU:HG2	1:C:488:PRO:HD3	1.92	0.51
1:C:228:ALA:HB1	1:C:242:LEU:HD21	1.91	0.51
1:A:228:ALA:HB1	1:A:242:LEU:HD21	1.91	0.51
1:A:288:LEU:HD23	1:A:311:ALA:HB2	1.91	0.51
1:A:526:GLU:OE2	1:A:540:TYR:OH	2.25	0.51
1:B:171:LEU:HB2	1:B:397:MET:HE1	1.93	0.51
1:D:171:LEU:HB2	1:D:397:MET:HE1	1.93	0.51
1:B:732:ASN:ND2	1:B:736:ASN:OD1	2.44	0.51
1:C:368:PHE:O	1:C:391:ASN:ND2	2.44	0.51
1:D:732:ASN:ND2	1:D:736:ASN:OD1	2.44	0.51
1:A:429:ASN:HD22	1:A:430:LEU:H	1.58	0.51
1:A:159:ASP:O	1:A:172:ARG:NH1	2.38	0.50
1:A:368:PHE:O	1:A:391:ASN:ND2	2.44	0.50
1:C:369:SER:HB3	1:C:389:VAL:HG22	1.93	0.50
1:C:625:LEU:O	1:C:629:ALA:N	2.44	0.50
1:A:625:LEU:O	1:A:629:ALA:N	2.44	0.50
1:A:250:GLU:HG2	1:A:488:PRO:HD3	1.92	0.50
1:C:789:ARG:NH2	1:C:790:THR:OG1	2.45	0.50
1:B:728:THR:HG23	1:B:731:ARG:H	1.77	0.50
1:D:288:LEU:HD23	1:D:311:ALA:HB2	1.93	0.50
1:A:789:ARG:NH2	1:A:790:THR:OG1	2.45	0.50
1:B:288:LEU:HD23	1:B:311:ALA:HB2	1.93	0.50
1:D:715:LEU:O	1:D:744:ARG:NH2	2.41	0.49
1:A:369:SER:HB3	1:A:389:VAL:HG22	1.93	0.49
1:D:728:THR:HG23	1:D:731:ARG:H	1.77	0.49
1:A:423:PRO:HG2	1:A:443:ASN:HB2	1.95	0.49
1:C:252:ARG:HH11	1:C:486:VAL:HG11	1.78	0.49
1:C:423:PRO:HG2	1:C:443:ASN:HB2	1.95	0.49
1:D:496:ILE:HG13	1:D:566:VAL:HG13	1.95	0.49
1:D:612:PHE:O	1:D:617:TRP:NE1	2.46	0.49
1:C:503:SER:HB3	1:C:750:ASP:HA	1.95	0.48
1:B:496:ILE:HG13	1:B:566:VAL:HG13	1.95	0.48
1:B:612:PHE:O	1:B:617:TRP:NE1	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:392:GLU:HG3	1:D:395:LYS:HD3	1.95	0.48
1:A:321:VAL:HG12	1:A:408:VAL:HG12	1.96	0.48
1:D:782:THR:HG21	1:D:837:TYR:HB3	1.96	0.48
1:B:178:TYR:CZ	1:B:182:HIS:HE1	2.32	0.48
1:A:252:ARG:HH11	1:A:486:VAL:HG11	1.78	0.47
1:C:321:VAL:HG12	1:C:408:VAL:HG12	1.96	0.47
1:A:608:PHE:HE1	1:B:687:ILE:HG21	1.80	0.47
1:C:708:ARG:HH12	1:D:706:THR:HG22	1.78	0.47
1:D:304:ASP:HA	1:D:307:GLN:HE21	1.79	0.47
1:B:782:THR:HG21	1:B:837:TYR:HB3	1.96	0.47
1:C:204:GLU:O	1:C:208:ASN:ND2	2.48	0.47
1:A:204:GLU:O	1:A:208:ASN:ND2	2.48	0.47
1:D:250:GLU:HG2	1:D:488:PRO:HD3	1.96	0.47
1:B:250:GLU:HG2	1:B:488:PRO:HD3	1.96	0.47
1:B:304:ASP:HA	1:B:307:GLN:HE21	1.79	0.47
1:B:853:LEU:HD12	1:C:610:LYS:HD3	1.97	0.47
1:D:178:TYR:CZ	1:D:182:HIS:HE1	2.32	0.47
1:B:197:ILE:HG13	1:B:251:SER:HB2	1.97	0.47
1:B:252:ARG:HH11	1:B:486:VAL:HG11	1.80	0.47
1:D:483:ARG:NH2	1:D:809:PRO:O	2.48	0.47
1:A:503:SER:HB3	1:A:750:ASP:HA	1.95	0.47
1:B:392:GLU:HG3	1:B:395:LYS:HD3	1.95	0.47
1:B:483:ARG:NH2	1:B:809:PRO:O	2.48	0.47
1:D:309:VAL:HG13	1:D:430:LEU:HD12	1.97	0.47
1:C:629:ALA:HA	1:C:632:TRP:HD1	1.80	0.46
1:B:776:TYR:HE2	3:B:1001:GLU:HB2	1.80	0.46
1:D:176:ASN:ND2	1:D:419:ASN:OD1	2.47	0.46
1:D:776:TYR:HE2	3:D:1001:GLU:HB2	1.80	0.46
1:A:309:VAL:HG13	1:A:430:LEU:HD12	1.97	0.46
1:D:197:ILE:HG13	1:D:251:SER:HB2	1.97	0.46
1:D:354:ARG:HG3	1:D:405:HIS:CD2	2.51	0.46
1:A:629:ALA:HA	1:A:632:TRP:HD1	1.80	0.46
1:B:309:VAL:HG13	1:B:430:LEU:HD12	1.97	0.46
1:C:135:SER:OG	1:C:157:ALA:O	2.34	0.45
1:C:369:SER:HB2	1:C:391:ASN:HD21	1.81	0.45
1:A:369:SER:HB2	1:A:391:ASN:HD21	1.81	0.45
1:D:252:ARG:HH11	1:D:486:VAL:HG11	1.80	0.45
1:C:309:VAL:HG13	1:C:430:LEU:HD12	1.97	0.45
1:A:579:ARG:NH1	1:B:585:GLN:OE1	2.49	0.45
1:A:290:THR:HG23	1:A:339:ASN:HB2	1.99	0.45
1:B:507:TYR:O	1:B:520:TYR:N	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:ALA:HB1	1:B:328:ARG:HE	1.82	0.44
1:C:290:THR:HG23	1:C:339:ASN:HB2	1.99	0.44
1:D:534:TYR:OH	1:D:813:ASP:OD2	2.23	0.44
1:B:354:ARG:HG3	1:B:405:HIS:CD2	2.51	0.44
1:A:708:ARG:NH2	1:A:849:GLU:OE2	2.50	0.44
1:B:222:SER:OG	1:B:223:ARG:N	2.50	0.44
1:B:625:LEU:O	1:B:629:ALA:N	2.51	0.44
1:D:200:PHE:HE1	1:D:227:LYS:HB3	1.83	0.44
1:B:176:ASN:ND2	1:B:419:ASN:OD1	2.47	0.44
1:B:200:PHE:HE1	1:B:227:LYS:HB3	1.83	0.44
1:C:708:ARG:NH2	1:C:849:GLU:OE2	2.50	0.44
1:D:625:LEU:O	1:D:629:ALA:N	2.51	0.44
1:A:352:VAL:O	1:A:356:LEU:N	2.47	0.44
1:D:222:SER:OG	1:D:223:ARG:N	2.50	0.44
1:A:112:PHE:HD1	1:B:144:VAL:HG12	1.80	0.43
1:D:296:GLU:OE2	1:D:333:ARG:NH2	2.51	0.43
1:A:135:SER:OG	1:A:157:ALA:O	2.34	0.43
1:A:178:TYR:CZ	1:A:182:HIS:HE1	2.36	0.43
1:D:172:ARG:HH21	1:D:176:ASN:HA	1.84	0.43
1:C:178:TYR:CZ	1:C:182:HIS:HE1	2.37	0.43
1:C:354:ARG:HG3	1:C:405:HIS:CD2	2.54	0.43
1:A:318:GLU:HA	1:A:322:LYS:HE2	2.00	0.43
1:D:83:ALA:HB1	1:D:328:ARG:HE	1.82	0.43
1:D:308:GLY:N	1:D:430:LEU:O	2.47	0.43
1:A:182:HIS:O	1:A:186:ASP:N	2.51	0.43
1:D:182:HIS:O	1:D:186:ASP:N	2.52	0.43
1:D:498:VAL:HG11	1:D:517:VAL:HG11	2.00	0.43
1:A:354:ARG:HG3	1:A:405:HIS:CD2	2.54	0.43
1:C:158:THR:HB	1:C:177:ASP:HB2	2.01	0.43
1:A:205:CYS:HB2	5:A:1004:GSH:SG2	2.58	0.43
1:A:421:VAL:HA	2:E:1:NAG:H81	2.01	0.43
1:B:296:GLU:OE2	1:B:333:ARG:NH2	2.51	0.43
1:D:257:HIS:HD2	1:D:285:THR:HG21	1.84	0.43
1:B:481:PRO:HA	1:B:482:PRO:HD3	1.86	0.42
1:B:182:HIS:O	1:B:186:ASP:N	2.52	0.42
1:B:257:HIS:HD2	1:B:285:THR:HG21	1.84	0.42
1:A:634:LEU:HG	1:A:674:GLY:HA3	2.01	0.42
1:A:498:VAL:HG11	1:A:517:VAL:HG11	2.02	0.42
1:B:498:VAL:HG11	1:B:517:VAL:HG11	2.00	0.42
1:B:526:GLU:OE2	1:B:540:TYR:OH	2.24	0.42
1:B:697:THR:HG22	1:C:694:ALA:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:498:VAL:HG11	1:C:517:VAL:HG11	2.02	0.42
1:A:158:THR:HB	1:A:177:ASP:HB2	2.01	0.42
1:A:558:GLU:OE1	1:A:563:ASN:ND2	2.40	0.42
1:C:68:THR:H	1:C:133:GLN:HE22	1.68	0.42
1:A:708:ARG:HH12	1:B:706:THR:HG22	1.84	0.42
1:C:757:ALA:HB1	1:C:767:VAL:HG22	2.01	0.42
1:C:182:HIS:O	1:C:186:ASP:N	2.51	0.42
1:C:318:GLU:HA	1:C:322:LYS:HE2	2.00	0.42
1:C:112:PHE:HD1	1:D:144:VAL:HG12	1.85	0.42
1:C:403:MET:HG3	1:C:405:HIS:H	1.85	0.42
1:B:172:ARG:HH21	1:B:176:ASN:HA	1.84	0.42
1:A:403:MET:HG3	1:A:405:HIS:H	1.85	0.41
1:A:608:PHE:CE1	1:B:687:ILE:HG21	2.55	0.41
1:D:526:GLU:OE2	1:D:540:TYR:OH	2.24	0.41
1:C:352:VAL:O	1:C:356:LEU:N	2.47	0.41
1:A:782:THR:HG23	1:A:839:HIS:HD2	1.85	0.41
1:C:634:LEU:HG	1:C:674:GLY:HA3	2.01	0.41
1:C:782:THR:HG23	1:C:839:HIS:HD2	1.85	0.41
1:D:634:LEU:HG	1:D:674:GLY:HA3	2.02	0.41
1:B:716:VAL:O	1:B:744:ARG:NH1	2.51	0.41
1:B:447:LEU:HD23	1:B:447:LEU:HA	1.93	0.41
1:D:507:TYR:O	1:D:520:TYR:N	2.42	0.41
1:C:79:PRO:O	1:C:83:ALA:N	2.53	0.41
1:C:862:PHE:HA	1:C:865:CYS:HB2	2.03	0.41
1:A:757:ALA:HB1	1:A:767:VAL:HG22	2.01	0.41
1:B:308:GLY:N	1:B:430:LEU:O	2.47	0.41
1:B:68:THR:O	1:B:74:GLY:HA3	2.21	0.41
1:B:135:SER:HA	1:B:138:ALA:HB3	2.03	0.41
1:D:135:SER:HA	1:D:138:ALA:HB3	2.03	0.41
1:B:730:ALA:HA	1:B:733:TYR:HB3	2.03	0.41
1:B:879:ARG:O	1:B:883:GLN:N	2.51	0.41
1:D:228:ALA:HB1	1:D:242:LEU:HD21	2.02	0.41
1:D:382:ILE:O	1:D:385:SER:OG	2.36	0.41
1:A:68:THR:H	1:A:133:GLN:HE22	1.68	0.40
1:B:713:ASP:OD1	1:B:713:ASP:N	2.54	0.40
1:C:79:PRO:HG2	1:C:334:PRO:HG3	2.03	0.40
1:D:730:ALA:HA	1:D:733:TYR:HB3	2.03	0.40
1:B:634:LEU:HG	1:B:674:GLY:HA3	2.02	0.40
1:A:91:ASP:OD2	1:A:93:SER:OG	2.34	0.40
1:B:115:THR:HA	1:B:141:ILE:HD11	2.03	0.40
1:D:115:THR:HA	1:D:141:ILE:HD11	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:PRO:HG2	1:A:334:PRO:HG3	2.03	0.40
1:D:68:THR:O	1:D:74:GLY:HA3	2.21	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	790/959 (82%)	734 (93%)	56 (7%)	0	100	100
1	B	778/959 (81%)	717 (92%)	61 (8%)	0	100	100
1	C	790/959 (82%)	733 (93%)	57 (7%)	0	100	100
1	D	778/959 (81%)	716 (92%)	62 (8%)	0	100	100
All	All	3136/3836 (82%)	2900 (92%)	236 (8%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	680/837 (81%)	675 (99%)	5 (1%)	76	78
1	B	670/837 (80%)	665 (99%)	5 (1%)	76	78
1	C	680/837 (81%)	677 (100%)	3 (0%)	84	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	670/837 (80%)	665 (99%)	5 (1%)	76	78
All	All	2700/3348 (81%)	2682 (99%)	18 (1%)	73	78

