Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:13 PM UTC

PDB ID	:	6HP0 / pdb_00006hp0
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 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:

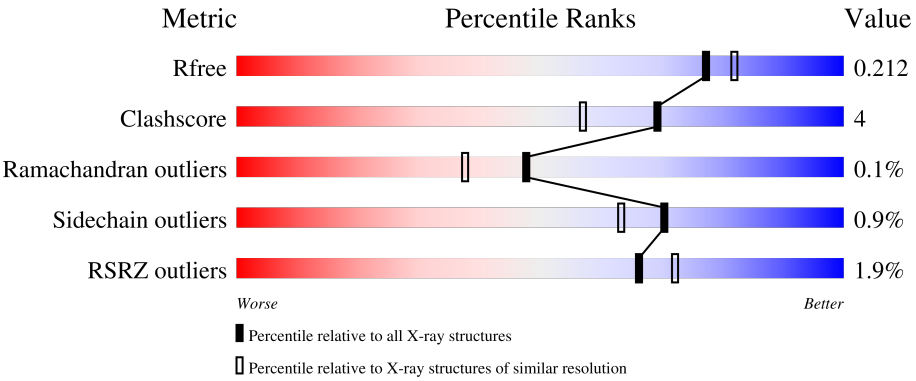
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 (i)

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}	180053	1220 (1.88-1.88)
Clashscore	190562	1234 (1.88-1.88)
Ramachandran outliers	187476	1222 (1.88-1.88)
Sidechain outliers	187428	1222 (1.88-1.88)
RSRZ outliers	180081	1220 (1.88-1.88)

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 <=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	2% 88% 10% ·
1	B	388	2% 87% 12% ·
1	C	388	2% 86% 12% ·
1	D	388	2% 87% 12% ·
2	E	3	33% 67%

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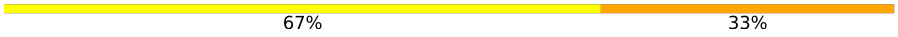
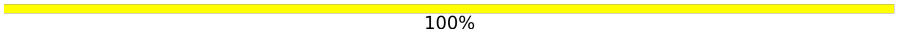
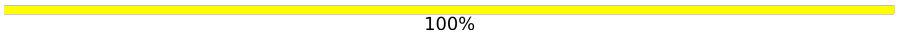
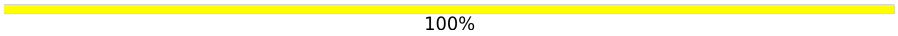
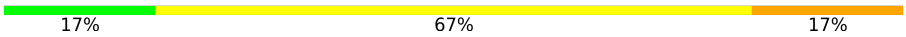
Mol	Chain	Length	Quality of chain
2	G	3	
2	H	3	
3	F	2	
3	J	2	
4	I	6	

2 Entry composition

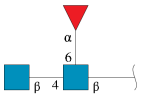
There are 10 unique types of molecules in this entry. The entry contains 14022 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.



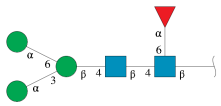
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	3	Total	C	N	O	0	0	0
			38	22	2	14			
2	G	3	Total	C	N	O	0	0	0
			38	22	2	14			
2	H	3	Total	C	N	O	0	0	0
			38	22	2	14			

- 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 24 14 1 9	0	0	0
3	J	2	Total C N O 24 14 1 9	0	0	0

- 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.

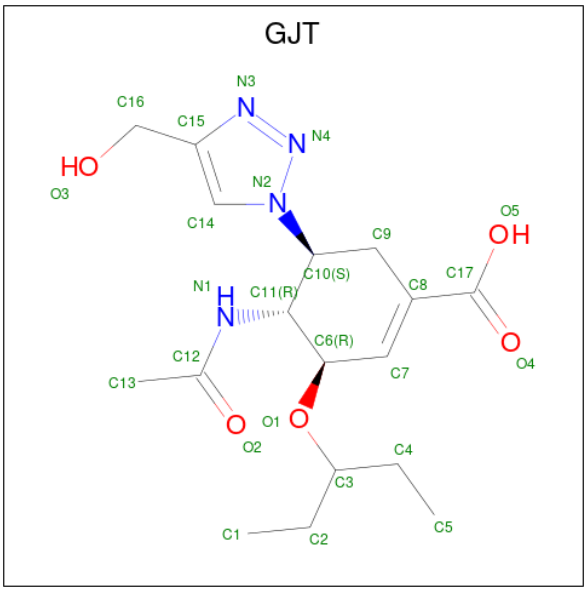


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	I	6	Total C N O 71 40 2 29	0	0	0

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

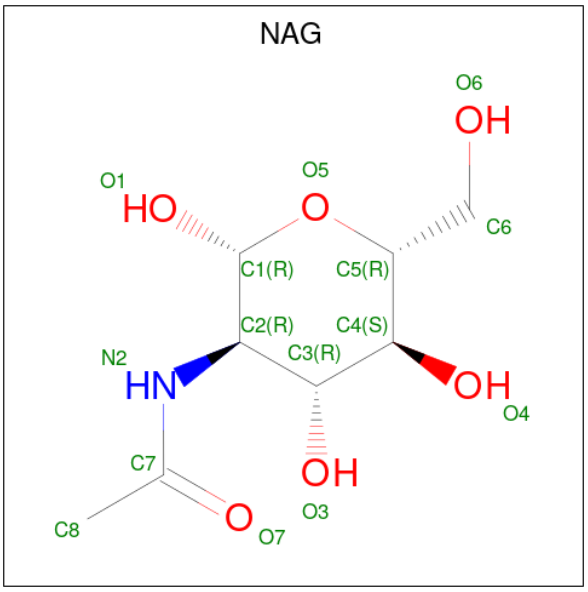
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total Ca 2 2	0	0
5	B	2	Total Ca 2 2	0	0
5	C	2	Total Ca 2 2	0	0
5	D	2	Total Ca 2 2	0	0

- 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 (CCD ID: GJT) (formula: $C_{17}H_{26}N_4O_5$).



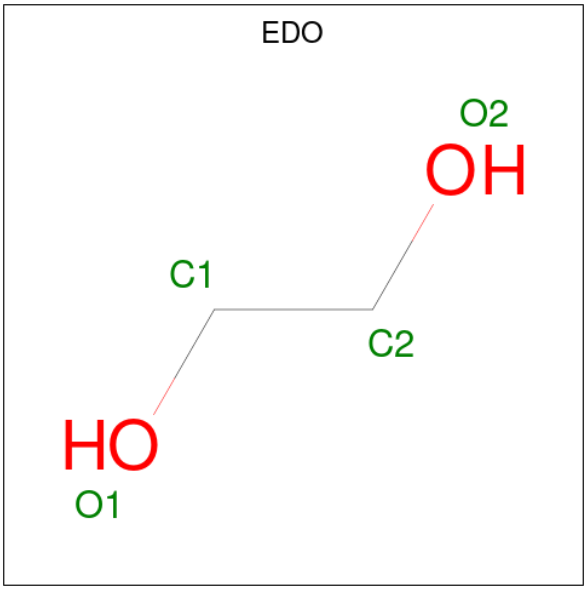
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			26	17	4	5		
6	B	1	Total	C	N	O	0	0
			26	17	4	5		
6	C	1	Total	C	N	O	0	0
			26	17	4	5		
6	D	1	Total	C	N	O	0	0
			26	17	4	5		

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



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

- Molecule 8 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

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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		
8	A	1	Total	C	O	0	0
			4	2	2		
8	A	1	Total	C	O	0	0
			4	2	2		
8	B	1	Total	C	O	0	0
			4	2	2		
8	B	1	Total	C	O	0	0
			4	2	2		
8	B	1	Total	C	O	0	0
			4	2	2		
8	B	1	Total	C	O	0	0
			4	2	2		
8	B	1	Total	C	O	0	0
			4	2	2		
8	B	1	Total	C	O	0	0
			4	2	2		
8	C	1	Total	C	O	0	0
			4	2	2		
8	C	1	Total	C	O	0	1
			8	4	4		
8	C	1	Total	C	O	0	0
			4	2	2		
8	D	1	Total	C	O	0	0
			4	2	2		
8	D	1	Total	C	O	0	0
			4	2	2		
8	D	1	Total	C	O	0	0
			4	2	2		
8	D	1	Total	C	O	0	0
			4	2	2		

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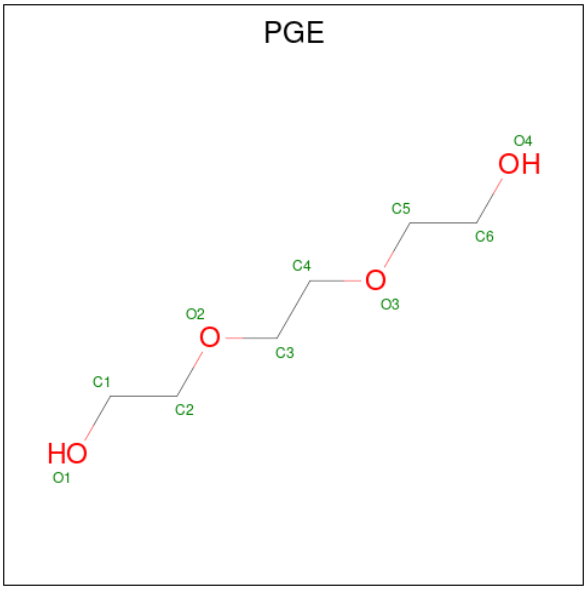
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	D	1	Total C O 4 2 2	0	0
8	D	1	Total C O 4 2 2	0	0

- Molecule 9 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



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

- Molecule 10 is water.

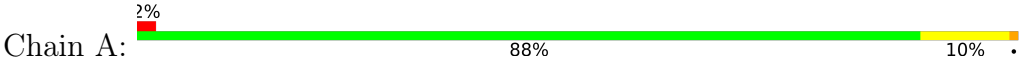
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	335	Total O 339 339	0	4
10	B	337	Total O 344 344	0	7
10	C	357	Total O 361 361	0	4
10	D	370	Total O 379 379	0	9

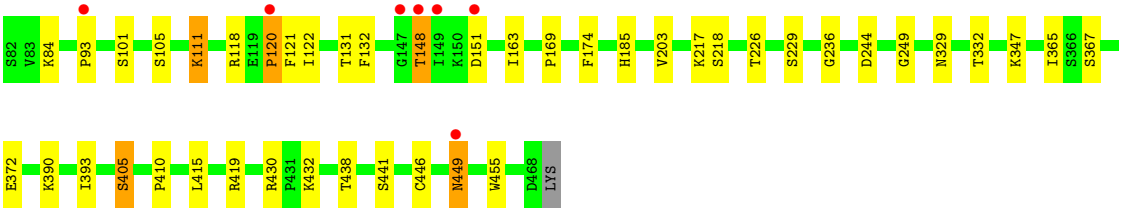
3 Residue-property plots (i)

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

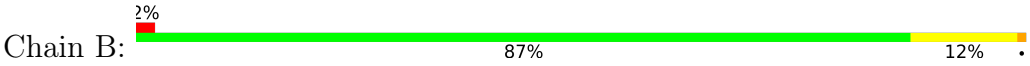
Chain A:

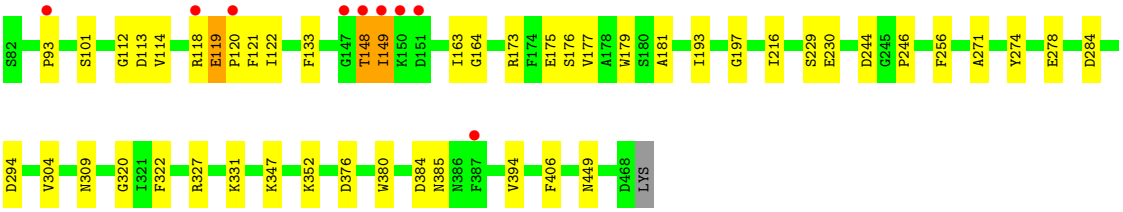




• Molecule 1: Neuraminidase

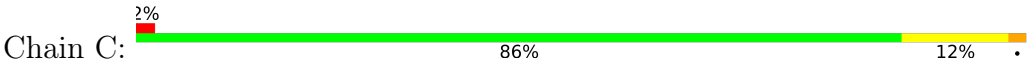
Chain B:

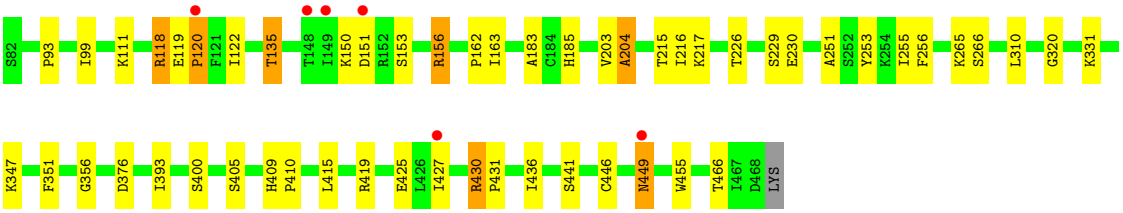




• Molecule 1: Neuraminidase

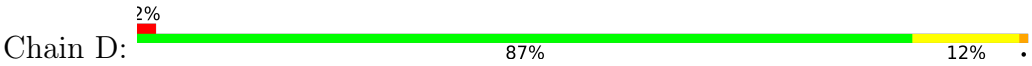
Chain C:





• Molecule 1: Neuraminidase

Chain D:

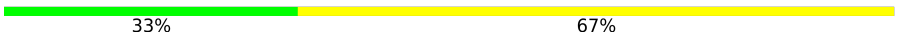






• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

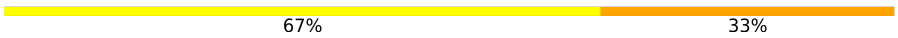
Chain E:





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

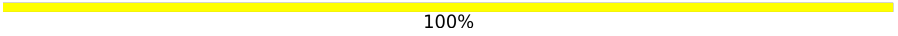
Chain G:





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

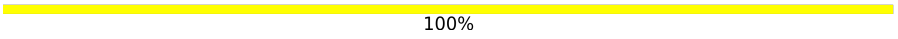
Chain H:





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

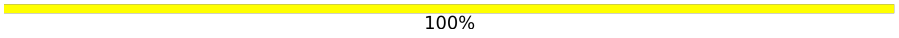
Chain F:





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

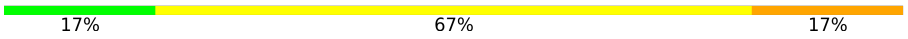
Chain J:

