



wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 15, 2024 – 10:21 AM EST

PDB ID : 3G0B
Title : Crystal structure of dipeptidyl peptidase IV in complex with TAK-322
Authors : Zhang, Z.; Wallace, M.B.; Feng, J.; Stafford, J.A.; Kaldor, S.W.; Shi, L.; Skene, R.J.; Aertgeerts, K.; Lee, B.; Jennings, A.; Xu, R.; Kassel, D.; Webb, D.R.; Gwaltney, S.L.
Deposited on : 2009-01-27
Resolution : 2.25 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

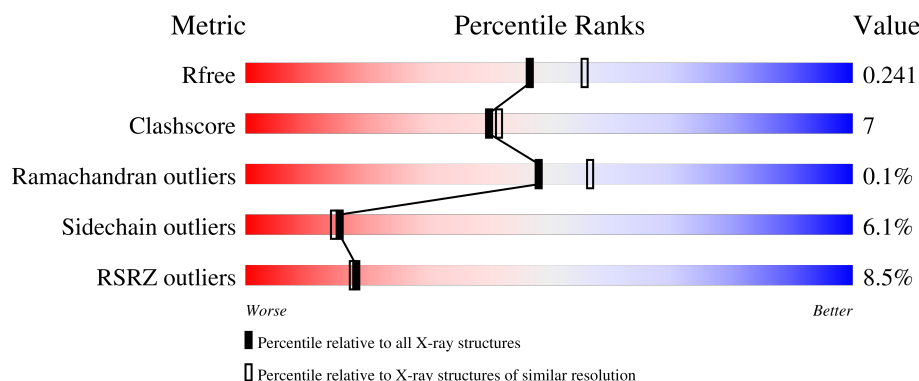
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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}	164625	1763 (2.26-2.26)
Clashscore	180529	1919 (2.26-2.26)
Ramachandran outliers	177936	1884 (2.26-2.26)
Sidechain outliers	177891	1885 (2.26-2.26)
RSRZ outliers	164620	1763 (2.26-2.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	740	<div> <div>5%</div> <div>79%</div> <div>17%</div> <div>• •</div> </div>
1	B	740	<div> <div>4%</div> <div>81%</div> <div>16%</div> <div>• •</div> </div>
1	C	740	<div> <div>19%</div> <div>79%</div> <div>17%</div> <div>• •</div> </div>
1	D	740	<div> <div>5%</div> <div>80%</div> <div>16%</div> <div>• •</div> </div>
2	E	2	<div> <div>100%</div> </div>

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Mol	Chain	Length	Quality of chain
2	F	2	 50%50%
2	G	2	 50%50%
2	H	2	 100%
2	I	2	 100%
2	J	2	 50%50%
2	K	2	 100%
2	L	2	 50%50%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	D	804	X	-	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 24992 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 Dipeptidyl peptidase 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	727	Total	C	N	O	S	0	0	0
			5957	3824	981	1126	26			
1	B	733	Total	C	N	O	S	0	0	0
			6013	3857	997	1133	26			
1	C	726	Total	C	N	O	S	0	0	0
			5946	3818	977	1125	26			
1	D	727	Total	C	N	O	S	0	0	0
			5957	3824	981	1126	26			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	27	ALA	-	expression tag	UNP P27487
A	28	ASP	-	expression tag	UNP P27487
A	29	PRO	-	expression tag	UNP P27487
A	30	GLY	-	expression tag	UNP P27487
A	31	GLY	-	expression tag	UNP P27487
A	32	SER	-	expression tag	UNP P27487
A	33	HIS	-	expression tag	UNP P27487
A	34	HIS	-	expression tag	UNP P27487
A	35	HIS	-	expression tag	UNP P27487
A	36	HIS	-	expression tag	UNP P27487
A	37	HIS	-	expression tag	UNP P27487
A	38	HIS	-	expression tag	UNP P27487
B	27	ALA	-	expression tag	UNP P27487
B	28	ASP	-	expression tag	UNP P27487
B	29	PRO	-	expression tag	UNP P27487
B	30	GLY	-	expression tag	UNP P27487
B	31	GLY	-	expression tag	UNP P27487
B	32	SER	-	expression tag	UNP P27487
B	33	HIS	-	expression tag	UNP P27487
B	34	HIS	-	expression tag	UNP P27487
B	35	HIS	-	expression tag	UNP P27487

