



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:48 PM UTC

PDB ID : 5NZN / pdb_00005nzn
Title : Complex of H275Y/S247N mutant variant of neuraminidase from H1N1 influenza virus with oseltamivir
Authors : Pachl, P.; Pokorna, J.
Deposited on : 2017-05-14
Resolution : 1.73 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 ⓘ](#)) 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

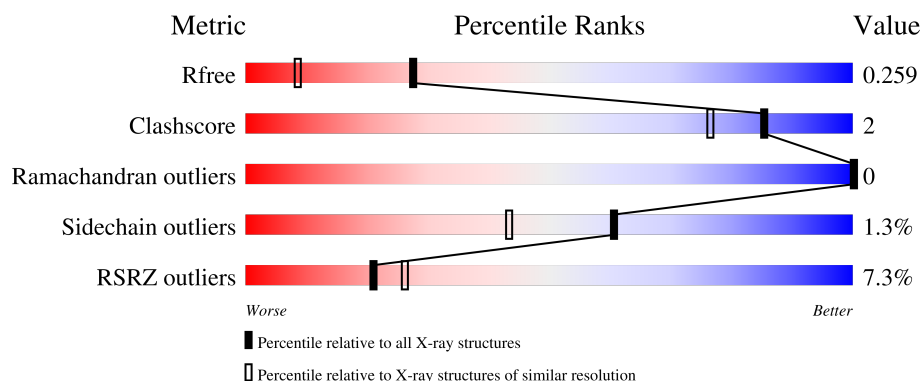
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.73 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.



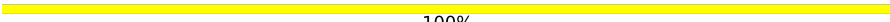
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1187 (1.74-1.74)
Clashscore	190562	1207 (1.74-1.74)
Ramachandran outliers	187476	1200 (1.74-1.74)
Sidechain outliers	187428	1200 (1.74-1.74)
RSRZ outliers	180081	1188 (1.74-1.74)

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	388	5% 91% 8%
1	B	388	11% 90% 10%
1	C	388	5% 94% 5%
1	D	388	8% 91% 8%
2	E	4	50% 50%

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Mol	Chain	Length	Quality of chain
3	F	2	 100%

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 13688 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.

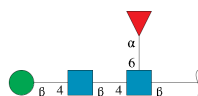
- Molecule 1 is a protein called Neuraminidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	387	Total	C	N	O	S	0	3	0
			3012	1891	519	581	21			
1	B	387	Total	C	N	O	S	0	1	0
			3003	1885	517	580	21			
1	C	387	Total	C	N	O	S	1	1	0
			3003	1885	517	580	21			
1	D	387	Total	C	N	O	S	0	1	0
			3003	1886	518	578	21			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	247	ASN	SER	engineered mutation	UNP W5R8B8
A	275	TYR	HIS	engineered mutation	UNP W5R8B8
B	247	ASN	SER	engineered mutation	UNP W5R8B8
B	275	TYR	HIS	engineered mutation	UNP W5R8B8
C	247	ASN	SER	engineered mutation	UNP W5R8B8
C	275	TYR	HIS	engineered mutation	UNP W5R8B8
D	247	ASN	SER	engineered mutation	UNP W5R8B8
D	275	TYR	HIS	engineered mutation	UNP W5R8B8

- Molecule 2 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	4	Total	C	N	O	0	0	0
			49	28	2	19			

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

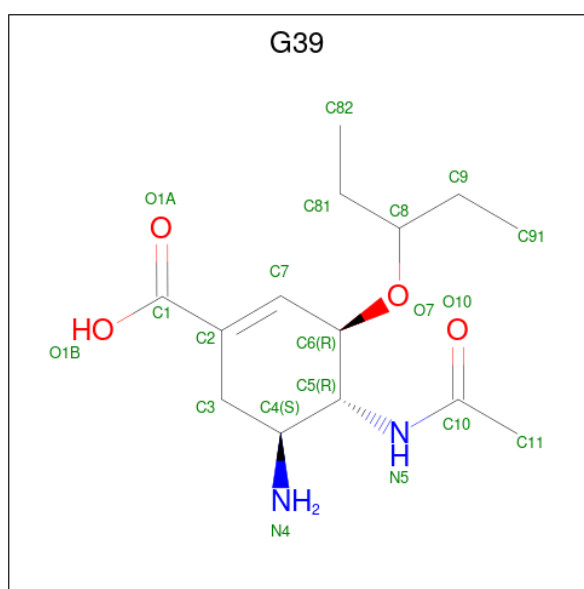


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	F	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

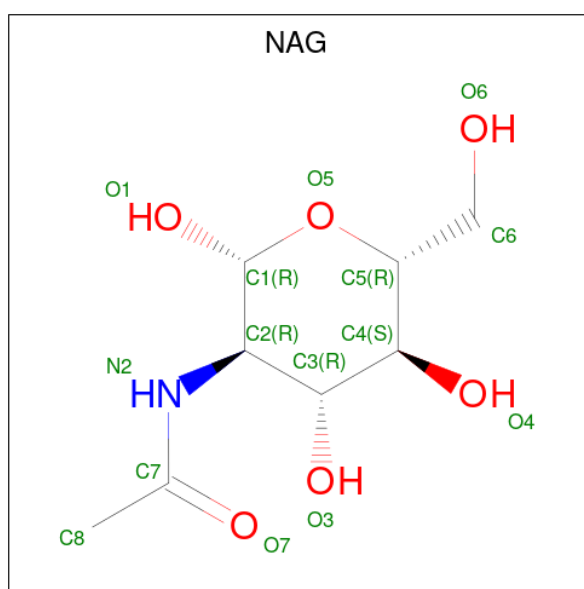
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Ca	0	0
			2	2		
4	B	2	Total	Ca	0	0
			2	2		
4	C	2	Total	Ca	0	0
			2	2		
4	D	2	Total	Ca	0	0
			2	2		

- Molecule 5 is (3R,4R,5S)-4-(acetlamino)-5-amino-3-(pentan-3-yloxy)cyclohex-1-ene-1-carboxylic acid (CCD ID: G39) (formula: C₁₄H₂₄N₂O₄).



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

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



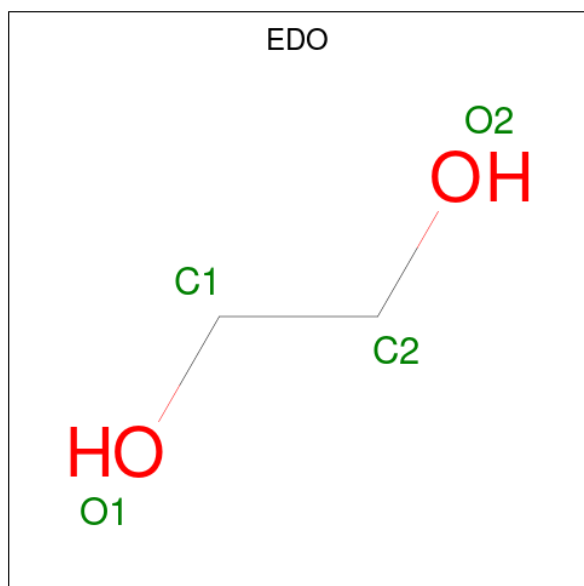
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	B	1	Total	C	N	O	0	0
			14	8	1	5		
6	B	1	Total	C	N	O	0	0
			14	8	1	5		
6	B	1	Total	C	N	O	0	0
			14	8	1	5		
6	C	1	Total	C	N	O	0	0
			14	8	1	5		
6	C	1	Total	C	N	O	0	0
			14	8	1	5		

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

- Molecule 7 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	2	2		
7	C	1	Total	C	O	0	0
			4	2	2		

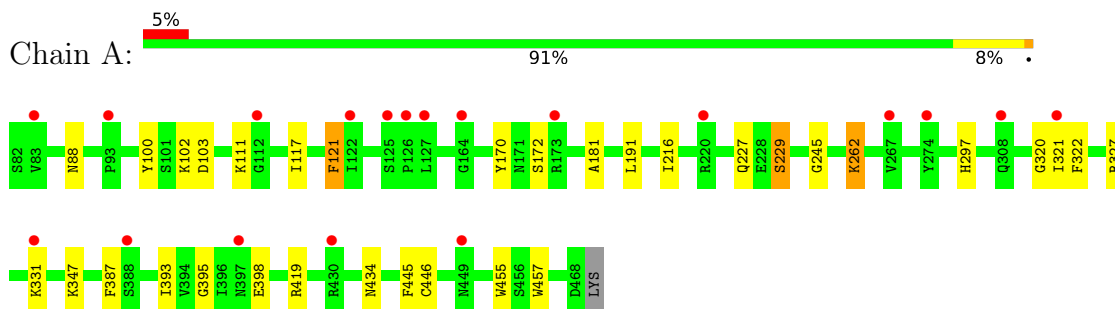
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	326	Total	O	0	1
			327	327		
8	B	351	Total	O	0	8
			359	359		
8	C	354	Total	O	0	6
			359	359		
8	D	331	Total	O	0	6
			337	337		