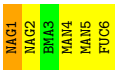




• Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:





4 Data and refinement statistics (i)

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 – 1.89	Depositor EDS
% Data completeness (in resolution range)	97.6 (48.34-1.88) 97.6 (48.34-1.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.82 (at 1.88Å)	Xtriage
Refinement program	REFMAC 5.8.0232	Depositor
R, R_{free}	0.185 , 0.222 (Not available) , 0.212	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)	0.37 , 50.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, EDO, GJT, CA, PGE, FUC, NAG, BMA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.22	8/3107 (0.3%)	1.35	12/4224 (0.3%)
1	B	1.20	6/3099 (0.2%)	1.30	7/4213 (0.2%)
1	C	1.22	9/3108 (0.3%)	1.32	8/4225 (0.2%)
1	D	1.25	12/3117 (0.4%)	1.34	5/4239 (0.1%)
All	All	1.22	35/12431 (0.3%)	1.33	32/16901 (0.2%)

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 (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	304	VAL	C-O	8.20	1.32	1.24
1	D	304	VAL	C-O	7.42	1.31	1.24
1	D	110	SER	C-O	6.92	1.32	1.24
1	D	196	SER	C-O	6.81	1.31	1.24
1	A	218	SER	CA-CB	-6.40	1.43	1.53
1	D	394	VAL	C-O	6.34	1.30	1.24
1	D	459	ASP	C-O	6.33	1.31	1.24
1	A	441	SER	C-O	6.25	1.32	1.23
1	D	255	ILE	C-O	6.17	1.31	1.24
1	A	405	SER	C-O	6.13	1.31	1.23
1	C	162	PRO	C-O	-6.07	1.16	1.23
1	C	351	PHE	C-O	6.05	1.30	1.24
1	C	405	SER	C-O	6.05	1.31	1.23
1	D	344[A]	ASN	C-O	5.92	1.31	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	344[B]	ASN	C-O	5.92	1.31	1.24
1	C	409	HIS	CE1-NE2	5.81	1.38	1.32
1	D	108	ILE	C-O	5.80	1.31	1.24
1	A	169	PRO	C-O	-5.69	1.16	1.24
1	B	278	GLU	C-O	5.68	1.30	1.23
1	D	440	GLY	C-O	5.64	1.30	1.23
1	A	185	HIS	CE1-NE2	5.62	1.38	1.32
1	C	185	HIS	CE1-NE2	5.56	1.38	1.32
1	B	246	PRO	C-O	-5.55	1.17	1.23
1	C	356	GLY	C-O	5.51	1.32	1.23
1	B	101	SER	C-O	5.41	1.30	1.23
1	D	223	ILE	C-O	5.40	1.30	1.24
1	A	249	GLY	C-O	5.35	1.30	1.24
1	B	114	VAL	C-O	-5.31	1.18	1.24
1	C	135	THR	C-O	-5.26	1.17	1.23
1	C	204	ALA	C-O	5.16	1.30	1.24
1	D	204	ALA	C-O	5.16	1.30	1.24
1	C	441	SER	C-O	5.11	1.31	1.23
1	A	105	SER	C-O	5.05	1.29	1.24
1	B	394	VAL	C-O	5.02	1.29	1.24
1	A	226	THR	C-O	5.01	1.29	1.24

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	120	PRO	N-CA-C	-8.82	98.18	111.41
1	A	449	ASN	CA-CB-CG	-8.72	103.88	112.60
1	C	120	PRO	N-CA-C	-7.17	100.66	111.41
1	D	394	VAL	CA-C-N	6.53	126.30	120.10
1	D	394	VAL	C-N-CA	6.53	126.30	120.10
1	A	148	THR	CA-C-N	6.51	129.00	120.60
1	A	148	THR	C-N-CA	6.51	129.00	120.60
1	A	393	ILE	CA-C-O	-6.49	115.02	120.80
1	D	376	ASP	CB-CA-C	6.37	116.83	110.33
1	C	430	ARG	CB-CA-C	6.26	119.25	109.42
1	B	133	PHE	O-C-N	6.09	129.49	123.46
1	D	459	ASP	CA-CB-CG	-5.94	106.66	112.60
1	C	226	THR	CA-C-N	5.65	127.78	120.44
1	C	226	THR	C-N-CA	5.65	127.78	120.44
1	A	121	PHE	CA-CB-CG	5.65	119.45	113.80
1	B	244	ASP	CA-CB-CG	5.57	118.17	112.60
1	C	393	ILE	O-C-N	5.50	126.22	121.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	121	PHE	CA-CB-CG	5.47	119.27	113.80
1	A	131	THR	CA-C-N	5.42	130.11	122.09
1	A	131	THR	C-N-CA	5.42	130.11	122.09
1	C	156	ARG	CG-CD-NE	-5.36	100.20	112.00
1	C	466	THR	CA-CB-OG1	-5.35	101.58	109.60
1	A	332	THR	CA-CB-OG1	-5.34	101.58	109.60
1	B	284	ASP	CB-CA-C	5.34	117.77	110.94
1	B	449	ASN	CA-CB-CG	-5.29	107.31	112.60
1	C	449	ASN	CA-CB-CG	-5.25	107.35	112.60
1	B	133	PHE	CA-C-O	-5.15	115.44	121.10
1	A	111	LYS	CB-CG-CD	5.12	123.07	111.30
1	D	228	GLU	N-CA-C	-5.11	106.34	112.58
1	A	393	ILE	O-C-N	5.11	125.91	121.98
1	B	93	PRO	N-CA-C	-5.04	102.71	111.32
1	A	244	ASP	CA-CB-CG	5.03	117.63	112.60

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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3010	0	2843	21	0
1	B	3005	0	2834	24	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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	86	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 4.

All (86) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:216:ILE:HD13	1:C:256:PHE:CE2	2.47	0.49
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:B:112:GLY:O	1:C:111:LYS:NZ	2.45	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:C:376:ASP:OD1	1:C:376:ASP:C	2.58	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:D:294:ASP:OD1	1:D:294:ASP:C	2.60	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O7	2:G:1:NAG:H3	2.18	0.43
1:A:430:ARG:HB2	1:A:438:THR:OG1	2.18	0.42
1:B:384:ASP:C	1:B:384:ASP:OD1	2.61	0.42
1:A:329:ASN:OD1	8:A:513:EDO:H22	2.20	0.42
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:B:294:ASP:C	1:B:294:ASP:OD1	2.64	0.40
1:B:331:LYS:O	1:B:385:ASN:HB3	2.22	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
1:B:376:ASP:C	1:B:376:ASP:OD1	2.65	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
1	B	389/388 (100%)	367 (94%)	21 (5%)	1 (0%)	36	26
1	C	321/388 (83%)	309 (96%)	12 (4%)	0	100	100
1	D	391/388 (101%)	370 (95%)	21 (5%)	0	100	100
All	All	1491/1552 (96%)	1419 (95%)	71 (5%)	1 (0%)	48	37

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	149	ILE

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	338/335 (101%)	335 (99%)	3 (1%)	70	63
1	B	336/335 (100%)	332 (99%)	4 (1%)	63	53
1	C	338/335 (101%)	337 (100%)	1 (0%)	86	82
1	D	339/335 (101%)	334 (98%)	5 (2%)	57	46
All	All	1351/1340 (101%)	1338 (99%)	13 (1%)	70	60

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	118	ARG
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

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Mol	Chain	Res	Type
1	C	118	ARG
1	D	118	ARG
1	D	148	THR
1	D	149	ILE
1	D	331	LYS
1	D	367	SER

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

Mol	Chain	Res	Type
1	A	341	ASN
1	A	355	ASN
1	B	329	ASN
1	B	341	ASN
1	C	308	GLN
1	C	325	ASN
1	C	355	ASN
1	C	449	ASN
1	D	104	ASN
1	D	136	GLN
1	D	221	ASN
1	D	329	ASN
1	D	341	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	0.63	0	17,19,21	1.73	4 (23%)
2	NAG	E	2	2	14,14,15	0.57	0	17,19,21	1.03	0
2	FUC	E	3	2	10,10,11	0.97	0	14,14,16	1.12	1 (7%)
3	NAG	F	1	3,1	14,14,15	1.13	1 (7%)	17,19,21	2.11	3 (17%)
3	FUC	F	2	3	10,10,11	0.99	0	14,14,16	1.05	1 (7%)
2	NAG	G	1	1,2	14,14,15	0.76	0	17,19,21	1.59	2 (11%)
2	NAG	G	2	2	14,14,15	0.60	0	17,19,21	1.41	2 (11%)
2	FUC	G	3	2	10,10,11	0.85	0	14,14,16	1.42	1 (7%)
2	NAG	H	1	1,2	14,14,15	0.93	1 (7%)	17,19,21	1.58	4 (23%)
2	NAG	H	2	2	14,14,15	0.67	0	17,19,21	1.28	2 (11%)
2	FUC	H	3	2	10,10,11	1.15	0	14,14,16	1.01	1 (7%)
4	NAG	I	1	4,1	14,14,15	0.95	1 (7%)	17,19,21	1.83	5 (29%)
4	NAG	I	2	4	14,14,15	0.65	0	17,19,21	1.16	1 (5%)
4	BMA	I	3	4	11,11,12	0.96	0	15,15,17	1.07	0
4	MAN	I	4	4	11,11,12	0.63	0	15,15,17	1.79	2 (13%)
4	MAN	I	5	4	11,11,12	0.98	1 (9%)	15,15,17	1.00	1 (6%)
4	FUC	I	6	4	10,10,11	0.78	0	14,14,16	2.03	4 (28%)
3	NAG	J	1	3,1	14,14,15	1.22	2 (14%)	17,19,21	1.81	4 (23%)
3	FUC	J	2	3	10,10,11	1.09	0	14,14,16	0.87	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	3,1	-	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	-	1/6/23/26	0/1/1/1
2	FUC	G	3	2	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	4,1	-	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
4	FUC	I	6	4	-	-	0/1/1/1
3	NAG	J	1	3,1	-	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	-2.68	1.41	1.46
2	H	1	NAG	C1-C2	2.62	1.55	1.52
3	J	1	NAG	C3-C2	2.33	1.57	1.52
3	F	1	NAG	C1-C2	-2.31	1.49	1.52
3	J	1	NAG	C1-C2	2.23	1.55	1.52
4	I	5	MAN	C2-C3	2.11	1.55	1.52

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	1	NAG	C1-O5-C5	5.85	120.03	112.19
2	E	1	NAG	C1-C2-N2	-4.72	103.00	110.43
3	J	1	NAG	C1-C2-N2	-4.48	103.37	110.43
4	I	6	FUC	O5-C5-C4	-4.38	101.68	109.55
4	I	1	NAG	C1-O5-C5	-4.23	106.51	112.19
4	I	4	MAN	O5-C5-C6	4.23	115.89	107.66
3	F	1	NAG	C2-N2-C7	4.18	128.50	122.90
2	G	1	NAG	C1-C2-N2	-4.13	103.92	110.43
4	I	4	MAN	C1-O5-C5	-4.11	106.67	112.19
4	I	1	NAG	C4-C3-C2	-3.77	105.49	111.02
3	J	1	NAG	O4-C4-C3	3.71	119.12	110.38
2	H	1	NAG	O5-C1-C2	-3.43	105.99	111.29
4	I	6	FUC	O5-C5-C6	3.38	114.73	107.40
2	H	2	NAG	C2-N2-C7	-3.36	118.40	122.90
2	G	3	FUC	C1-C2-C3	3.33	114.50	109.64
2	H	1	NAG	C4-C3-C2	-3.18	106.36	111.02
3	F	1	NAG	C1-C2-N2	-3.07	105.59	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	I	6	FUC	O3-C3-C2	-2.76	104.42	110.05
4	I	6	FUC	O3-C3-C4	2.75	116.87	110.38
2	E	3	FUC	O5-C5-C4	2.71	114.42	109.55
2	G	1	NAG	O5-C5-C4	-2.67	104.33	110.83
2	H	3	FUC	C3-C4-C5	2.63	113.81	109.81
2	G	2	NAG	C4-C3-C2	-2.59	107.23	111.02
2	H	1	NAG	O3-C3-C2	2.56	114.71	109.40
2	E	1	NAG	O7-C7-N2	-2.56	117.46	121.98
2	G	2	NAG	C3-C4-C5	-2.49	105.72	110.23
4	I	1	NAG	C2-N2-C7	-2.45	119.61	122.90
4	I	5	MAN	O5-C1-C2	2.42	116.56	110.79
2	H	1	NAG	C1-O5-C5	2.33	115.31	112.19
3	F	2	FUC	O5-C5-C6	2.32	112.43	107.40
4	I	1	NAG	O7-C7-C8	-2.23	118.08	122.05
2	E	1	NAG	C8-C7-N2	2.20	119.77	116.12
4	I	2	NAG	C1-O5-C5	-2.13	109.34	112.19
3	J	1	NAG	O5-C5-C4	-2.12	105.68	110.83
3	J	1	NAG	C2-N2-C7	2.09	125.70	122.90
2	E	1	NAG	C1-O5-C5	-2.07	109.41	112.19
2	H	2	NAG	O4-C4-C5	2.02	114.30	109.32
3	J	2	FUC	C1-C2-C3	2.01	112.58	109.64
4	I	1	NAG	C3-C4-C5	-2.01	106.59	110.23

There are no chirality outliers.

