



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2020 – 08:32 AM BST

PDB ID : 6HP0
Title : Complex of Neuraminidase from H1N1 Influenza Virus in Complex with Oseltamivir Triazol Derivative
Authors : Pachl, P.; Pokorna, J.
Deposited on : 2018-09-19
Resolution : 1.88 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

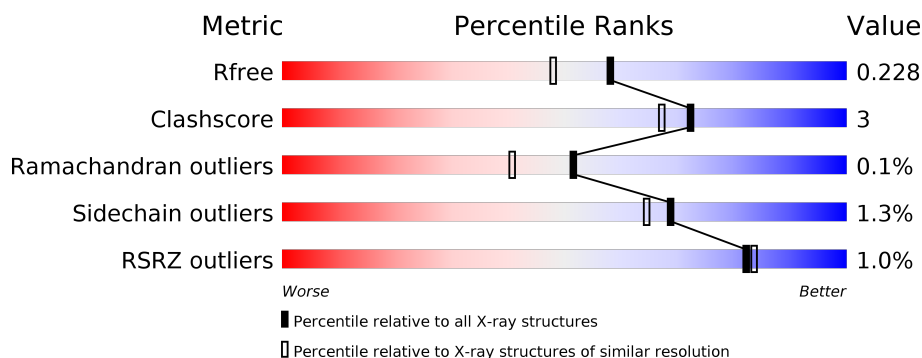
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.88 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.



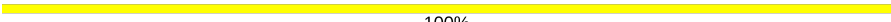
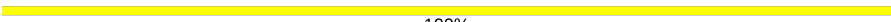
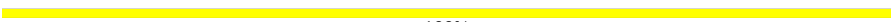
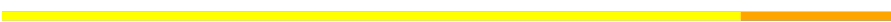
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	9470 (1.90-1.86)
Clashscore	141614	10282 (1.90-1.86)
Ramachandran outliers	138981	10152 (1.90-1.86)
Sidechain outliers	138945	10152 (1.90-1.86)
RSRZ outliers	127900	9303 (1.90-1.86)

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 style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 90%, green 9%, grey 0%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 90% 9% </div> </div>
1	B	388	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, orange 1%, yellow 90%, green 9%, grey 0%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 2% 90% 9% </div> </div>
1	C	388	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 87%, green 12%, grey 0%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 87% 12% </div> </div>
1	D	388	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 89%, green 11%, grey 0%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 89% 11% </div> </div>
2	E	3	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, yellow 33%, orange 67%, grey 0%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 33% 67% </div> </div>
2	G	3	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, yellow 67%, orange 33%, grey 0%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 67% 33% </div> </div>

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Mol	Chain	Length	Quality of chain
2	H	3	 100%
3	F	2	 100%
3	J	2	 100%
4	I	6	 83% 17%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	H	2	-	-	-	X

2 Entry composition [i](#)

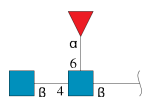
There are 10 unique types of molecules in this entry. The entry contains 14022 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	5	0
			3010	1890	517	582	21			
1	B	387	Total	C	N	O	S	0	4	0
			3005	1886	519	579	21			
1	C	387	Total	C	N	O	S	0	6	0
			3011	1890	518	582	21			
1	D	387	Total	C	N	O	S	0	6	0
			3017	1896	518	582	21			

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



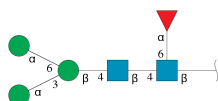
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	3	Total	C	N	O	0	0	0
			38	22	2	14			
2	G	3	Total	C	N	O	0	0	0
			38	22	2	14			
2	H	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 3 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	F	2	Total	C	N	O	0	0	0
			24	14	1	9			
3	J	2	Total	C	N	O	0	0	0
			24	14	1	9			

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[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.

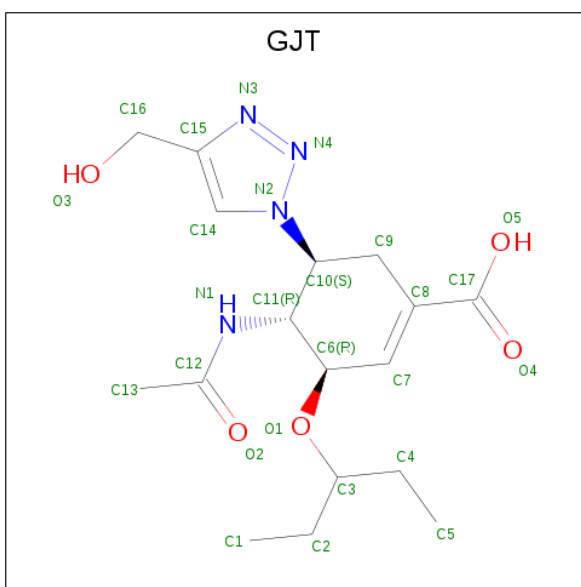


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	I	6	Total	C	N	O	0	0	0
			71	40	2	29			

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

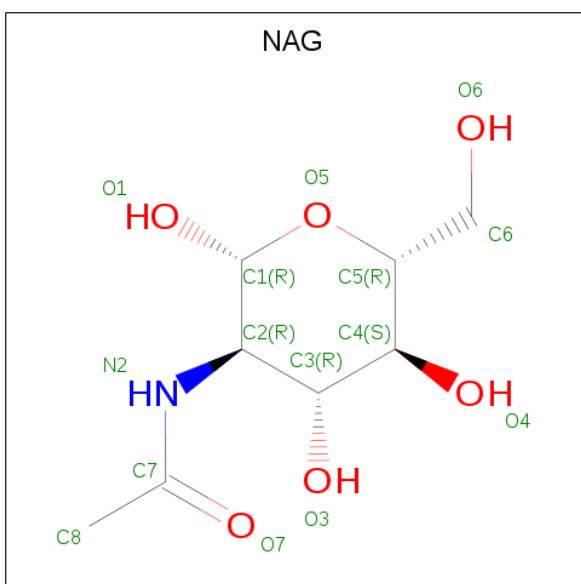
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	2	Total	Ca	0	0
			2	2		
5	A	2	Total	Ca	0	0
			2	2		
5	D	2	Total	Ca	0	0
			2	2		
5	C	2	Total	Ca	0	0
			2	2		

- Molecule 6 is (3 {R},4 {R},5 {S})-4-acetamido-5-[4-(hydroxymethyl)-1,2,3-triazol-1-yl]-3-pentan-3-yloxy-cyclohexene-1-carboxylic acid (three-letter code: GJT) (formula: C₁₇H₂₆N₄O₅).



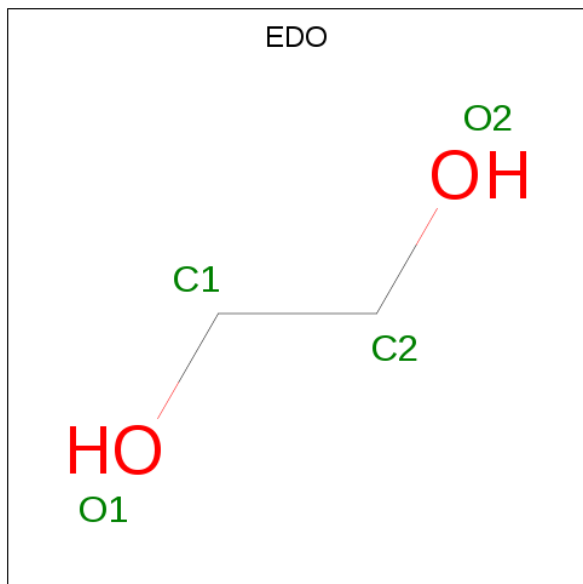
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			26	17	4	5		
6	B	1	Total	C	N	O	0	0
			26	17	4	5		
6	C	1	Total	C	N	O	0	0
			26	17	4	5		
6	D	1	Total	C	N	O	0	0
			26	17	4	5		

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 8 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

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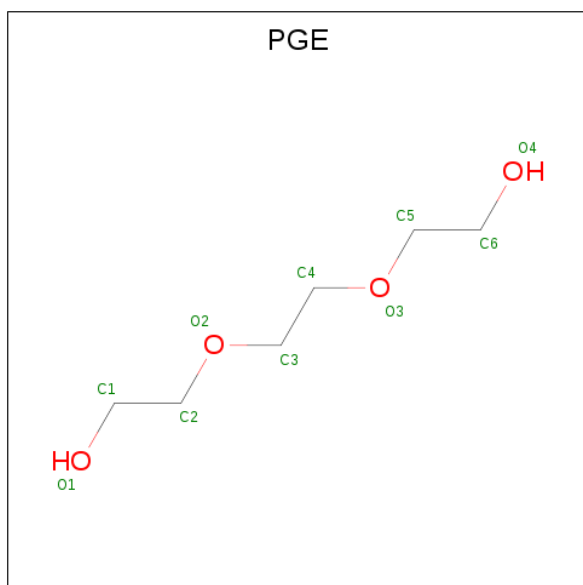
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total 4	C 2	O 2	0	0
8	A	1	Total 4	C 2	O 2	0	0
8	A	1	Total 4	C 2	O 2	0	0
8	A	1	Total 4	C 2	O 2	0	0
8	A	1	Total 4	C 2	O 2	0	0
8	A	1	Total 4	C 2	O 2	0	0
8	A	1	Total 4	C 2	O 2	0	0
8	A	1	Total 4	C 2	O 2	0	0
8	B	1	Total 4	C 2	O 2	0	0
8	B	1	Total 4	C 2	O 2	0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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	D	1	Total	C	O	0	0
			4	2	2		
8	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 9 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	D	1	Total	C	O	0	0
			7	4	3		

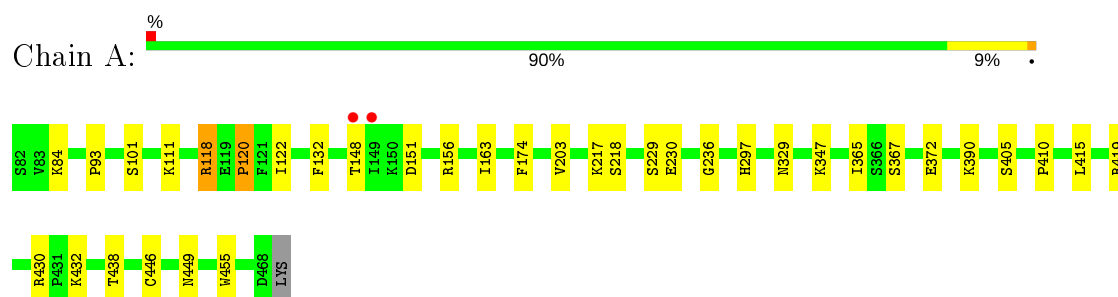
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	335	Total	O	0	4
			339	339		
10	B	337	Total	O	0	7
			344	344		
10	C	357	Total	O	0	4
			361	361		
10	D	370	Total	O	0	9
			379	379		

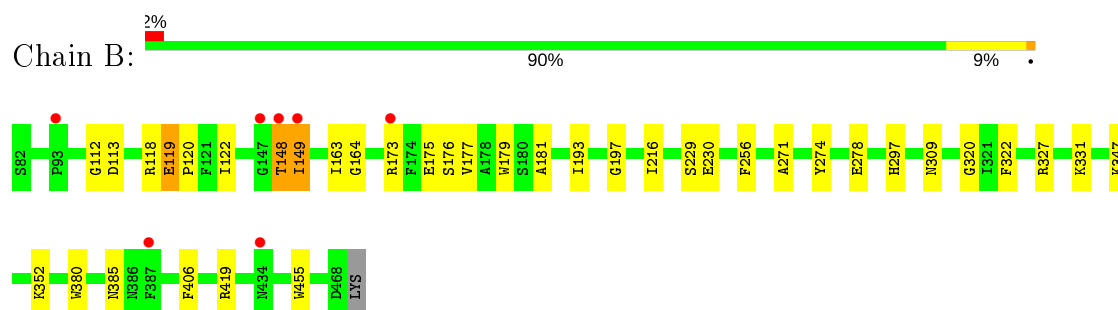
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

