



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 08:45 AM BST

PDB ID : 5NZN
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 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

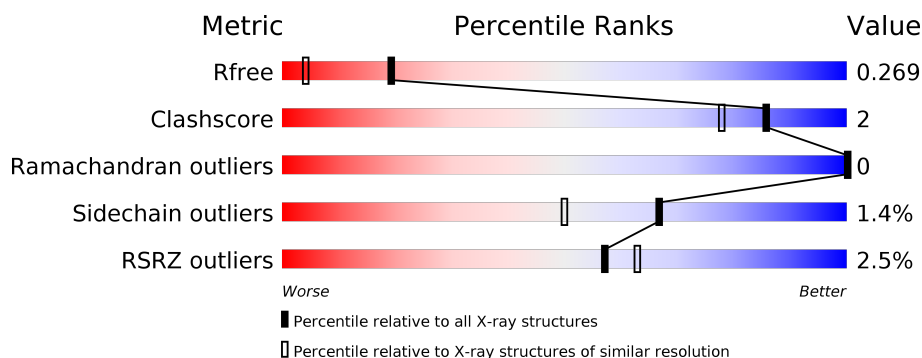
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.73 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}	130704	3764 (1.76-1.72)
Clashscore	141614	3923 (1.76-1.72)
Ramachandran outliers	138981	3878 (1.76-1.72)
Sidechain outliers	138945	3878 (1.76-1.72)
RSRZ outliers	127900	3705 (1.76-1.72)

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	388	<div> <div>2%</div> <div> <div></div> <div>93%</div> <div>7%</div> </div> </div>
1	B	388	<div> <div>3%</div> <div> <div></div> <div>94%</div> <div>6%</div> </div> </div>
1	C	388	<div> <div>3%</div> <div> <div></div> <div>93%</div> <div>7%</div> </div> </div>
1	D	388	<div> <div>2%</div> <div> <div></div> <div>91%</div> <div>8%</div> </div> </div>
2	E	4	<div> <div></div> <div> <div>50%</div> <div>50%</div> </div> </div>
3	F	2	<div> <div></div> <div>100%</div> </div>

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
3	NAG	F	2	-	-	-	X
6	NAG	C	509	-	-	-	X

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.

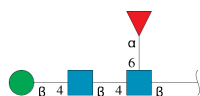
- Molecule 1 is a protein called Neuraminidase.

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.

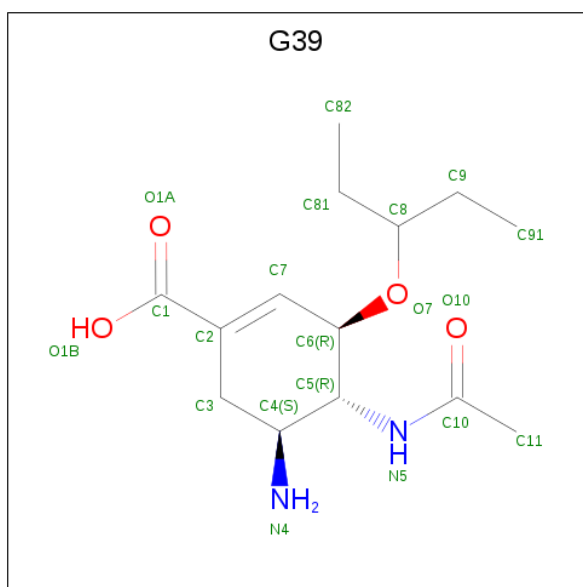


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	F	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

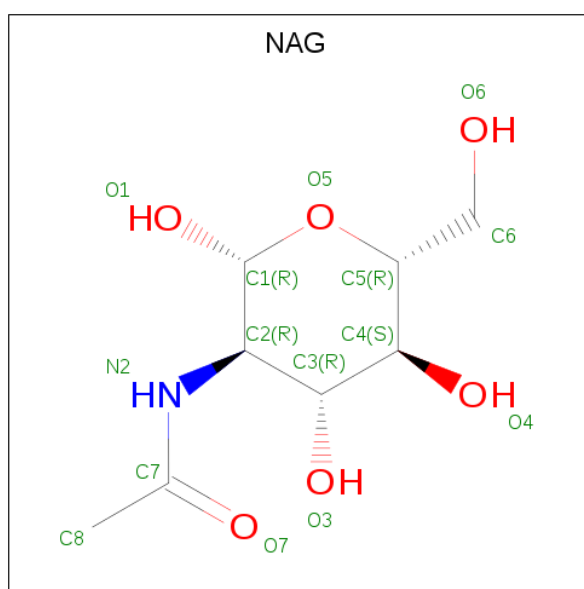
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total	Ca	0	0
			2	2		
4	A	2	Total	Ca	0	0
			2	2		
4	D	2	Total	Ca	0	0
			2	2		
4	C	2	Total	Ca	0	0
			2	2		

- Molecule 5 is (3R,4R,5S)-4-(acetamino)-5-amino-3-(pentan-3-yloxy)cyclohex-1-ene-1-carboxylic acid (three-letter code: 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 (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		

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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 (three-letter code: 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		

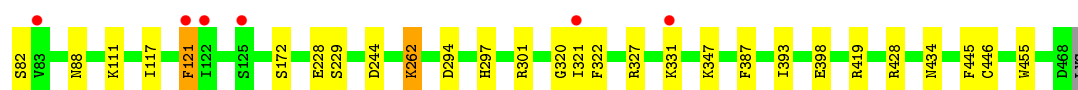
- Molecule 8 is water.

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		

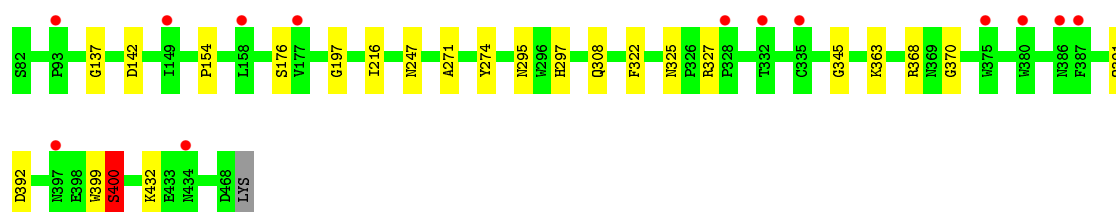
3 Residue-property plots [i](#)

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.

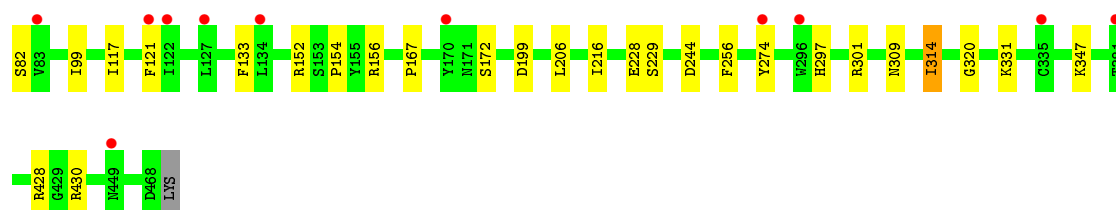
• Molecule 1: Neuraminidase



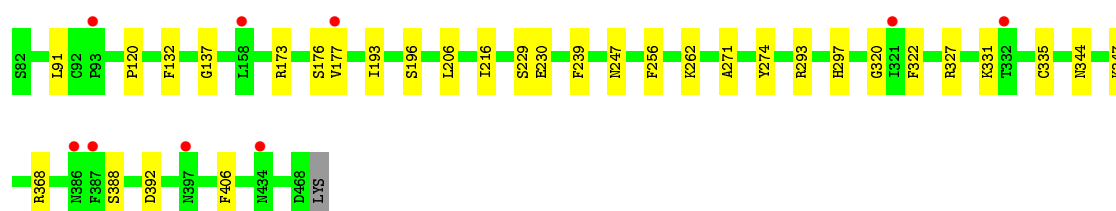
• Molecule 1: Neuraminidase



• Molecule 1: Neuraminidase



• Molecule 1: Neuraminidase



- Molecule 2: 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

Chain E:  50% 50%

NAG1
NAG2
BNA3
FUC4

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

Chain F:  100%

NAG1
NAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	85.78 Å 127.54 Å 96.77 Å 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) 99.4 (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 1.73 Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.229 , 0.261 0.237 , 0.269	Depositor DCC
R_{free} test set	2253 reflections (1.05%)	wwPDB-VP
Wilson B-factor (Å ²)	15.6	Xtriage
Anisotropy	0.094	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 53.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	13688	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage'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, NAG, G39, CA, EDO, FUC