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Chain	Residue	Modelled	Actual	Comment	Reference
B	36	HIS	-	expression tag	UNP P27487
B	37	HIS	-	expression tag	UNP P27487
B	38	HIS	-	expression tag	UNP P27487
C	27	ALA	-	expression tag	UNP P27487
C	28	ASP	-	expression tag	UNP P27487
C	29	PRO	-	expression tag	UNP P27487
C	30	GLY	-	expression tag	UNP P27487
C	31	GLY	-	expression tag	UNP P27487
C	32	SER	-	expression tag	UNP P27487
C	33	HIS	-	expression tag	UNP P27487
C	34	HIS	-	expression tag	UNP P27487
C	35	HIS	-	expression tag	UNP P27487
C	36	HIS	-	expression tag	UNP P27487
C	37	HIS	-	expression tag	UNP P27487
C	38	HIS	-	expression tag	UNP P27487
D	27	ALA	-	expression tag	UNP P27487
D	28	ASP	-	expression tag	UNP P27487
D	29	PRO	-	expression tag	UNP P27487
D	30	GLY	-	expression tag	UNP P27487
D	31	GLY	-	expression tag	UNP P27487
D	32	SER	-	expression tag	UNP P27487
D	33	HIS	-	expression tag	UNP P27487
D	34	HIS	-	expression tag	UNP P27487
D	35	HIS	-	expression tag	UNP P27487
D	36	HIS	-	expression tag	UNP P27487
D	37	HIS	-	expression tag	UNP P27487
D	38	HIS	-	expression tag	UNP P27487

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



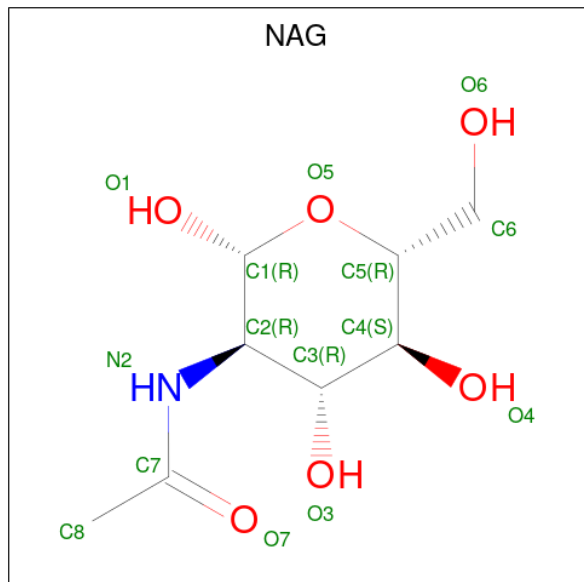
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	G	2	Total	C	N	O	0	0	0
			28	16	2	10			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	K	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	L	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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[illegible]

- ## T22
-
- The chemical structure of T22 is a complex molecule featuring a central pyridine ring (N15) substituted with three distinct groups:
- A 4-aminocyclohexyl group attached at the 2-position (C6) via the nitrogen atom (N7). The cyclohexane ring consists of carbons C8, C9, C10, C11(R), C14, and C16. An amino group (N13, H₂N) is attached to C11(R) with a dashed bond.
 - A 2-cyano-1-phenylethyl group attached at the 3-position (C16) via the carbon atom (C17). The ethyl chain consists of C16 and C22, with a nitrile group (N24) attached to C22. A phenyl ring is attached to C17, consisting of carbons C18, C19, C20, and C21.
 - A 2-oxo-1-methylpropyl group attached at the 4-position (C3) via the nitrogen atom (N2). The propyl chain consists of C3, C5, and C6, with a carbonyl group (O4) attached to C3 and a methyl group (C1) attached to N2. An additional oxygen atom (O26) is shown double-bonded to C6.
- The pyridine ring (N15) also has a carbon atom (C25) at the 5-position, which is part of a carbonyl group (O26) and is connected to the 2-position (C6).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			25	18	5	2		
4	B	1	Total	C	N	O	0	0
			25	18	5	2		
4	C	1	Total	C	N	O	0	0
			25	18	5	2		
4	D	1	Total	C	N	O	0	0
			25	18	5	2		