All (13) torsion outliers are listed below:

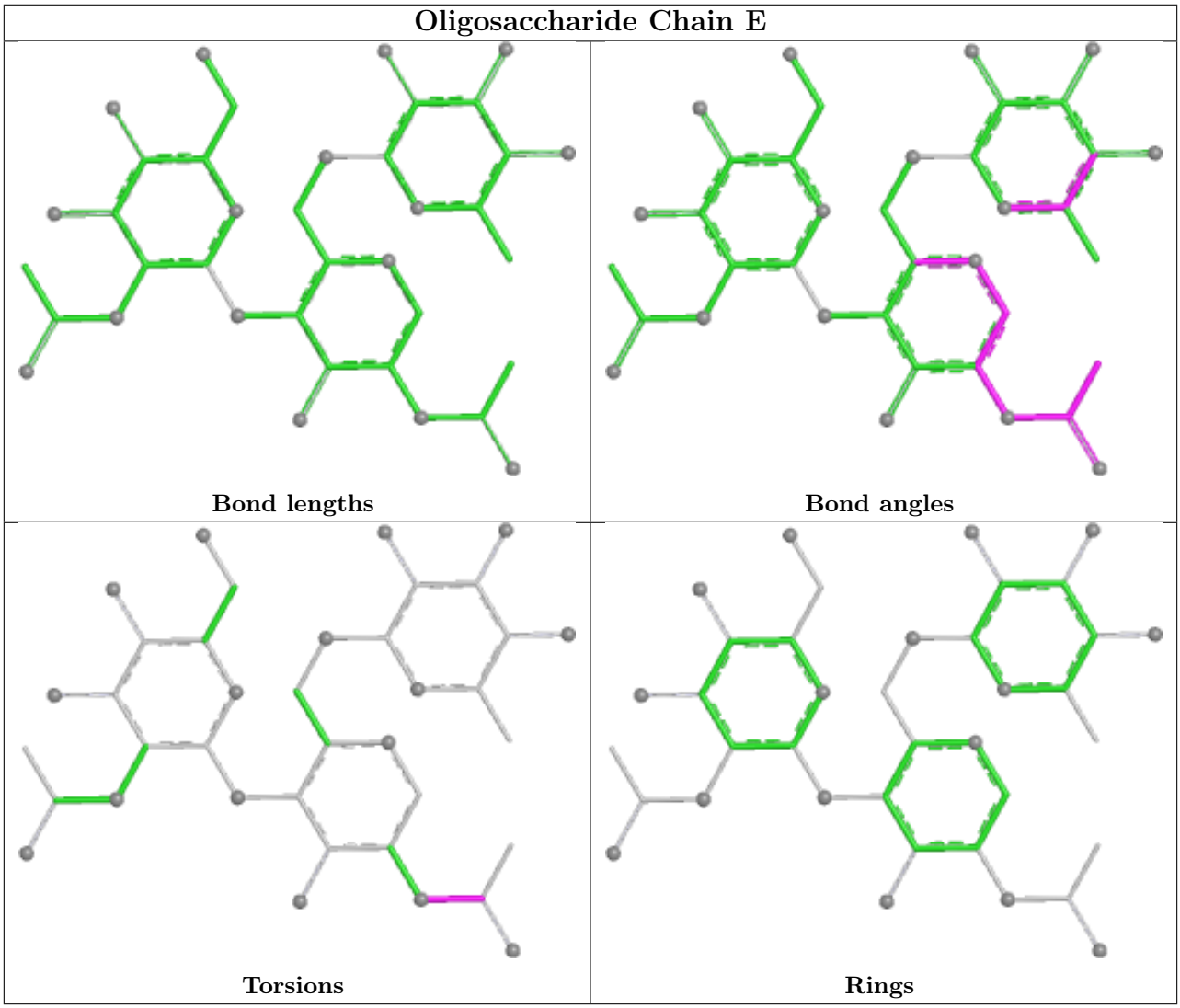
Mol	Chain	Res	Type	Atoms
2	E	1	NAG	C8-C7-N2-C2
2	E	1	NAG	O7-C7-N2-C2
2	G	1	NAG	C3-C2-N2-C7
2	H	1	NAG	C1-C2-N2-C7
4	I	4	MAN	O5-C5-C6-O6
2	G	1	NAG	C8-C7-N2-C2
3	J	1	NAG	C8-C7-N2-C2
4	I	4	MAN	C4-C5-C6-O6
3	F	1	NAG	C4-C5-C6-O6
3	J	1	NAG	C3-C2-N2-C7
3	J	1	NAG	O7-C7-N2-C2
2	G	1	NAG	O7-C7-N2-C2
2	G	2	NAG	C1-C2-N2-C7

There are no ring outliers.

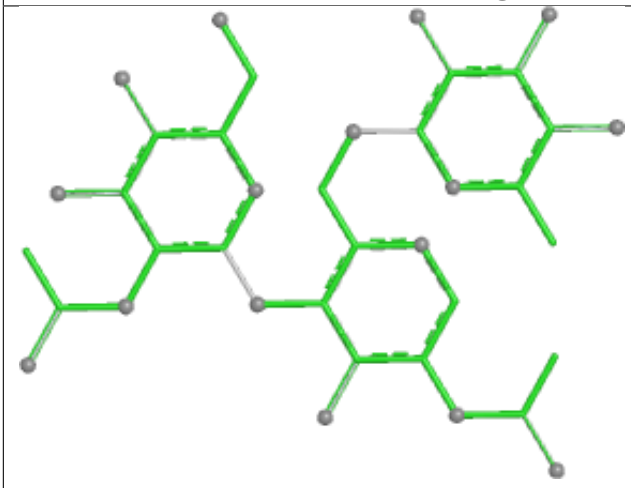
2 monomers are involved in 2 short contacts:

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

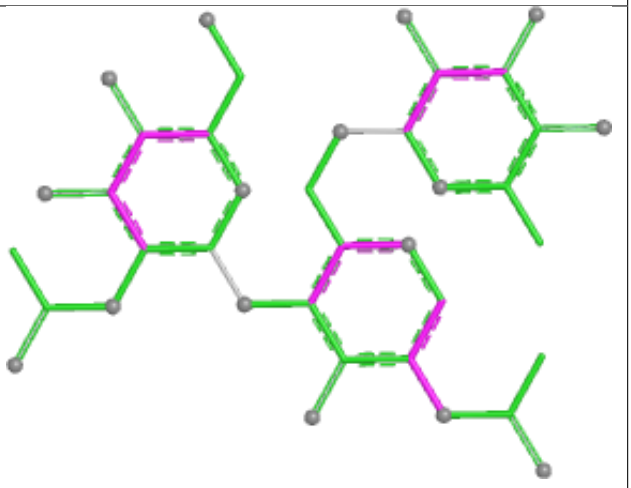
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



