



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2020 – 06:17 AM BST

PDB ID : 4B7R
Title : H1N1 2009 Pandemic Influenza Virus: Resistance of the I223R Neuraminidase Mutant Explained by Kinetic and Structural Analysis
Authors : Liu, J.; van der Vries, E.; Vachieri, S.G.; Xiong, X.; Collins, P.J.; Walker, P.A.; Haire, L.F.; Hay, A.J.; Schutten, M.; Osterhaus, A.D.M.E.; Martin, S.R.; Boucher, C.A.B.; Skehel, J.J.; Gamblin, S.J.
Deposited on : 2012-08-21
Resolution : 1.90 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

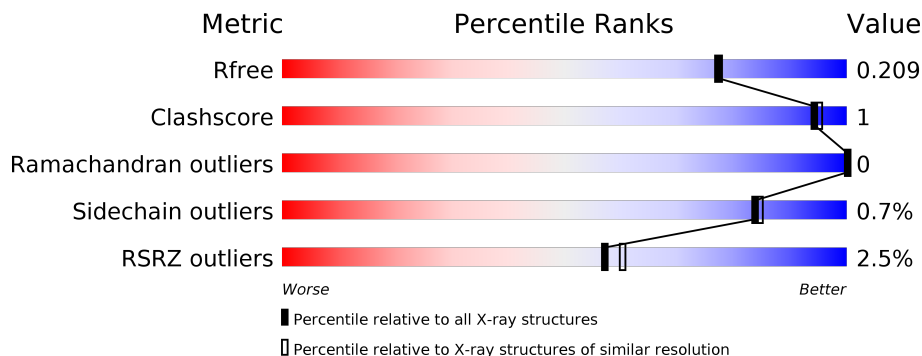
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 on the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	387	<p>3% 96%</p>
1	B	387	<p>3% 97%</p>
1	C	387	<p>% 96%</p>
1	D	387	<p>3% 96%</p>
2	E	2	<p>50% 50%</p>

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
2	NAG	E	2	-	-	-	X
6	NAG	B	1235	-	-	-	X
6	NAG	C	1235	-	-	-	X
6	NAG	C	1386	-	-	-	X
6	NAG	D	1235	-	-	-	X

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 13276 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 NEURAMINIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	387	2994	1880	517	576	21	0	0	0
1	B	387	2994	1880	517	576	21	0	0	0
1	C	387	2994	1880	517	576	21	0	0	0
1	D	387	2994	1880	517	576	21	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	351	PHE	TYR	variant	UNP C7FH46
B	351	PHE	TYR	variant	UNP C7FH46
C	351	PHE	TYR	variant	UNP C7FH46
D	351	PHE	TYR	variant	UNP C7FH46

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

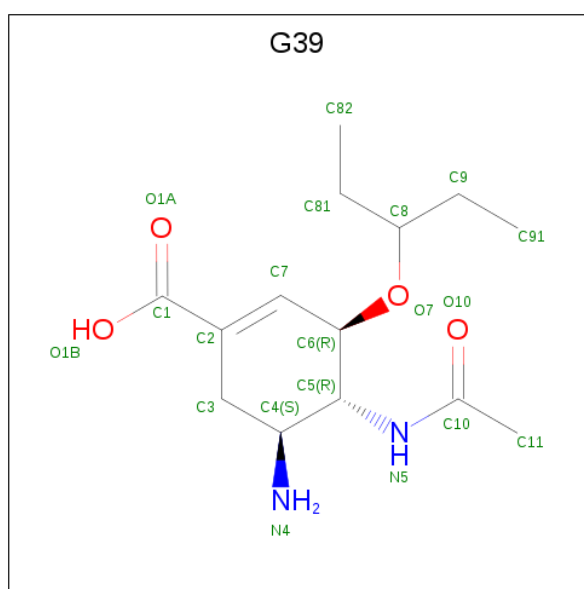


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	E	2	28	16	2	10	0	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

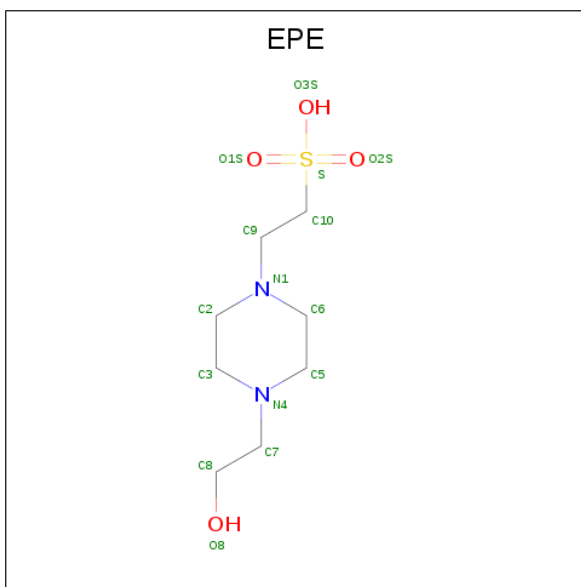
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	2	Total Ca 2 2	0	0
3	A	2	Total Ca 2 2	0	0
3	D	2	Total Ca 2 2	0	0
3	C	2	Total Ca 2 2	0	0

- Molecule 4 is (3R,4R,5S)-4-(acetylamino)-5-amino-3-(pentan-3-yloxy)cyclohex-1-ene-1-carboxylic acid (three-letter code: G39) (formula: C₁₄H₂₄N₂O₄).



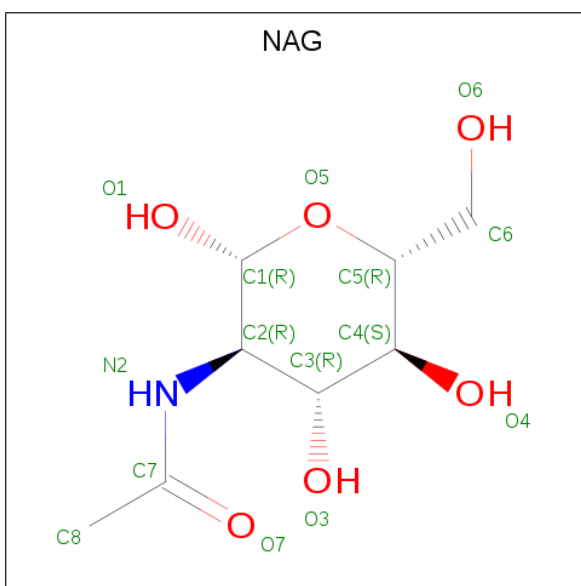
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 20 14 2 4	0	0
4	B	1	Total C N O 20 14 2 4	0	0
4	C	1	Total C N O 20 14 2 4	0	0
4	D	1	Total C N O 20 14 2 4	0	0

- Molecule 5 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C₈H₁₈N₂O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
5	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
5	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
5	C	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
5	D	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

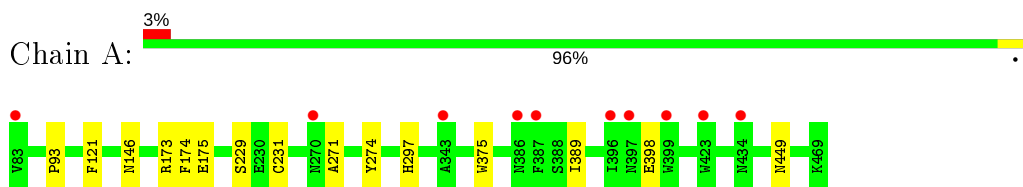
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	225	Total	O	0	0
			225	225		
7	B	252	Total	O	0	0
			252	252		
7	C	265	Total	O	0	0
			265	265		
7	D	214	Total	O	0	0
			214	214		

