



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:48 AM UTC

PDB ID : 5NWE / pdb_00005nwe
Title : Complex of H275Y mutant variant of neuraminidase from H1N1 influenza virus with oseltamivir
Authors : Pachl, P.; Pokorna, J.
Deposited on : 2017-05-05
Resolution : 2.00 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

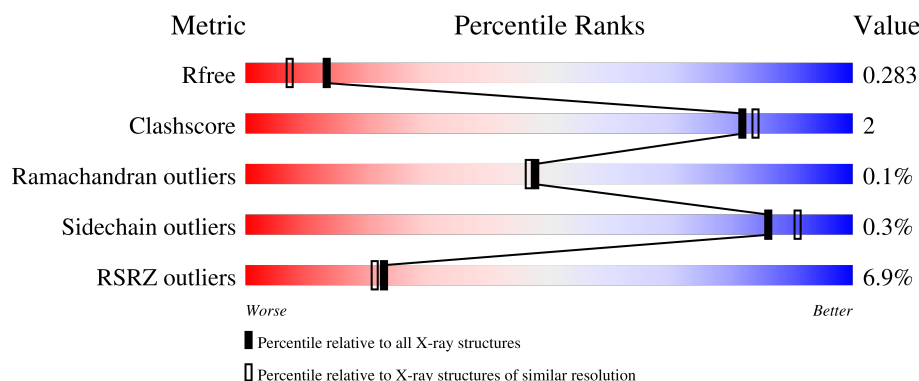
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

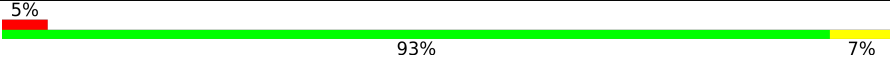
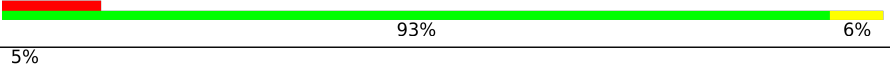
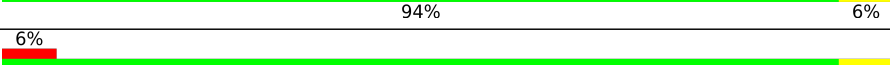
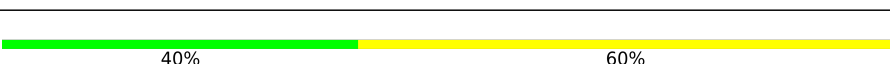
The reported resolution of this entry is 2.00 Å.

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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	
1	B	388	
1	C	388	
1	D	388	
2	E	5	

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Mol	Chain	Length	Quality of chain
3	F	2	 100%

2 Entry composition [i](#)

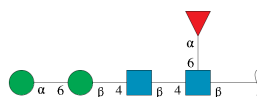
There are 7 unique types of molecules in this entry. The entry contains 13704 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	388	Total	C	N	O	S	0	0	0
			3002	1886	516	579	21			
1	B	388	Total	C	N	O	S	0	0	0
			3002	1886	516	579	21			
1	C	388	Total	C	N	O	S	0	0	0
			3002	1886	516	579	21			
1	D	388	Total	C	N	O	S	0	0	0
			3002	1886	516	579	21			

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-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	5	Total	C	N	O	0	0	0
			60	34	2	24			

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

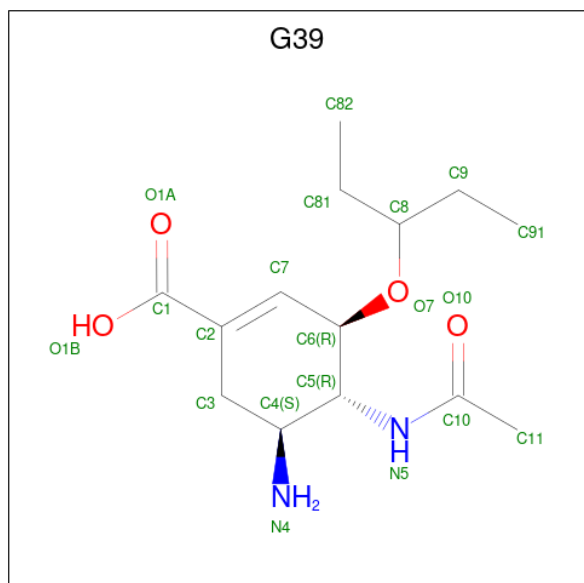


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	F	2	Total	C	N	O	0	0	0
			28	16	2	10			

- 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-(acetylamino)-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: C₈H₁₅NO₆).



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	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	345	Total	O	0	0
			345	345		
7	B	359	Total	O	0	0
			359	359		

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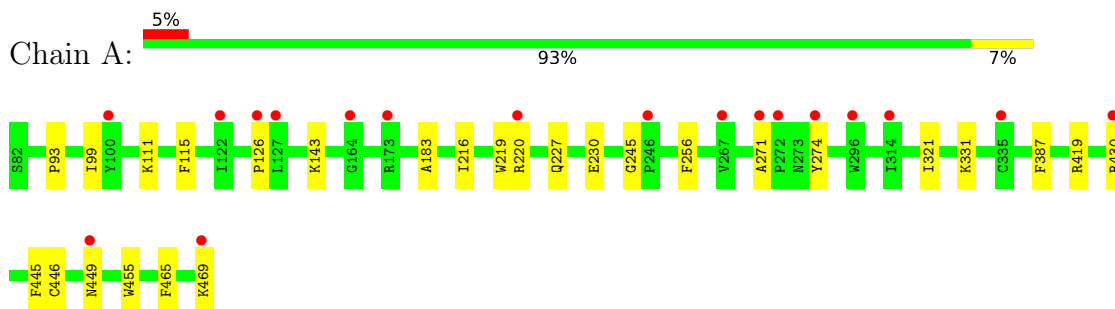
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	341	Total 341	O 341	0	0
7	D	335	Total 335	O 335	0	0

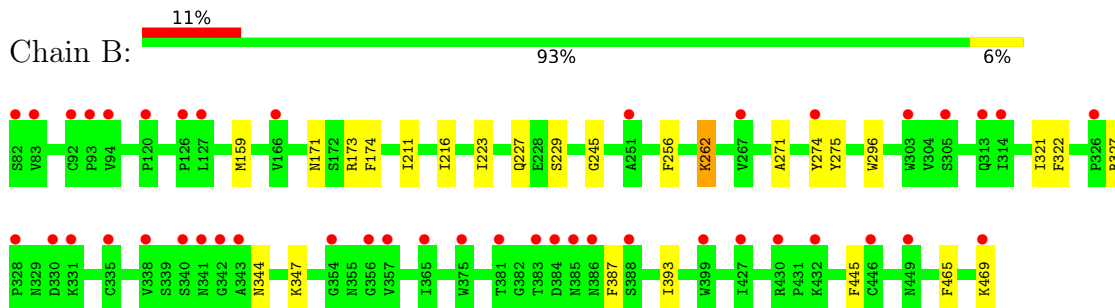
3 Residue-property plots

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.

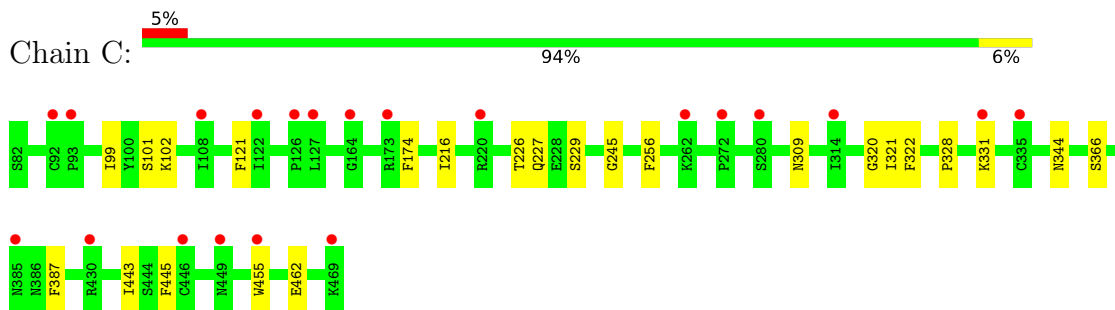
• Molecule 1: Neuraminidase



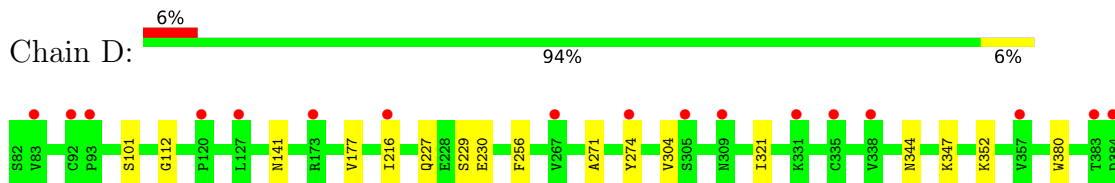
• Molecule 1: Neuraminidase

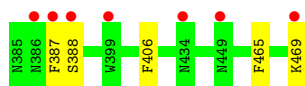


• Molecule 1: Neuraminidase



• Molecule 1: Neuraminidase





- Molecule 2: alpha-D-mannopyranose-(1-6)-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: 40% 60%