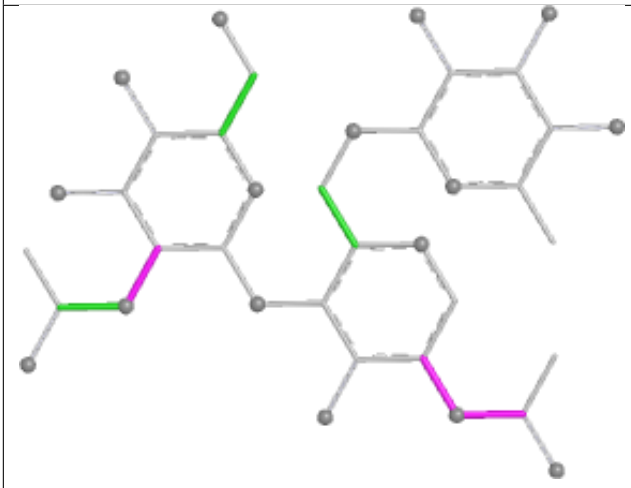
Oligosaccharide Chain G



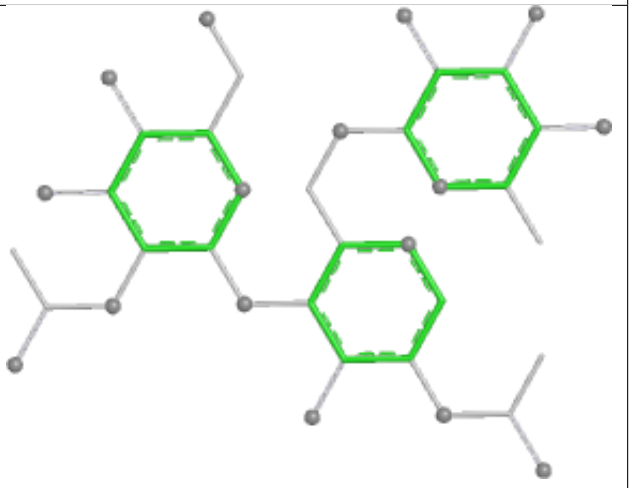
Bond lengths



Bond angles

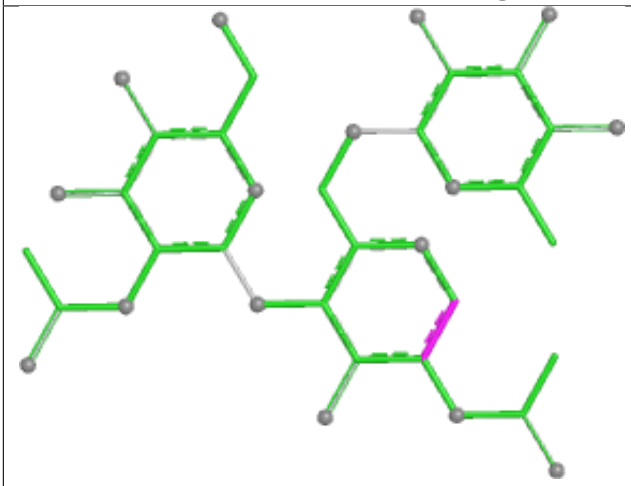


Torsions

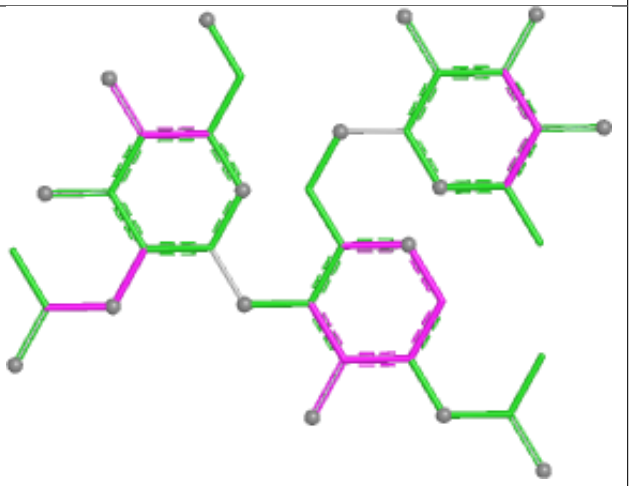


Rings

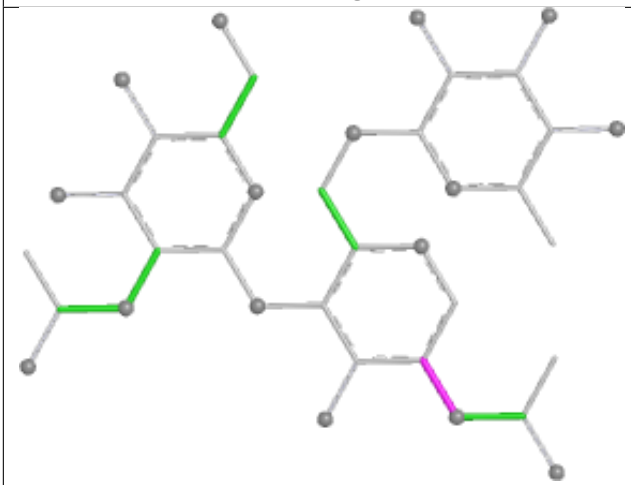
Oligosaccharide Chain H



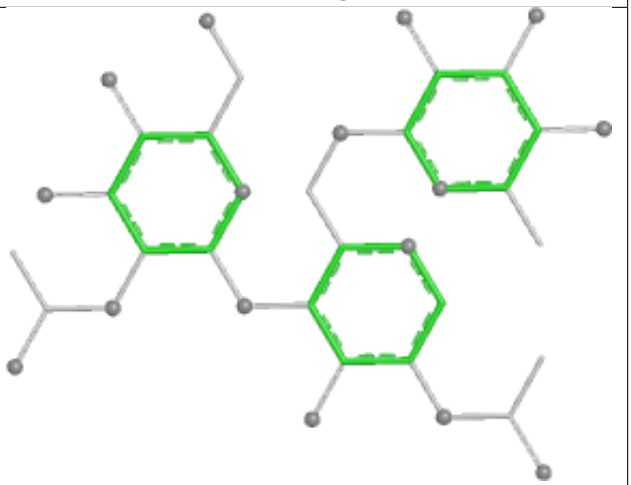
Bond lengths



Bond angles

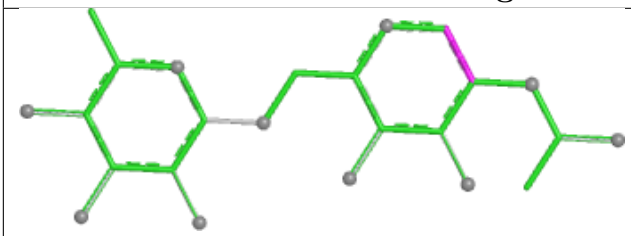


Torsions

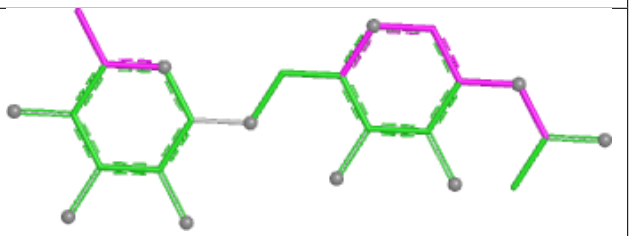


Rings

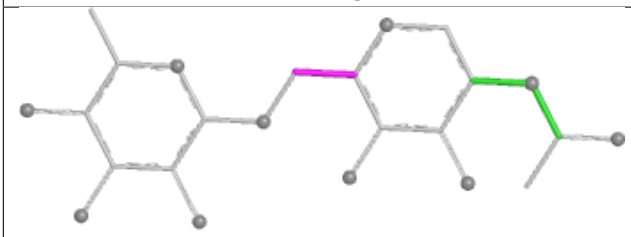
Oligosaccharide Chain F



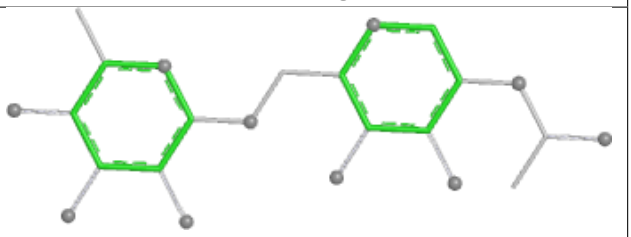
Bond lengths



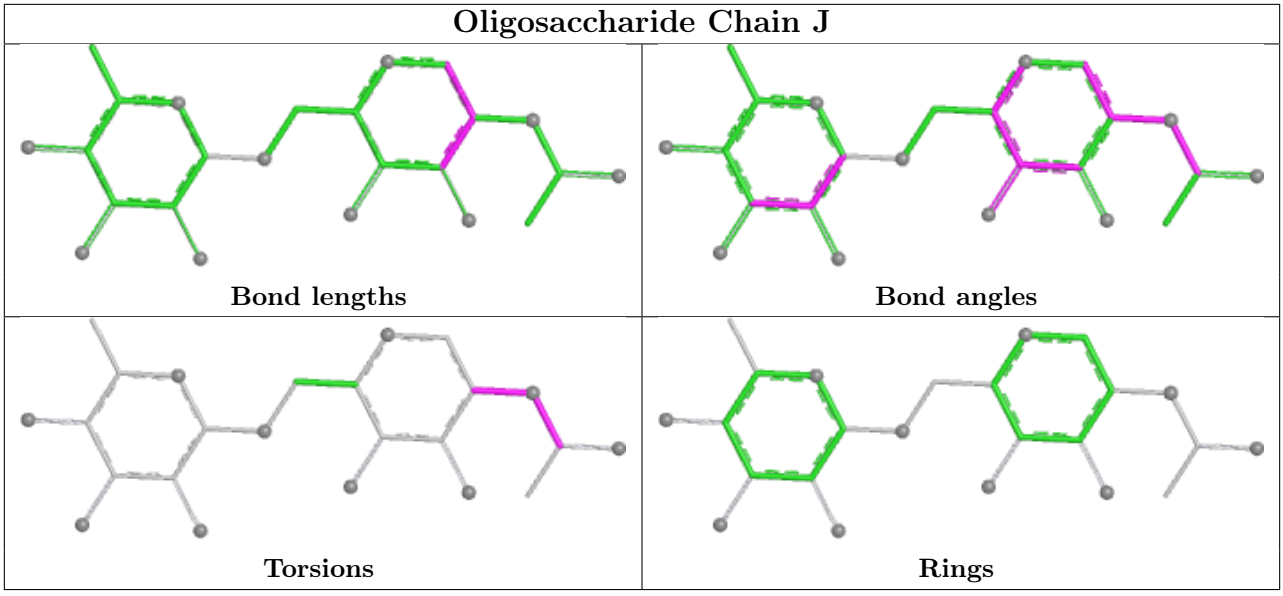
Bond angles

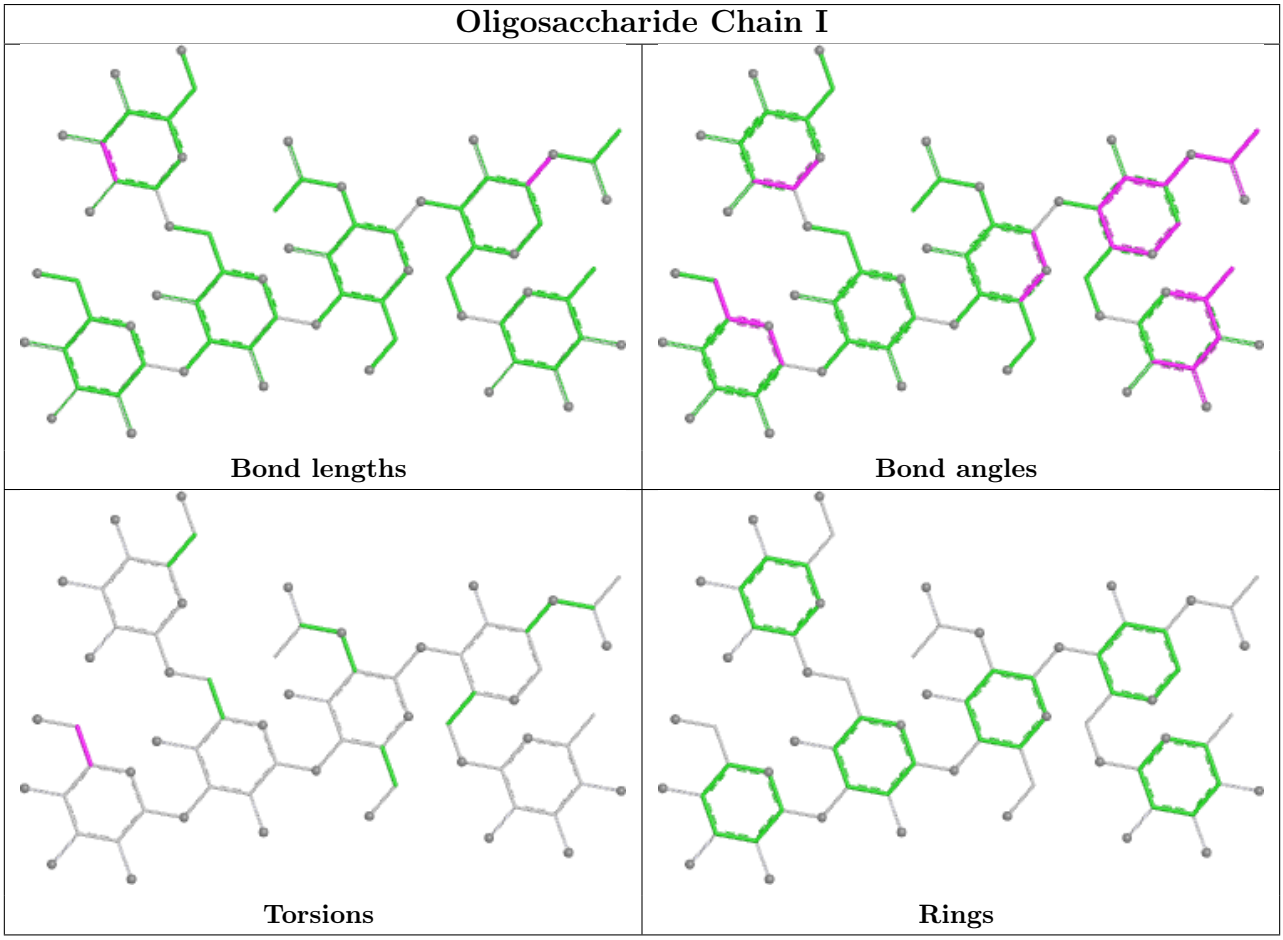


Torsions



Rings





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	C	516	-	3,3,3	0.24	0	2,2,2	0.37	0
9	PGE	D	514	-	6,6,9	0.22	0	5,5,8	0.29	0
8	EDO	A	518	-	3,3,3	0.40	0	2,2,2	0.19	0
8	EDO	B	513	-	3,3,3	0.14	0	2,2,2	0.13	0
8	EDO	D	510	-	3,3,3	0.32	0	2,2,2	0.13	0
8	EDO	D	511	-	3,3,3	0.19	0	2,2,2	0.25	0
8	EDO	A	510	-	3,3,3	0.16	0	2,2,2	0.21	0
8	EDO	A	513	-	3,3,3	0.38	0	2,2,2	0.37	0
6	GJT	B	503	-	26,27,27	0.93	1 (3%)	29,37,37	1.40	4 (13%)
6	GJT	C	503	-	26,27,27	0.87	1 (3%)	29,37,37	1.45	5 (17%)
7	NAG	D	507	1	14,14,15	0.87	1 (7%)	17,19,21	1.23	3 (17%)
7	NAG	B	508	1	14,14,15	0.93	1 (7%)	17,19,21	2.26	6 (35%)
8	EDO	D	509	-	3,3,3	0.47	0	2,2,2	0.47	0
8	EDO	D	513	-	3,3,3	0.47	0	2,2,2	0.10	0
8	EDO	A	515	-	3,3,3	0.14	0	2,2,2	0.50	0
8	EDO	A	516	-	3,3,3	0.25	0	2,2,2	0.48	0
8	EDO	A	511	-	3,3,3	0.78	0	2,2,2	0.84	0
7	NAG	C	513	1	14,14,15	0.93	0	17,19,21	1.29	2 (11%)
8	EDO	B	514	-	3,3,3	0.61	0	2,2,2	0.58	0
8	EDO	A	521	-	3,3,3	0.34	0	2,2,2	0.27	0
8	EDO	C	515[A]	-	3,3,3	0.17	0	2,2,2	0.40	0
8	EDO	D	508	-	3,3,3	0.27	0	2,2,2	0.33	0
7	NAG	D	506	1	14,14,15	0.77	0	17,19,21	1.70	3 (17%)
8	EDO	A	519	-	3,3,3	0.57	0	2,2,2	0.42	0
6	GJT	D	503	-	26,27,27	1.33	5 (19%)	29,37,37	1.69	7 (24%)
8	EDO	B	512	-	3,3,3	0.14	0	2,2,2	0.20	0
8	EDO	A	522	-	3,3,3	0.23	0	2,2,2	0.27	0
8	EDO	A	514	-	3,3,3	0.62	0	2,2,2	0.37	0
8	EDO	B	509	-	3,3,3	0.14	0	2,2,2	0.21	0
8	EDO	B	511	-	3,3,3	0.20	0	2,2,2	0.25	0
8	EDO	D	512	-	3,3,3	0.10	0	2,2,2	0.08	0
8	EDO	C	514	-	3,3,3	0.23	0	2,2,2	0.17	0
8	EDO	B	510	-	3,3,3	0.14	0	2,2,2	0.56	0
8	EDO	A	517	-	3,3,3	0.50	0	2,2,2	0.04	0
8	EDO	A	512	-	3,3,3	0.26	0	2,2,2	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	EDO	A	520	-	3,3,3	0.44	0	2,2,2	0.54	0
8	EDO	A	523	-	3,3,3	0.12	0	2,2,2	0.16	0
6	GJT	A	503	-	26,27,27	1.08	2 (7%)	29,37,37	1.40	5 (17%)
7	NAG	A	509	1	14,14,15	0.90	0	17,19,21	1.19	1 (5%)
7	NAG	B	507	1	14,14,15	0.87	0	17,19,21	1.40	3 (17%)
8	EDO	C	515[B]	-	3,3,3	0.29	0	2,2,2	0.57	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	EDO	C	516	-	-	1/1/1/1	-
9	PGE	D	514	-	-	2/4/4/7	-
8	EDO	A	518	-	-	1/1/1/1	-
8	EDO	B	513	-	-	1/1/1/1	-
8	EDO	D	510	-	-	0/1/1/1	-
8	EDO	D	511	-	-	1/1/1/1	-
8	EDO	A	510	-	-	1/1/1/1	-
8	EDO	A	513	-	-	1/1/1/1	-
6	GJT	B	503	-	-	2/22/38/38	0/2/2/2
6	GJT	C	503	-	-	3/22/38/38	0/2/2/2
7	NAG	D	507	1	-	0/6/23/26	0/1/1/1
7	NAG	B	508	1	-	2/6/23/26	0/1/1/1
8	EDO	D	509	-	-	1/1/1/1	-
8	EDO	D	513	-	-	1/1/1/1	-
8	EDO	A	515	-	-	1/1/1/1	-
8	EDO	A	516	-	-	1/1/1/1	-
8	EDO	A	511	-	-	0/1/1/1	-
7	NAG	C	513	1	-	0/6/23/26	0/1/1/1
8	EDO	B	514	-	-	1/1/1/1	-
8	EDO	A	521	-	-	1/1/1/1	-
8	EDO	C	515[A]	-	-	1/1/1/1	-
8	EDO	D	508	-	-	1/1/1/1	-
7	NAG	D	506	1	-	2/6/23/26	0/1/1/1
8	EDO	A	519	-	-	1/1/1/1	-
6	GJT	D	503	-	-	4/22/38/38	0/2/2/2
8	EDO	B	512	-	-	1/1/1/1	-
8	EDO	A	522	-	-	1/1/1/1	-
8	EDO	A	514	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	EDO	B	509	-	-	1/1/1/1	-
8	EDO	B	511	-	-	1/1/1/1	-
8	EDO	D	512	-	-	1/1/1/1	-
8	EDO	C	514	-	-	1/1/1/1	-
8	EDO	B	510	-	-	1/1/1/1	-
8	EDO	A	517	-	-	1/1/1/1	-
8	EDO	A	512	-	-	1/1/1/1	-
8	EDO	A	520	-	-	1/1/1/1	-
8	EDO	A	523	-	-	1/1/1/1	-
6	GJT	A	503	-	-	4/22/38/38	0/2/2/2
7	NAG	A	509	1	-	0/6/23/26	0/1/1/1
7	NAG	B	507	1	-	0/6/23/26	0/1/1/1
8	EDO	C	515[B]	-	-	1/1/1/1	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	503	GJT	C9-C10	-3.54	1.48	1.54
6	A	503	GJT	C11-C10	3.53	1.57	1.53
6	B	503	GJT	O5-C17	-2.90	1.22	1.30
6	C	503	GJT	O4-C17	2.90	1.29	1.22
6	D	503	GJT	C10-N2	-2.79	1.43	1.47
6	D	503	GJT	O5-C17	-2.75	1.23	1.30
6	A	503	GJT	O4-C17	2.45	1.28	1.22
6	D	503	GJT	C16-C15	-2.33	1.48	1.50
7	B	508	NAG	O5-C1	2.22	1.47	1.43
7	D	507	NAG	C1-C2	2.21	1.55	1.52
6	D	503	GJT	O4-C17	2.21	1.28	1.22

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	508	NAG	C1-O5-C5	4.90	118.75	112.19
7	D	506	NAG	C1-O5-C5	4.51	118.23	112.19
6	D	503	GJT	C10-N2-N4	-4.17	115.77	120.80
6	B	503	GJT	C10-C9-C8	4.03	114.29	109.72
7	B	508	NAG	C6-C5-C4	-3.64	104.09	113.02
7	B	507	NAG	C1-O5-C5	3.51	116.89	112.19
6	D	503	GJT	C10-N2-C14	3.38	133.53	128.46
6	C	503	GJT	C10-N2-C14	3.34	133.48	128.46
7	B	508	NAG	C1-C2-N2	-3.29	105.25	110.43
7	B	508	NAG	O7-C7-N2	-3.29	116.17	121.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	D	503	GJT	C9-C8-C17	3.15	122.76	116.99
6	C	503	GJT	C14-N2-N4	-3.05	107.75	110.63
7	D	506	NAG	C3-C4-C5	-2.88	105.01	110.23
7	C	513	NAG	C3-C4-C5	-2.87	105.02	110.23
7	D	506	NAG	O4-C4-C5	2.86	116.36	109.32
6	D	503	GJT	O1-C3-C4	-2.78	97.34	108.87
6	A	503	GJT	N2-N4-N3	2.78	109.44	107.09
6	A	503	GJT	C14-N2-N4	-2.61	108.17	110.63
6	C	503	GJT	C9-C8-C17	2.58	121.71	116.99
6	D	503	GJT	C16-C15-N3	-2.51	117.46	121.62
6	A	503	GJT	C9-C8-C17	2.51	121.59	116.99
6	D	503	GJT	C9-C8-C7	-2.49	119.17	122.25
6	B	503	GJT	O1-C3-C4	-2.48	98.57	108.87
6	B	503	GJT	O5-C17-C8	2.44	120.60	115.43
7	D	507	NAG	C1-O5-C5	2.39	115.39	112.19
7	A	509	NAG	C1-O5-C5	2.39	115.39	112.19
6	D	503	GJT	C10-C9-C8	2.37	112.40	109.72
6	C	503	GJT	N2-N4-N3	2.35	109.08	107.09
7	B	507	NAG	O5-C5-C6	2.35	112.23	107.66
7	B	507	NAG	O3-C3-C2	-2.32	104.59	109.40
7	B	508	NAG	C8-C7-N2	2.29	119.92	116.12
6	A	503	GJT	C10-C9-C8	2.23	112.24	109.72
7	D	507	NAG	C3-C4-C5	-2.19	106.26	110.23
7	B	508	NAG	O5-C1-C2	2.17	114.65	111.29
6	C	503	GJT	C10-C9-C8	2.16	112.17	109.72
6	A	503	GJT	O3-C16-C15	-2.16	107.30	111.79
7	C	513	NAG	O5-C1-C2	2.07	114.50	111.29
7	D	507	NAG	O3-C3-C4	2.03	115.16	110.38
6	B	503	GJT	O5-C17-O4	-2.02	119.10	123.90

There are no chirality outliers.