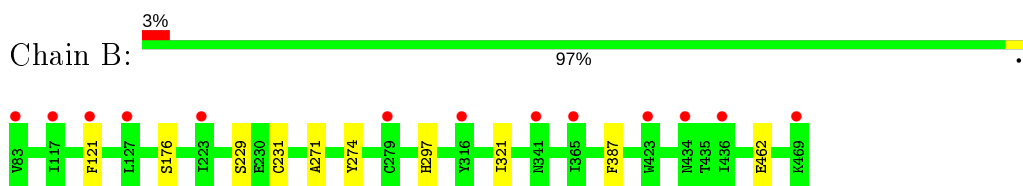
3 Residue-property plots [i](#)

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 electron 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

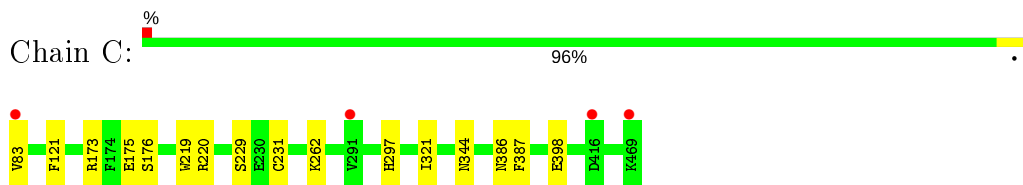
- Molecule 1: NEURAMINIDASE



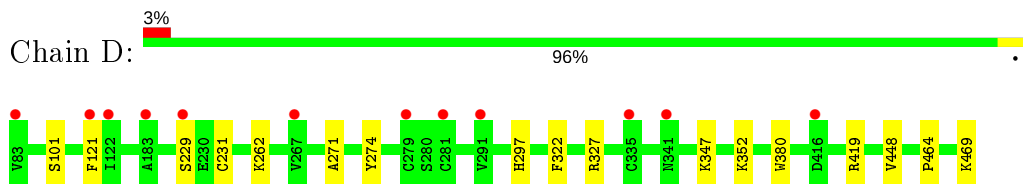
- Molecule 1: NEURAMINIDASE



- Molecule 1: NEURAMINIDASE



- Molecule 1: NEURAMINIDASE



- 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, α , β , γ	82.65Å 148.82Å 166.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.82 – 1.90 29.76 – 1.88	Depositor EDS
% Data completeness (in resolution range)	99.7 (29.82-1.90) 98.4 (29.76-1.88)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.15 (at 1.88Å)	Xtrriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.146 , 0.173 0.187 , 0.209	Depositor DCC
R_{free} test set	8190 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	26.0	Xtrriage
Anisotropy	0.751	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 41.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	13276	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.90% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: G39, CA, EPE, 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	0.35	0/3076	0.53	0/4180
1	B	0.37	0/3076	0.55	0/4180
1	C	0.40	0/3076	0.56	0/4180
1	D	0.38	0/3076	0.55	0/4180
All	All	0.38	0/12304	0.55	0/16720

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	2994	0	2827	8	0
1	B	2994	0	2827	4	0
1	C	2994	0	2827	9	1
1	D	2994	0	2827	9	0
2	E	28	0	25	1	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	20	0	23	0	0
4	B	20	0	23	0	0
4	C	20	0	23	0	0
4	D	20	0	23	0	0
5	A	15	0	17	0	0
5	B	15	0	17	0	0
5	C	15	0	17	0	0
5	D	15	0	17	0	0
6	A	28	0	26	1	0
6	B	42	0	39	1	0
6	C	56	0	52	1	0
6	D	42	0	39	0	0
7	A	225	0	0	1	1
7	B	252	0	0	2	1
7	C	265	0	0	5	0
7	D	214	0	0	0	1
All	All	13276	0	11649	32	2

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 1.

All (32) 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:398:GLU:OE1	7:A:2195:HOH:O	2.11	0.69
1:D:464:PRO:HG2	1:D:469:LYS:HE2	1.76	0.68
1:A:93:PRO:O	1:A:449:ASN:ND2	2.27	0.67
1:C:387:PHE:O	7:C:2219:HOH:O	2.14	0.67
7:C:2239:HOH:O	1:D:262:LYS:NZ	2.29	0.64
7:B:2226:HOH:O	1:C:262:LYS:NZ	2.22	0.61
1:C:83:VAL:N	7:C:2002:HOH:O	2.37	0.56
1:C:398:GLU:OE1	7:C:2227:HOH:O	2.18	0.54
1:A:146:ASN:HD22	2:E:1:NAG:H83	1.77	0.49
1:A:173:ARG:HD2	1:A:175:GLU:OE2	2.13	0.49
1:B:121:PHE:CG	1:B:229:SER:HA	2.47	0.48
1:D:271:ALA:HB1	1:D:274:TYR:HB2	1.95	0.48
1:A:375:TRP:HB3	1:A:389:ILE:HB	1.96	0.47
1:C:173:ARG:HD2	1:C:175:GLU:OE2	2.14	0.47
1:C:121:PHE:CG	1:C:229:SER:HA	2.51	0.45
1:D:352:LYS:HD2	1:D:380:TRP:CE2	2.53	0.44
1:D:121:PHE:CG	1:D:229:SER:HA	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:419:ARG:HH21	1:D:448:VAL:HG12	1.82	0.44
1:C:219:TRP:CD1	1:C:220:ARG:HG2	2.53	0.44
1:B:462:GLU:HG2	7:B:2125:HOH:O	2.18	0.43
1:B:321:ILE:CD1	1:B:387:PHE:HB3	2.49	0.43
1:C:321:ILE:HD11	1:C:387:PHE:HB3	1.99	0.43
6:B:1235:NAG:H2	6:B:1235:NAG:H83	1.91	0.43
1:D:229:SER:HB3	1:D:347:LYS:HE2	2.00	0.43
1:A:271:ALA:HB1	1:A:274:TYR:HB2	2.01	0.43
1:B:271:ALA:HB1	1:B:274:TYR:HB2	2.01	0.43
1:D:322:PHE:HB2	1:D:327:ARG:HD2	2.01	0.42
1:A:121:PHE:CG	1:A:229:SER:HA	2.55	0.41
6:A:1235:NAG:H83	6:A:1235:NAG:H2	1.89	0.41
6:C:1235:NAG:H83	6:C:1235:NAG:H2	1.93	0.41
1:C:344:ASN:HB3	7:C:2194:HOH:O	2.20	0.41
1:A:174:PHE:CZ	1:D:101:SER:HA	2.57	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:2161:HOH:O	7:D:2163:HOH:O[2_555]	1.97	0.23
1:C:386:ASN:ND2	7:A:2123:HOH:O[3_544]	2.15	0.05

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	385/387 (100%)	371 (96%)	14 (4%)	0	100	100
1	B	385/387 (100%)	373 (97%)	12 (3%)	0	100	100
1	C	385/387 (100%)	369 (96%)	16 (4%)	0	100	100
1	D	385/387 (100%)	368 (96%)	17 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1540/1548 (100%)	1481 (96%)	59 (4%)	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 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	334/334 (100%)	332 (99%)	2 (1%)	86	87
1	B	334/334 (100%)	331 (99%)	3 (1%)	78	79
1	C	334/334 (100%)	331 (99%)	3 (1%)	78	79
1	D	334/334 (100%)	332 (99%)	2 (1%)	86	87
All	All	1336/1336 (100%)	1326 (99%)	10 (1%)	84	84

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	231	CYS
1	A	297	HIS
1	B	176	SER
1	B	231	CYS
1	B	297	HIS
1	C	176	SER
1	C	231	CYS
1	C	297	HIS
1	D	231	CYS
1	D	297	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	386	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](#)

2 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	0.47	0	17,19,21	1.35	1 (5%)
2	NAG	E	2	2	14,14,15	0.53	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
2	NAG	E	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1	NAG	C1-O5-C5	4.43	118.20	112.19

There are no chirality outliers.