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	0.98	3/3102 (0.1%)	0.94	4/4216 (0.1%)
1	B	1.02	1/3085 (0.0%)	0.91	0/4194
1	C	1.00	3/3085 (0.1%)	0.98	10/4194 (0.2%)
1	D	0.96	1/3088 (0.0%)	0.92	5/4197 (0.1%)
All	All	0.99	8/12360 (0.1%)	0.94	19/16801 (0.1%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	314	ILE	CB-CG1	7.34	1.74	1.54
1	B	400	SER	CB-OG	-7.05	1.33	1.42
1	C	228	GLU	CD-OE1	6.58	1.32	1.25
1	A	228	GLU	CD-OE1	5.72	1.31	1.25
1	C	172	SER	CA-CB	-5.51	1.44	1.52
1	A	172	SER	CA-CB	-5.26	1.45	1.52
1	D	196	SER	CB-OG	5.10	1.48	1.42
1	A	121	PHE	CG-CD2	-5.05	1.31	1.38

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	430	ARG	NE-CZ-NH2	-8.00	116.30	120.30
1	D	368	ARG	NE-CZ-NH2	-7.94	116.33	120.30
1	C	430	ARG	NE-CZ-NH1	7.88	124.24	120.30
1	C	199	ASP	CB-CG-OD1	7.29	124.86	118.30
1	A	244	ASP	CB-CG-OD1	6.29	123.96	118.30
1	C	244	ASP	CB-CG-OD1	6.07	123.76	118.30
1	C	301	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	C	199	ASP	CB-CG-OD2	-5.96	112.94	118.30
1	D	392	ASP	CB-CG-OD1	5.90	123.61	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	428	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	A	294	ASP	CB-CG-OD2	-5.55	113.31	118.30
1	A	428	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	A	301	ARG	NE-CZ-NH1	5.35	122.97	120.30
1	C	152	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	D	293	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	D	173	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	C	428	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	C	156	ARG	NE-CZ-NH1	-5.08	117.76	120.30
1	D	91	LEU	CA-CB-CG	5.00	126.80	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3012	0	2843	14	0
1	B	3003	0	2827	15	0
1	C	3003	0	2827	12	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	4	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:C:309[B]:ASN:OD1	8:C:601:HOH:O	1.70	1.08
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:CA	1:C:314:ILE:CG1	2.71	0.68
7:A:506:EDO:H12	1:B:154:PRO:HG3	1.79	0.63
1:C:314:ILE:CG2	1:C:314:ILE:CG1	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
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: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: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:239:PHE:HA	1:D:256:PHE:O	2.16	0.45
1:D:229:SER:HB3	1:D:347:LYS:HE2	1.98	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
7:C:510:EDO:C2	8:C:604:HOH:O	2.56	0.44
1:A:455:TRP:CE3	1:B:197:GLY:HA2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:363:LYS:NZ	1:B:392:ASP:OD1	2.37	0.43
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:D:120:PRO:HA	1:D:132:PHE:O	2.19	0.42
1:C:99:ILE:HD13	1:D:177:VAL:HG11	2.01	0.42
1:C:206:LEU:HD12	1:C:206:LEU:N	2.34	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:B:368:ARG:C	1:B:400:SER:HB3	2.40	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: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:B:370:GLY:O	1:B:400:SER:OG	2.31	0.41
1:A:262:LYS:HB3	1:A:262:LYS:HE3	1.83	0.40
1:C:133:PHE:CE2	1:C:167:PRO:HB3	2.57	0.40
1:C:121:PHE:CG	1:C:229:SER:HA	2.57	0.40
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 ⓘ

5.3.1 Protein backbone ⓘ

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 ⓘ

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%)	59	38
1	B	335/335 (100%)	330 (98%)	5 (2%)	65	47
1	C	335/335 (100%)	331 (99%)	4 (1%)	71	56
1	D	335/335 (100%)	330 (98%)	5 (2%)	65	47
All	All	1342/1340 (100%)	1322 (98%)	20 (2%)	67	47

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	SER
1	A	117	ILE
1	A	262	LYS
1	A	297	HIS
1	A	331[A]	LYS
1	A	331[B]	LYS
1	B	176	SER
1	B	216	ILE
1	B	247	ASN
1	B	297	HIS

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Mol	Chain	Res	Type
1	B	400	SER
1	C	82	SER
1	C	117	ILE
1	C	154	PRO
1	C	297	HIS
1	D	176	SER
1	D	216	ILE
1	D	247	ASN
1	D	297	HIS
1	D	388	SER

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

Mol	Chain	Res	Type
1	D	344	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	0.61	0	17,19,21	0.72	0
2	NAG	E	2	2	14,14,15	0.59	0	17,19,21	0.99	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BMA	E	3	2	11,11,12	0.97	0	15,15,17	0.82	0
2	FUC	E	4	2	10,10,11	0.98	0	14,14,16	1.96	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	0.59	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	4.74	115.49	109.67
2	E	2	NAG	O5-C5-C6	3.42	112.57	107.20
2	E	4	FUC	O5-C5-C6	2.96	113.69	107.33
2	E	4	FUC	O2-C2-C3	-2.93	104.27	110.14
3	F	1	NAG	O3-C3-C2	-2.48	104.34	109.47
3	F	1	NAG	C2-N2-C7	-2.27	119.67	122.90
2	E	4	FUC	O5-C5-C4	2.22	113.50	109.52
3	F	2	NAG	O4-C4-C3	2.09	115.18	110.35

There are no chirality outliers.