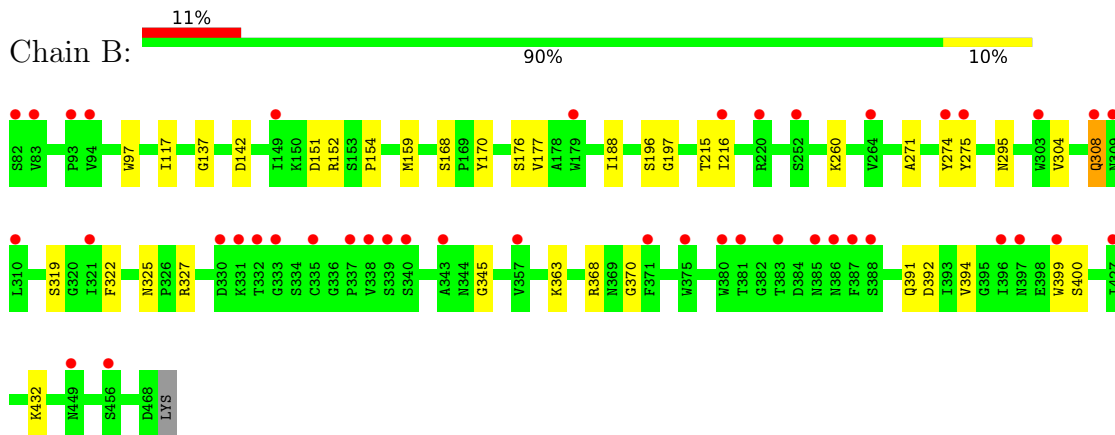
3 Residue-property plots

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

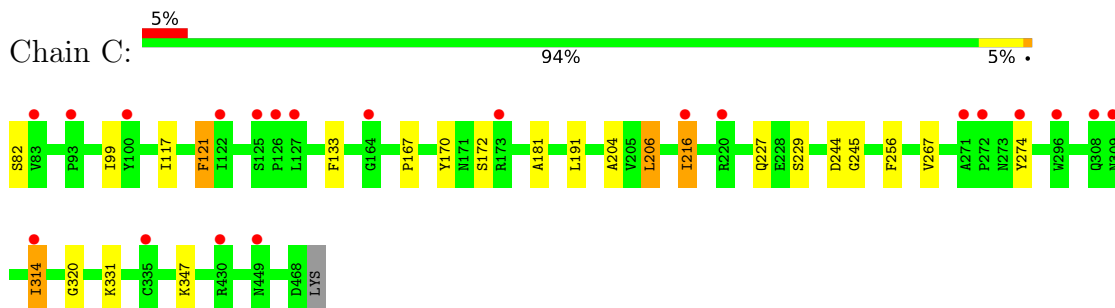
- Molecule 1: Neuraminidase



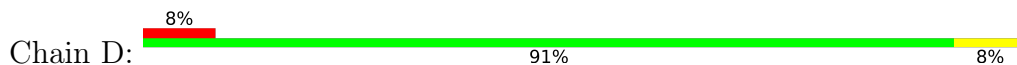
- Molecule 1: Neuraminidase

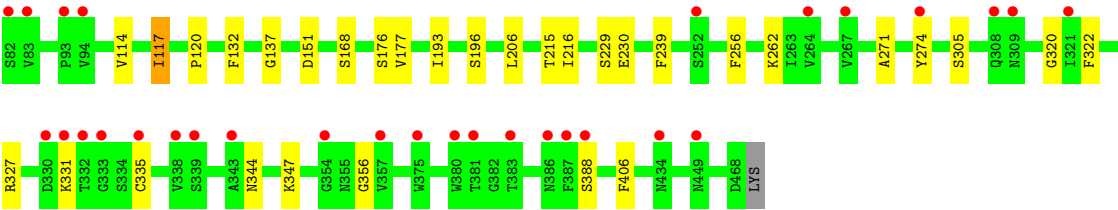


- Molecule 1: Neuraminidase



- Molecule 1: Neuraminidase





• Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	85.78Å 127.54Å 96.77Å 90.00° 93.24° 90.00°	Depositor
Resolution (Å)	48.31 – 1.73 48.31 – 1.73	Depositor EDS
% Data completeness (in resolution range)	99.4 (48.31-1.73) 99.5 (48.31-1.73)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 1.73Å)	Xtrriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.229 , 0.261 (Not available) , 0.259	Depositor DCC
R_{free} test set	2253 reflections (1.05%)	wwPDB-VP
Wilson B-factor (Å ²)	15.6	Xtrriage
Anisotropy	0.094	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 48.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	13688	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 27.87 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.0375e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: BMA, G39, FUC, NAG, EDO, CA

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	1.24	8/3102 (0.3%)	1.07	6/4216 (0.1%)
1	B	1.29	11/3085 (0.4%)	1.10	3/4194 (0.1%)
1	C	1.23	8/3085 (0.3%)	1.08	4/4194 (0.1%)
1	D	1.22	6/3088 (0.2%)	1.06	3/4197 (0.1%)
All	All	1.25	33/12360 (0.3%)	1.08	16/16801 (0.1%)

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	314	ILE	CB-CG1	10.58	1.74	1.53
1	D	114	VAL	C-O	-9.29	1.14	1.24
1	B	394	VAL	C-O	6.76	1.30	1.24
1	C	191	LEU	C-O	-6.62	1.16	1.24
1	A	191	LEU	C-O	-6.44	1.16	1.24
1	B	196	SER	C-O	6.18	1.31	1.24
1	D	305	SER	N-CA	-6.17	1.38	1.45
1	C	172	SER	CA-CB	-6.11	1.44	1.53
1	B	152	ARG	C-O	6.07	1.30	1.24
1	D	196	SER	C-O	5.92	1.30	1.24
1	A	121	PHE	C-O	5.86	1.30	1.23
1	A	172	SER	CA-CB	-5.85	1.45	1.53
1	A	100	TYR	CA-C	5.77	1.58	1.52
1	D	356	GLY	N-CA	5.75	1.50	1.44
1	C	121	PHE	C-O	5.75	1.30	1.23
1	A	170	TYR	N-CA	5.66	1.53	1.46
1	A	102	LYS	CA-C	-5.60	1.45	1.52
1	A	457	TRP	CA-C	5.57	1.58	1.52
1	B	159	MET	C-O	-5.57	1.16	1.23
1	B	215	THR	C-O	-5.52	1.17	1.23
1	B	170	TYR	CA-C	-5.51	1.45	1.52
1	B	319	SER	CA-C	-5.39	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	215	THR	C-O	-5.37	1.17	1.23
1	B	97	TRP	C-O	-5.30	1.18	1.24
1	C	170	TYR	N-CA	5.24	1.52	1.46
1	C	206	LEU	CA-C	5.24	1.59	1.52
1	C	204	ALA	N-CA	-5.23	1.39	1.46
1	B	177	VAL	C-O	-5.14	1.18	1.24
1	D	117	ILE	C-O	5.13	1.29	1.23
1	B	304	VAL	C-O	5.03	1.29	1.23
1	C	244	ASP	C-O	-5.02	1.18	1.23
1	A	229	SER	N-CA	-5.01	1.40	1.46
1	B	260	LYS	N-CA	-5.00	1.39	1.46

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	227	GLN	N-CA-C	7.13	119.05	111.28
1	B	151	ASP	N-CA-C	7.00	118.99	111.36
1	B	168	SER	CA-C-N	-6.92	112.68	119.87
1	B	168	SER	C-N-CA	-6.92	112.68	119.87
1	C	227	GLN	N-CA-C	6.33	118.17	111.28
1	D	168	SER	CA-C-N	-5.69	113.95	119.87
1	D	168	SER	C-N-CA	-5.69	113.95	119.87
1	A	181	ALA	N-CA-C	5.65	117.65	109.07
1	A	245	GLY	CA-C-N	5.43	125.43	119.89
1	A	245	GLY	C-N-CA	5.43	125.43	119.89
1	A	103	ASP	N-CA-C	5.26	119.97	113.50
1	C	181	ALA	N-CA-C	5.22	117.00	109.07
1	A	395	GLY	N-CA-C	-5.08	104.95	113.02
1	C	245	GLY	CA-C-N	5.08	125.07	119.89
1	C	245	GLY	C-N-CA	5.08	125.07	119.89
1	D	151	ASP	N-CA-C	5.01	117.85	111.69

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	3012	0	2843	14	0
1	B	3003	0	2827	16	0
1	C	3003	0	2827	11	0
1	D	3003	0	2836	14	0
2	E	49	0	43	0	0
3	F	28	0	25	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
5	A	20	0	23	0	0
5	B	20	0	23	1	0
5	C	20	0	23	0	0
5	D	20	0	23	0	0
6	A	28	0	26	0	0
6	B	42	0	39	0	0
6	C	28	0	26	0	0
6	D	14	0	13	0	0
7	A	4	0	6	1	0
7	C	4	0	6	2	0
8	A	327	0	0	4	2
8	B	359	0	0	3	1
8	C	359	0	0	3	2
8	D	337	0	0	3	1
All	All	13688	0	11609	53	3

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 2.