All (4) torsion outliers are listed below:

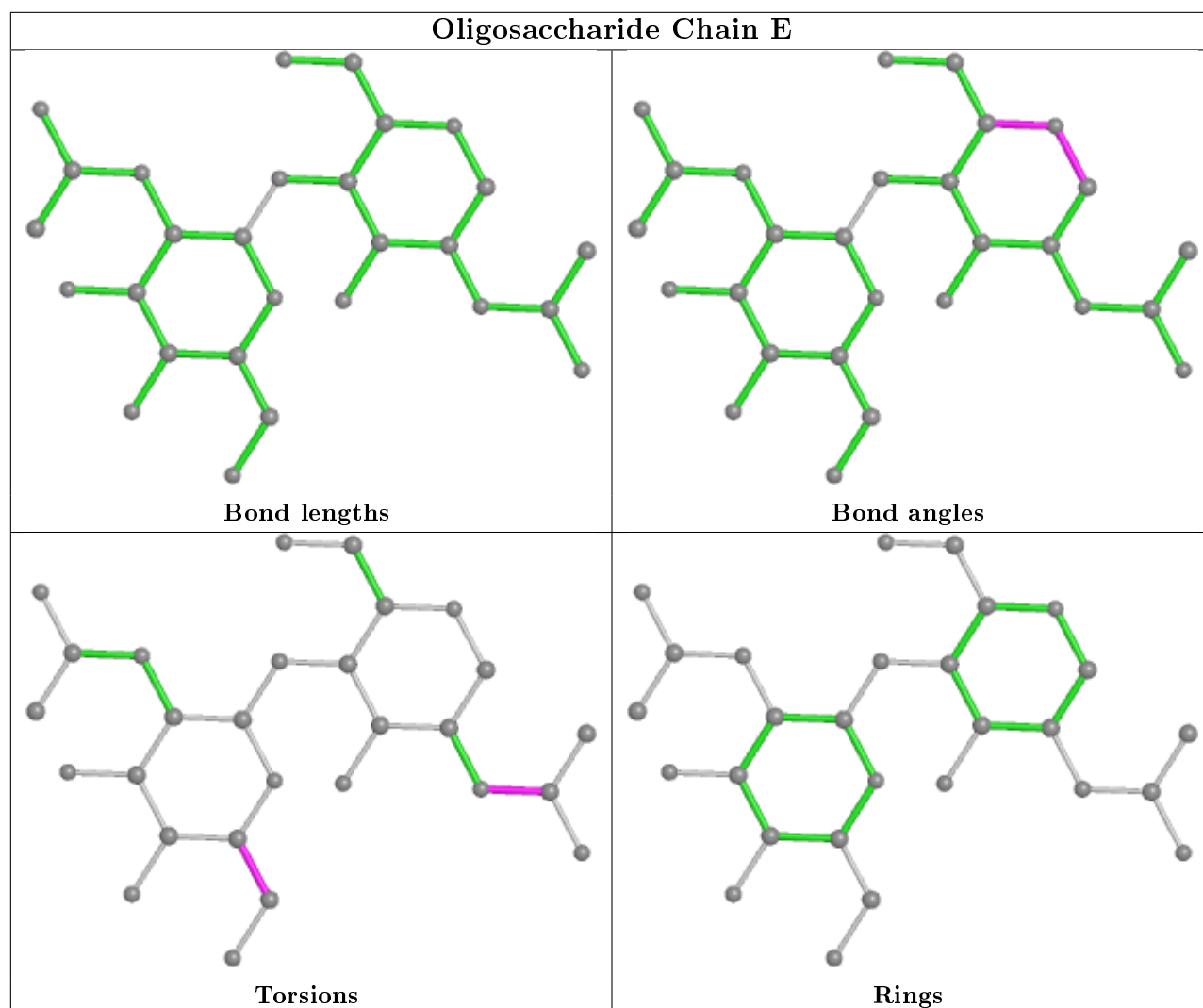
Mol	Chain	Res	Type	Atoms
2	E	1	NAG	C8-C7-N2-C2
2	E	1	NAG	O7-C7-N2-C2
2	E	2	NAG	C4-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
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

Of 28 ligands modelled in this entry, 8 are monoatomic - leaving 20 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	D	1088	1	14,14,15	0.48	0	17,19,21	0.75	0
6	NAG	D	1146	1	14,14,15	0.59	0	17,19,21	0.95	1 (5%)
6	NAG	B	1088	1	14,14,15	0.49	0	17,19,21	1.17	1 (5%)
5	EPE	C	901	-	15,15,15	0.85	1 (6%)	18,20,20	1.69	5 (27%)
6	NAG	C	1146	1	14,14,15	0.51	0	17,19,21	0.93	1 (5%)
6	NAG	C	1088	1	14,14,15	0.50	0	17,19,21	0.73	0
6	NAG	C	1386	-	14,14,15	0.45	0	17,19,21	1.18	2 (11%)
6	NAG	A	1235	1	14,14,15	0.44	0	17,19,21	0.95	1 (5%)
4	G39	C	801	-	17,20,20	2.95	4 (23%)	15,27,27	2.44	2 (13%)
4	G39	A	801	-	17,20,20	3.07	4 (23%)	15,27,27	2.44	3 (20%)
6	NAG	C	1235	1	14,14,15	0.47	0	17,19,21	0.90	1 (5%)
5	EPE	B	901	-	15,15,15	0.94	1 (6%)	18,20,20	1.82	5 (27%)
6	NAG	B	1235	1	14,14,15	0.44	0	17,19,21	1.56	3 (17%)
5	EPE	A	901	-	15,15,15	0.85	1 (6%)	18,20,20	1.66	5 (27%)
4	G39	D	801	-	17,20,20	2.93	4 (23%)	15,27,27	2.49	1 (6%)
6	NAG	B	1146	1	14,14,15	0.58	0	17,19,21	0.77	0
4	G39	B	801	-	17,20,20	3.06	4 (23%)	15,27,27	2.43	2 (13%)
6	NAG	D	1235	1	14,14,15	0.58	0	17,19,21	1.10	1 (5%)
5	EPE	D	901	-	15,15,15	0.85	1 (6%)	18,20,20	1.67	5 (27%)
6	NAG	A	1088	1	14,14,15	0.47	0	17,19,21	0.76	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
6	NAG	D	1088	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	D	1146	1	-	0/6/23/26	0/1/1/1
6	NAG	B	1088	1	-	3/6/23/26	0/1/1/1
5	EPE	C	901	-	-	1/9/19/19	0/1/1/1
6	NAG	C	1146	1	-	0/6/23/26	0/1/1/1
6	NAG	C	1088	1	-	2/6/23/26	0/1/1/1
6	NAG	C	1386	-	-	2/6/23/26	0/1/1/1
6	NAG	A	1235	1	-	2/6/23/26	0/1/1/1
4	G39	C	801	-	-	1/12/32/32	0/1/1/1
4	G39	A	801	-	-	1/12/32/32	0/1/1/1
6	NAG	C	1235	1	-	2/6/23/26	0/1/1/1
5	EPE	B	901	-	-	1/9/19/19	0/1/1/1
6	NAG	B	1235	1	-	3/6/23/26	0/1/1/1
5	EPE	A	901	-	-	1/9/19/19	0/1/1/1
4	G39	D	801	-	-	1/12/32/32	0/1/1/1
6	NAG	B	1146	1	-	0/6/23/26	0/1/1/1
4	G39	B	801	-	-	1/12/32/32	0/1/1/1
6	NAG	D	1235	1	-	0/6/23/26	0/1/1/1
5	EPE	D	901	-	-	1/9/19/19	0/1/1/1
6	NAG	A	1088	1	-	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)
4	A	801	G39	C7-C2	11.44	1.50	1.34
4	B	801	G39	C7-C2	11.32	1.50	1.34
4	C	801	G39	C7-C2	10.94	1.49	1.34
4	D	801	G39	C7-C2	10.86	1.49	1.34
5	B	901	EPE	C10-S	3.17	1.82	1.77
4	A	801	G39	C10-N5	3.02	1.44	1.34
4	B	801	G39	O7-C8	-2.97	1.40	1.44
5	A	901	EPE	C10-S	2.89	1.81	1.77
5	D	901	EPE	C10-S	2.87	1.81	1.77
5	C	901	EPE	C10-S	2.83	1.81	1.77
4	B	801	G39	C10-N5	2.75	1.43	1.34
4	D	801	G39	C10-N5	2.75	1.43	1.34
4	C	801	G39	C10-N5	2.73	1.43	1.34
4	A	801	G39	O7-C8	-2.67	1.41	1.44
4	D	801	G39	O7-C8	-2.60	1.41	1.44
4	C	801	G39	O7-C8	-2.57	1.41	1.44
4	A	801	G39	C6-C7	2.17	1.53	1.50
4	B	801	G39	O7-C6	-2.16	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	801	G39	C6-C7	2.13	1.53	1.50
4	D	801	G39	O7-C6	-2.09	1.39	1.44

