



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:36 AM UTC

PDB ID : 4B7R / pdb_00004b7r
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references](#) ①) 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

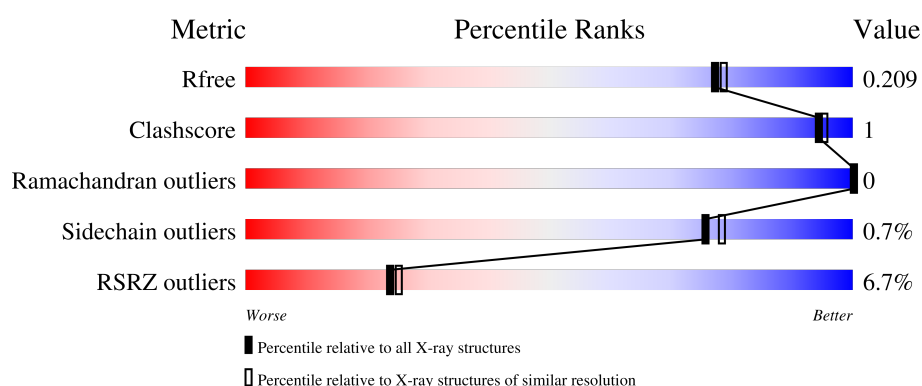
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (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 of 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	10% 96% .
1	B	387	13% 97% .
1	C	387	% 96% .
1	D	387	2% 95% 5%
2	E	2	50% 50%

2 Entry composition

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
1	A	387	Total	C	N	O	S	0	0	0
			2994	1880	517	576	21			
1	B	387	Total	C	N	O	S	0	0	0
			2994	1880	517	576	21			
1	C	387	Total	C	N	O	S	0	0	0
			2994	1880	517	576	21			
1	D	387	Total	C	N	O	S	0	0	0
			2994	1880	517	576	21			

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.

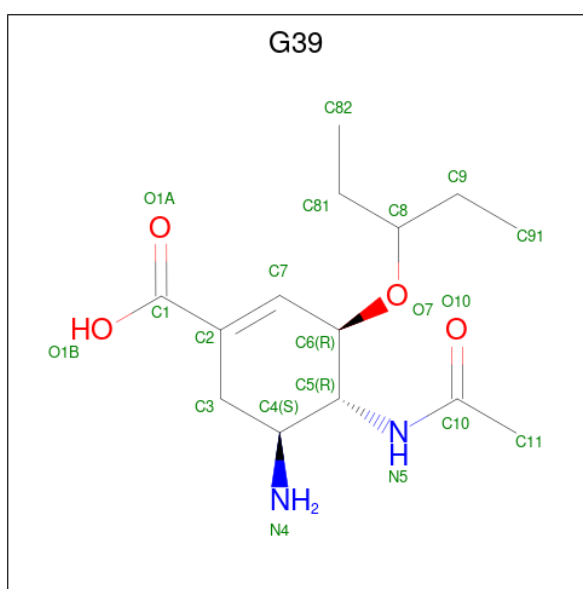


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Ca 2 2	0	0
3	B	2	Total Ca 2 2	0	0
3	C	2	Total Ca 2 2	0	0
3	D	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 (CCD ID: G39) (formula: C₁₄H₂₄N₂O₄).



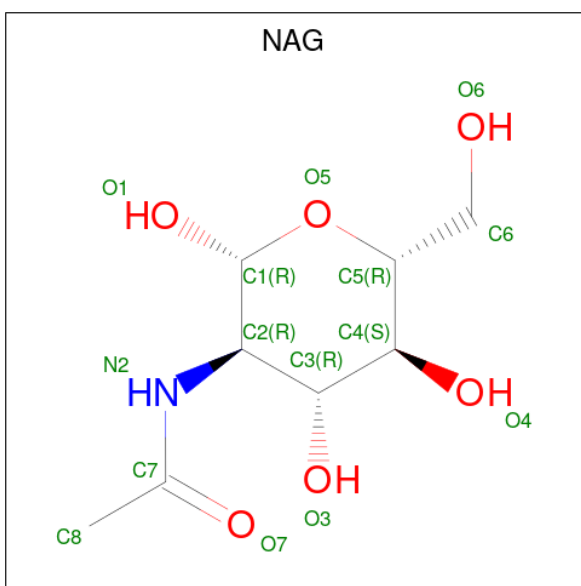
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 20 14 2 4	0	0
4	B	1	Total C N O 20 14 2 4	0	0
4	C	1	Total C N O 20 14 2 4	0	0
4	D	1	Total C N O 20 14 2 4	0	0

- Molecule 5 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: C₈H₁₈N₂O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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 (CCD ID: 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		

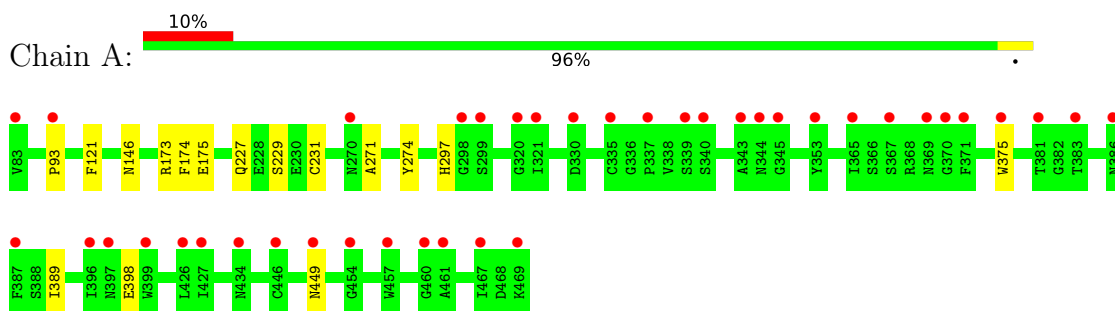
- Molecule 7 is water.

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		

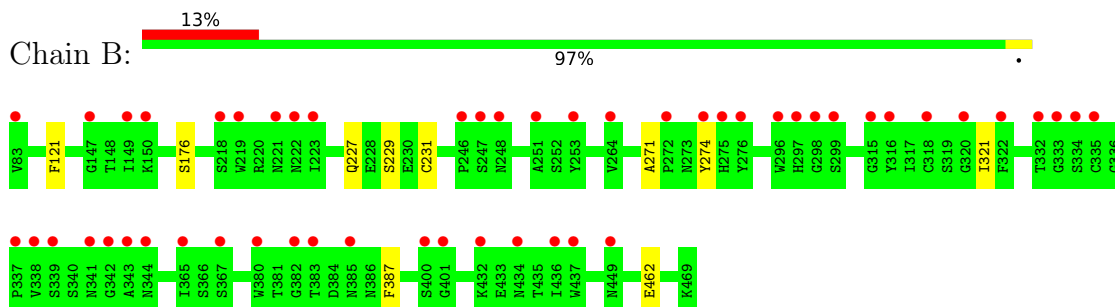
3 Residue-property plots [i](#)

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.