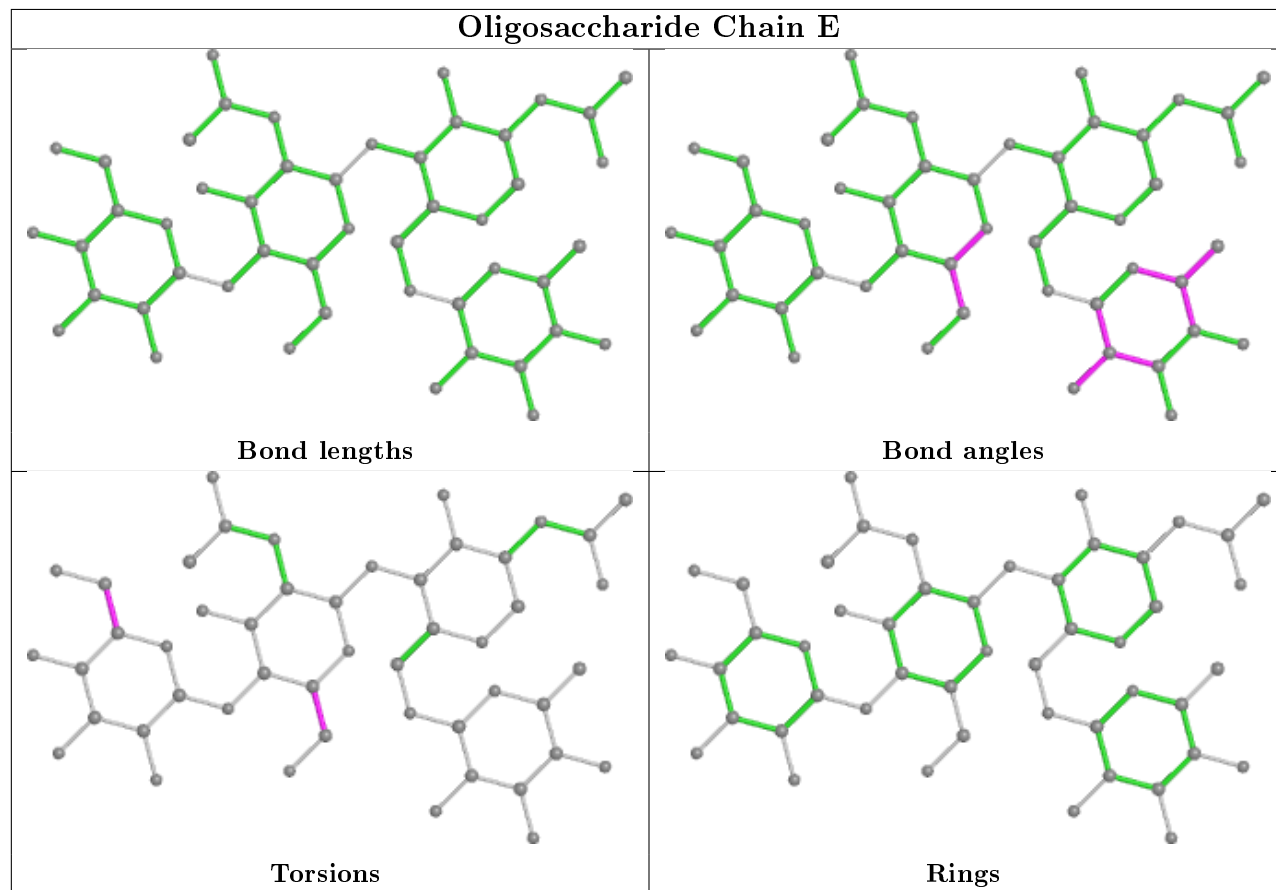
All (5) torsion outliers are listed below:

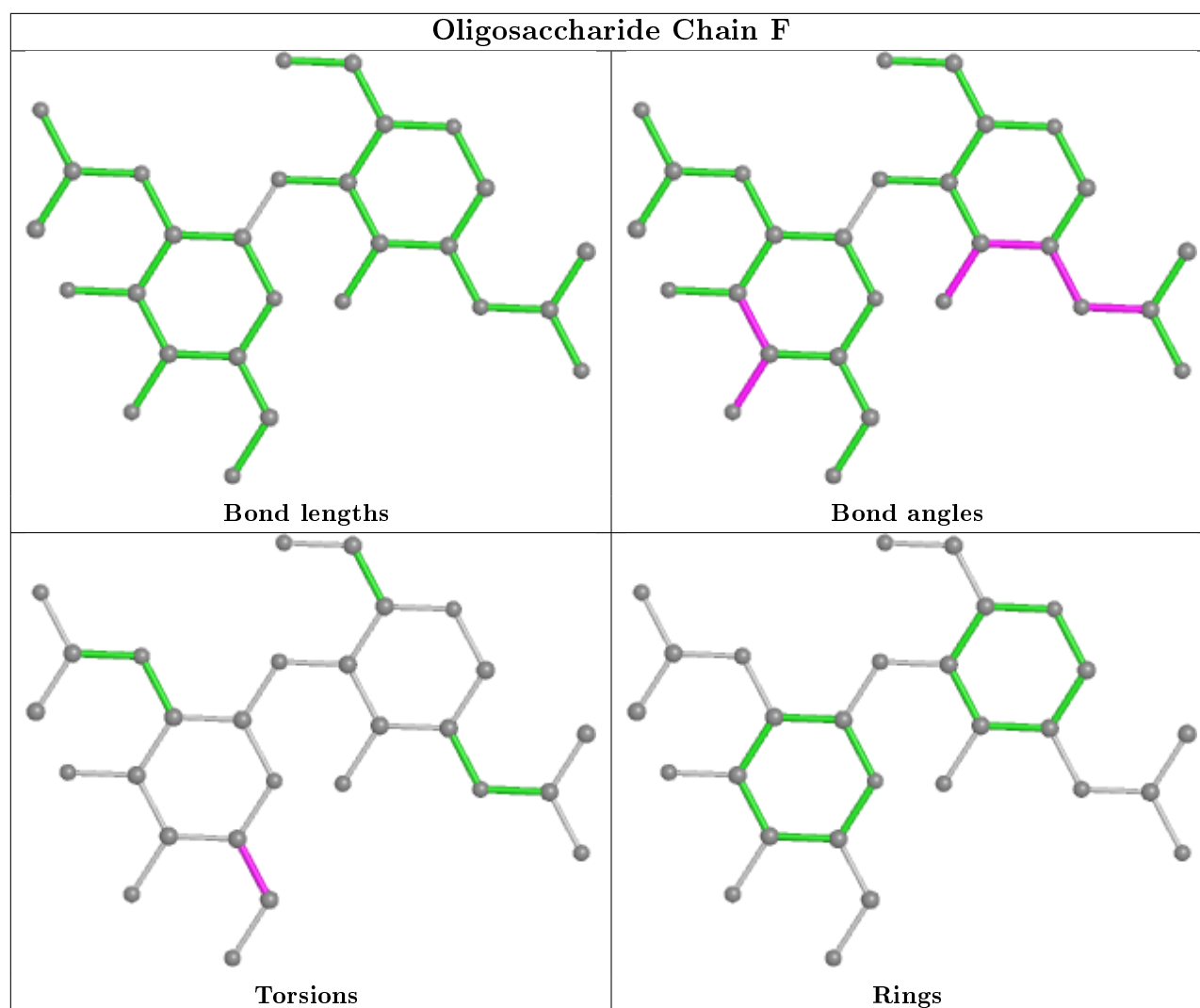
Mol	Chain	Res	Type	Atoms
2	E	2	NAG	O5-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6
2	E	3	BMA	C4-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6

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	$\# Z > 2$
6	NAG	C	504	1	14,14,15	0.56	0	17,19,21	2.76	5 (29%)
6	NAG	A	504	1	14,14,15	0.58	0	17,19,21	1.08	0
5	G39	D	503	-	17,20,20	1.19	3 (17%)	15,27,27	1.22	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	D	506	1	14,14,15	0.46	0	17,19,21	1.03	1 (5%)
6	NAG	B	505	1	14,14,15	0.89	1 (7%)	17,19,21	2.11	5 (29%)
6	NAG	C	509	1	14,14,15	0.57	0	17,19,21	1.00	1 (5%)
5	G39	A	503	-	17,20,20	1.03	1 (5%)	15,27,27	1.16	1 (6%)
5	G39	B	503	-	17,20,20	1.01	1 (5%)	15,27,27	0.83	0
5	G39	C	503	-	17,20,20	0.95	0	15,27,27	1.30	2 (13%)
7	EDO	C	510	-	3,3,3	0.43	0	2,2,2	0.37	0
7	EDO	A	506	-	3,3,3	1.55	0	2,2,2	0.88	0
6	NAG	B	506	1	14,14,15	0.52	0	17,19,21	0.74	0
6	NAG	B	504	1	14,14,15	0.64	0	17,19,21	2.55	5 (29%)
6	NAG	A	505	1	14,14,15	0.54	0	17,19,21	1.74	4 (23%)