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	108	ASN
1	A	273	LEU
1	A	566	VAL
1	A	835	LEU
1	A	853	LEU
1	B	309	VAL
1	B	566	VAL
1	B	609	LEU
1	B	686	LEU
1	B	835	LEU
1	C	273	LEU
1	C	566	VAL
1	C	853	LEU
1	D	309	VAL
1	D	566	VAL
1	D	609	LEU
1	D	686	LEU
1	D	835	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (63) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	GLN
1	A	89	ASN
1	A	175	GLN
1	A	307	GLN
1	A	331	ASN
1	A	365	ASN
1	A	391	ASN
1	A	466	ASN
1	A	557	ASN
1	A	689	ASN
1	A	704	GLN
1	A	732	ASN
1	A	736	ASN

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Mol	Chain	Res	Type
1	A	759	GLN
1	A	805	GLN
1	A	839	HIS
1	B	89	ASN
1	B	139	HIS
1	B	307	GLN
1	B	331	ASN
1	B	339	ASN
1	B	365	ASN
1	B	383	GLN
1	B	405	HIS
1	B	444	HIS
1	B	451	HIS
1	B	466	ASN
1	B	557	ASN
1	B	732	ASN
1	B	759	GLN
1	C	56	GLN
1	C	89	ASN
1	C	105	GLN
1	C	120	GLN
1	C	139	HIS
1	C	175	GLN
1	C	307	GLN
1	C	331	ASN
1	C	365	ASN
1	C	391	ASN
1	C	451	HIS
1	C	466	ASN
1	C	557	ASN
1	C	689	ASN
1	C	704	GLN
1	C	732	ASN
1	C	736	ASN
1	C	759	GLN
1	C	805	GLN
1	C	839	HIS
1	D	89	ASN
1	D	139	HIS
1	D	307	GLN
1	D	331	ASN
1	D	365	ASN

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Mol	Chain	Res	Type
1	D	383	GLN
1	D	405	HIS
1	D	444	HIS
1	D	451	HIS
1	D	466	ASN
1	D	557	ASN
1	D	732	ASN
1	D	759	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

16 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	$\# Z > 2$
2	NAG	E	1	1,2	14,14,15	0.27	0	17,19,21	0.70	1 (5%)
2	NAG	E	2	2	14,14,15	0.26	0	17,19,21	0.51	0
2	NAG	F	1	1,2	14,14,15	1.11	1 (7%)	17,19,21	1.43	2 (11%)
2	NAG	F	2	2	14,14,15	0.70	0	17,19,21	0.40	0
2	NAG	G	1	1,2	14,14,15	0.91	1 (7%)	17,19,21	0.73	1 (5%)
2	NAG	G	2	2	14,14,15	0.33	0	17,19,21	0.51	0
2	NAG	H	1	1,2	14,14,15	0.27	0	17,19,21	0.77	1 (5%)
2	NAG	H	2	2	14,14,15	0.45	0	17,19,21	0.51	0
2	NAG	I	1	1,2	14,14,15	0.29	0	17,19,21	0.70	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	I	2	2	14,14,15	0.27	0	17,19,21	0.50	0
2	NAG	J	1	1,2	14,14,15	1.07	1 (7%)	17,19,21	1.40	2 (11%)
2	NAG	J	2	2	14,14,15	0.73	1 (7%)	17,19,21	0.42	0
2	NAG	K	1	1,2	14,14,15	1.01	1 (7%)	17,19,21	0.81	1 (5%)
2	NAG	K	2	2	14,14,15	0.35	0	17,19,21	0.50	0
2	NAG	L	1	1,2	14,14,15	0.29	0	17,19,21	0.80	1 (5%)
2	NAG	L	2	2	14,14,15	0.47	0	17,19,21	0.52	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	NAG	E	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	NAG	F	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1
2	NAG	G	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	2/6/23/26	0/1/1/1
2	NAG	H	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	H	2	2	-	3/6/23/26	0/1/1/1
2	NAG	I	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	I	2	2	-	2/6/23/26	0/1/1/1
2	NAG	J	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	J	2	2	-	2/6/23/26	0/1/1/1
2	NAG	K	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	K	2	2	-	2/6/23/26	0/1/1/1
2	NAG	L	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	L	2	2	-	3/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1	NAG	O5-C1	-3.56	1.37	1.43
2	K	1	NAG	O5-C1	-3.43	1.37	1.43
2	J	1	NAG	O5-C1	-3.40	1.38	1.43
2	G	1	NAG	O5-C1	-3.03	1.38	1.43
2	J	2	NAG	C1-C2	2.08	1.55	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1	NAG	C3-C4-C5	4.12	117.70	110.23
2	J	1	NAG	C3-C4-C5	4.03	117.55	110.23
2	L	1	NAG	C1-O5-C5	2.84	116.00	112.19
2	J	1	NAG	C4-C3-C2	2.84	115.17	111.02
2	F	1	NAG	C4-C3-C2	2.83	115.17	111.02
2	H	1	NAG	C1-O5-C5	2.72	115.84	112.19
2	E	1	NAG	C1-O5-C5	2.37	115.36	112.19
2	K	1	NAG	C4-C3-C2	2.35	114.46	111.02
2	I	1	NAG	C1-O5-C5	2.33	115.31	112.19
2	G	1	NAG	C4-C3-C2	2.08	114.07	111.02

There are no chirality outliers.

All (23) torsion outliers are listed below:

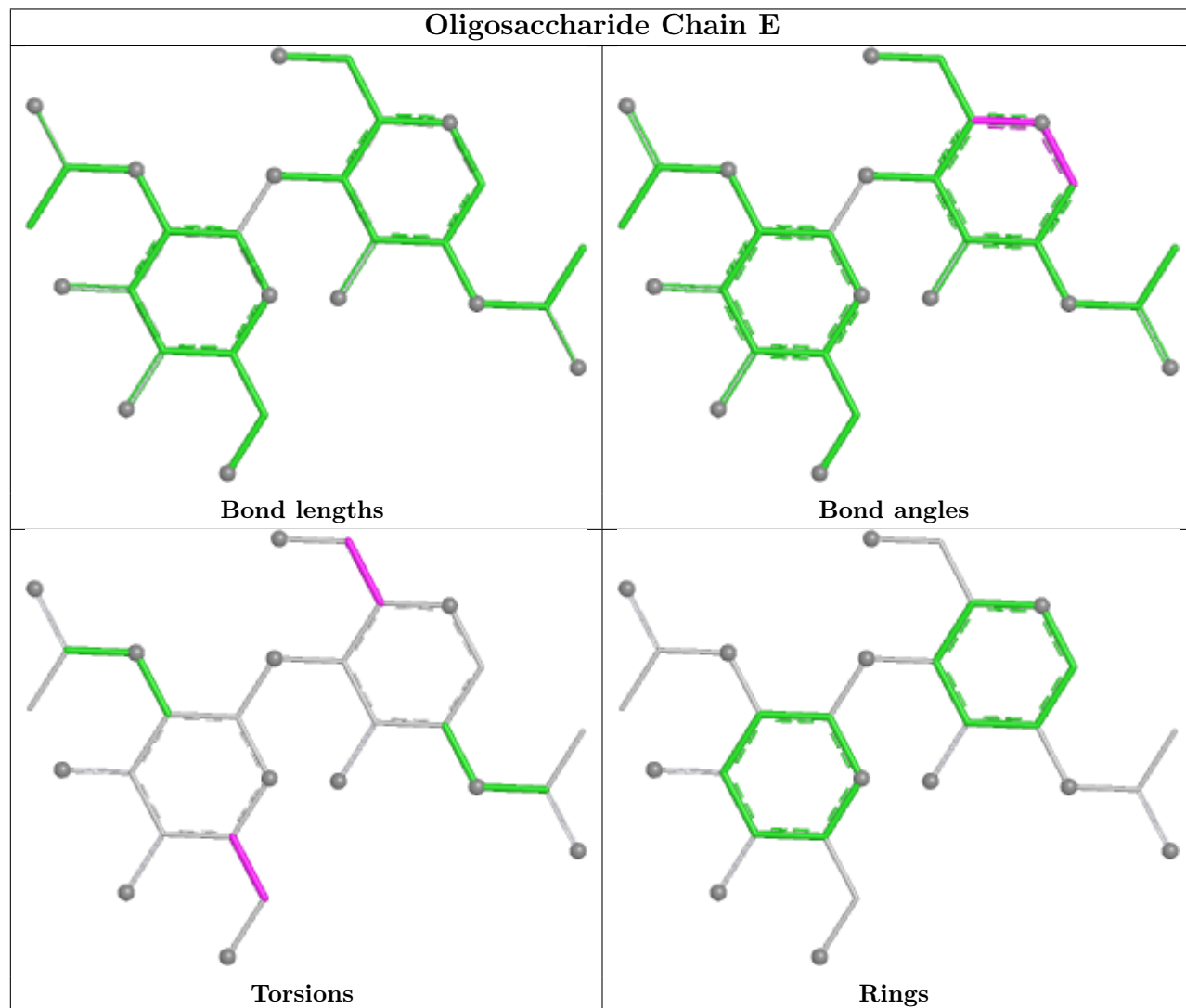
Mol	Chain	Res	Type	Atoms
2	E	2	NAG	O5-C5-C6-O6
2	J	2	NAG	O5-C5-C6-O6
2	I	2	NAG	O5-C5-C6-O6
2	F	2	NAG	O5-C5-C6-O6
2	J	2	NAG	C4-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
2	I	2	NAG	C4-C5-C6-O6
2	F	2	NAG	C4-C5-C6-O6
2	H	2	NAG	C8-C7-N2-C2
2	H	2	NAG	O7-C7-N2-C2
2	L	2	NAG	C8-C7-N2-C2
2	L	2	NAG	O7-C7-N2-C2
2	G	2	NAG	O5-C5-C6-O6
2	G	2	NAG	C4-C5-C6-O6
2	K	2	NAG	O5-C5-C6-O6
2	K	2	NAG	C4-C5-C6-O6
2	L	2	NAG	O5-C5-C6-O6
2	H	2	NAG	O5-C5-C6-O6
2	L	1	NAG	C4-C5-C6-O6
2	H	1	NAG	C4-C5-C6-O6
2	L	1	NAG	O5-C5-C6-O6
2	H	1	NAG	O5-C5-C6-O6
2	E	1	NAG	C4-C5-C6-O6

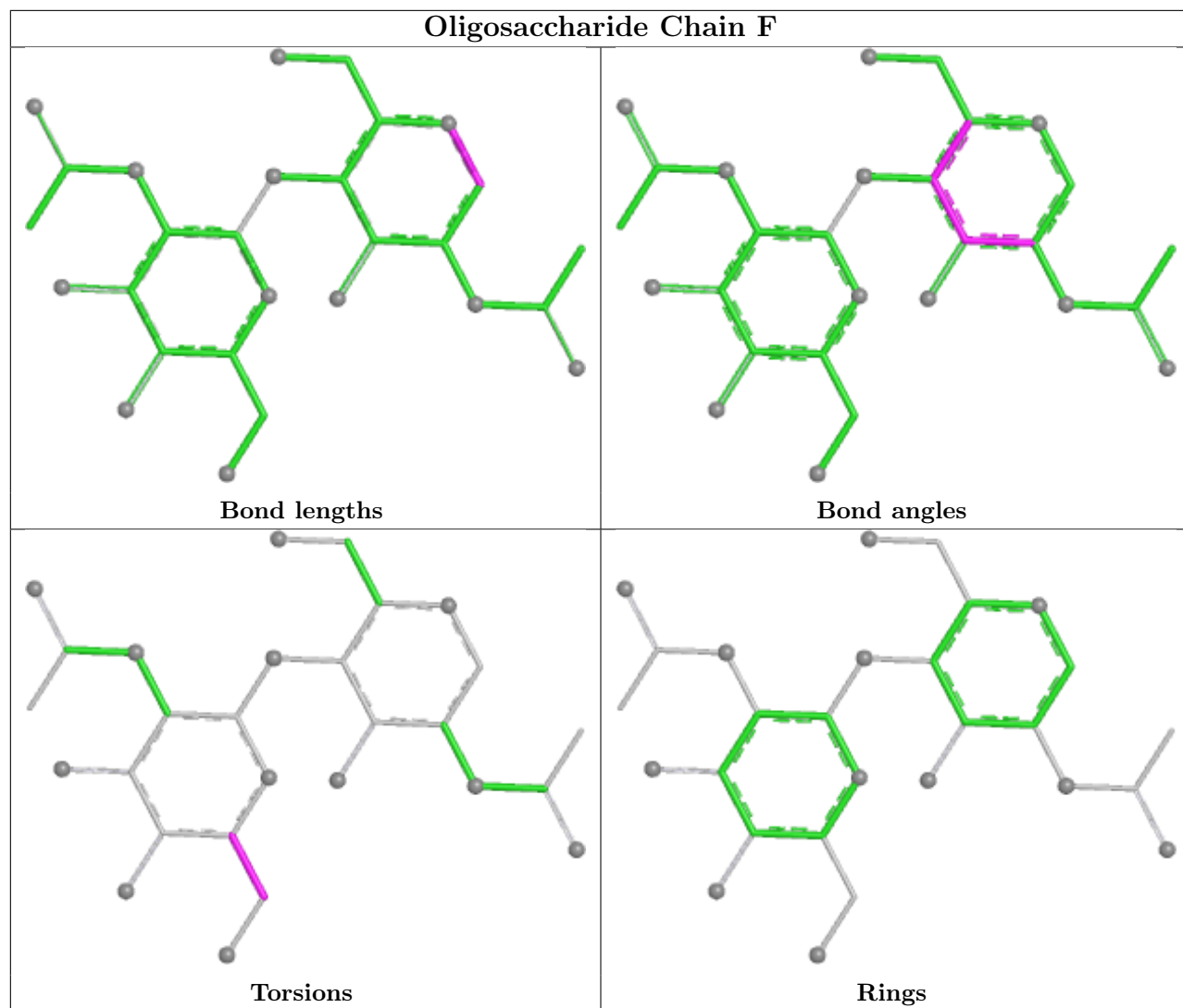
There are no ring outliers.