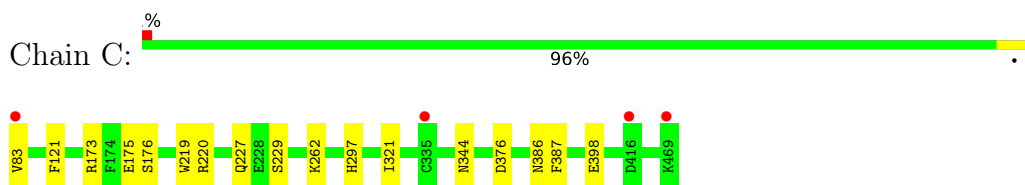
• Molecule 1: NEURAMINIDASE



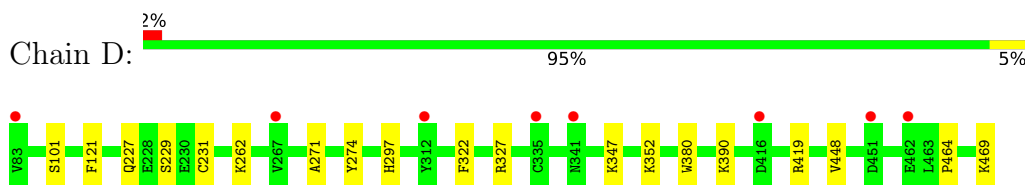
• Molecule 1: NEURAMINIDASE



• Molecule 1: NEURAMINIDASE



• Molecule 1: NEURAMINIDASE



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

Chain E:



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 29.82 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.7 (29.82-1.90) 99.7 (29.82-1.90)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.15 (at 1.88Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.146 , 0.173 0.188 , 0.209	Depositor DCC
R_{free} test set	8190 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	26.0	Xtriage
Anisotropy	0.751	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 36.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
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

Xtriage'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: EPE, G39, CA, 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	0.41	0/3076	0.76	1/4180 (0.0%)
1	B	0.44	0/3076	0.77	1/4180 (0.0%)
1	C	0.46	0/3076	0.78	3/4180 (0.1%)
1	D	0.44	0/3076	0.76	1/4180 (0.0%)
All	All	0.44	0/12304	0.77	6/16720 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	227	GLN	N-CA-C	6.47	118.41	111.36
1	C	227	GLN	N-CA-C	6.45	118.39	111.36
1	B	227	GLN	N-CA-C	6.43	118.37	111.36
1	C	376	ASP	CA-C-N	5.54	125.21	119.56
1	C	376	ASP	C-N-CA	5.54	125.21	119.56
1	A	227	GLN	N-CA-C	5.52	117.38	111.36

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:H83	6:B:1235:NAG:H2	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
1:C:344:ASN:HB3	7:C:2194:HOH:O	2.20	0.41
6:C:1235:NAG:H83	6:C:1235:NAG:H2	1.93	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
All	All	1540/1548 (100%)	1481 (96%)	59 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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%)	78	81
1	B	334/334 (100%)	332 (99%)	2 (1%)	78	81
1	C	334/334 (100%)	332 (99%)	2 (1%)	78	81
1	D	334/334 (100%)	331 (99%)	3 (1%)	70	73
All	All	1336/1336 (100%)	1327 (99%)	9 (1%)	76	78

All (9) 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	C	176	SER
1	C	297	HIS
1	D	231	CYS
1	D	297	HIS
1	D	390	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	341	ASN
1	C	386	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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	2,1	14,14,15	0.47	0	17,19,21	1.37	1 (5%)
2	NAG	E	2	2	14,14,15	0.52	0	17,19,21	0.66	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	2,1	-	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($^{\circ}$)	Ideal($^{\circ}$)
2	E	1	NAG	C1-O5-C5	4.49	118.20	112.19

There are no chirality outliers.

All (4) torsion outliers are listed below:

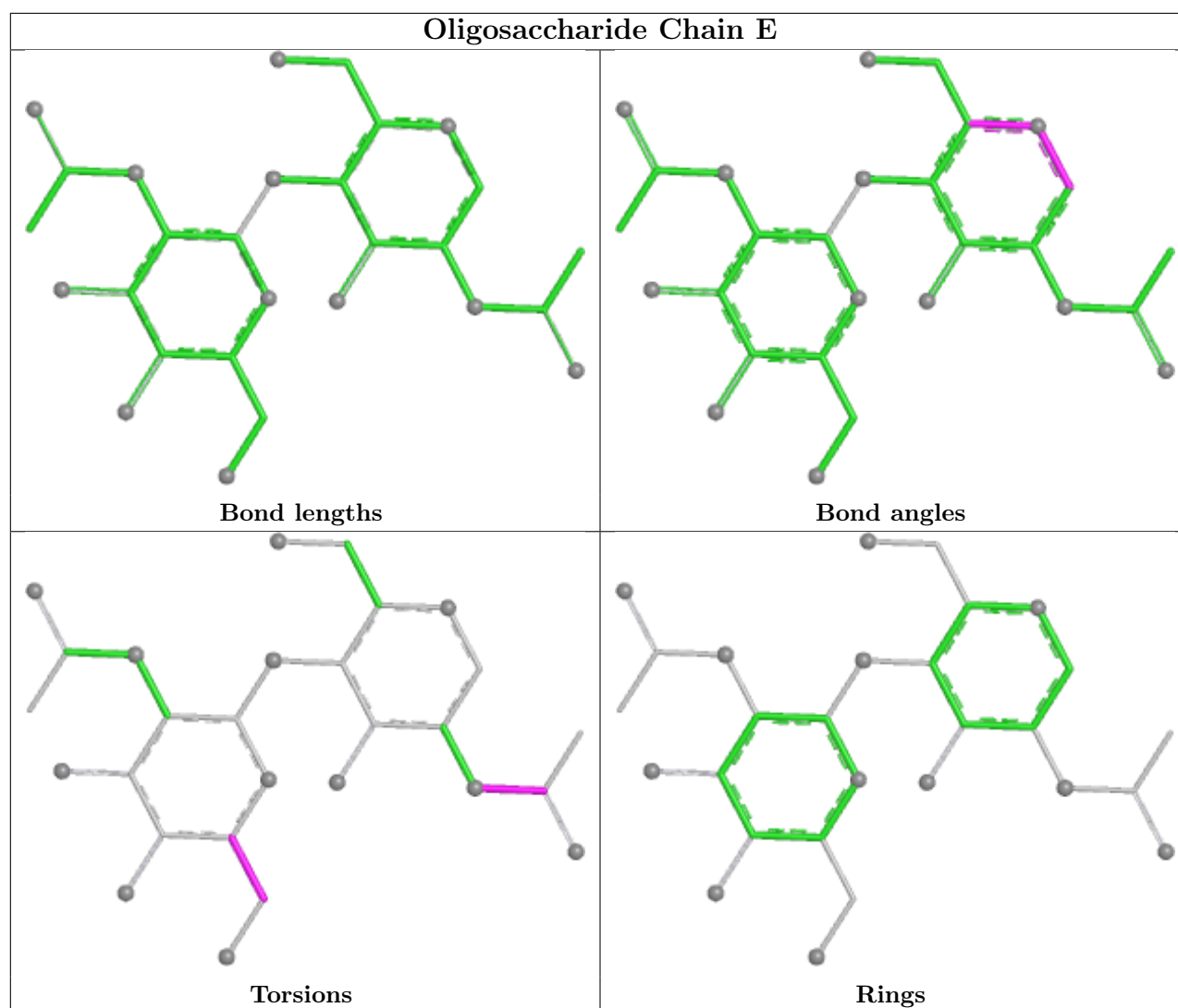
Mol	Chain	Res	Type	Atoms
2	E	1	NAG	C8-C7-N2-C2
2	E	1	NAG	O7-C7-N2-C2
2	E	2	NAG	C4-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6

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 [i](#)

