



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:30 AM UTC

PDB ID : 5CFB / pdb\_00005cfb  
Title : Crystal Structure of Human Glycine Receptor alpha-3 Bound to Strychnine  
Authors : Shaffer, P.L.; Huang, X.; Chen, H.  
Deposited on : 2015-07-08  
Resolution : 3.04 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

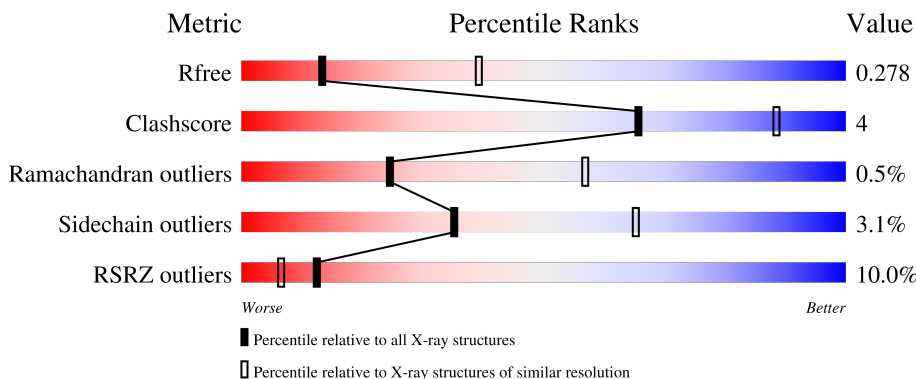
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.04 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)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	3685 (3.08-3.00)
Clashscore	190562	4007 (3.08-3.00)
Ramachandran outliers	187476	3834 (3.08-3.00)
Sidechain outliers	187428	3836 (3.08-3.00)
RSRZ outliers	180081	3684 (3.08-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	362	 9% 85% 9% • 6%
1	B	362	 9% 83% 10% 6%
1	C	362	 12% 83% 9% • 7%
1	D	362	 9% 78% 12% • 9%
1	E	362	 8% 82% 11% 6%

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Mol	Chain	Length	Quality of chain
2	F	2	 50% 50%
2	G	2	 50% 50%

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13540 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Glycine receptor subunit alpha-3, Glycine receptor subunit alpha-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	339	Total 2685	C 1748	N 428	O 490	S 19	0	0	0
1	B	339	Total 2676	C 1743	N 425	O 490	S 18	0	0	0
1	C	336	Total 2644	C 1719	N 421	O 486	S 18	0	0	0
1	D	331	Total 2626	C 1711	N 417	O 480	S 18	0	0	0
1	E	339	Total 2686	C 1752	N 426	O 490	S 18	0	0	0

There are 55 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	310	ALA	-	linker	UNP O75311
A	311	GLY	-	linker	UNP O75311
A	312	THR	-	linker	UNP O75311
A	355	TRP	-	expression tag	UNP O75311
A	356	SER	-	expression tag	UNP O75311
A	357	HIS	-	expression tag	UNP O75311
A	358	PRO	-	expression tag	UNP O75311
A	359	GLN	-	expression tag	UNP O75311
A	360	PHE	-	expression tag	UNP O75311
A	361	GLU	-	expression tag	UNP O75311
A	362	LYS	-	expression tag	UNP O75311
B	310	ALA	-	linker	UNP O75311
B	311	GLY	-	linker	UNP O75311
B	312	THR	-	linker	UNP O75311
B	355	TRP	-	expression tag	UNP O75311
B	356	SER	-	expression tag	UNP O75311
B	357	HIS	-	expression tag	UNP O75311
B	358	PRO	-	expression tag	UNP O75311

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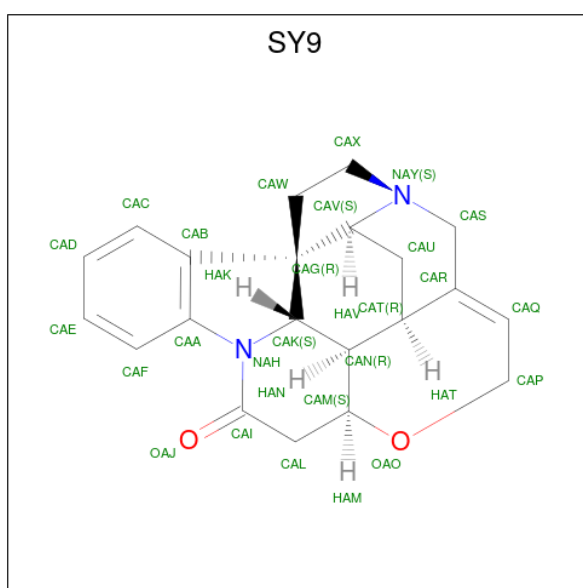
Chain	Residue	Modelled	Actual	Comment	Reference
B	359	GLN	-	expression tag	UNP O75311
B	360	PHE	-	expression tag	UNP O75311
B	361	GLU	-	expression tag	UNP O75311
B	362	LYS	-	expression tag	UNP O75311
C	310	ALA	-	linker	UNP O75311
C	311	GLY	-	linker	UNP O75311
C	312	THR	-	linker	UNP O75311
C	355	TRP	-	expression tag	UNP O75311
C	356	SER	-	expression tag	UNP O75311
C	357	HIS	-	expression tag	UNP O75311
C	358	PRO	-	expression tag	UNP O75311
C	359	GLN	-	expression tag	UNP O75311
C	360	PHE	-	expression tag	UNP O75311
C	361	GLU	-	expression tag	UNP O75311
C	362	LYS	-	expression tag	UNP O75311
D	310	ALA	-	linker	UNP O75311
D	311	GLY	-	linker	UNP O75311
D	312	THR	-	linker	UNP O75311
D	355	TRP	-	expression tag	UNP O75311
D	356	SER	-	expression tag	UNP O75311
D	357	HIS	-	expression tag	UNP O75311
D	358	PRO	-	expression tag	UNP O75311
D	359	GLN	-	expression tag	UNP O75311
D	360	PHE	-	expression tag	UNP O75311
D	361	GLU	-	expression tag	UNP O75311
D	362	LYS	-	expression tag	UNP O75311
E	310	ALA	-	linker	UNP O75311
E	311	GLY	-	linker	UNP O75311
E	312	THR	-	linker	UNP O75311
E	355	TRP	-	expression tag	UNP O75311
E	356	SER	-	expression tag	UNP O75311
E	357	HIS	-	expression tag	UNP O75311
E	358	PRO	-	expression tag	UNP O75311
E	359	GLN	-	expression tag	UNP O75311
E	360	PHE	-	expression tag	UNP O75311
E	361	GLU	-	expression tag	UNP O75311
E	362	LYS	-	expression tag	UNP O75311

- 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				ZeroOcc	AltConf	Trace
2	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	G	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is STRYCHNINE (CCD ID: SY9) (formula: C<sub>21</sub>H<sub>22</sub>N<sub>2</sub>O<sub>2</sub>).



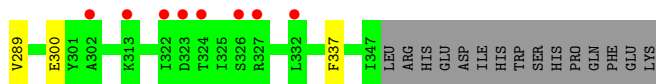
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			25	21	2	2		
3	B	1	Total	C	N	O	0	0
			25	21	2	2		
3	C	1	Total	C	N	O	0	0
			25	21	2	2		
3	D	1	Total	C	N	O	0	0
			25	21	2	2		
3	E	1	Total	C	N	O	0	0
			25	21	2	2		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).

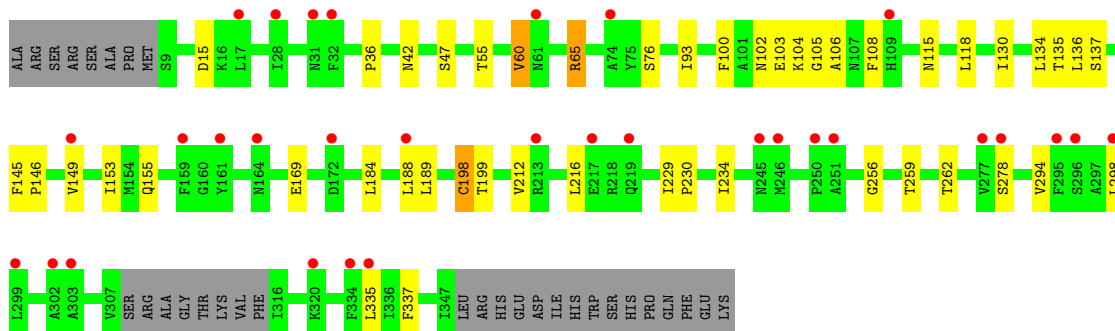
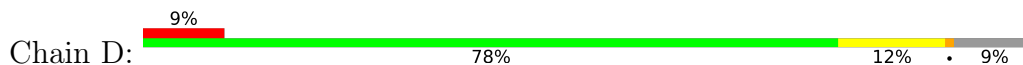


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	Total 14	8	1	5	0	0
4	B	1	Total 14	8	1	5	0	0
4	E	1	Total 14	8	1	5	0	0

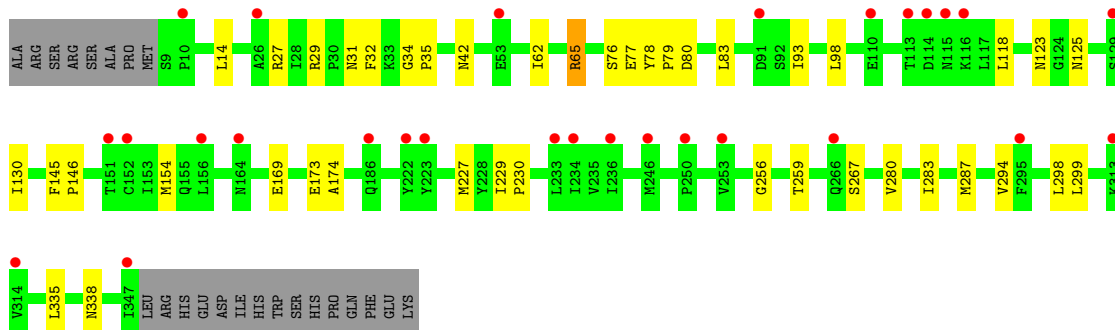
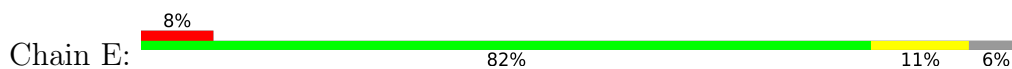




- Molecule 1: Glycine receptor subunit alpha-3, Glycine receptor subunit alpha-3



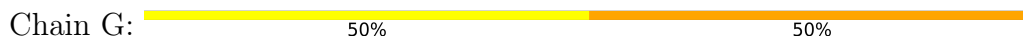
- Molecule 1: Glycine receptor subunit alpha-3, Glycine receptor subunit alpha-3



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



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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	140.24Å 143.20Å 180.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.04 50.00 – 3.04	Depositor EDS
% Data completeness (in resolution range)	96.8 (50.00-3.04) 96.8 (50.00-3.04)	Depositor EDS
$R_{merge}$	0.20	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.72 (at 3.07Å)	Xtrriage
Refinement program	REFMAC 5.8.0073	Depositor
R, $R_{free}$	0.260 , 0.283 0.258 , 0.278	Depositor DCC
$R_{free}$ test set	3426 reflections (4.51%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	97.8	Xtrriage
Anisotropy	0.565	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 88.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.015 for k,h,-l	Xtrriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	13540	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	124.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SY9, NAG