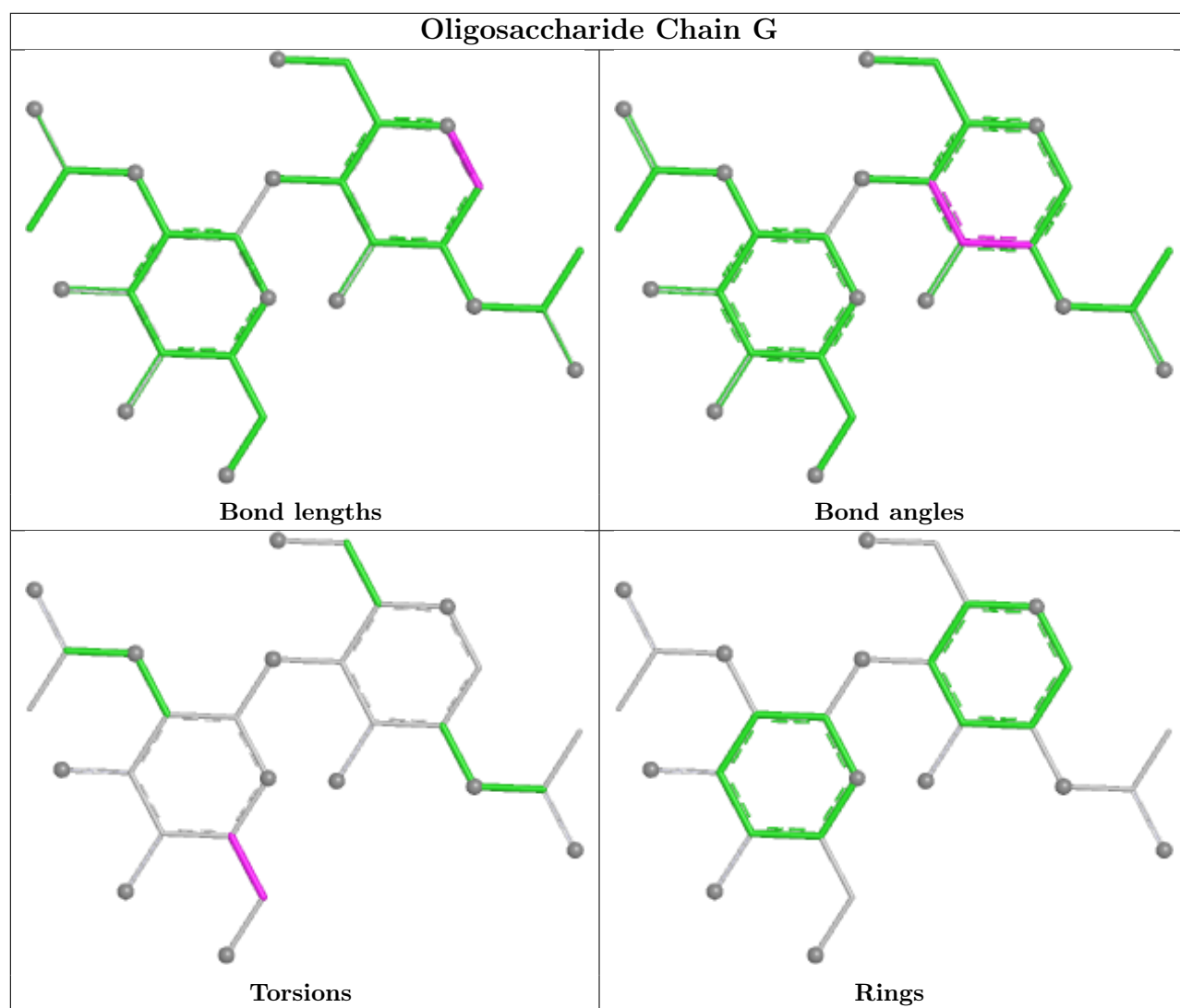
1 monomer is involved in 1 short contact:

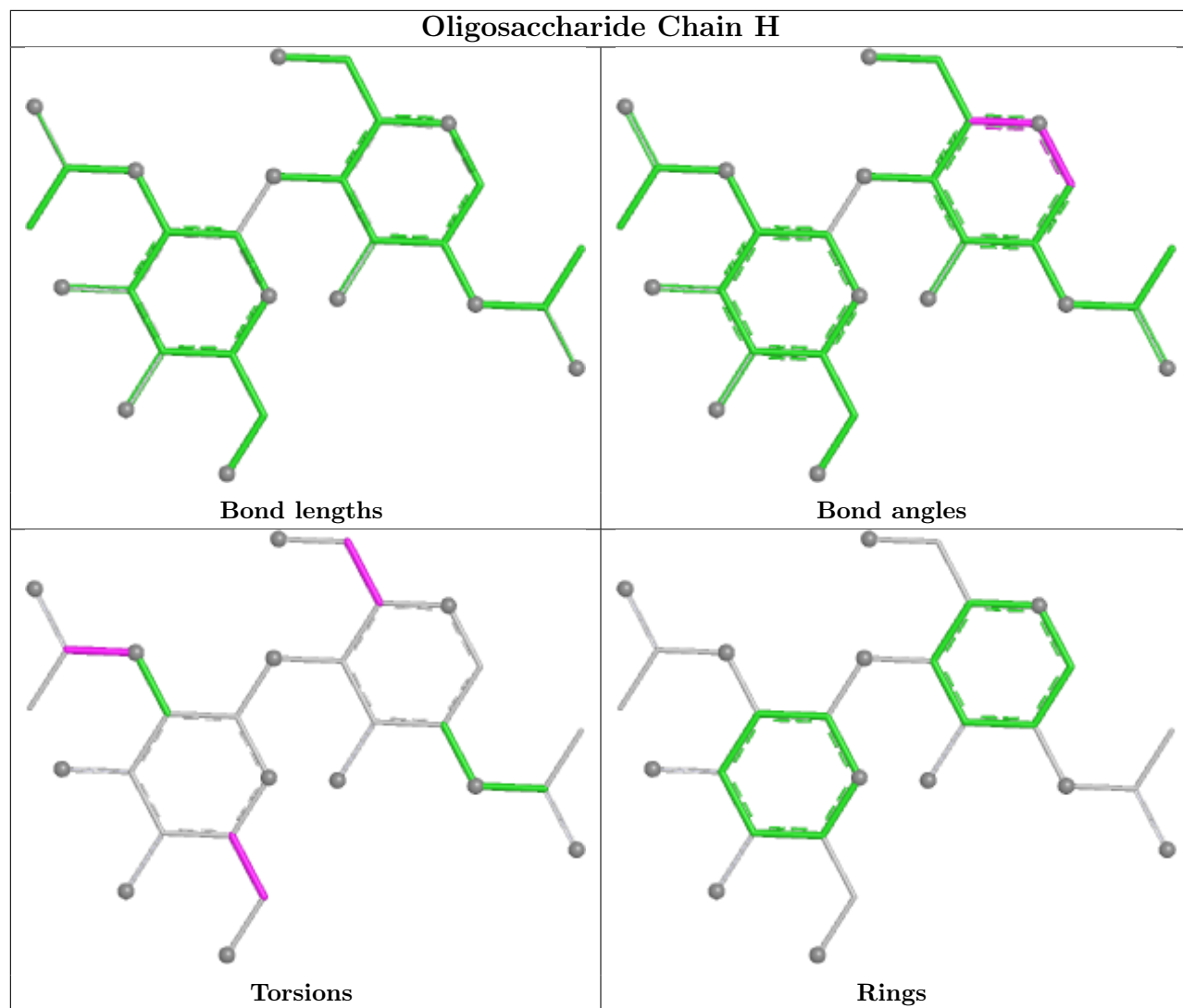
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1	NAG	1	0

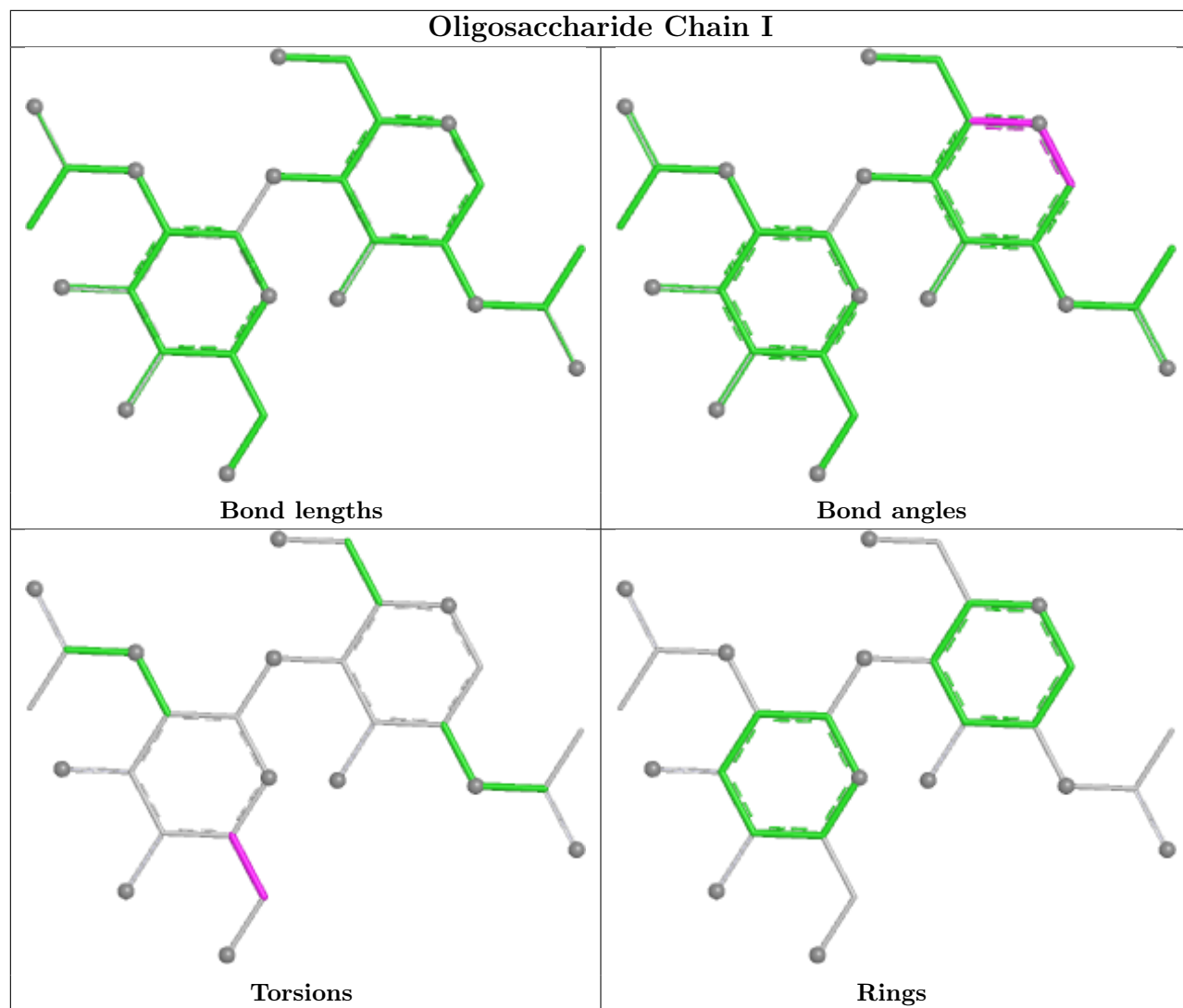
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