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

Chain F: 100%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	85.47Å 126.61Å 96.56Å 90.00° 93.49° 90.00°	Depositor
Resolution (Å)	48.19 – 2.00 48.19 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.8 (48.19-2.00) 99.3 (48.19-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.80 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.235 , 0.277 0.240 , 0.283	Depositor DCC
R_{free} test set	2100 reflections (1.53%)	wwPDB-VP
Wilson B-factor (Å ²)	21.3	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 47.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	13704	wwPDB-VP
Average B, all atoms (Å ²)	23.0	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 27.43 % 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 2.2017e-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: MAN, BMA, FUC, 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	0.92	2/3084 (0.1%)	0.91	4/4191 (0.1%)
1	B	0.92	0/3084	0.93	3/4191 (0.1%)
1	C	0.91	2/3084 (0.1%)	0.92	3/4191 (0.1%)
1	D	0.88	1/3084 (0.0%)	0.89	1/4191 (0.0%)
All	All	0.91	5/12336 (0.0%)	0.91	11/16764 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	455	TRP	C-O	-8.63	1.17	1.24
1	A	455	TRP	C-O	-6.20	1.19	1.24
1	C	226	THR	CA-C	5.24	1.58	1.53
1	D	304	VAL	C-O	5.11	1.29	1.23
1	A	115	PHE	CA-C	-5.07	1.46	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	227	GLN	N-CA-C	6.75	118.64	111.28
1	D	227	GLN	N-CA-C	6.73	118.61	111.28
1	B	227	GLN	N-CA-C	6.53	118.48	111.36
1	C	245	GLY	CA-C-N	6.45	126.42	119.78
1	C	245	GLY	C-N-CA	6.45	126.42	119.78
1	C	227	GLN	N-CA-C	6.44	119.13	111.33
1	A	245	GLY	CA-C-N	5.64	125.59	119.78
1	A	245	GLY	C-N-CA	5.64	125.59	119.78
1	A	143	LYS	N-CA-C	5.17	116.92	111.28
1	B	245	GLY	CA-C-N	5.16	125.07	119.76
1	B	245	GLY	C-N-CA	5.16	125.07	119.76

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	3002	0	2834	14	1
1	B	3002	0	2834	21	0
1	C	3002	0	2834	14	1
1	D	3002	0	2834	15	0
2	E	60	0	52	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	0	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	42	0	39	0	0
7	A	345	0	0	2	0
7	B	359	0	0	7	0
7	C	341	0	0	7	0
7	D	335	0	0	4	0
All	All	13704	0	11635	59	1

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 (59) 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:159:MET:HE1	7:C:824:HOH:O	1.84	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:274:TYR:CE1	7:D:856:HOH:O	2.43	0.71
1:A:126:PRO:O	7:A:601:HOH:O	2.10	0.68
1:C:102:LYS:HG3	1:C:443:ILE:HG22	1.76	0.67
1:B:275:TYR:CD2	7:B:604:HOH:O	2.51	0.61
1:B:275:TYR:CE2	7:B:604:HOH:O	2.53	0.61
1:B:262:LYS:HG2	7:B:928:HOH:O	2.02	0.59
1:A:111:LYS:NZ	1:D:112:GLY:O	2.35	0.58
1:B:229:SER:HB3	1:B:347:LYS:HE2	1.89	0.53
1:A:321:ILE:HD11	1:A:387:PHE:HB3	1.91	0.51
1:B:296:TRP:N	7:B:604:HOH:O	2.45	0.50
1:B:344:ASN:HB3	7:B:813:HOH:O	2.13	0.48
1:C:331:LYS:HE3	7:C:862:HOH:O	2.13	0.48
1:C:216:ILE:HD13	1:C:256:PHE:CE2	2.49	0.48
1:D:216:ILE:HD13	1:D:256:PHE:CE2	2.49	0.48
1:C:309:ASN:HB3	7:C:626:HOH:O	2.13	0.48
1:B:211:ILE:HG13	7:C:817:HOH:O	2.13	0.47
1:C:462:GLU:HB2	7:C:884:HOH:O	2.13	0.47
1:D:465:PHE:O	1:D:469:LYS:HG3	2.14	0.47
1:D:321:ILE:CD1	1:D:387:PHE:HB3	2.44	0.47
1:B:321:ILE:CD1	1:B:387:PHE:HB3	2.45	0.47
1:D:344:ASN:HB3	7:D:836:HOH:O	2.15	0.46
1:B:321:ILE:HD11	1:B:387:PHE:HB3	1.97	0.46
1:A:99:ILE:HA	1:A:445:PHE:CD2	2.51	0.45
1:D:141:ASN:ND2	7:D:611:HOH:O	2.48	0.45
1:C:102:LYS:HG3	1:C:443:ILE:CG2	2.44	0.45
1:A:219:TRP:CD1	1:A:220:ARG:HG2	2.51	0.45
1:C:344:ASN:HB3	7:C:705:HOH:O	2.16	0.45
1:B:275:TYR:CZ	7:B:604:HOH:O	2.70	0.45
1:C:121:PHE:CG	1:C:229:SER:HA	2.52	0.45
1:B:271:ALA:HB1	1:B:274:TYR:HB2	1.99	0.44
1:D:271:ALA:HB1	1:D:274:TYR:HB2	1.99	0.44
1:A:321:ILE:CD1	1:A:387:PHE:HB3	2.47	0.44
1:D:230:GLU:OE2	1:D:406:PHE:HA	2.17	0.44
1:A:99:ILE:HD13	1:D:177:VAL:HG11	1.99	0.44
1:D:274:TYR:CZ	7:D:856:HOH:O	2.62	0.44
1:B:275:TYR:CG	7:B:604:HOH:O	2.70	0.43
1:B:275:TYR:CD1	1:B:275:TYR:C	2.96	0.43
1:C:321:ILE:HD11	1:C:387:PHE:HB3	2.00	0.43
1:A:465:PHE:O	1:A:469:LYS:HG3	2.19	0.43
1:A:99:ILE:HG12	1:D:177:VAL:HG21	2.00	0.43
1:B:465:PHE:O	1:B:469:LYS:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:216:ILE:HD13	1:B:256:PHE:CE2	2.55	0.42
1:A:183:ALA:O	1:A:230:GLU:HA	2.20	0.42
1:A:93:PRO:O	1:A:449:ASN:ND2	2.50	0.42
1:B:174:PHE:CZ	1:C:101:SER:HA	2.55	0.41
1:B:211:ILE:CG1	7:C:817:HOH:O	2.67	0.41
1:A:216:ILE:HD13	1:A:256:PHE:CE2	2.55	0.41
7:A:730:HOH:O	1:B:171:ASN:CB	2.69	0.41
1:A:419:ARG:HD3	1:A:446:CYS:HB3	2.02	0.41
1:B:322:PHE:HB2	1:B:327:ARG:HD2	2.03	0.41
1:B:393:ILE:HG23	1:B:445:PHE:CZ	2.56	0.41
1:C:99:ILE:HA	1:C:445:PHE:CD2	2.56	0.40
1:C:174:PHE:CZ	1:D:101:SER:HA	2.56	0.40
1:C:320:GLY:HA3	1:C:331:LYS:O	2.20	0.40
1:C:322:PHE:CE2	1:C:328:PRO:HG2	2.57	0.40
1:D:352:LYS:HE2	1:D:380:TRP:CD1	2.55	0.40
1:A:271:ALA:HB1	1:A:274:TYR:HB2	2.03	0.40
1:D:229:SER:HB3	1:D:347:LYS:HE2	2.02	0.40

All (1) 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)
1:A:430:ARG:NH1	1:C:366:SER:OG[2_556]	1.97	0.23

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	386/388 (100%)	367 (95%)	19 (5%)	0	100	100
1	B	386/388 (100%)	368 (95%)	17 (4%)	1 (0%)	36	35
1	C	386/388 (100%)	370 (96%)	16 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	386/388 (100%)	369 (96%)	17 (4%)	0	100	100
All	All	1544/1552 (100%)	1474 (96%)	69 (4%)	1 (0%)	48	46

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	223	ILE

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	335/335 (100%)	334 (100%)	1 (0%)	86	91
1	B	335/335 (100%)	333 (99%)	2 (1%)	78	85
1	C	335/335 (100%)	335 (100%)	0	100	100
1	D	335/335 (100%)	334 (100%)	1 (0%)	86	91
All	All	1340/1340 (100%)	1336 (100%)	4 (0%)	86	91