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	801	G39	C6-C7-C2	-9.11	107.89	122.57
4	B	801	G39	C6-C7-C2	-8.67	108.60	122.57
4	C	801	G39	C6-C7-C2	-8.46	108.93	122.57
4	A	801	G39	C6-C7-C2	-8.28	109.22	122.57
6	B	1235	NAG	C1-O5-C5	4.62	118.45	112.19
5	B	901	EPE	C5-N4-C3	4.11	118.08	108.83
5	D	901	EPE	C5-N4-C3	4.02	117.88	108.83
5	A	901	EPE	C5-N4-C3	3.82	117.43	108.83
5	C	901	EPE	C5-N4-C3	3.51	116.72	108.83
5	A	901	EPE	C7-N4-C5	3.36	119.84	111.23
6	B	1088	NAG	C1-O5-C5	3.33	116.71	112.19
5	C	901	EPE	C7-N4-C5	3.30	119.68	111.23
5	D	901	EPE	C7-N4-C5	3.22	119.46	111.23
5	B	901	EPE	C7-N4-C5	3.14	119.27	111.23
6	D	1146	NAG	C1-O5-C5	2.96	116.20	112.19
5	C	901	EPE	O1S-S-C10	2.91	110.41	106.92
5	B	901	EPE	C7-N4-C3	2.58	117.84	111.23
5	B	901	EPE	O1S-S-C10	2.58	110.02	106.92
6	A	1235	NAG	C1-O5-C5	2.58	115.68	112.19
4	C	801	G39	C4-C3-C2	-2.54	106.74	109.75
4	A	801	G39	C4-C3-C2	-2.53	106.75	109.75
6	C	1235	NAG	C1-O5-C5	2.49	115.56	112.19
6	D	1235	NAG	O5-C5-C6	2.38	110.93	107.20
5	A	901	EPE	O1S-S-C10	2.36	109.76	106.92
6	B	1235	NAG	O5-C5-C6	2.35	110.89	107.20
6	C	1386	NAG	C1-O5-C5	2.32	115.34	112.19
5	A	901	EPE	C7-N4-C3	2.32	117.17	111.23
5	D	901	EPE	C7-N4-C3	2.30	117.11	111.23
5	D	901	EPE	O2S-S-C10	2.29	109.67	106.92
6	B	1235	NAG	C3-C4-C5	2.24	114.24	110.24
4	A	801	G39	C3-C2-C7	-2.16	115.72	119.87
6	C	1386	NAG	O5-C1-C2	-2.12	107.94	111.29
6	C	1146	NAG	O5-C5-C6	2.12	110.52	107.20
5	D	901	EPE	O3S-S-C10	2.11	109.17	105.77
5	C	901	EPE	O3S-S-C10	2.09	109.16	105.77
5	C	901	EPE	C7-N4-C3	2.09	116.57	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	801	G39	C3-C2-C7	-2.05	115.92	119.87
5	B	901	EPE	O3S-S-C10	2.02	109.03	105.77
5	A	901	EPE	O3S-S-C10	2.00	109.00	105.77

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	901	EPE	C8-C7-N4-C5
5	C	901	EPE	C8-C7-N4-C5
6	C	1386	NAG	C8-C7-N2-C2
6	C	1386	NAG	O7-C7-N2-C2
6	C	1235	NAG	C8-C7-N2-C2
6	C	1235	NAG	O7-C7-N2-C2
6	B	1235	NAG	C8-C7-N2-C2
6	B	1235	NAG	O7-C7-N2-C2
5	A	901	EPE	C8-C7-N4-C5
6	B	1088	NAG	C1-C2-N2-C7
6	B	1088	NAG	C8-C7-N2-C2
6	B	1088	NAG	O7-C7-N2-C2
6	A	1235	NAG	C8-C7-N2-C2
6	A	1235	NAG	O7-C7-N2-C2
5	D	901	EPE	C8-C7-N4-C5
6	D	1088	NAG	C8-C7-N2-C2
6	D	1088	NAG	O7-C7-N2-C2
6	C	1088	NAG	C8-C7-N2-C2
6	C	1088	NAG	O7-C7-N2-C2
6	A	1088	NAG	C8-C7-N2-C2
6	A	1088	NAG	O7-C7-N2-C2
4	B	801	G39	C81-C8-O7-C6
4	D	801	G39	C81-C8-O7-C6
4	C	801	G39	C81-C8-O7-C6
4	A	801	G39	C81-C8-O7-C6
6	B	1235	NAG	O5-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 3 short contacts:

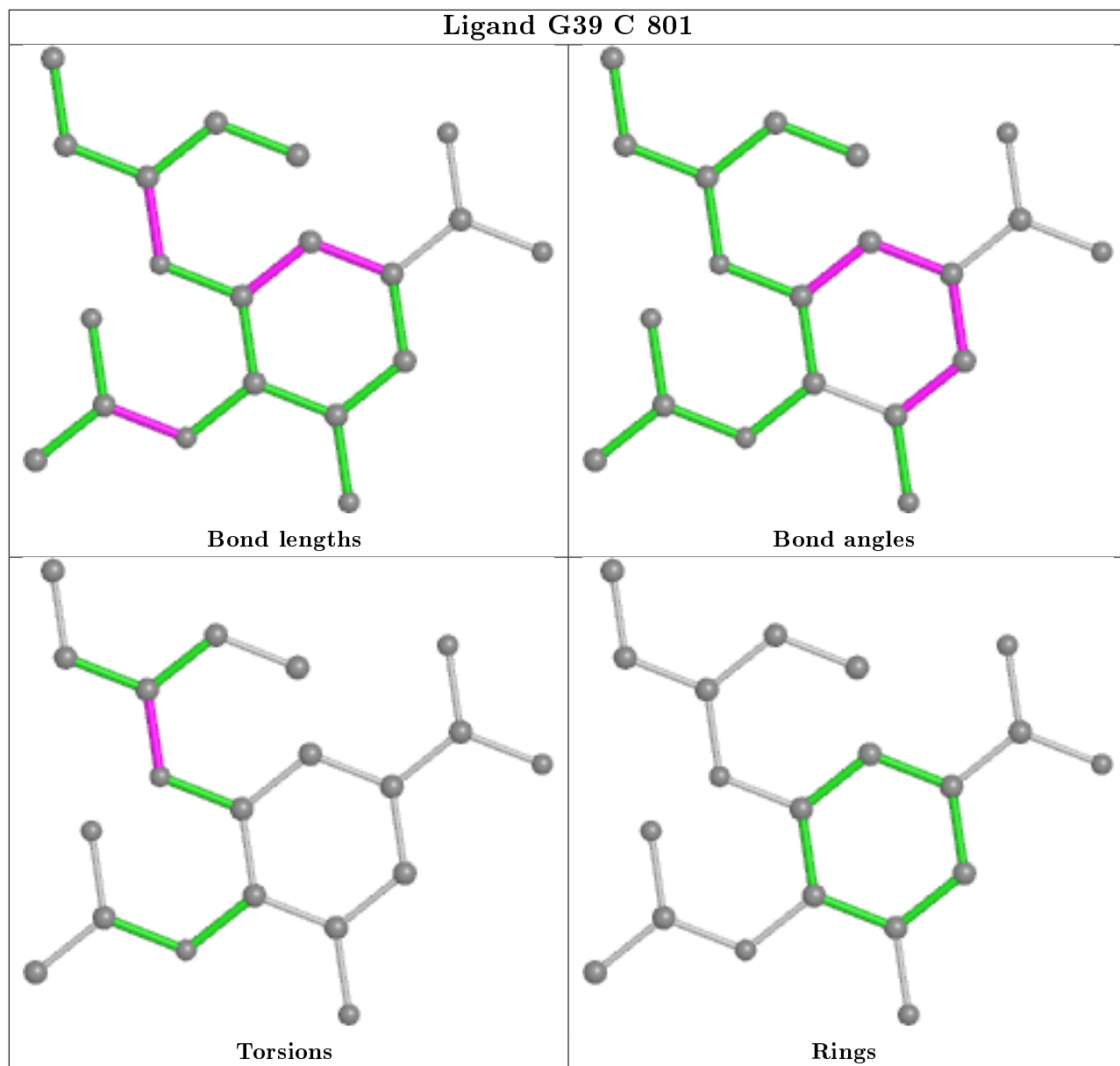
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1235	NAG	1	0
6	C	1235	NAG	1	0