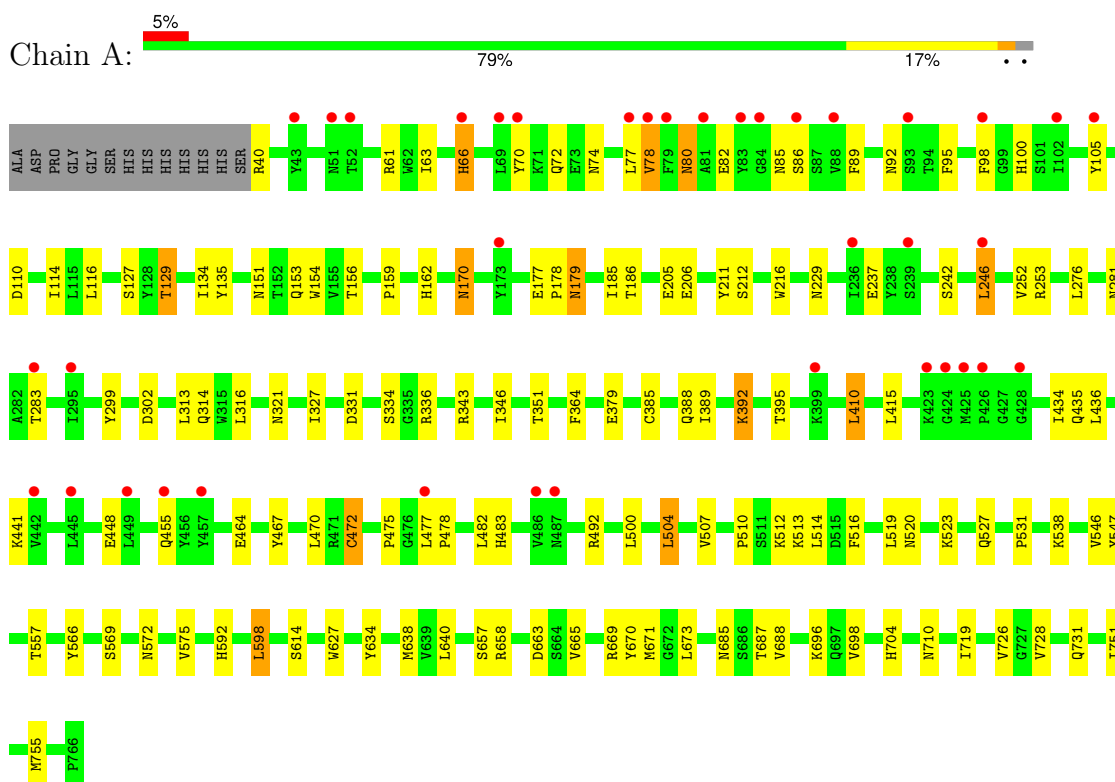
- Molecule 5 is water.

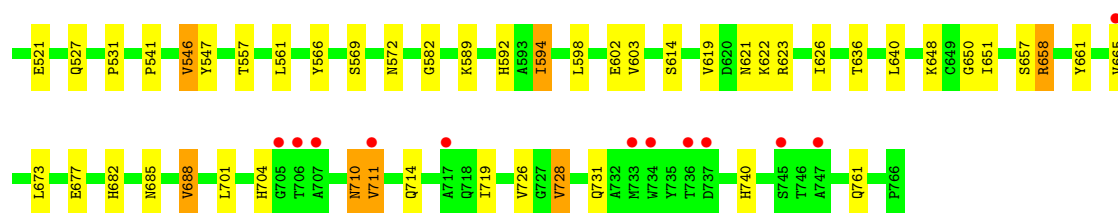
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	166	Total	O	0	0
			166	166		
5	B	166	Total	O	0	0
			166	166		
5	C	80	Total	O	0	0
			80	80		
5	D	145	Total	O	0	0
			145	145		

3 Residue-property plots [i](#)

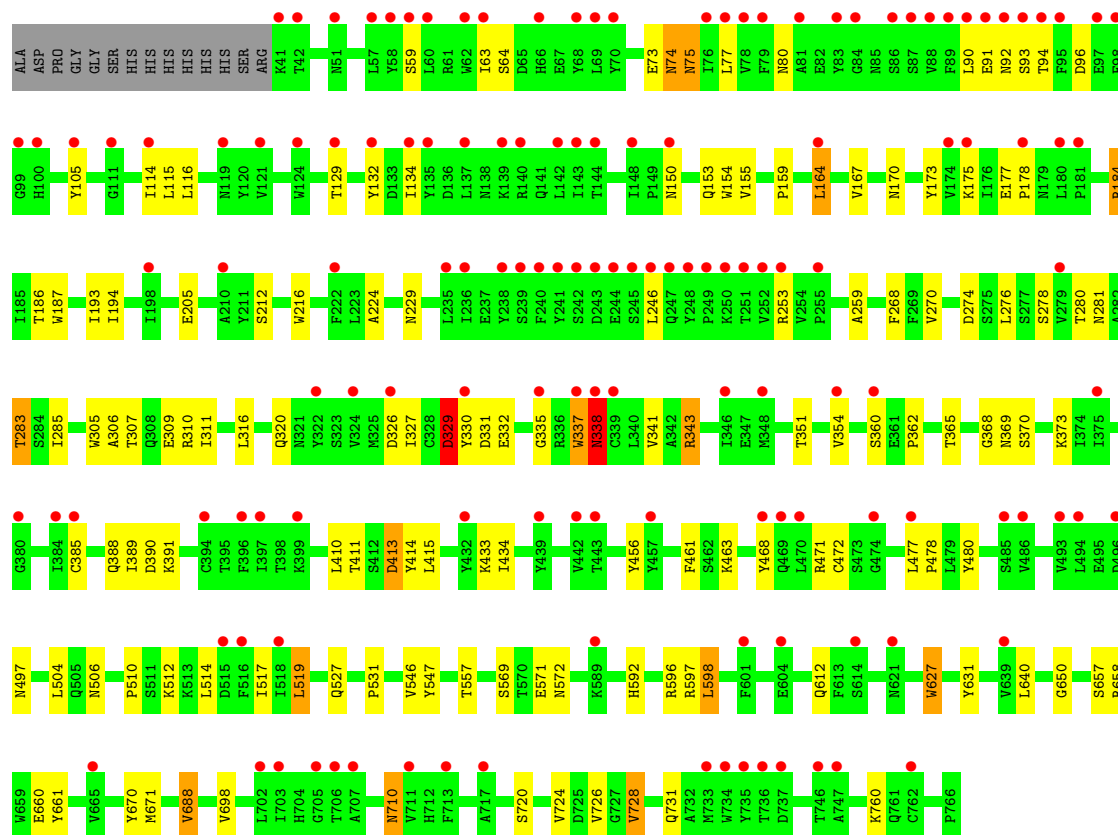
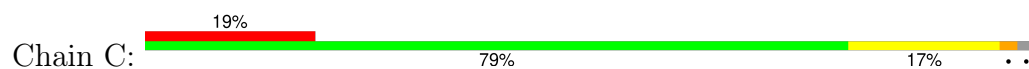
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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: Dipeptidyl peptidase 4