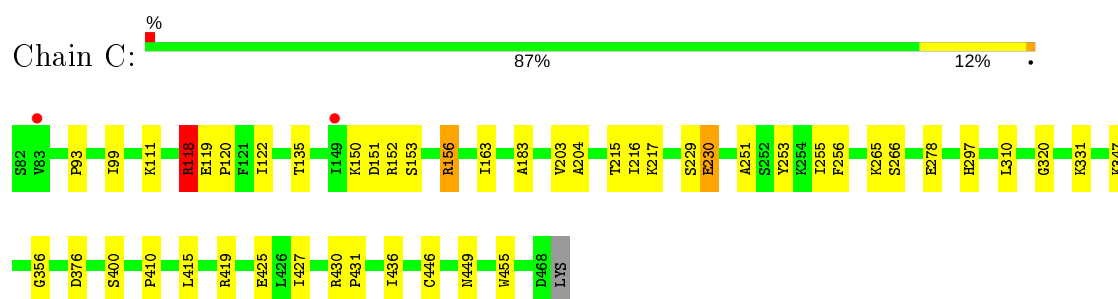
• Molecule 1: Neuraminidase



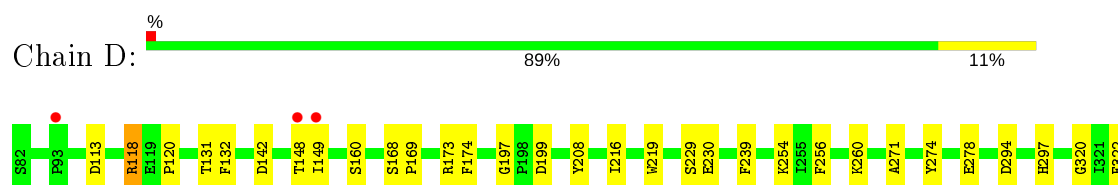
• Molecule 1: Neuraminidase

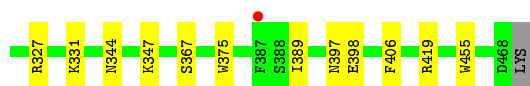


• Molecule 1: Neuraminidase



• Molecule 1: Neuraminidase





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

Chain E: 33% 67%



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

Chain G: 67% 33%



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

Chain H: 100%



- Molecule 3: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F: 100%



- Molecule 3: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J: 100%



- Molecule 4: alpha-D-mannopyranose-(1-3)-[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 I: 83% 17%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	85.84Å 126.86Å 96.91Å 90.00° 93.93° 90.00°	Depositor
Resolution (Å)	48.34 – 1.88 48.34 – 1.88	Depositor EDS
% Data completeness (in resolution range)	97.6 (48.34-1.88) 97.6 (48.34-1.88)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 1.88Å)	Xtriage
Refinement program	REFMAC 5.8.0232	Depositor
R, R_{free}	0.185 , 0.222 0.193 , 0.228	Depositor DCC
R_{free} test set	1626 reflections (1.00%)	wwPDB-VP
Wilson B-factor (Å ²)	20.9	Xtriage
Anisotropy	0.090	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 55.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14022	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.28% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PGE, NAG, GJT, EDO, BMA, FUC, CA, MAN

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	0.89	2/3107 (0.1%)	1.01	4/4224 (0.1%)
1	B	0.85	1/3099 (0.0%)	0.93	1/4213 (0.0%)
1	C	0.88	3/3108 (0.1%)	0.98	3/4225 (0.1%)
1	D	0.90	2/3117 (0.1%)	0.98	4/4239 (0.1%)
All	All	0.88	8/12431 (0.1%)	0.98	12/16901 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	278	GLU	CD-OE2	7.21	1.33	1.25
1	A	218	SER	CA-CB	-6.36	1.43	1.52
1	A	230	GLU	CD-OE1	6.24	1.32	1.25
1	D	398	GLU	CD-OE1	6.00	1.32	1.25
1	C	230	GLU	CD-OE1	5.36	1.31	1.25
1	C	356	GLY	C-O	5.25	1.32	1.23
1	D	278	GLU	CD-OE2	5.22	1.31	1.25
1	C	278	GLU	CD-OE2	5.06	1.31	1.25

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	118	ARG	NE-CZ-NH1	10.41	125.51	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	118	ARG	NE-CZ-NH2	-7.06	116.77	120.30
1	D	419	ARG	NE-CZ-NH2	-6.90	116.85	120.30
1	C	118	ARG	NE-CZ-NH2	6.40	123.50	120.30
1	D	344[A]	ASN	CB-CA-C	6.09	122.59	110.40
1	D	344[B]	ASN	CB-CA-C	6.09	122.59	110.40
1	D	173	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	C	152	ARG	NE-CZ-NH1	5.95	123.27	120.30
1	C	156	ARG	CG-CD-NE	-5.52	100.20	111.80
1	A	156	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	A	120	PRO	N-CA-C	-5.35	98.18	112.10
1	B	419	ARG	NE-CZ-NH2	-5.05	117.78	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	405	SER	Peptide

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	3010	0	2843	21	0
1	B	3005	0	2834	21	0
1	C	3011	0	2844	26	0
1	D	3017	0	2855	22	0
2	E	38	0	34	0	0
2	G	38	0	34	1	0
2	H	38	0	34	0	0
3	F	24	0	22	0	0
3	J	24	0	22	0	0
4	I	71	0	61	1	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
5	C	2	0	0	0	0
5	D	2	0	0	0	0
6	A	26	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	26	0	0	1	0
6	C	26	0	0	0	0
6	D	26	0	0	0	0
7	A	14	0	13	0	0
7	B	28	0	26	0	0
7	C	14	0	13	0	0
7	D	28	0	26	0	0
8	A	56	0	84	3	0
8	B	24	0	36	0	0
8	C	16	0	24	0	0
8	D	24	0	36	2	0
9	D	7	0	9	1	0
10	A	339	0	0	0	0
10	B	344	0	0	1	0
10	C	361	0	0	0	0
10	D	379	0	0	2	0
All	All	14022	0	11850	83	0

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 3.

All (83) 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:93:PRO:O	1:C:449:ASN:ND2	2.25	0.69
1:A:148:THR:HG23	1:A:151:ASP:HB2	1.77	0.66
1:C:151:ASP:OD2	1:C:153:SER:HB3	1.98	0.64
1:C:150:LYS:O	1:C:151:ASP:HB2	2.03	0.59
1:D:229:SER:HB3	1:D:347:LYS:HE2	1.85	0.58
1:C:229:SER:HB3	1:C:347:LYS:HE2	1.85	0.57
1:B:309:ASN:HB3	10:B:839:HOH:O	2.07	0.55
1:B:173[A]:ARG:NE	1:B:175:GLU:OE2	2.37	0.54
1:A:93:PRO:O	1:A:449:ASN:ND2	2.33	0.54
1:D:397:ASN:O	9:D:514:PGE:H3	2.08	0.54
1:B:320:GLY:HA3	1:B:331:LYS:O	2.09	0.53
1:A:122:ILE:HD13	1:A:163:ILE:HD12	1.91	0.52
1:D:322:PHE:HB2	1:D:327:ARG:HD2	1.92	0.51
1:D:320:GLY:HA3	1:D:331:LYS:O	2.12	0.50
1:B:216:ILE:HD13	1:B:256:PHE:CE2	2.47	0.50
1:B:112:GLY:O	1:C:111:LYS:NZ	2.45	0.49
1:C:216:ILE:HD13	1:C:256:PHE:CE2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:229:SER:HB3	1:B:347:LYS:HE2	1.95	0.49
1:A:419:ARG:HD3	1:A:446:CYS:HB3	1.96	0.48
1:C:203:VAL:HG22	1:C:217:LYS:HG3	1.95	0.48
1:A:120:PRO:HA	1:A:132:PHE:O	2.14	0.48
1:C:320:GLY:HA3	1:C:331:LYS:O	2.14	0.48
1:A:455:TRP:CE3	1:D:197:GLY:HA2	2.48	0.47
1:D:120:PRO:HA	1:D:132:PHE:O	2.14	0.47
1:A:365:ILE:CG2	8:A:513:EDO:H11	2.45	0.47
1:B:230:GLU:OE2	1:B:406:PHE:HA	2.15	0.47
1:B:322:PHE:HB2	1:B:327:ARG:HD2	1.97	0.46
1:B:197:GLY:HA2	1:C:455:TRP:CE3	2.51	0.46
1:D:199:ASP:HB3	8:D:511:EDO:H22	1.97	0.46
1:B:119:GLU:N	1:B:120:PRO:CD	2.79	0.46
1:A:111:LYS:HE2	1:D:113:ASP:OD1	2.15	0.46
1:B:148:THR:O	1:B:149:ILE:CB	2.64	0.46
1:C:265:LYS:HG2	1:C:310:LEU:HD12	1.98	0.46
1:D:208:TYR:CZ	1:D:260:LYS:HD3	2.51	0.46
1:D:118:ARG:HG3	10:D:853:HOH:O	2.16	0.45
1:A:101:SER:HA	1:D:174:PHE:CZ	2.51	0.45
1:A:372:GLU:OE1	1:A:390[A]:LYS:NZ	2.38	0.45
1:B:352:LYS:HE2	1:B:380:TRP:CD1	2.52	0.45
1:C:436:ILE:HG21	4:I:1:NAG:H82	1.98	0.45
1:D:131:THR:O	1:D:160:SER:HA	2.17	0.45
1:B:179:TRP:O	6:B:503:GJT:O3	2.35	0.45
1:C:119:GLU:N	1:C:120:PRO:CD	2.81	0.45
1:C:135:THR:O	1:C:156:ARG:HA	2.17	0.44
1:A:174:PHE:CG	1:B:164:GLY:HA3	2.52	0.44
1:C:410:PRO:HB3	1:C:415:LEU:O	2.17	0.44
1:A:84:LYS:HD2	1:A:236:GLY:HA3	1.99	0.44
1:B:113:ASP:OD1	1:C:111:LYS:HE2	2.18	0.44
1:A:122:ILE:HD13	1:A:163:ILE:CD1	2.48	0.44
1:D:219:TRP:CE2	1:D:254:LYS:HE3	2.53	0.44
1:C:255:ILE:O	1:C:266:SER:HA	2.18	0.44
1:C:122:ILE:HD13	1:C:163:ILE:CD1	2.48	0.43
1:C:118:ARG:NE	1:C:425:GLU:OE2	2.50	0.43
1:D:168[B]:SER:OG	1:D:169:PRO:HD2	2.18	0.43
1:B:177:VAL:HG11	1:C:99:ILE:HD13	2.00	0.43
1:B:122[B]:ILE:HD13	1:B:163:ILE:CD1	2.49	0.43
2:G:1:NAG:H3	2:G:1:NAG:O7	2.18	0.43
1:A:430:ARG:HB2	1:A:438:THR:OG1	2.18	0.42
1:A:329:ASN:OD1	8:A:513:EDO:H22	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:449:ASN:ND2	8:A:510:EDO:O2	2.52	0.42
1:D:239:PHE:HA	1:D:256:PHE:O	2.18	0.42
1:C:400:SER:O	1:C:427:ILE:HG22	2.18	0.42
1:A:410:PRO:HB3	1:A:415:LEU:O	2.20	0.42
1:A:432:LYS:HA	1:A:432:LYS:HD3	1.91	0.42
1:C:419:ARG:HD3	1:C:446:CYS:HB3	2.02	0.42
1:A:111:LYS:HB2	1:D:142:ASP:HB2	2.02	0.41
1:C:251:ALA:HB3	1:C:253:TYR:CE1	2.55	0.41
1:D:216:ILE:HD13	1:D:256:PHE:CE2	2.55	0.41
1:C:430:ARG:HA	1:C:431:PRO:HA	1.78	0.41
1:D:271:ALA:HB1	1:D:274:TYR:HB2	2.02	0.41
1:D:375:TRP:HB3	1:D:389:ILE:HB	2.02	0.41
1:A:229:SER:HB3	1:A:347:LYS:HE2	2.01	0.41
1:C:204:ALA:O	1:C:215:THR:HA	2.20	0.41
1:D:230:GLU:OE2	1:D:406:PHE:HA	2.20	0.41
1:A:203:VAL:HG22	1:A:217:LYS:HG3	2.03	0.41
1:B:271:ALA:HB1	1:B:274:TYR:HB2	2.03	0.41
8:D:509:EDO:H11	10:D:812:HOH:O	2.19	0.41
1:B:181:ALA:HA	1:B:193:ILE:O	2.20	0.40
1:D:294:ASP:OD1	1:D:294:ASP:C	2.60	0.40
1:B:331:LYS:O	1:B:385:ASN:HB3	2.22	0.40
1:C:376:ASP:OD1	1:C:376:ASP:C	2.58	0.40
1:C:183:ALA:O	1:C:230:GLU:HA	2.22	0.40
1:B:122[B]:ILE:HD13	1:B:163:ILE:HD11	2.04	0.40

There are no symmetry-related clashes.