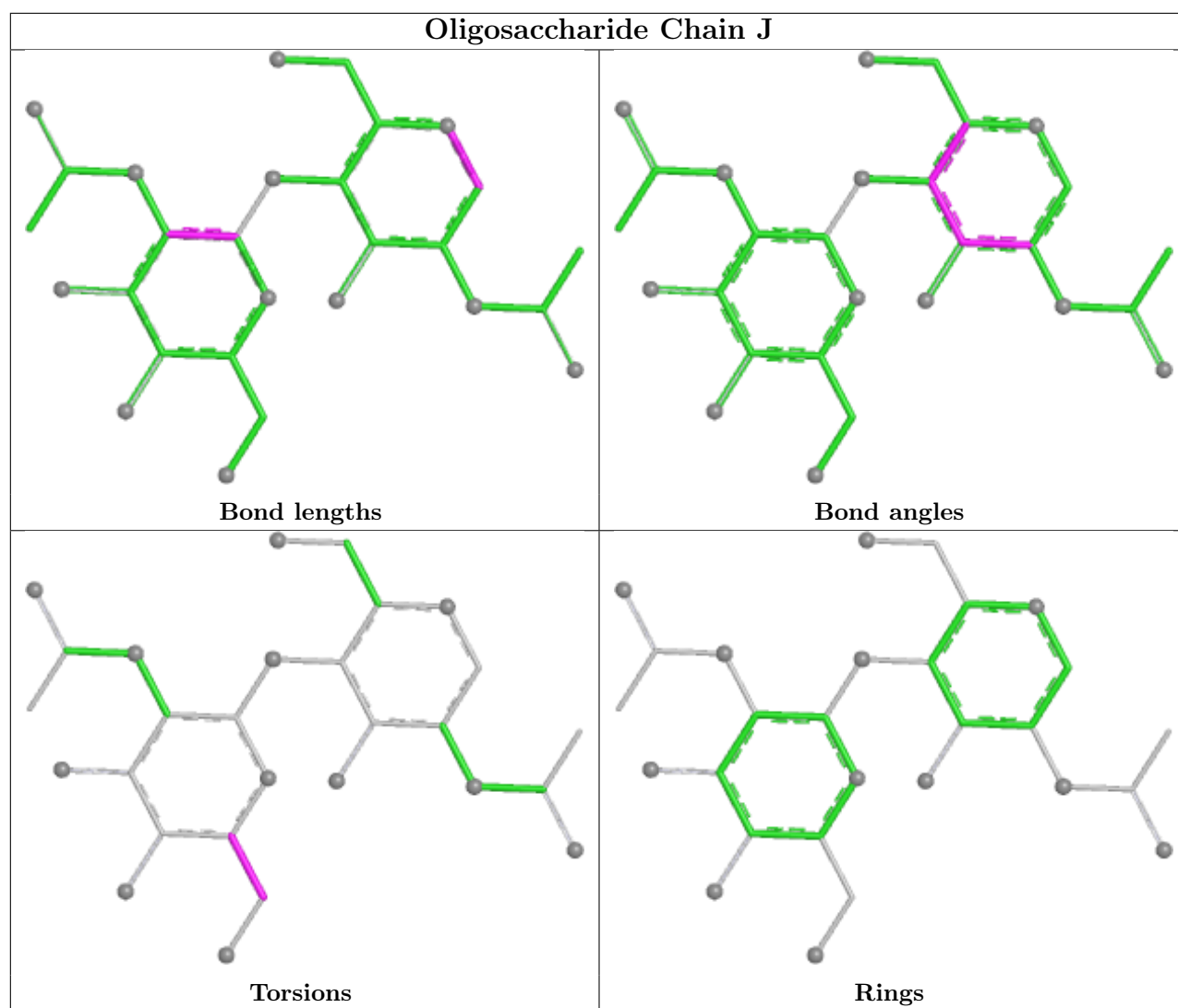


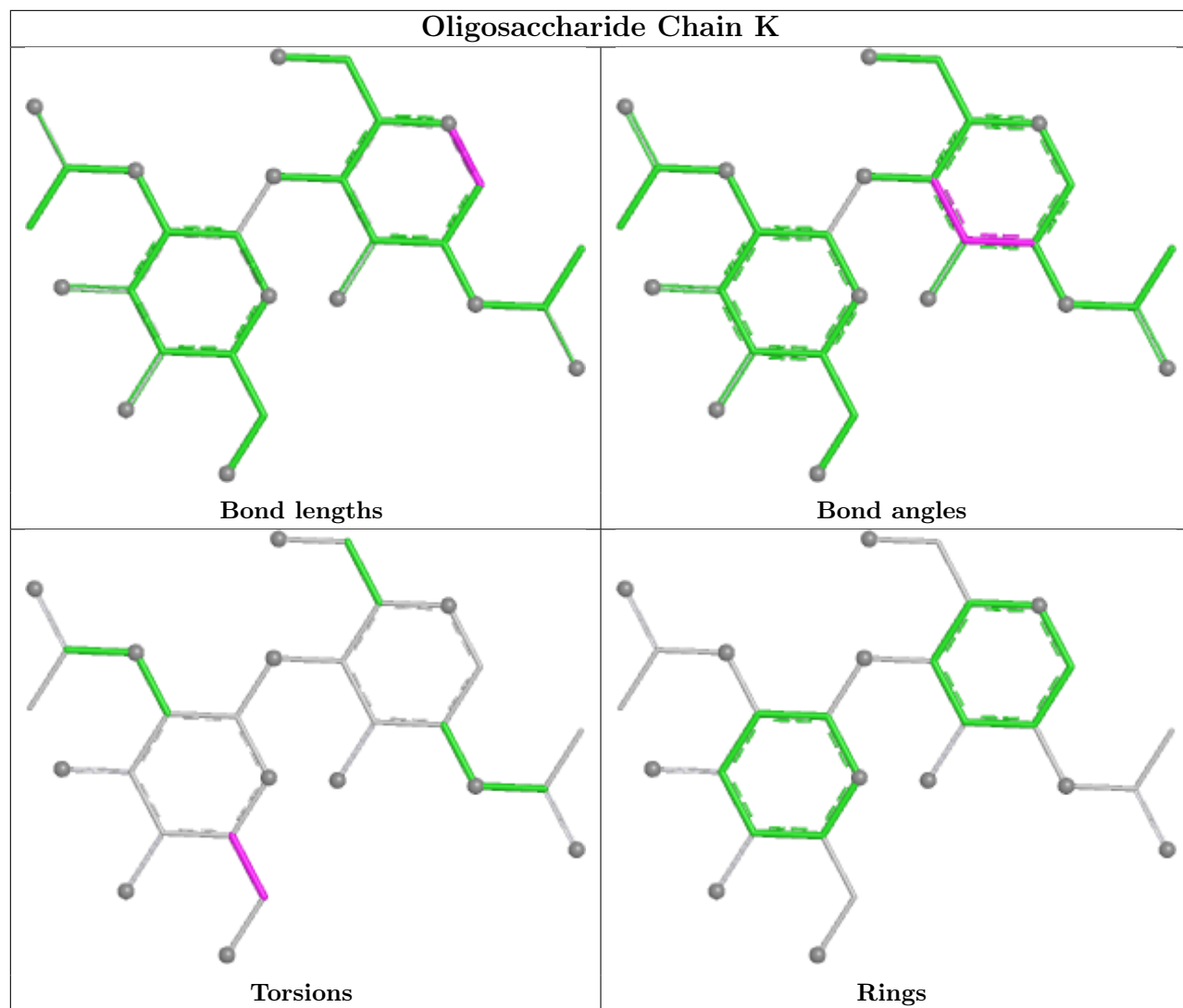


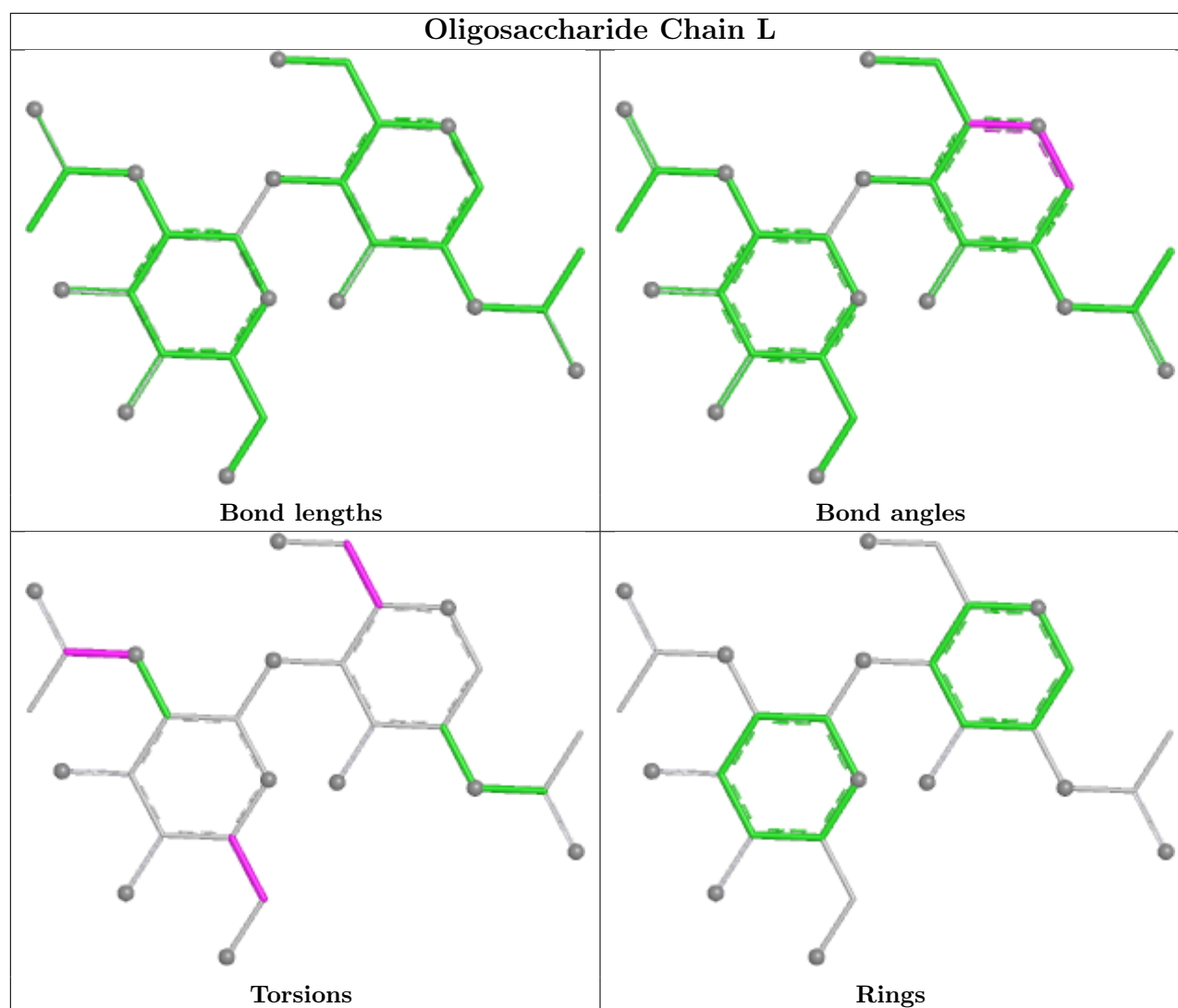












5.6 Ligand geometry [i](#)

16 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	D	1003	1	14,14,15	0.23	0	17,19,21	0.62	0
4	NAG	C	1003	1	14,14,15	0.19	0	17,19,21	0.60	0
3	GLU	A	1001	-	8,9,9	1.15	1 (12%)	8,11,11	1.27	1 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GSH	B	1004	-	18,19,19	2.02	4 (22%)	21,24,24	1.51	2 (9%)
4	NAG	B	1003	1	14,14,15	0.23	0	17,19,21	0.60	0
5	GSH	D	1004	-	18,19,19	2.03	4 (22%)	21,24,24	1.57	2 (9%)
3	GLU	B	1001	-	8,9,9	1.18	1 (12%)	8,11,11	1.42	1 (12%)
3	GLU	C	1001	-	8,9,9	1.16	1 (12%)	8,11,11	1.28	1 (12%)
5	GSH	C	1004	-	18,19,19	2.05	4 (22%)	21,24,24	1.30	3 (14%)
5	GSH	A	1004	-	18,19,19	2.07	4 (22%)	21,24,24	1.40	3 (14%)
4	NAG	B	1002	1	14,14,15	0.40	0	17,19,21	1.35	2 (11%)
4	NAG	D	1002	1	14,14,15	0.40	0	17,19,21	1.37	2 (11%)
4	NAG	A	1003	1	14,14,15	0.20	0	17,19,21	0.61	0
4	NAG	A	1002	1	14,14,15	0.50	0	17,19,21	1.22	1 (5%)
3	GLU	D	1001	-	8,9,9	1.17	1 (12%)	8,11,11	1.41	1 (12%)
4	NAG	C	1002	1	14,14,15	0.33	0	17,19,21	0.71	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	D	1003	1	-	4/6/23/26	0/1/1/1
4	NAG	C	1003	1	-	4/6/23/26	0/1/1/1
3	GLU	A	1001	-	-	1/9/9/9	-
5	GSH	B	1004	-	-	10/24/24/24	-
4	NAG	B	1003	1	-	4/6/23/26	0/1/1/1
5	GSH	D	1004	-	-	9/24/24/24	-
3	GLU	B	1001	-	-	2/9/9/9	-
3	GLU	C	1001	-	-	1/9/9/9	-
5	GSH	C	1004	-	-	8/24/24/24	-
5	GSH	A	1004	-	-	8/24/24/24	-
4	NAG	B	1002	1	1/1/5/7	4/6/23/26	0/1/1/1
4	NAG	D	1002	1	1/1/5/7	4/6/23/26	0/1/1/1
4	NAG	A	1003	1	-	4/6/23/26	0/1/1/1
4	NAG	A	1002	1	-	4/6/23/26	0/1/1/1
3	GLU	D	1001	-	-	2/9/9/9	-
4	NAG	C	1002	1	1/1/5/7	2/6/23/26	0/1/1/1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1004	GSH	CD1-N2	5.43	1.45	1.34
5	C	1004	GSH	CD1-N2	5.41	1.45	1.34
5	B	1004	GSH	CD1-N2	5.21	1.45	1.34
5	D	1004	GSH	CD1-N2	5.20	1.45	1.34
5	A	1004	GSH	C2-N3	5.01	1.45	1.33
5	C	1004	GSH	C2-N3	4.96	1.45	1.33
5	D	1004	GSH	C2-N3	4.93	1.45	1.33
5	B	1004	GSH	C2-N3	4.92	1.45	1.33
5	D	1004	GSH	OE1-CD1	-2.84	1.17	1.23
5	B	1004	GSH	OE1-CD1	-2.72	1.17	1.23
5	A	1004	GSH	OE1-CD1	-2.58	1.18	1.23
5	A	1004	GSH	O2-C2	-2.58	1.18	1.23
5	C	1004	GSH	O2-C2	-2.53	1.18	1.23
5	C	1004	GSH	OE1-CD1	-2.52	1.18	1.23
5	B	1004	GSH	O2-C2	-2.48	1.18	1.23
5	D	1004	GSH	O2-C2	-2.46	1.18	1.23
3	C	1001	GLU	OXT-C	-2.42	1.22	1.30
3	A	1001	GLU	OXT-C	-2.41	1.23	1.30
3	D	1001	GLU	OXT-C	-2.38	1.23	1.30
3	B	1001	GLU	OXT-C	-2.37	1.23	1.30