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	331	LYS
1	B	173	ARG
1	B	262	LYS
1	D	388	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	313	GLN
1	A	325	ASN
1	A	341	ASN
1	B	136	GLN

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Mol	Chain	Res	Type
1	B	270	ASN
1	C	341	ASN
1	C	344	ASN
1	C	434	ASN
1	D	136	GLN
1	D	325	ASN
1	D	329	ASN
1	D	341	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

7 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	0.57	0	17,19,21	1.25	2 (11%)
2	NAG	E	2	2	14,14,15	0.35	0	17,19,21	0.85	0
2	BMA	E	3	2	11,11,12	0.58	0	15,15,17	0.88	0
2	MAN	E	4	2	11,11,12	0.66	0	15,15,17	1.02	1 (6%)
2	FUC	E	5	2	10,10,11	0.48	0	14,14,16	1.50	3 (21%)
3	NAG	F	1	1,3	14,14,15	0.66	0	17,19,21	2.33	3 (17%)
3	NAG	F	2	3	14,14,15	0.53	0	17,19,21	1.11	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	2,1	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
2	BMA	E	3	2	-	2/2/19/22	0/1/1/1
2	MAN	E	4	2	-	1/2/19/22	0/1/1/1
2	FUC	E	5	2	-	-	0/1/1/1
3	NAG	F	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	F	2	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	1	NAG	C1-C2-N2	-7.40	98.77	110.43
3	F	1	NAG	C1-O5-C5	4.45	118.14	112.19
2	E	5	FUC	O5-C5-C6	2.71	113.28	107.40
2	E	5	FUC	O5-C5-C4	-2.65	104.78	109.55
2	E	1	NAG	O5-C1-C2	2.36	114.94	111.29
2	E	4	MAN	O6-C6-C5	-2.27	103.59	111.33
2	E	1	NAG	C1-O5-C5	-2.13	109.33	112.19
3	F	1	NAG	C8-C7-N2	-2.12	112.59	116.12
2	E	5	FUC	O5-C1-C2	-2.04	105.93	110.79
3	F	2	NAG	C1-O5-C5	2.03	114.91	112.19

There are no chirality outliers.

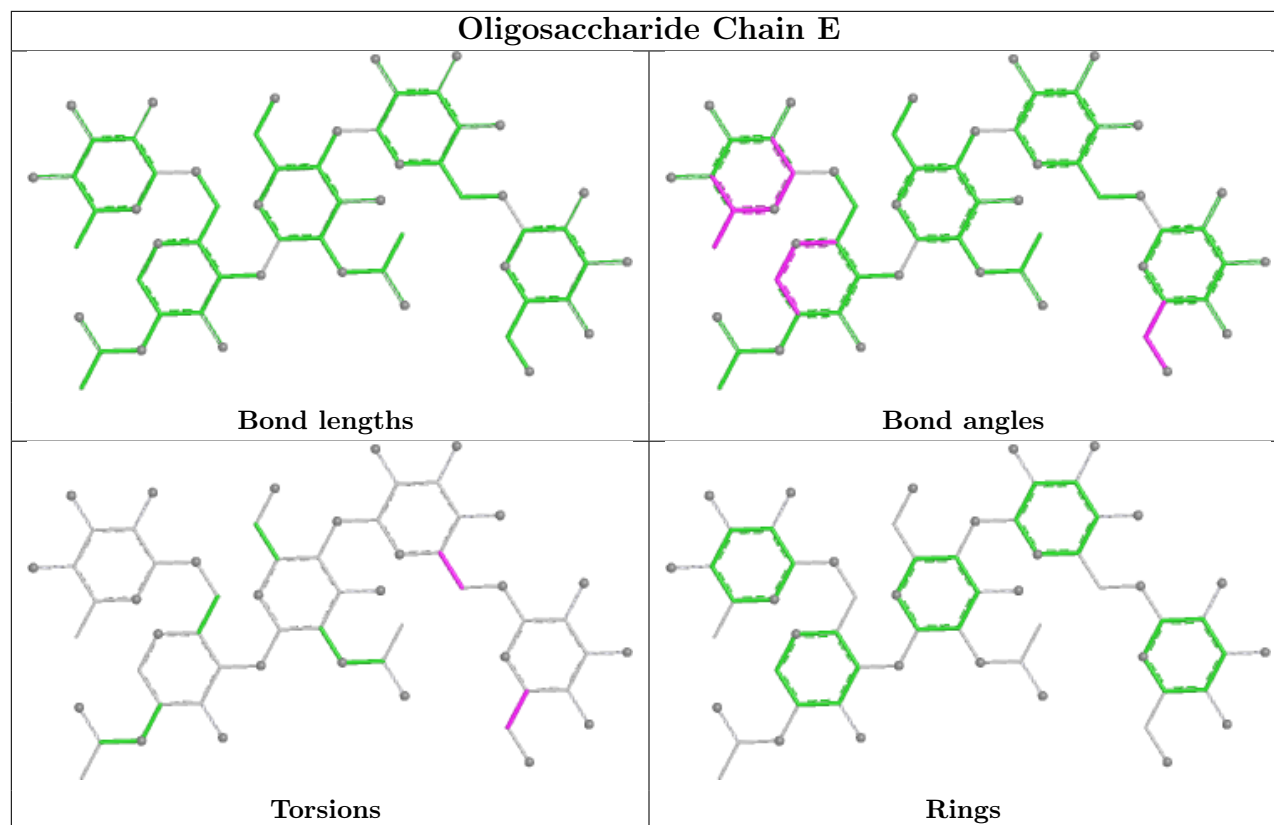
All (5) torsion outliers are listed below:

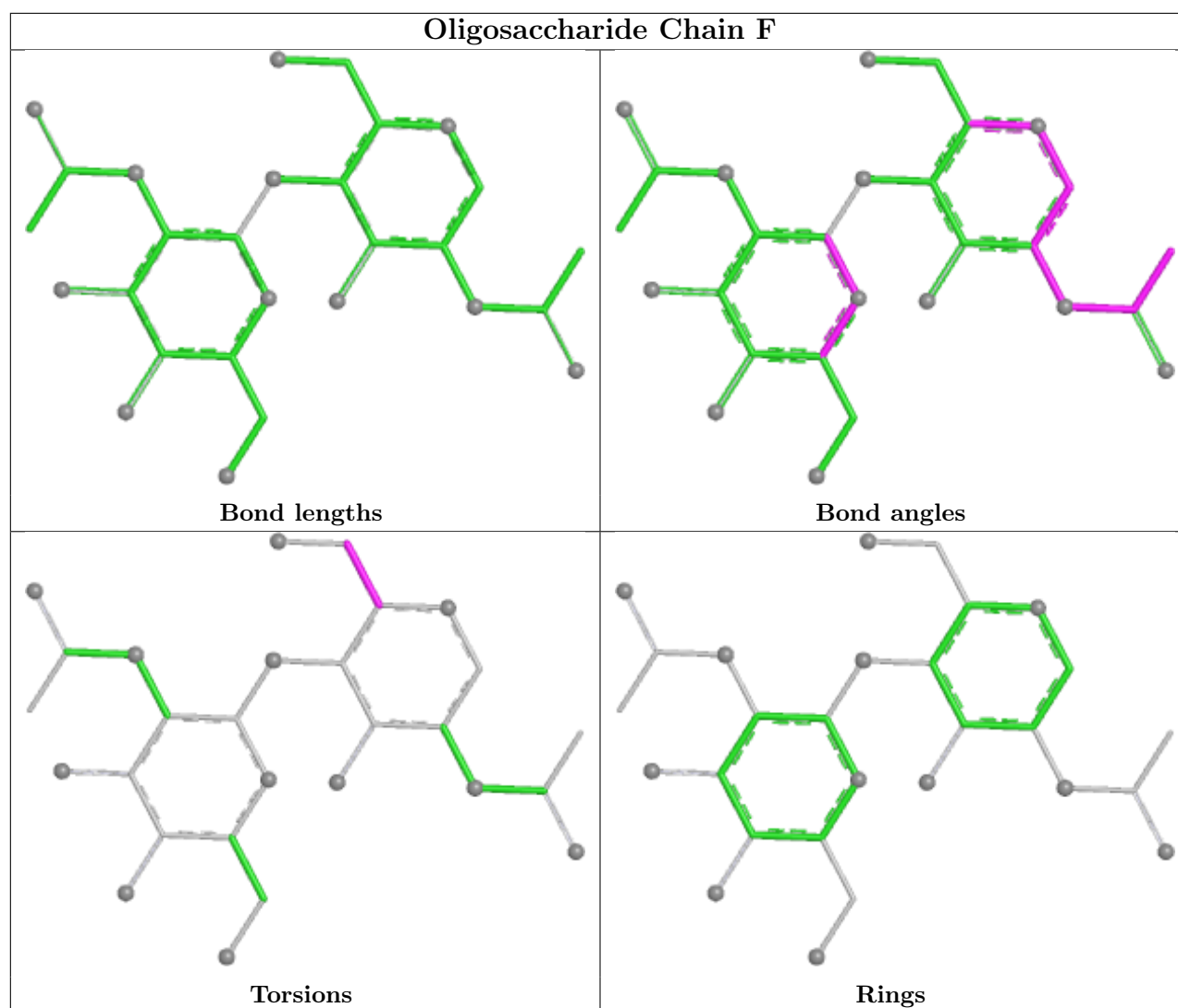
Mol	Chain	Res	Type	Atoms
3	F	1	NAG	C4-C5-C6-O6
3	F	1	NAG	O5-C5-C6-O6
2	E	4	MAN	C4-C5-C6-O6
2	E	3	BMA	O5-C5-C6-O6
2	E	3	BMA	C4-C5-C6-O6