All (53) 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:B:392:ASP:HB3	8:B:614:HOH:O	1.80	0.80
7:C:510:EDO:H21	8:C:604:HOH:O	1.92	0.69
1:C:314:ILE:CG1	1:C:314:ILE:CA	2.71	0.68
7:A:506:EDO:H12	1:B:154:PRO:HG3	1.79	0.63
1:C:314:ILE:CG1	1:C:314:ILE:CG2	2.76	0.63
8:C:854:HOH:O	1:D:137:GLY:HA2	2.06	0.55
1:B:322:PHE:HB2	1:B:327:ARG:HD2	1.92	0.52
1:B:391:GLN:HG3	8:B:874:HOH:O	2.11	0.51
1:A:398:GLU:OE1	8:A:601:HOH:O	2.18	0.49
1:D:320:GLY:HA3	1:D:331:LYS:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:344:ASN:ND2	8:D:604:HOH:O	2.42	0.49
1:A:88:ASN:ND2	8:A:605:HOH:O	2.46	0.49
1:B:363:LYS:NZ	1:B:392:ASP:OD1	2.37	0.49
1:C:99:ILE:HG12	1:D:177:VAL:HG21	1.95	0.49
1:A:419:ARG:HD3	1:A:446:CYS:HB3	1.95	0.48
1:D:271:ALA:HB1	1:D:274:TYR:HB2	1.96	0.47
1:D:335:CYS:HB3	8:D:681:HOH:O	2.15	0.47
1:A:322:PHE:HB2	1:A:327:ARG:HD2	1.97	0.46
1:B:368:ARG:C	1:B:400:SER:HB3	2.40	0.46
1:B:399:TRP:CH2	1:B:432:LYS:HB3	2.51	0.46
1:C:320:GLY:HA3	1:C:331:LYS:O	2.16	0.45
1:A:321:ILE:HD11	1:A:387:PHE:HB3	1.98	0.45
1:B:271:ALA:HB1	1:B:274:TYR:HB2	1.97	0.45
1:D:229:SER:HB3	1:D:347:LYS:HE2	1.98	0.45
1:D:239:PHE:HA	1:D:256:PHE:O	2.16	0.45
1:B:295:ASN:ND2	5:B:503:G39:H911	2.32	0.44
1:A:229:SER:HB3	1:A:347:LYS:HE2	1.99	0.44
1:A:455:TRP:CE3	1:B:197:GLY:HA2	2.53	0.44
1:D:193:ILE:HG12	1:D:206:LEU:HG	1.99	0.44
1:D:230:GLU:OE2	1:D:406:PHE:HA	2.18	0.44
1:C:229:SER:HB3	1:C:347:LYS:HE2	2.00	0.43
1:B:308:GLN:OE1	8:B:601:HOH:O	2.22	0.43
1:C:99:ILE:HD13	1:D:177:VAL:HG11	2.01	0.42
1:D:120:PRO:HA	1:D:132:PHE:O	2.19	0.42
1:C:206:LEU:HD12	1:C:206:LEU:N	2.34	0.42
7:C:510:EDO:C2	8:C:604:HOH:O	2.56	0.42
1:D:262:LYS:HD3	8:D:884:HOH:O	2.17	0.42
1:B:325:ASN:O	1:B:345:GLY:HA2	2.18	0.42
1:A:321:ILE:CD1	1:A:387:PHE:HB3	2.48	0.42
1:A:393:ILE:HG23	1:A:445:PHE:CZ	2.55	0.42
1:C:216:ILE:HD13	1:C:256:PHE:CE2	2.55	0.41
8:A:853:HOH:O	1:B:137:GLY:HA2	2.18	0.41
1:A:121:PHE:CG	1:A:229:SER:HA	2.56	0.41
1:A:434:ASN:ND2	8:A:603:HOH:O	2.43	0.41
1:B:275:TYR:CD1	1:B:275:TYR:C	2.99	0.41
1:B:370:GLY:O	1:B:400:SER:OG	2.31	0.41
1:C:274:TYR:CZ	1:C:314:ILE:HD12	2.56	0.41
1:D:322:PHE:HB2	1:D:327:ARG:HD2	2.03	0.41
1:A:262:LYS:HE3	1:A:262:LYS:HB3	1.83	0.40
1:C:121:PHE:CG	1:C:229:SER:HA	2.57	0.40
1:C:133:PHE:CE2	1:C:167:PRO:HB3	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:LYS:HB2	1:B:142:ASP:HB2	2.04	0.40

All (3) 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)
8:A:620:HOH:O	8:D:675:HOH:O[2_646]	0.75	1.45
8:B:750:HOH:O	8:C:615:HOH:O[2_545]	1.33	0.87
8:A:608:HOH:O	8:C:631:HOH:O[2_645]	1.84	0.36

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	388/388 (100%)	374 (96%)	14 (4%)	0	100	100
1	B	386/388 (100%)	370 (96%)	16 (4%)	0	100	100
1	C	386/388 (100%)	368 (95%)	18 (5%)	0	100	100
1	D	386/388 (100%)	372 (96%)	14 (4%)	0	100	100
All	All	1546/1552 (100%)	1484 (96%)	62 (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	337/335 (101%)	331 (98%)	6 (2%)	51	30
1	B	335/335 (100%)	330 (98%)	5 (2%)	57	38
1	C	335/335 (100%)	331 (99%)	4 (1%)	63	47
1	D	335/335 (100%)	331 (99%)	4 (1%)	63	47
All	All	1342/1340 (100%)	1323 (99%)	19 (1%)	61	41

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	117	ILE
1	A	216	ILE
1	A	262	LYS
1	A	297	HIS
1	A	331[A]	LYS
1	A	331[B]	LYS
1	B	117	ILE
1	B	176	SER
1	B	188	ILE
1	B	216	ILE
1	B	308	GLN
1	C	82	SER
1	C	117	ILE
1	C	216	ILE
1	C	267	VAL
1	D	117	ILE
1	D	176	SER
1	D	216	ILE
1	D	388	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	221	ASN
1	A	355	ASN
1	B	104	ASN
1	B	325	ASN
1	B	329	ASN
1	B	341	ASN
1	B	355	ASN
1	B	449	ASN

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Mol	Chain	Res	Type
1	C	355	ASN
1	C	449	ASN
1	D	344	ASN
1	D	355	ASN
1	D	449	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 ⓘ

6 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	0.60	0	17,19,21	0.72	0
2	NAG	E	2	2	14,14,15	0.60	0	17,19,21	0.82	1 (5%)
2	BMA	E	3	2	11,11,12	0.96	0	15,15,17	0.75	0
2	FUC	E	4	2	10,10,11	0.97	0	14,14,16	1.81	4 (28%)
3	NAG	F	1	1,3	14,14,15	0.63	0	17,19,21	1.21	2 (11%)
3	NAG	F	2	3	14,14,15	0.60	0	17,19,21	1.06	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
2	NAG	E	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	BMA	E	3	2	-	1/2/19/22	0/1/1/1
2	FUC	E	4	2	-	-	0/1/1/1
3	NAG	F	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	4	FUC	C1-C2-C3	4.02	115.49	109.64
2	E	4	FUC	O5-C5-C6	2.90	113.69	107.40
2	E	4	FUC	O2-C2-C3	-2.84	104.27	110.15
2	E	2	NAG	O5-C5-C6	2.52	112.57	107.66
3	F	1	NAG	O3-C3-C2	-2.43	104.34	109.40
3	F	1	NAG	C2-N2-C7	-2.41	119.67	122.90
2	E	4	FUC	O5-C5-C4	2.19	113.50	109.55
3	F	2	NAG	O4-C4-C3	2.04	115.18	110.38

There are no chirality outliers.

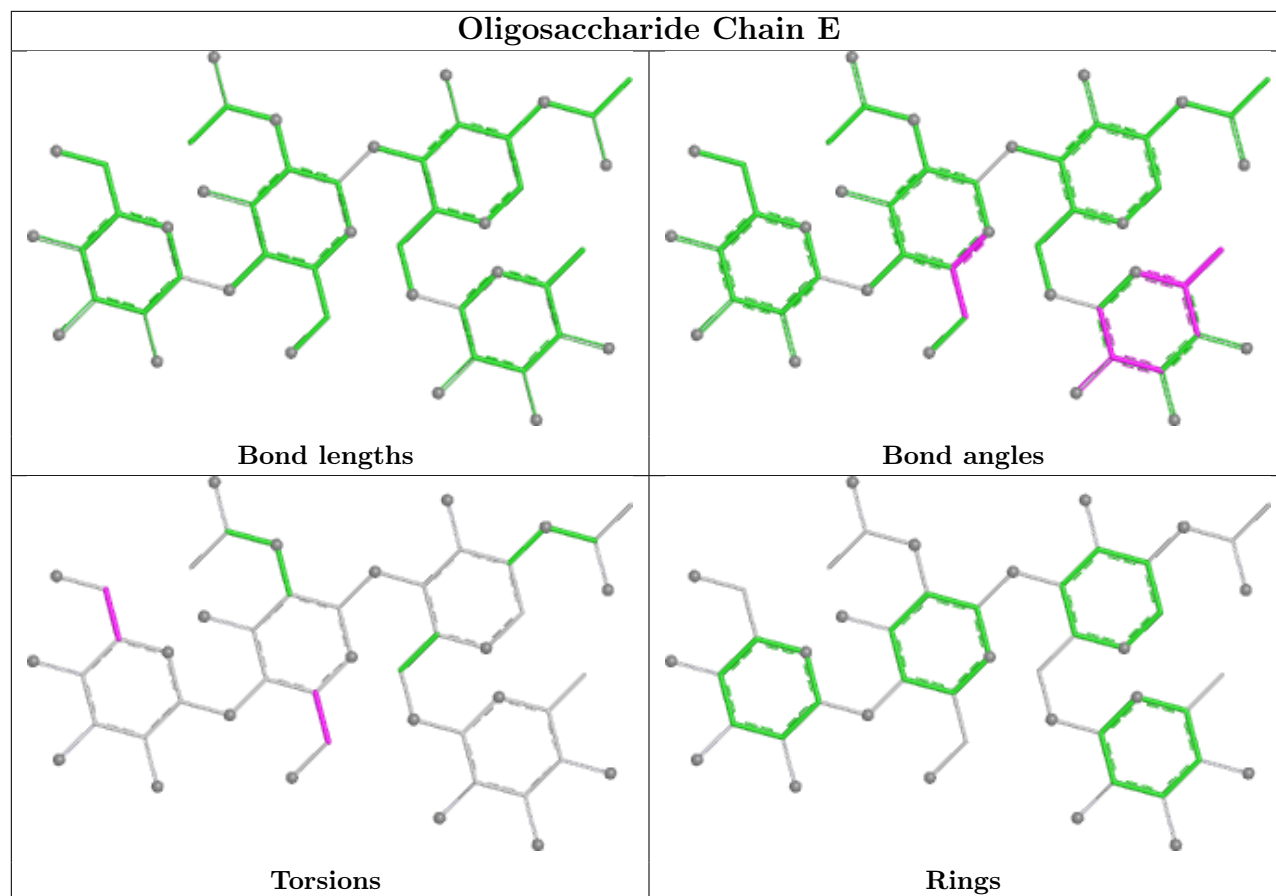
All (5) torsion outliers are listed below:

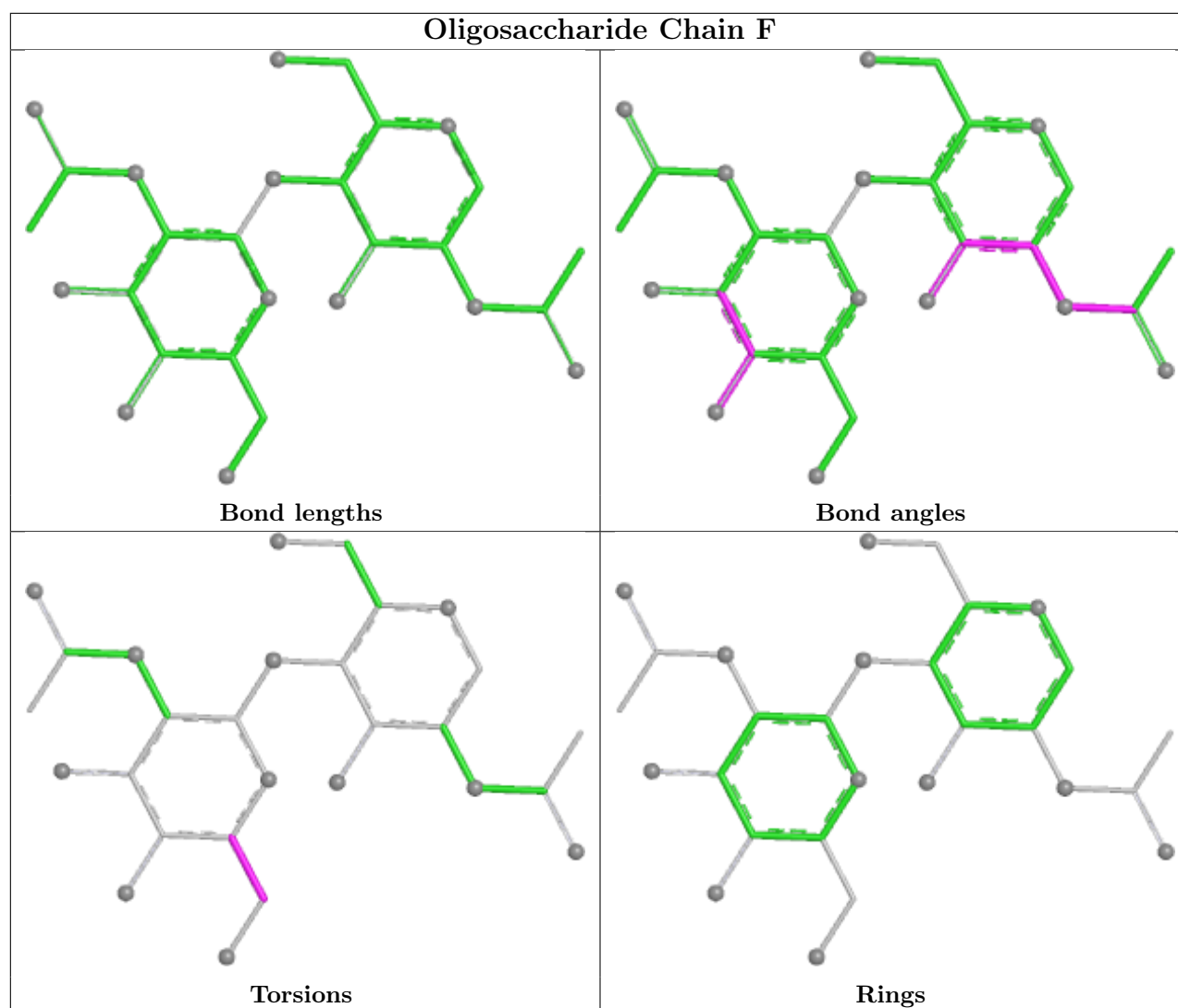
Mol	Chain	Res	Type	Atoms
2	E	2	NAG	O5-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
2	E	3	BMA	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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 22 ligands modelled in this entry, 8 are monoatomic - leaving 14 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	$\# Z > 2$
5	G39	D	503	-	19,20,20	1.16	3 (15%)	20,27,27	1.47	4 (20%)
6	NAG	B	506	1	14,14,15	0.52	0	17,19,21	0.70	0
6	NAG	C	509	1	14,14,15	0.58	0	17,19,21	1.01	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	B	505	1	14,14,15	0.92	1 (7%)	17,19,21	2.11	5 (29%)
6	NAG	A	504	1	14,14,15	0.60	0	17,19,21	1.05	0
6	NAG	A	505	1	14,14,15	0.55	0	17,19,21	1.76	4 (23%)
7	EDO	C	510	-	3,3,3	0.42	0	2,2,2	0.33	0
5	G39	B	503	-	19,20,20	1.07	3 (15%)	20,27,27	1.17	2 (10%)
6	NAG	D	506	1	14,14,15	0.47	0	17,19,21	1.05	1 (5%)
5	G39	C	503	-	19,20,20	0.93	0	20,27,27	1.74	5 (25%)
7	EDO	A	506	-	3,3,3	1.53	0	2,2,2	0.77	0
5	G39	A	503	-	19,20,20	1.14	2 (10%)	20,27,27	1.40	2 (10%)
6	NAG	B	504	1	14,14,15	0.64	0	17,19,21	2.68	5 (29%)
6	NAG	C	504	1	14,14,15	0.57	0	17,19,21	2.93	5 (29%)

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
5	G39	D	503	-	-	0/16/32/32	0/1/1/1
6	NAG	B	506	1	-	2/6/23/26	0/1/1/1
6	NAG	C	509	1	-	0/6/23/26	0/1/1/1
6	NAG	B	505	1	-	0/6/23/26	0/1/1/1
6	NAG	A	504	1	-	0/6/23/26	0/1/1/1
6	NAG	A	505	1	-	0/6/23/26	0/1/1/1
7	EDO	C	510	-	-	1/1/1/1	-
5	G39	B	503	-	-	0/16/32/32	0/1/1/1
6	NAG	D	506	1	-	0/6/23/26	0/1/1/1
5	G39	C	503	-	-	0/16/32/32	0/1/1/1
7	EDO	A	506	-	-	1/1/1/1	-
5	G39	A	503	-	-	0/16/32/32	0/1/1/1
6	NAG	B	504	1	-	2/6/23/26	0/1/1/1
6	NAG	C	504	1	-	2/6/23/26	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	503	G39	C6-C7	2.84	1.54	1.50
5	B	503	G39	O7-C8	2.52	1.48	1.44
5	A	503	G39	O1A-C1	2.43	1.28	1.22
5	D	503	G39	O10-C10	-2.37	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	503	G39	C6-C7	2.26	1.53	1.50
5	D	503	G39	O1A-C1	2.23	1.28	1.22
6	B	505	NAG	C1-C2	2.22	1.55	1.52
5	B	503	G39	O1A-C1	2.04	1.27	1.22
5	B	503	G39	O10-C10	-2.02	1.18	1.23

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	504	NAG	C1-C2-N2	-8.94	96.34	110.43
6	B	504	NAG	C1-C2-N2	-8.56	96.94	110.43
6	C	504	NAG	C2-N2-C7	6.43	131.51	122.90
6	B	505	NAG	C4-C3-C2	-4.91	103.83	111.02
5	C	503	G39	O1A-C1-C2	-3.83	114.93	121.64
5	A	503	G39	C6-C5-N5	-3.77	106.91	111.13
6	B	505	NAG	C3-C4-C5	-3.74	103.46	110.23
5	A	503	G39	C4-C3-C2	3.60	113.79	109.72
5	D	503	G39	C4-C3-C2	3.57	113.76	109.72
5	C	503	G39	C4-C3-C2	3.51	113.69	109.72
6	B	504	NAG	O5-C1-C2	3.24	116.30	111.29
6	B	504	NAG	C4-C3-C2	3.18	115.68	111.02
6	A	505	NAG	C1-O5-C5	3.13	116.38	112.19
6	A	505	NAG	C4-C3-C2	-3.12	106.45	111.02
6	A	505	NAG	O5-C1-C2	-2.94	106.74	111.29
6	B	505	NAG	O4-C4-C5	2.84	116.33	109.32
6	C	504	NAG	O7-C7-N2	2.81	126.94	121.98
5	C	503	G39	O1B-C1-C2	2.79	121.33	115.43
5	D	503	G39	O1A-C1-C2	-2.77	116.78	121.64
6	B	504	NAG	C3-C4-C5	2.63	115.00	110.23
6	C	509	NAG	O5-C1-C2	-2.60	107.27	111.29
6	C	504	NAG	C8-C7-N2	-2.57	111.86	116.12
5	D	503	G39	O10-C10-C11	-2.45	117.68	122.05
5	D	503	G39	O1B-C1-C2	2.29	120.27	115.43
5	C	503	G39	C6-C5-N5	-2.29	108.56	111.13
5	B	503	G39	C7-C2-C1	-2.24	116.92	119.99
6	C	504	NAG	O3-C3-C4	-2.23	105.12	110.38
6	A	505	NAG	O4-C4-C5	2.19	114.72	109.32
6	B	505	NAG	O3-C3-C2	2.18	113.92	109.40
6	B	505	NAG	O7-C7-N2	2.16	125.80	121.98
6	B	504	NAG	C2-N2-C7	2.15	125.78	122.90
5	C	503	G39	O10-C10-N5	2.13	125.75	121.98
5	B	503	G39	C3-C2-C1	2.13	120.89	116.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	506	NAG	C1-O5-C5	-2.09	109.39	112.19