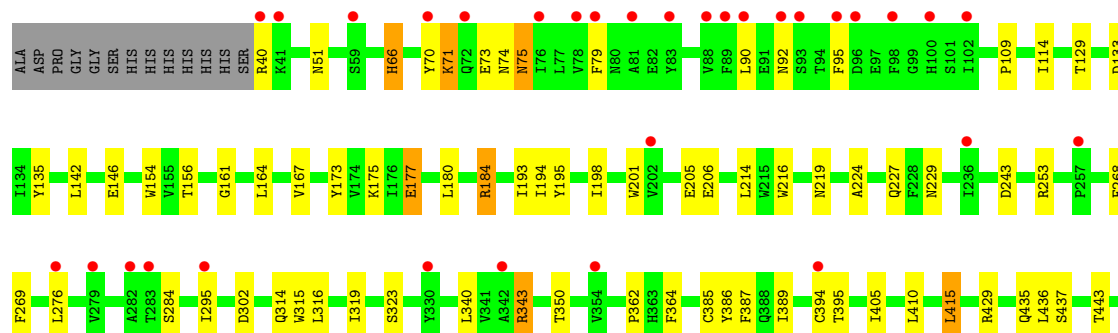
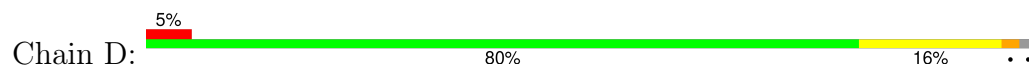


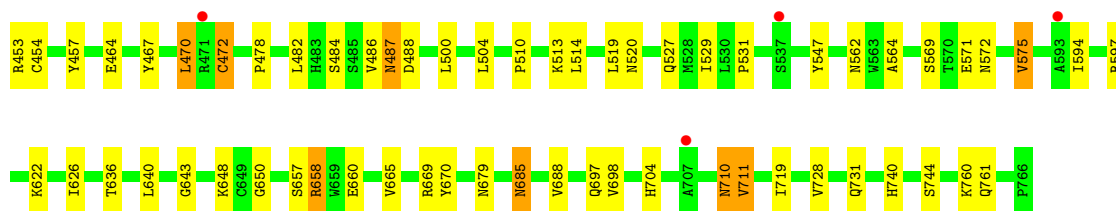


● Molecule 1: Dipeptidyl peptidase 4



● Molecule 1: Dipeptidyl peptidase 4





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

Chain E: 100%



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

Chain F: 50% 50%



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

Chain G: 50% 50%



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

Chain H: 100%



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

Chain I: 100%



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

Chain J: 50% 50%



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

Chain K:  100%



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

Chain L:  50% 50%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	121.69Å 122.40Å 144.01Å 90.00° 114.72° 90.00°	Depositor
Resolution (Å)	35.00 – 2.25 35.00 – 2.25	Depositor EDS
% Data completeness (in resolution range)	97.0 (35.00-2.25) 97.3 (35.00-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.207 , 0.242 0.204 , 0.241	Depositor DCC
R_{free} test set	8843 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	45.1	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 37.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.035 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	24992	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.15% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, T22