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	0.43	0/2755	0.69	0/3759
1	B	0.42	0/2746	0.68	0/3749
1	C	0.43	0/2710	0.71	0/3696
1	D	0.50	0/2694	0.75	0/3676
1	E	0.44	0/2757	0.70	0/3762
All	All	0.44	0/13662	0.71	0/18642

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2685	0	2603	18	0
1	B	2676	0	2585	22	0
1	C	2644	0	2561	20	0
1	D	2626	0	2542	22	0
1	E	2686	0	2603	23	0
2	F	28	0	25	1	0
2	G	28	0	25	1	0
3	A	25	0	22	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	25	0	22	0	0
3	C	25	0	22	0	0
3	D	25	0	22	0	0
3	E	25	0	22	0	0
4	A	14	0	13	2	0
4	B	14	0	13	2	0
4	E	14	0	13	0	0
All	All	13540	0	13093	102	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 (102) 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:D:189:LEU:HD12	1:D:216:LEU:HD23	1.72	0.71
1:A:42:ASN:HD21	1:A:65:ARG:HD2	1.57	0.70
1:B:42:ASN:HD21	1:B:65:ARG:HD2	1.62	0.65
1:D:42:ASN:HD21	1:D:65:ARG:HD2	1.63	0.64
1:C:42:ASN:HD21	1:C:65:ARG:HD2	1.63	0.62
1:B:108:PHE:CE1	1:B:130:ILE:HD11	2.36	0.61
1:A:227:MET:HG2	1:A:283:ILE:HD11	1.86	0.58
1:B:257:ILE:HG12	1:C:258:THR:HG21	1.87	0.56
1:D:93:ILE:HD13	1:D:118:LEU:HD21	1.87	0.56
1:D:189:LEU:HD12	1:D:216:LEU:CD2	2.35	0.56
1:E:42:ASN:HD21	1:E:65:ARG:HD2	1.71	0.56
1:E:93:ILE:HD13	1:E:118:LEU:HD21	1.87	0.55
1:B:257:ILE:HG23	1:C:258:THR:HG22	1.90	0.54
1:D:55:THR:O	1:D:104:LYS:NZ	2.41	0.54
1:B:63:PHE:CZ	1:B:131:ARG:HD2	2.43	0.54
1:B:173:GLU:O	1:B:174:ALA:C	2.51	0.53
1:D:108:PHE:CE1	1:D:130:ILE:HD11	2.44	0.53
4:B:601:NAG:H83	4:B:601:NAG:H3	1.91	0.52
1:D:259:THR:HG22	1:D:294:VAL:HG13	1.92	0.52
1:C:29:ARG:NH2	1:C:35:PRO:O	2.45	0.49
1:B:63:PHE:CE1	1:B:131:ARG:HD2	2.47	0.49
1:D:100:PHE:HA	1:D:155:GLN:O	2.12	0.49
1:C:58:TYR:CE1	1:C:152:CYS:HB3	2.48	0.49
1:D:229:ILE:HB	1:D:230:PRO:HD3	1.93	0.48
1:B:108:PHE:HE1	1:B:130:ILE:HD11	1.75	0.48
1:D:105:GLY:O	1:D:135:THR:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:14:LEU:HG	1:E:83:LEU:HD23	1.94	0.48
1:D:256:GLY:HA3	1:D:298:LEU:HD13	1.96	0.48
1:C:36:PRO:O	2:F:1:NAG:H82	2.13	0.48
1:E:31:ASN:O	1:E:32:PHE:C	2.56	0.48
1:A:229:ILE:HB	1:A:230:PRO:HD3	1.95	0.48
1:B:98:LEU:HD23	1:B:98:LEU:C	2.38	0.47
1:A:225:ILE:HD12	1:E:280:VAL:HG21	1.95	0.47
1:A:304:VAL:HG21	1:A:323:ASP:OD1	2.14	0.47
1:E:259:THR:HG22	1:E:294:VAL:HG13	1.97	0.47
1:C:24:TYR:CE2	1:C:73:LEU:HD21	2.49	0.47
1:B:229:ILE:HB	1:B:230:PRO:HD3	1.96	0.47
1:A:29:ARG:NH2	1:A:35:PRO:O	2.48	0.47
1:C:220:MET:O	1:C:221:GLY:C	2.58	0.47
1:A:36:PRO:O	4:A:502:NAG:H82	2.15	0.47
1:D:198:CYS:O	1:D:199:THR:C	2.57	0.47
1:C:170:TRP:CD1	1:C:195:LEU:HD22	2.51	0.46
1:E:229:ILE:HB	1:E:230:PRO:HD3	1.98	0.46
1:C:227:MET:HE3	1:C:227:MET:HA	1.98	0.46
1:D:189:LEU:CD1	1:D:216:LEU:CD2	2.94	0.46
1:A:220:MET:O	1:A:221:GLY:C	2.58	0.46
1:A:235:VAL:O	1:A:238:SER:OG	2.29	0.46
1:E:98:LEU:C	1:E:98:LEU:HD23	2.41	0.46
4:A:502:NAG:H83	4:A:502:NAG:H3	1.98	0.46
1:D:153:ILE:HD12	1:D:155:GLN:HG3	1.98	0.46
1:E:173:GLU:O	1:E:174:ALA:C	2.59	0.46
1:C:63:PHE:CZ	1:C:131:ARG:HD2	2.52	0.45
1:C:83:LEU:HD12	1:C:120:ILE:HD11	1.97	0.45
1:C:289:VAL:HG11	1:C:337:PHE:CZ	2.52	0.45
1:E:29:ARG:NH2	1:E:35:PRO:O	2.49	0.45
1:E:77:GLU:OE1	1:E:77:GLU:N	2.49	0.45
1:E:62:ILE:HD13	1:E:154:MET:HE1	1.99	0.45
1:B:267:SER:O	1:B:271:ARG:HG3	2.17	0.45
1:D:188:LEU:O	1:D:216:LEU:HA	2.16	0.45
1:A:260:VAL:HG22	1:A:294:VAL:HG12	1.99	0.44
1:C:198:CYS:O	1:C:199:THR:C	2.60	0.44
1:A:153:ILE:HG22	1:A:213:ARG:HG2	1.99	0.44
1:D:60:VAL:HG12	1:D:134:LEU:HB2	1.99	0.44
1:A:249:ALA:N	1:A:250:PRO:CD	2.81	0.44
1:C:98:LEU:HD23	1:C:99:PHE:N	2.32	0.44
1:A:11:SER:HB3	1:E:27:ARG:CZ	2.48	0.44
1:B:77:GLU:OE1	1:B:77:GLU:N	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:ARG:NH1	1:A:165:ASP:OD2	2.51	0.44
1:E:267:SER:HA	1:E:287:MET:HE2	1.99	0.44
1:A:237:LEU:O	1:A:240:VAL:HG22	2.17	0.43
1:C:254:ALA:O	1:C:258:THR:HG23	2.17	0.43
1:B:230:PRO:CB	1:B:266:GLN:HE22	2.31	0.43
1:B:42:ASN:ND2	1:B:65:ARG:HD2	2.32	0.43
1:B:83:LEU:HD12	1:B:120:ILE:HD11	2.01	0.43
1:C:289:VAL:HG11	1:C:337:PHE:CE2	2.54	0.43
1:B:85:LEU:HD23	1:B:118:LEU:HD23	2.01	0.42
1:C:156:LEU:N	1:C:156:LEU:HD12	2.35	0.42
1:D:102:ASN:O	1:D:136:LEU:HA	2.19	0.42
1:B:198:CYS:O	1:B:199:THR:C	2.62	0.42
1:E:256:GLY:HA3	1:E:298:LEU:HD13	2.01	0.42
1:A:225:ILE:HD12	1:E:280:VAL:CG2	2.50	0.42
1:B:73:LEU:HD11	1:B:93:ILE:HD11	2.01	0.42
1:B:108:PHE:CD1	1:B:130:ILE:HD11	2.54	0.42
1:E:123:ASN:OD1	1:E:125:ASN:ND2	2.52	0.42
1:E:145:PHE:HA	1:E:146:PRO:HA	1.85	0.41
1:D:115:ASN:HD22	1:D:115:ASN:N	2.17	0.41
1:E:78:TYR:CG	1:E:79:PRO:HD2	2.55	0.41
1:D:36:PRO:O	2:G:1:NAG:H82	2.21	0.41
1:A:237:LEU:HD21	1:E:299:LEU:HD13	2.01	0.41
1:E:31:ASN:O	1:E:34:GLY:N	2.54	0.41
1:A:108:PHE:CE1	1:A:130:ILE:HD11	2.55	0.41
1:D:145:PHE:HA	1:D:146:PRO:HA	1.91	0.41
1:B:230:PRO:HB3	1:B:266:GLN:HE22	1.86	0.41
1:C:227:MET:SD	1:C:270:SER:HB3	2.61	0.41
1:E:227:MET:HE2	1:E:287:MET:HE1	2.03	0.41
1:B:229:ILE:HB	1:B:230:PRO:CD	2.51	0.40
1:D:106:ALA:HB1	1:D:134:LEU:HD23	2.04	0.40
1:D:234:ILE:HD11	1:D:262:THR:HG22	2.02	0.40
1:E:146:PRO:HD3	1:E:283:ILE:HB	2.01	0.40
4:B:601:NAG:H3	4:B:601:NAG:C8	2.52	0.40
1:C:60:VAL:HG12	1:C:134:LEU:HB2	2.02	0.40
1:B:237:LEU:O	1:B:240:VAL:HG22	2.20	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 X-ray entries followed by that with respect to entries of similar resolution.

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	337/362 (93%)	321 (95%)	15 (4%)	1 (0%)	36	67
1	B	337/362 (93%)	314 (93%)	21 (6%)	2 (1%)	21	53
1	C	332/362 (92%)	313 (94%)	16 (5%)	3 (1%)	14	44
1	D	327/362 (90%)	309 (94%)	17 (5%)	1 (0%)	36	67
1	E	337/362 (93%)	322 (96%)	14 (4%)	1 (0%)	36	67
All	All	1670/1810 (92%)	1579 (95%)	83 (5%)	8 (0%)	24	57

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	221	GLY
1	B	221	GLY
1	B	248	ALA
1	C	221	GLY
1	C	76	SER
1	C	227	MET
1	D	76	SER
1	E	76	SER

### 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 X-ray entries followed by that with respect to entries of similar resolution.