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	504	1	-	1/6/23/26	0/1/1/1
6	NAG	A	504	1	-	0/6/23/26	0/1/1/1
5	G39	D	503	-	-	0/12/32/32	0/1/1/1
6	NAG	D	506	1	-	0/6/23/26	0/1/1/1
6	NAG	B	505	1	-	0/6/23/26	0/1/1/1
6	NAG	C	509	1	-	0/6/23/26	0/1/1/1
5	G39	A	503	-	-	0/12/32/32	0/1/1/1
5	G39	B	503	-	-	0/12/32/32	0/1/1/1
5	G39	C	503	-	-	0/12/32/32	0/1/1/1
7	EDO	C	510	-	-	1/1/1/1	-
7	EDO	A	506	-	-	1/1/1/1	-
6	NAG	B	506	1	-	2/6/23/26	0/1/1/1
6	NAG	B	504	1	-	2/6/23/26	0/1/1/1
6	NAG	A	505	1	-	0/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	503	G39	C6-C7	2.73	1.54	1.50
5	D	503	G39	C3-C2	2.49	1.54	1.50
5	B	503	G39	O7-C8	2.42	1.48	1.44
5	D	503	G39	O10-C10	-2.34	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	503	G39	C6-C7	2.17	1.53	1.50
6	B	505	NAG	C1-C2	2.03	1.55	1.52

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	504	NAG	C1-C2-N2	-8.28	96.34	110.49
6	B	504	NAG	C1-C2-N2	-7.93	96.94	110.49
6	C	504	NAG	C2-N2-C7	6.05	131.51	122.90
6	B	505	NAG	C4-C3-C2	-4.91	103.83	111.02
6	B	505	NAG	C3-C4-C5	-3.80	103.46	110.24
5	A	503	G39	C4-C3-C2	3.41	113.79	109.75
5	D	503	G39	C4-C3-C2	3.39	113.76	109.75
5	C	503	G39	C4-C3-C2	3.33	113.69	109.75
6	B	504	NAG	C4-C3-C2	3.18	115.68	111.02
6	B	504	NAG	O5-C1-C2	3.18	116.30	111.29
6	A	505	NAG	C4-C3-C2	-3.12	106.45	111.02
6	A	505	NAG	C1-O5-C5	3.09	116.38	112.19
6	A	505	NAG	O5-C1-C2	-2.88	106.74	111.29
6	B	505	NAG	O4-C4-C5	2.83	116.33	109.30
6	C	504	NAG	O7-C7-N2	2.72	126.94	121.95
6	B	504	NAG	C3-C4-C5	2.67	115.00	110.24
6	C	509	NAG	O5-C1-C2	-2.54	107.27	111.29
6	C	504	NAG	C8-C7-N2	-2.51	111.86	116.10
5	D	503	G39	O10-C10-C11	-2.36	117.68	122.06
6	C	504	NAG	O3-C3-C4	-2.26	105.12	110.35
6	A	505	NAG	O4-C4-C5	2.18	114.72	109.30
6	B	505	NAG	O3-C3-C2	2.15	113.92	109.47
6	B	505	NAG	O7-C7-N2	2.09	125.80	121.95
6	D	506	NAG	C1-O5-C5	-2.07	109.39	112.19
5	C	503	G39	O10-C10-N5	2.06	125.75	121.95
6	B	504	NAG	C2-N2-C7	2.02	125.78	122.90

There are no chirality outliers.

All (7) 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

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Mol	Chain	Res	Type	Atoms
7	C	510	EDO	O1-C1-C2-O2
6	B	506	NAG	O5-C5-C6-O6

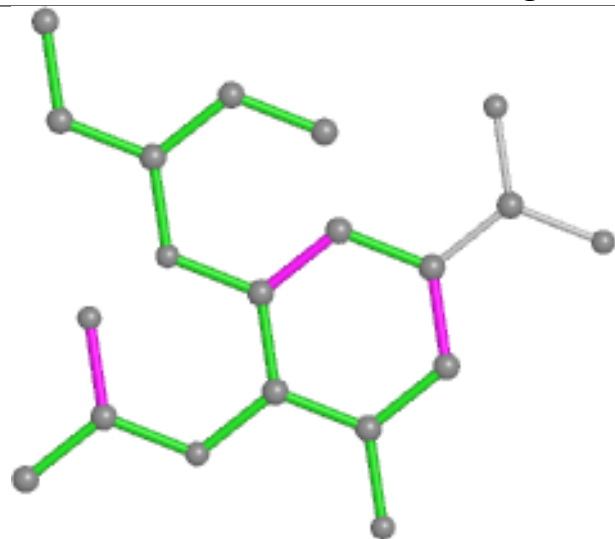
There are no ring outliers.

3 monomers are involved in 4 short contacts:

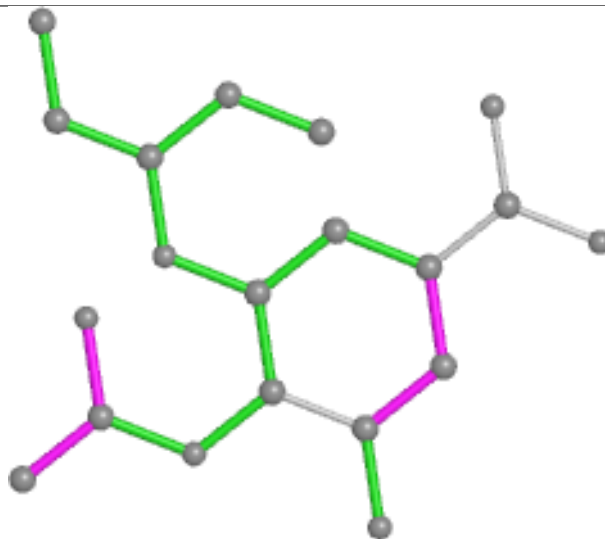
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	503	G39	1	0
7	C	510	EDO	2	0
7	A	506	EDO	1	0

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.