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	390/388 (100%)	373 (96%)	17 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	389/388 (100%)	367 (94%)	21 (5%)	1 (0%)	41	30
1	C	391/388 (101%)	374 (96%)	17 (4%)	0	100	100
1	D	391/388 (101%)	370 (95%)	21 (5%)	0	100	100
All	All	1561/1552 (101%)	1484 (95%)	76 (5%)	1 (0%)	51	41

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	149	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	338/335 (101%)	334 (99%)	4 (1%)	71	67
1	B	336/335 (100%)	330 (98%)	6 (2%)	59	52
1	C	338/335 (101%)	336 (99%)	2 (1%)	86	86
1	D	339/335 (101%)	333 (98%)	6 (2%)	59	52
All	All	1351/1340 (101%)	1333 (99%)	18 (1%)	69	64

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	118	ARG
1	A	297	HIS
1	A	367[A]	SER
1	A	367[B]	SER
1	B	118	ARG
1	B	119	GLU
1	B	148	THR
1	B	176	SER
1	B	297	HIS
1	B	455	TRP

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Mol	Chain	Res	Type
1	C	118	ARG
1	C	297	HIS
1	D	118	ARG
1	D	148	THR
1	D	149	ILE
1	D	297	HIS
1	D	367	SER
1	D	455	TRP

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

Mol	Chain	Res	Type
1	C	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 ⓘ

19 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	1.70	5 (29%)
2	NAG	E	2	2	14,14,15	0.58	0	17,19,21	1.01	0
2	FUC	E	3	2	10,10,11	0.97	0	14,14,16	1.18	1 (7%)
3	NAG	F	1	1,3	14,14,15	1.09	1 (7%)	17,19,21	2.10	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	FUC	F	2	3	10,10,11	1.00	0	14,14,16	1.09	1 (7%)
2	NAG	G	1	1,2	14,14,15	0.73	0	17,19,21	1.54	2 (11%)
2	NAG	G	2	2	14,14,15	0.58	0	17,19,21	1.47	3 (17%)
2	FUC	G	3	2	10,10,11	0.86	0	14,14,16	1.62	3 (21%)
2	NAG	H	1	1,2	14,14,15	0.88	1 (7%)	17,19,21	1.60	4 (23%)
2	NAG	H	2	2	14,14,15	0.67	0	17,19,21	1.24	2 (11%)
2	FUC	H	3	2	10,10,11	1.17	0	14,14,16	1.05	1 (7%)
4	NAG	I	1	1,4	14,14,15	0.93	1 (7%)	17,19,21	1.81	5 (29%)
4	NAG	I	2	4	14,14,15	0.67	0	17,19,21	1.16	1 (5%)
4	BMA	I	3	4	11,11,12	0.98	0	15,15,17	1.19	1 (6%)
4	MAN	I	4	4	11,11,12	0.64	0	15,15,17	2.03	3 (20%)
4	MAN	I	5	4	11,11,12	1.01	1 (9%)	15,15,17	1.25	1 (6%)
4	FUC	I	6	4	10,10,11	0.78	0	14,14,16	2.10	4 (28%)
3	NAG	J	1	1,3	14,14,15	1.19	2 (14%)	17,19,21	1.82	4 (23%)
3	FUC	J	2	3	10,10,11	1.10	0	14,14,16	1.00	1 (7%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	E	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
2	FUC	E	3	2	-	-	0/1/1/1
3	NAG	F	1	1,3	-	1/6/23/26	0/1/1/1
3	FUC	F	2	3	-	-	0/1/1/1
2	NAG	G	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	G	2	2	-	0/6/23/26	0/1/1/1
2	FUC	G	3	2	-	-	0/1/1/1
2	NAG	H	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	H	2	2	-	0/6/23/26	0/1/1/1
2	FUC	H	3	2	-	-	0/1/1/1
4	NAG	I	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	I	2	4	-	0/6/23/26	0/1/1/1
4	BMA	I	3	4	-	0/2/19/22	0/1/1/1
4	MAN	I	4	4	-	2/2/19/22	0/1/1/1
4	MAN	I	5	4	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FUC	I	6	4	-	-	0/1/1/1
3	NAG	J	1	1,3	-	3/6/23/26	0/1/1/1
3	FUC	J	2	3	-	-	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	1	NAG	C2-N2	-2.64	1.41	1.46
2	H	1	NAG	C1-C2	2.39	1.55	1.52
3	J	1	NAG	C3-C2	2.30	1.57	1.52
4	I	5	MAN	C2-C3	2.18	1.55	1.52
3	F	1	NAG	C1-C2	-2.10	1.49	1.52
3	J	1	NAG	C1-C2	2.04	1.55	1.52

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	1	NAG	C1-O5-C5	5.78	120.03	112.19
4	I	4	MAN	O5-C5-C6	5.54	115.89	107.20
2	E	1	NAG	C1-C2-N2	-4.38	103.00	110.49
4	I	6	FUC	O5-C5-C4	-4.37	101.68	109.52
4	I	1	NAG	C1-O5-C5	-4.19	106.51	112.19
3	J	1	NAG	C1-C2-N2	-4.17	103.37	110.49
4	I	4	MAN	C1-O5-C5	-4.07	106.67	112.19
2	G	3	FUC	C1-C2-C3	3.93	114.50	109.67
3	F	1	NAG	C2-N2-C7	3.93	128.50	122.90
2	G	1	NAG	C1-C2-N2	-3.84	103.92	110.49
3	J	1	NAG	O4-C4-C3	3.80	119.12	110.35
4	I	1	NAG	C4-C3-C2	-3.77	105.49	111.02
4	I	5	MAN	O5-C1-C2	3.75	116.56	110.77
4	I	6	FUC	O5-C5-C6	3.44	114.73	107.33
2	H	1	NAG	O5-C1-C2	-3.36	105.99	111.29
2	H	1	NAG	C4-C3-C2	-3.18	106.36	111.02
2	H	2	NAG	C2-N2-C7	-3.17	118.40	122.90
4	I	6	FUC	O3-C3-C2	-2.91	104.42	109.99
3	F	1	NAG	C1-C2-N2	-2.87	105.59	110.49
4	I	6	FUC	O3-C3-C4	2.82	116.87	110.35
2	G	2	NAG	O5-C5-C6	2.75	111.52	107.20
2	E	3	FUC	O5-C5-C4	2.73	114.42	109.52
3	F	1	NAG	O5-C5-C6	2.73	111.49	107.20
2	G	1	NAG	O5-C5-C4	-2.67	104.33	110.83
2	H	3	FUC	C3-C4-C5	2.59	113.81	109.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	2	NAG	C4-C3-C2	-2.59	107.23	111.02
2	H	1	NAG	O3-C3-C2	2.54	114.71	109.47
2	G	2	NAG	C3-C4-C5	-2.54	105.72	110.24
4	I	3	BMA	O5-C5-C6	2.51	111.14	107.20
2	E	1	NAG	O7-C7-N2	-2.44	117.46	121.95
3	J	1	NAG	O5-C5-C6	2.40	110.97	107.20
3	F	2	FUC	O5-C5-C6	2.37	112.43	107.33
3	J	2	FUC	C1-C2-C3	2.37	112.58	109.67
4	I	1	NAG	C2-N2-C7	-2.31	119.61	122.90
2	H	1	NAG	C1-O5-C5	2.30	115.31	112.19
2	G	3	FUC	O5-C1-C2	2.20	114.17	110.77
2	E	1	NAG	C8-C7-N2	2.17	119.77	116.10
2	G	3	FUC	C1-O5-C5	2.15	117.64	112.78
4	I	1	NAG	O7-C7-C8	-2.14	118.08	122.06
3	J	1	NAG	O5-C5-C4	-2.12	105.68	110.83
4	I	2	NAG	C1-O5-C5	-2.11	109.34	112.19
2	E	1	NAG	O5-C5-C6	2.10	110.50	107.20
2	E	1	NAG	C1-O5-C5	-2.05	109.41	112.19
4	I	4	MAN	C6-C5-C4	-2.05	108.19	113.00
4	I	1	NAG	C3-C4-C5	-2.05	106.59	110.24
2	H	2	NAG	O4-C4-C5	2.01	114.30	109.30

There are no chirality outliers.

All (12) torsion outliers are listed below:

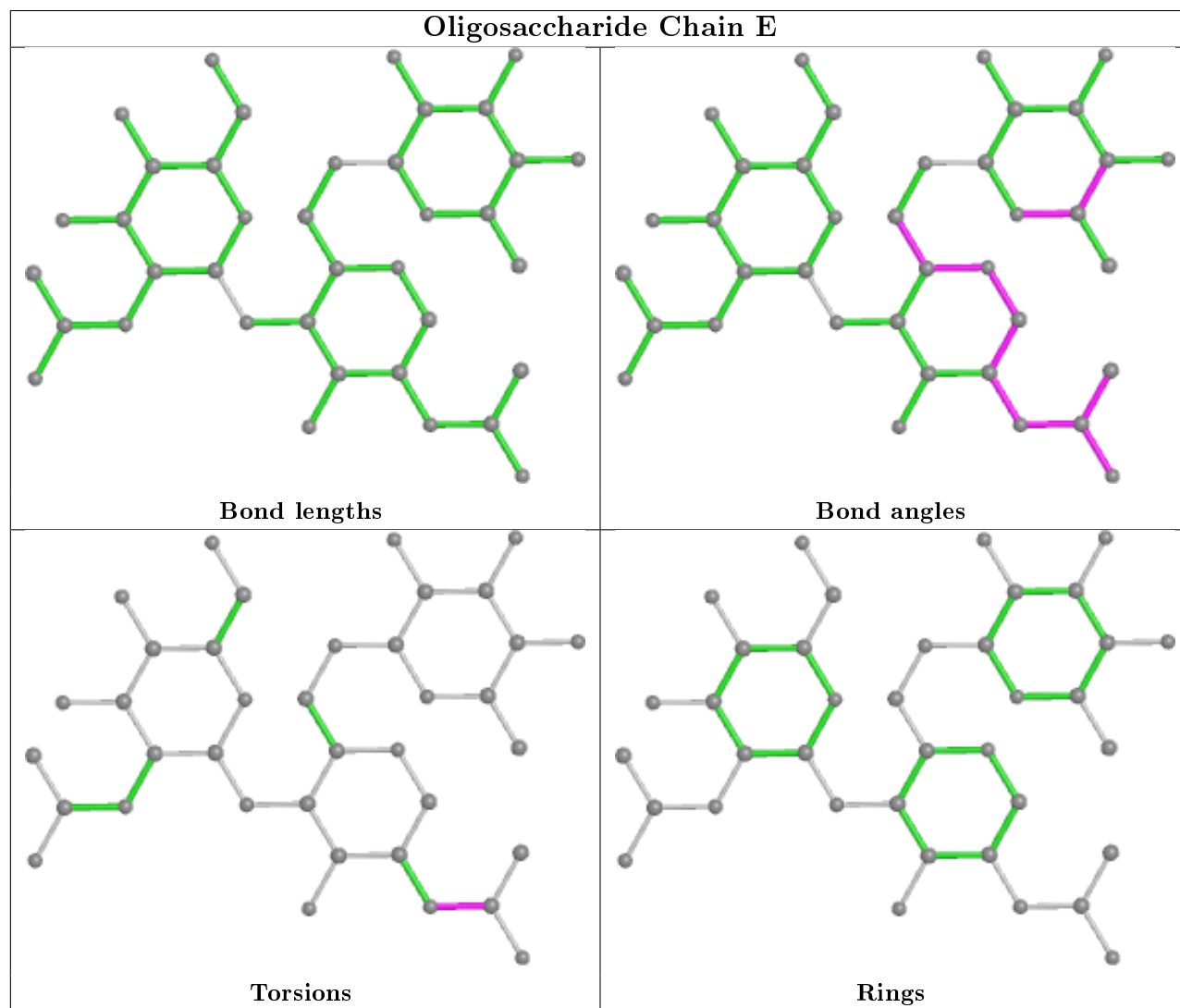
Mol	Chain	Res	Type	Atoms
2	G	1	NAG	C3-C2-N2-C7
2	E	1	NAG	C8-C7-N2-C2
2	E	1	NAG	O7-C7-N2-C2
4	I	4	MAN	O5-C5-C6-O6
3	J	1	NAG	C8-C7-N2-C2
2	G	1	NAG	C8-C7-N2-C2
4	I	4	MAN	C4-C5-C6-O6
2	H	1	NAG	C1-C2-N2-C7
3	F	1	NAG	C4-C5-C6-O6
3	J	1	NAG	C3-C2-N2-C7
3	J	1	NAG	O7-C7-N2-C2
2	G	1	NAG	O7-C7-N2-C2

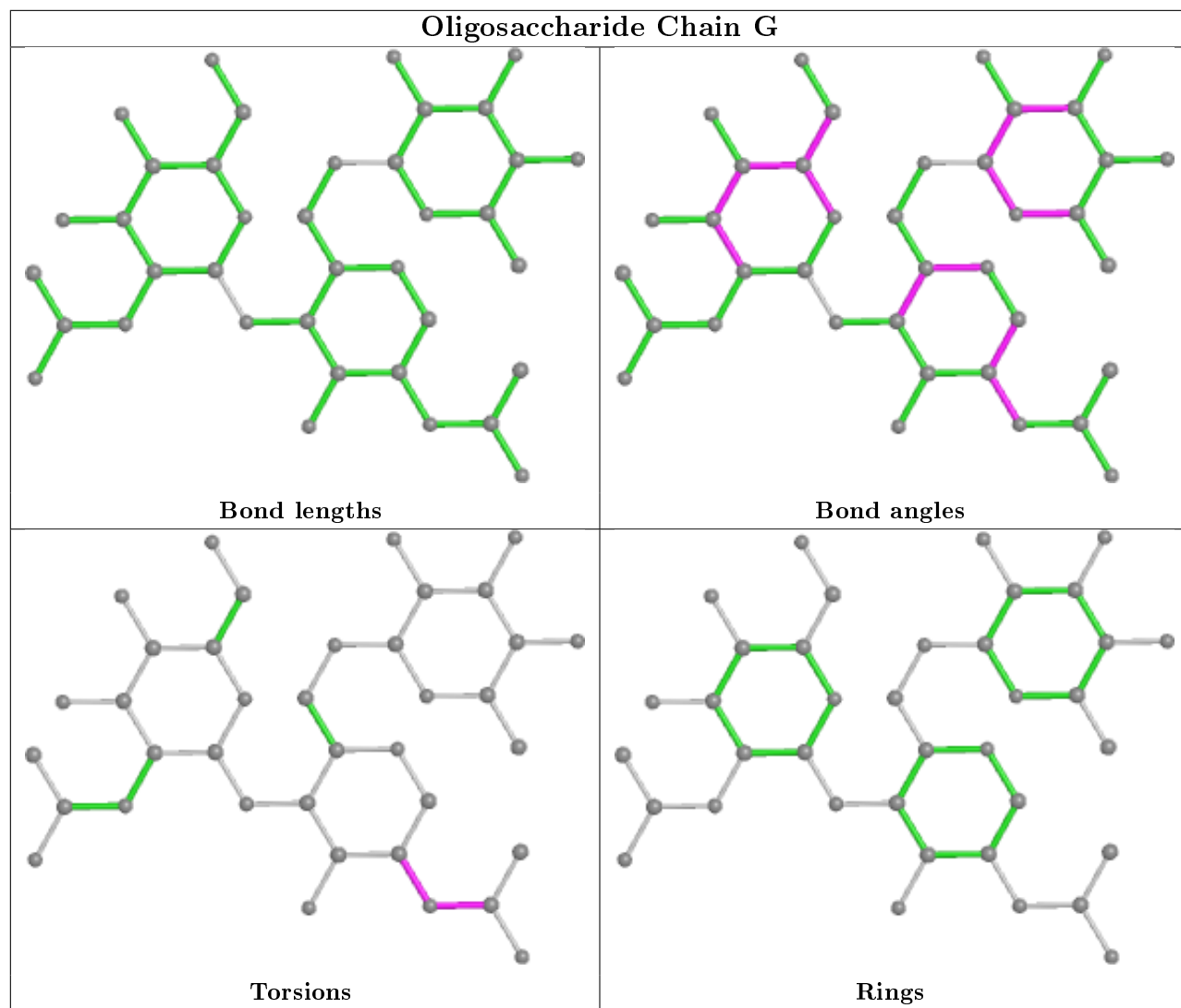
There are no ring outliers.