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	291/326 (89%)	285 (98%)	6 (2%)	47	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	289/326 (89%)	279 (96%)	10 (4%)	32	62
1	C	286/326 (88%)	278 (97%)	8 (3%)	38	67
1	D	285/326 (87%)	271 (95%)	14 (5%)	22	53
1	E	291/326 (89%)	285 (98%)	6 (2%)	47	72
All	All	1442/1630 (88%)	1398 (97%)	44 (3%)	35	65

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	LEU
1	A	53	GLU
1	A	65	ARG
1	A	84	ASP
1	A	110	GLU
1	A	118	LEU
1	B	65	ARG
1	B	95	LYS
1	B	117	LEU
1	B	164	ASN
1	B	169	GLU
1	B	220	MET
1	B	291	LEU
1	B	300	GLU
1	B	335	LEU
1	B	347	ILE
1	C	53	GLU
1	C	65	ARG
1	C	103	GLU
1	C	133	THR
1	C	137	SER
1	C	198	CYS
1	C	225	ILE
1	C	300	GLU
1	D	15	ASP
1	D	47	SER
1	D	60	VAL
1	D	65	ARG
1	D	103	GLU
1	D	137	SER
1	D	149	VAL
1	D	169	GLU

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Mol	Chain	Res	Type
1	D	184	LEU
1	D	198	CYS
1	D	212	VAL
1	D	278	SER
1	D	335	LEU
1	D	337	PHE
1	E	65	ARG
1	E	80	ASP
1	E	130	ILE
1	E	169	GLU
1	E	335	LEU
1	E	338	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	ASN
1	A	69	ASN
1	A	125	ASN
1	A	144	ASN
1	A	219	GLN
1	B	42	ASN
1	B	107	ASN
1	B	125	ASN
1	B	266	GLN
1	B	305	ASN
1	C	42	ASN
1	C	61	ASN
1	C	69	ASN
1	C	125	ASN
1	C	226	GLN
1	D	61	ASN
1	D	219	GLN
1	D	266	GLN
1	D	338	ASN
1	E	61	ASN
1	E	69	ASN
1	E	186	GLN
1	E	266	GLN
1	E	305	ASN
1	E	338	ASN

### 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](#)

4 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	F	1	1,2	14,14,15	0.52	0	17,19,21	2.23	7 (41%)
2	NAG	F	2	2	14,14,15	0.47	0	17,19,21	0.76	0
2	NAG	G	1	1,2	14,14,15	0.39	0	17,19,21	2.67	7 (41%)
2	NAG	G	2	2	14,14,15	0.51	0	17,19,21	1.37	3 (17%)

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	F	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1
2	NAG	G	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	G	2	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	1	NAG	C1-O5-C5	7.48	122.21	112.19
2	G	1	NAG	C2-N2-C7	4.57	129.03	122.90
2	F	1	NAG	C2-N2-C7	4.43	128.83	122.90
2	F	1	NAG	C1-C2-N2	3.67	116.22	110.43
2	G	2	NAG	C8-C7-N2	3.55	122.00	116.12
2	F	1	NAG	O5-C1-C2	-3.51	105.86	111.29
2	F	1	NAG	C8-C7-N2	3.20	121.43	116.12
2	F	1	NAG	C4-C3-C2	-3.18	106.36	111.02
2	G	1	NAG	C8-C7-N2	3.06	121.19	116.12
2	G	1	NAG	O5-C5-C4	2.82	117.70	110.83
2	F	1	NAG	C1-O5-C5	2.75	115.88	112.19
2	G	1	NAG	C4-C3-C2	-2.62	107.18	111.02
2	G	2	NAG	C2-N2-C7	2.58	126.35	122.90
2	F	1	NAG	O7-C7-C8	-2.55	117.52	122.05
2	G	2	NAG	O7-C7-C8	-2.37	117.83	122.05
2	G	1	NAG	O7-C7-C8	-2.30	117.97	122.05
2	G	1	NAG	O5-C1-C2	-2.00	108.19	111.29

There are no chirality outliers.

All (12) torsion outliers are listed below:

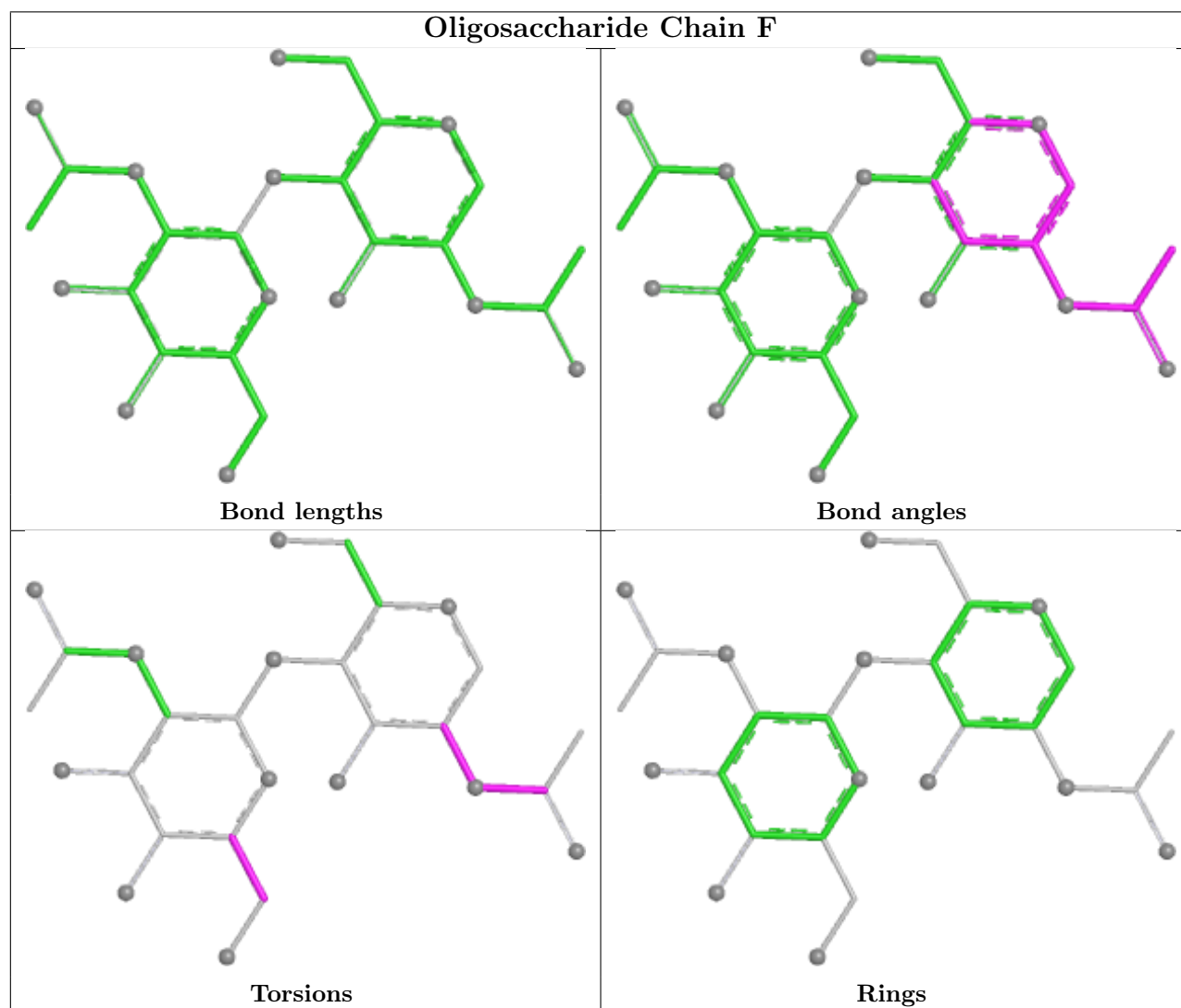
Mol	Chain	Res	Type	Atoms
2	G	1	NAG	C3-C2-N2-C7
2	F	1	NAG	C8-C7-N2-C2
2	F	1	NAG	O7-C7-N2-C2
2	G	1	NAG	C8-C7-N2-C2
2	G	1	NAG	O7-C7-N2-C2
2	G	2	NAG	C8-C7-N2-C2
2	G	2	NAG	O7-C7-N2-C2
2	F	2	NAG	O5-C5-C6-O6
2	G	1	NAG	C4-C5-C6-O6
2	F	2	NAG	C4-C5-C6-O6
2	F	1	NAG	C1-C2-N2-C7
2	F	1	NAG	C3-C2-N2-C7

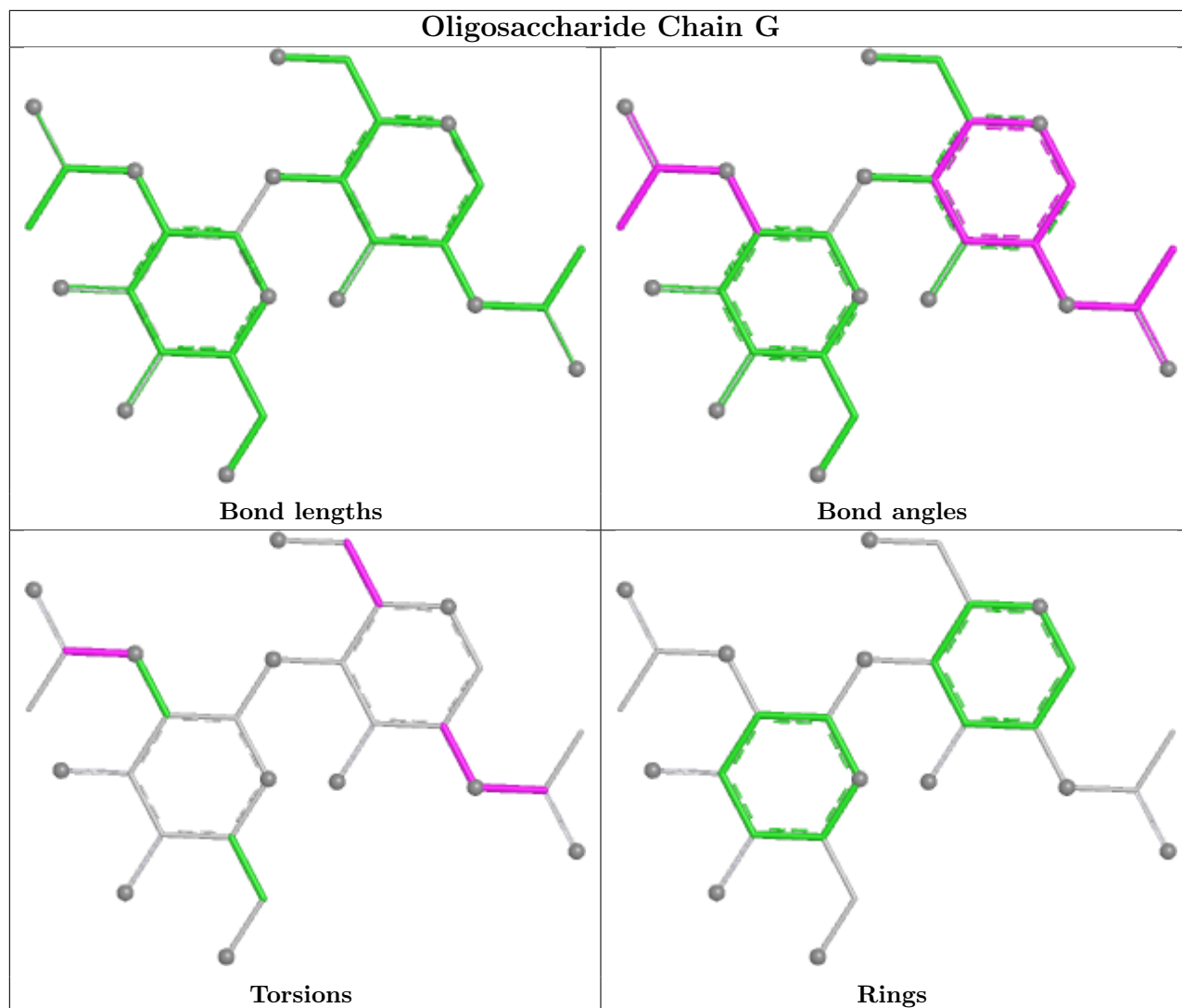
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	1	NAG	1	0
2	F	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](#)