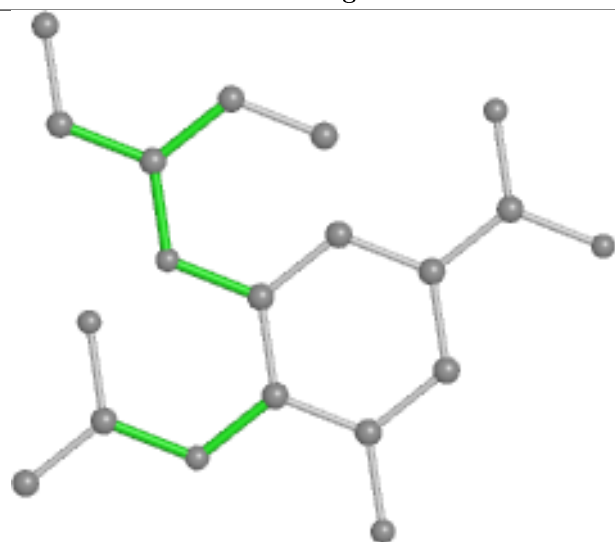
Ligand G39 D 503



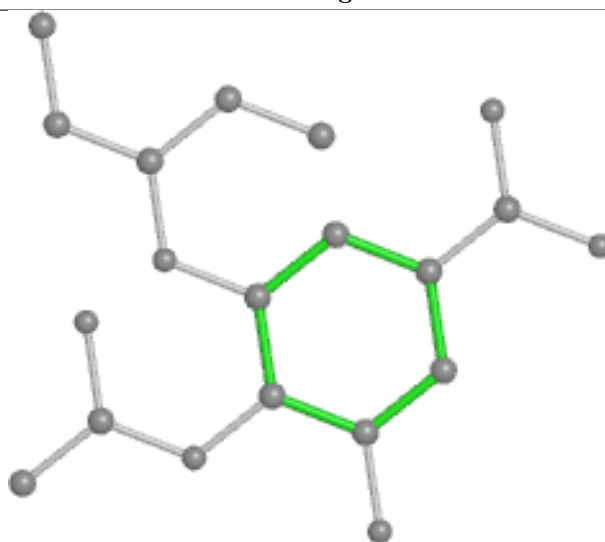
Bond lengths



Bond angles

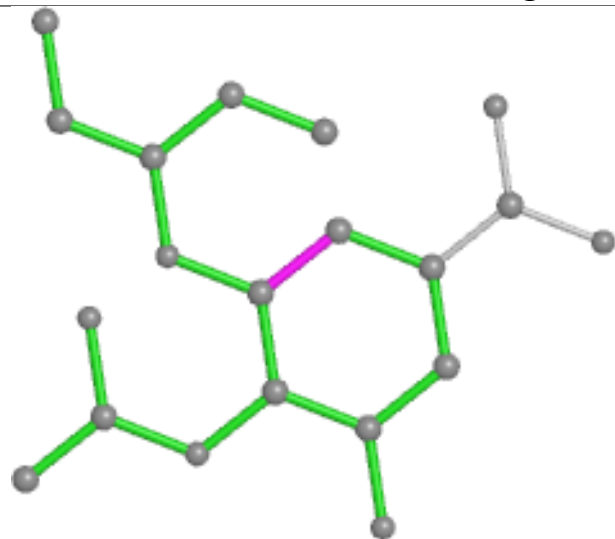


Torsions

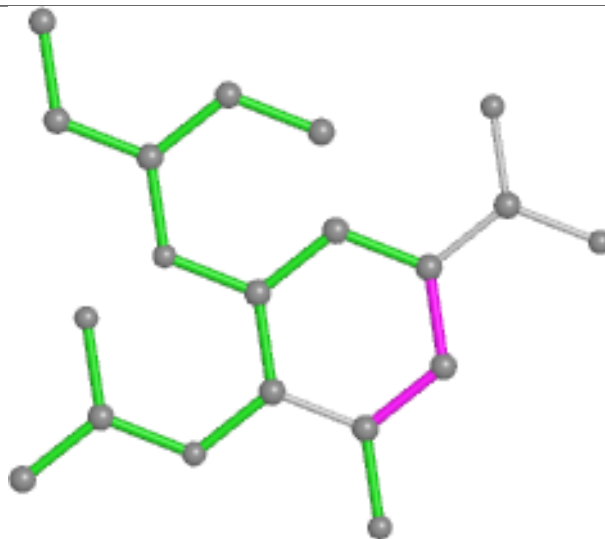


Rings

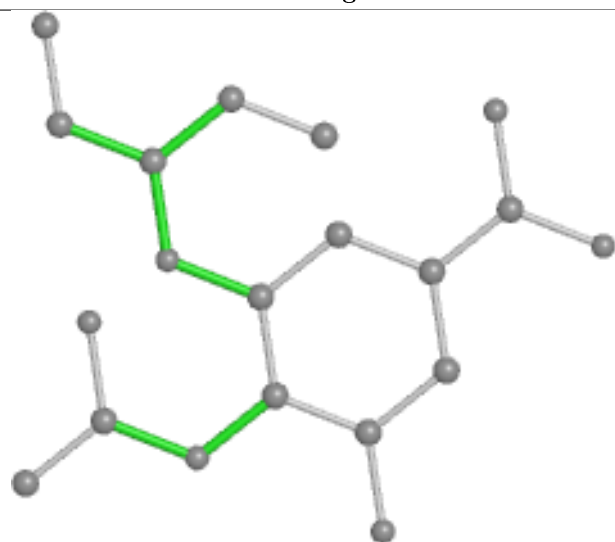
Ligand G39 A 503



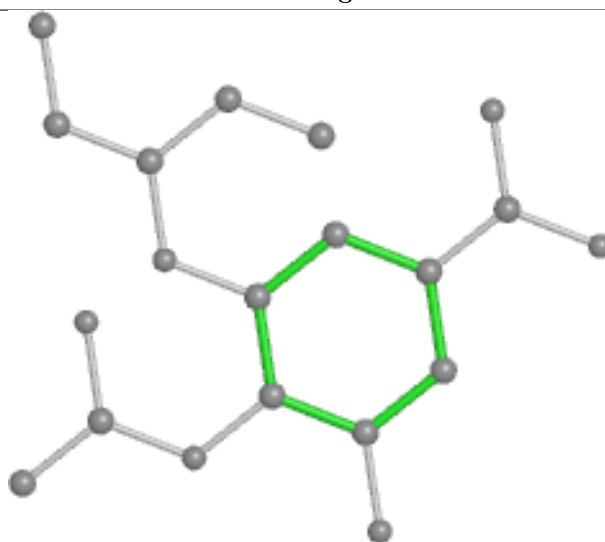
Bond lengths



Bond angles

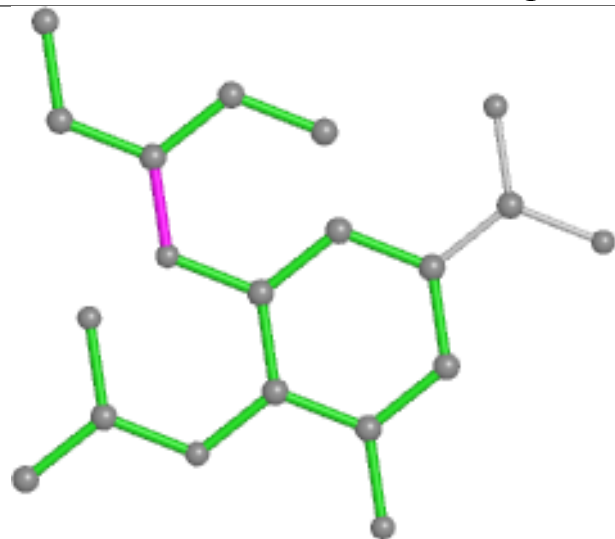


Torsions

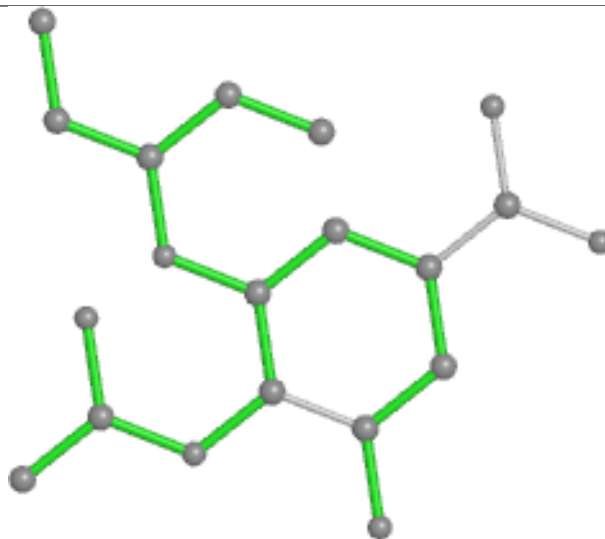


Rings

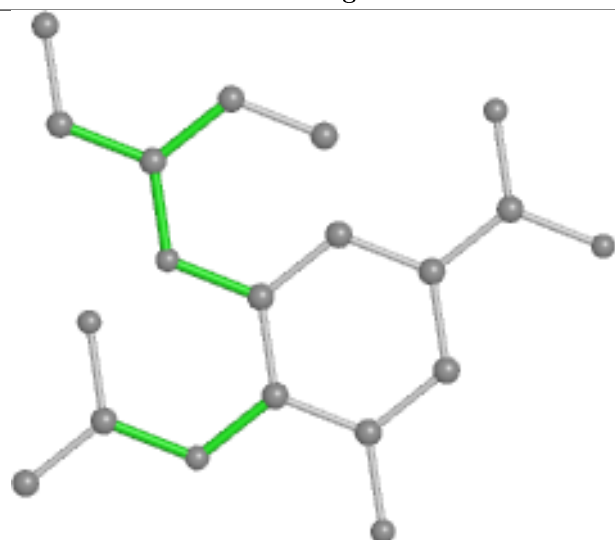
Ligand G39 B 503



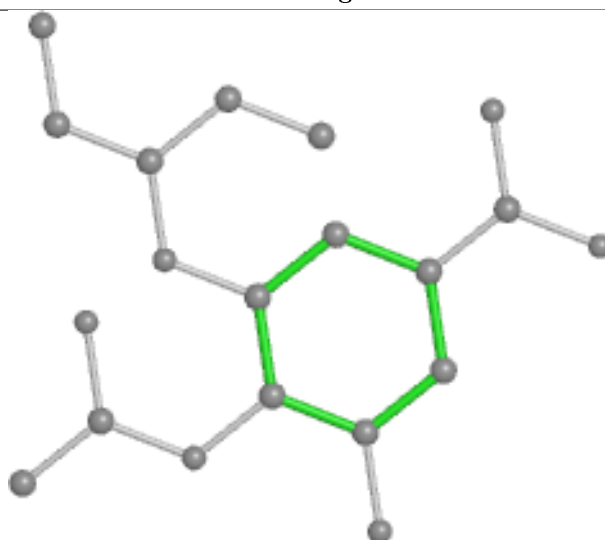
Bond lengths



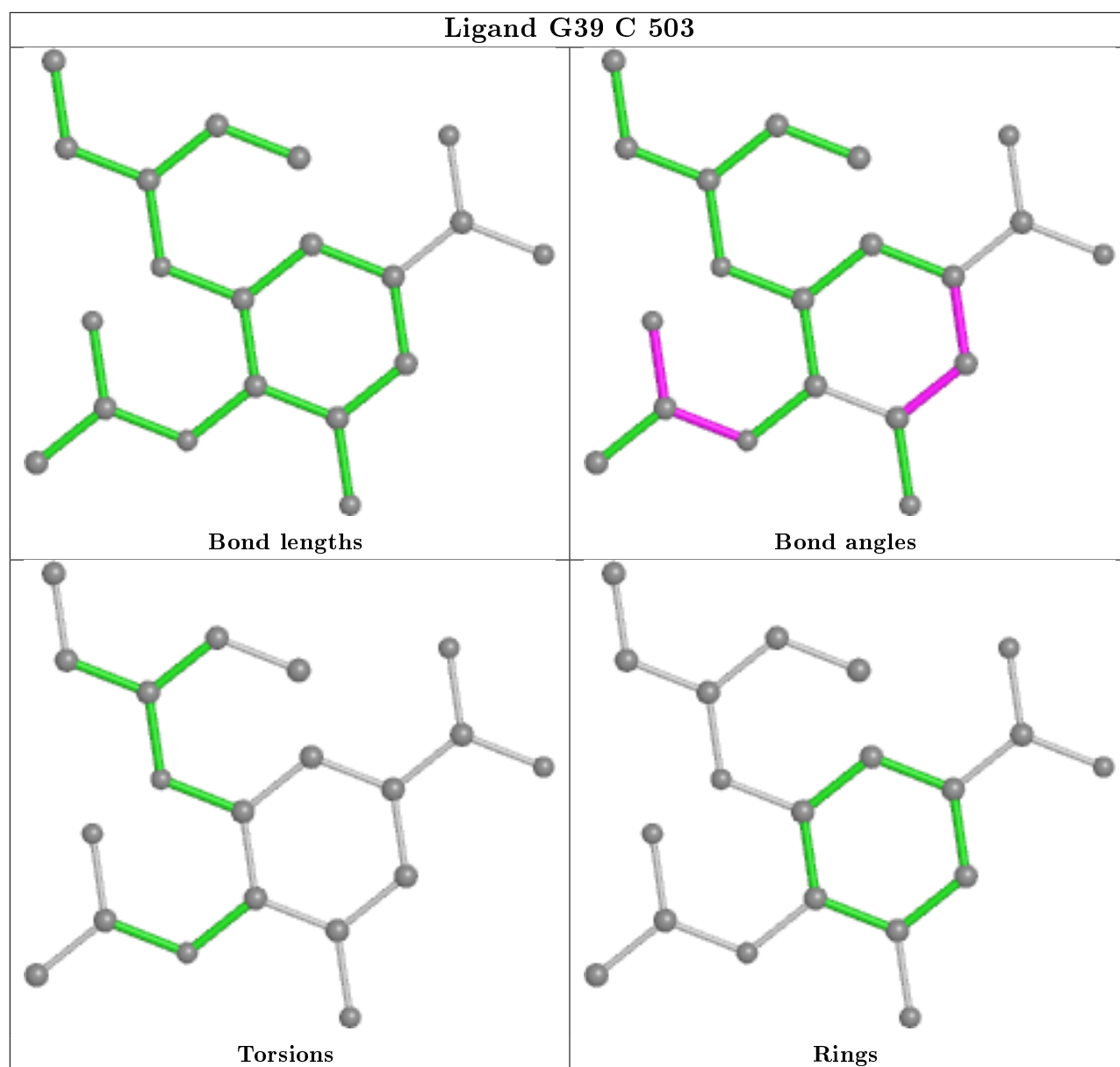
Bond angles



Torsions



Rings



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%)	0.30	6 (1%) 72 78	9, 15, 24, 36	0
1	B	387/388 (99%)	0.58	13 (3%) 45 51	10, 17, 27, 37	0
1	C	387/388 (99%)	0.38	11 (2%) 53 58	9, 15, 25, 34	1 (0%)