All (47) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	503	GJT	N3-C15-C16-O3
7	B	508	NAG	C8-C7-N2-C2
7	B	508	NAG	O7-C7-N2-C2
9	D	514	PGE	O1-C1-C2-O2
7	D	506	NAG	C4-C5-C6-O6
8	A	512	EDO	O1-C1-C2-O2
8	A	516	EDO	O1-C1-C2-O2
8	A	519	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
8	A	522	EDO	O1-C1-C2-O2
7	D	506	NAG	O5-C5-C6-O6
8	A	520	EDO	O1-C1-C2-O2
8	A	523	EDO	O1-C1-C2-O2
8	B	514	EDO	O1-C1-C2-O2
8	C	515[A]	EDO	O1-C1-C2-O2
8	D	512	EDO	O1-C1-C2-O2
8	A	521	EDO	O1-C1-C2-O2
6	D	503	GJT	C1-C2-C3-C4
8	B	512	EDO	O1-C1-C2-O2
8	D	508	EDO	O1-C1-C2-O2
6	D	503	GJT	N3-C15-C16-O3
9	D	514	PGE	O2-C3-C4-O3
6	A	503	GJT	C14-C15-C16-O3
6	C	503	GJT	C14-C15-C16-O3
6	D	503	GJT	C14-C15-C16-O3
6	A	503	GJT	C11-C6-O1-C3
8	A	514	EDO	O1-C1-C2-O2
8	A	515	EDO	O1-C1-C2-O2
8	B	513	EDO	O1-C1-C2-O2
6	B	503	GJT	C1-C2-C3-C4
8	B	510	EDO	O1-C1-C2-O2
8	C	514	EDO	O1-C1-C2-O2
8	C	516	EDO	O1-C1-C2-O2
8	D	509	EDO	O1-C1-C2-O2
8	A	510	EDO	O1-C1-C2-O2
8	A	513	EDO	O1-C1-C2-O2
8	B	511	EDO	O1-C1-C2-O2
8	D	511	EDO	O1-C1-C2-O2
8	C	515[B]	EDO	O1-C1-C2-O2
8	D	513	EDO	O1-C1-C2-O2
6	A	503	GJT	C9-C10-N2-C14
6	A	503	GJT	N3-C15-C16-O3
6	B	503	GJT	C2-C3-O1-C6
8	A	517	EDO	O1-C1-C2-O2
8	B	509	EDO	O1-C1-C2-O2
6	C	503	GJT	C11-C6-O1-C3
6	D	503	GJT	C11-C6-O1-C3
8	A	518	EDO	O1-C1-C2-O2

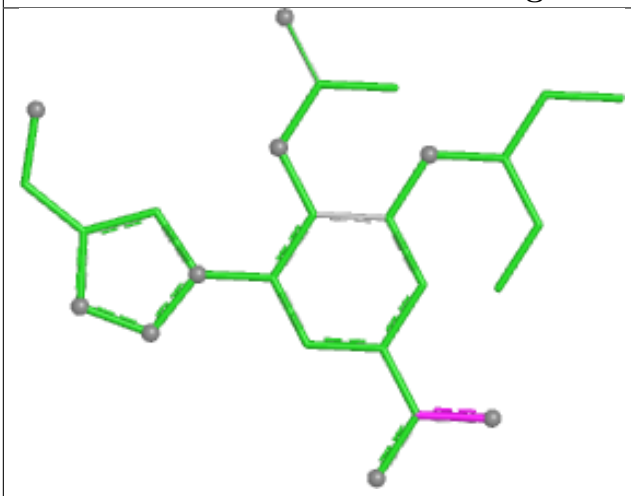
There are no ring outliers.

6 monomers are involved in 7 short contacts:

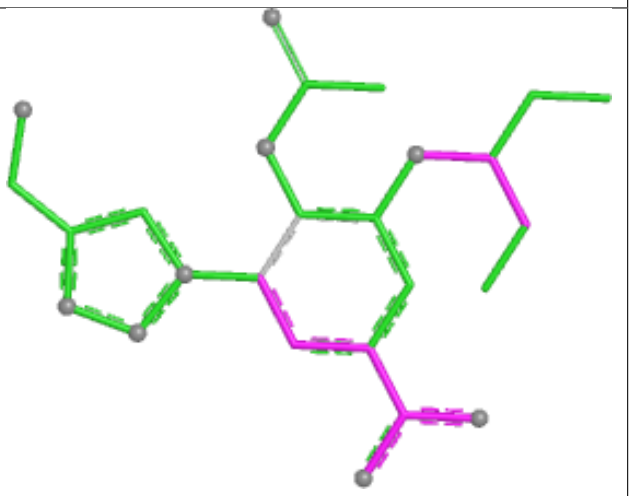
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	D	514	PGE	1	0
8	D	511	EDO	1	0
8	A	510	EDO	1	0
8	A	513	EDO	2	0
6	B	503	GJT	1	0
8	D	509	EDO	1	0