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1002	NAG	C1-O5-C5	-4.28	106.46	112.19
4	B	1002	NAG	C1-O5-C5	-3.87	107.00	112.19
5	D	1004	GSH	CA2-CB2-SG2	-3.75	109.93	114.16
5	A	1004	GSH	CA2-CB2-SG2	-3.64	110.06	114.16
5	B	1004	GSH	CA2-CB2-SG2	-3.61	110.09	114.16
4	A	1002	NAG	C1-O5-C5	-3.57	107.40	112.19
5	C	1004	GSH	CA2-CB2-SG2	-3.00	110.78	114.16
3	B	1001	GLU	OXT-C-O	-2.95	117.38	124.08
5	D	1004	GSH	CG1-CD1-N2	2.95	121.06	115.86
3	D	1001	GLU	OXT-C-O	-2.94	117.41	124.08
3	C	1001	GLU	OXT-C-O	-2.89	117.52	124.08
3	A	1001	GLU	OXT-C-O	-2.88	117.55	124.08
5	B	1004	GSH	CG1-CD1-N2	2.64	120.51	115.86
5	A	1004	GSH	CG1-CD1-N2	2.21	119.75	115.86
4	B	1002	NAG	O5-C1-C2	-2.12	108.01	111.29
5	C	1004	GSH	O31-C3-CA3	2.08	120.70	112.81
5	A	1004	GSH	O31-C3-CA3	2.03	120.52	112.81
5	C	1004	GSH	CG1-CD1-N2	2.02	119.43	115.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1002	NAG	O5-C1-C2	-2.01	108.18	111.29

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	B	1002	NAG	C1
4	C	1002	NAG	C1
4	D	1002	NAG	C1

All (71) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	1002	NAG	C8-C7-N2-C2
4	C	1002	NAG	O7-C7-N2-C2
5	A	1004	GSH	N2-CA2-CB2-SG2
5	A	1004	GSH	C2-CA2-CB2-SG2
5	B	1004	GSH	O12-C1-CA1-N1
5	B	1004	GSH	N2-CA2-CB2-SG2
5	B	1004	GSH	C2-CA2-CB2-SG2
5	C	1004	GSH	N2-CA2-CB2-SG2
5	C	1004	GSH	C2-CA2-CB2-SG2
5	D	1004	GSH	O12-C1-CA1-N1
5	D	1004	GSH	N2-CA2-CB2-SG2
5	D	1004	GSH	C2-CA2-CB2-SG2
4	D	1003	NAG	O5-C5-C6-O6
4	B	1003	NAG	O5-C5-C6-O6
4	A	1003	NAG	O5-C5-C6-O6
4	C	1003	NAG	O5-C5-C6-O6
4	D	1003	NAG	C4-C5-C6-O6
4	B	1003	NAG	C4-C5-C6-O6
4	B	1002	NAG	C8-C7-N2-C2
4	B	1002	NAG	O7-C7-N2-C2
4	A	1003	NAG	C4-C5-C6-O6
5	C	1004	GSH	CA1-CB1-CG1-CD1
4	D	1002	NAG	C8-C7-N2-C2
4	C	1003	NAG	C4-C5-C6-O6
4	A	1003	NAG	C8-C7-N2-C2
4	A	1003	NAG	O7-C7-N2-C2
4	B	1003	NAG	C8-C7-N2-C2
4	B	1003	NAG	O7-C7-N2-C2
4	C	1003	NAG	C8-C7-N2-C2
4	C	1003	NAG	O7-C7-N2-C2

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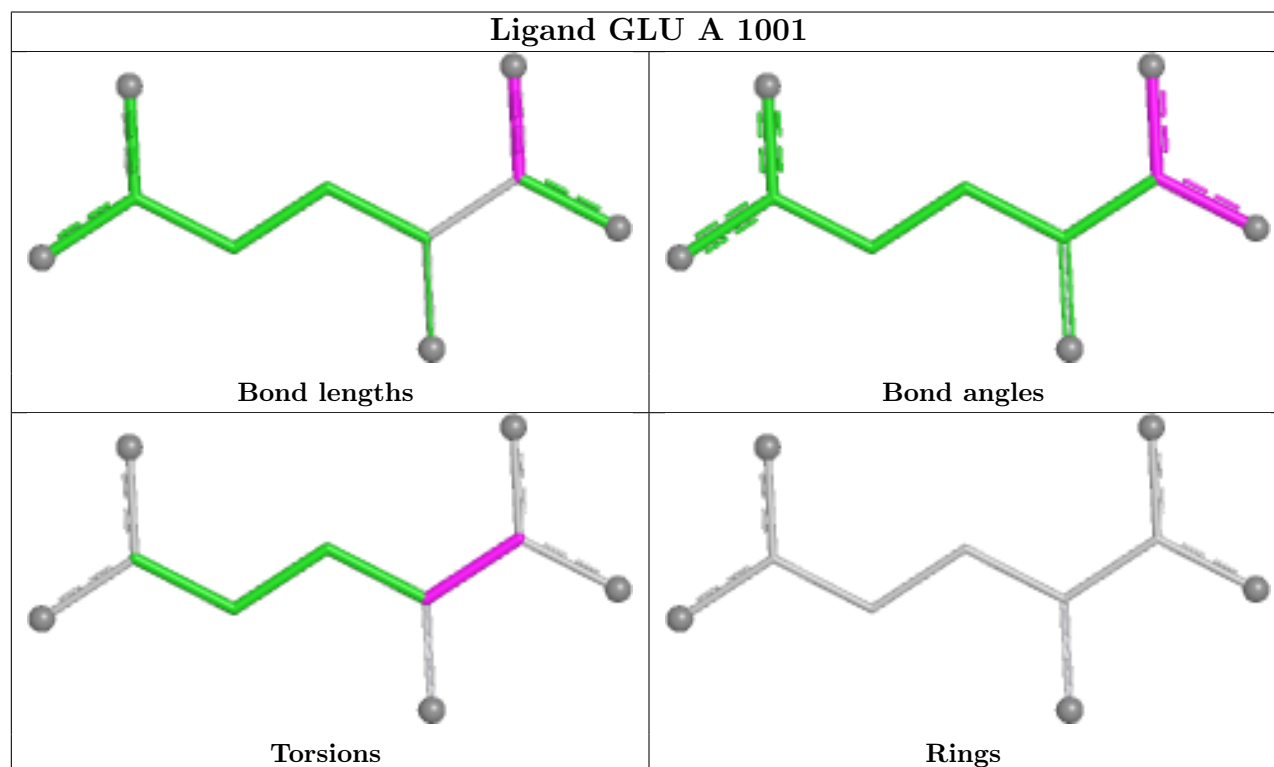
Mol	Chain	Res	Type	Atoms
4	D	1002	NAG	O7-C7-N2-C2
4	D	1003	NAG	C8-C7-N2-C2
4	D	1003	NAG	O7-C7-N2-C2
5	D	1004	GSH	O11-C1-CA1-N1
5	C	1004	GSH	O31-C3-CA3-N3
4	B	1002	NAG	C4-C5-C6-O6
5	B	1004	GSH	O11-C1-CA1-N1
4	D	1002	NAG	C4-C5-C6-O6
4	A	1002	NAG	C4-C5-C6-O6
4	A	1002	NAG	C8-C7-N2-C2
5	A	1004	GSH	O31-C3-CA3-N3
4	B	1002	NAG	O5-C5-C6-O6
4	A	1002	NAG	O5-C5-C6-O6
5	A	1004	GSH	O11-C1-CA1-N1
4	D	1002	NAG	O5-C5-C6-O6
4	A	1002	NAG	O7-C7-N2-C2
5	C	1004	GSH	O11-C1-CA1-N1
5	A	1004	GSH	CA1-CB1-CG1-CD1
5	A	1004	GSH	O32-C3-CA3-N3
5	C	1004	GSH	O32-C3-CA3-N3
5	D	1004	GSH	O11-C1-CA1-CB1
5	B	1004	GSH	O11-C1-CA1-CB1
5	D	1004	GSH	O12-C1-CA1-CB1
5	B	1004	GSH	O12-C1-CA1-CB1
5	D	1004	GSH	O2-C2-CA2-N2
5	B	1004	GSH	O2-C2-CA2-N2
3	B	1001	GLU	OE2-CD-CG-CB
3	D	1001	GLU	OE2-CD-CG-CB
5	C	1004	GSH	O12-C1-CA1-CB1
3	B	1001	GLU	OE1-CD-CG-CB
3	D	1001	GLU	OE1-CD-CG-CB
5	D	1004	GSH	N3-C2-CA2-N2
5	B	1004	GSH	O2-C2-CA2-CB2
5	D	1004	GSH	O2-C2-CA2-CB2
5	A	1004	GSH	O12-C1-CA1-CB1
5	B	1004	GSH	N3-C2-CA2-N2
5	B	1004	GSH	CA1-CB1-CG1-CD1
5	A	1004	GSH	O11-C1-CA1-CB1
5	C	1004	GSH	O11-C1-CA1-CB1
3	A	1001	GLU	OXT-C-CA-N
3	C	1001	GLU	OXT-C-CA-N