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	$\# Z > 2$
6	NAG	D	505	1	14,14,15	0.73	0	17,19,21	0.85	0
6	NAG	D	506	1	14,14,15	0.45	0	17,19,21	0.85	1 (5%)
6	NAG	B	505	1	14,14,15	1.06	2 (14%)	17,19,21	1.53	5 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	B	506	1	14,14,15	0.57	0	17,19,21	1.14	1 (5%)
6	NAG	C	506	1	14,14,15	0.51	0	17,19,21	1.07	2 (11%)
6	NAG	A	504	1	14,14,15	0.69	0	17,19,21	1.07	1 (5%)
6	NAG	B	504	1	14,14,15	0.57	0	17,19,21	1.12	1 (5%)
6	NAG	C	507	1	14,14,15	0.47	0	17,19,21	0.80	1 (5%)
5	G39	B	503	-	19,20,20	1.11	1 (5%)	20,27,27	1.68	4 (20%)
6	NAG	D	504	1	14,14,15	0.69	0	17,19,21	1.95	2 (11%)
6	NAG	A	510	1	14,14,15	0.36	0	17,19,21	0.79	0
5	G39	C	503	-	19,20,20	1.01	1 (5%)	20,27,27	1.41	1 (5%)
5	G39	D	503	-	19,20,20	1.23	2 (10%)	20,27,27	1.69	3 (15%)
5	G39	A	503	-	19,20,20	0.82	1 (5%)	20,27,27	1.52	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	D	505	1	-	0/6/23/26	0/1/1/1
6	NAG	D	506	1	-	0/6/23/26	0/1/1/1
6	NAG	B	505	1	-	2/6/23/26	0/1/1/1
6	NAG	B	506	1	-	0/6/23/26	0/1/1/1
6	NAG	C	506	1	-	2/6/23/26	0/1/1/1
6	NAG	A	504	1	-	0/6/23/26	0/1/1/1
6	NAG	B	504	1	-	0/6/23/26	0/1/1/1
6	NAG	C	507	1	-	0/6/23/26	0/1/1/1
5	G39	B	503	-	-	0/16/32/32	0/1/1/1
6	NAG	D	504	1	-	0/6/23/26	0/1/1/1
6	NAG	A	510	1	-	0/6/23/26	0/1/1/1
5	G39	C	503	-	-	0/16/32/32	0/1/1/1
5	G39	D	503	-	-	1/16/32/32	0/1/1/1
5	G39	A	503	-	-	0/16/32/32	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	503	G39	C6-C7	3.31	1.54	1.50
5	B	503	G39	C6-C7	3.00	1.54	1.50
5	D	503	G39	O1A-C1	2.53	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	505	NAG	C1-C2	2.34	1.55	1.52
5	A	503	G39	C6-C7	2.09	1.53	1.50
5	C	503	G39	C6-C7	2.07	1.53	1.50
6	B	505	NAG	C3-C2	2.03	1.56	1.52

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	504	NAG	C1-C2-N2	-6.47	100.23	110.43
5	D	503	G39	C4-C3-C2	5.50	115.95	109.72
5	B	503	G39	C4-C3-C2	5.14	115.54	109.72
5	C	503	G39	C4-C3-C2	5.06	115.45	109.72
5	A	503	G39	C4-C3-C2	4.69	115.03	109.72
5	B	503	G39	O1B-C1-C2	2.77	121.27	115.43
5	B	503	G39	O1B-C1-O1A	-2.72	117.42	123.90
6	B	505	NAG	C1-O5-C5	2.46	115.48	112.19
6	B	505	NAG	C3-C4-C5	-2.41	105.86	110.23
6	C	507	NAG	C1-O5-C5	2.40	115.41	112.19
6	B	504	NAG	C1-C2-N2	-2.35	106.74	110.43
5	D	503	G39	C3-C2-C7	-2.32	119.38	122.25
6	B	505	NAG	O5-C5-C4	-2.28	105.27	110.83
5	D	503	G39	O1B-C1-O1A	-2.25	118.53	123.90
5	B	503	G39	C3-C2-C7	-2.22	119.51	122.25
6	B	505	NAG	O4-C4-C5	2.20	114.73	109.32
6	A	504	NAG	O3-C3-C4	-2.17	105.25	110.38
6	C	506	NAG	O5-C1-C2	2.10	114.54	111.29
6	D	504	NAG	O3-C3-C4	-2.08	105.47	110.38
6	C	506	NAG	O7-C7-N2	2.05	125.60	121.98
6	B	505	NAG	C1-C2-N2	-2.03	107.23	110.43
6	B	506	NAG	C4-C3-C2	-2.03	108.05	111.02
6	D	506	NAG	C1-C2-N2	-2.01	107.27	110.43

There are no chirality outliers.

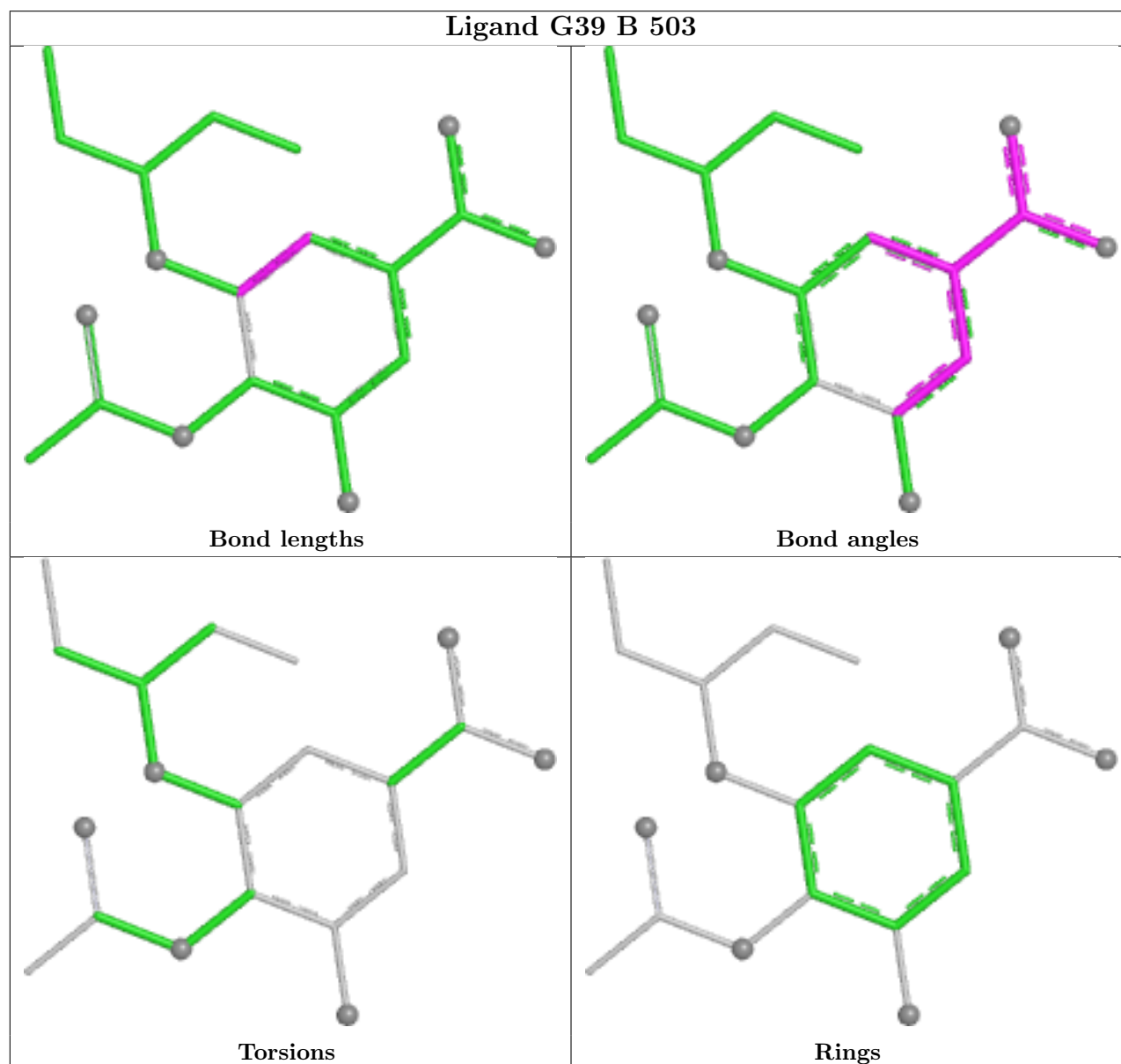
All (5) torsion outliers are listed below:

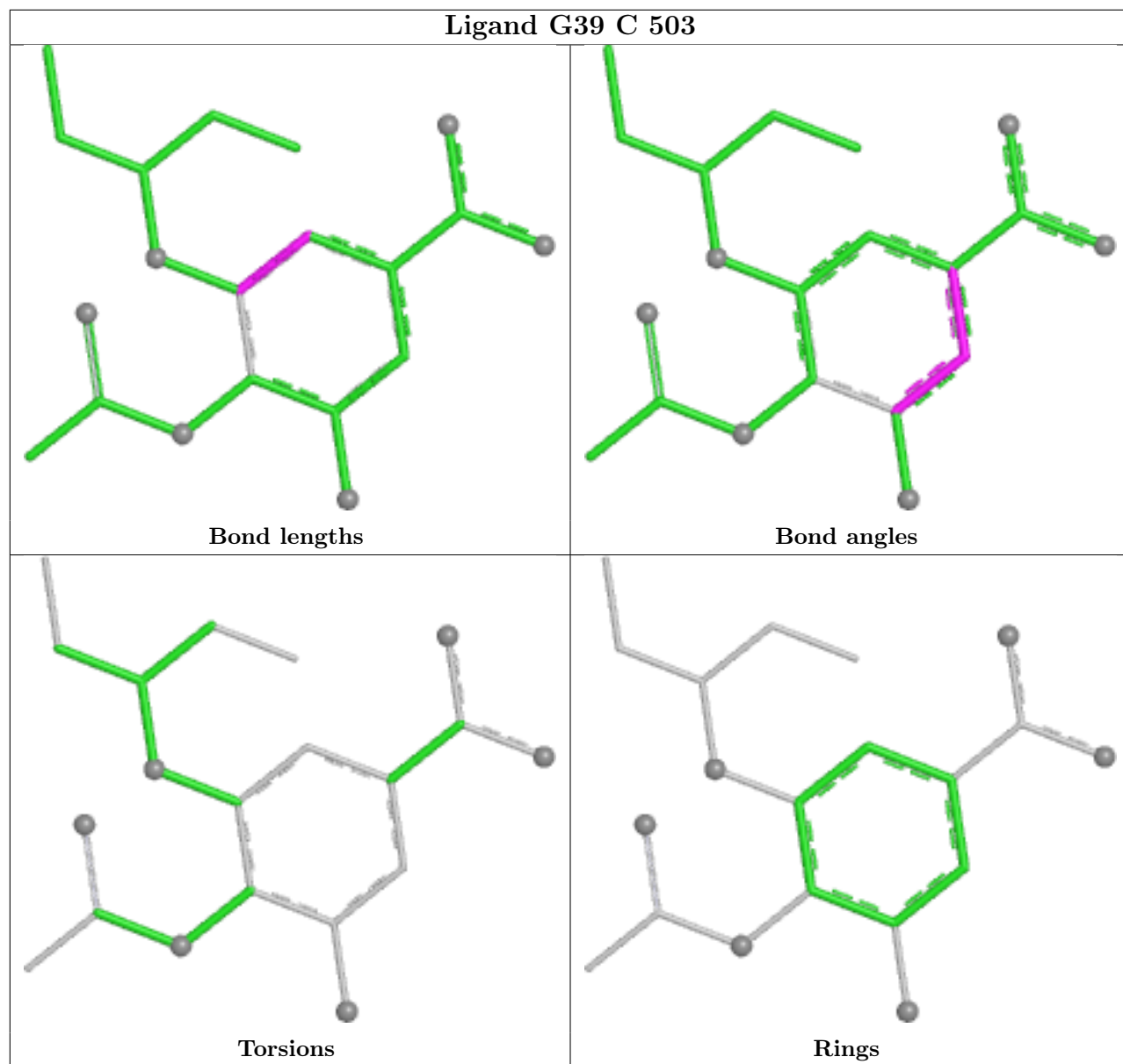
Mol	Chain	Res	Type	Atoms
6	C	506	NAG	O5-C5-C6-O6
6	C	506	NAG	C4-C5-C6-O6
6	B	505	NAG	C4-C5-C6-O6
6	B	505	NAG	O5-C5-C6-O6
5	D	503	G39	O7-C8-C81-C82

There are no ring outliers.

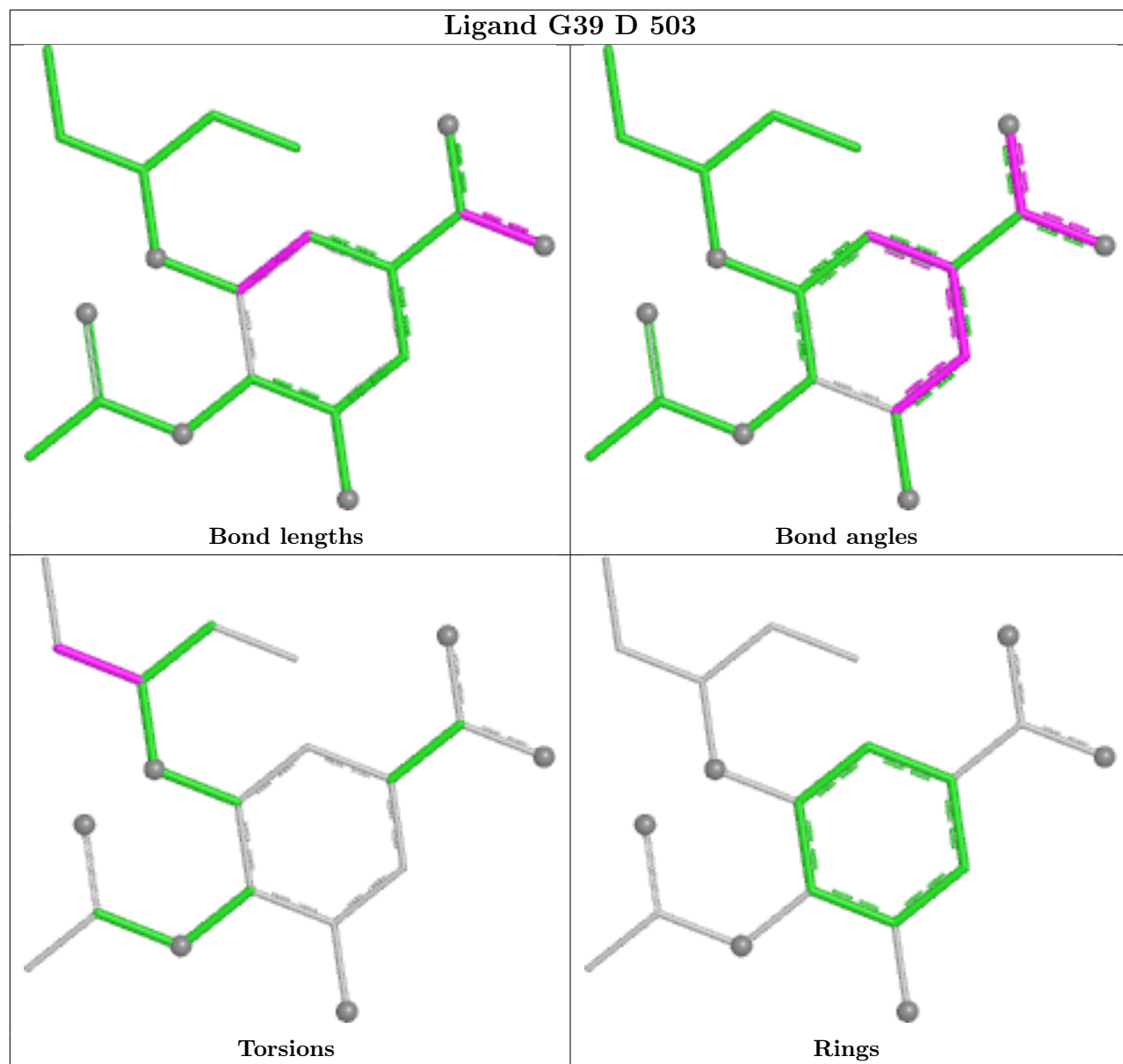
No monomer is involved in short contacts.