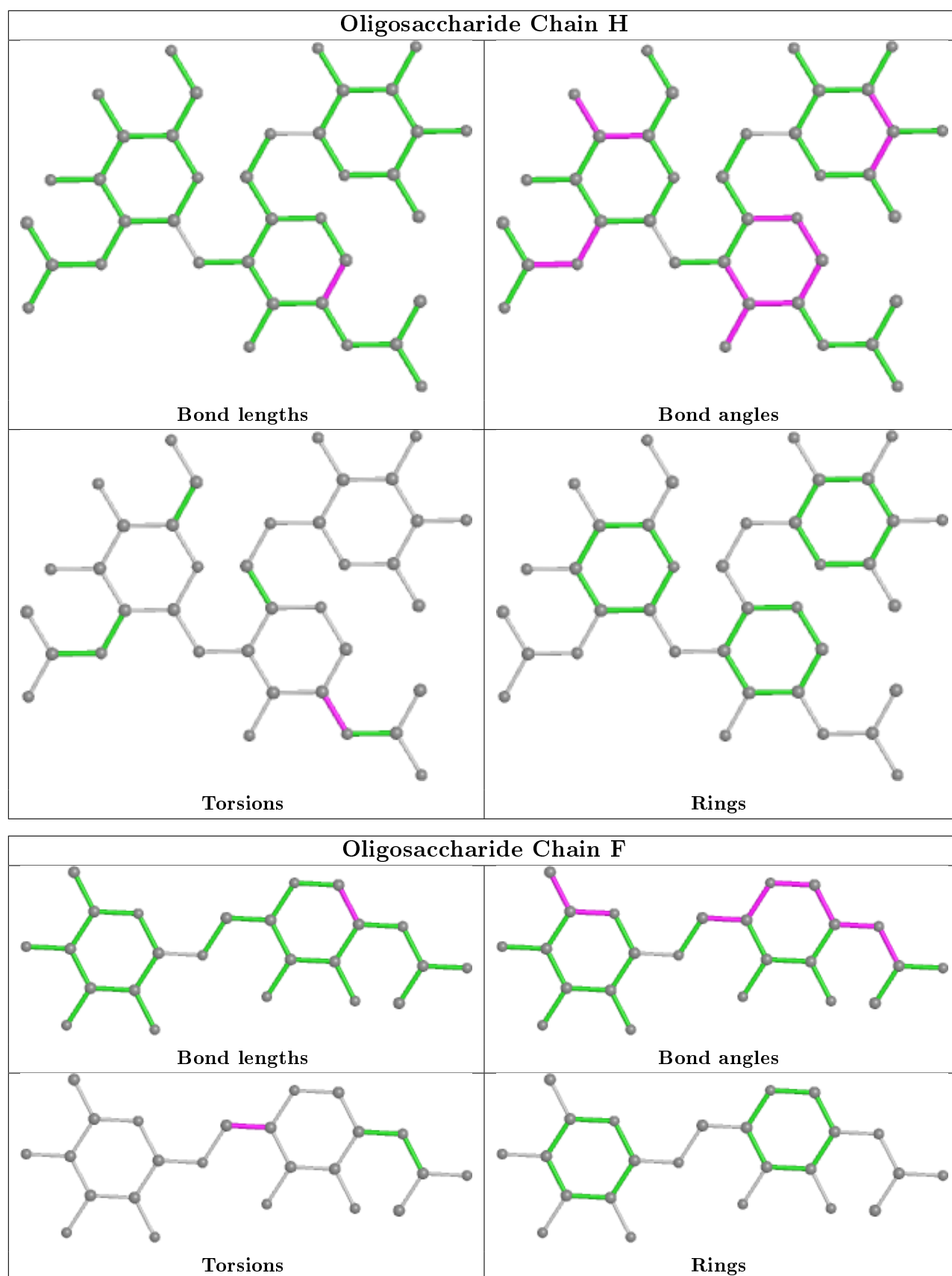
2 monomers are involved in 2 short contacts:

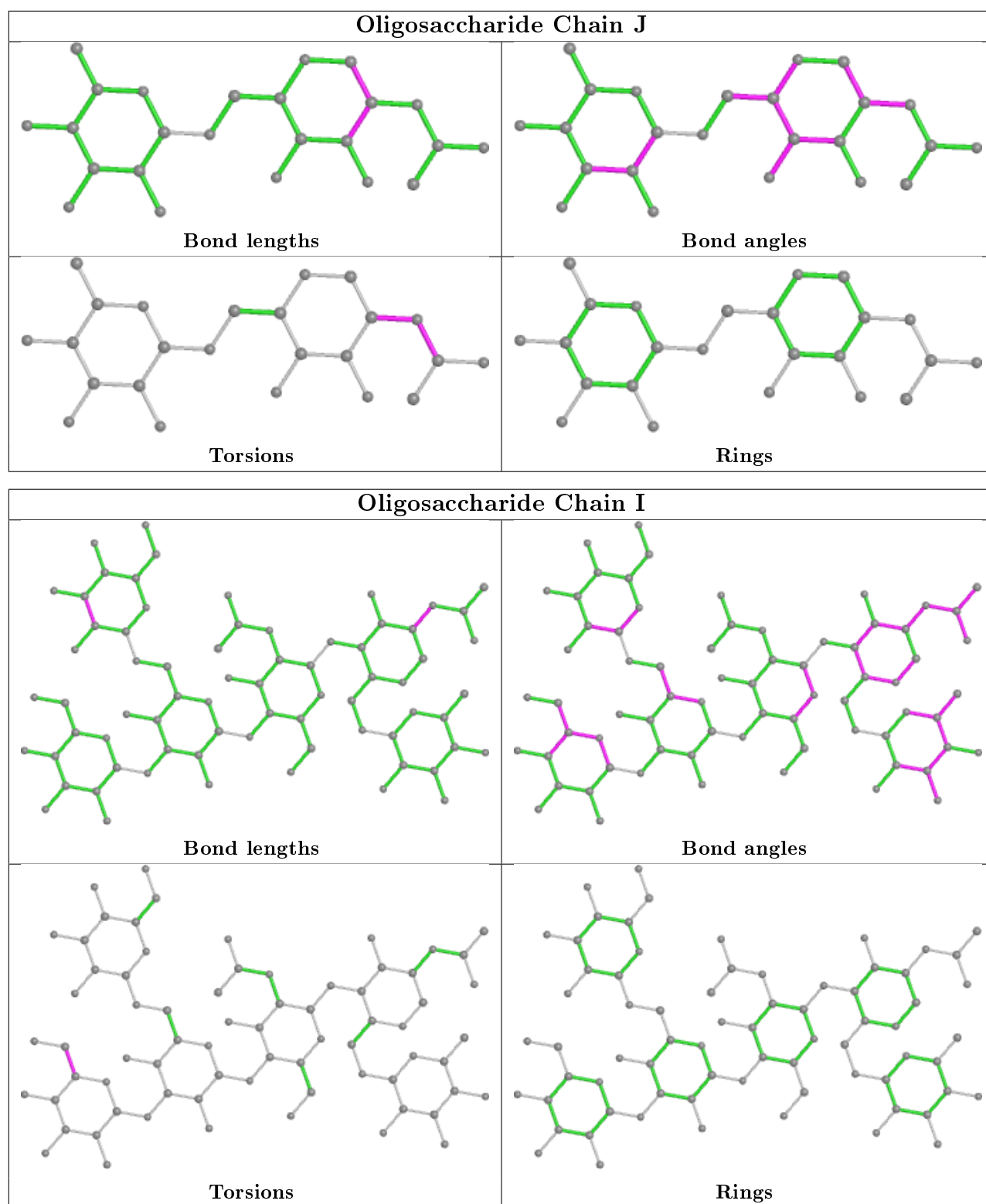
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	I	1	NAG	1	0
2	G	1	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.









5.6 Ligand geometry [i](#)

Of 49 ligands modelled in this entry, 8 are monoatomic - leaving 41 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$
8	EDO	A	519	-	3,3,3	0.60	0	2,2,2	0.44	0
8	EDO	A	510	-	3,3,3	0.15	0	2,2,2	0.18	0
8	EDO	A	511	-	3,3,3	0.79	0	2,2,2	0.96	0
8	EDO	A	514	-	3,3,3	0.63	0	2,2,2	0.46	0
8	EDO	B	511	-	3,3,3	0.20	0	2,2,2	0.22	0
8	EDO	A	515	-	3,3,3	0.14	0	2,2,2	0.47	0
8	EDO	C	515[B]	-	3,3,3	0.31	0	2,2,2	0.67	0
8	EDO	B	512	-	3,3,3	0.14	0	2,2,2	0.16	0
8	EDO	C	515[A]	-	3,3,3	0.17	0	2,2,2	0.49	0
8	EDO	D	510	-	3,3,3	0.32	0	2,2,2	0.07	0
7	NAG	D	506	1	14,14,15	0.75	0	17,19,21	1.69	3 (17%)
6	GJT	B	503	-	24,27,27	0.93	2 (8%)	18,37,37	1.58	4 (22%)
7	NAG	D	507	1	14,14,15	0.84	1 (7%)	17,19,21	1.28	4 (23%)
8	EDO	A	518	-	3,3,3	0.39	0	2,2,2	0.14	0
6	GJT	C	503	-	24,27,27	0.85	0	18,37,37	2.31	3 (16%)
8	EDO	A	521	-	3,3,3	0.34	0	2,2,2	0.22	0
8	EDO	D	508	-	3,3,3	0.27	0	2,2,2	0.29	0
8	EDO	A	520	-	3,3,3	0.43	0	2,2,2	0.64	0
8	EDO	C	514	-	3,3,3	0.23	0	2,2,2	0.15	0
8	EDO	D	509	-	3,3,3	0.47	0	2,2,2	0.57	0
8	EDO	B	513	-	3,3,3	0.15	0	2,2,2	0.13	0
8	EDO	C	516	-	3,3,3	0.24	0	2,2,2	0.37	0
8	EDO	A	522	-	3,3,3	0.24	0	2,2,2	0.35	0
8	EDO	A	513	-	3,3,3	0.39	0	2,2,2	0.45	0
7	NAG	B	508	1	14,14,15	0.94	1 (7%)	17,19,21	2.26	7 (41%)
7	NAG	B	507	1	14,14,15	0.88	0	17,19,21	1.48	3 (17%)
8	EDO	B	509	-	3,3,3	0.14	0	2,2,2	0.22	0
8	EDO	D	511	-	3,3,3	0.20	0	2,2,2	0.27	0
9	PGE	D	514	-	6,6,9	0.22	0	5,5,8	0.30	0
7	NAG	A	509	1	14,14,15	0.89	0	17,19,21	1.21	1 (5%)
8	EDO	D	513	-	3,3,3	0.47	0	2,2,2	0.16	0
7	NAG	C	513	1	14,14,15	0.93	0	17,19,21	1.37	3 (17%)
8	EDO	A	517	-	3,3,3	0.49	0	2,2,2	0.04	0
8	EDO	D	512	-	3,3,3	0.10	0	2,2,2	0.14	0
8	EDO	A	523	-	3,3,3	0.12	0	2,2,2	0.11	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	EDO	A	512	-	3,3,3	0.26	0	2,2,2	0.50	0
6	GJT	D	503	-	24,27,27	1.43	2 (8%)	18,37,37	2.44	4 (22%)
8	EDO	B	510	-	3,3,3	0.16	0	2,2,2	0.52	0
8	EDO	A	516	-	3,3,3	0.26	0	2,2,2	0.47	0
8	EDO	B	514	-	3,3,3	0.61	0	2,2,2	0.68	0
6	GJT	A	503	-	24,27,27	1.14	2 (8%)	18,37,37	1.77	3 (16%)