8 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$
3	SY9	A	501	-	31,31,31	1.57	5 (16%)	51,51,51	2.15	15 (29%)
3	SY9	E	501	-	31,31,31	1.51	3 (9%)	51,51,51	2.20	13 (25%)
4	NAG	B	601	1	14,14,15	0.49	0	17,19,21	1.58	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	SY9	C	501	-	31,31,31	1.59	4 (12%)	51,51,51	2.18	15 (29%)
4	NAG	A	502	1	14,14,15	0.52	0	17,19,21	1.70	5 (29%)
3	SY9	D	501	-	31,31,31	1.56	4 (12%)	51,51,51	2.18	15 (29%)
4	NAG	E	601	1	14,14,15	0.46	0	17,19,21	2.91	6 (35%)
3	SY9	B	501	-	31,31,31	1.47	3 (9%)	51,51,51	2.35	16 (31%)

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	B	601	1	-	3/6/23/26	0/1/1/1
4	NAG	E	601	1	-	5/6/23/26	0/1/1/1
4	NAG	A	502	1	-	5/6/23/26	0/1/1/1

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	501	SY9	CAP-CAQ	-6.17	1.38	1.50
3	A	501	SY9	CAP-CAQ	-6.09	1.38	1.50
3	C	501	SY9	CAP-CAQ	-6.07	1.38	1.50
3	E	501	SY9	CAP-CAQ	-6.07	1.38	1.50
3	B	501	SY9	CAP-CAQ	-5.64	1.39	1.50
3	B	501	SY9	CAQ-CAR	2.92	1.38	1.33
3	C	501	SY9	CAQ-CAR	2.80	1.38	1.33
3	D	501	SY9	CAQ-CAR	2.79	1.38	1.33
3	E	501	SY9	CAQ-CAR	2.71	1.38	1.33
3	A	501	SY9	CAQ-CAR	2.70	1.38	1.33
3	C	501	SY9	CAL-CAM	2.60	1.59	1.53
3	D	501	SY9	CAL-CAI	2.59	1.55	1.51
3	C	501	SY9	CAL-CAI	2.48	1.54	1.51
3	A	501	SY9	CAL-CAI	2.45	1.54	1.51
3	A	501	SY9	CAI-NAH	2.41	1.41	1.36
3	E	501	SY9	CAL-CAI	2.35	1.54	1.51
3	A	501	SY9	CAL-CAM	2.15	1.58	1.53
3	D	501	SY9	CAI-NAH	2.13	1.40	1.36
3	B	501	SY9	CAI-NAH	2.10	1.40	1.36

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	501	SY9	CAS-CAR-CAQ	-9.06	114.72	123.07
3	D	501	SY9	CAS-CAR-CAQ	-8.93	114.84	123.07
3	E	501	SY9	CAS-CAR-CAQ	-8.92	114.85	123.07
3	A	501	SY9	CAS-CAR-CAQ	-8.88	114.89	123.07
4	E	601	NAG	C1-O5-C5	8.84	124.03	112.19
3	B	501	SY9	CAS-CAR-CAQ	-8.25	115.47	123.07
3	D	501	SY9	CAA-NAH-CAI	5.78	133.03	125.45
3	A	501	SY9	CAA-NAH-CAI	5.70	132.93	125.45
3	B	501	SY9	OAO-CAM-CAN	5.70	119.37	114.39
3	B	501	SY9	CAA-NAH-CAI	5.58	132.77	125.45
3	C	501	SY9	CAA-NAH-CAI	5.52	132.68	125.45
3	E	501	SY9	CAA-NAH-CAI	5.49	132.65	125.45
3	D	501	SY9	CAN-CAK-NAH	-4.82	101.87	106.08
4	E	601	NAG	C2-N2-C7	4.52	128.95	122.90
3	E	501	SY9	CAN-CAK-NAH	-4.45	102.20	106.08
3	B	501	SY9	CAN-CAK-NAH	-4.39	102.24	106.08
3	C	501	SY9	OAO-CAM-CAN	4.11	117.98	114.39
4	E	601	NAG	C8-C7-N2	4.09	122.91	116.12
4	A	502	NAG	C2-N2-C7	3.93	128.17	122.90
3	A	501	SY9	CAS-NAY-CAX	-3.66	106.55	112.58
3	B	501	SY9	OAO-CAP-CAQ	3.60	118.73	111.51
4	B	601	NAG	C2-N2-C7	3.59	127.71	122.90
3	A	501	SY9	CAN-CAK-NAH	-3.54	102.99	106.08
3	B	501	SY9	CAM-CAL-CAI	-3.47	112.30	117.12
3	B	501	SY9	CAN-CAT-CAR	-3.36	111.14	114.36
3	E	501	SY9	CAS-NAY-CAX	-3.35	107.06	112.58
3	C	501	SY9	CAN-CAK-NAH	-3.28	103.22	106.08
3	B	501	SY9	CAS-NAY-CAX	-3.27	107.20	112.58
3	E	501	SY9	OAO-CAM-CAN	3.17	117.16	114.39
3	E	501	SY9	CAM-CAL-CAI	-3.04	112.89	117.12
3	B	501	SY9	OAO-CAM-CAL	-3.01	101.03	104.49
3	A	501	SY9	OAO-CAP-CAQ	2.99	117.50	111.51
3	B	501	SY9	CAK-CAG-CAV	2.98	116.71	113.82
4	A	502	NAG	O5-C1-C2	-2.96	106.70	111.29
3	A	501	SY9	CAT-CAR-CAQ	2.93	126.37	122.67
3	A	501	SY9	CAK-CAG-CAV	2.92	116.66	113.82
4	A	502	NAG	C8-C7-N2	2.86	120.87	116.12
3	D	501	SY9	CAM-CAL-CAI	-2.84	113.17	117.12
3	D	501	SY9	CAT-CAR-CAQ	2.83	126.23	122.67
3	C	501	SY9	CAM-CAL-CAI	-2.80	113.23	117.12
4	B	601	NAG	O5-C1-C2	-2.77	107.00	111.29
3	B	501	SY9	CAS-CAR-CAT	2.76	119.85	114.01
4	E	601	NAG	O5-C5-C4	2.73	117.46	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	501	SY9	CAK-CAG-CAV	2.72	116.47	113.82
3	D	501	SY9	CAN-CAT-CAR	-2.72	111.75	114.36
3	C	501	SY9	CAF-CAA-CAB	-2.71	119.14	121.76
3	C	501	SY9	CAS-NAY-CAX	-2.70	108.14	112.58
3	E	501	SY9	CAN-CAT-CAR	-2.70	111.77	114.36
4	E	601	NAG	O7-C7-C8	-2.68	117.28	122.05
3	C	501	SY9	CAS-CAR-CAT	2.67	119.66	114.01
3	C	501	SY9	CAK-NAH-CAI	-2.65	115.23	119.23
3	D	501	SY9	CAK-NAH-CAI	-2.65	115.23	119.23
3	C	501	SY9	CAK-CAG-CAV	2.63	116.37	113.82
3	C	501	SY9	OAO-CAP-CAQ	2.63	116.77	111.51
3	B	501	SY9	CAK-NAH-CAI	-2.60	115.30	119.23
3	E	501	SY9	CAS-CAR-CAT	2.60	119.51	114.01
3	E	501	SY9	OAO-CAP-CAQ	2.60	116.72	111.51
3	B	501	SY9	CAF-CAA-CAB	-2.55	119.30	121.76
3	D	501	SY9	CAF-CAA-CAB	-2.53	119.31	121.76
3	D	501	SY9	CAS-NAY-CAX	-2.47	108.52	112.58
3	A	501	SY9	CAM-CAL-CAI	-2.43	113.75	117.12
3	E	501	SY9	CAK-NAH-CAI	-2.41	115.58	119.23
3	D	501	SY9	OAO-CAP-CAQ	2.41	116.33	111.51
3	E	501	SY9	CAF-CAA-CAB	-2.40	119.44	121.76
3	C	501	SY9	CAP-OAO-CAM	2.38	117.32	114.86
3	B	501	SY9	CAW-CAG-CAB	-2.38	108.03	112.36
3	A	501	SY9	CAF-CAA-CAB	-2.37	119.47	121.76
3	E	501	SY9	CAT-CAR-CAQ	2.36	125.64	122.67
4	B	601	NAG	C8-C7-N2	2.36	120.03	116.12
3	C	501	SY9	CAT-CAR-CAQ	2.33	125.61	122.67
3	D	501	SY9	CAS-CAR-CAT	2.32	118.92	114.01
3	A	501	SY9	CAK-NAH-CAI	-2.30	115.75	119.23
4	A	502	NAG	O7-C7-C8	-2.28	118.00	122.05
4	E	601	NAG	C1-C2-N2	2.27	114.00	110.43
3	A	501	SY9	CAL-CAI-NAH	2.24	119.15	115.41
3	A	501	SY9	CAW-CAG-CAB	-2.24	108.28	112.36
3	A	501	SY9	CAS-CAR-CAT	2.24	118.74	114.01
3	B	501	SY9	CAS-NAY-CAV	2.21	115.09	113.05
3	D	501	SY9	CAU-CAT-CAR	-2.21	106.57	109.12
3	D	501	SY9	CAK-CAG-CAV	2.20	115.96	113.82
3	B	501	SY9	CAM-CAN-CAK	2.17	109.47	107.46
3	C	501	SY9	CAU-CAT-CAR	-2.16	106.62	109.12
4	B	601	NAG	O7-C7-C8	-2.16	118.21	122.05
3	C	501	SY9	CAN-CAT-CAR	-2.16	112.29	114.36
3	A	501	SY9	CAU-CAT-CAR	-2.11	106.68	109.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	501	SY9	CAR-CAS-NAY	-2.10	108.85	112.86
4	A	502	NAG	C1-O5-C5	2.08	114.98	112.19
3	A	501	SY9	CAR-CAS-NAY	-2.04	108.96	112.86
3	D	501	SY9	CAL-CAI-NAH	2.02	118.78	115.41

There are no chirality outliers.

All (13) torsion outliers are listed below:

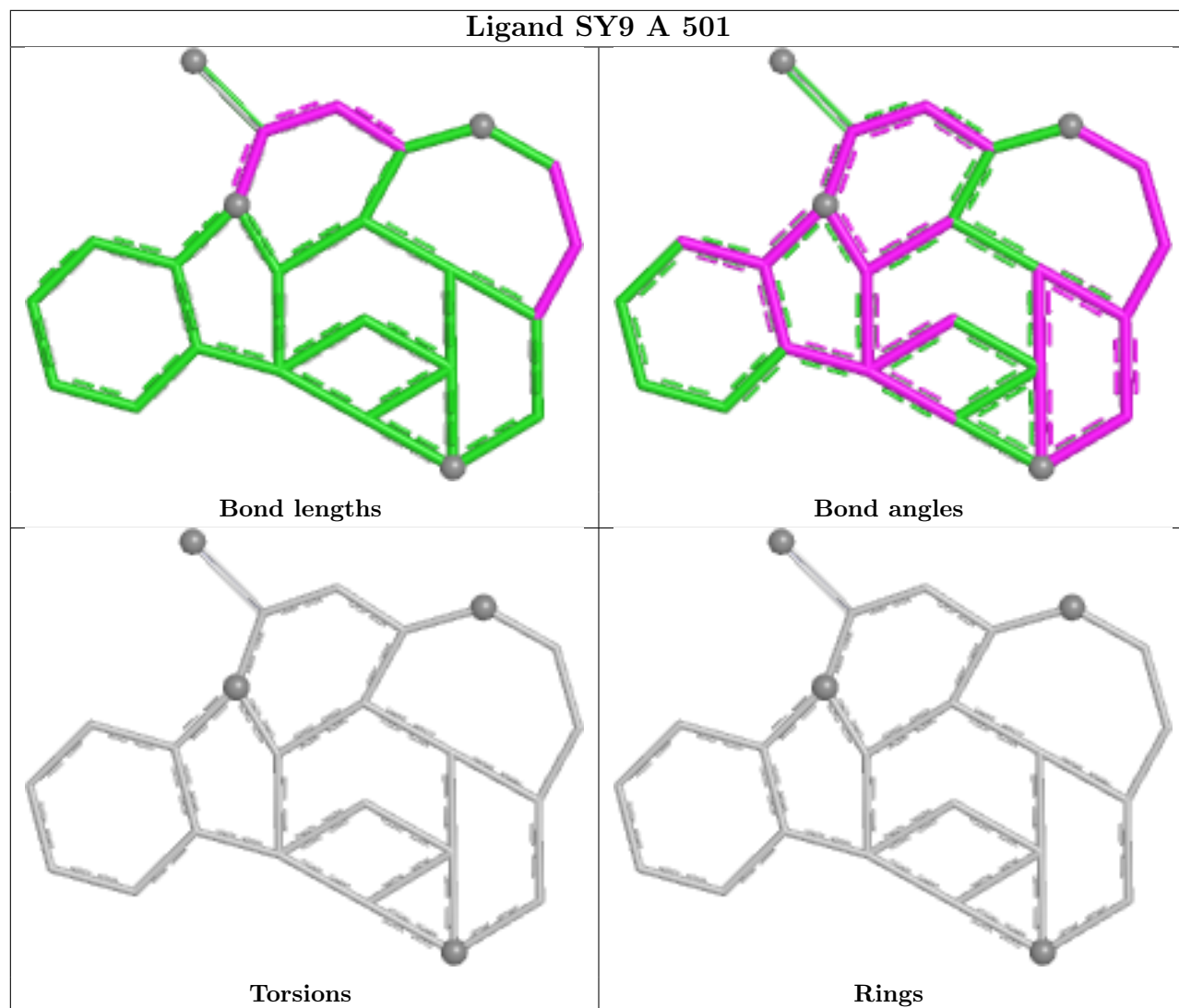
Mol	Chain	Res	Type	Atoms
4	A	502	NAG	O5-C5-C6-O6
4	A	502	NAG	C4-C5-C6-O6
4	A	502	NAG	C8-C7-N2-C2
4	A	502	NAG	O7-C7-N2-C2
4	B	601	NAG	C8-C7-N2-C2
4	B	601	NAG	O7-C7-N2-C2
4	E	601	NAG	C8-C7-N2-C2
4	E	601	NAG	O7-C7-N2-C2
4	A	502	NAG	C3-C2-N2-C7
4	B	601	NAG	C3-C2-N2-C7
4	E	601	NAG	C1-C2-N2-C7
4	E	601	NAG	O5-C5-C6-O6
4	E	601	NAG	C3-C2-N2-C7

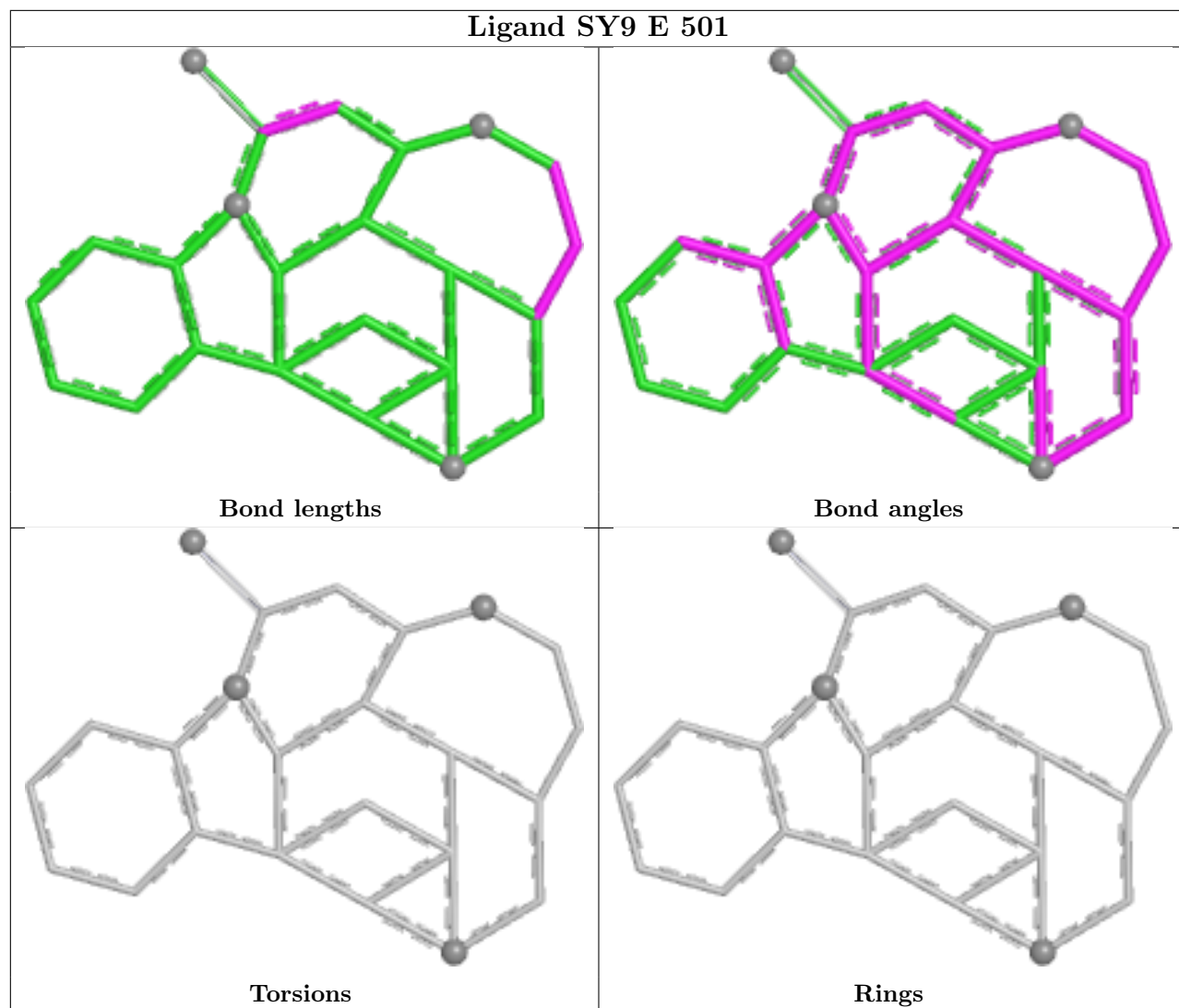
There are no ring outliers.

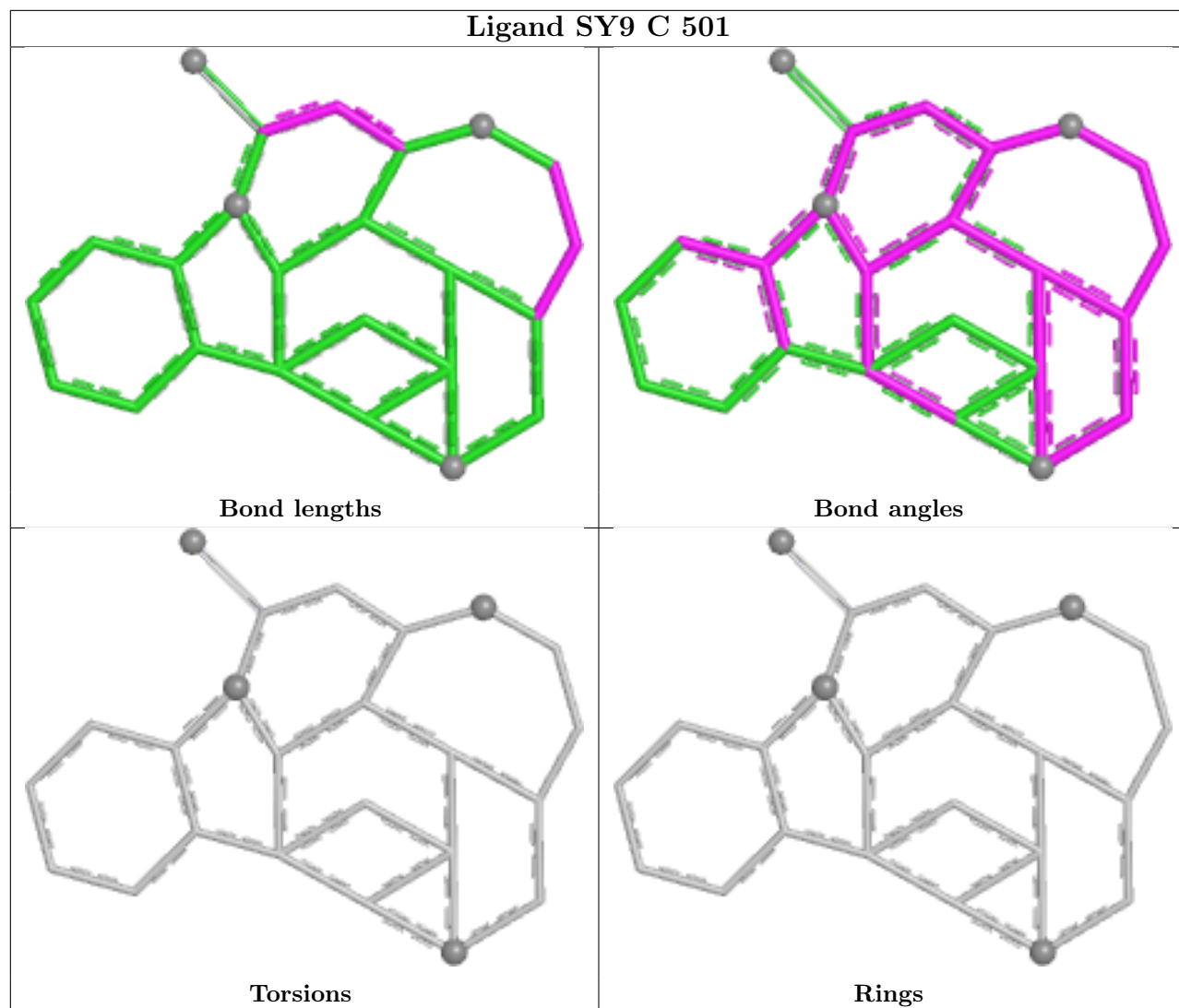
2 monomers are involved in 4 short contacts:

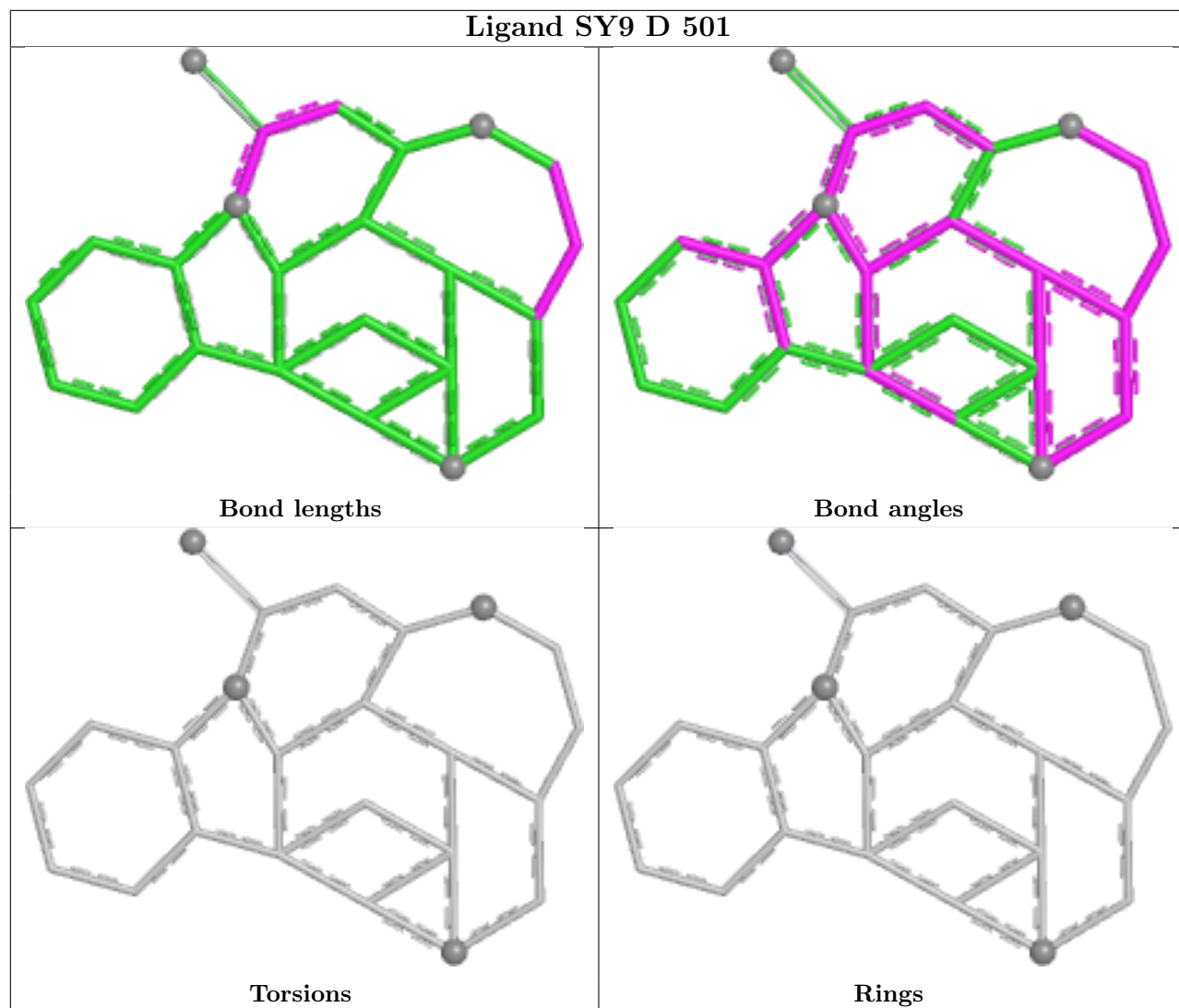
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	601	NAG	2	0
4	A	502	NAG	2	0

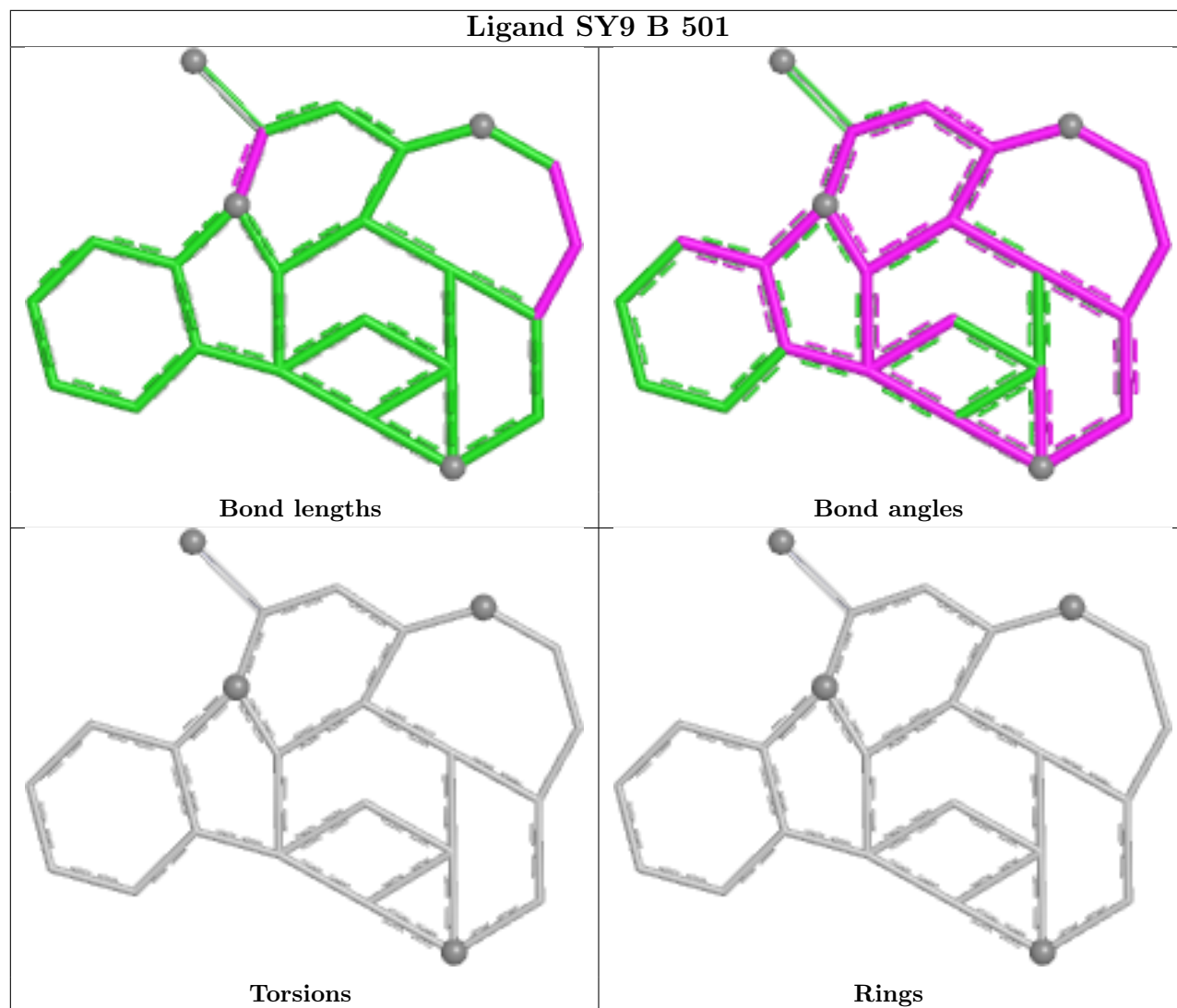
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











## 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 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	339/362 (93%)	0.47	32 (9%) 14 7	65, 126, 174, 207	0
1	B	339/362 (93%)	0.47	32 (9%) 14 7	77, 119, 164, 182	0
1	C	336/362 (92%)	0.70	45 (13%) 7 4	71, 115, 216, 247	0
1	D	331/362 (91%)	0.63	31 (9%) 14 7	36, 116, 199, 233	0
1	E	339/362 (93%)	0.46	28 (8%) 17 9	68, 116, 196, 232	0
All	All	1684/1810 (93%)	0.54	168 (9%) 12 6	36, 119, 190, 247	0

All (168) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	129	SER	8.2
1	D	302	ALA	8.1
1	C	63	PHE	7.5
1	C	324	THR	7.2
1	D	295	PHE	6.8
1	E	115	ASN	6.8
1	C	64	LEU	6.5
1	D	299	LEU	6.3
1	A	249	ALA	6.3
1	A	250	PRO	6.1
1	E	164	ASN	5.9
1	A	199	THR	5.7
1	C	323	ASP	5.6
1	C	128	TYR	5.5
1	C	41	CYS	5.5
1	C	46	ASN	5.3
1	D	303	ALA	5.3
1	B	225	ILE	5.3
1	A	197	TYR	5.1
1	C	248	ALA	5.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	60	VAL	4.9
1	C	130	ILE	4.8
1	E	110	GLU	4.8
1	B	230	PRO	4.8
1	C	246	MET	4.7
1	C	322	ILE	4.7
1	A	295	PHE	4.6
1	B	123	ASN	4.4
1	D	32	PHE	4.2
1	A	284	ASP	4.2
1	C	91	ASP	4.1
1	C	201	HIS	4.1
1	A	198	CYS	4.1
1	E	114	ASP	3.9
1	A	280	VAL	3.9
1	B	217	GLU	3.9
1	B	266	GLN	3.9
1	A	81	ASP	3.9
1	D	250	PRO	3.8
1	C	327	ARG	3.7
1	D	296	SER	3.7
1	C	42	ASN	3.6
1	E	314	VAL	3.6
1	D	188	LEU	3.6
1	D	246	MET	3.6
1	C	188	LEU	3.5
1	C	131	ARG	3.5
1	D	159	PHE	3.5
1	B	203	ASN	3.5
1	C	132	LEU	3.4
1	C	251	ALA	3.4
1	A	164	ASN	3.4
1	C	270	SER	3.4
1	C	217	GLU	3.4
1	D	161	TYR	3.4
1	E	313	LYS	3.3
1	D	149	VAL	3.3
1	A	311	GLY	3.3
1	A	188	LEU	3.3
1	D	217	GLU	3.3
1	A	251	ALA	3.2
1	B	127	LEU	3.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	317	ASP	3.1
1	E	152	CYS	3.1
1	D	245	ASN	3.1
1	B	26	ALA	3.1
1	A	163	MET	3.1
1	C	62	ILE	3.1
1	E	236	ILE	3.1
1	C	66	GLN	3.0
1	D	219	GLN	3.0
1	E	223	TYR	3.0
1	E	234	ILE	3.0
1	B	224	LEU	3.0
1	C	65	ARG	2.9
1	A	114	ASP	2.9
1	B	229	ILE	2.8
1	B	208	THR	2.8
1	E	250	PRO	2.8
1	C	326	SER	2.8
1	C	44	PHE	2.7
1	E	91	ASP	2.7
1	C	266	GLN	2.7
1	A	217	GLU	2.7
1	D	109	HIS	2.7
1	B	9	SER	2.7
1	B	202	TYR	2.7
1	B	46	ASN	2.7
1	E	116	LYS	2.6
1	B	162	THR	2.6
1	E	233	LEU	2.6
1	B	234	ILE	2.6
1	A	335	LEU	2.6
1	B	226	GLN	2.6
1	C	164	ASN	2.5
1	D	277	VAL	2.5
1	C	43	ILE	2.5
1	C	241	SER	2.5
1	E	151	THR	2.5
1	B	61	ASN	2.5
1	C	141	ASP	2.5
1	D	164	ASN	2.5
1	B	295	PHE	2.5
1	D	213	ARG	2.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	298	LEU	2.5
1	D	335	LEU	2.5
1	E	26	ALA	2.5
1	E	10	PRO	2.5
1	B	172	ASP	2.4
1	C	265	THR	2.4
1	E	222	TYR	2.4
1	B	31	ASN	2.4
1	E	295	PHE	2.4
1	A	310	ALA	2.4
1	B	189	LEU	2.4
1	C	233	LEU	2.4
1	E	186	GLN	2.3
1	C	267	SER	2.3
1	D	334	PHE	2.3
1	B	62	ILE	2.3
1	A	219	GLN	2.3
1	C	204	THR	2.3
1	E	129	SER	2.3
1	A	237	LEU	2.3
1	E	53	GLU	2.3
1	B	227	MET	2.3
1	D	61	ASN	2.3
1	C	219	GLN	2.3
1	C	232	LEU	2.2
1	A	246	MET	2.2
1	E	156	LEU	2.2
1	A	260	VAL	2.2
1	E	113	THR	2.1
1	D	28	ILE	2.1
1	B	214	PHE	2.1
1	C	302	ALA	2.1
1	B	270	SER	2.1
1	B	69	ASN	2.1
1	D	31	ASN	2.1
1	B	204	THR	2.1
1	E	246	MET	2.1
1	E	266	GLN	2.1
1	B	35	PRO	2.1
1	D	278	SER	2.1
1	A	107	ASN	2.1
1	A	80	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	134	LEU	2.1
1	C	81	ASP	2.1
1	E	347	ILE	2.1
1	A	128	TYR	2.1
1	A	312	THR	2.1
1	C	252	ARG	2.1
1	C	332	LEU	2.1
1	A	288	ALA	2.1
1	D	251	ALA	2.1
1	D	320	LYS	2.0
1	C	203	ASN	2.0
1	A	247	ASP	2.0
1	D	74	ALA	2.0
1	D	172	ASP	2.0
1	B	250	PRO	2.0
1	C	53	GLU	2.0
1	E	253	VAL	2.0
1	A	28	ILE	2.0
1	A	279	TYR	2.0
1	A	330	PHE	2.0
1	C	313	LYS	2.0
1	D	17	LEU	2.0