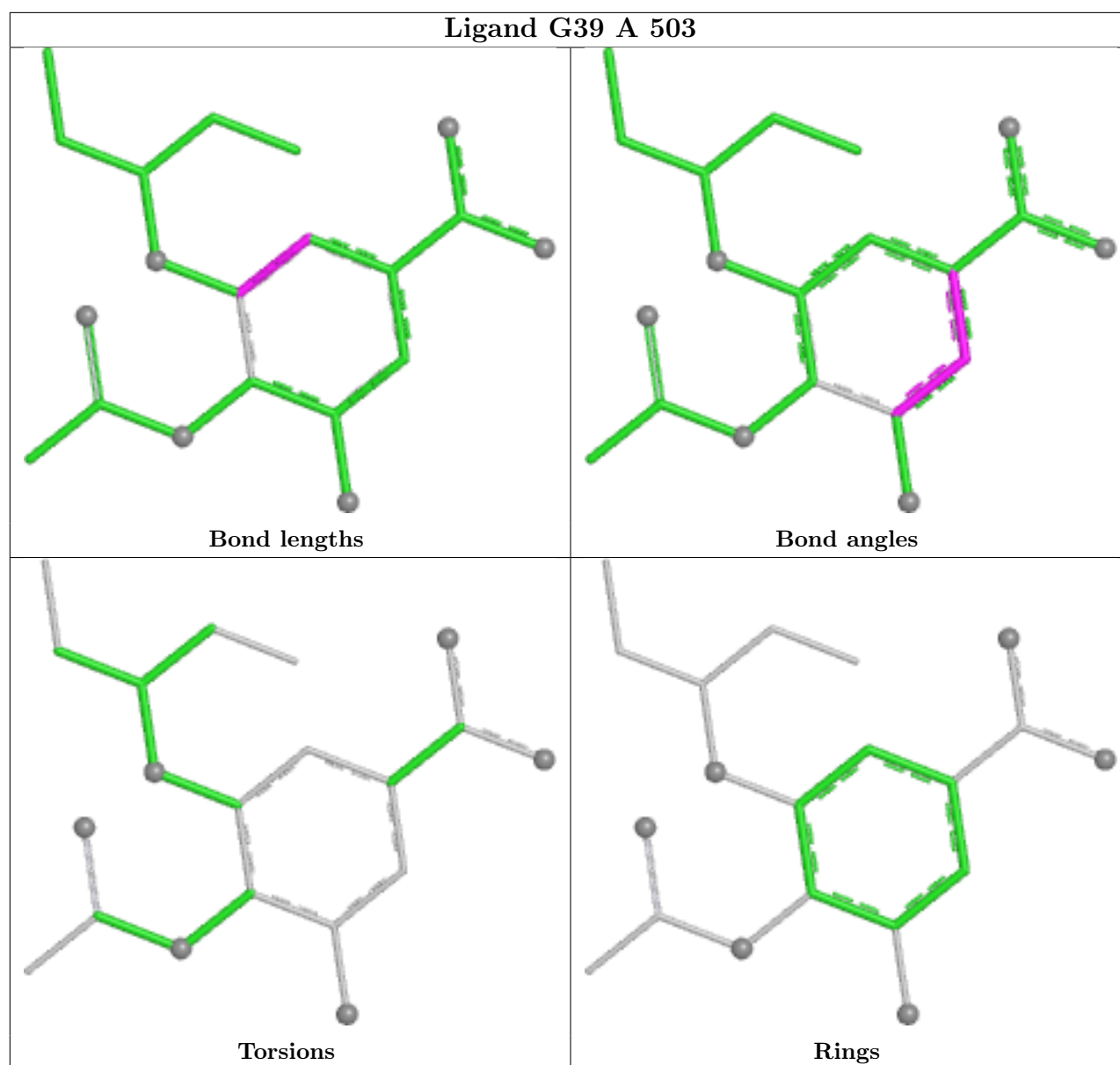
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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





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	388/388 (100%)	0.75	18 (4%) 37 36	14, 21, 32, 54	0
1	B	388/388 (100%)	1.00	44 (11%) 10 9	13, 22, 35, 55	0
1	C	388/388 (100%)	0.67	21 (5%) 31 30	14, 20, 30, 59	0
1	D	388/388 (100%)	0.77	24 (6%) 26 25	13, 22, 35, 54	0
All	All	1552/1552 (100%)	0.80	107 (6%) 23 21	13, 21, 34, 59	0

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	469	LYS	6.2
1	B	335	CYS	4.1
1	A	469	LYS	4.0
1	C	430	ARG	3.8
1	B	338	VAL	3.6
1	D	335	CYS	3.6
1	B	386	ASN	3.6
1	B	331	LYS	3.5
1	A	430	ARG	3.4
1	C	164	GLY	3.4
1	D	331	LYS	3.3
1	D	274	TYR	3.3
1	A	164	GLY	3.1
1	A	267	VAL	3.1
1	B	274	TYR	3.0
1	C	449	ASN	3.0
1	D	469	LYS	3.0
1	A	127	LEU	3.0
1	B	343	ALA	2.9
1	B	449	ASN	2.9
1	D	386	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	469	LYS	2.9
1	A	220	ARG	2.9
1	C	335	CYS	2.9
1	B	384	ASP	2.9
1	B	93	PRO	2.9
1	B	399	TRP	2.9
1	B	381	THR	2.8
1	C	122	ILE	2.8
1	C	173	ARG	2.7
1	D	93	PRO	2.7
1	B	357	VAL	2.7
1	D	338	VAL	2.7
1	B	356	GLY	2.7
1	A	449	ASN	2.6
1	A	173	ARG	2.6
1	C	331	LYS	2.6
1	B	330	ASP	2.6
1	C	127	LEU	2.6
1	D	388	SER	2.6
1	A	274	TYR	2.5
1	B	340	SER	2.5
1	B	354	GLY	2.5
1	C	314	ILE	2.5
1	D	434	ASN	2.5
1	A	126	PRO	2.4
1	B	341	ASN	2.4
1	A	296	TRP	2.4
1	B	375	TRP	2.4
1	C	280	SER	2.4
1	C	92	CYS	2.4
1	D	309	ASN	2.4
1	D	449	ASN	2.4
1	D	384	ASP	2.4
1	B	83	VAL	2.4
1	B	314	ILE	2.3
1	D	357	VAL	2.3
1	D	92	CYS	2.3
1	D	387	PHE	2.3
1	B	82	SER	2.3
1	B	328	PRO	2.3
1	C	126	PRO	2.3
1	D	127	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	365	ILE	2.3
1	B	120	PRO	2.3
1	B	342	GLY	2.3
1	D	305	SER	2.2
1	D	383	THR	2.2
1	B	432	LYS	2.2
1	B	126	PRO	2.2
1	B	251	ALA	2.2
1	A	335	CYS	2.2
1	B	446	CYS	2.2
1	B	430	ARG	2.2
1	B	303	TRP	2.2
1	D	399	TRP	2.2
1	A	246	PRO	2.1
1	B	427	ILE	2.1
1	D	83	VAL	2.1
1	B	305	SER	2.1
1	C	272	PRO	2.1
1	C	108	ILE	2.1
1	D	267	VAL	2.1
1	A	100	TYR	2.1
1	D	120	PRO	2.1
1	C	446	CYS	2.1
1	A	272	PRO	2.1
1	B	326	PRO	2.1
1	A	314	ILE	2.1
1	C	262	LYS	2.1
1	D	216	ILE	2.1
1	B	94	VAL	2.1
1	B	267	VAL	2.1
1	A	271	ALA	2.1
1	B	92	CYS	2.0
1	B	313	GLN	2.0
1	C	220	ARG	2.0
1	B	383	THR	2.0
1	A	122	ILE	2.0
1	B	166	VAL	2.0
1	B	388	SER	2.0
1	C	455	TRP	2.0
1	B	385	ASN	2.0
1	C	385	ASN	2.0
1	B	127	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	173	ARG	2.0
1	C	93	PRO	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](#)

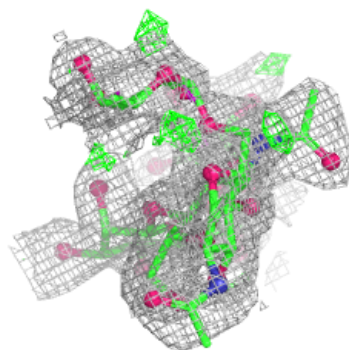
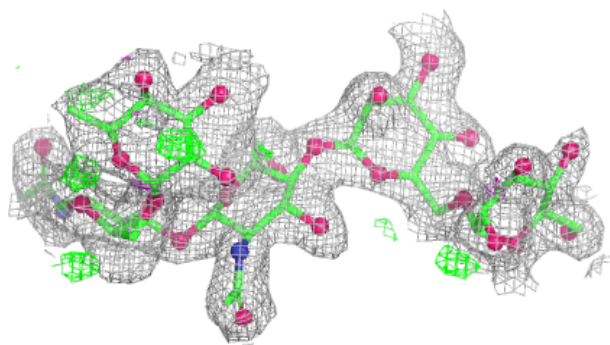
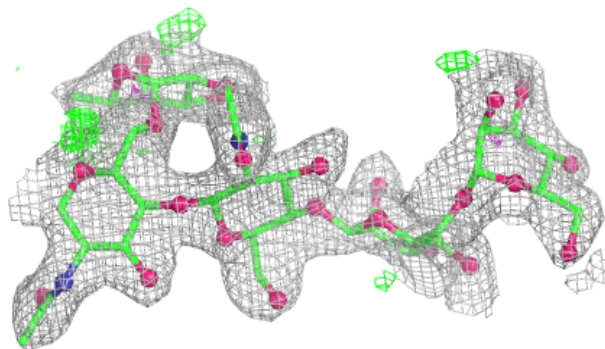
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists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