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	504	NAG	C3-C2-N2-C7
6	B	504	NAG	O5-C5-C6-O6
6	B	504	NAG	C4-C5-C6-O6
7	A	506	EDO	O1-C1-C2-O2
6	B	506	NAG	C4-C5-C6-O6
6	C	504	NAG	C1-C2-N2-C7
7	C	510	EDO	O1-C1-C2-O2
6	B	506	NAG	O5-C5-C6-O6

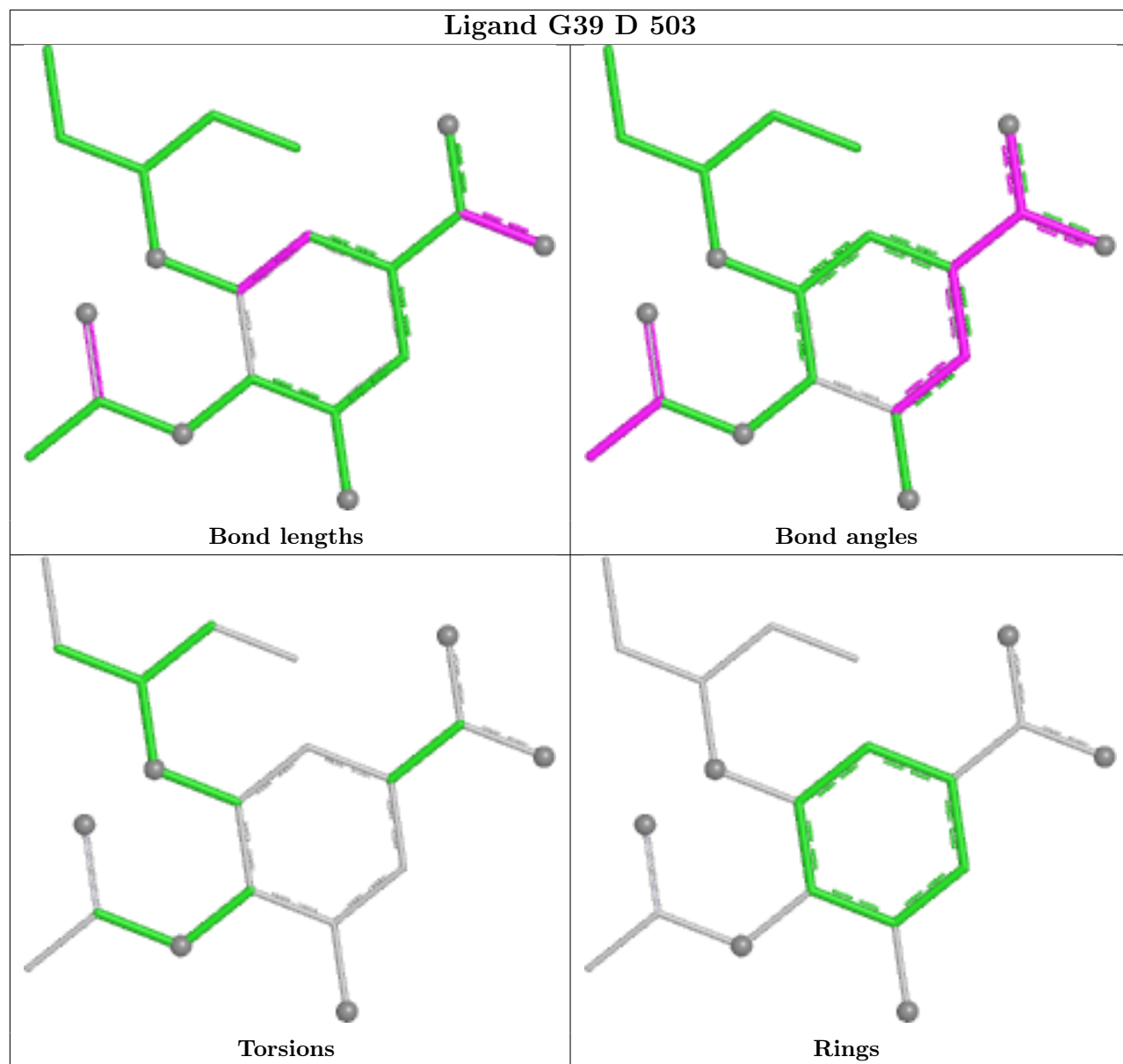
There are no ring outliers.

3 monomers are involved in 4 short contacts:

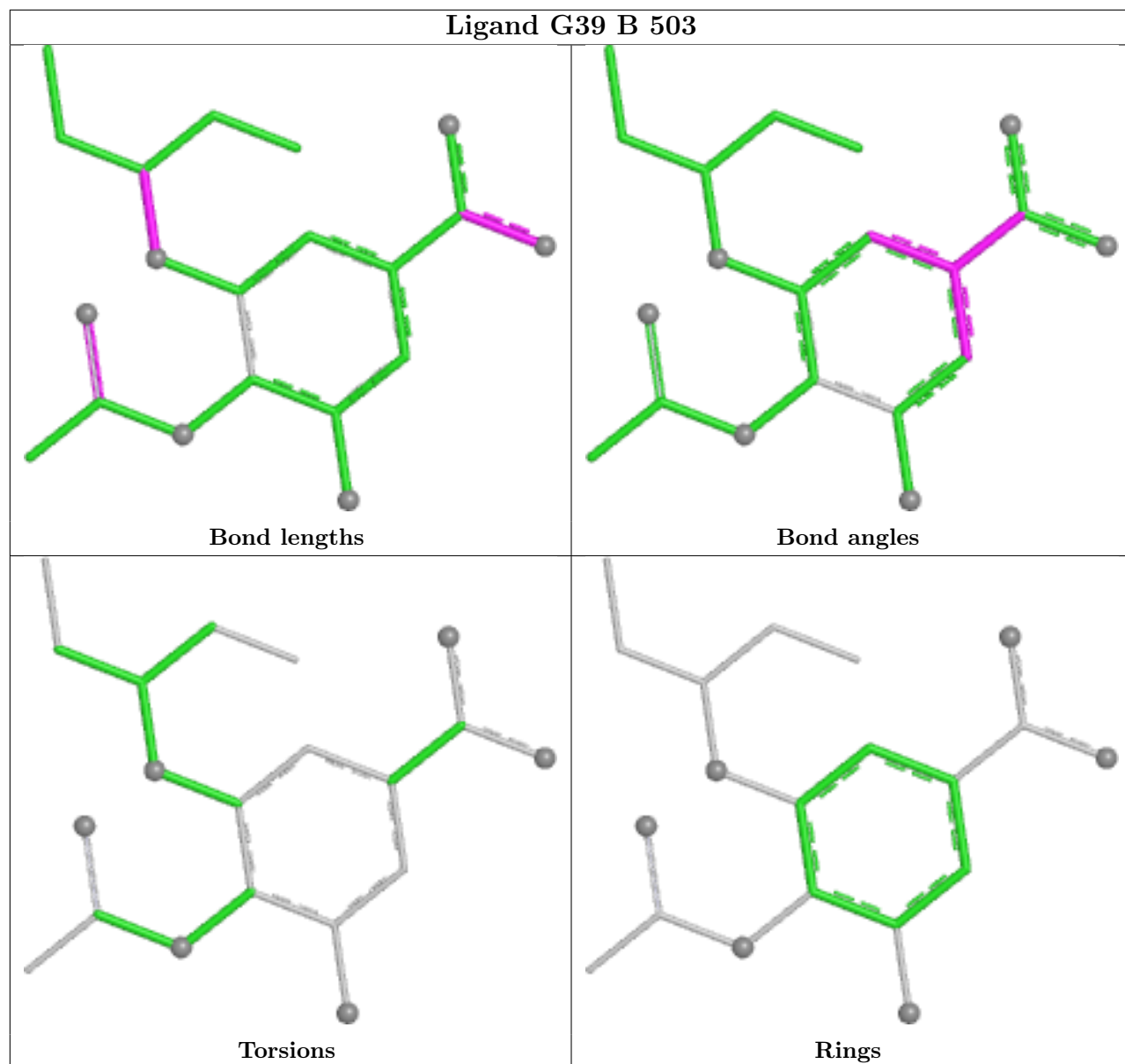
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	510	EDO	2	0
5	B	503	G39	1	0
7	A	506	EDO	1	0

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.