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	0.49	0/6129	0.63	0/8336
1	B	0.48	0/6190	0.63	2/8419 (0.0%)
1	C	0.82	23/6118 (0.4%)	0.67	9/8322 (0.1%)
1	D	0.48	0/6129	0.62	1/8336 (0.0%)
All	All	0.59	23/24566 (0.1%)	0.64	12/33413 (0.0%)

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	C	0	1

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	338	ASN	CG-ND2	22.47	1.89	1.32
1	C	329	ASP	CG-OD1	17.61	1.65	1.25
1	C	343	ARG	CZ-NH2	17.20	1.55	1.33
1	C	177	GLU	CD-OE2	13.47	1.40	1.25
1	C	177	GLU	CD-OE1	11.77	1.38	1.25

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	329	ASP	CB-CG-OD1	-19.59	100.67	118.30
1	C	343	ARG	NE-CZ-NH1	-10.23	115.19	120.30
1	C	274	ASP	CB-CG-OD2	-7.27	111.75	118.30
1	C	329	ASP	OD1-CG-OD2	6.81	136.24	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	415	LEU	CA-CB-CG	6.75	130.83	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	338	ASN	Sidechain

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	5957	0	5679	84	0
1	B	6013	0	5720	73	0
1	C	5946	0	5666	84	0
1	D	5957	0	5676	83	0
2	E	28	0	25	0	0
2	F	28	0	25	2	0
2	G	28	0	25	1	0
2	H	28	0	25	3	0
2	I	28	0	25	0	0
2	J	28	0	25	2	0
2	K	28	0	25	2	0
2	L	28	0	25	5	0
3	A	56	0	52	4	0
3	B	56	0	52	5	0
3	C	56	0	52	3	0
3	D	70	0	65	4	0
4	A	25	0	21	1	0
4	B	25	0	21	1	0
4	C	25	0	21	1	0
4	D	25	0	21	1	0
5	A	166	0	0	0	0
5	B	166	0	0	0	0
5	C	80	0	0	0	0
5	D	145	0	0	1	0
All	All	24992	0	23246	312	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 7.

The worst 5 of 312 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:A:229:ASN:HD21	2:F:1:NAG:C1	1.12	1.58
1:C:329:ASP:CG	1:C:329:ASP:OD1	1.65	1.31
1:C:338:ASN:ND2	1:C:338:ASN:CG	1.89	1.26
1:A:229:ASN:ND2	2:F:1:NAG:C1	1.95	1.25
1:D:229:ASN:HD21	2:L:1:NAG:C1	1.69	1.04

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	725/740 (98%)	697 (96%)	28 (4%)	0	100	100
1	B	731/740 (99%)	704 (96%)	26 (4%)	1 (0%)	48	57
1	C	724/740 (98%)	690 (95%)	32 (4%)	2 (0%)	37	41
1	D	725/740 (98%)	692 (95%)	33 (5%)	0	100	100
All	All	2905/2960 (98%)	2783 (96%)	119 (4%)	3 (0%)	48	57

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	714	GLN
1	C	73	GLU
1	C	463	LYS

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	652/662 (98%)	613 (94%)	39 (6%)	16	15
1	B	658/662 (99%)	610 (93%)	48 (7%)	11	10
1	C	651/662 (98%)	617 (95%)	34 (5%)	19	20
1	D	652/662 (98%)	613 (94%)	39 (6%)	16	15
All	All	2613/2648 (99%)	2453 (94%)	160 (6%)	15	14

5 of 160 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	597	ARG
1	D	470	LEU
1	C	710	ASN
1	D	243	ASP
1	D	575	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 67 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	196	ASN
1	D	344	GLN
1	D	710	ASN
1	B	281	ASN
1	B	229	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