1	D	387/388 (99%)	0.45	9 (2%) 60 66	10, 17, 27, 38	0
All	All	1548/1552 (99%)	0.42	39 (2%) 57 63	9, 16, 26, 38	1 (0%)

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	93	PRO	3.9
1	D	386	ASN	3.2
1	D	434	ASN	3.1
1	B	93	PRO	2.9
1	A	83	VAL	2.8
1	B	335	CYS	2.8
1	A	321	ILE	2.7
1	C	122	ILE	2.5
1	B	397	ASN	2.5
1	C	274	TYR	2.5
1	C	121	PHE	2.5
1	B	149	ILE	2.5
1	C	296	TRP	2.5
1	B	386	ASN	2.4
1	C	381	THR	2.4
1	B	375	TRP	2.4
1	C	335	CYS	2.3
1	D	158	LEU	2.3
1	B	332	THR	2.2
1	C	449	ASN	2.2
1	A	331[A]	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	83	VAL	2.2
1	A	122	ILE	2.2
1	D	332	THR	2.1
1	A	125	SER	2.1
1	D	321	ILE	2.1
1	B	434	ASN	2.1
1	B	177	VAL	2.1
1	B	158	LEU	2.1
1	C	134	LEU	2.1
1	C	170	TYR	2.1
1	A	121	PHE	2.1
1	B	328	PRO	2.0
1	D	177	VAL	2.0
1	C	127	LEU	2.0
1	B	387	PHE	2.0
1	D	387	PHE	2.0
1	B	380	TRP	2.0
1	D	397	ASN	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 ⓘ