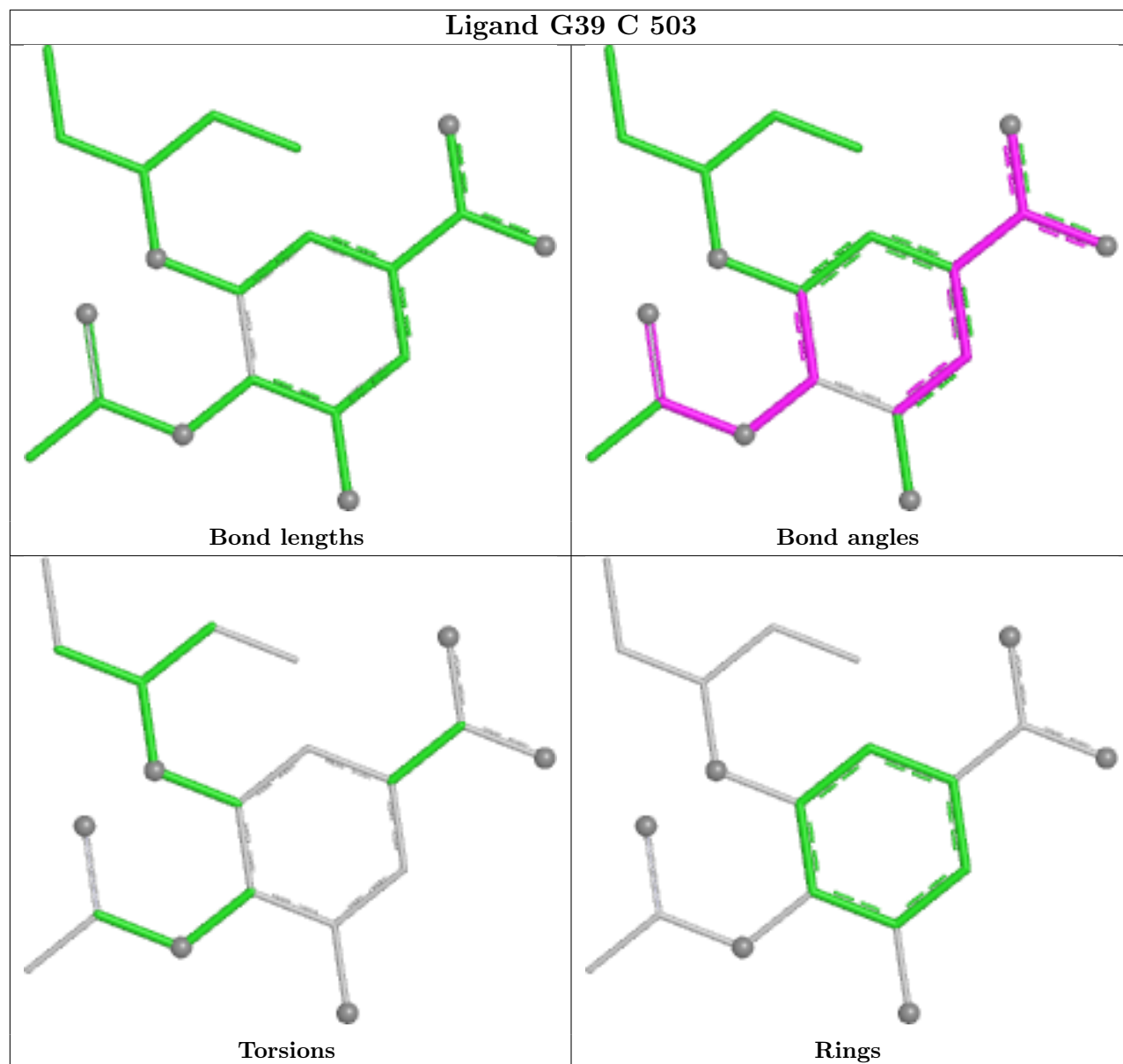
Ligand G39 D 503

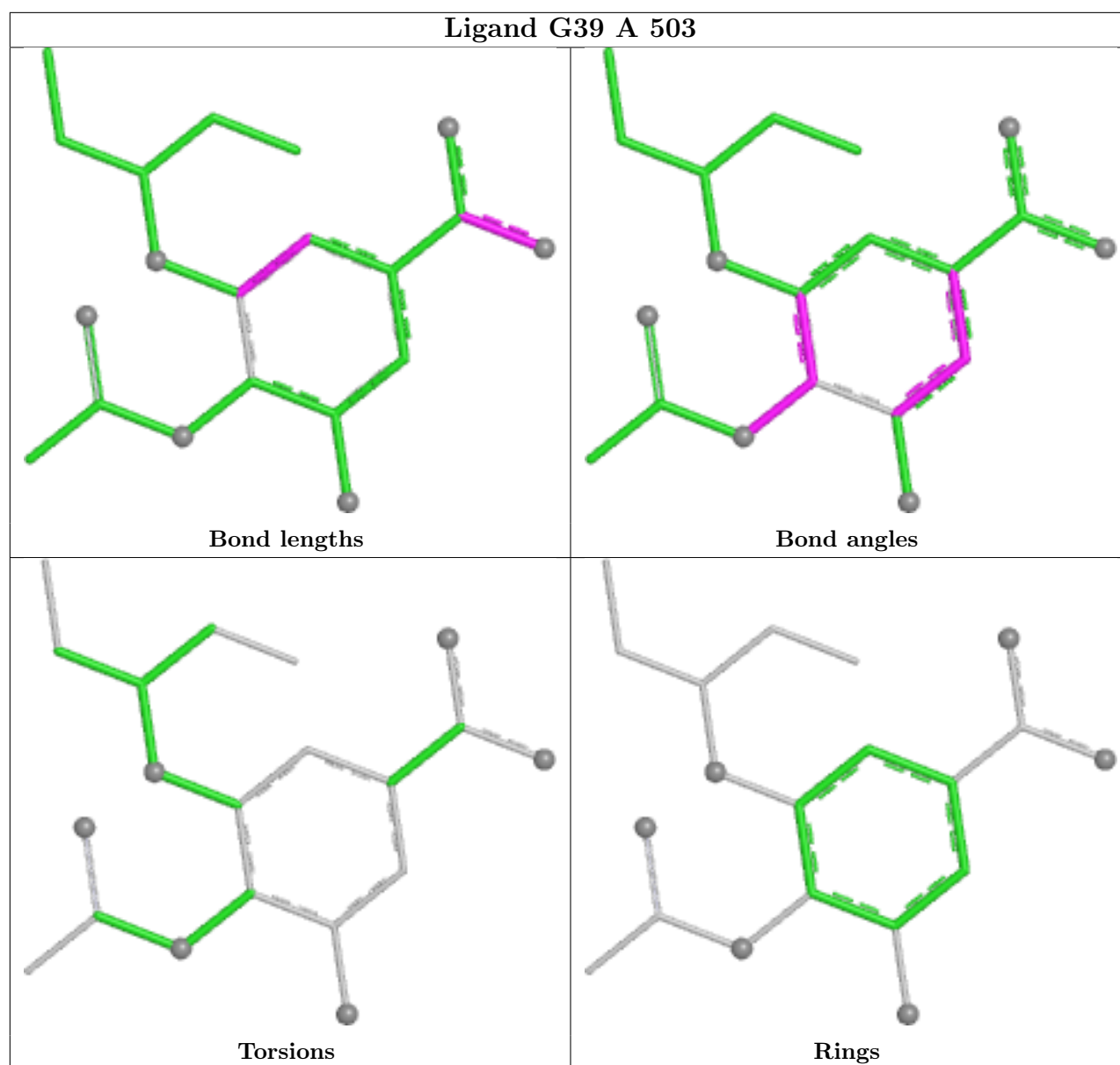


Ligand G39 B 503



Ligand G39 C 503





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	387/388 (99%)	0.54	19 (4%)	35	42	8, 15, 24, 36	3 (0%)
1	B	387/388 (99%)	0.96	43 (11%)	10	14	10, 17, 27, 37	1 (0%)
1	C	387/388 (99%)	0.65	21 (5%)	31	38	9, 15, 25, 34	2 (0%)
1	D	387/388 (99%)	0.75	30 (7%)	19	24	10, 17, 27, 38	1 (0%)
All	All	1548/1552 (99%)	0.73	113 (7%)	21	26	8, 16, 26, 38	7 (0%)

All (113) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	335	CYS	4.3
1	B	338	VAL	3.8
1	C	430	ARG	3.7
1	A	125	SER	3.5
1	B	331	LYS	3.5
1	C	127	LEU	3.4
1	C	220	ARG	3.3
1	B	149	ILE	3.3
1	B	216	ILE	3.3
1	D	331	LYS	3.2
1	B	309	ASN	3.2
1	D	388	SER	3.2
1	B	332	THR	3.2
1	C	93	PRO	3.1
1	D	381	THR	3.1
1	B	388	SER	3.1
1	C	125	SER	3.1
1	B	330	ASP	3.1
1	A	164	GLY	3.0
1	C	274	TYR	3.0
1	D	93	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	386	ASN	3.0
1	A	430	ARG	3.0
1	D	335	CYS	3.0
1	A	126	PRO	3.0
1	D	386	ASN	2.9
1	B	340	SER	2.9
1	D	94	VAL	2.9
1	B	357	VAL	2.9
1	A	321	ILE	2.9
1	A	220	ARG	2.8
1	A	93	PRO	2.8
1	B	380	TRP	2.8
1	B	383	THR	2.8
1	B	385	ASN	2.8
1	C	449	ASN	2.8
1	A	308	GLN	2.8
1	D	309	ASN	2.8
1	B	397	ASN	2.7
1	C	296	TRP	2.7
1	C	335	CYS	2.7
1	B	82	SER	2.7
1	B	333	GLY	2.7
1	B	337	PRO	2.7
1	A	274	TYR	2.7
1	D	308	GLN	2.7
1	B	93	PRO	2.7
1	A	127	LEU	2.7
1	B	264	VAL	2.6
1	B	252	SER	2.6
1	D	267	VAL	2.6
1	D	338	VAL	2.6
1	C	122	ILE	2.6
1	D	82	SER	2.6
1	B	381	THR	2.5
1	A	449	ASN	2.5
1	D	274	TYR	2.5
1	B	83	VAL	2.5
1	B	343	ALA	2.5
1	D	387	PHE	2.5
1	B	308	GLN	2.5
1	C	126	PRO	2.5
1	D	332	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	375	TRP	2.5
1	B	310	LEU	2.5
1	D	330	ASP	2.5
1	C	216	ILE	2.5
1	B	399	TRP	2.4
1	D	339	SER	2.4
1	B	387	PHE	2.4
1	C	164	GLY	2.4
1	C	272	PRO	2.4
1	C	309[A]	ASN	2.4
1	C	314	ILE	2.4
1	D	83	VAL	2.4
1	C	271	ALA	2.3
1	A	331[A]	LYS	2.3
1	B	449	ASN	2.3
1	C	100	TYR	2.3
1	A	397	ASN	2.3
1	D	321	ILE	2.3
1	D	449	ASN	2.3
1	B	339	SER	2.3
1	D	375	TRP	2.3
1	D	380	TRP	2.3
1	A	83	VAL	2.3
1	B	274	TYR	2.3
1	A	267	VAL	2.3
1	C	83	VAL	2.3
1	D	264	VAL	2.3
1	D	343	ALA	2.2
1	B	321	ILE	2.2
1	C	308	GLN	2.2
1	B	94	VAL	2.2
1	B	456	SER	2.2
1	D	333	GLY	2.2
1	B	427	ILE	2.2
1	D	354	GLY	2.2
1	B	275	TYR	2.2
1	B	396	ILE	2.2
1	D	357	VAL	2.1
1	B	179	TRP	2.1
1	A	173	ARG	2.1
1	A	388	SER	2.1
1	B	303	TRP	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	173	ARG	2.1
1	B	371	PHE	2.1
1	A	122	ILE	2.1
1	D	383	THR	2.1
1	B	220	ARG	2.0
1	A	112	GLY	2.0
1	D	434	ASN	2.0
1	D	252	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](#)