16 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	NAG	E	1	2,1	14,14,15	0.53	0	17,19,21	1.84	3 (17%)
2	NAG	E	2	2	14,14,15	0.59	0	17,19,21	1.19	1 (5%)
2	NAG	F	1	2	14,14,15	0.70	0	17,19,21	1.34	1 (5%)
2	NAG	F	2	2	14,14,15	0.44	0	17,19,21	1.55	3 (17%)
2	NAG	G	1	2	14,14,15	0.59	0	17,19,21	1.51	3 (17%)
2	NAG	G	2	2	14,14,15	0.55	0	17,19,21	0.65	0
2	NAG	H	1	2	14,14,15	0.54	0	17,19,21	1.66	4 (23%)
2	NAG	H	2	2	14,14,15	0.66	0	17,19,21	1.18	1 (5%)
2	NAG	I	1	2	14,14,15	0.51	0	17,19,21	0.89	0
2	NAG	I	2	2	14,14,15	0.49	0	17,19,21	0.82	0
2	NAG	J	1	2	14,14,15	0.69	0	17,19,21	1.15	2 (11%)
2	NAG	J	2	2	14,14,15	0.52	0	17,19,21	1.18	3 (17%)
2	NAG	K	1	2	14,14,15	0.60	0	17,19,21	0.94	0
2	NAG	K	2	2	14,14,15	0.52	0	17,19,21	1.63	3 (17%)
2	NAG	L	1	2	14,14,15	0.64	0	17,19,21	1.64	2 (11%)
2	NAG	L	2	2	14,14,15	0.54	0	17,19,21	1.41	3 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	E	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	E	2	2	-	4/6/23/26	0/1/1/1
2	NAG	F	1	2	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	4/6/23/26	0/1/1/1
2	NAG	G	1	2	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	G	2	2	-	4/6/23/26	0/1/1/1
2	NAG	H	1	2	-	2/6/23/26	0/1/1/1
2	NAG	H	2	2	-	3/6/23/26	0/1/1/1
2	NAG	I	1	2	-	4/6/23/26	0/1/1/1
2	NAG	I	2	2	-	4/6/23/26	0/1/1/1
2	NAG	J	1	2	-	0/6/23/26	0/1/1/1
2	NAG	J	2	2	-	4/6/23/26	0/1/1/1
2	NAG	K	1	2	-	0/6/23/26	0/1/1/1
2	NAG	K	2	2	-	2/6/23/26	0/1/1/1
2	NAG	L	1	2	-	2/6/23/26	0/1/1/1
2	NAG	L	2	2	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1	NAG	C1-O5-C5	5.72	119.85	112.19
2	K	2	NAG	C1-O5-C5	4.64	118.41	112.19
2	F	2	NAG	C1-O5-C5	4.64	118.40	112.19
2	L	1	NAG	O5-C1-C2	-4.06	105.01	111.29
2	L	1	NAG	C3-C4-C5	4.06	117.59	110.23

There are no chirality outliers.

5 of 44 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	1	NAG	C8-C7-N2-C2
2	G	1	NAG	O7-C7-N2-C2
2	G	2	NAG	C8-C7-N2-C2
2	G	2	NAG	O7-C7-N2-C2
2	H	2	NAG	C3-C2-N2-C7

There are no ring outliers.

7 monomers are involved in 15 short contacts:

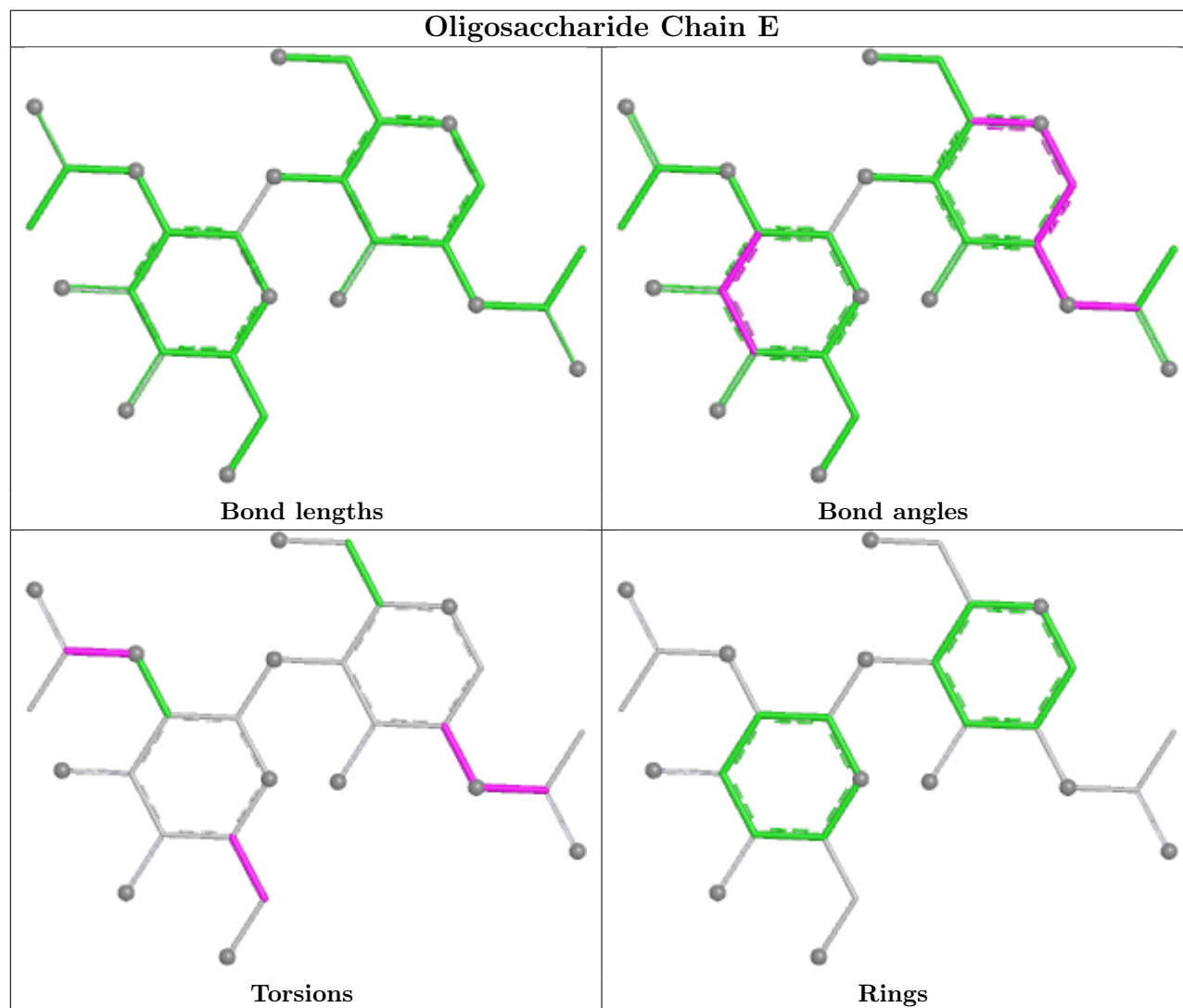
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	1	NAG	1	0
2	F	1	NAG	2	0
2	H	2	NAG	1	0