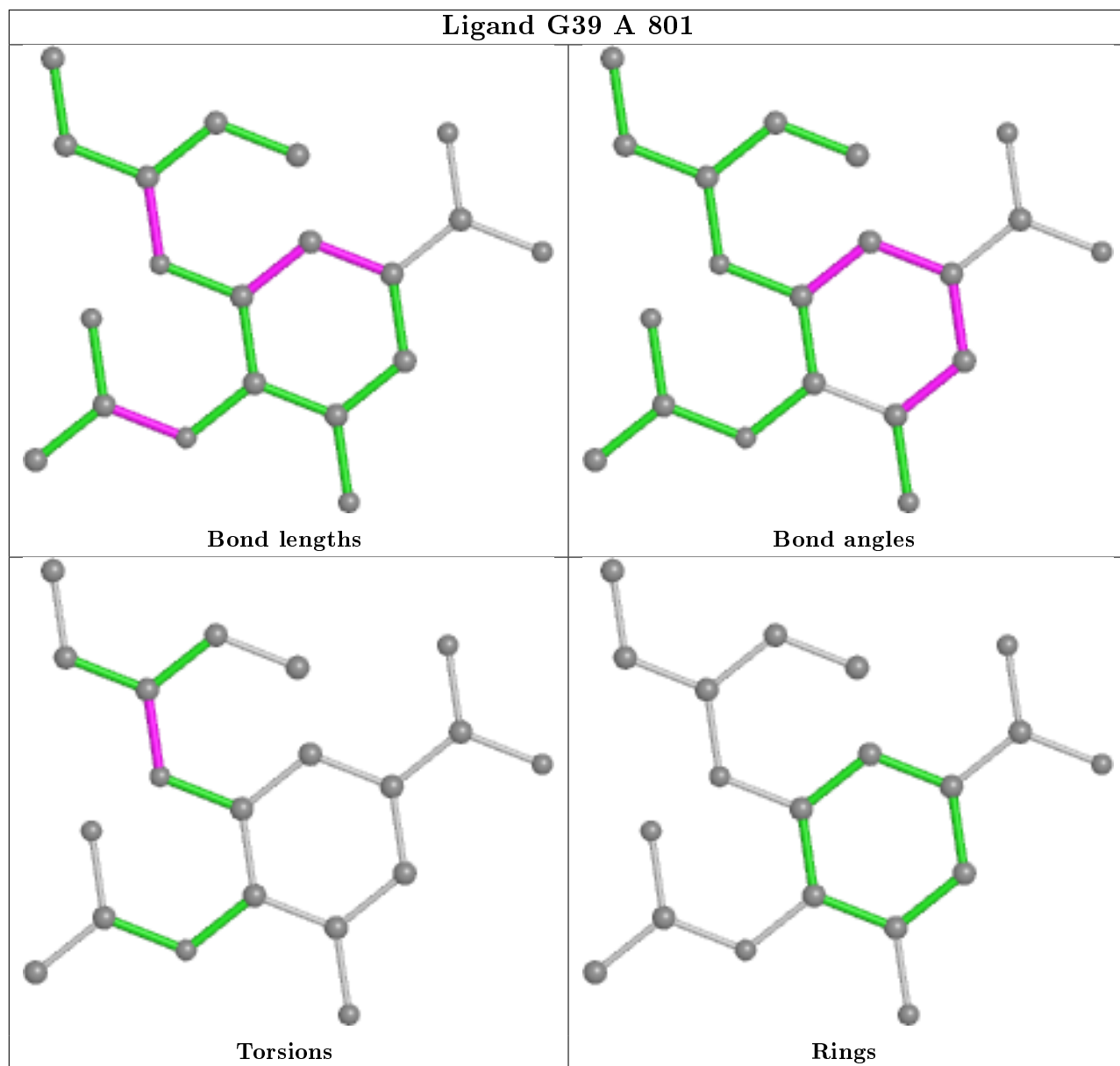
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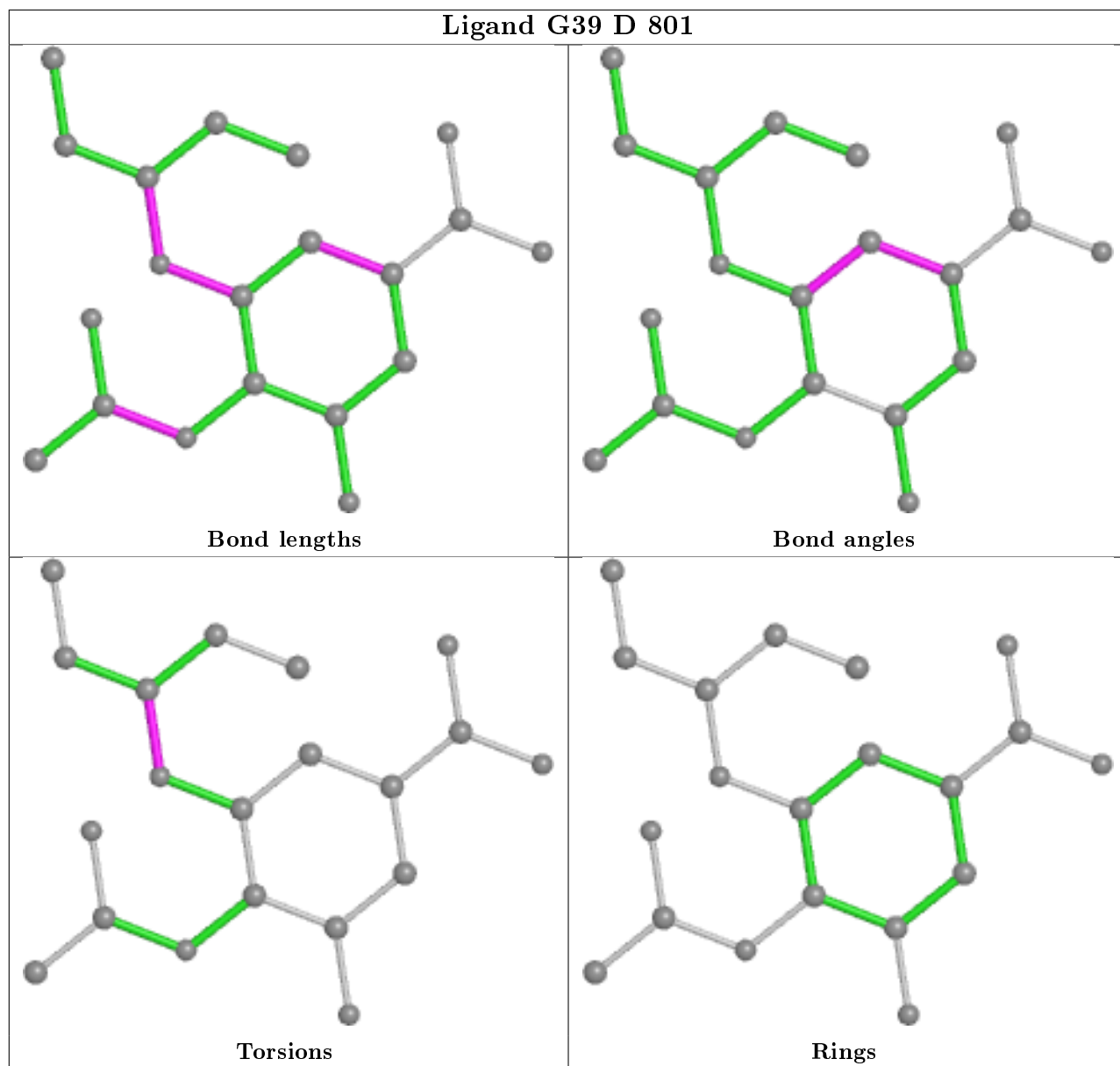
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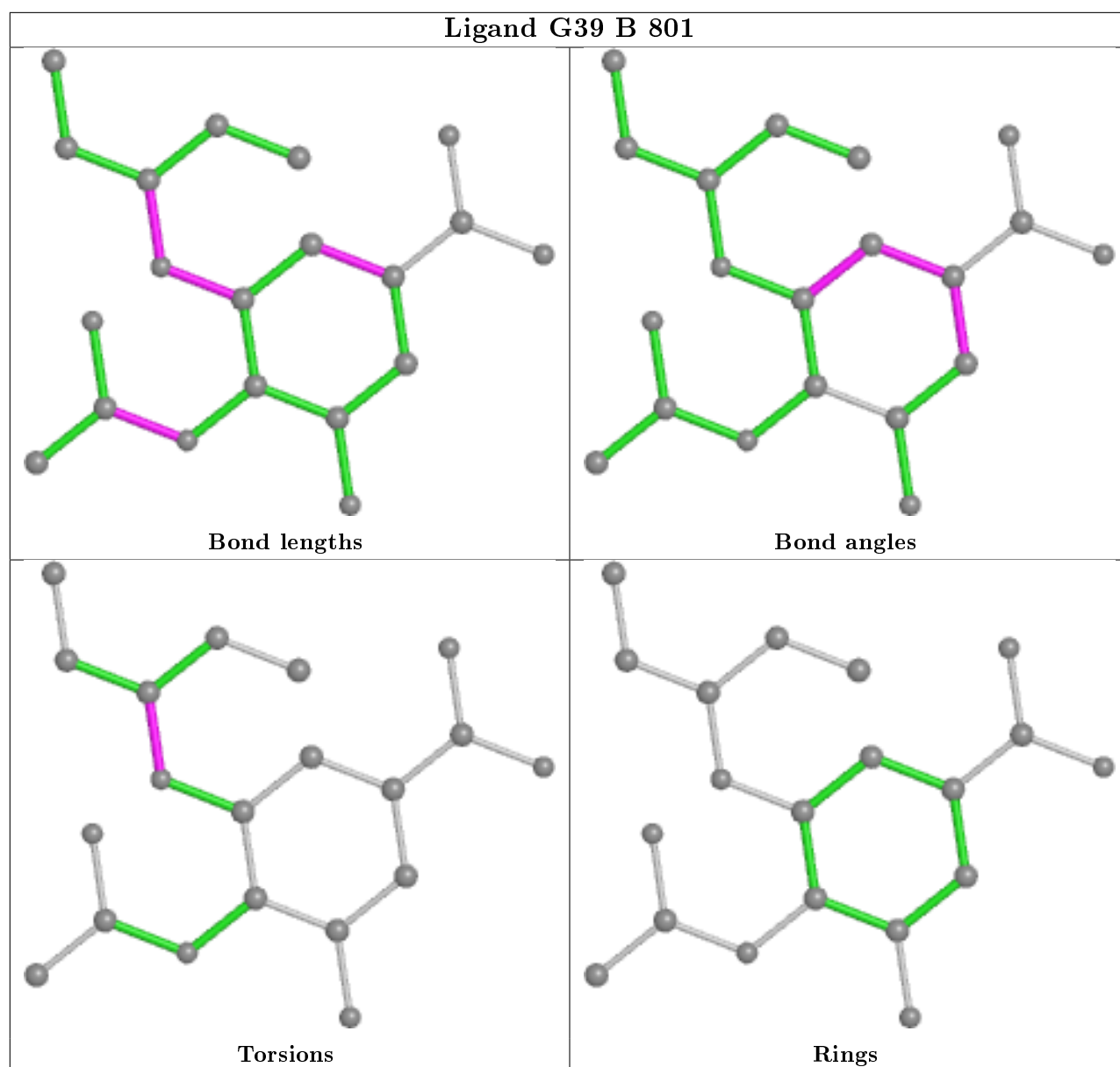
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	1235	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for 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, 95th 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 ²)	Q<0.9
1	A	387/387 (100%)	0.43	10 (2%) 56 58	20, 30, 47, 61	0
1	B	387/387 (100%)	0.61	13 (3%) 45 48	19, 26, 38, 56	0
1	C	387/387 (100%)	0.01	4 (1%) 82 84	19, 25, 39, 56	0
1	D	387/387 (100%)	0.17	12 (3%) 49 51	19, 27, 42, 57	0