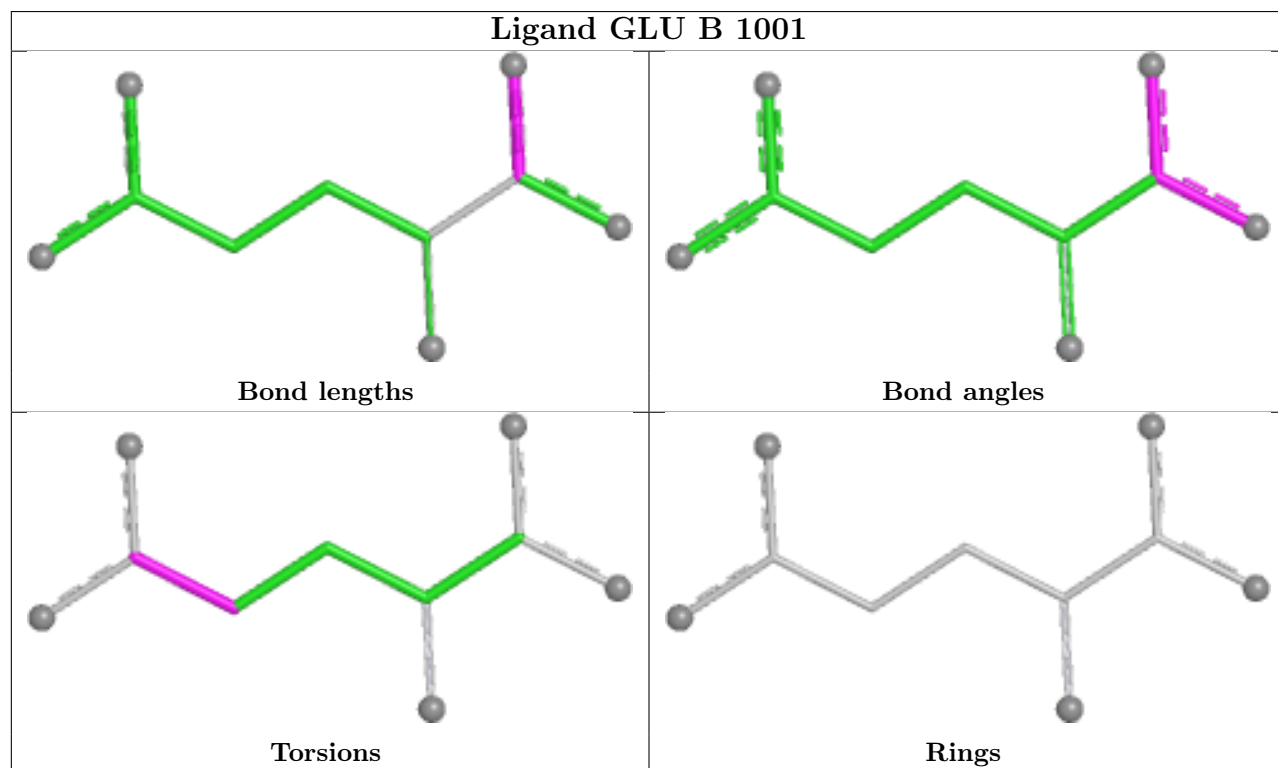
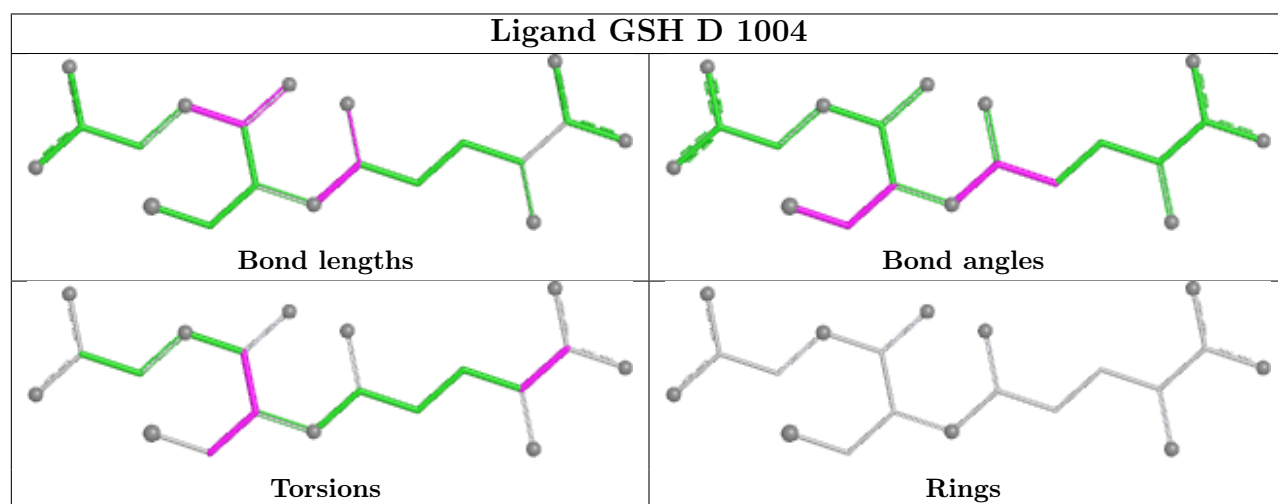
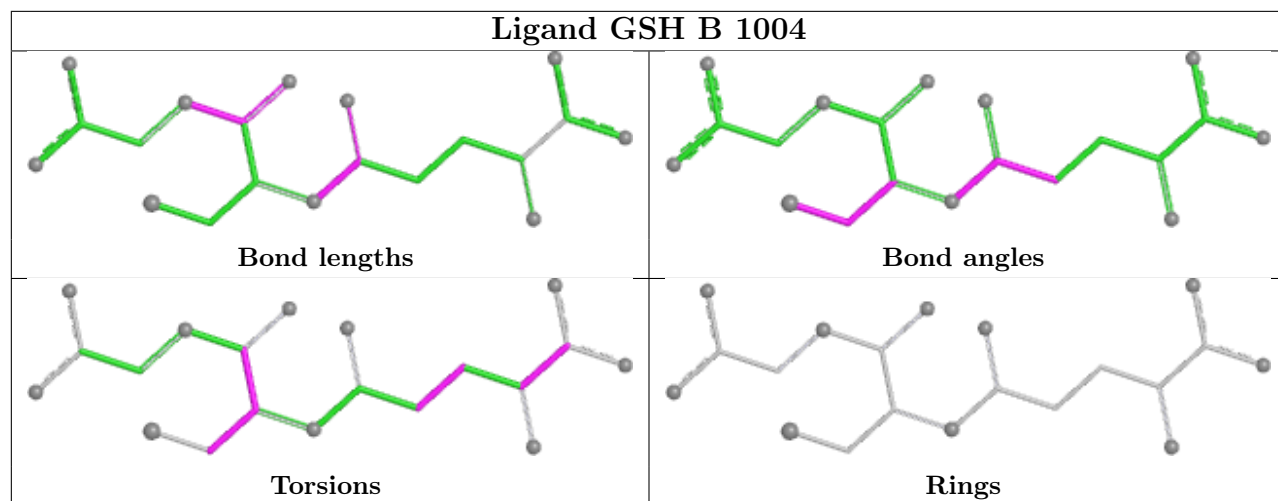
There are no ring outliers.

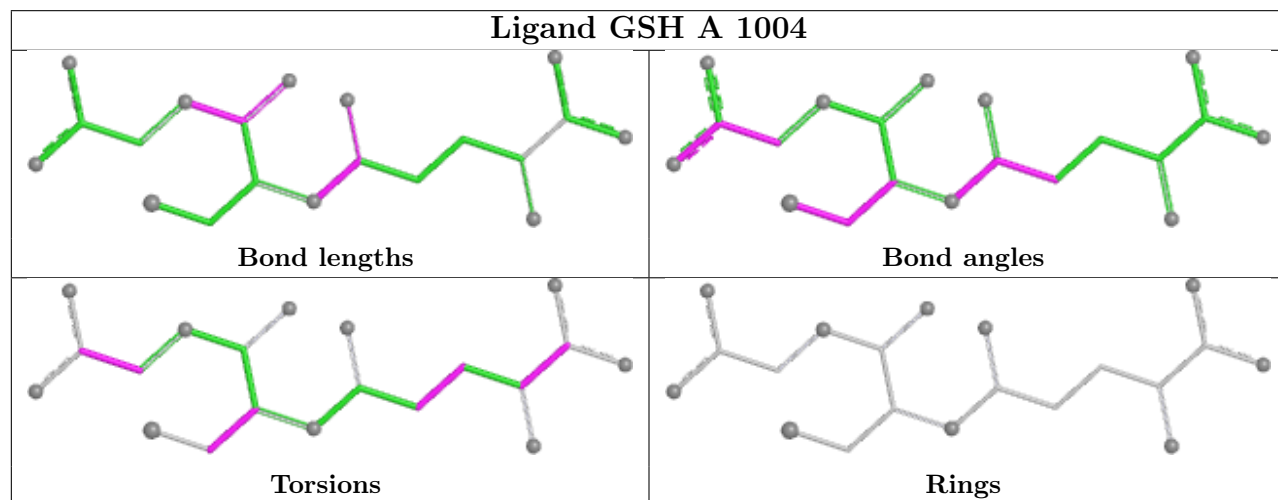
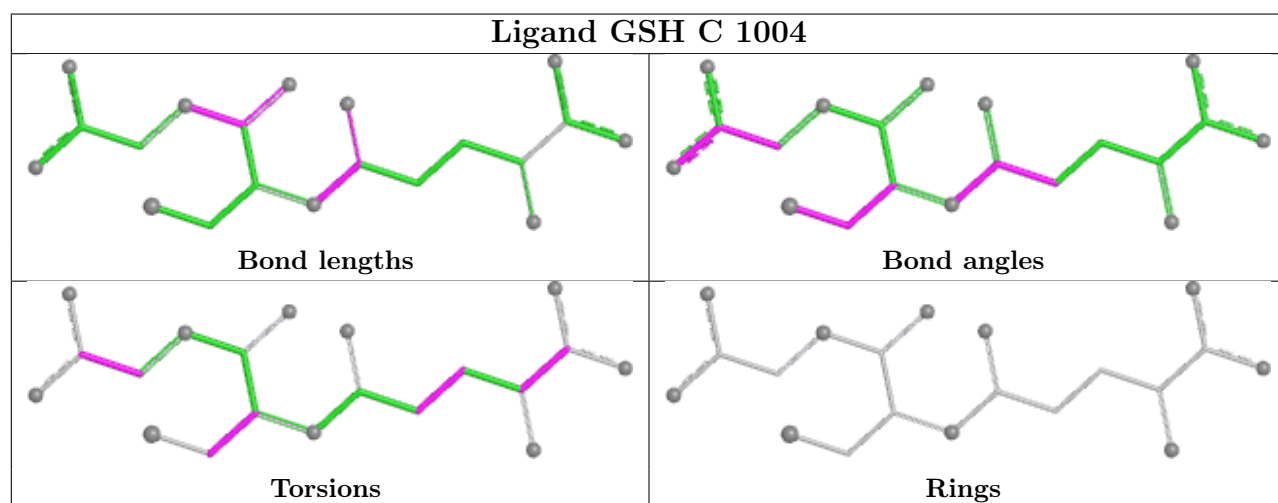
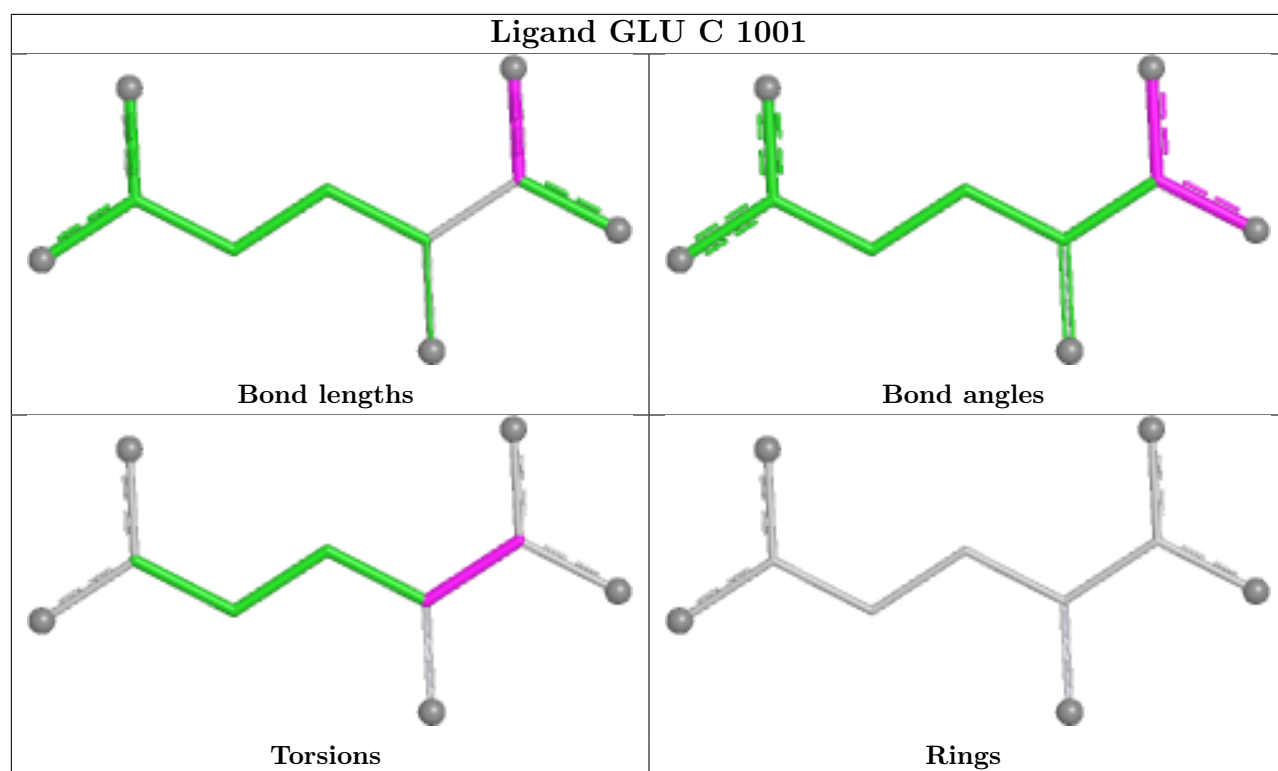
8 monomers are involved in 12 short contacts:

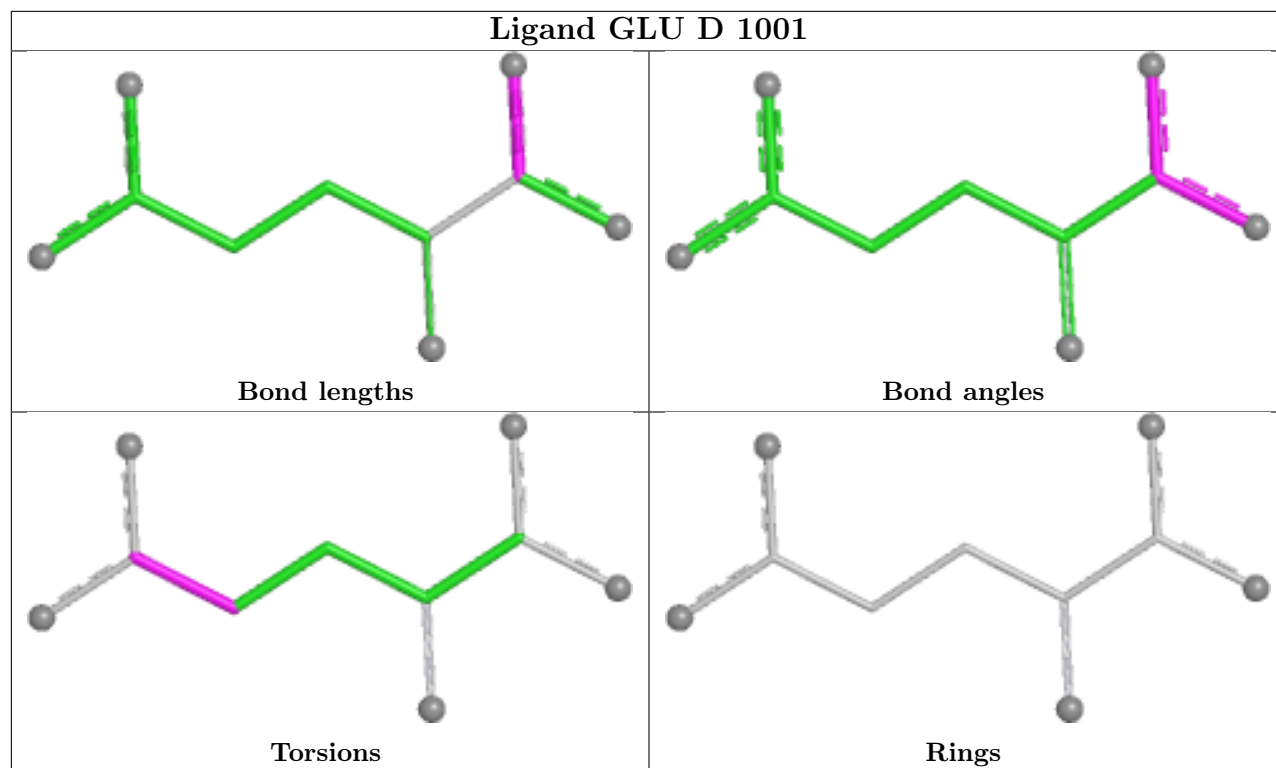
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1001	GLU	1	0
5	B	1004	GSH	1	0
5	D	1004	GSH	1	0
3	B	1001	GLU	1	0
3	C	1001	GLU	1	0
5	C	1004	GSH	3	0
5	A	1004	GSH	3	0
3	D	1001	GLU	1	0

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









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.

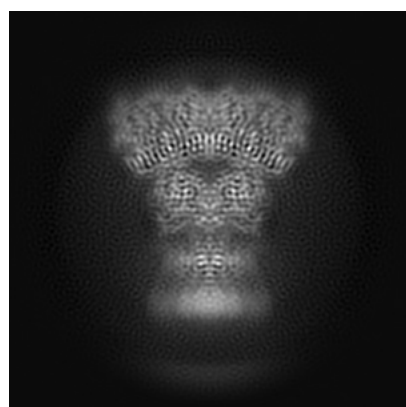
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23606. These allow visual inspection of the internal detail of the map and identification of artifacts.

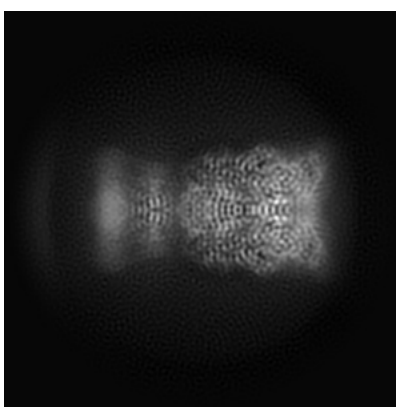
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

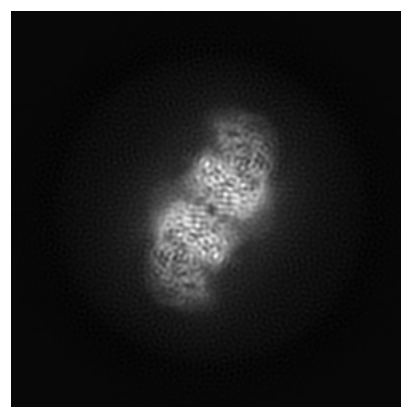
6.1.1 Primary map



X



Y

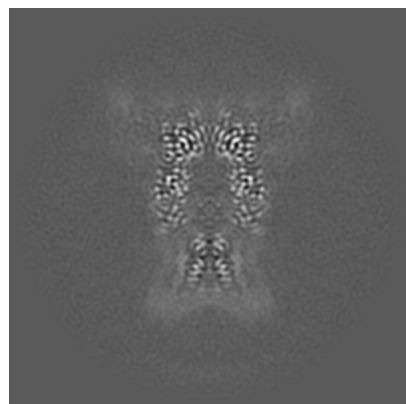


Z

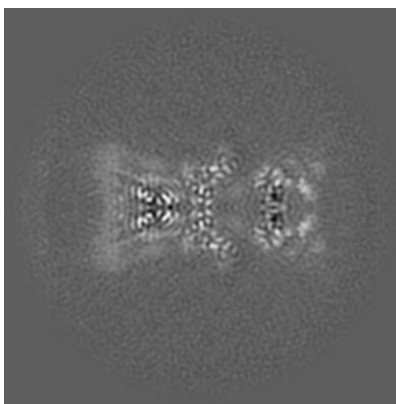
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

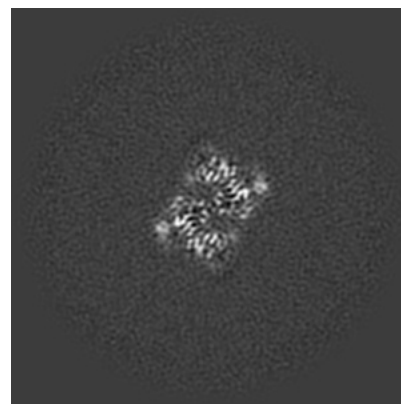
6.2.1 Primary map



X Index: 180



Y Index: 180

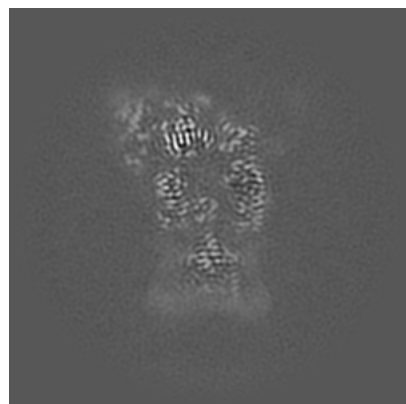


Z Index: 180

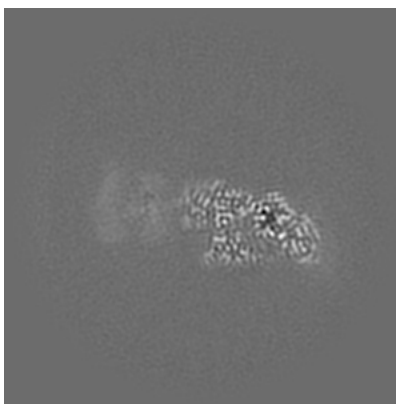
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

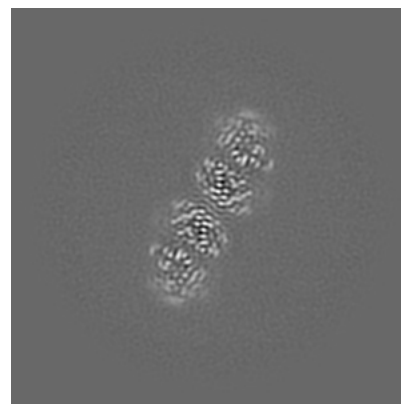
6.3.1 Primary map



X Index: 172



Y Index: 152

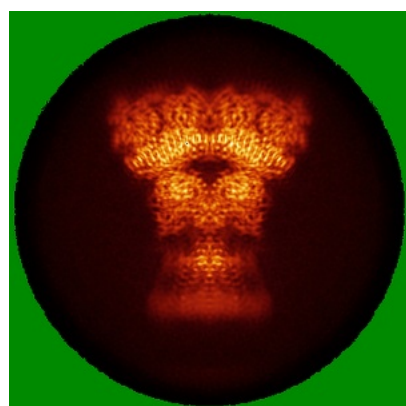


Z Index: 243

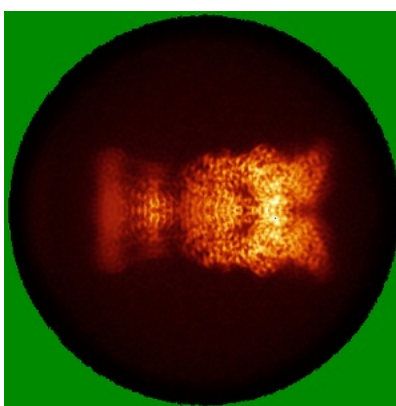
The images above show the largest variance slices of the map in three orthogonal directions.

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

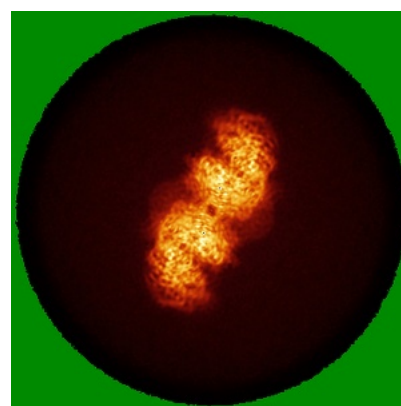
6.4.1 Primary map



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.