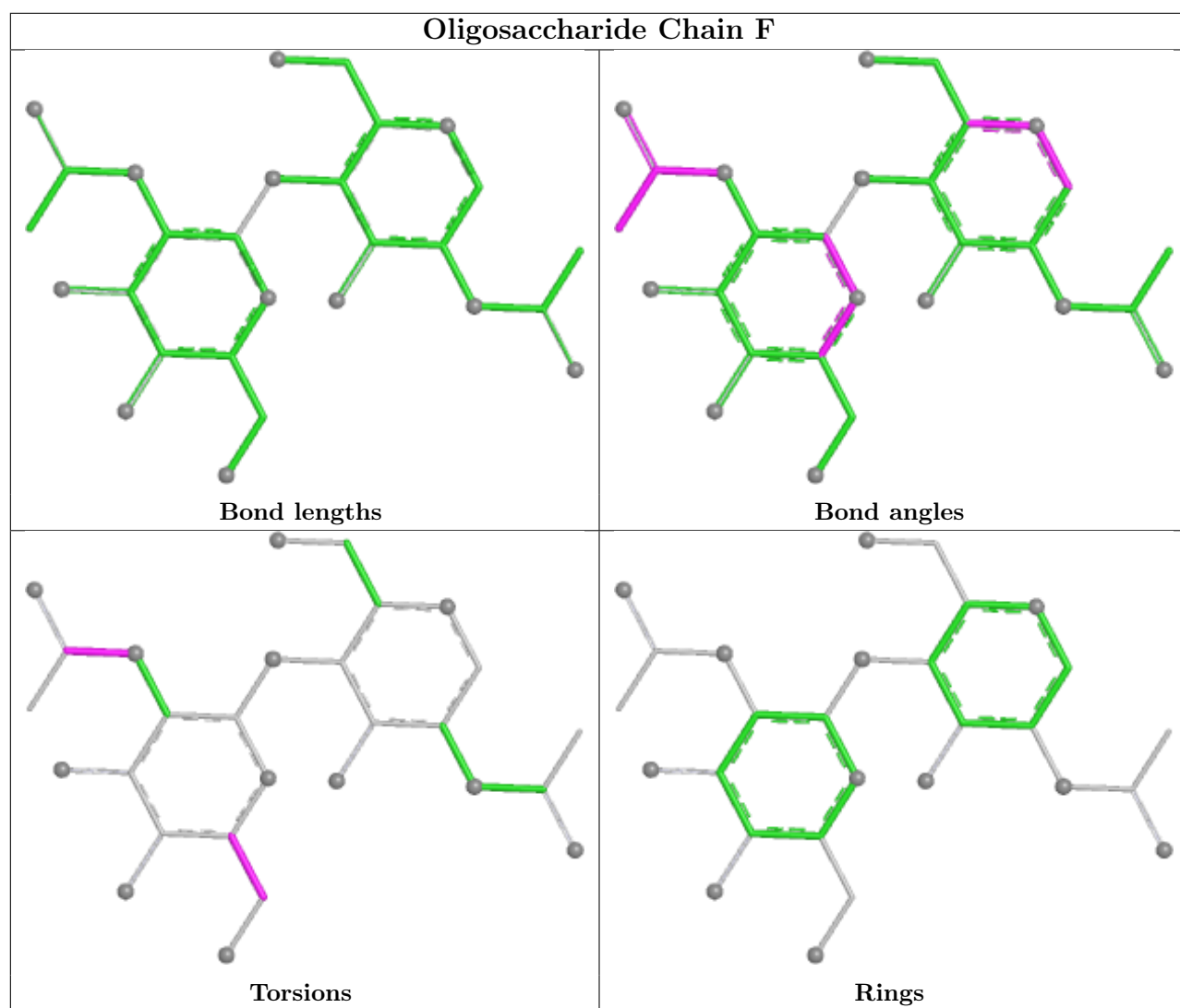
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