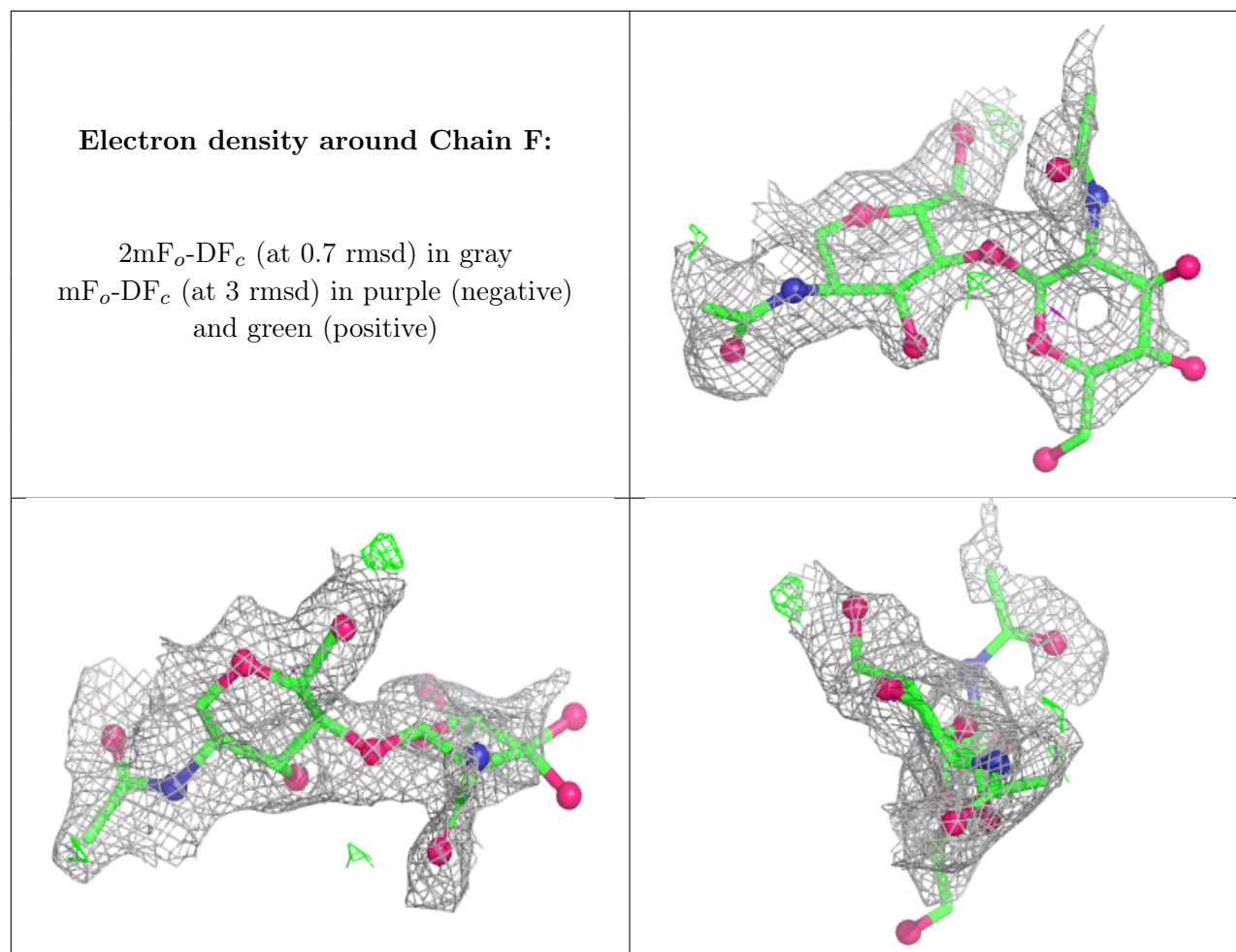
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAG	F	2	14/15	0.47	0.18	47,51,55,56	0
3	NAG	F	1	14/15	0.70	0.15	35,36,40,43	0
2	FUC	E	5	10/11	0.76	0.15	29,34,35,36	0
2	BMA	E	3	11/12	0.81	0.13	39,41,42,43	0
2	MAN	E	4	11/12	0.84	0.12	39,40,41,42	0
2	NAG	E	1	14/15	0.85	0.11	26,29,32,33	0
2	NAG	E	2	14/15	0.88	0.11	32,33,37,38	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(Å ²)	Q<0.9
6	NAG	B	506	14/15	0.56	0.16	43,46,48,53	0
6	NAG	D	506	14/15	0.60	0.17	42,46,48,51	0
6	NAG	D	504	14/15	0.62	0.17	44,47,52,53	0
6	NAG	B	505	14/15	0.64	0.20	37,45,51,52	0
6	NAG	A	510	14/15	0.68	0.15	41,46,50,50	0
6	NAG	B	504	14/15	0.70	0.15	41,46,49,50	0
6	NAG	C	507	14/15	0.70	0.15	43,48,49,52	0
6	NAG	A	504	14/15	0.73	0.14	33,36,39,42	0
6	NAG	D	505	14/15	0.79	0.12	28,34,36,42	0
6	NAG	C	506	14/15	0.82	0.12	31,33,37,38	0
5	G39	B	503	20/20	0.88	0.12	18,21,27,27	0

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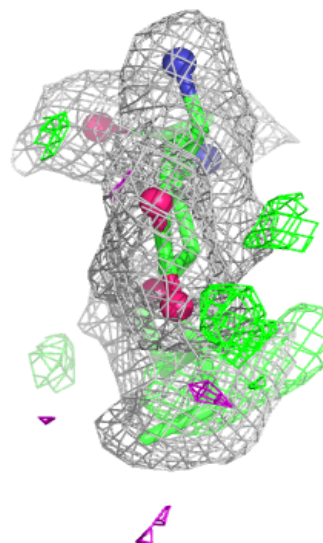
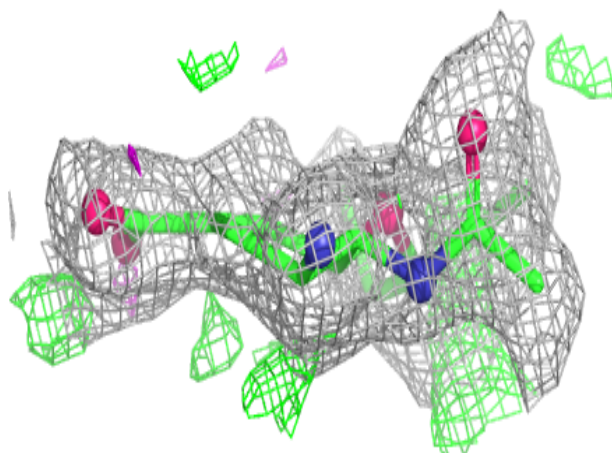
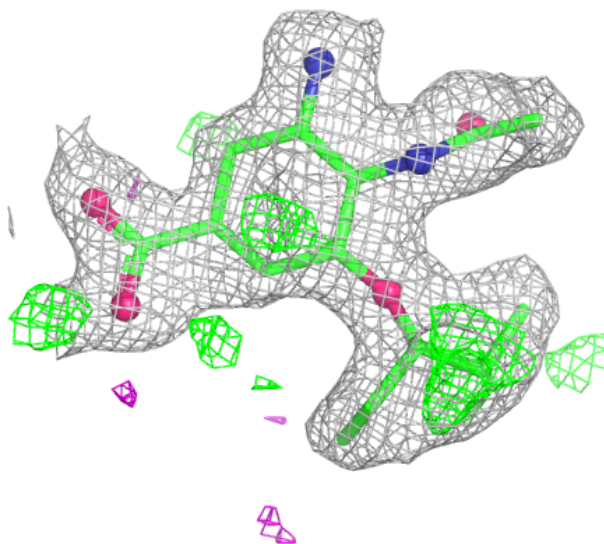
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	G39	D	503	20/20	0.88	0.11	17,21,24,24	0
5	G39	A	503	20/20	0.90	0.10	15,20,27,29	0
5	G39	C	503	20/20	0.91	0.10	14,20,25,26	0
4	CA	B	502	1/1	0.96	0.10	42,42,42,42	0
4	CA	D	502	1/1	0.97	0.11	37,37,37,37	0
4	CA	A	502	1/1	0.98	0.05	36,36,36,36	0
4	CA	B	501	1/1	0.98	0.03	23,23,23,23	0
4	CA	D	501	1/1	0.99	0.02	23,23,23,23	0
4	CA	A	501	1/1	0.99	0.02	18,18,18,18	0
4	CA	C	501	1/1	0.99	0.03	16,16,16,16	0
4	CA	C	502	1/1	0.99	0.06	31,31,31,31	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.