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
8	EDO	A	519	-	-	1/1/1/1	-
8	EDO	A	510	-	-	1/1/1/1	-
8	EDO	A	511	-	-	0/1/1/1	-
8	EDO	A	514	-	-	1/1/1/1	-
8	EDO	B	511	-	-	1/1/1/1	-
8	EDO	A	515	-	-	1/1/1/1	-
8	EDO	C	515[B]	-	-	1/1/1/1	-
8	EDO	B	512	-	-	1/1/1/1	-
8	EDO	C	515[A]	-	-	1/1/1/1	-
8	EDO	D	510	-	-	0/1/1/1	-
7	NAG	D	506	1	-	2/6/23/26	0/1/1/1
6	GJT	B	503	-	-	2/12/38/38	0/2/2/2
7	NAG	D	507	1	-	0/6/23/26	0/1/1/1
8	EDO	A	518	-	-	1/1/1/1	-
6	GJT	C	503	-	-	0/12/38/38	0/2/2/2
8	EDO	A	521	-	-	1/1/1/1	-
8	EDO	D	508	-	-	1/1/1/1	-
8	EDO	A	520	-	-	1/1/1/1	-
8	EDO	C	514	-	-	1/1/1/1	-
8	EDO	D	509	-	-	1/1/1/1	-
8	EDO	B	513	-	-	1/1/1/1	-
8	EDO	C	516	-	-	1/1/1/1	-
8	EDO	A	522	-	-	1/1/1/1	-
8	EDO	A	513	-	-	1/1/1/1	-
7	NAG	B	508	1	-	2/6/23/26	0/1/1/1
7	NAG	B	507	1	-	0/6/23/26	0/1/1/1
8	EDO	B	509	-	-	1/1/1/1	-
8	EDO	D	511	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	PGE	D	514	-	-	2/4/4/7	-
7	NAG	A	509	1	-	0/6/23/26	0/1/1/1
8	EDO	D	513	-	-	1/1/1/1	-
7	NAG	C	513	1	-	0/6/23/26	0/1/1/1
8	EDO	A	517	-	-	1/1/1/1	-
8	EDO	D	512	-	-	1/1/1/1	-
8	EDO	A	523	-	-	1/1/1/1	-
8	EDO	A	512	-	-	1/1/1/1	-
6	GJT	D	503	-	-	1/12/38/38	0/2/2/2
8	EDO	B	510	-	-	1/1/1/1	-
8	EDO	A	516	-	-	1/1/1/1	-
8	EDO	B	514	-	-	1/1/1/1	-
6	GJT	A	503	-	-	0/12/38/38	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	503	GJT	C9-C10	-4.93	1.48	1.53
6	D	503	GJT	C10-N2	-3.62	1.43	1.49
6	A	503	GJT	C11-C10	3.58	1.57	1.53
7	B	508	NAG	O5-C1	2.32	1.47	1.43
6	B	503	GJT	C15-N3	2.30	1.37	1.34
6	A	503	GJT	C9-C10	-2.20	1.50	1.53
6	B	503	GJT	C10-N2	-2.12	1.46	1.49
7	D	507	NAG	C1-C2	2.02	1.55	1.52

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	503	GJT	C14-N2-C10	9.09	133.53	125.48
6	C	503	GJT	C14-N2-C10	9.03	133.48	125.48
6	A	503	GJT	C14-N2-C10	5.81	130.63	125.48
7	B	508	NAG	C1-O5-C5	4.84	118.75	112.19
7	D	506	NAG	C1-O5-C5	4.45	118.23	112.19
6	B	503	GJT	C10-C9-C8	3.86	114.29	109.78
7	B	508	NAG	C6-C5-C4	-3.81	104.09	113.00
7	B	507	NAG	C1-O5-C5	3.47	116.89	112.19
7	B	507	NAG	O5-C5-C6	3.21	112.23	107.20
7	B	508	NAG	O7-C7-N2	-3.15	116.17	121.95
7	B	508	NAG	C1-C2-N2	-3.07	105.25	110.49
6	B	503	GJT	C14-C15-N3	-3.01	106.86	111.34
7	D	506	NAG	C3-C4-C5	-2.93	105.01	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	513	NAG	C3-C4-C5	-2.92	105.02	110.24
7	D	506	NAG	O4-C4-C5	2.85	116.36	109.30
6	B	503	GJT	C14-N2-C10	2.81	127.97	125.48
6	D	503	GJT	O1-C3-C4	-2.62	97.34	109.00
7	C	513	NAG	O5-C5-C6	2.48	111.09	107.20
7	D	507	NAG	C1-O5-C5	2.36	115.39	112.19
7	A	509	NAG	C1-O5-C5	2.36	115.39	112.19
7	B	507	NAG	O3-C3-C2	-2.36	104.59	109.47
6	B	503	GJT	O1-C3-C4	-2.34	98.57	109.00
7	B	508	NAG	O5-C5-C6	2.34	110.87	107.20
7	B	508	NAG	C8-C7-N2	2.26	119.92	116.10
6	D	503	GJT	C10-C9-C8	2.24	112.40	109.78
7	D	507	NAG	C3-C4-C5	-2.23	106.26	110.24
6	C	503	GJT	C14-C15-N3	-2.23	108.03	111.34
6	A	503	GJT	O3-C16-C15	-2.18	107.30	112.10
7	B	508	NAG	O5-C1-C2	2.13	114.65	111.29
6	A	503	GJT	C10-C9-C8	2.11	112.24	109.78
7	D	507	NAG	O3-C3-C4	2.08	115.16	110.35
7	D	507	NAG	O5-C5-C6	2.07	110.45	107.20
6	C	503	GJT	C10-C9-C8	2.04	112.17	109.78
7	C	513	NAG	O5-C1-C2	2.03	114.50	111.29
6	D	503	GJT	C15-C14-N2	-2.02	104.23	107.35

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	D	514	PGE	O1-C1-C2-O2
7	B	508	NAG	C8-C7-N2-C2
7	B	508	NAG	O7-C7-N2-C2
7	D	506	NAG	C4-C5-C6-O6
8	A	519	EDO	O1-C1-C2-O2
8	A	520	EDO	O1-C1-C2-O2
8	A	523	EDO	O1-C1-C2-O2
8	A	522	EDO	O1-C1-C2-O2
8	D	512	EDO	O1-C1-C2-O2
8	A	512	EDO	O1-C1-C2-O2
8	A	516	EDO	O1-C1-C2-O2
8	B	514	EDO	O1-C1-C2-O2
7	D	506	NAG	O5-C5-C6-O6
8	C	515[A]	EDO	O1-C1-C2-O2
8	A	521	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
8	A	514	EDO	O1-C1-C2-O2
8	B	512	EDO	O1-C1-C2-O2
8	D	508	EDO	O1-C1-C2-O2
6	D	503	GJT	C1-C2-C3-C4
9	D	514	PGE	O2-C3-C4-O3
8	C	516	EDO	O1-C1-C2-O2
8	A	510	EDO	O1-C1-C2-O2
8	A	515	EDO	O1-C1-C2-O2
8	C	514	EDO	O1-C1-C2-O2
8	D	509	EDO	O1-C1-C2-O2
8	B	513	EDO	O1-C1-C2-O2
8	A	513	EDO	O1-C1-C2-O2
8	D	511	EDO	O1-C1-C2-O2
8	B	510	EDO	O1-C1-C2-O2
6	B	503	GJT	C2-C3-O1-C6
6	B	503	GJT	C1-C2-C3-C4
8	C	515[B]	EDO	O1-C1-C2-O2
8	B	511	EDO	O1-C1-C2-O2
8	B	509	EDO	O1-C1-C2-O2
8	A	517	EDO	O1-C1-C2-O2
8	A	518	EDO	O1-C1-C2-O2
8	D	513	EDO	O1-C1-C2-O2

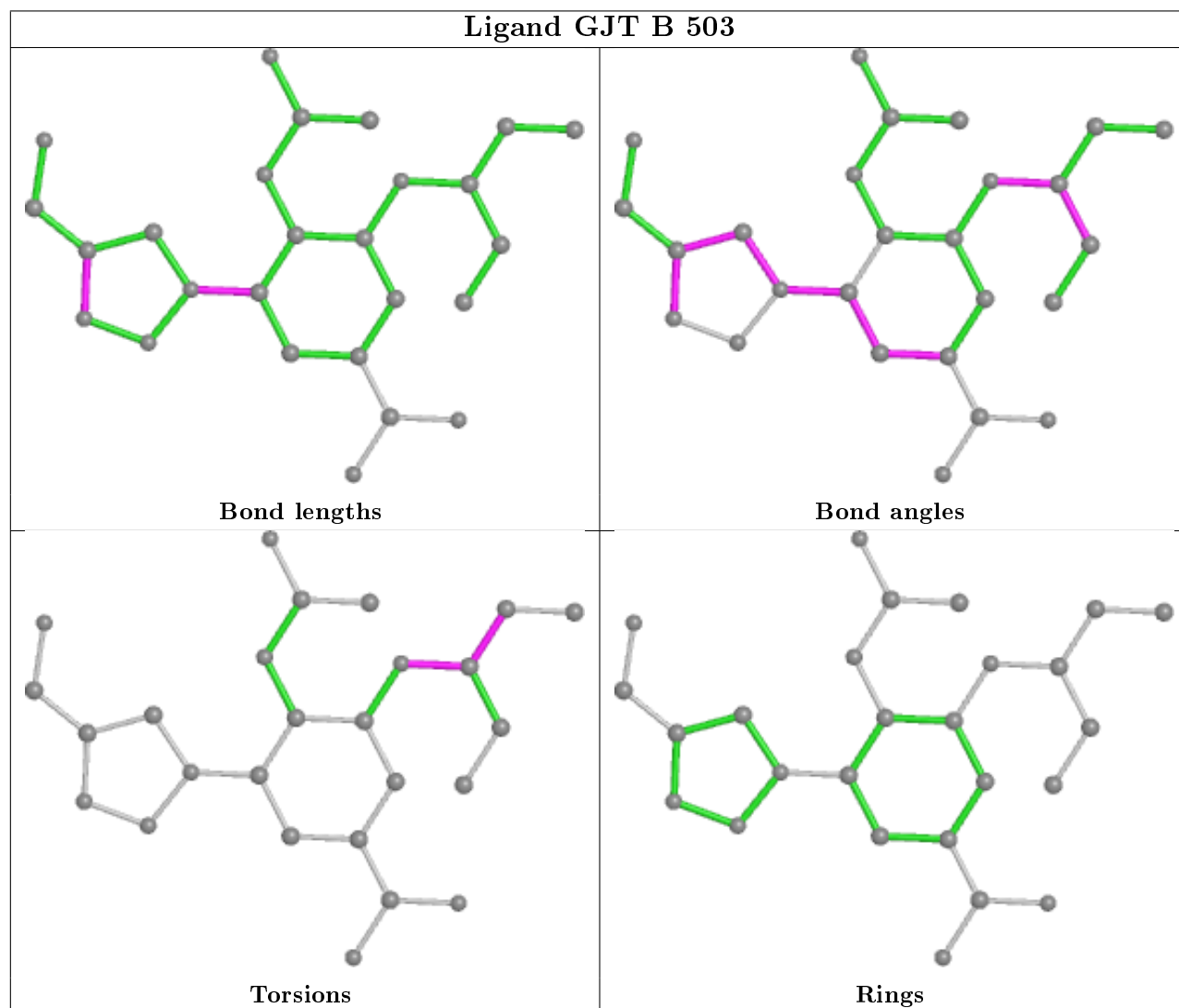
There are no ring outliers.