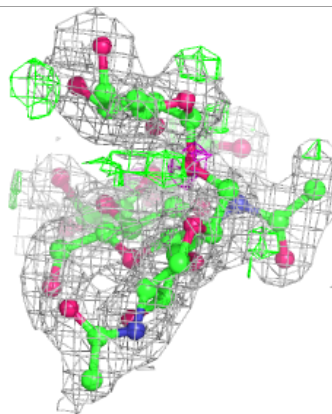
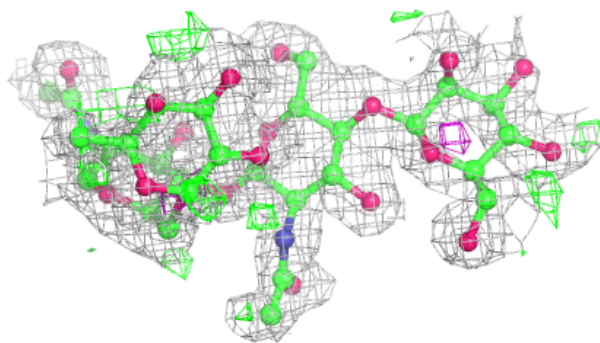
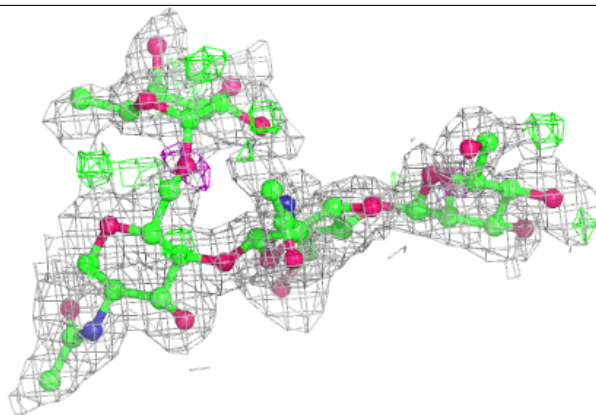
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

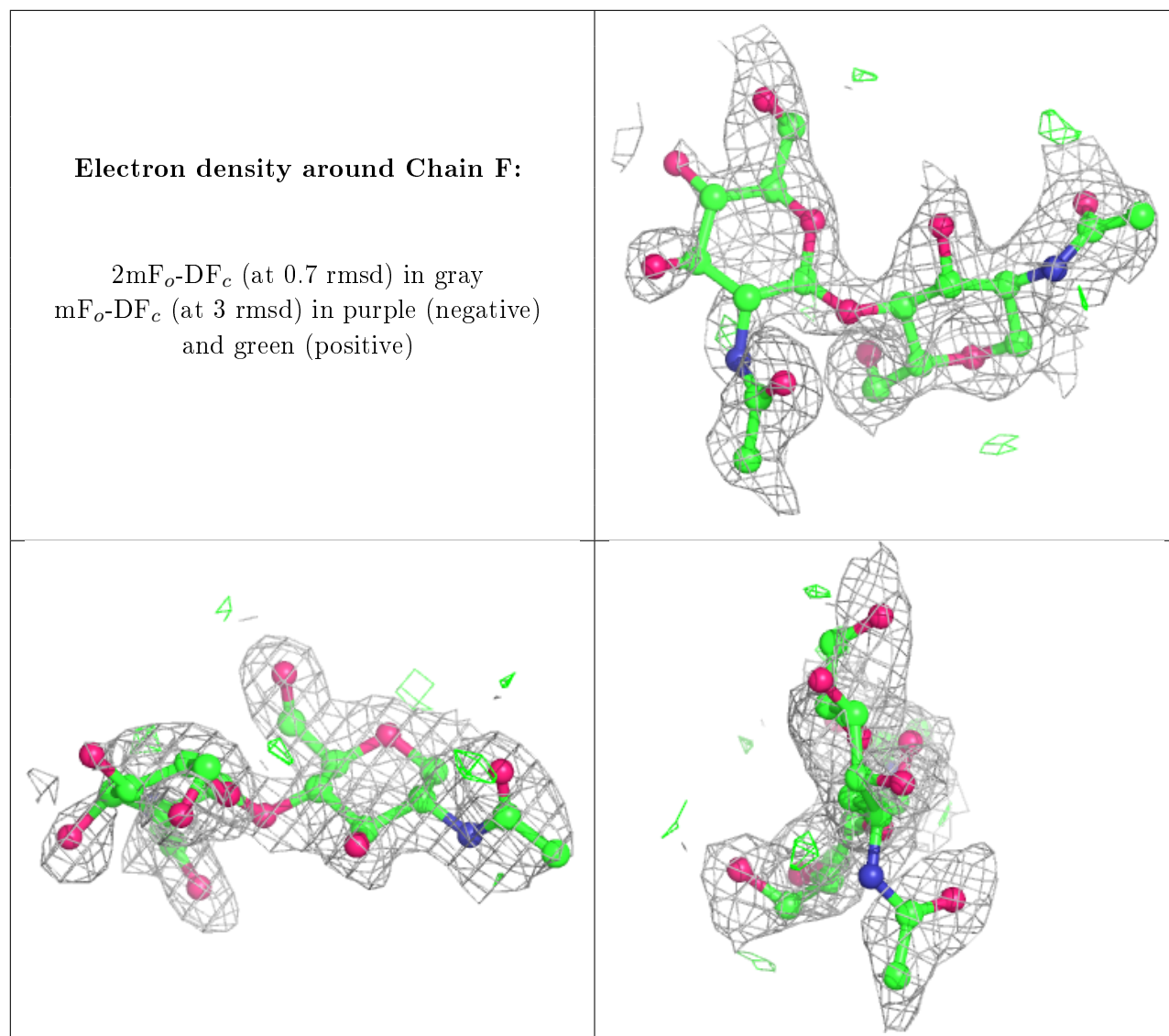
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	F	2	14/15	0.62	0.41	37,44,46,48	0
2	BMA	E	3	11/12	0.63	0.29	32,38,40,46	0
2	FUC	E	4	10/11	0.77	0.21	30,32,32,37	0
3	NAG	F	1	14/15	0.79	0.25	31,37,38,44	0
2	NAG	E	1	14/15	0.81	0.16	24,29,33,34	0
2	NAG	E	2	14/15	0.87	0.15	28,30,32,38	0

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 ⓘ

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	505	14/15	0.56	0.28	35,40,41,42	0
6	NAG	B	504	14/15	0.69	0.31	37,41,45,46	0
6	NAG	C	504	14/15	0.69	0.35	36,42,45,47	0
6	NAG	C	509	14/15	0.76	0.45	35,40,42,44	0
7	EDO	C	510	4/4	0.78	0.14	24,26,26,29	0
6	NAG	A	505	14/15	0.79	0.40	35,38,43,44	0
6	NAG	B	506	14/15	0.82	0.35	32,37,40,41	0

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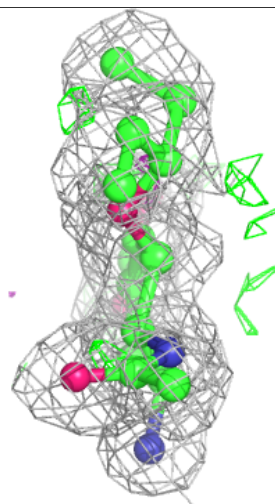
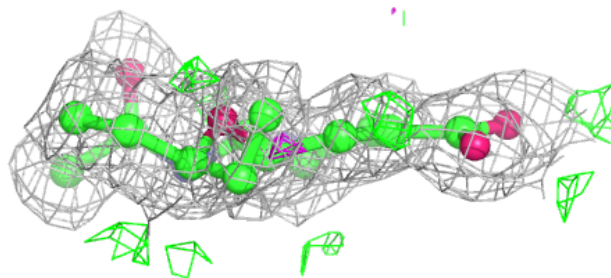
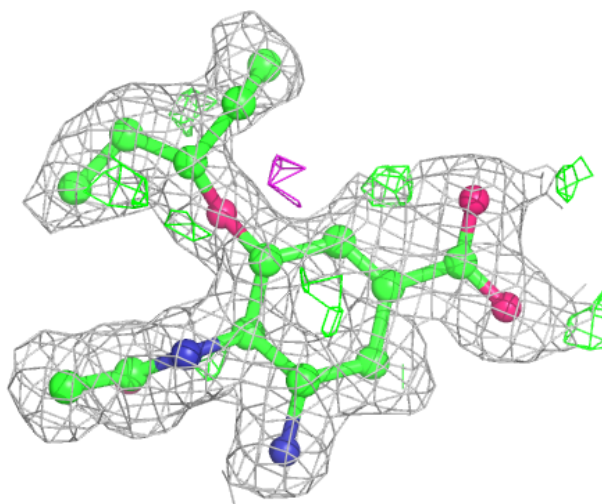
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	EDO	A	506	4/4	0.82	0.13	21,23,24,25	0
6	NAG	D	506	14/15	0.82	0.37	33,38,41,43	0
6	NAG	A	504	14/15	0.83	0.24	32,37,41,42	0
5	G39	D	503	20/20	0.89	0.13	13,16,23,24	0
5	G39	B	503	20/20	0.90	0.13	11,15,24,26	0
5	G39	C	503	20/20	0.91	0.12	11,14,21,24	0
5	G39	A	503	20/20	0.93	0.11	10,14,22,24	0
4	CA	B	502	1/1	0.96	0.10	26,26,26,26	0
4	CA	B	501	1/1	0.96	0.05	20,20,20,20	0
4	CA	C	502	1/1	0.97	0.07	21,21,21,21	0
4	CA	D	502	1/1	0.97	0.08	25,25,25,25	0
4	CA	A	502	1/1	0.97	0.05	20,20,20,20	0
4	CA	D	501	1/1	0.98	0.04	19,19,19,19	0
4	CA	A	501	1/1	0.99	0.04	14,14,14,14	0
4	CA	C	501	1/1	0.99	0.04	15,15,15,15	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.