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	C	1386	-	14,14,15	0.44	0	17,19,21	1.19	2 (11%)
5	EPE	D	901	-	15,15,15	0.84	1 (6%)	19,20,20	1.57	3 (15%)
4	G39	A	801	-	19,20,20	2.23	5 (26%)	20,27,27	2.81	5 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	G39	B	801	-	19,20,20	2.22	4 (21%)	20,27,27	2.71	3 (15%)
6	NAG	C	1235	1	14,14,15	0.46	0	17,19,21	0.88	1 (5%)
6	NAG	D	1088	1	14,14,15	0.48	0	17,19,21	0.71	1 (5%)
5	EPE	C	901	-	15,15,15	0.84	1 (6%)	19,20,20	1.57	4 (21%)
4	G39	C	801	-	19,20,20	2.14	5 (26%)	20,27,27	2.72	4 (20%)
5	EPE	B	901	-	15,15,15	0.94	1 (6%)	19,20,20	1.72	4 (21%)
6	NAG	C	1146	1	14,14,15	0.51	0	17,19,21	0.87	0
6	NAG	A	1088	1	14,14,15	0.46	0	17,19,21	0.73	0
6	NAG	B	1146	1	14,14,15	0.58	0	17,19,21	0.75	0
6	NAG	B	1088	1	14,14,15	0.49	0	17,19,21	1.18	1 (5%)
4	G39	D	801	-	19,20,20	2.13	5 (26%)	20,27,27	2.72	3 (15%)
5	EPE	A	901	-	15,15,15	0.85	1 (6%)	19,20,20	1.56	4 (21%)
6	NAG	D	1235	1	14,14,15	0.58	0	17,19,21	1.03	0
6	NAG	B	1235	1	14,14,15	0.43	0	17,19,21	1.53	2 (11%)
6	NAG	C	1088	1	14,14,15	0.49	0	17,19,21	0.69	0
6	NAG	D	1146	1	14,14,15	0.60	0	17,19,21	0.96	1 (5%)
6	NAG	A	1235	1	14,14,15	0.43	0	17,19,21	0.95	1 (5%)

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	C	1386	-	-	2/6/23/26	0/1/1/1
5	EPE	D	901	-	-	1/9/19/19	0/1/1/1
4	G39	A	801	-	-	4/16/32/32	0/1/1/1
4	G39	B	801	-	-	4/16/32/32	0/1/1/1
6	NAG	C	1235	1	-	2/6/23/26	0/1/1/1
6	NAG	D	1088	1	-	2/6/23/26	0/1/1/1
5	EPE	C	901	-	-	1/9/19/19	0/1/1/1
4	G39	C	801	-	-	4/16/32/32	0/1/1/1
5	EPE	B	901	-	-	1/9/19/19	0/1/1/1
6	NAG	C	1146	1	-	0/6/23/26	0/1/1/1
6	NAG	A	1088	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1146	1	-	1/6/23/26	0/1/1/1
6	NAG	B	1088	1	-	3/6/23/26	0/1/1/1
4	G39	D	801	-	-	4/16/32/32	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EPE	A	901	-	-	1/9/19/19	0/1/1/1
6	NAG	D	1235	1	-	0/6/23/26	0/1/1/1
6	NAG	B	1235	1	-	3/6/23/26	0/1/1/1
6	NAG	C	1088	1	-	2/6/23/26	0/1/1/1
6	NAG	D	1146	1	-	0/6/23/26	0/1/1/1
6	NAG	A	1235	1	-	2/6/23/26	0/1/1/1

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	801	G39	C7-C2	7.55	1.50	1.33
4	B	801	G39	C7-C2	7.47	1.50	1.33
4	C	801	G39	C7-C2	7.22	1.49	1.33
4	D	801	G39	C7-C2	7.17	1.49	1.33
4	A	801	G39	C10-N5	3.22	1.44	1.34
5	B	901	EPE	C10-S	3.16	1.82	1.77
4	B	801	G39	O7-C8	-3.11	1.40	1.44
4	B	801	G39	C10-N5	2.94	1.43	1.34
4	D	801	G39	C10-N5	2.93	1.43	1.34
4	C	801	G39	C10-N5	2.90	1.43	1.34
5	A	901	EPE	C10-S	2.87	1.81	1.77
5	D	901	EPE	C10-S	2.85	1.81	1.77
5	C	901	EPE	C10-S	2.81	1.81	1.77
4	A	801	G39	O7-C8	-2.79	1.41	1.44
4	D	801	G39	O7-C8	-2.71	1.41	1.44
4	C	801	G39	O7-C8	-2.69	1.41	1.44
4	B	801	G39	O7-C6	-2.34	1.39	1.44
4	D	801	G39	O7-C6	-2.27	1.39	1.44
4	A	801	G39	C6-C7	2.26	1.53	1.50
4	C	801	G39	C6-C7	2.22	1.53	1.50
4	C	801	G39	O7-C6	-2.14	1.39	1.44
4	A	801	G39	O7-C6	-2.13	1.39	1.44
4	D	801	G39	C6-C7	2.07	1.53	1.50

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	801	G39	C6-C7-C2	-9.50	107.89	122.66
4	B	801	G39	C6-C7-C2	-9.04	108.60	122.66
4	C	801	G39	C6-C7-C2	-8.83	108.93	122.66
4	A	801	G39	C6-C7-C2	-8.64	109.22	122.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	801	G39	C7-C2-C1	-5.55	112.40	119.99
4	C	801	G39	C7-C2-C1	-5.38	112.63	119.99
4	A	801	G39	C3-C2-C7	-5.30	115.72	122.25
4	B	801	G39	C3-C2-C7	-5.13	115.92	122.25
4	D	801	G39	C7-C2-C1	-5.05	113.08	119.99
4	B	801	G39	C7-C2-C1	-4.72	113.53	119.99
4	C	801	G39	C3-C2-C7	-4.69	116.46	122.25
6	B	1235	NAG	C1-O5-C5	4.68	118.45	112.19
5	B	901	EPE	C5-N4-C3	4.29	118.08	108.84
4	D	801	G39	C3-C2-C7	-4.29	116.96	122.25
5	D	901	EPE	C5-N4-C3	4.20	117.88	108.84
5	A	901	EPE	C5-N4-C3	3.99	117.43	108.84
5	C	901	EPE	C5-N4-C3	3.66	116.72	108.84
6	B	1088	NAG	C1-O5-C5	3.37	116.71	112.19
5	A	901	EPE	C7-N4-C5	3.23	119.84	111.24
5	C	901	EPE	C7-N4-C5	3.17	119.68	111.24
5	D	901	EPE	C7-N4-C5	3.09	119.46	111.24
5	B	901	EPE	C7-N4-C5	3.01	119.27	111.24
6	D	1146	NAG	C1-O5-C5	3.00	116.20	112.19
4	C	801	G39	C4-C3-C2	-2.62	106.74	109.72
4	A	801	G39	C4-C3-C2	-2.62	106.75	109.72
6	A	1235	NAG	C1-O5-C5	2.61	115.68	112.19
6	C	1235	NAG	C1-O5-C5	2.52	115.56	112.19
5	B	901	EPE	C7-N4-C3	2.48	117.84	111.24
5	C	901	EPE	O1S-S-C10	2.44	110.41	106.73
6	C	1386	NAG	C1-O5-C5	2.35	115.34	112.19
5	A	901	EPE	C7-N4-C3	2.22	117.17	111.24
4	A	801	G39	C6-C5-N5	-2.22	108.65	111.13
6	B	1235	NAG	C3-C4-C5	2.21	114.24	110.23
5	D	901	EPE	C7-N4-C3	2.20	117.11	111.24
5	B	901	EPE	O1S-S-C10	2.18	110.02	106.73
6	C	1386	NAG	O5-C1-C2	-2.17	107.94	111.29
6	D	1088	NAG	C1-O5-C5	2.01	114.89	112.19
5	A	901	EPE	O1S-S-C10	2.01	109.76	106.73
5	C	901	EPE	C7-N4-C3	2.00	116.57	111.24