All	All	1548/1548 (100%)	0.31	39 (2%) 57 60	19, 27, 42, 61	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	434	ASN	3.4
1	A	387	PHE	3.4
1	D	416	ASP	3.4
1	B	83	VAL	3.1
1	A	397	ASN	3.0
1	D	335	CYS	2.8
1	B	117	ILE	2.7
1	C	83	VAL	2.7
1	D	121	PHE	2.7
1	B	434	ASN	2.6
1	D	83	VAL	2.6
1	C	416	ASP	2.6
1	B	436	ILE	2.6
1	D	291	VAL	2.6
1	A	83	VAL	2.5
1	B	469	LYS	2.5
1	A	396	ILE	2.4
1	B	279	CYS	2.4
1	C	469	LYS	2.3
1	D	341	ASN	2.3
1	A	399	TRP	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	122	ILE	2.3
1	D	279	CYS	2.3
1	D	281	CYS	2.3
1	A	423	TRP	2.3
1	D	267	VAL	2.3
1	B	316	TYR	2.2
1	A	343	ALA	2.2
1	B	127	LEU	2.2
1	B	365	ILE	2.1
1	C	291	VAL	2.1
1	B	121	PHE	2.1
1	B	341	ASN	2.1
1	D	183	ALA	2.1
1	B	423	TRP	2.0
1	B	223	ILE	2.0
1	A	270	ASN	2.0
1	A	386	ASN	2.0
1	D	229	SER	2.0