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

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

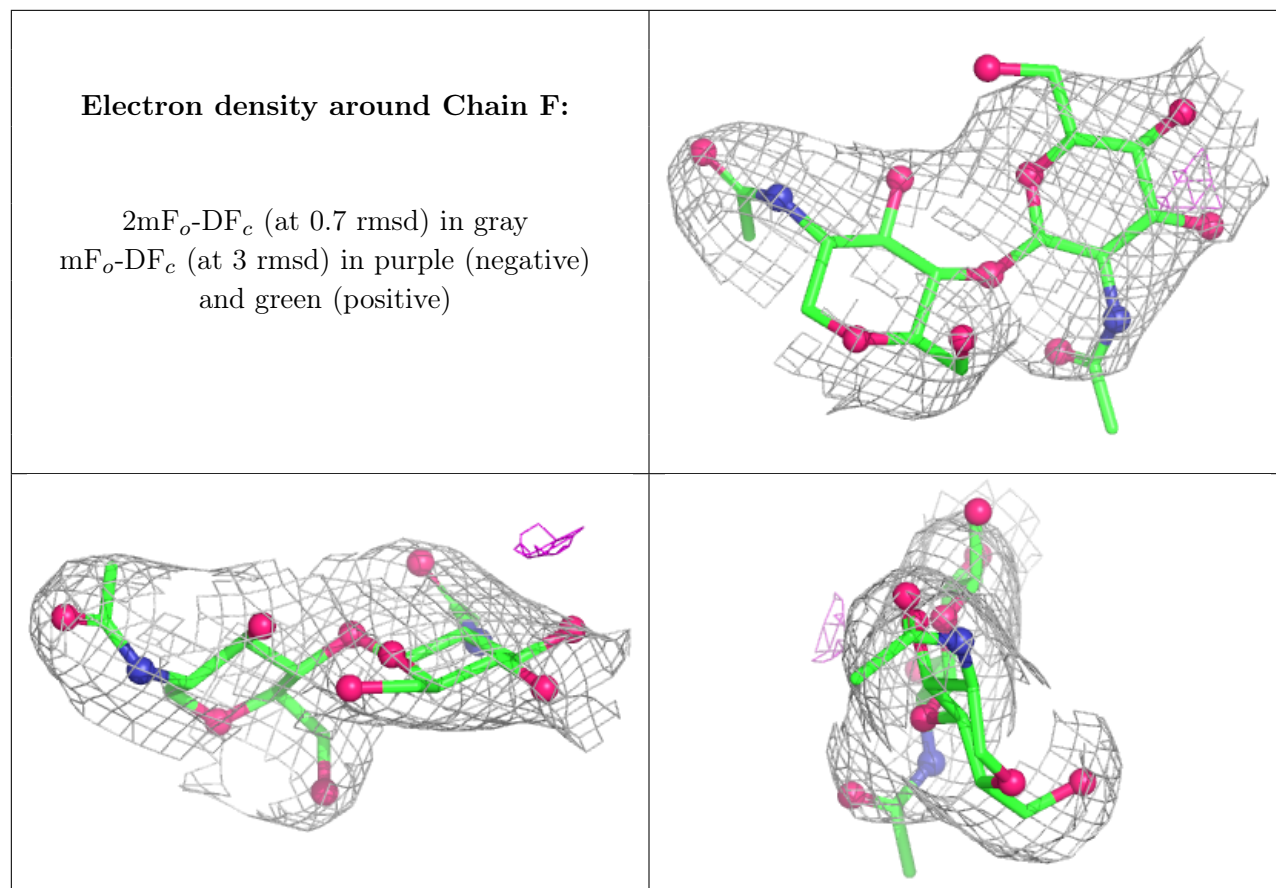
## 6.3 Carbohydrates [\(i\)](#)

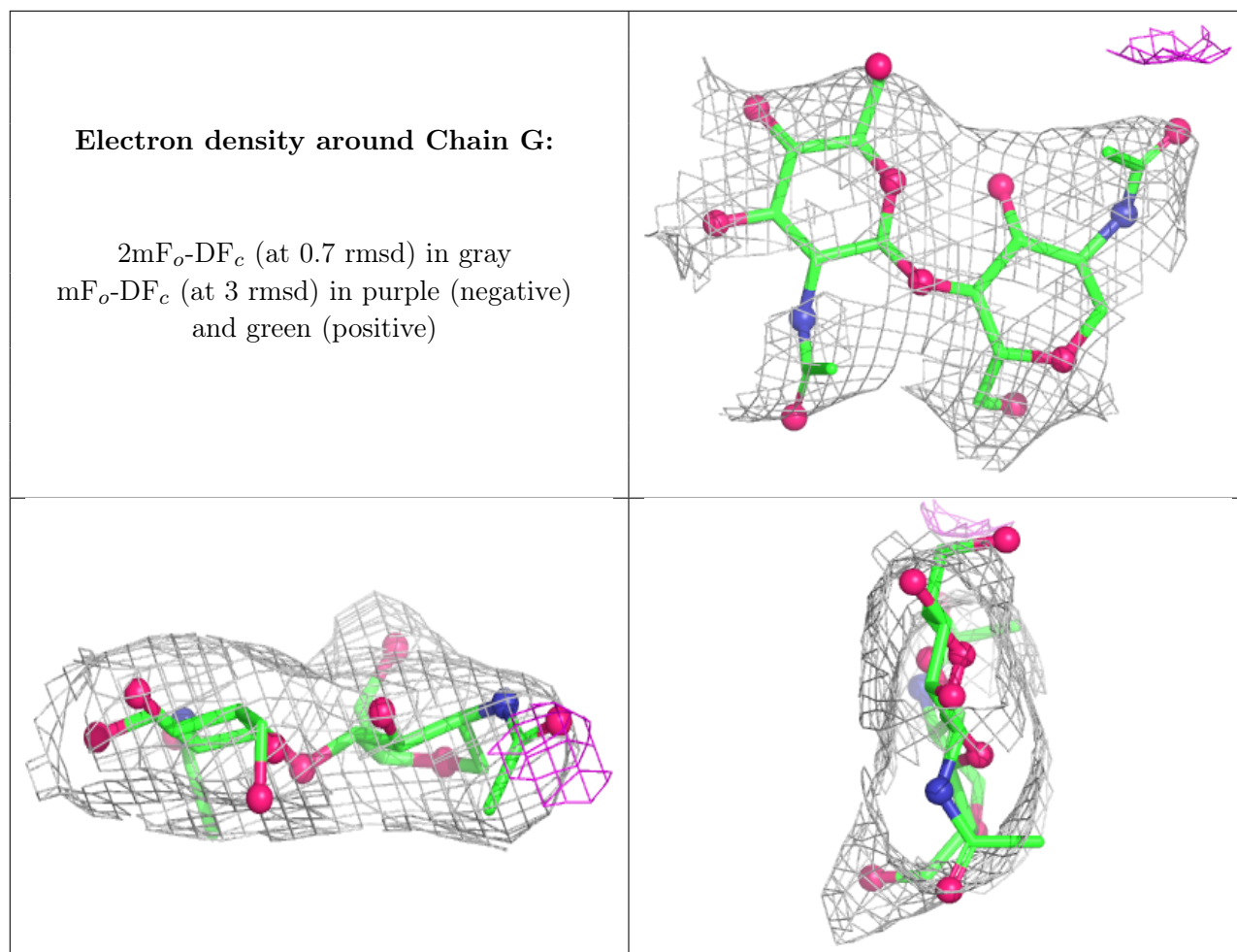
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	NAG	F	2	14/15	0.75	0.12	135,140,143,144	0
2	NAG	G	2	14/15	0.75	0.11	151,159,165,166	0
2	NAG	F	1	14/15	0.84	0.10	114,127,132,136	0
2	NAG	G	1	14/15	0.85	0.10	114,127,133,146	0

The following is a graphical depiction of the model fit to experimental electron density for oligosac-

charide. Each fit is shown from different orientation to approximate a three-dimensional view.





## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

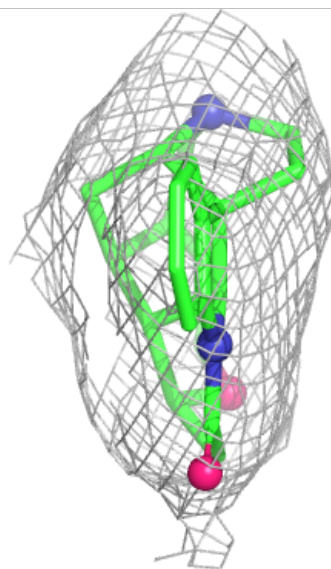
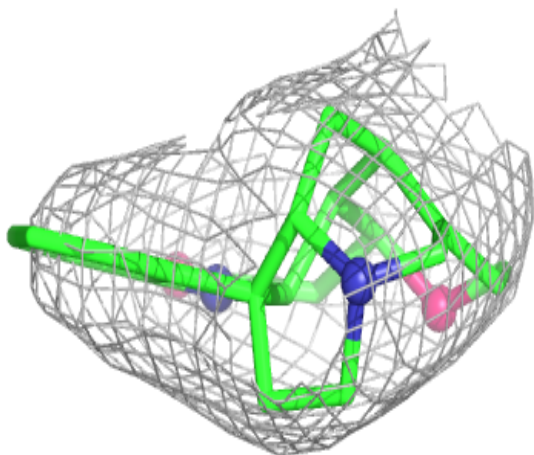
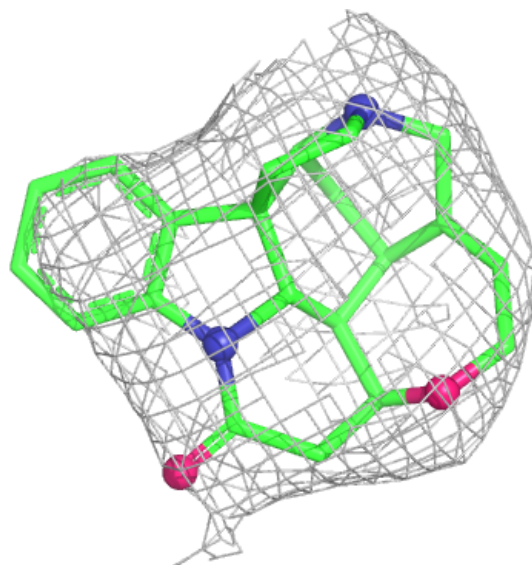
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	NAG	E	601	14/15	0.65	0.15	153,165,179,184	0
4	NAG	B	601	14/15	0.71	0.13	126,143,148,154	0
4	NAG	A	502	14/15	0.75	0.10	123,135,145,146	0
3	SY9	E	501	25/25	0.94	0.14	114,119,125,126	0
3	SY9	B	501	25/25	0.95	0.12	101,105,112,114	0
3	SY9	C	501	25/25	0.95	0.11	95,102,112,122	0
3	SY9	A	501	25/25	0.97	0.10	103,108,114,117	0
3	SY9	D	501	25/25	0.97	0.09	91,103,108,112	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