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	801	G39	O1B-C1-C2-C7
4	B	801	G39	O1B-C1-C2-C7

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Mol	Chain	Res	Type	Atoms
4	C	801	G39	O1B-C1-C2-C7
4	D	801	G39	O1B-C1-C2-C7
5	A	901	EPE	C8-C7-N4-C5
5	B	901	EPE	C8-C7-N4-C5
5	C	901	EPE	C8-C7-N4-C5
5	D	901	EPE	C8-C7-N4-C5
6	A	1235	NAG	C8-C7-N2-C2
6	A	1235	NAG	O7-C7-N2-C2
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	B	1235	NAG	C8-C7-N2-C2
6	B	1235	NAG	O7-C7-N2-C2
6	C	1235	NAG	C8-C7-N2-C2
6	C	1235	NAG	O7-C7-N2-C2
6	C	1386	NAG	C8-C7-N2-C2
6	C	1386	NAG	O7-C7-N2-C2
6	D	1088	NAG	C8-C7-N2-C2
6	D	1088	NAG	O7-C7-N2-C2
6	A	1088	NAG	C8-C7-N2-C2
6	A	1088	NAG	O7-C7-N2-C2
6	C	1088	NAG	C8-C7-N2-C2
6	C	1088	NAG	O7-C7-N2-C2
6	B	1235	NAG	O5-C5-C6-O6
4	A	801	G39	O1A-C1-C2-C7
4	B	801	G39	O1A-C1-C2-C7
4	D	801	G39	O1A-C1-C2-C7
4	A	801	G39	C81-C8-O7-C6
4	B	801	G39	C81-C8-O7-C6
4	C	801	G39	C81-C8-O7-C6
4	D	801	G39	C81-C8-O7-C6
4	B	801	G39	C5-C6-O7-C8
4	C	801	G39	O1A-C1-C2-C7
6	B	1146	NAG	C1-C2-N2-C7
4	A	801	G39	C5-C6-O7-C8
4	C	801	G39	C5-C6-O7-C8
4	D	801	G39	C5-C6-O7-C8

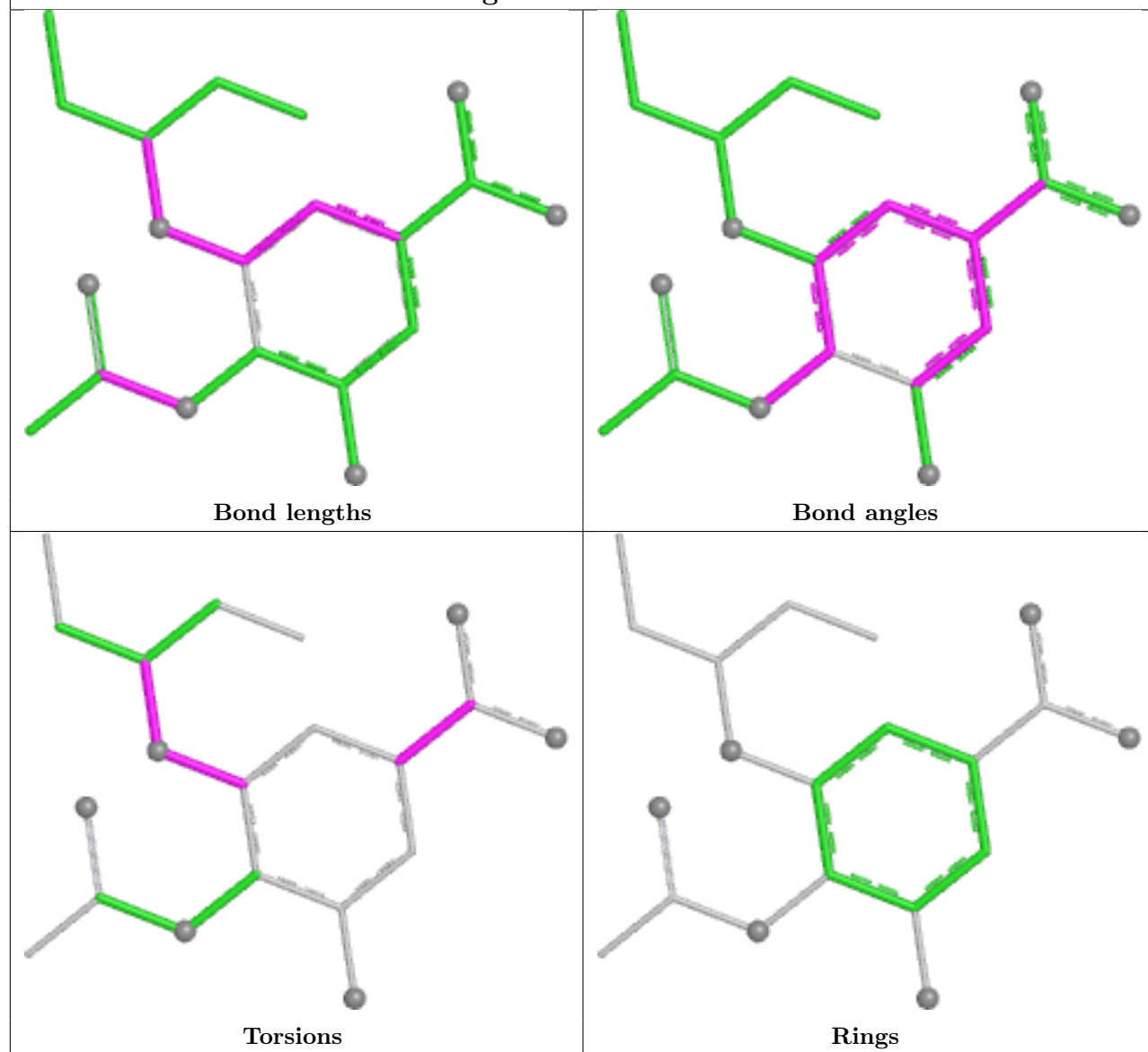
There are no ring outliers.

3 monomers are involved in 3 short contacts:

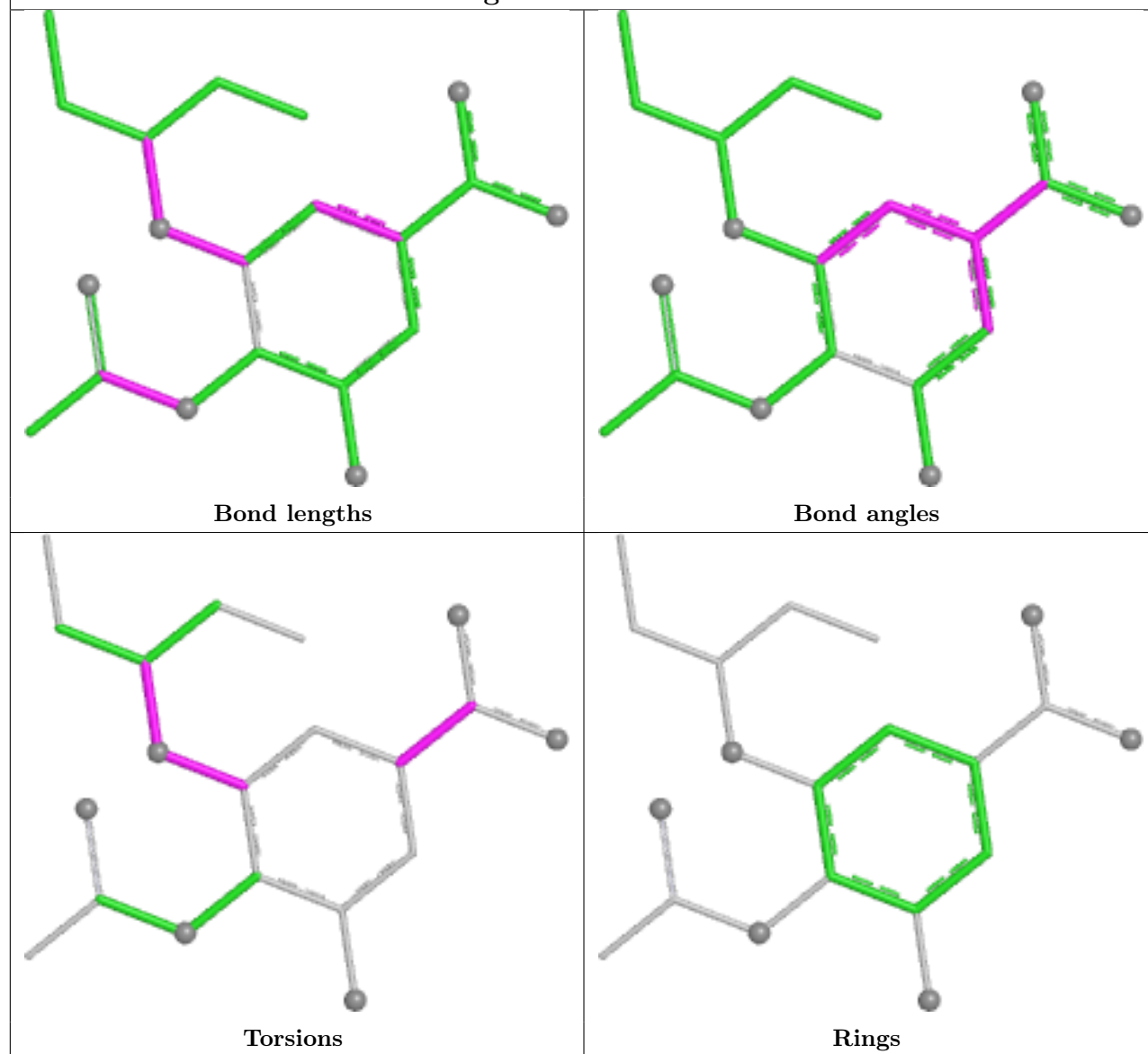
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	1235	NAG	1	0
6	B	1235	NAG	1	0
6	A	1235	NAG	1	0

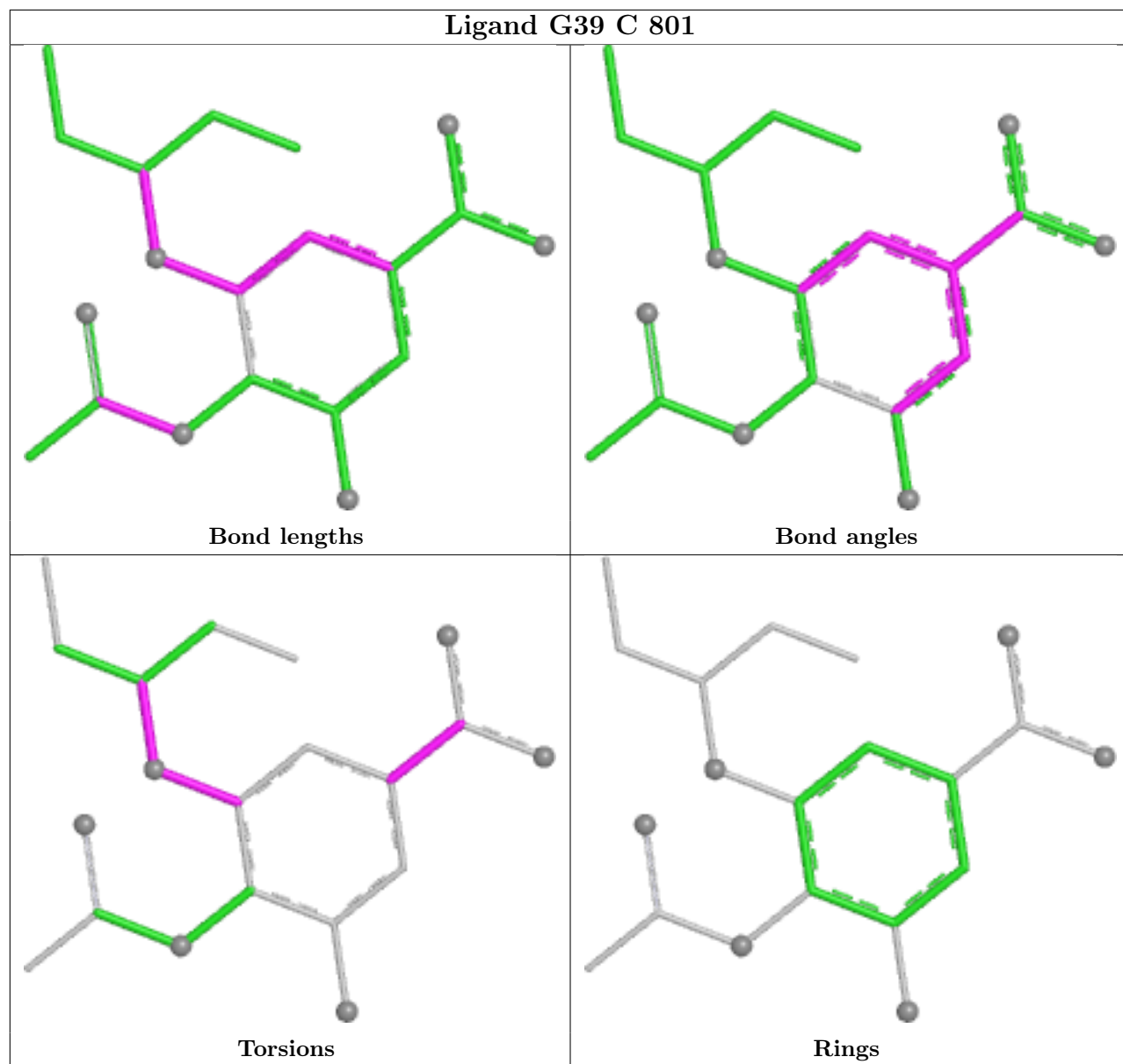
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