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

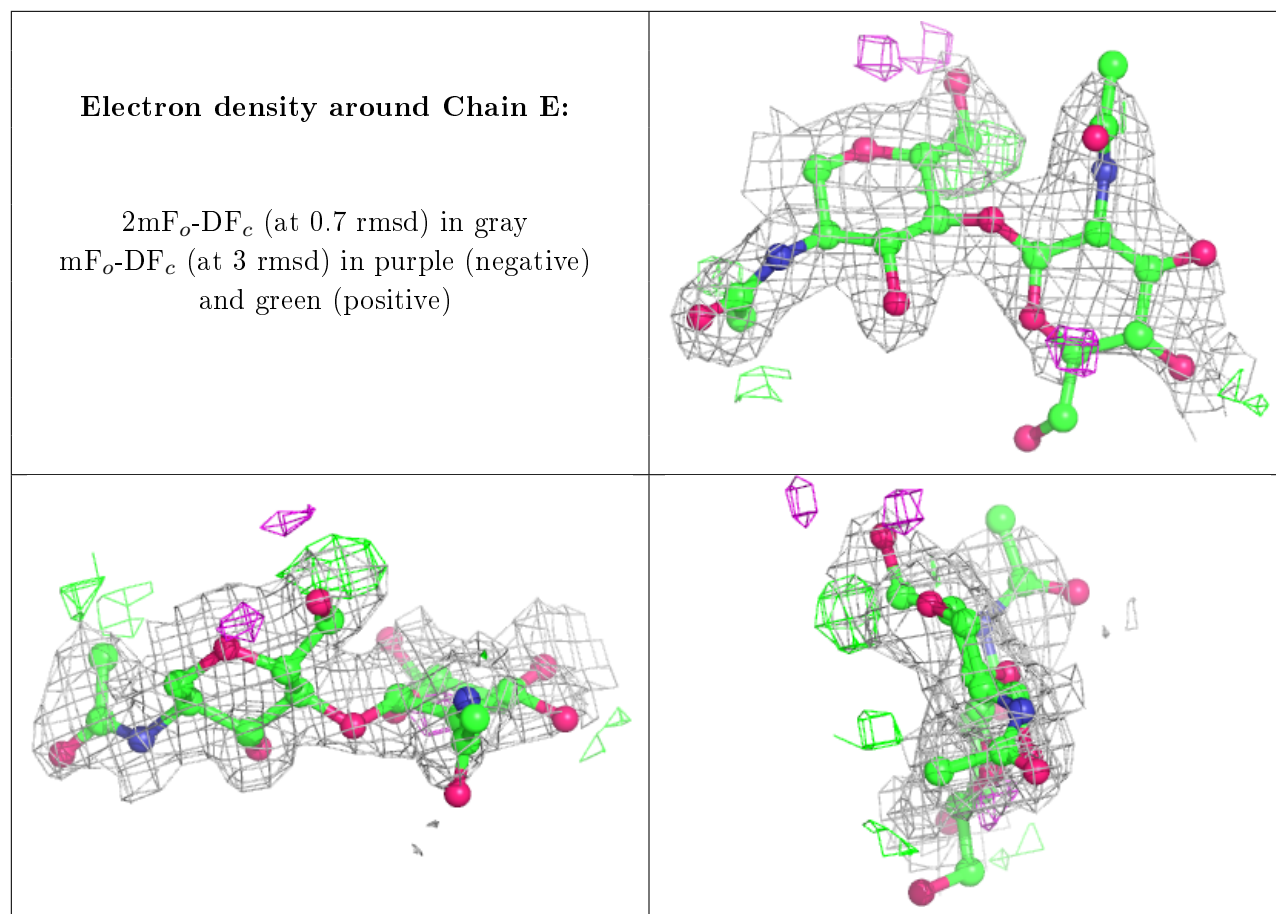
There are no non-standard protein/DNA/RNA residues in this entry.

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, 95th 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 ²)	Q<0.9
2	NAG	E	2	14/15	0.78	0.50	62,73,83,86	0
2	NAG	E	1	14/15	0.86	0.29	31,44,54,54	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. 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, 95th 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 ²)	Q<0.9
6	NAG	C	1386	14/15	0.48	0.49	95,102,104,104	0
6	NAG	B	1235	14/15	0.55	0.46	74,89,92,93	0
3	CA	A	502	1/1	0.70	0.15	59,59,59,59	0
5	EPE	B	901	15/15	0.73	0.25	40,51,57,63	0
6	NAG	C	1235	14/15	0.77	0.46	56,73,80,85	0
6	NAG	A	1235	14/15	0.77	0.33	71,80,87,89	0
6	NAG	D	1235	14/15	0.78	0.51	62,75,85,88	0
4	G39	B	801	20/20	0.80	0.22	22,25,33,35	0
6	NAG	A	1088	14/15	0.80	0.36	61,78,87,89	0
6	NAG	D	1088	14/15	0.82	0.39	60,75,82,82	0
3	CA	B	501	1/1	0.82	0.13	24,24,24,24	0
6	NAG	C	1088	14/15	0.84	0.37	53,66,73,74	0

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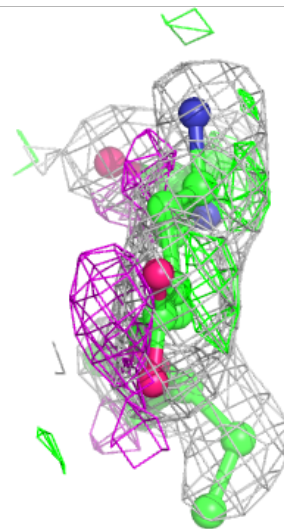
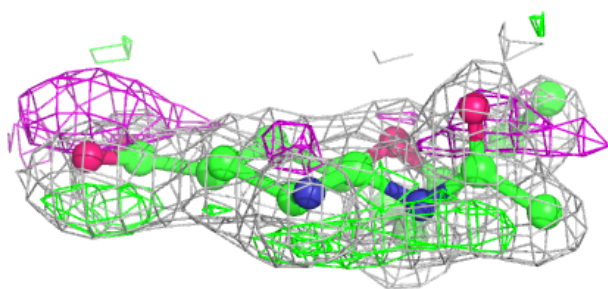
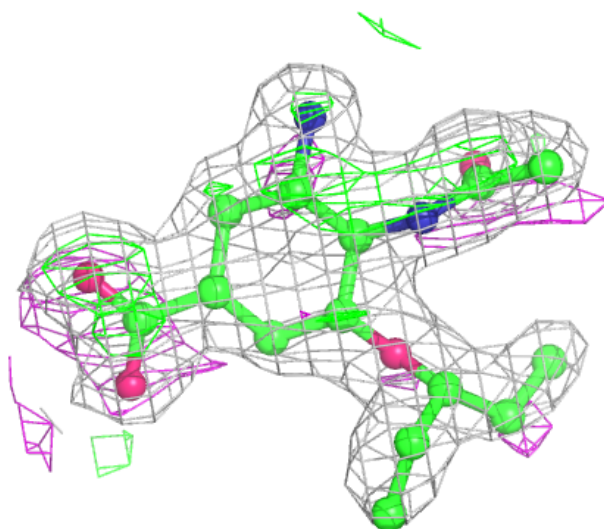
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	CA	B	502	1/1	0.85	0.12	49,49,49,49	0
6	NAG	C	1146	14/15	0.85	0.28	37,47,59,59	0
6	NAG	B	1146	14/15	0.85	0.30	39,55,74,74	0
6	NAG	B	1088	14/15	0.86	0.34	59,76,90,96	0
6	NAG	D	1146	14/15	0.88	0.30	39,50,61,64	0
5	EPE	A	901	15/15	0.88	0.20	46,56,68,76	0
4	G39	A	801	20/20	0.89	0.14	23,28,36,39	0
5	EPE	C	901	15/15	0.90	0.18	36,44,52,54	0
3	CA	D	502	1/1	0.91	0.28	57,57,57,57	0
3	CA	A	501	1/1	0.93	0.09	34,34,34,34	0
3	CA	C	502	1/1	0.94	0.14	49,49,49,49	0
5	EPE	D	901	15/15	0.94	0.15	32,37,47,48	0
4	G39	C	801	20/20	0.95	0.12	21,23,32,34	0
4	G39	D	801	20/20	0.96	0.09	21,25,36,38	0
3	CA	D	501	1/1	0.98	0.08	30,30,30,30	0
3	CA	C	501	1/1	0.98	0.06	25,25,25,25	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.