6 monomers are involved in 7 short contacts:

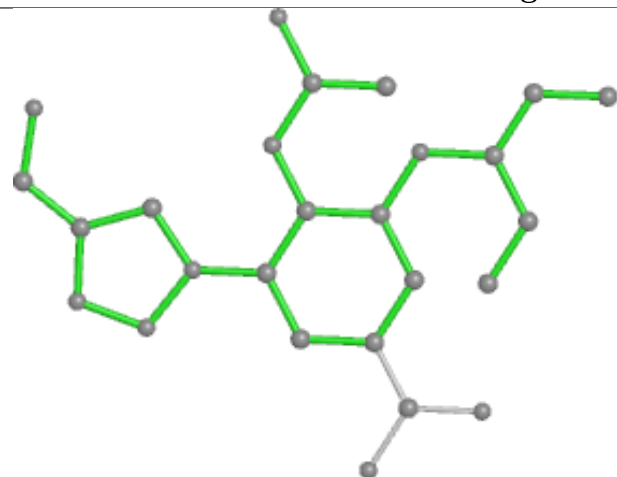
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	510	EDO	1	0
6	B	503	GJT	1	0
8	D	509	EDO	1	0
8	A	513	EDO	2	0
8	D	511	EDO	1	0
9	D	514	PGE	1	0

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

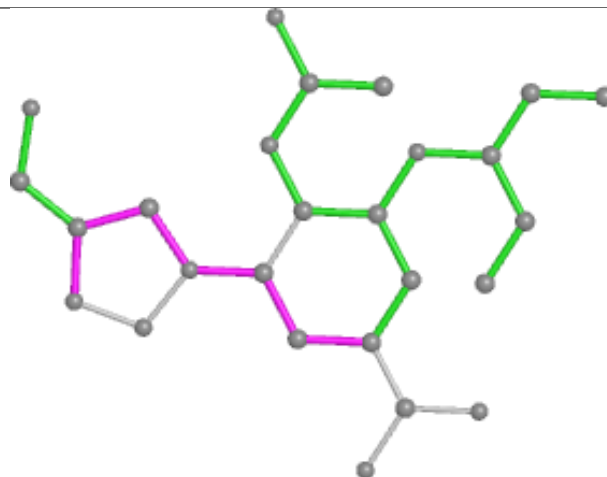
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



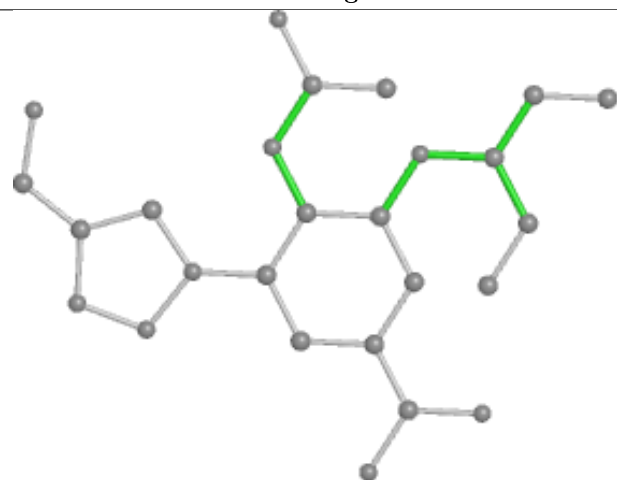
Ligand GJT C 503



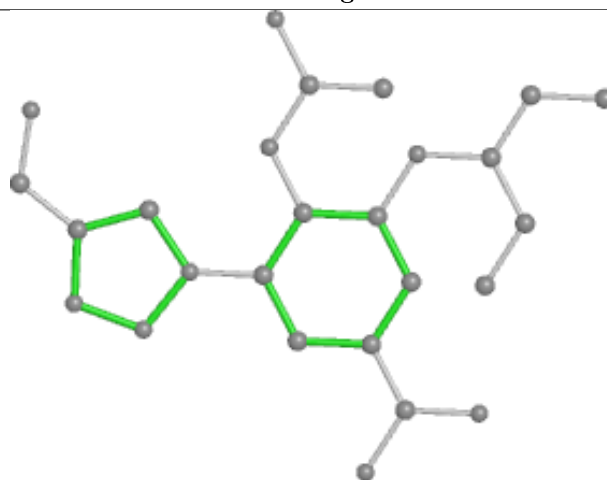
Bond lengths



Bond angles

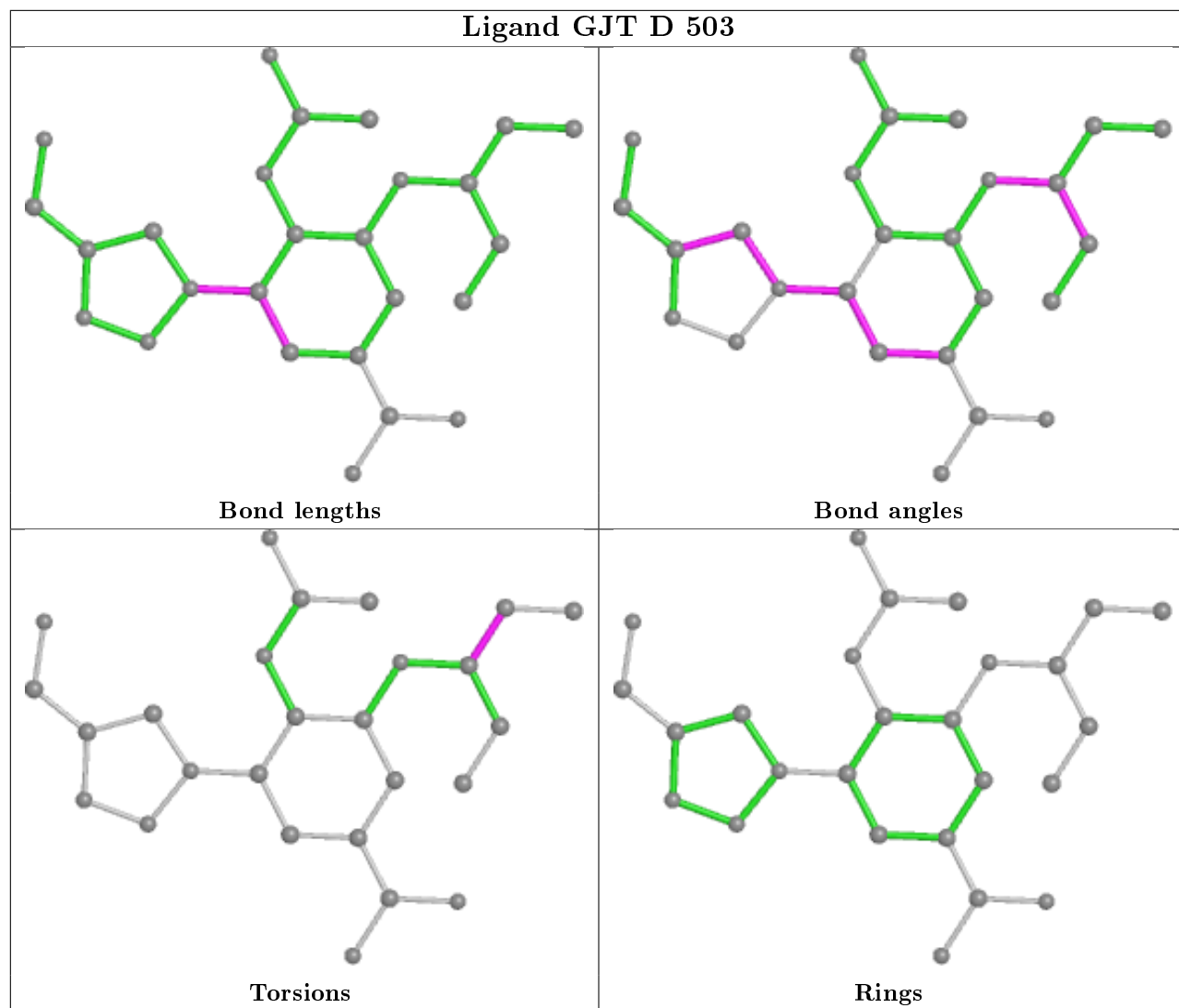


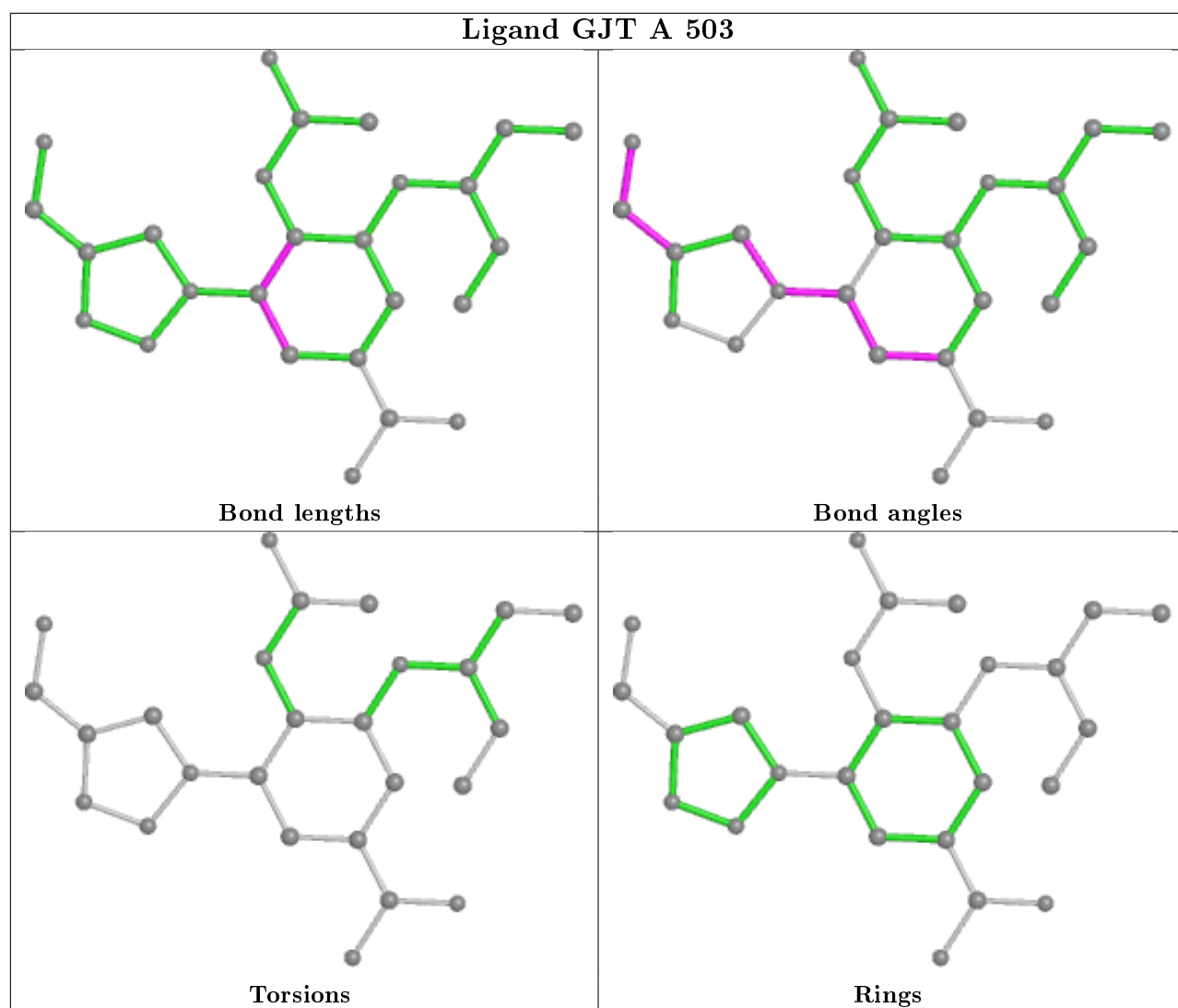
Torsions



Rings

Ligand GJT 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	387/388 (99%)	-0.24	2 (0%) 91 91	14, 20, 32, 60	0
1	B	387/388 (99%)	-0.11	7 (1%) 68 70	15, 21, 34, 80	0
1	C	387/388 (99%)	-0.24	2 (0%) 91 91	15, 20, 32, 63	0
1	D	387/388 (99%)	-0.11	4 (1%) 82 83	15, 21, 34, 63	0
All	All	1548/1552 (99%)	-0.17	15 (0%) 82 83	14, 21, 33, 80	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	148	THR	7.6
1	B	149	ILE	7.1
1	D	149	ILE	5.6
1	A	149	ILE	4.3
1	D	148	THR	3.1
1	B	173[A]	ARG	2.7
1	D	93	PRO	2.6
1	B	387	PHE	2.5
1	A	148	THR	2.4
1	D	387	PHE	2.4
1	B	147	GLY	2.4
1	B	434[A]	ASN	2.3
1	C	83	VAL	2.3
1	B	93	PRO	2.3
1	C	149	ILE	2.3

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 ⓘ

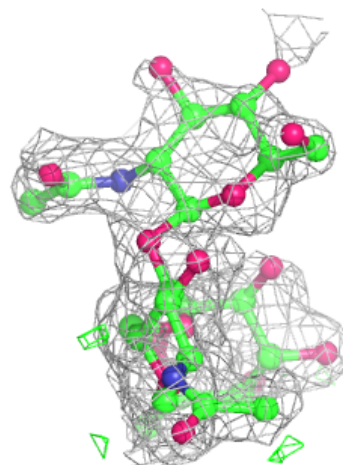
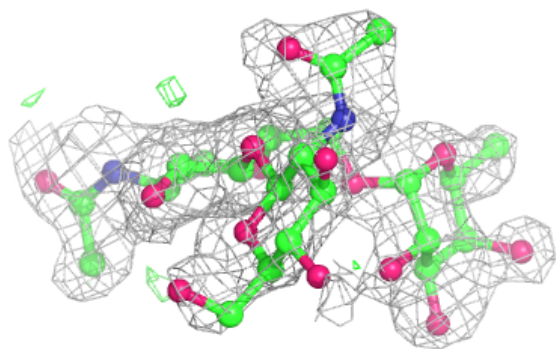
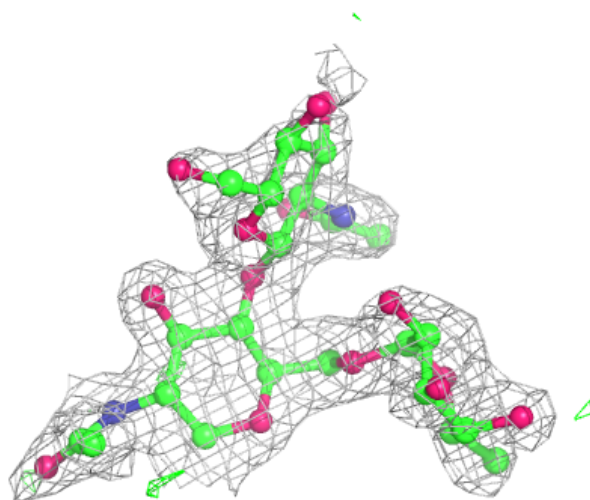
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists 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	FUC	F	2	10/11	0.70	0.32	49,58,62,65	0
2	FUC	G	3	10/11	0.74	0.36	49,54,58,59	0
2	FUC	E	3	10/11	0.77	0.39	50,55,58,61	0
2	FUC	H	3	10/11	0.78	0.38	46,54,57,60	0
3	NAG	J	1	14/15	0.78	0.28	47,57,66,67	0
2	NAG	H	2	14/15	0.79	0.44	56,68,80,82	0
2	NAG	E	2	14/15	0.81	0.41	54,61,68,74	0
3	FUC	J	2	10/11	0.82	0.31	45,49,52,52	0
2	NAG	G	1	14/15	0.83	0.32	45,57,63,65	0
2	NAG	E	1	14/15	0.84	0.26	38,45,52,52	0
4	MAN	I	4	11/12	0.85	0.33	49,54,62,76	0
2	NAG	G	2	14/15	0.87	0.38	56,63,69,72	0
3	NAG	F	1	14/15	0.87	0.19	42,50,57,65	0
4	FUC	I	6	10/11	0.88	0.19	34,40,49,50	0
2	NAG	H	1	14/15	0.90	0.28	44,51,65,69	0
4	BMA	I	3	11/12	0.90	0.17	30,35,40,43	0
4	MAN	I	5	11/12	0.91	0.19	29,33,37,37	0
4	NAG	I	2	14/15	0.95	0.11	26,29,32,34	0
4	NAG	I	1	14/15	0.96	0.10	25,27,31,34	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.