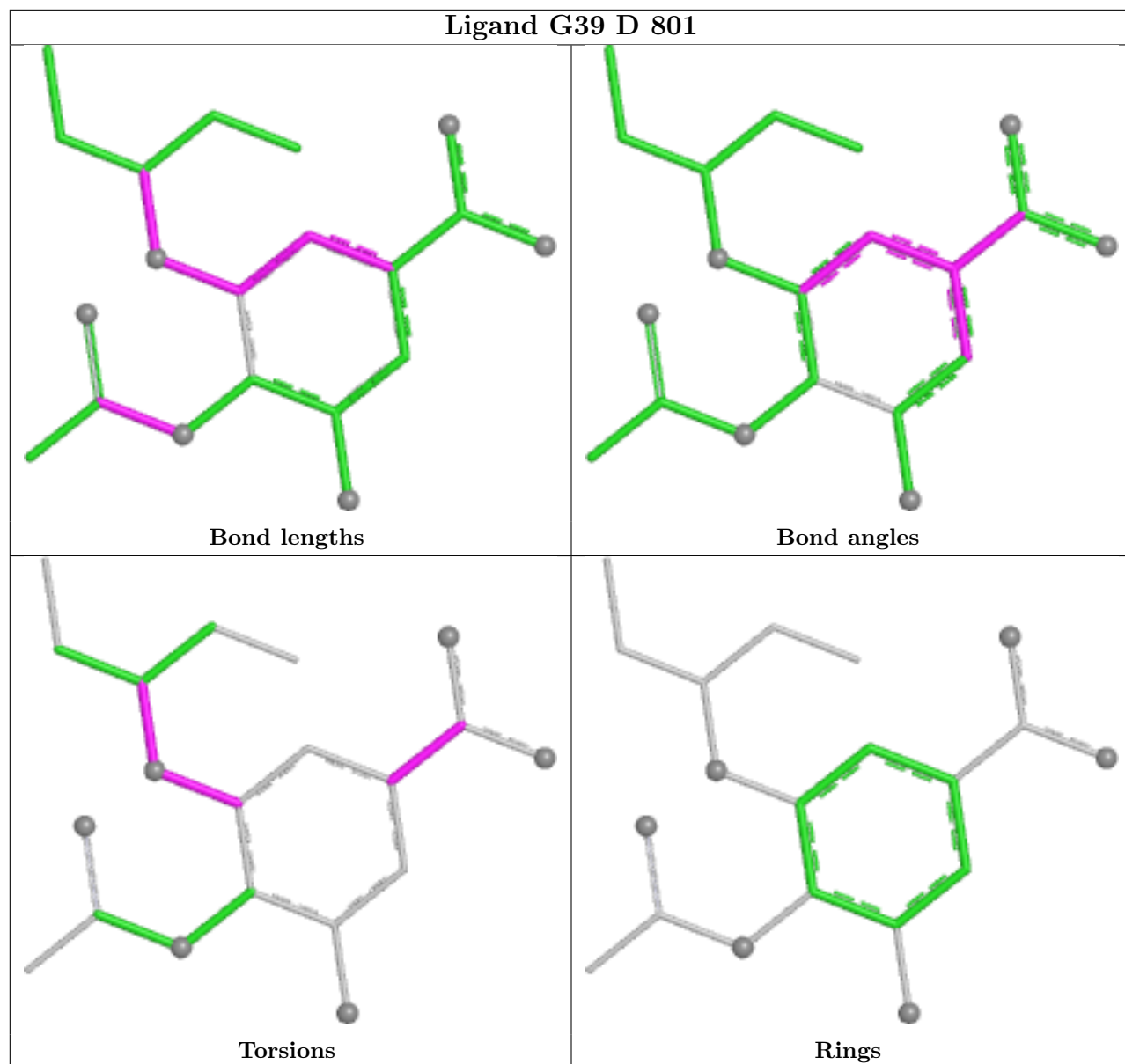
Ligand G39 A 801



Ligand G39 B 801







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%)	0.81	40 (10%) 12 12	20, 30, 47, 61	0
1	B	387/387 (100%)	1.09	52 (13%) 7 7	19, 26, 38, 56	0
1	C	387/387 (100%)	0.03	4 (1%) 79 82	19, 25, 38, 56	0
1	D	387/387 (100%)	0.22	8 (2%) 63 67	19, 27, 42, 57	0
All	All	1548/1548 (100%)	0.54	104 (6%) 24 25	19, 27, 42, 61	0

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	332	THR	3.9
1	A	83	VAL	3.7
1	B	337	PRO	3.7
1	B	341	ASN	3.5
1	D	335	CYS	3.5
1	A	335	CYS	3.3
1	B	339	SER	3.3
1	B	316	TYR	3.3
1	C	83	VAL	3.3
1	B	343	ALA	3.2
1	B	333	GLY	3.2
1	C	335	CYS	3.0
1	A	396	ILE	3.0
1	A	370	GLY	3.0
1	A	399	TRP	2.9
1	A	339	SER	2.9
1	B	315	GLY	2.9
1	B	275	HIS	2.9
1	B	251	ALA	2.9
1	B	247	SER	2.9
1	B	401	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	367	SER	2.8
1	B	296	TRP	2.8
1	A	397	ASN	2.8
1	A	387	PHE	2.8
1	B	149	ILE	2.8
1	B	246	PRO	2.7
1	B	338	VAL	2.7
1	B	437	TRP	2.7
1	B	83	VAL	2.7
1	B	274	TYR	2.6
1	B	335	CYS	2.6
1	A	449	ASN	2.6
1	B	344	ASN	2.6
1	B	436	ILE	2.6
1	C	469	LYS	2.6
1	B	400	SER	2.6
1	A	381	THR	2.6
1	B	320	GLY	2.5
1	B	365	ILE	2.5
1	A	369	ASN	2.5
1	B	221	ASN	2.5
1	B	218	SER	2.5
1	D	462	GLU	2.5
1	B	276	TYR	2.5
1	B	298	GLY	2.5
1	B	385	ASN	2.5
1	D	267	VAL	2.5
1	B	322	PHE	2.4
1	A	365	ILE	2.4
1	A	345	GLY	2.4
1	C	416	ASP	2.4
1	B	318	CYS	2.4
1	A	383	THR	2.4
1	B	434	ASN	2.4
1	A	454	GLY	2.4
1	B	223	ILE	2.3
1	B	264	VAL	2.3
1	D	83	VAL	2.3
1	A	270	ASN	2.3
1	B	449	ASN	2.3
1	A	337	PRO	2.3
1	B	272	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	432	LYS	2.3
1	B	299	SER	2.3
1	B	334	SER	2.3
1	D	451	ASP	2.3
1	A	460	GLY	2.3
1	A	93	PRO	2.2
1	B	342	GLY	2.2
1	A	340	SER	2.2
1	A	321	ILE	2.2
1	D	341	ASN	2.2
1	A	427	ILE	2.2
1	B	147	GLY	2.2
1	A	371	PHE	2.2
1	A	434	ASN	2.2
1	B	150	LYS	2.2
1	D	416	ASP	2.2
1	A	343	ALA	2.2
1	A	461	ALA	2.2
1	A	353	TYR	2.1
1	B	367	SER	2.1
1	A	320	GLY	2.1
1	A	386	ASN	2.1
1	B	248	ASN	2.1
1	A	467	ILE	2.1
1	B	219	TRP	2.1
1	B	380	TRP	2.1
1	A	298	GLY	2.1
1	A	469	LYS	2.1
1	D	312	TYR	2.1
1	A	375	TRP	2.1
1	A	457	TRP	2.1
1	B	297	HIS	2.1
1	A	299	SER	2.0
1	B	383	THR	2.0
1	B	382	GLY	2.0
1	A	426	LEU	2.0
1	A	446	CYS	2.0
1	A	330	ASP	2.0
1	A	344	ASN	2.0
1	B	222	ASN	2.0
1	B	253	TYR	2.0