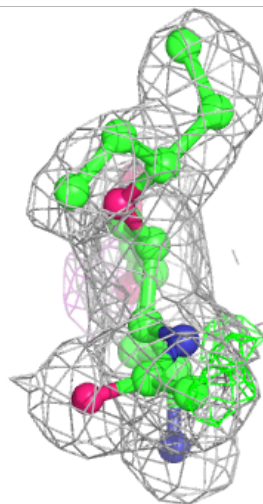
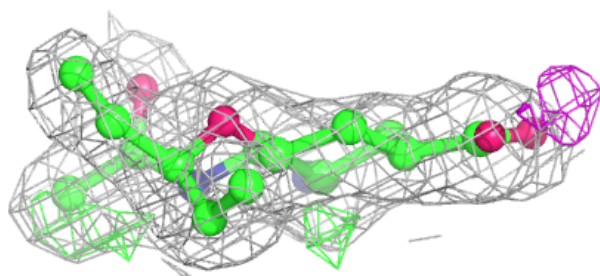
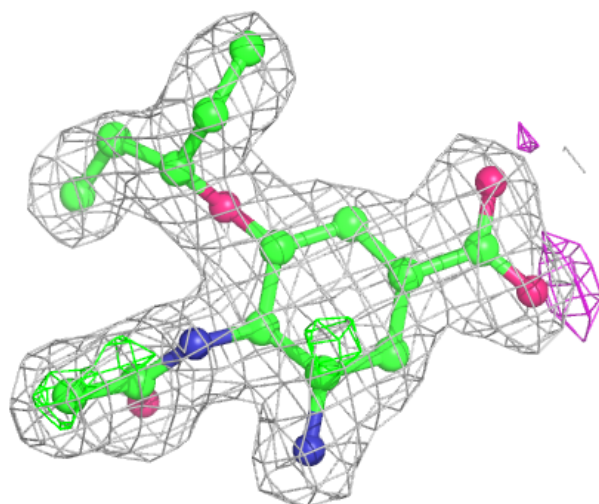
Electron density around G39 B 801:

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



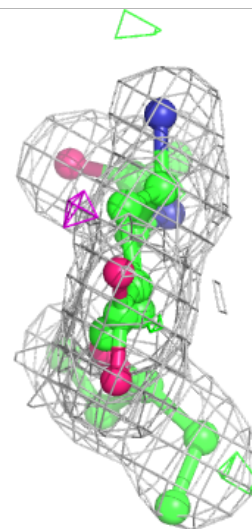
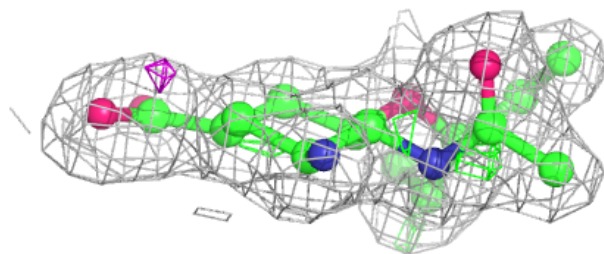
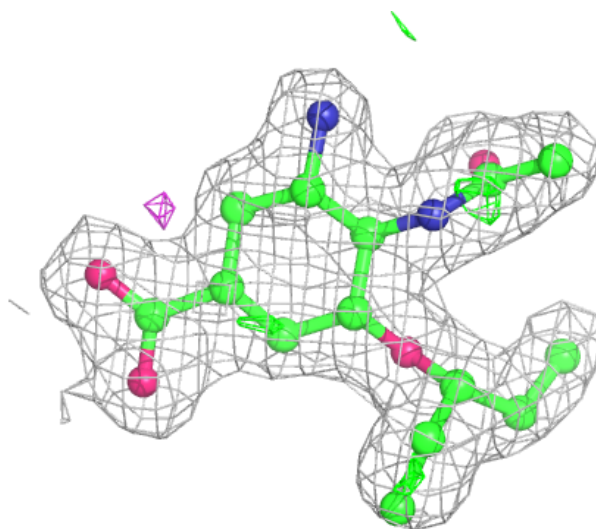
Electron density around G39 A 801:

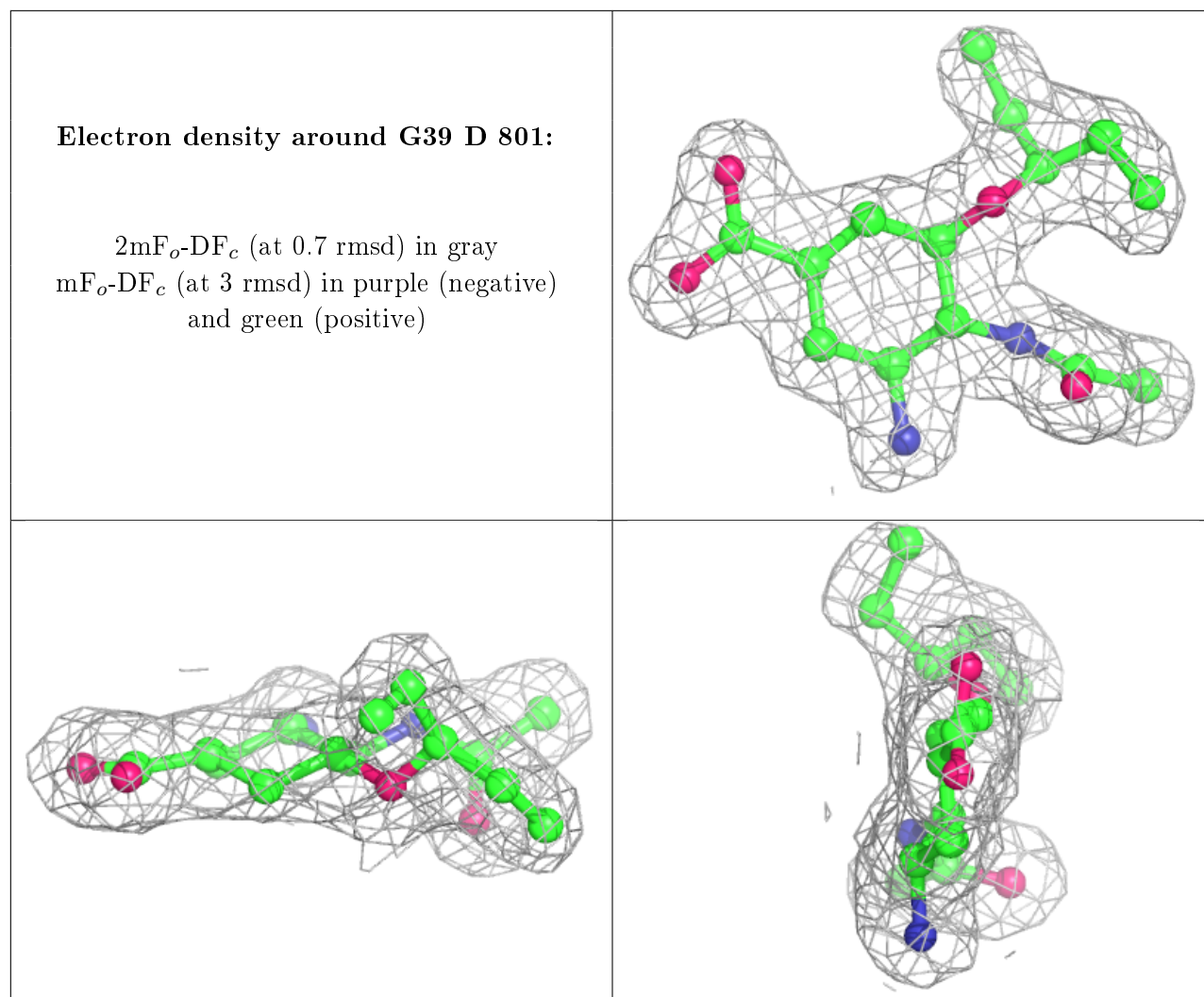
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around G39 C 801:

$2mF_o-DF_c$ (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.