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

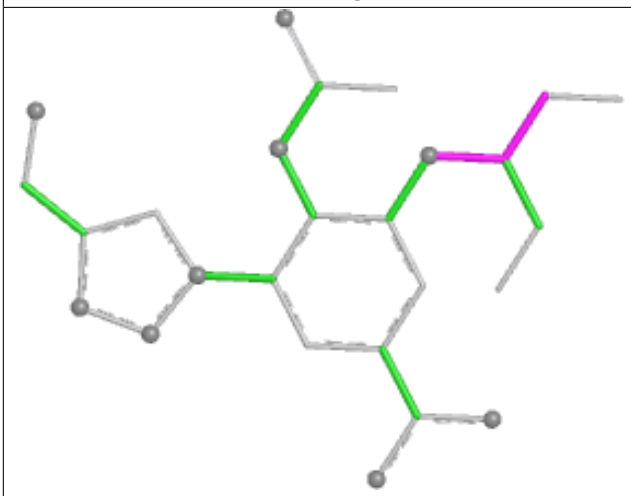
Ligand GJT B 503



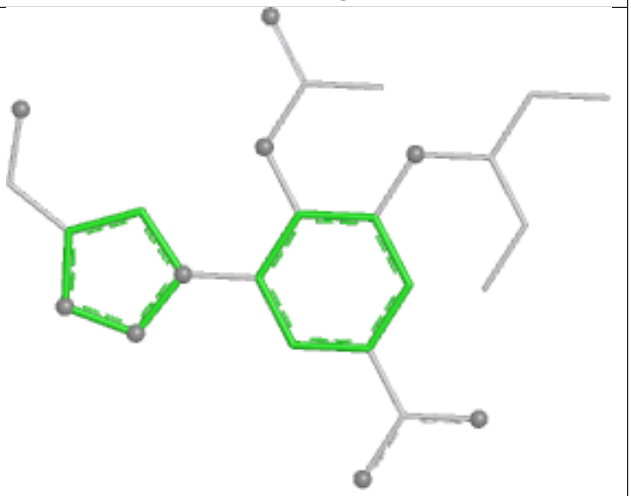
Bond lengths



Bond angles

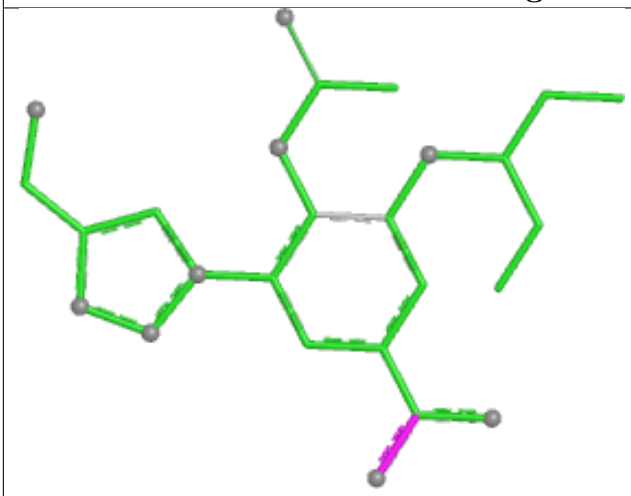


Torsions

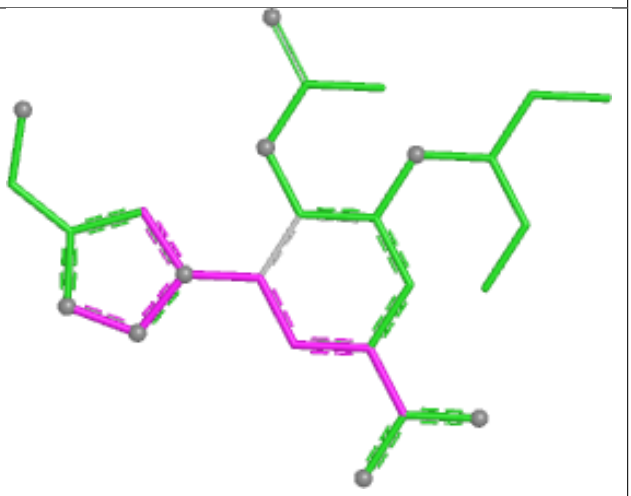


Rings

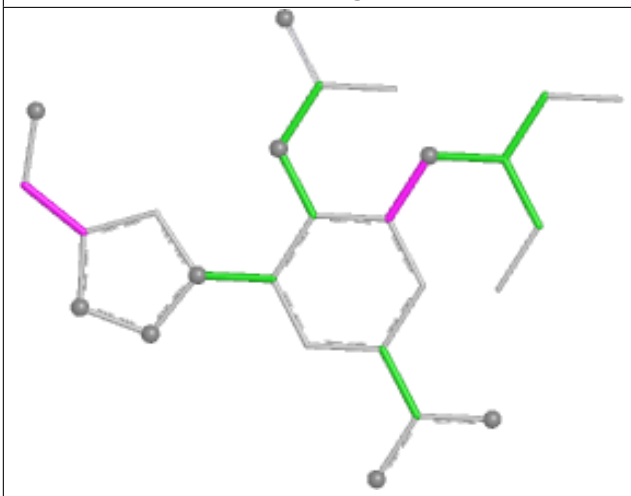
Ligand GJT C 503



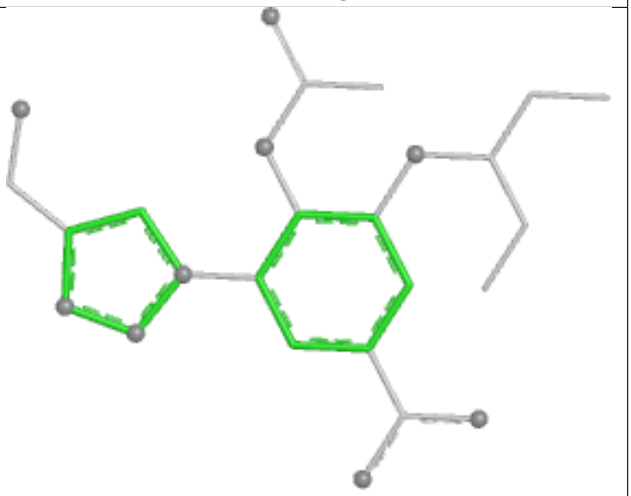
Bond lengths



Bond angles

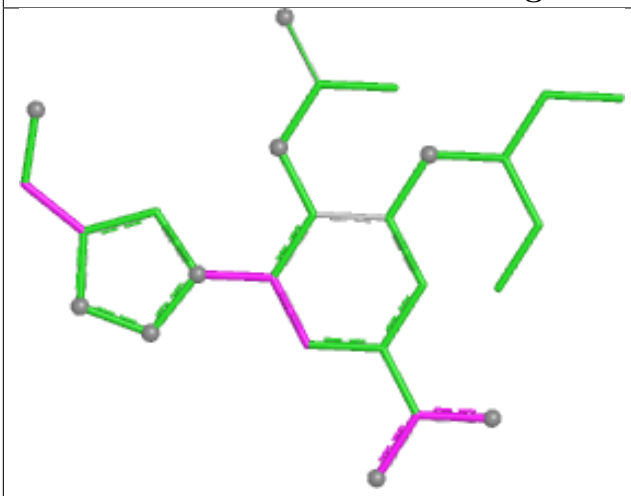


Torsions

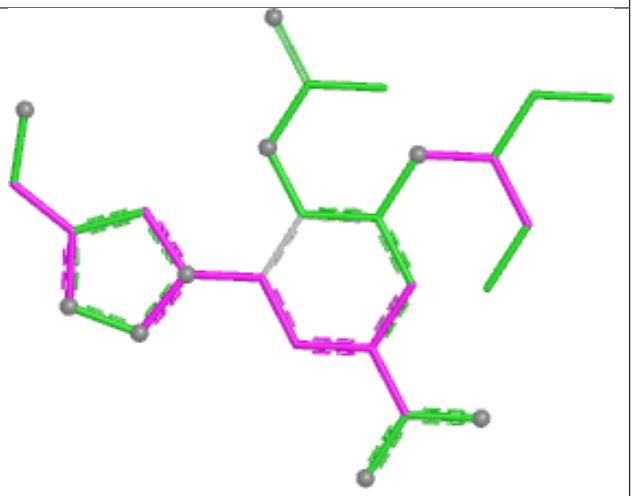


Rings

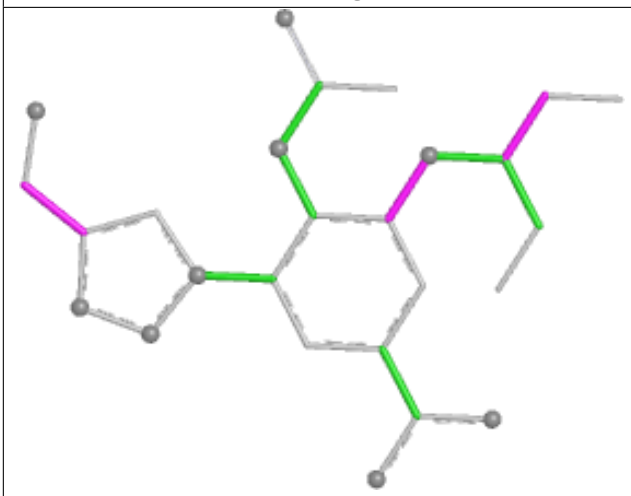
Ligand GJT D 503



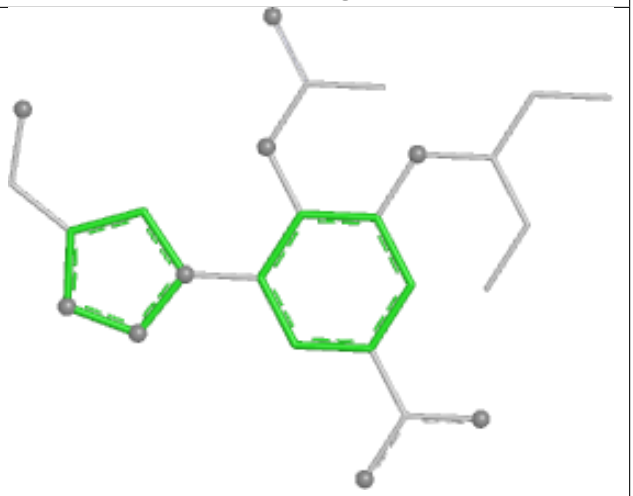
Bond lengths



Bond angles

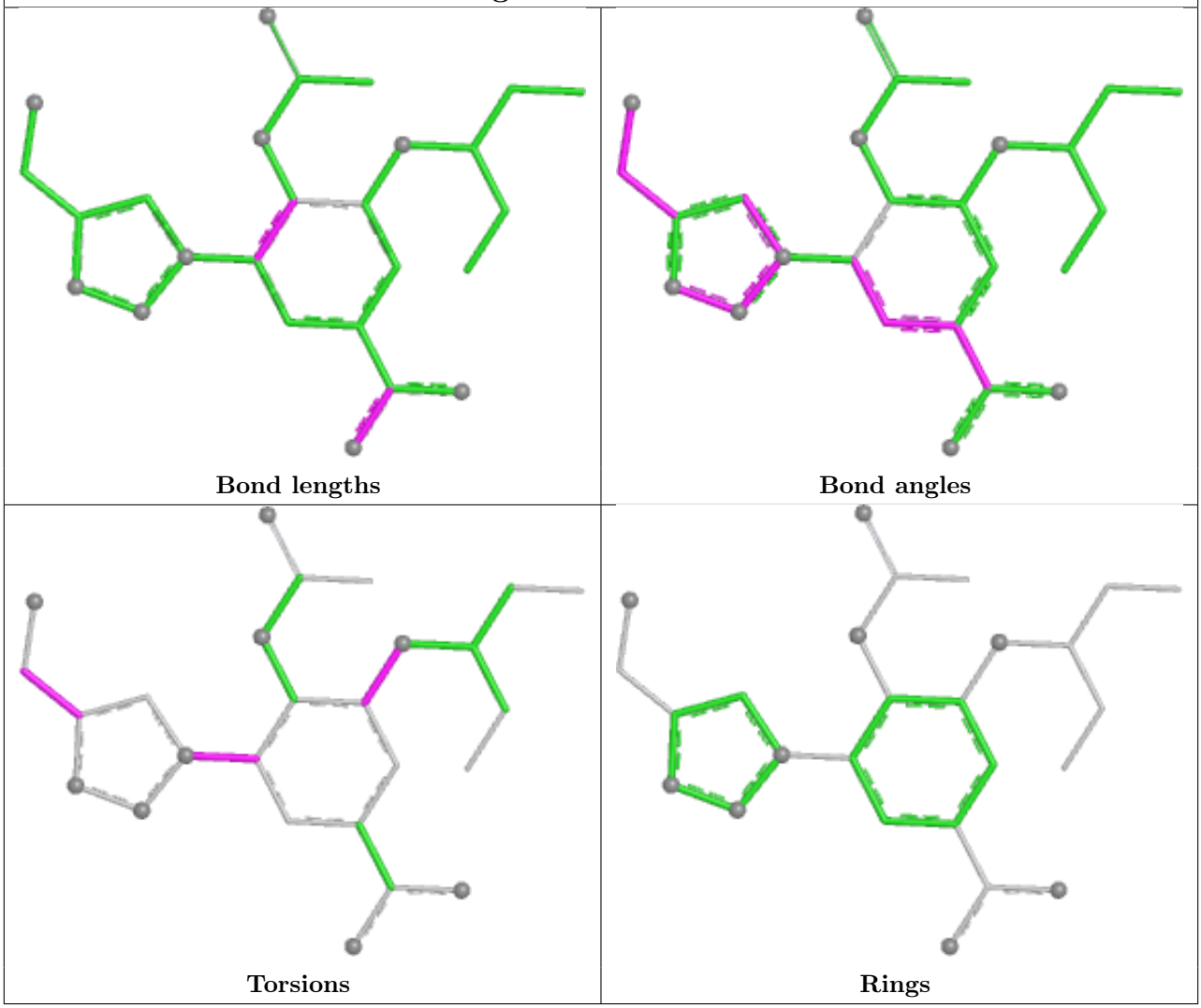


Torsions



Rings

Ligand GJT A 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%)	-0.02	7 (1%)	67	73	11, 20, 32, 60	5 (1%)
1	B	387/388 (99%)	0.11	9 (2%)	61	67	10, 21, 34, 80	4 (1%)
1	C	387/388 (99%)	-0.02	6 (1%)	70	75	11, 20, 32, 63	6 (1%)
1	D	387/388 (99%)	0.17	7 (1%)	67	73	11, 21, 34, 63	6 (1%)
All	All	1548/1552 (99%)	0.06	29 (1%)	66	72	10, 21, 33, 80	21 (1%)

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	149	ILE	7.9
1	D	149	ILE	7.3
1	B	148	THR	6.5
1	D	148	THR	5.5
1	C	149	ILE	5.5
1	A	149	ILE	5.3
1	B	147	GLY	4.1
1	C	427	ILE	3.5
1	A	148	THR	3.4
1	A	147	GLY	3.1
1	B	150	LYS	3.0
1	D	93	PRO	2.9
1	C	151	ASP	2.8
1	B	93	PRO	2.7
1	A	449	ASN	2.7
1	C	148	THR	2.5
1	A	93	PRO	2.5
1	B	151	ASP	2.4
1	A	120	PRO	2.4
1	B	120	PRO	2.4
1	D	147	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	120	PRO	2.3
1	D	150	LYS	2.3
1	D	163	ILE	2.2
1	A	151	ASP	2.2
1	C	449	ASN	2.2
1	B	118	ARG	2.1
1	B	387	PHE	2.0
1	D	216	ILE	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)

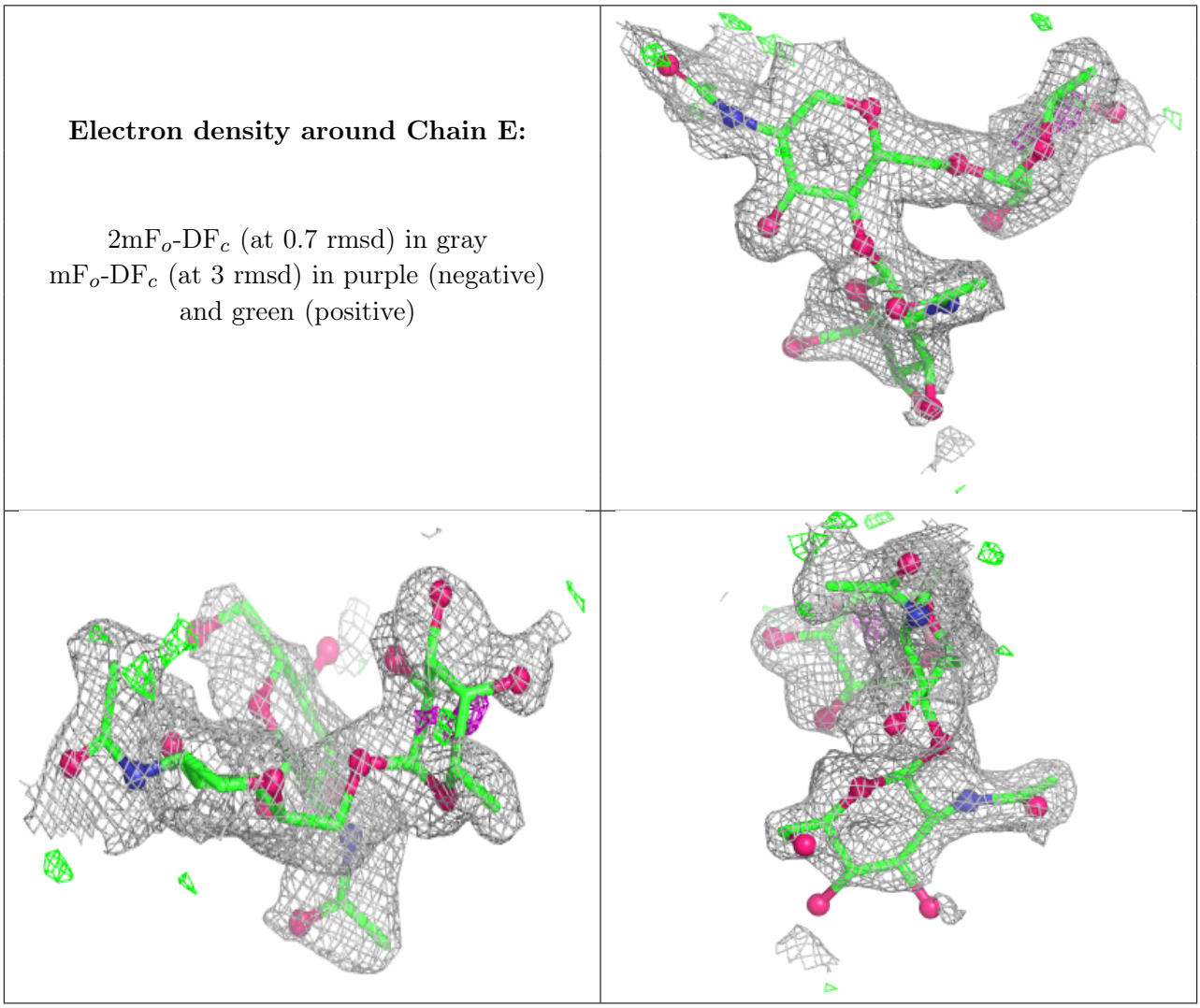
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	J	1	14/15	0.65	0.16	47,57,66,67	0
3	FUC	F	2	10/11	0.68	0.20	49,58,62,65	0
2	NAG	H	2	14/15	0.72	0.16	56,68,80,82	0
2	FUC	G	3	10/11	0.74	0.15	49,54,58,59	0
2	NAG	E	2	14/15	0.74	0.14	54,61,68,74	0
3	NAG	F	1	14/15	0.76	0.15	42,50,57,65	0
2	FUC	E	3	10/11	0.76	0.15	50,55,58,61	0
2	FUC	H	3	10/11	0.76	0.16	46,54,57,60	0
2	NAG	E	1	14/15	0.77	0.12	38,45,52,52	0
2	NAG	H	1	14/15	0.78	0.14	44,51,65,69	0
2	NAG	G	1	14/15	0.78	0.13	45,57,63,65	0
2	NAG	G	2	14/15	0.79	0.13	56,63,69,72	0
4	FUC	I	6	10/11	0.80	0.15	34,40,49,50	0
4	MAN	I	4	11/12	0.82	0.13	49,54,62,76	0
3	FUC	J	2	10/11	0.82	0.14	45,49,52,52	0
4	BMA	I	3	11/12	0.89	0.10	30,35,40,43	0
4	MAN	I	5	11/12	0.92	0.09	29,33,37,37	0
4	NAG	I	2	14/15	0.92	0.08	26,29,32,34	0
4	NAG	I	1	14/15	0.94	0.08	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.