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

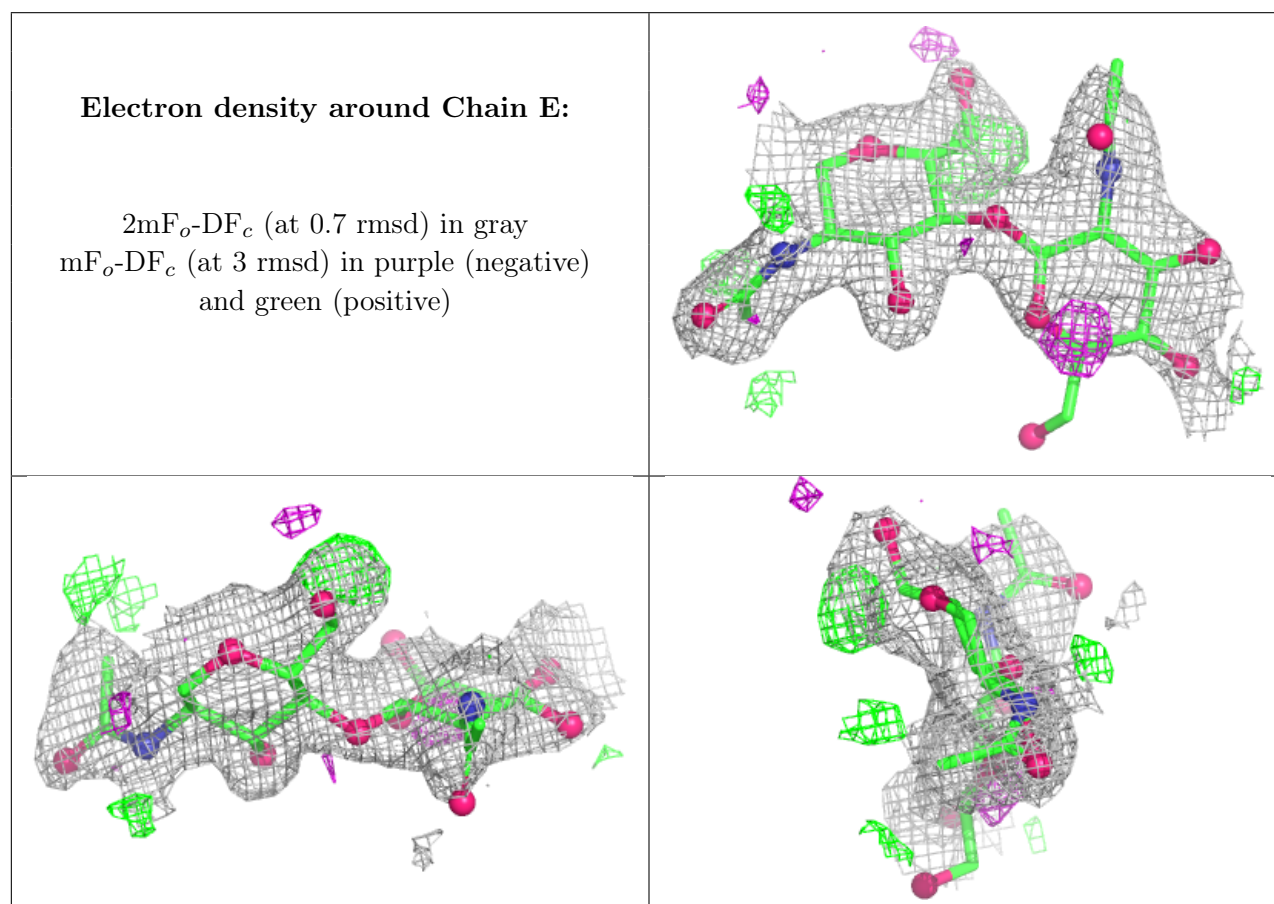
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

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	0.64	0.17	62,73,83,86	0
2	NAG	E	1	14/15	0.76	0.13	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 ⓘ

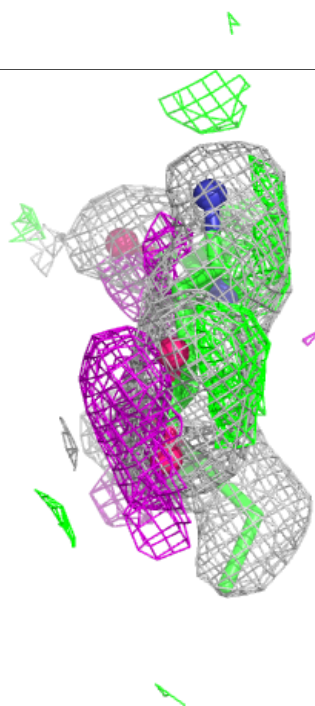
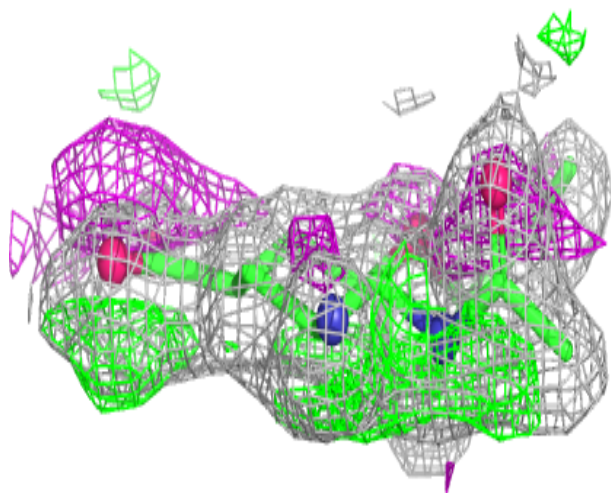
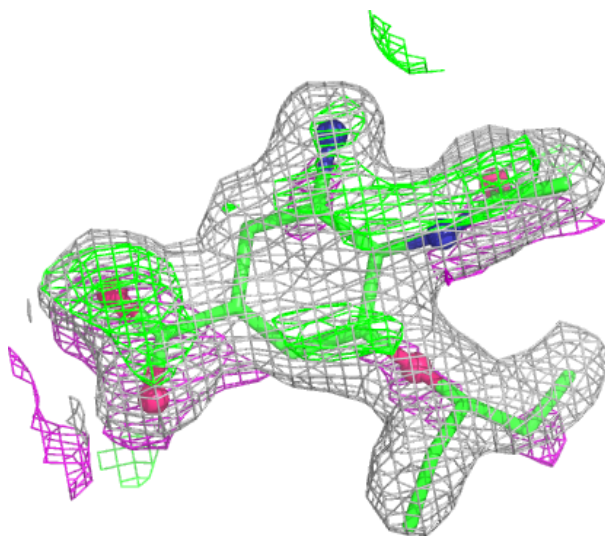
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	B	1235	14/15	0.34	0.20	74,89,92,93	0
6	NAG	C	1235	14/15	0.47	0.18	56,73,80,85	0
6	NAG	A	1235	14/15	0.54	0.18	71,80,87,89	0
6	NAG	D	1235	14/15	0.56	0.16	62,75,85,88	0
6	NAG	C	1386	14/15	0.57	0.23	95,102,104,104	0
6	NAG	A	1088	14/15	0.58	0.17	61,78,87,89	0
6	NAG	D	1088	14/15	0.65	0.17	60,75,82,82	0
6	NAG	B	1088	14/15	0.69	0.19	59,76,90,96	0
6	NAG	C	1088	14/15	0.71	0.14	53,66,73,74	0
5	EPE	B	901	15/15	0.75	0.19	40,51,57,63	0
3	CA	B	501	1/1	0.79	0.11	24,24,24,24	0
4	G39	B	801	20/20	0.79	0.17	22,25,33,35	0
6	NAG	B	1146	14/15	0.82	0.13	39,55,74,74	0
5	EPE	A	901	15/15	0.83	0.16	46,56,68,76	0
6	NAG	C	1146	14/15	0.83	0.11	37,47,59,59	0
6	NAG	D	1146	14/15	0.86	0.10	39,50,61,64	0
4	G39	A	801	20/20	0.88	0.11	23,28,36,39	0
3	CA	A	502	1/1	0.88	0.15	59,59,59,59	0
5	EPE	C	901	15/15	0.88	0.13	36,44,52,54	0
3	CA	D	502	1/1	0.92	0.18	57,57,57,57	0
3	CA	A	501	1/1	0.92	0.09	34,34,34,34	0
3	CA	B	502	1/1	0.92	0.15	49,49,49,49	0
5	EPE	D	901	15/15	0.92	0.10	32,37,47,48	0
4	G39	C	801	20/20	0.94	0.08	21,23,32,34	0
3	CA	C	502	1/1	0.95	0.15	49,49,49,49	0
4	G39	D	801	20/20	0.95	0.07	21,25,36,38	0
3	CA	D	501	1/1	0.96	0.07	30,30,30,30	0
3	CA	C	501	1/1	0.98	0.03	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.