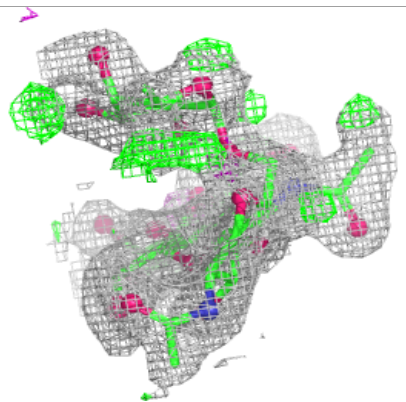
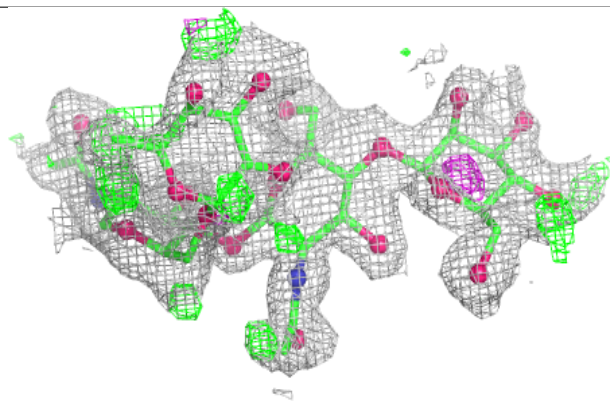
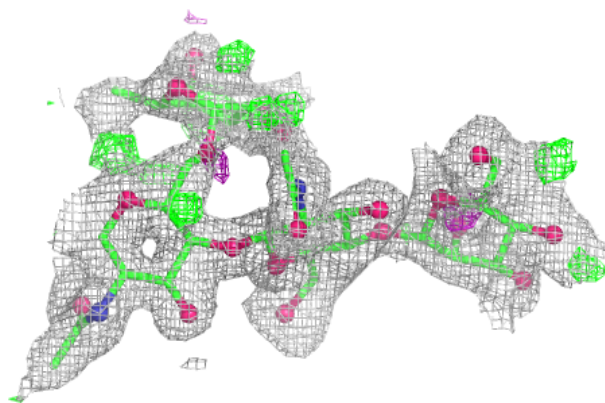
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

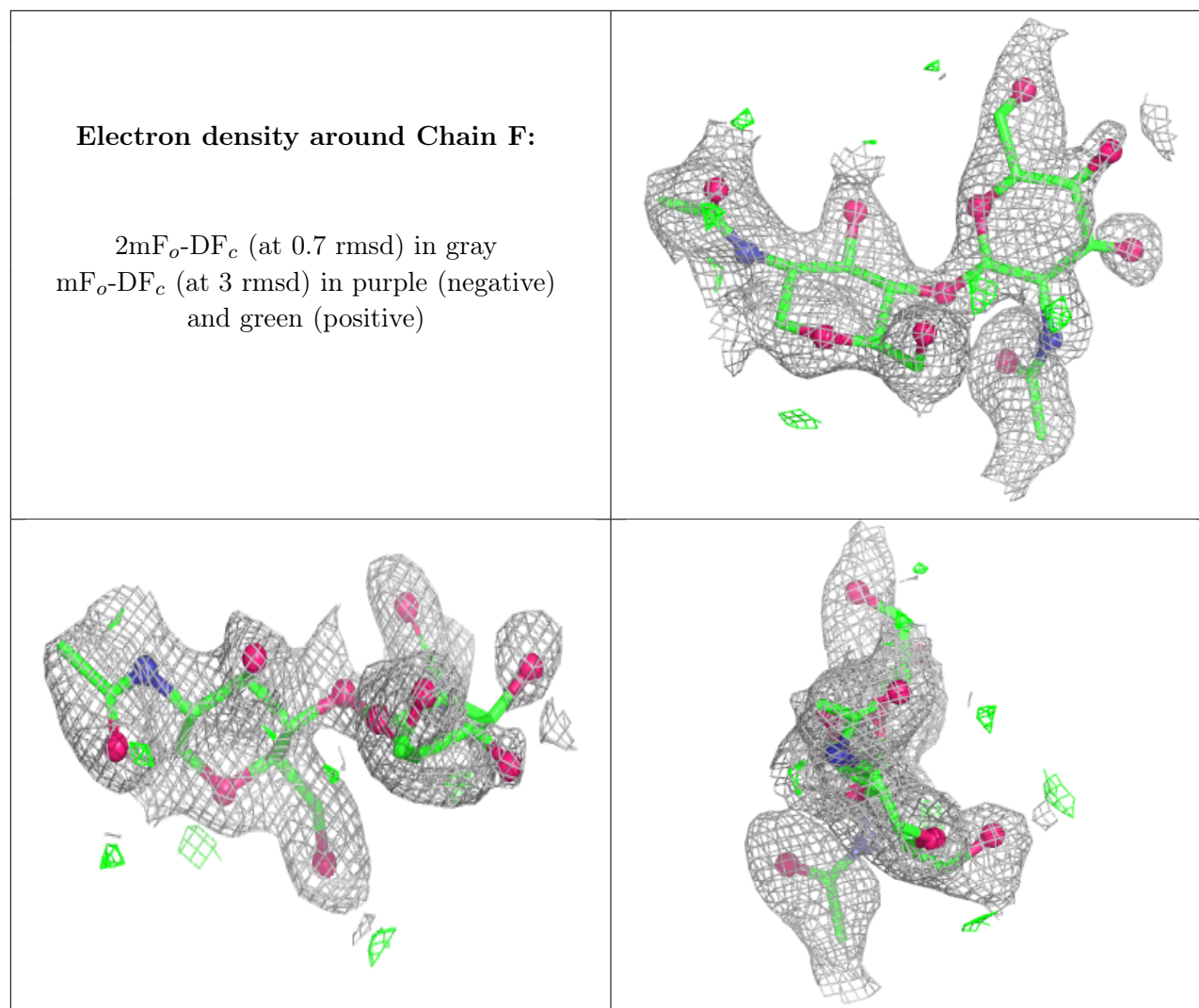
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAG	F	2	14/15	0.62	0.21	37,44,46,48	0
2	BMA	E	3	11/12	0.69	0.17	32,38,40,46	0
2	FUC	E	4	10/11	0.75	0.17	30,32,32,37	0
3	NAG	F	1	14/15	0.82	0.13	31,37,38,44	0
2	NAG	E	1	14/15	0.82	0.15	24,29,33,34	0
2	NAG	E	2	14/15	0.85	0.13	28,30,32,38	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.

Electron density around Chain E:

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





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($\text{\AA}^2$)	Q<0.9
6	NAG	B	505	14/15	0.61	0.23	35,40,41,42	0
6	NAG	C	504	14/15	0.64	0.18	36,42,45,47	0
6	NAG	B	504	14/15	0.66	0.17	37,41,45,46	0
6	NAG	A	505	14/15	0.73	0.15	35,38,43,44	0
6	NAG	C	509	14/15	0.73	0.15	35,40,42,44	0
6	NAG	D	506	14/15	0.75	0.16	33,38,41,43	0
6	NAG	A	504	14/15	0.79	0.15	32,37,41,42	0
6	NAG	B	506	14/15	0.81	0.14	32,37,40,41	0