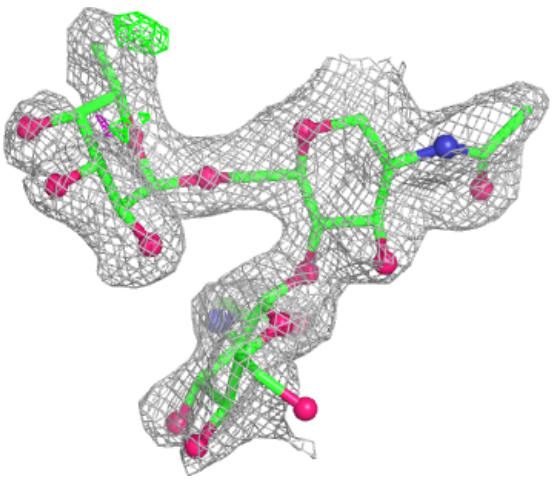
Electron density around Chain E:

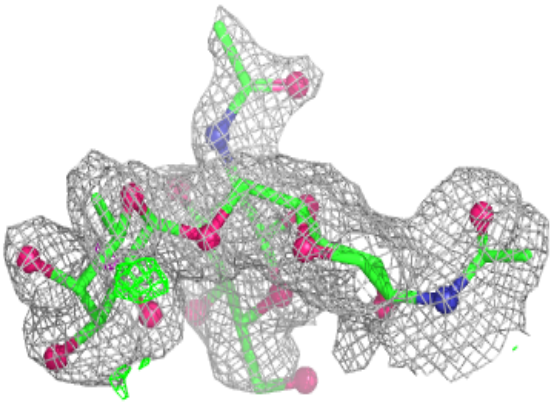
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

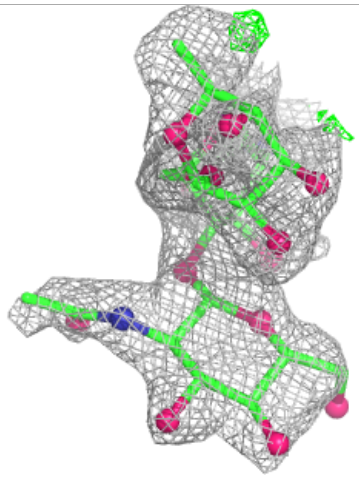


Electron density around Chain G:

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

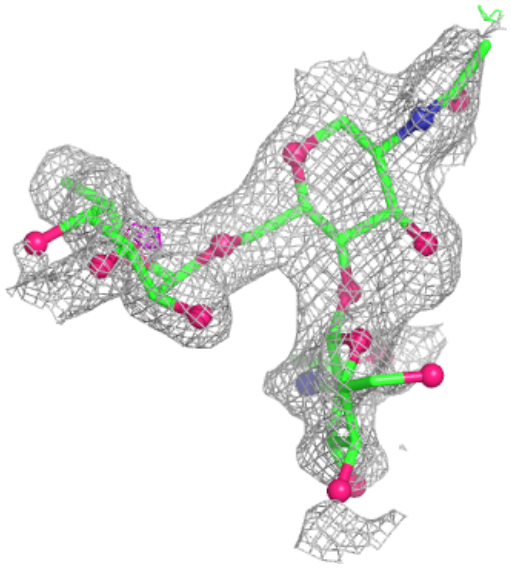


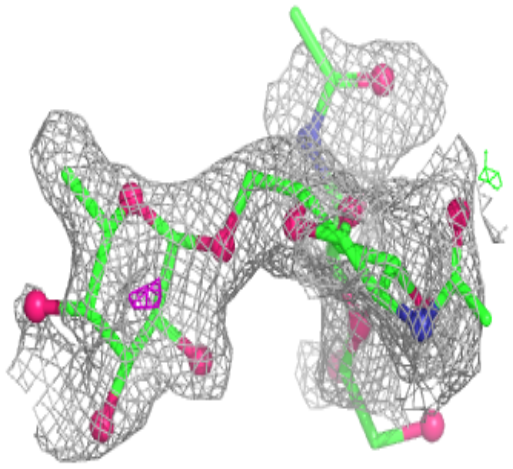


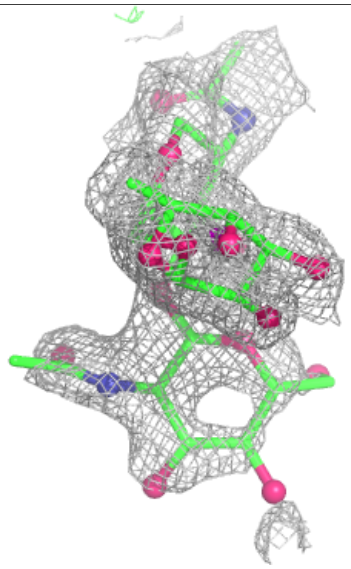


Electron density around Chain H:

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

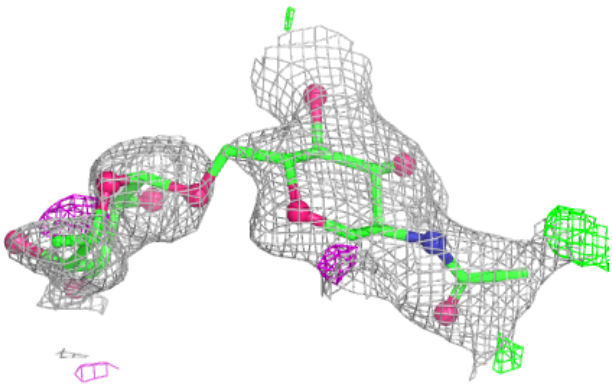


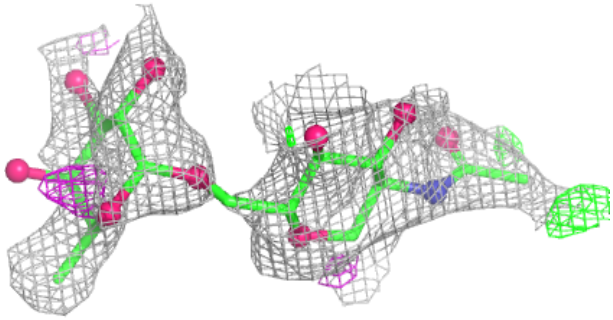


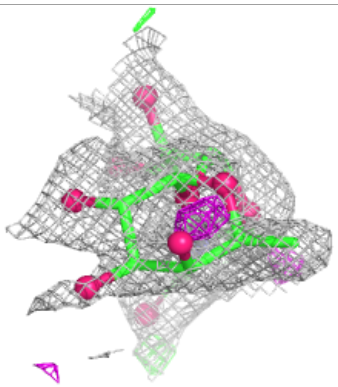


Electron density around Chain F:

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

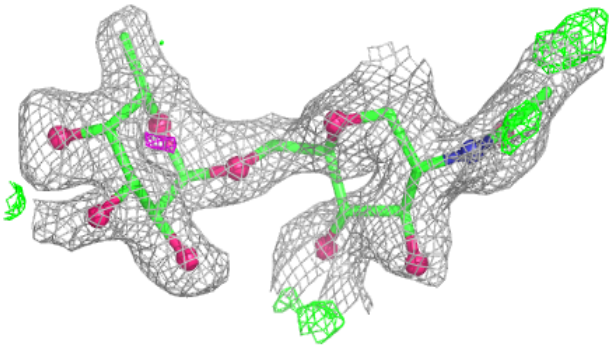


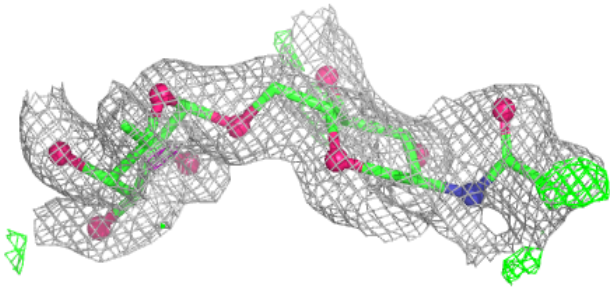


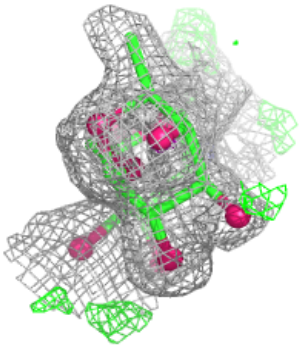


Electron density around Chain J:

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

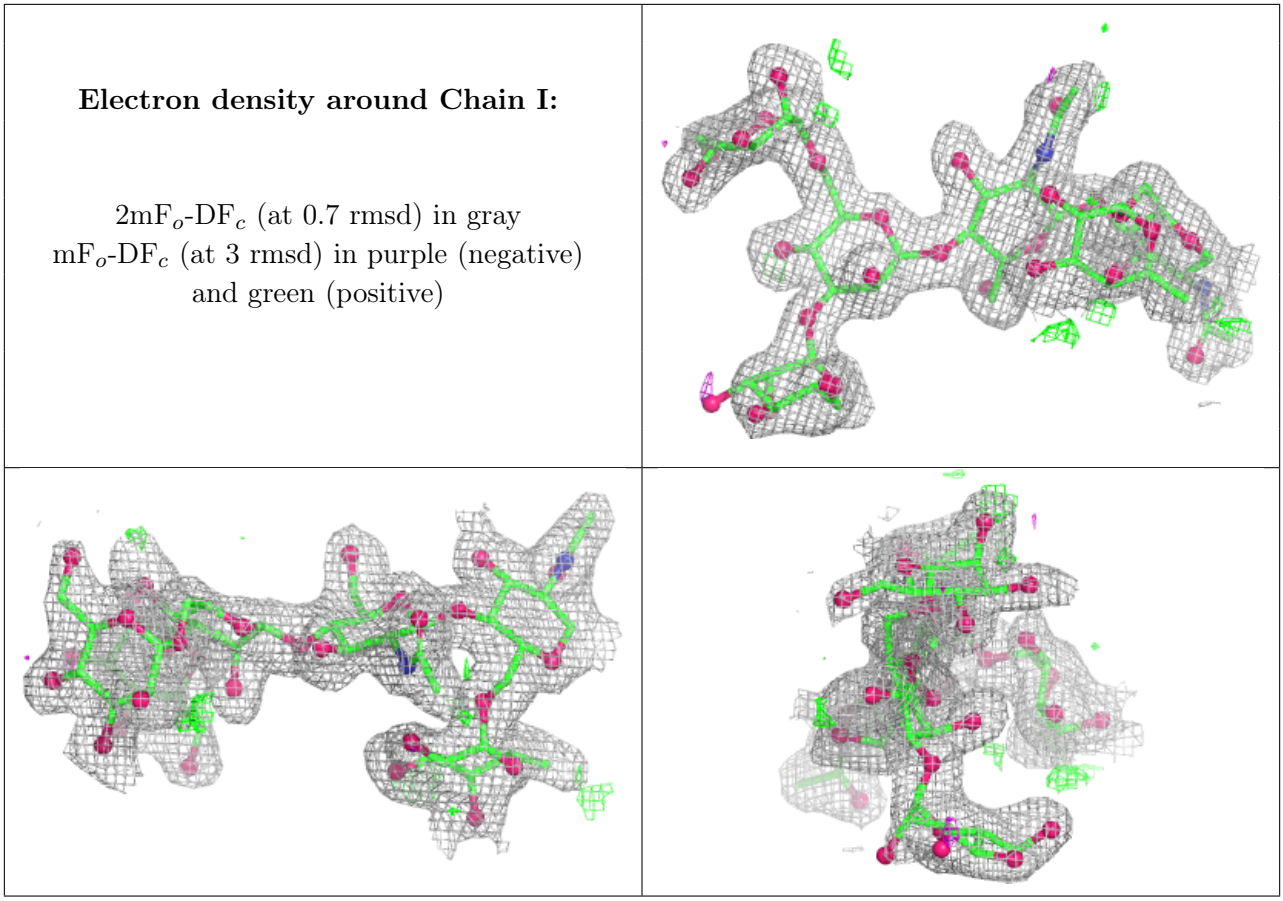






Electron density around Chain I:

$2mF_o$-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	0.60	0.22	45,49,51,51	0
7	NAG	B	508	14/15	0.61	0.17	42,52,60,69	0
7	NAG	D	506	14/15	0.63	0.19	56,63,71,74	0
8	EDO	B	511	4/4	0.67	0.21	52,53,53,59	0
8	EDO	D	513	4/4	0.68	0.17	45,46,46,47	0
7	NAG	D	507	14/15	0.72	0.15	48,54,60,63	0
7	NAG	A	509	14/15	0.72	0.15	46,50,53,55	0
8	EDO	A	521	4/4	0.74	0.18	42,47,48,48	0
8	EDO	B	513	4/4	0.74	0.16	48,49,53,55	0
8	EDO	A	523	4/4	0.74	0.22	48,48,52,53	0
8	EDO	A	518	4/4	0.75	0.16	34,39,39,42	0
9	PGE	D	514	7/10	0.75	0.15	40,41,45,46	0
8	EDO	A	519	4/4	0.76	0.19	40,40,41,48	0

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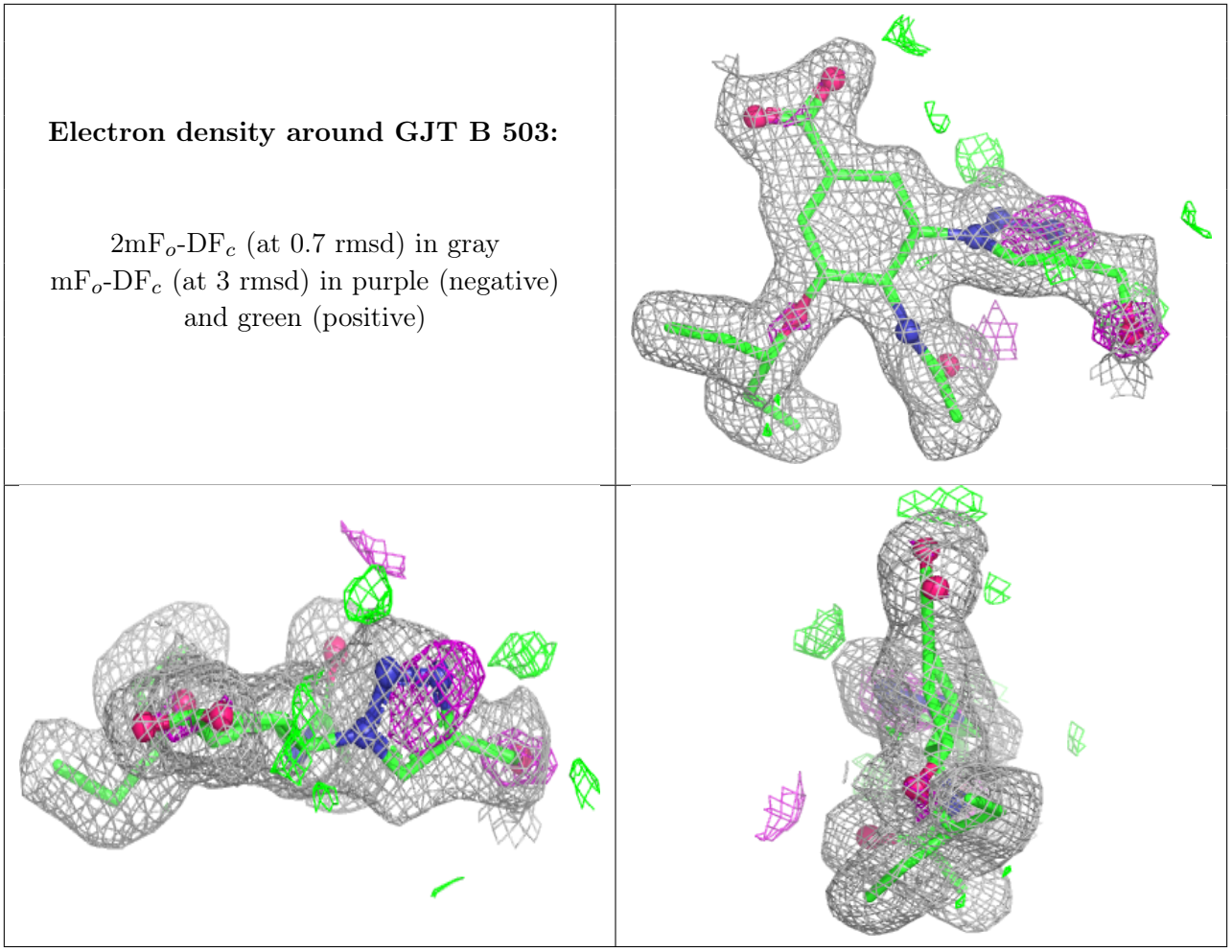
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	NAG	B	507	14/15	0.76	0.16	51,57,63,65	0
8	EDO	A	522	4/4	0.76	0.16	47,51,52,54	0
8	EDO	A	511	4/4	0.76	0.20	38,43,45,46	0
8	EDO	D	512	4/4	0.77	0.16	51,53,55,59	0
8	EDO	A	512	4/4	0.77	0.20	47,53,59,60	0
8	EDO	D	508	4/4	0.77	0.21	44,46,47,54	0
8	EDO	B	512	4/4	0.78	0.19	51,52,52,60	0
7	NAG	C	513	14/15	0.78	0.13	45,51,55,57	0
8	EDO	B	509	4/4	0.80	0.16	47,52,52,54	0
8	EDO	C	515[A]	4/4	0.82	0.20	30,33,35,37	4
8	EDO	C	515[B]	4/4	0.82	0.20	23,29,32,33	4
8	EDO	A	510	4/4	0.84	0.15	42,49,51,53	0
8	EDO	B	514	4/4	0.84	0.16	45,46,46,51	0
8	EDO	A	516	4/4	0.84	0.16	34,38,41,43	0
8	EDO	A	520	4/4	0.84	0.16	43,47,48,50	0
8	EDO	A	517	4/4	0.85	0.17	38,44,44,52	0
8	EDO	C	516	4/4	0.86	0.14	32,40,44,50	0
8	EDO	C	514	4/4	0.86	0.15	40,41,43,46	0
8	EDO	D	509	4/4	0.86	0.13	32,35,38,38	0
8	EDO	B	510	4/4	0.87	0.15	31,37,42,43	0
8	EDO	A	515	4/4	0.87	0.14	39,39,40,41	0
8	EDO	D	510	4/4	0.88	0.15	32,35,36,43	0
8	EDO	A	513	4/4	0.88	0.13	30,31,39,44	0
6	GJT	B	503	26/26	0.91	0.09	14,17,22,27	0
8	EDO	D	511	4/4	0.92	0.14	29,32,33,34	0
6	GJT	D	503	26/26	0.92	0.08	13,16,19,20	0
6	GJT	A	503	26/26	0.93	0.08	12,15,20,24	0
6	GJT	C	503	26/26	0.93	0.07	14,15,19,24	0
5	CA	B	502	1/1	0.96	0.11	42,42,42,42	0
5	CA	D	502	1/1	0.97	0.17	41,41,41,41	0
5	CA	A	502	1/1	0.97	0.10	34,34,34,34	0
5	CA	B	501	1/1	0.99	0.02	22,22,22,22	0
5	CA	C	502	1/1	0.99	0.09	35,35,35,35	0
5	CA	D	501	1/1	0.99	0.02	20,20,20,20	0
5	CA	A	501	1/1	1.00	0.02	17,17,17,17	0
5	CA	C	501	1/1	1.00	0.02	19,19,19,19	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.