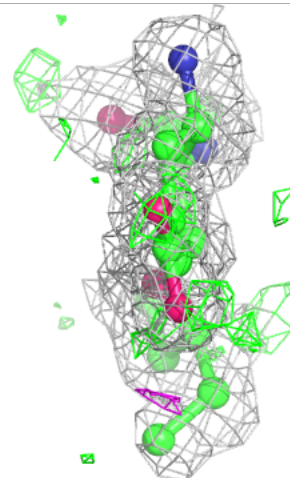
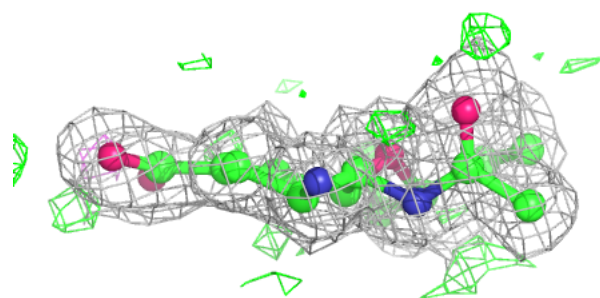
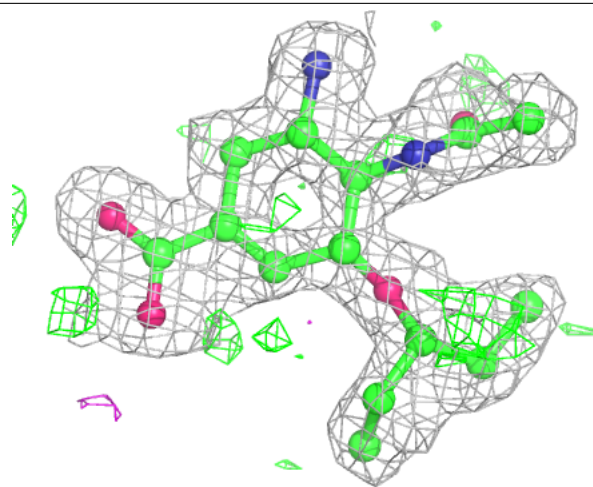
Electron density around G39 D 503:

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



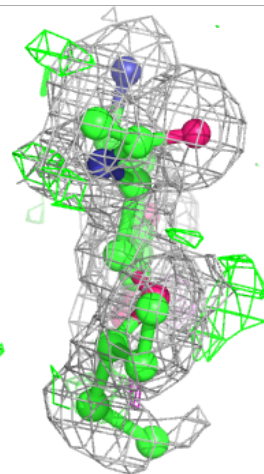
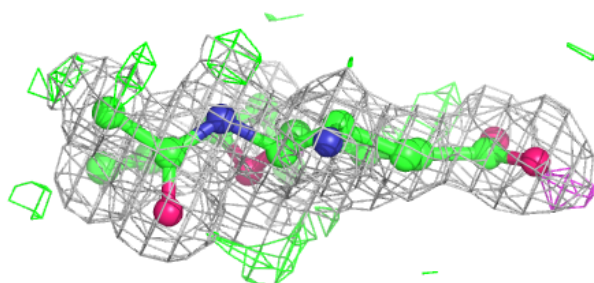
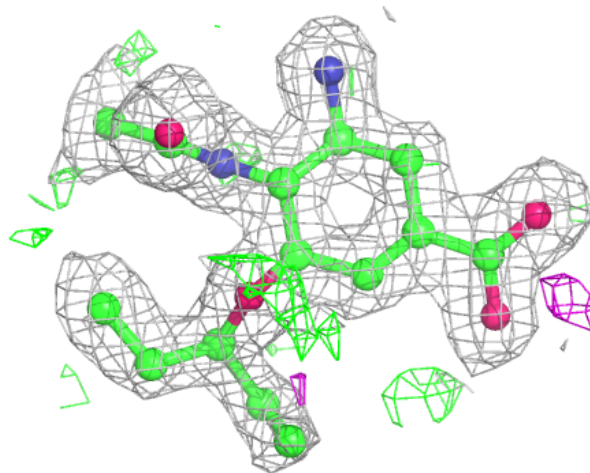
Electron density around G39 B 503:

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



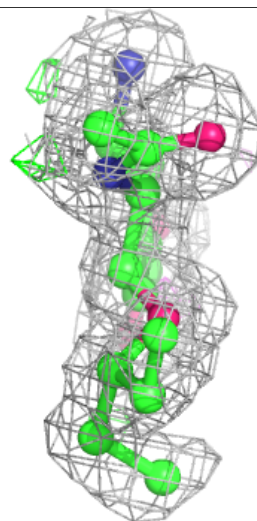
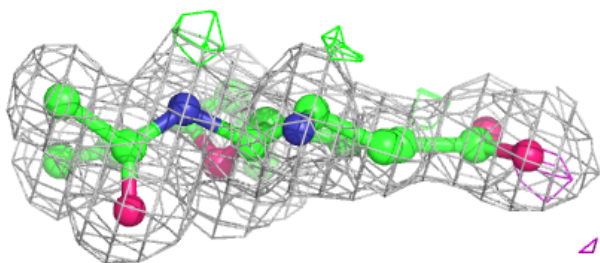
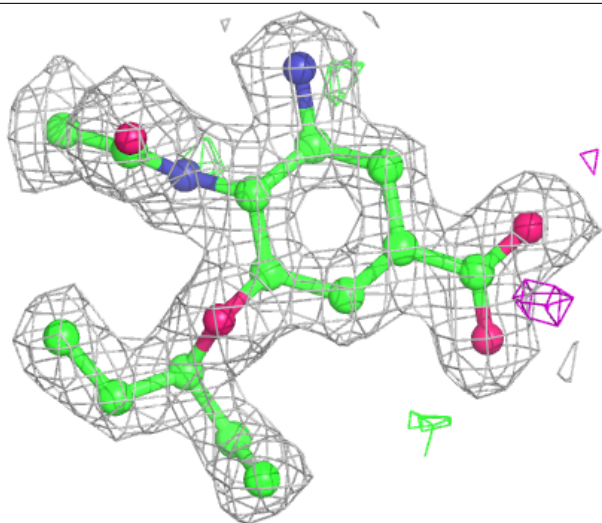
Electron density around G39 C 503:

$2mF_o-DF_c$ (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 [i](#)

There are no such residues in this entry.