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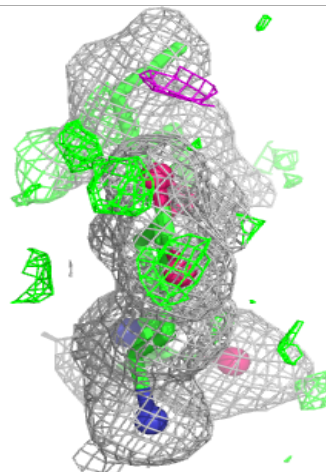
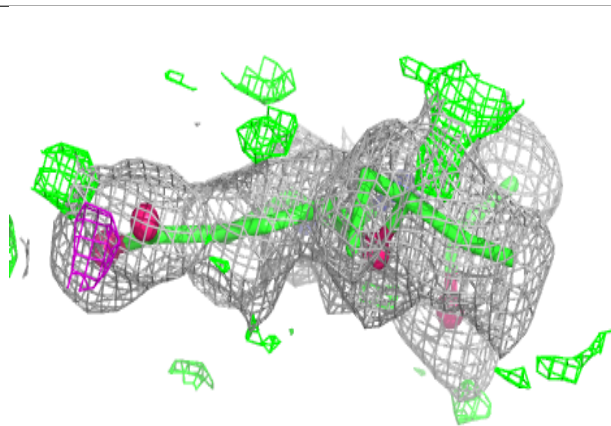
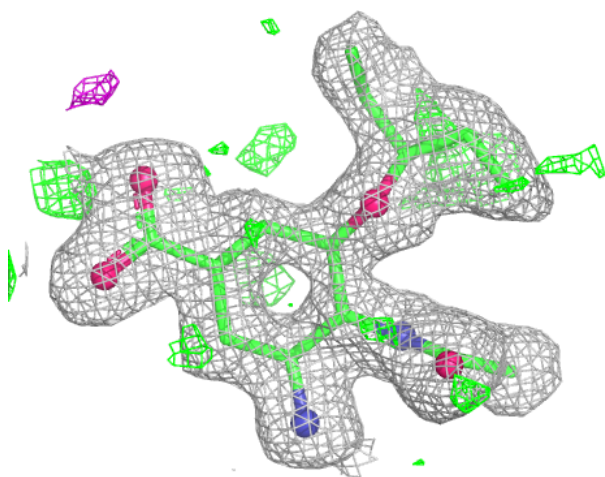
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	EDO	C	510	4/4	0.83	0.15	24,26,26,29	0
7	EDO	A	506	4/4	0.84	0.15	21,23,24,25	0
5	G39	B	503	20/20	0.91	0.11	11,15,24,26	0
5	G39	D	503	20/20	0.91	0.11	13,16,23,24	0
5	G39	C	503	20/20	0.93	0.09	11,14,21,24	0
5	G39	A	503	20/20	0.94	0.09	10,14,22,24	0
4	CA	B	502	1/1	0.95	0.10	26,26,26,26	0
4	CA	B	501	1/1	0.96	0.05	20,20,20,20	0
4	CA	D	502	1/1	0.97	0.09	25,25,25,25	0
4	CA	A	502	1/1	0.97	0.05	20,20,20,20	0
4	CA	C	502	1/1	0.97	0.08	21,21,21,21	0
4	CA	D	501	1/1	0.98	0.04	19,19,19,19	0
4	CA	C	501	1/1	0.99	0.04	15,15,15,15	0
4	CA	A	501	1/1	0.99	0.06	14,14,14,14	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.

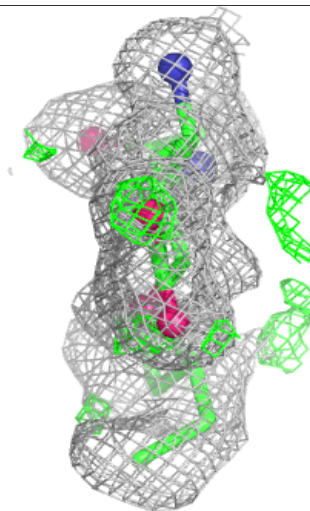
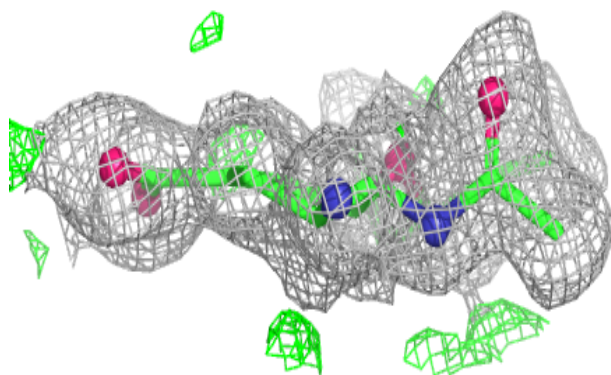
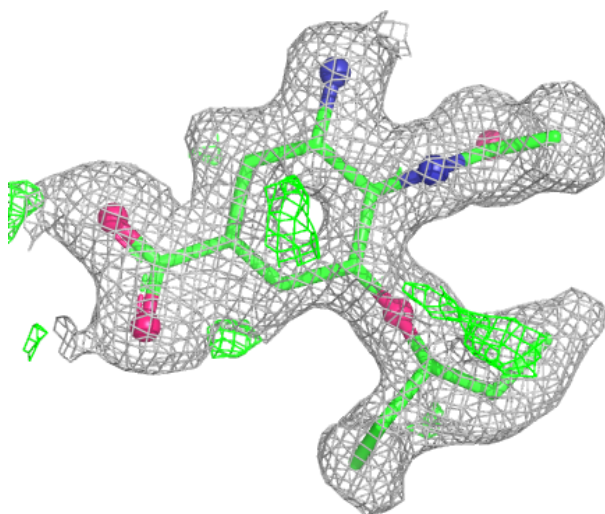
Electron density around G39 B 503:

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



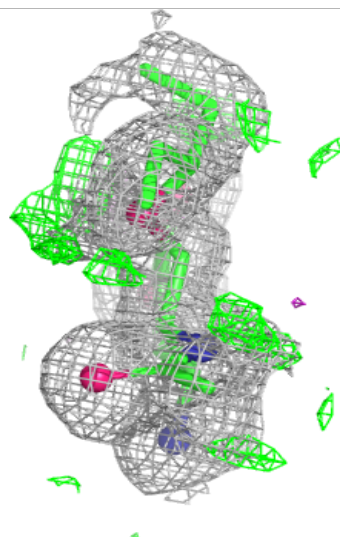
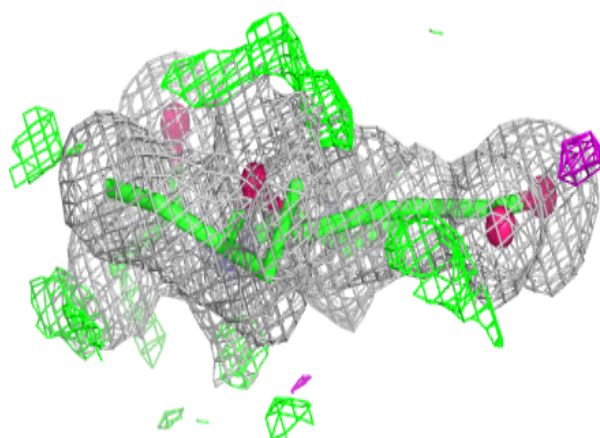
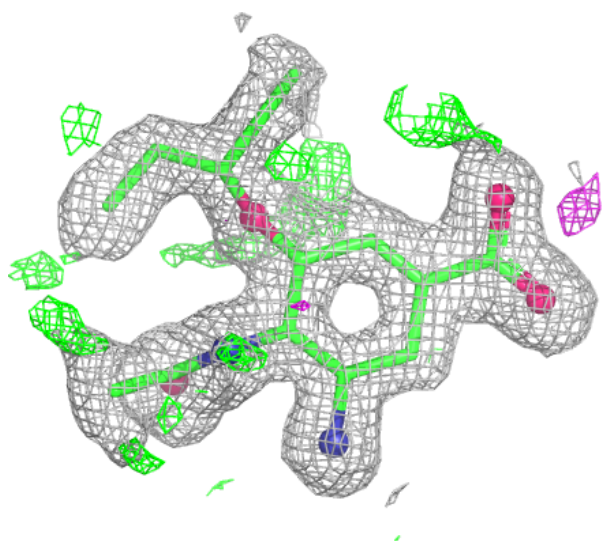
Electron density around G39 D 503:

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



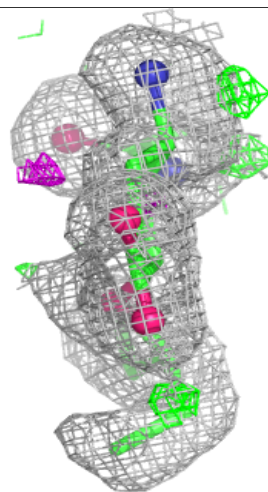
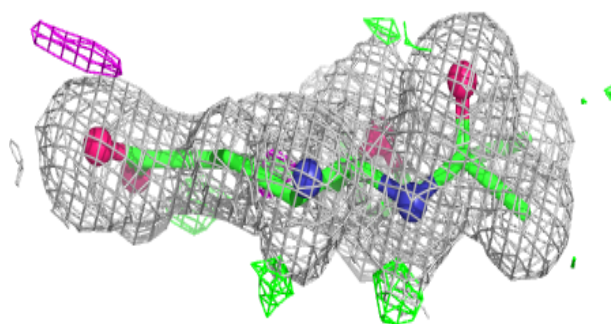
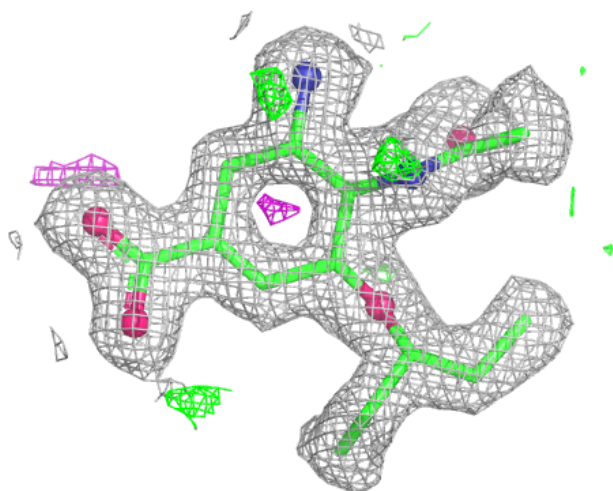
Electron density around G39 C 503:

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



Electron density around G39 A 503:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.