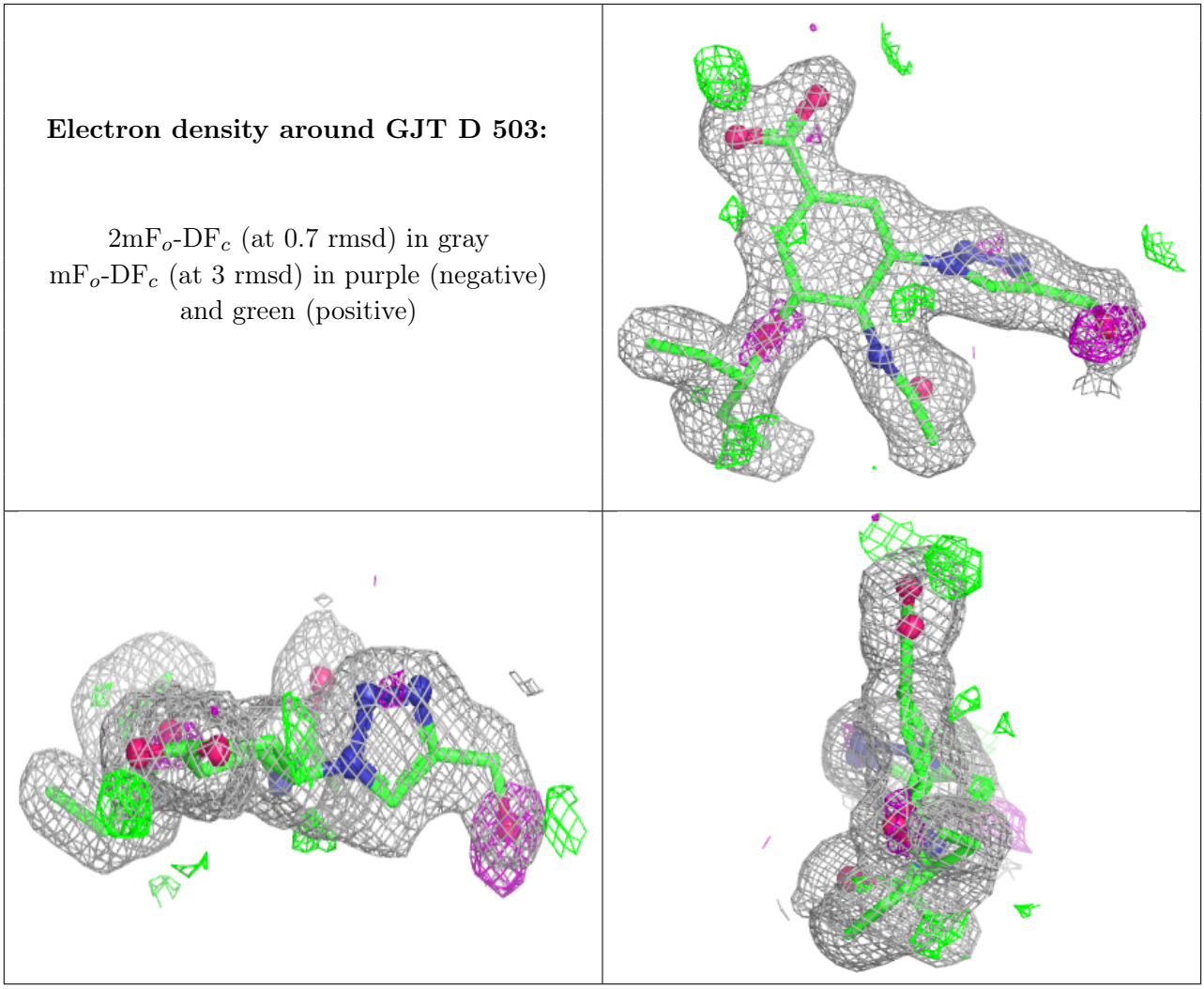
Electron density around GJT B 503:

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



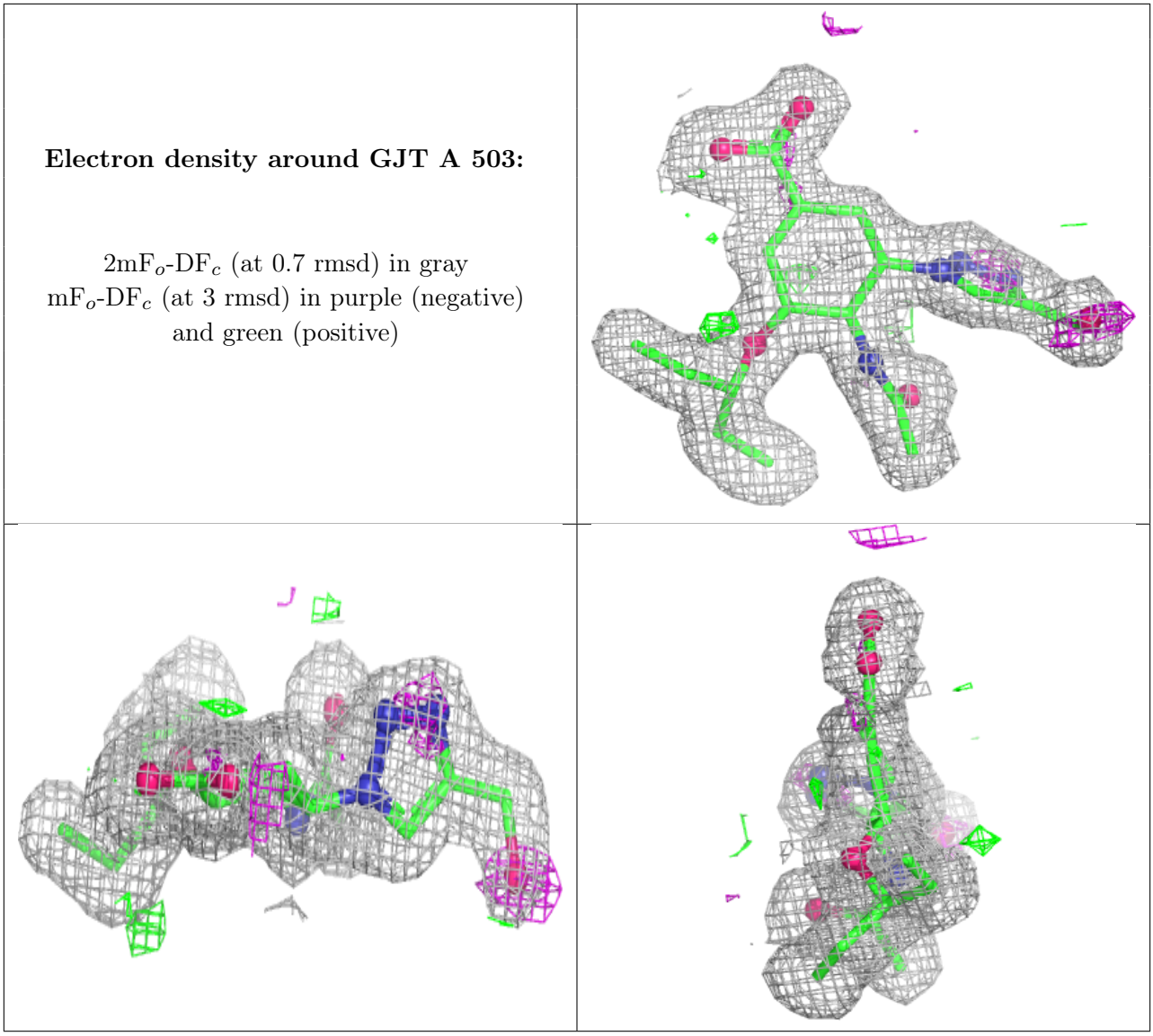
Electron density around GJT D 503:

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



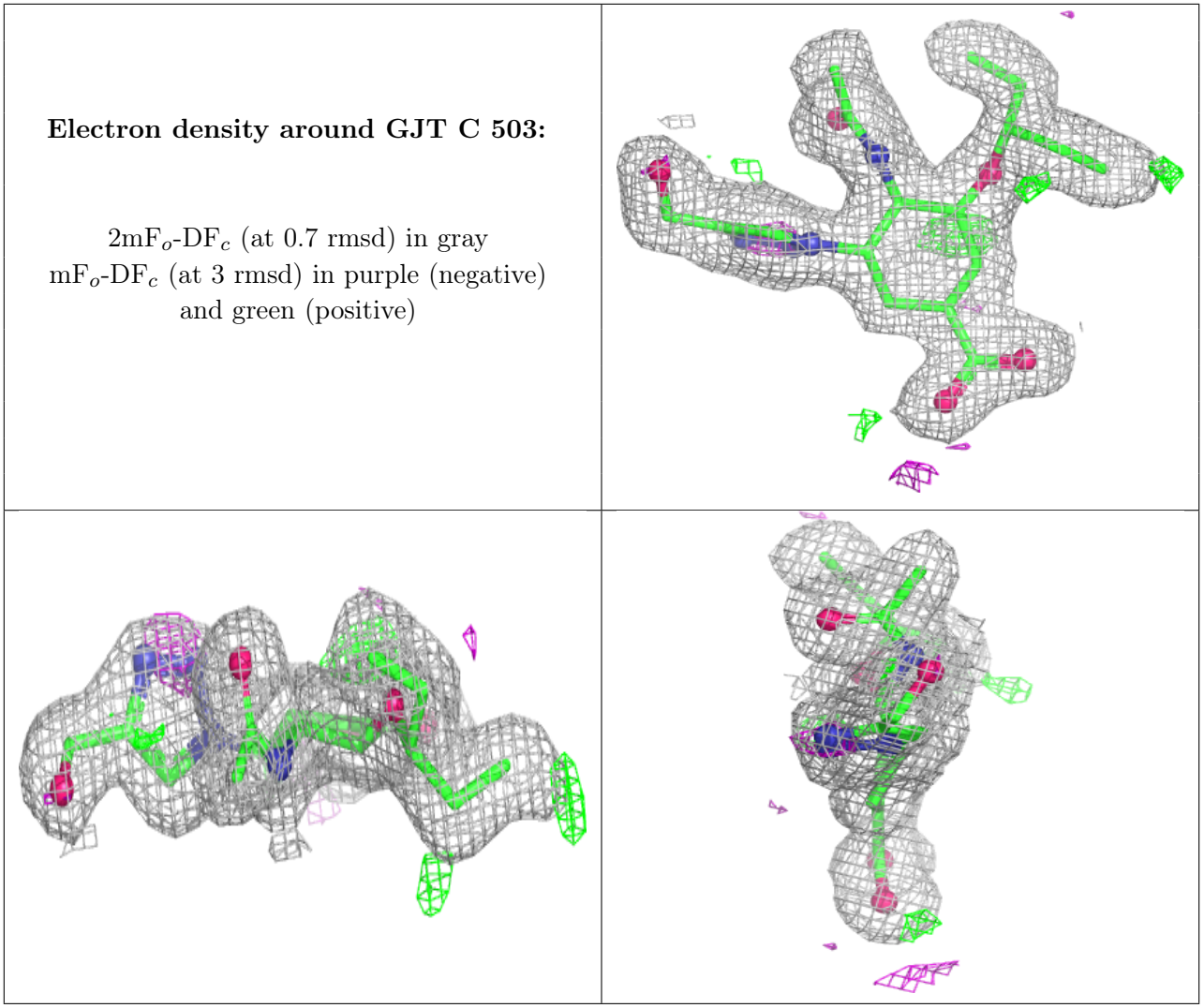
Electron density around GJT A 503:

$2mF_o$-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.