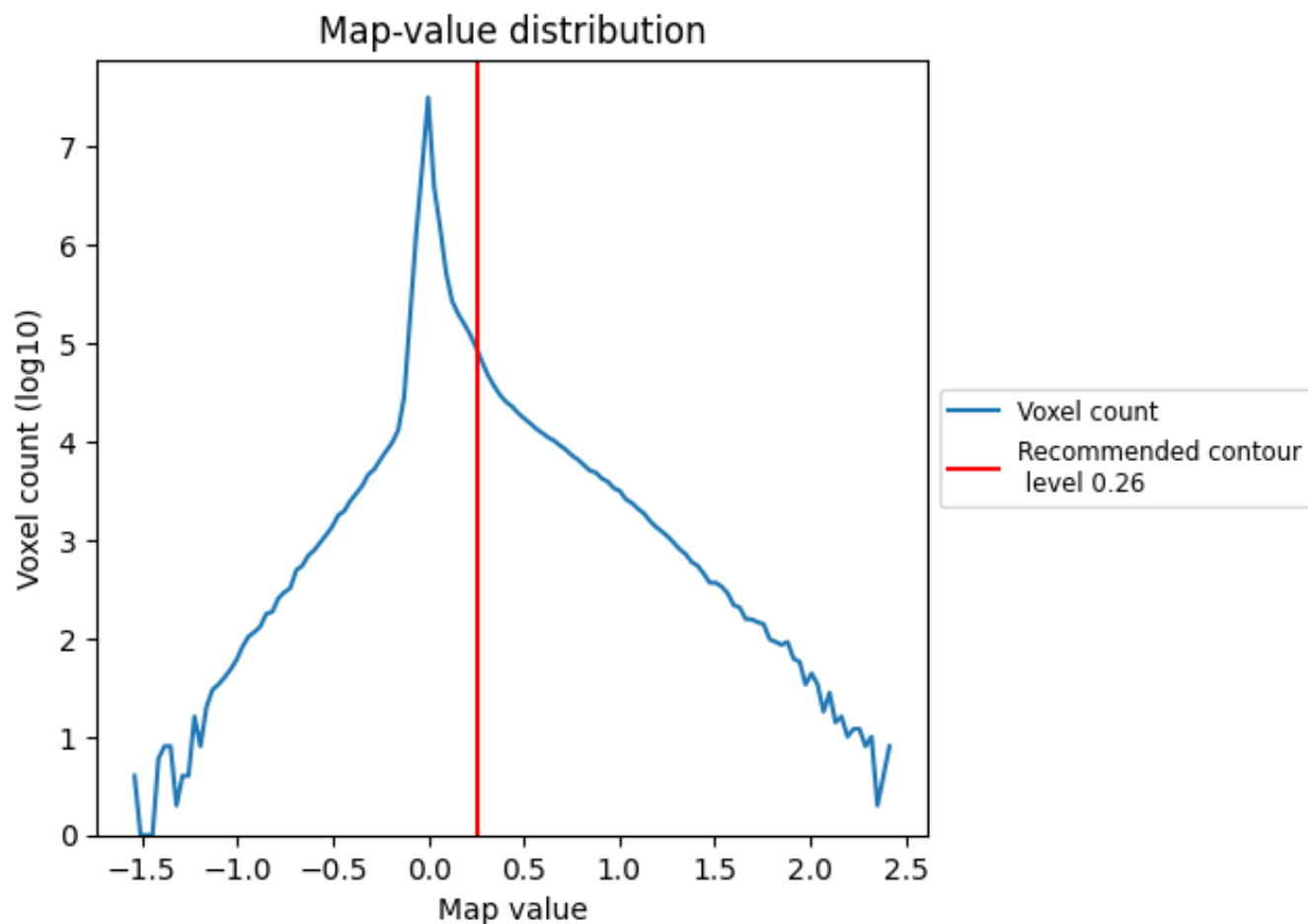
6.6 Mask visualisation

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

7 Map analysis [i](#)

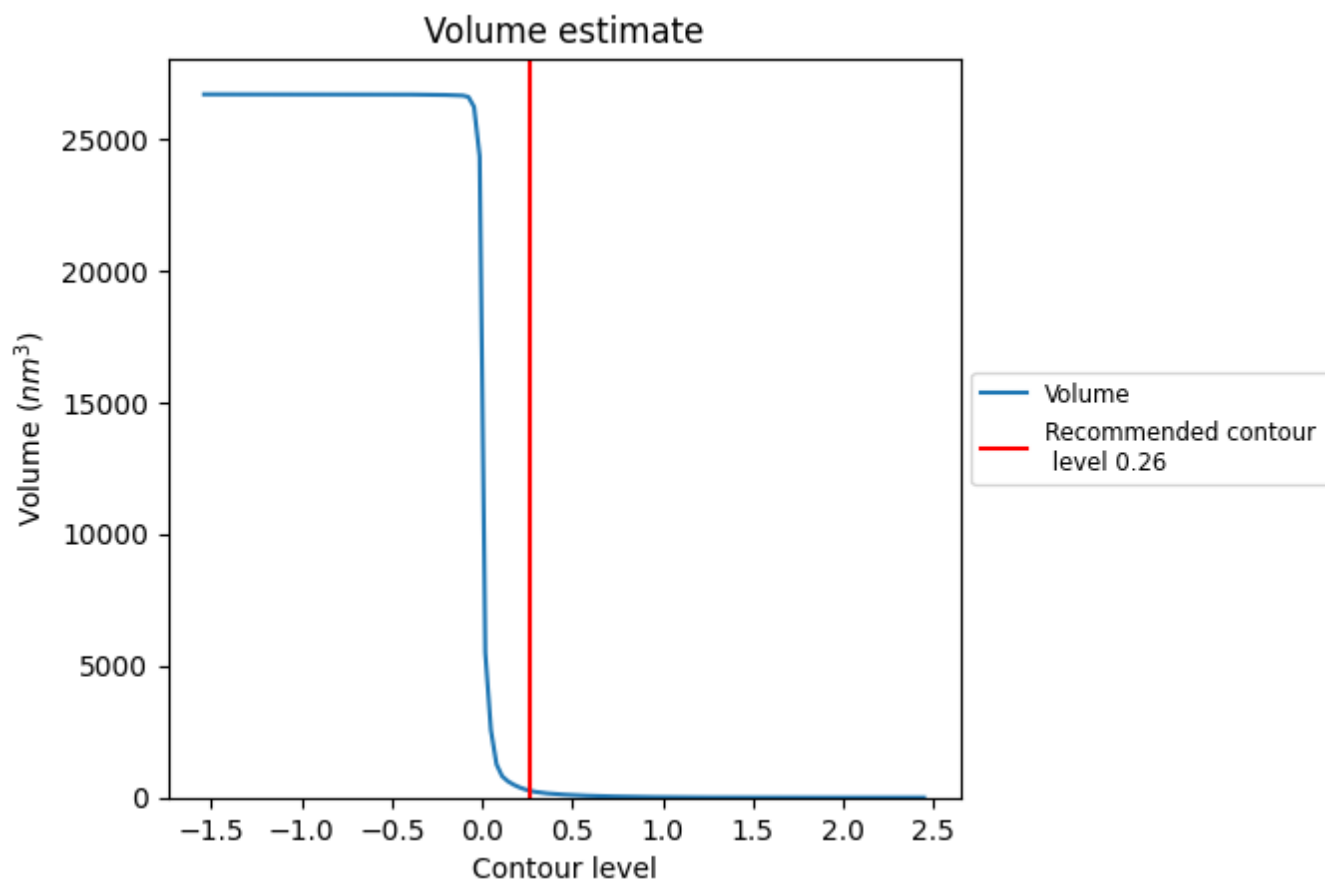
This section contains the results of statistical analysis of the map.

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.

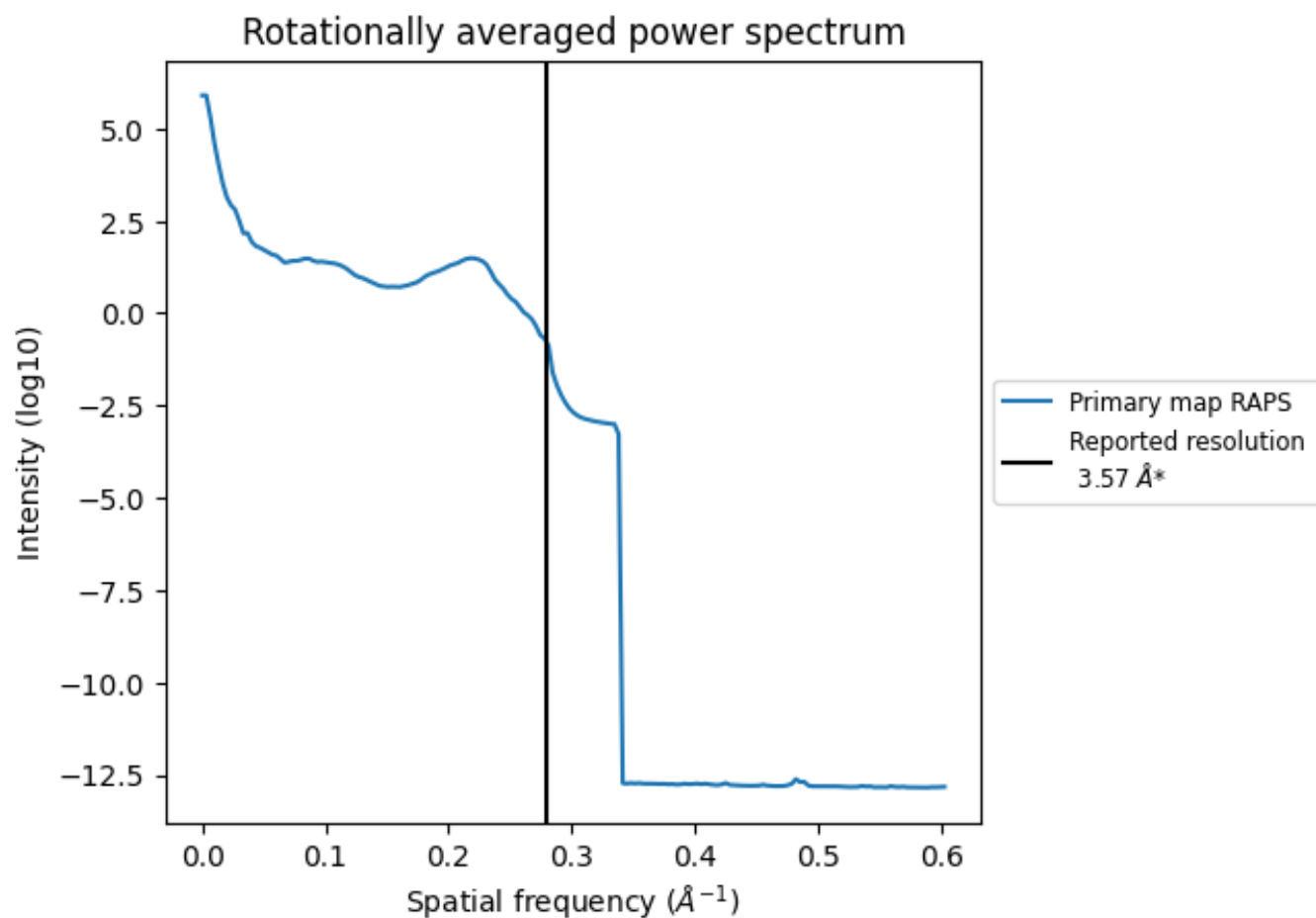
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 269 nm^3 ; this corresponds to an approximate mass of 243 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 0.280 Å⁻¹

8 Fourier-Shell correlation ⓘ

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

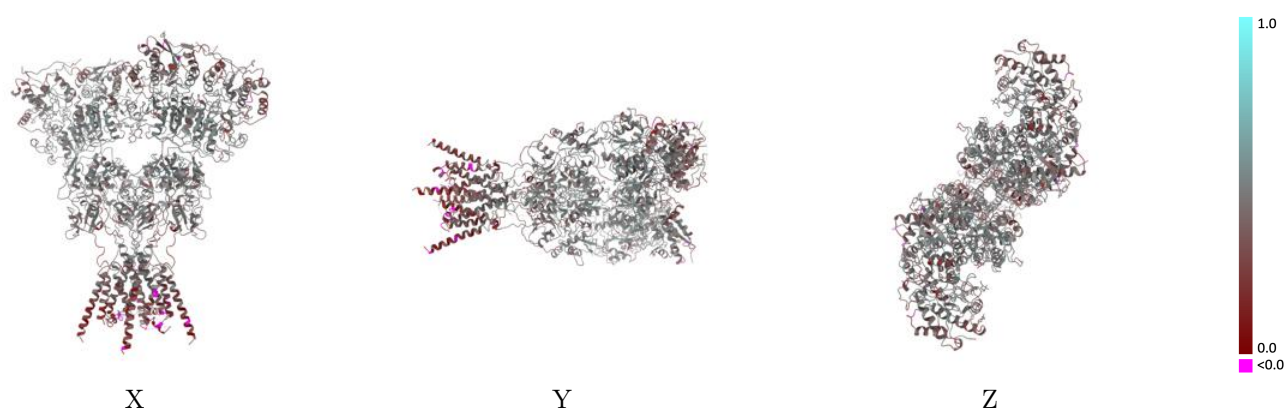
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-23606 and PDB model 7LZH. 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](#)

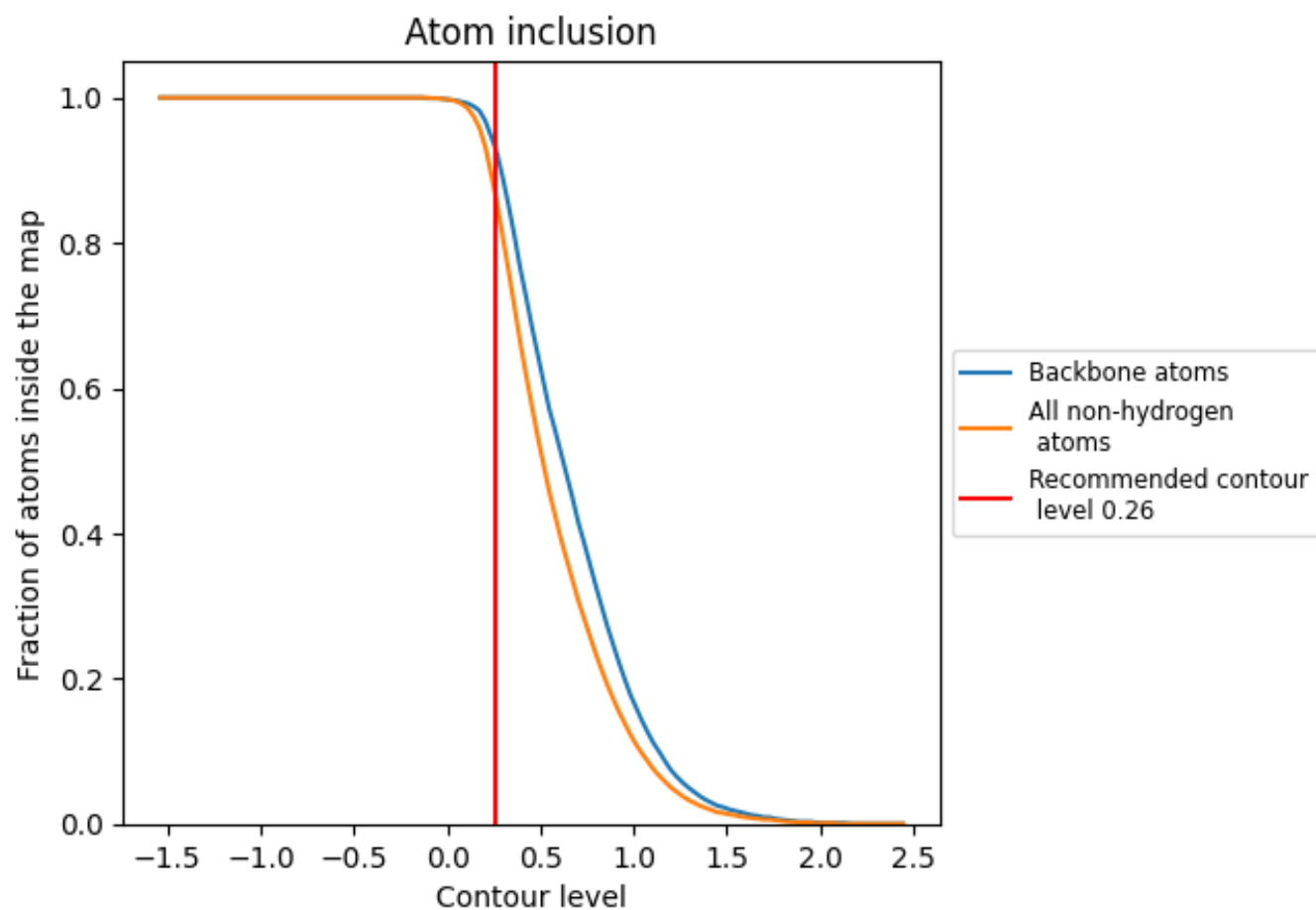


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 86% 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 (0.26) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8650	0.4240
A	0.8670	0.4250
B	0.8640	0.4210
C	0.8620	0.4210
D	0.8680	0.4270
E	0.8930	0.4490
F	0.9290	0.4830
G	0.7860	0.3710
H	0.9290	0.4470
I	0.8930	0.4510
J	0.9290	0.4950
K	0.8210	0.3700
L	0.9290	0.4320