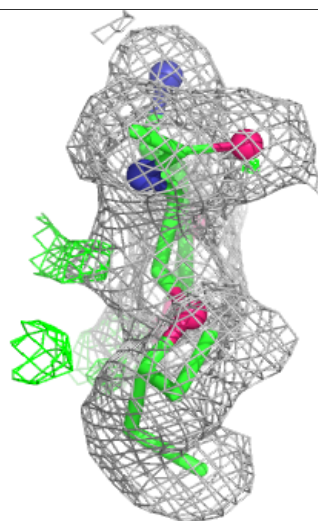
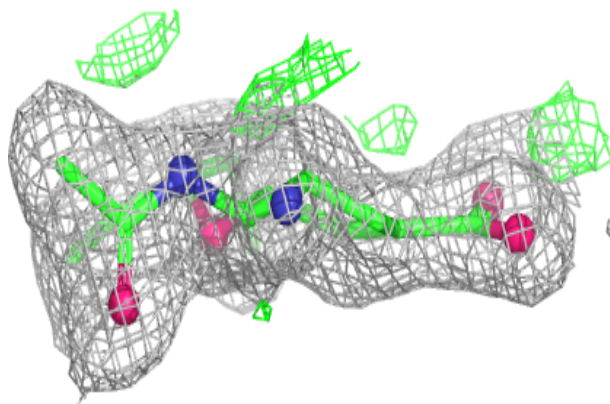
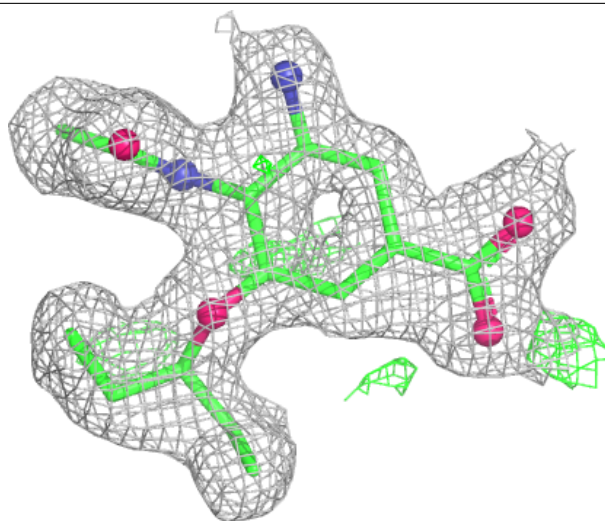
Electron density around G39 B 503:

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



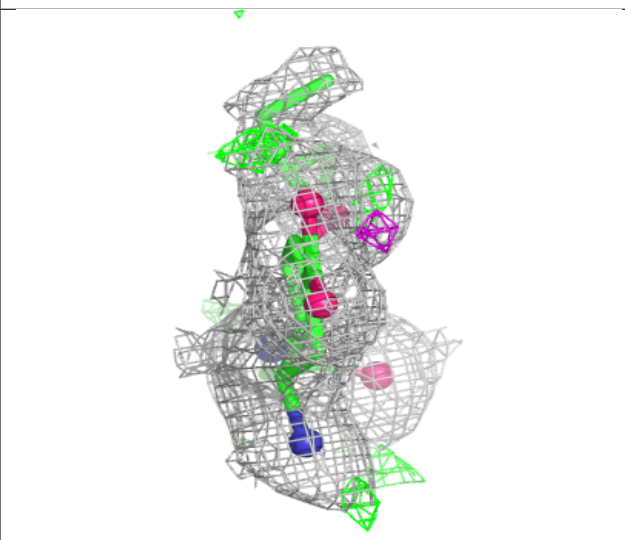
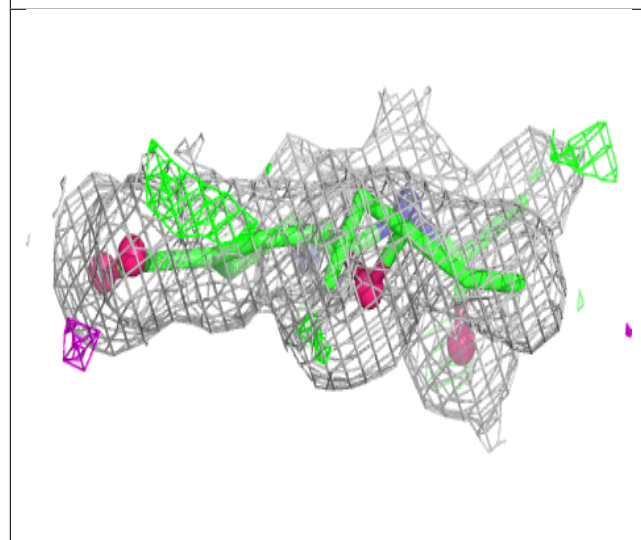
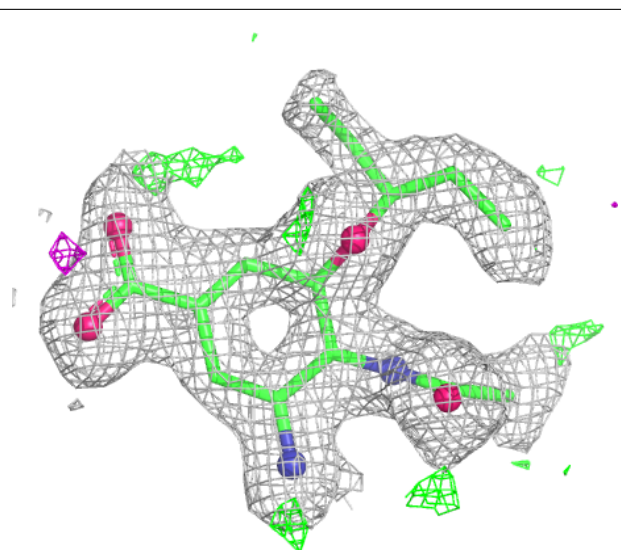
Electron density around G39 D 503:

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



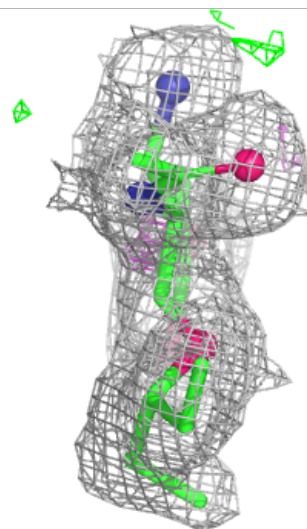
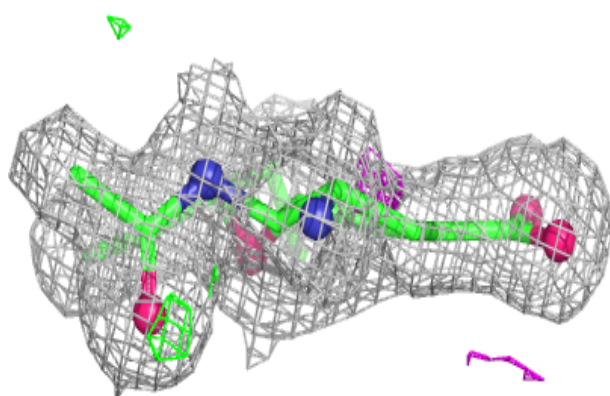
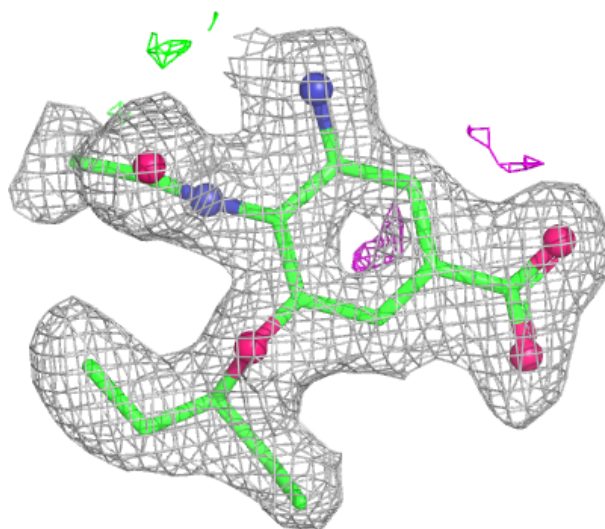
Electron density around G39 A 503:

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



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)



6.5 Other polymers ⓘ

There are no such residues in this entry.