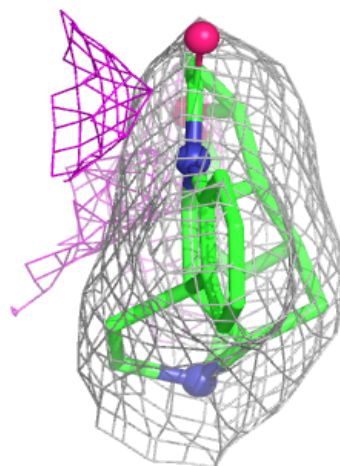
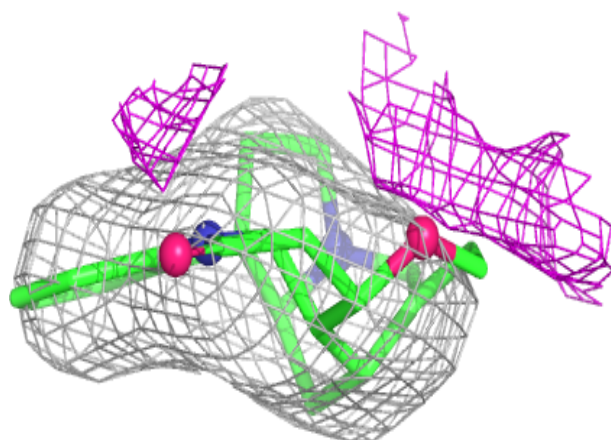
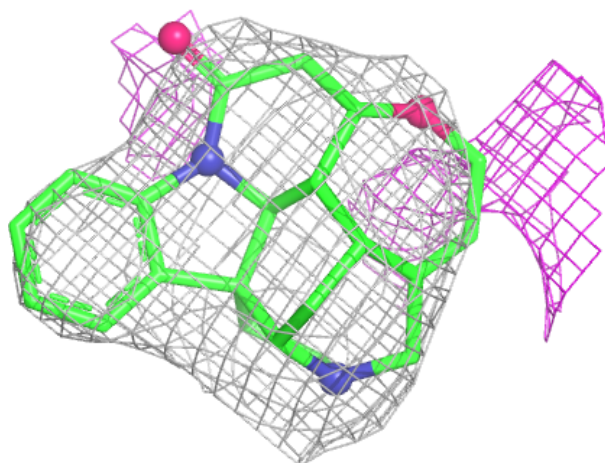
**Electron density around SY9 E 501:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



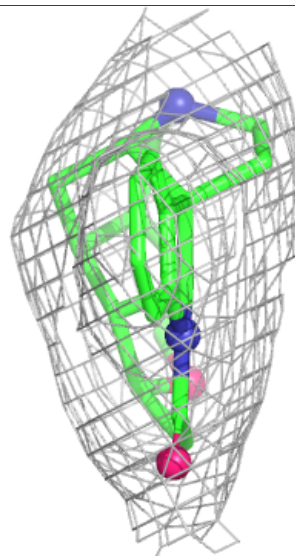
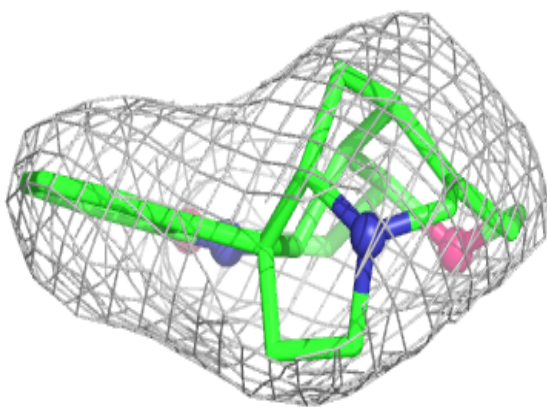
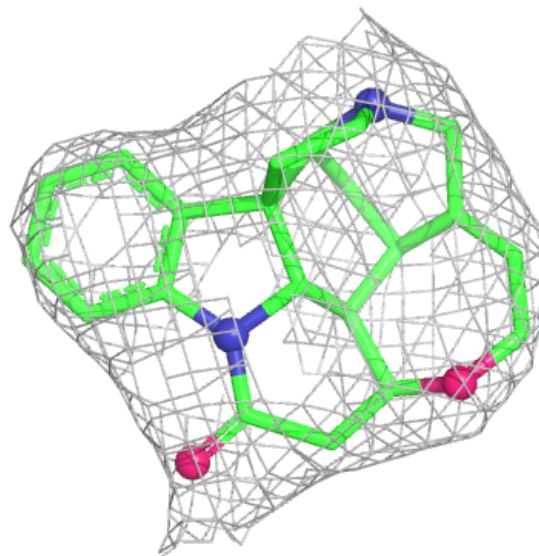
**Electron density around SY9 B 501:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



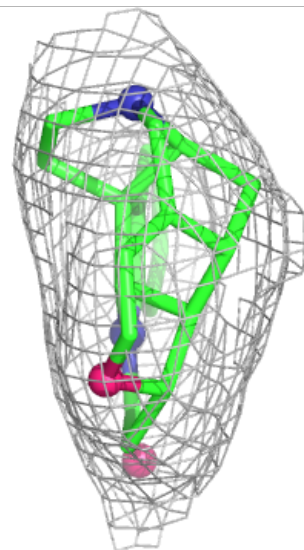
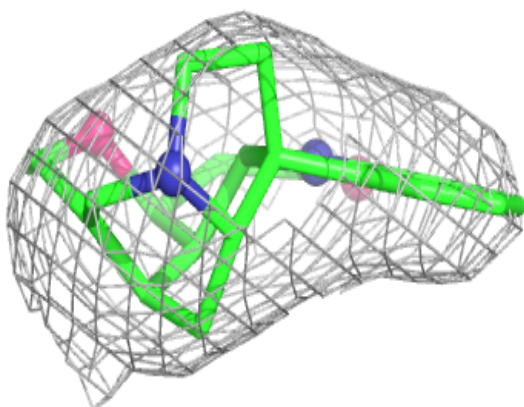
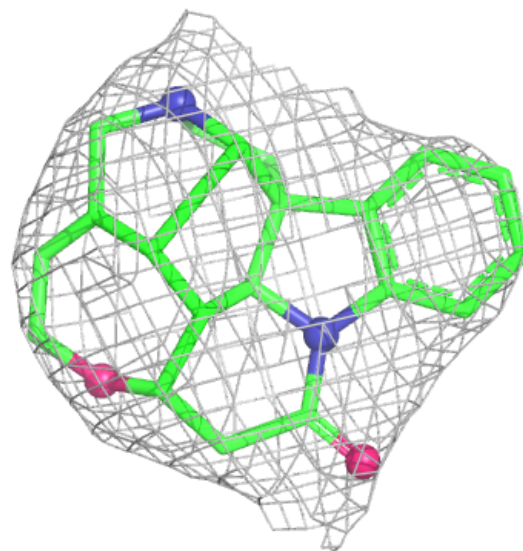
**Electron density around SY9 C 501:**

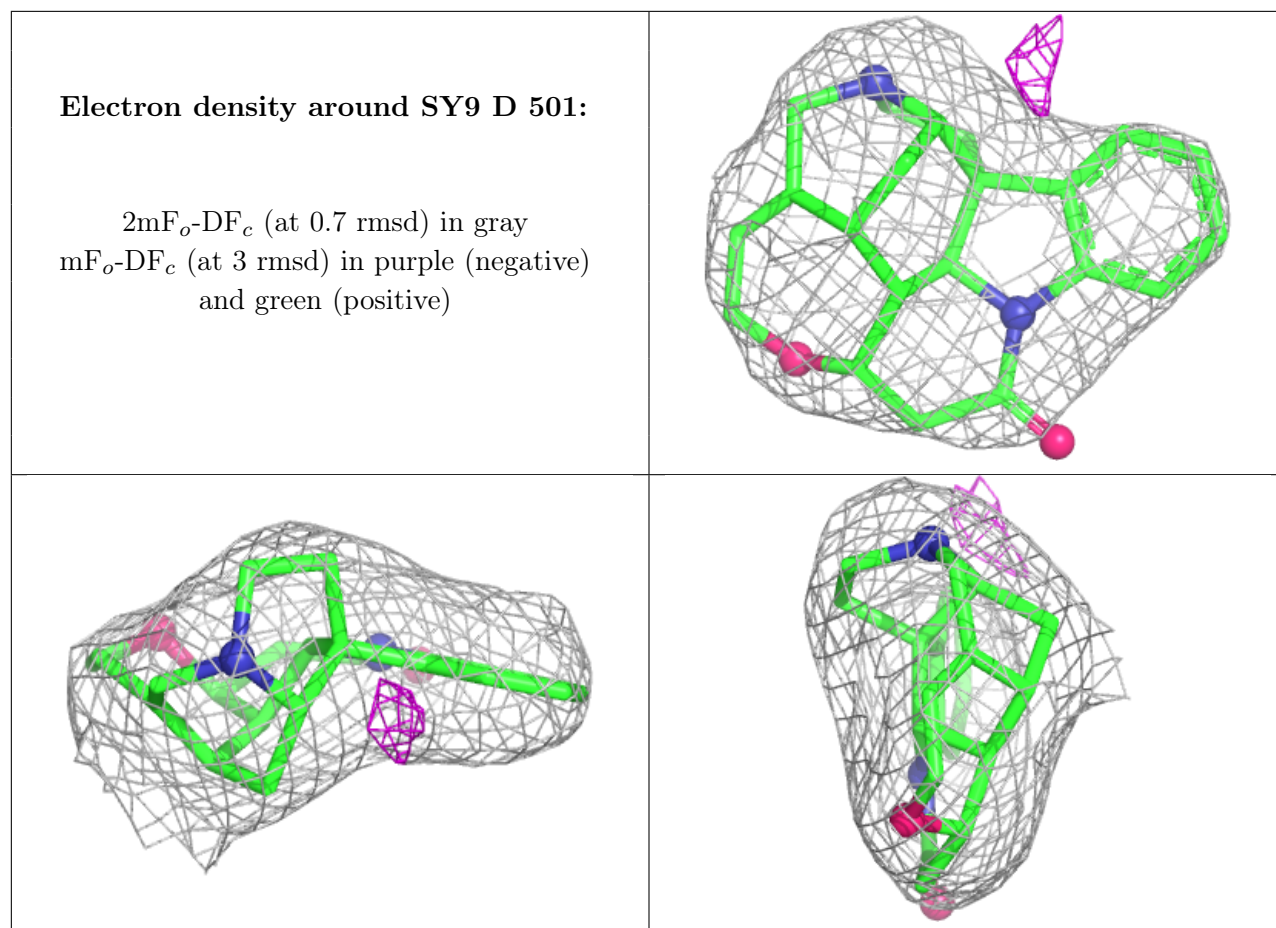
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around SY9 A 501:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.