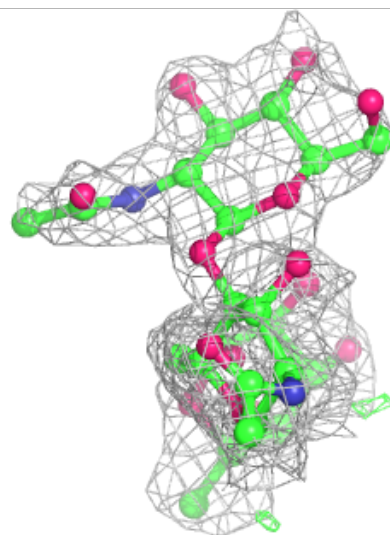
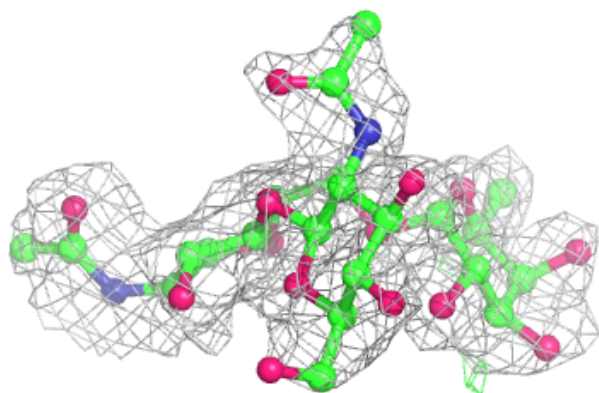
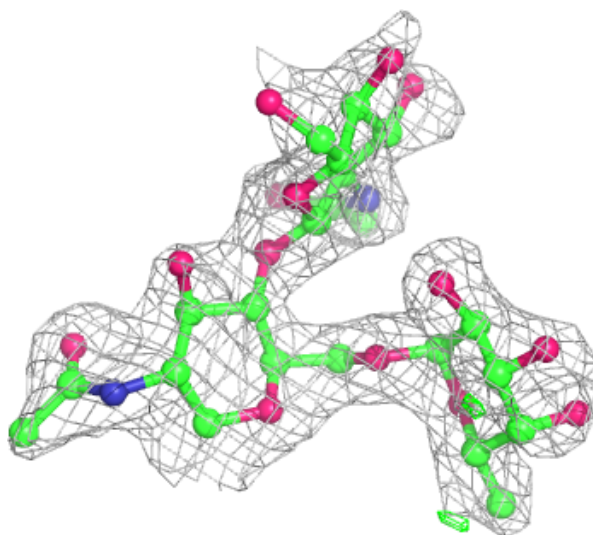
Electron density around Chain E:

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



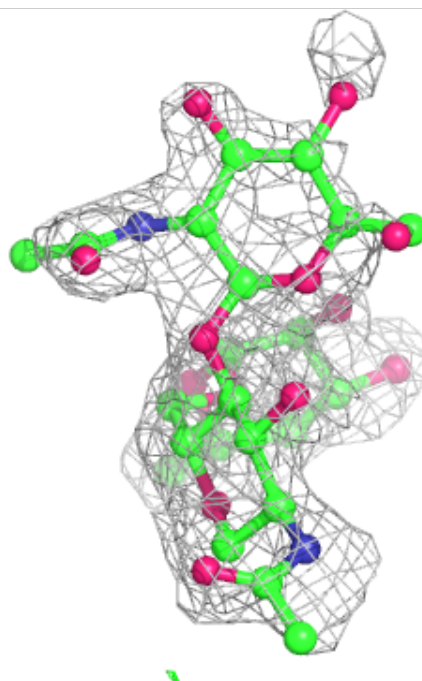
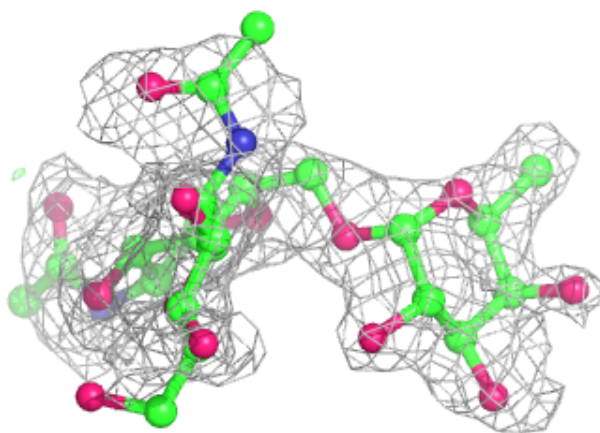
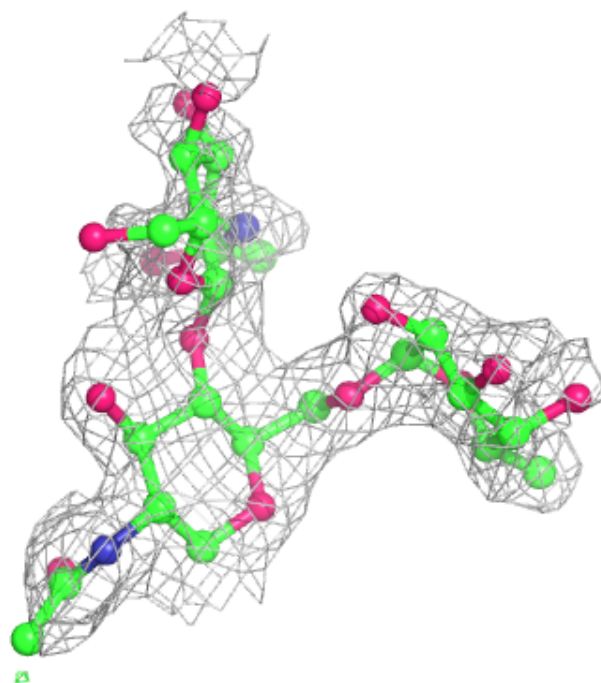
Electron density around Chain G:

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



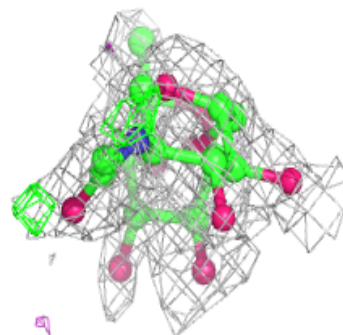
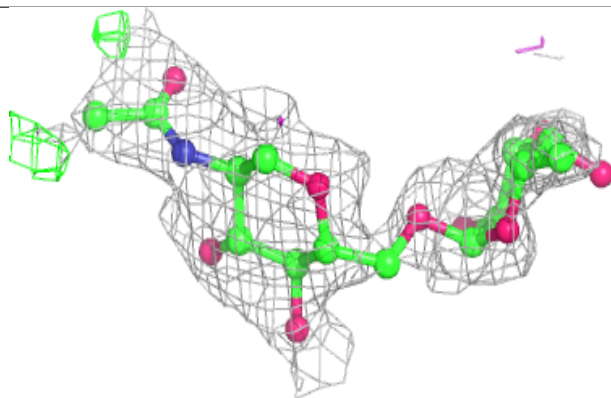
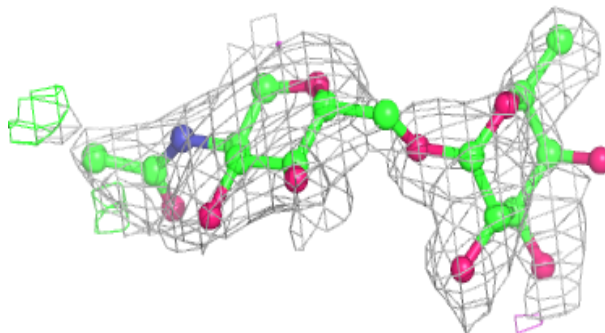
Electron density around Chain H:

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

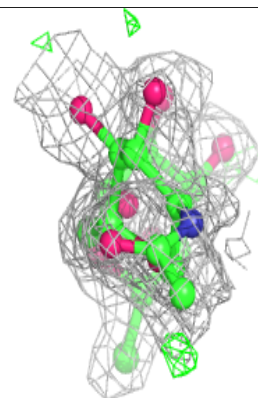
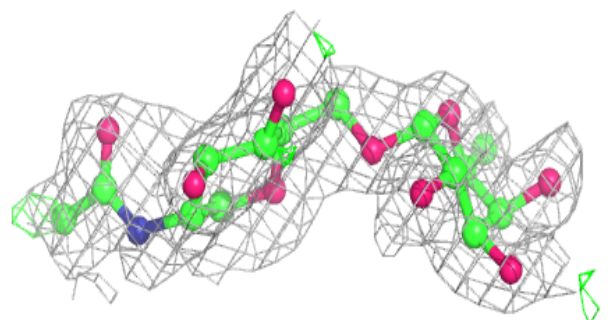
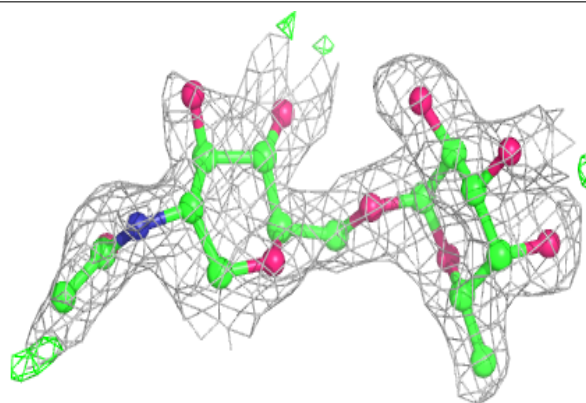


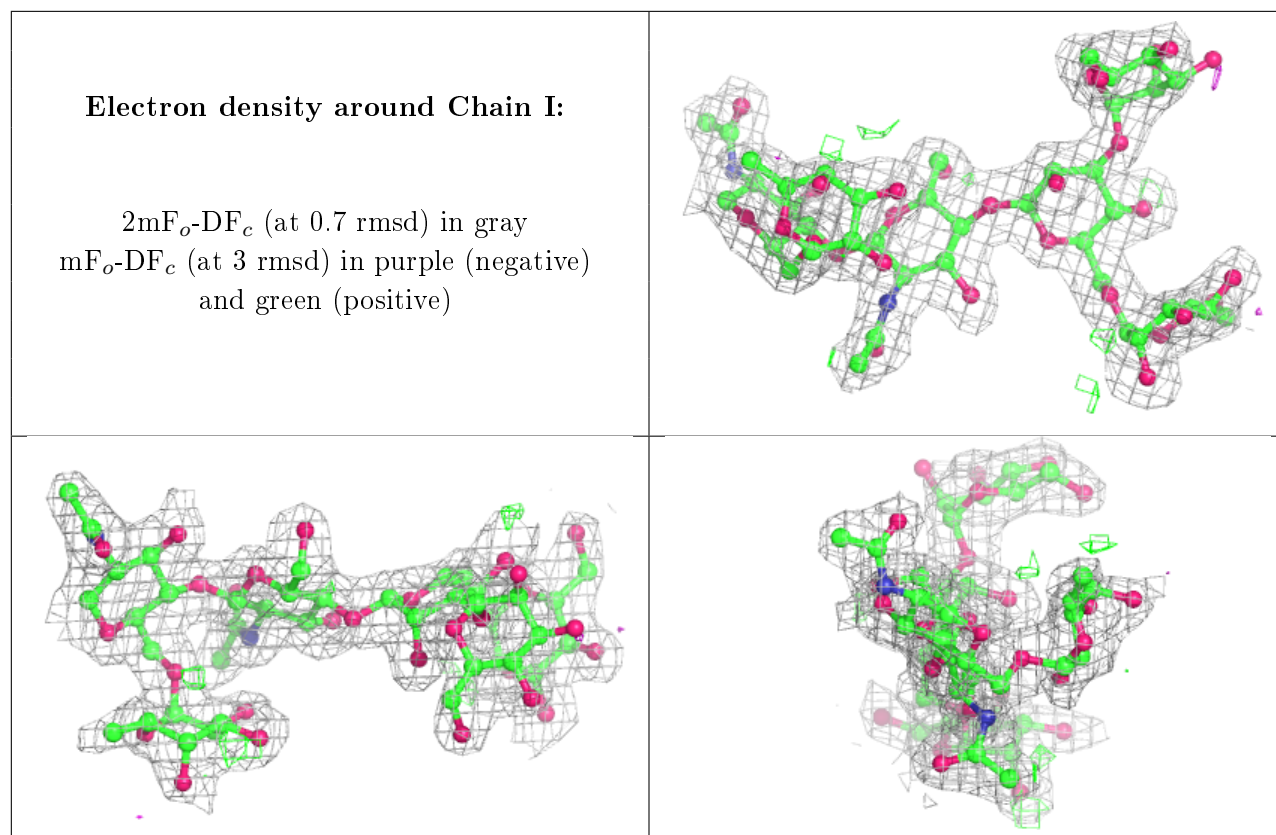
Electron density around Chain F:

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

**Electron density around Chain J:**

$2mF_o-DF_c$ (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
8	EDO	A	514	4/4	0.58	0.22	45,49,51,51	0
7	NAG	D	506	14/15	0.68	0.28	56,63,71,74	0
8	EDO	A	519	4/4	0.70	0.21	40,40,41,48	0
8	EDO	A	522	4/4	0.70	0.29	47,51,52,54	0
8	EDO	D	513	4/4	0.70	0.32	45,46,46,47	0
7	NAG	B	508	14/15	0.71	0.37	42,52,60,69	0
8	EDO	B	514	4/4	0.71	0.38	45,46,46,51	0
8	EDO	A	520	4/4	0.73	0.18	43,47,48,50	0
8	EDO	A	512	4/4	0.74	0.20	47,53,59,60	0
7	NAG	D	507	14/15	0.77	0.33	48,54,60,63	0
8	EDO	A	511	4/4	0.80	0.15	38,43,45,46	0
7	NAG	C	513	14/15	0.80	0.39	45,51,55,57	0
8	EDO	A	523	4/4	0.80	0.25	48,48,52,53	0
7	NAG	A	509	14/15	0.80	0.38	46,50,53,55	0

Continued on next page...

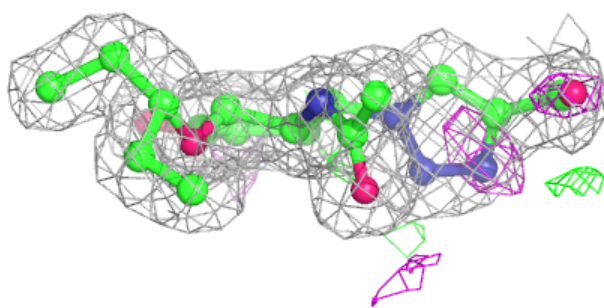
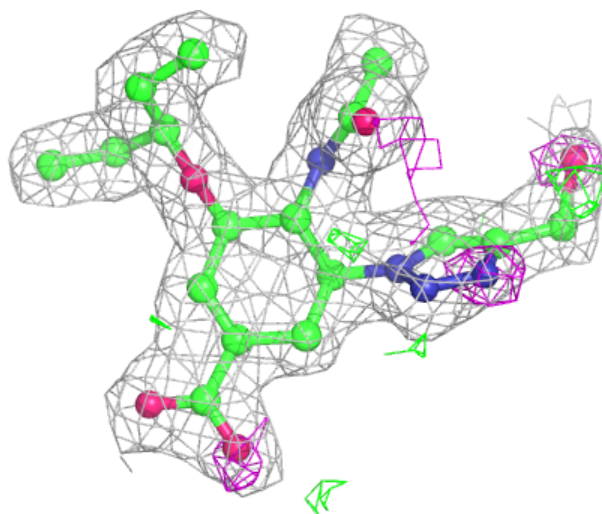
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	EDO	B	511	4/4	0.81	0.12	52,53,53,59	0
8	EDO	A	521	4/4	0.82	0.21	42,47,48,48	0
8	EDO	A	518	4/4	0.83	0.13	34,39,39,42	0
8	EDO	B	513	4/4	0.84	0.21	48,49,53,55	0
8	EDO	A	513	4/4	0.85	0.14	30,31,39,44	0
8	EDO	C	515[B]	4/4	0.85	0.21	23,29,32,33	4
7	NAG	B	507	14/15	0.85	0.27	51,57,63,65	0
8	EDO	C	515[A]	4/4	0.85	0.21	30,33,35,37	4
8	EDO	B	512	4/4	0.86	0.16	51,52,52,60	0
9	PGE	D	514	7/10	0.87	0.27	40,41,45,46	0
8	EDO	D	509	4/4	0.88	0.23	32,35,38,38	0
8	EDO	D	512	4/4	0.89	0.23	51,53,55,59	0
8	EDO	C	514	4/4	0.89	0.12	40,41,43,46	0
8	EDO	A	516	4/4	0.89	0.13	34,38,41,43	0
8	EDO	D	510	4/4	0.89	0.24	32,35,36,43	0
8	EDO	D	508	4/4	0.90	0.16	44,46,47,54	0
8	EDO	A	517	4/4	0.91	0.15	38,44,44,52	0
8	EDO	B	510	4/4	0.91	0.19	31,37,42,43	0
8	EDO	C	516	4/4	0.92	0.14	32,40,44,50	0
8	EDO	A	510	4/4	0.92	0.17	42,49,51,53	0
8	EDO	A	515	4/4	0.92	0.12	39,39,40,41	0
6	GJT	B	503	26/26	0.93	0.11	14,17,22,27	0
8	EDO	B	509	4/4	0.93	0.30	47,52,52,54	0
6	GJT	D	503	26/26	0.94	0.10	13,16,19,20	0
8	EDO	D	511	4/4	0.94	0.22	29,32,33,34	0
6	GJT	A	503	26/26	0.95	0.09	12,15,20,24	0
6	GJT	C	503	26/26	0.96	0.08	14,15,19,24	0
5	CA	B	502	1/1	0.97	0.10	42,42,42,42	0
5	CA	D	502	1/1	0.97	0.16	41,41,41,41	0
5	CA	A	502	1/1	0.98	0.13	34,34,34,34	0
5	CA	C	502	1/1	0.99	0.12	35,35,35,35	0
5	CA	D	501	1/1	1.00	0.04	20,20,20,20	0
5	CA	B	501	1/1	1.00	0.03	22,22,22,22	0
5	CA	C	501	1/1	1.00	0.04	19,19,19,19	0
5	CA	A	501	1/1	1.00	0.04	17,17,17,17	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.

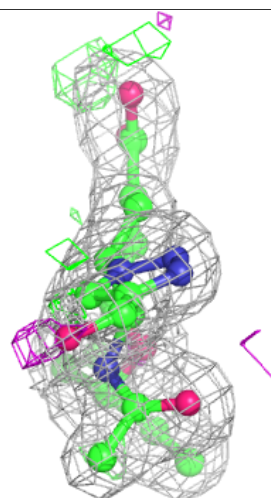
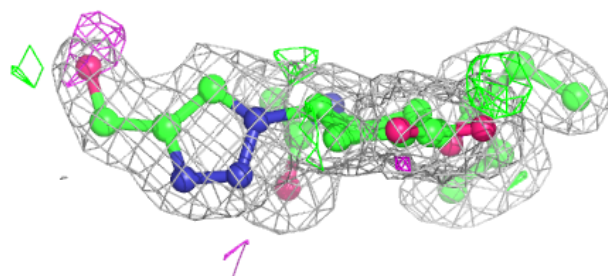
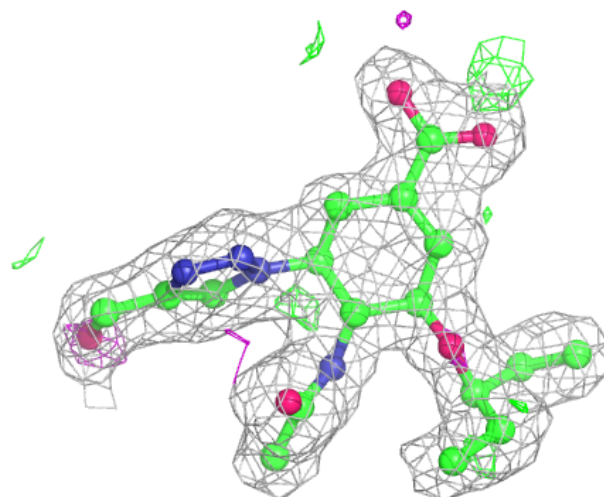
Electron density around GJT B 503:

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



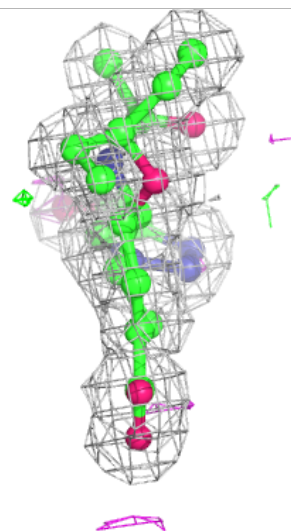
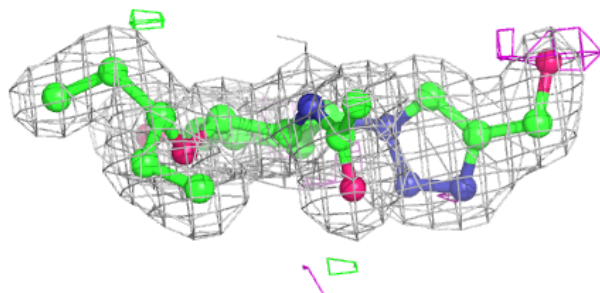
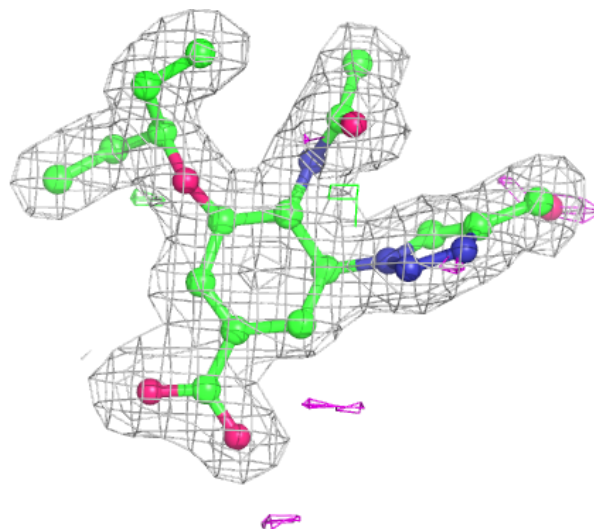
Electron density around GJT D 503:

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



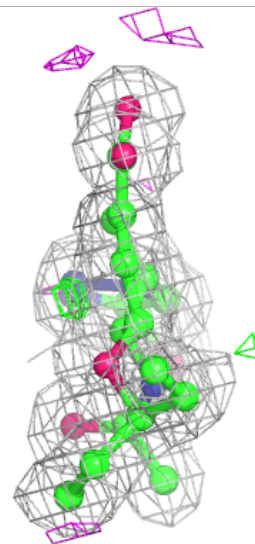
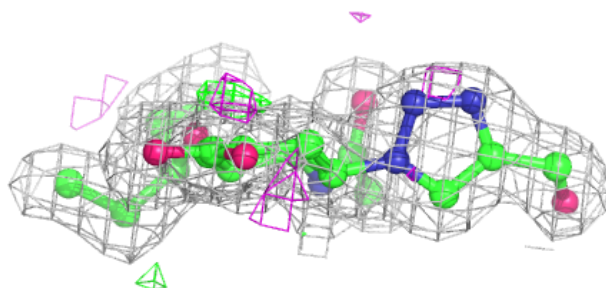
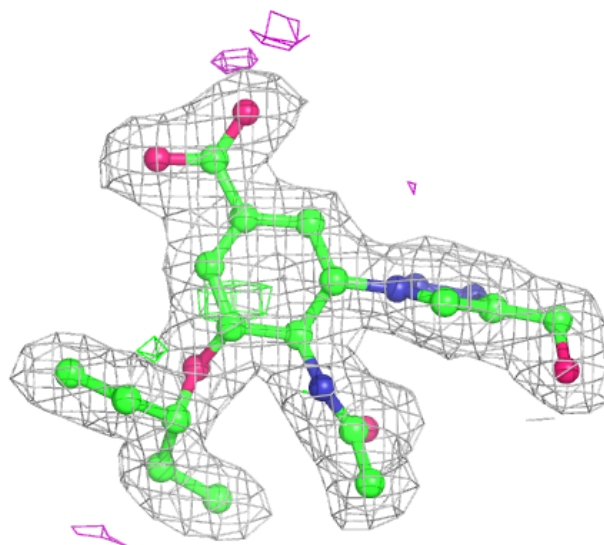
Electron density around GJT A 503:

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



Electron density around GJT 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.