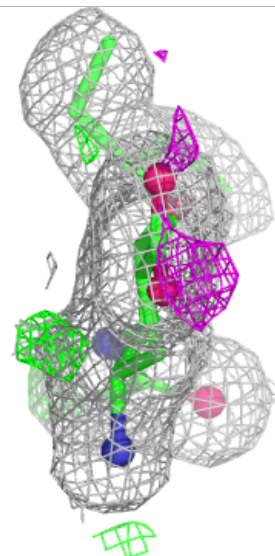
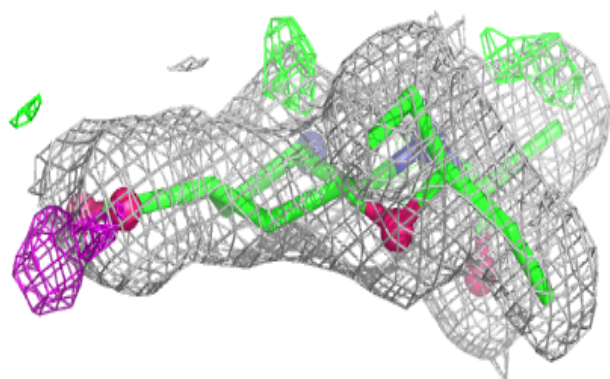
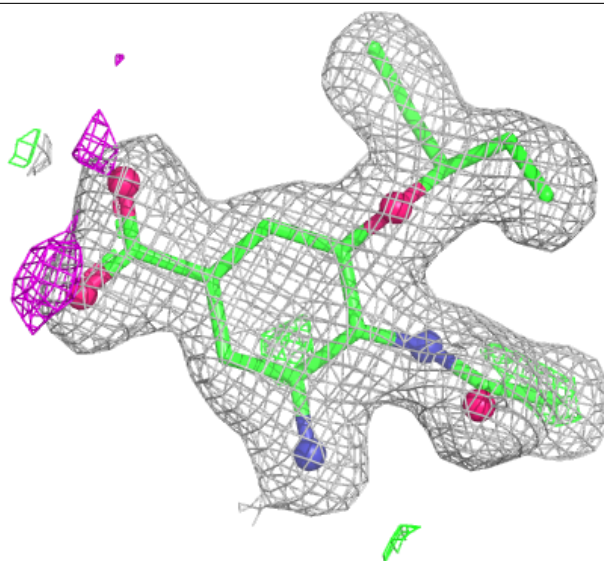
Electron density around G39 B 801:

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



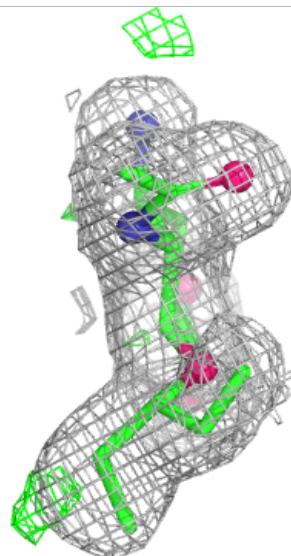
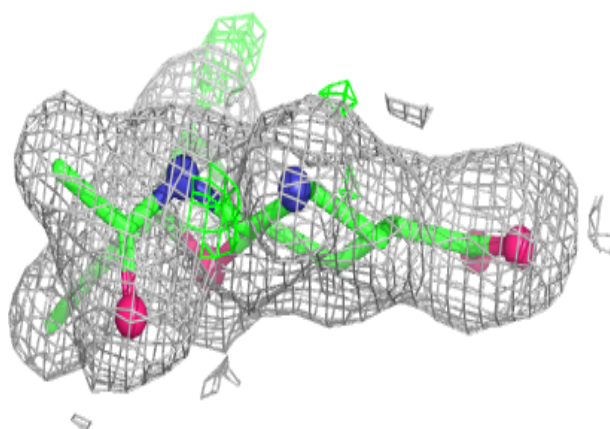
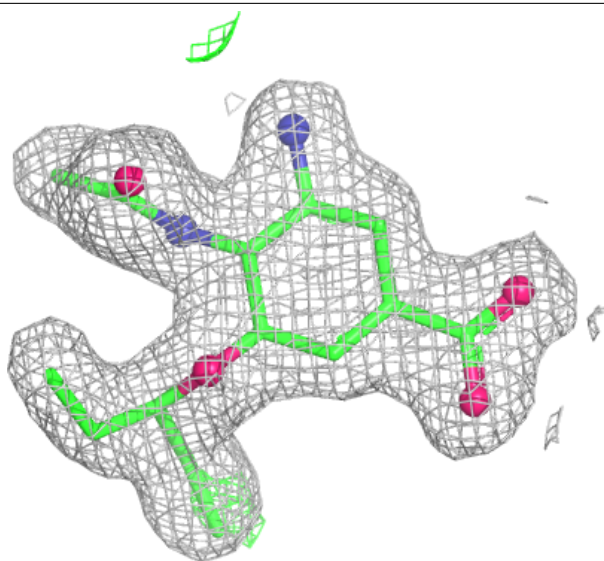
Electron density around G39 A 801:

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



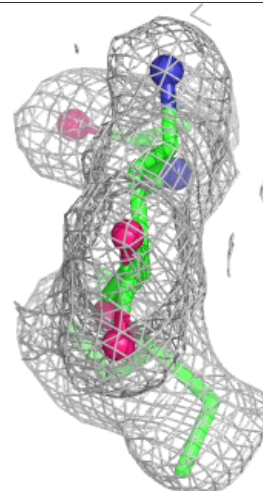
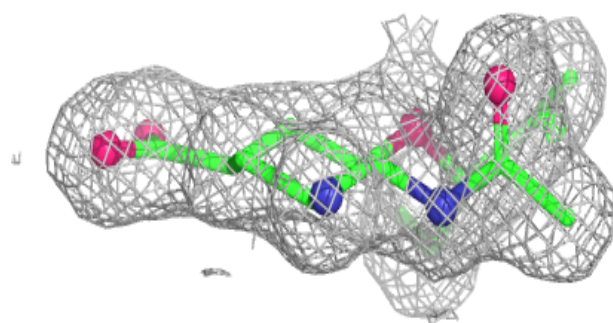
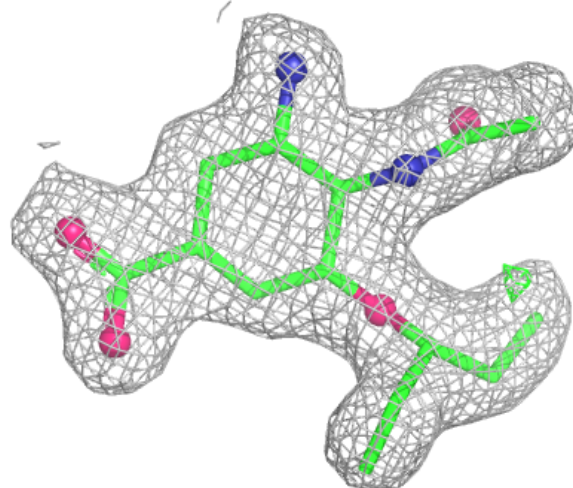
Electron density around G39 C 801:

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



Electron density around G39 D 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.