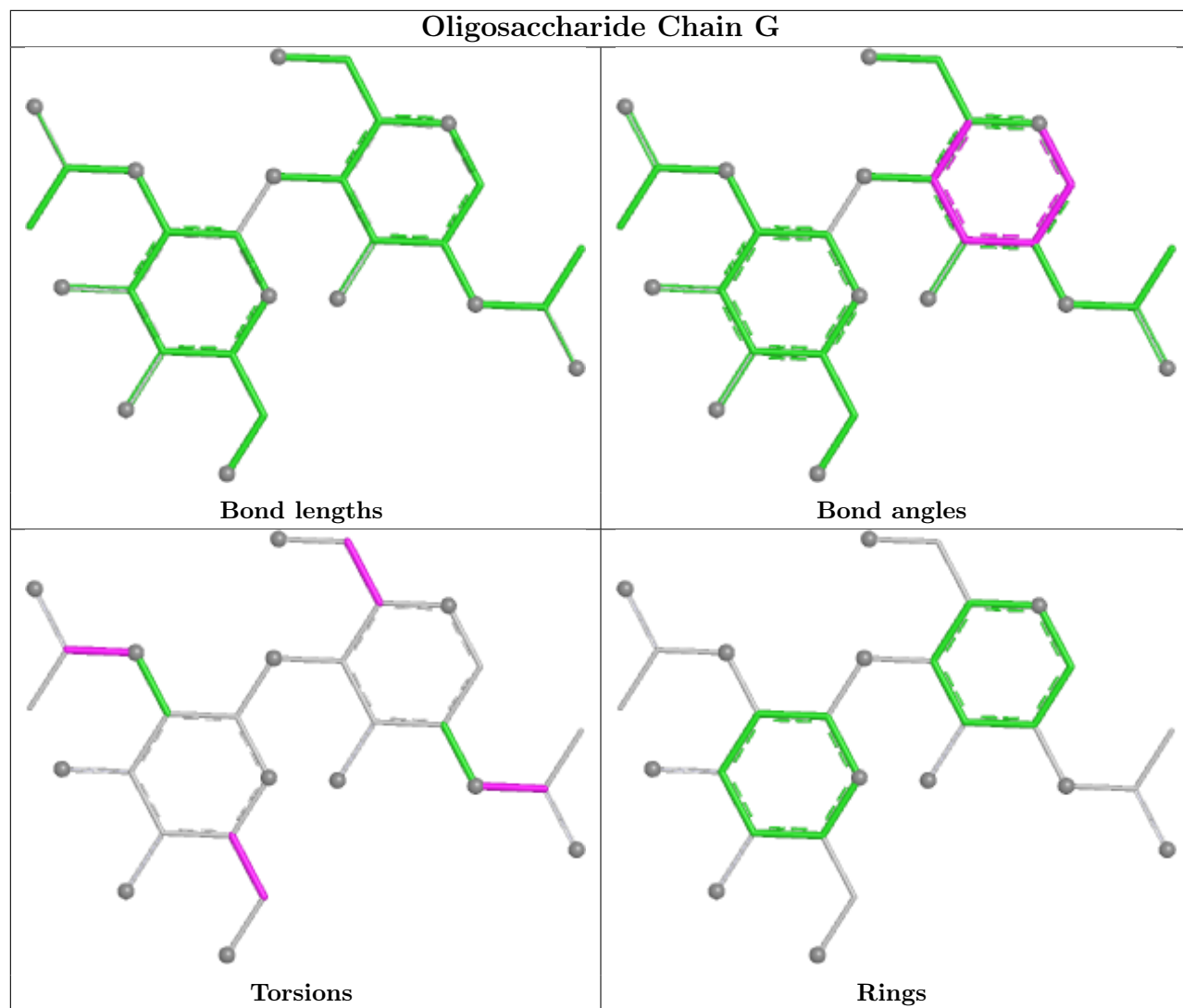
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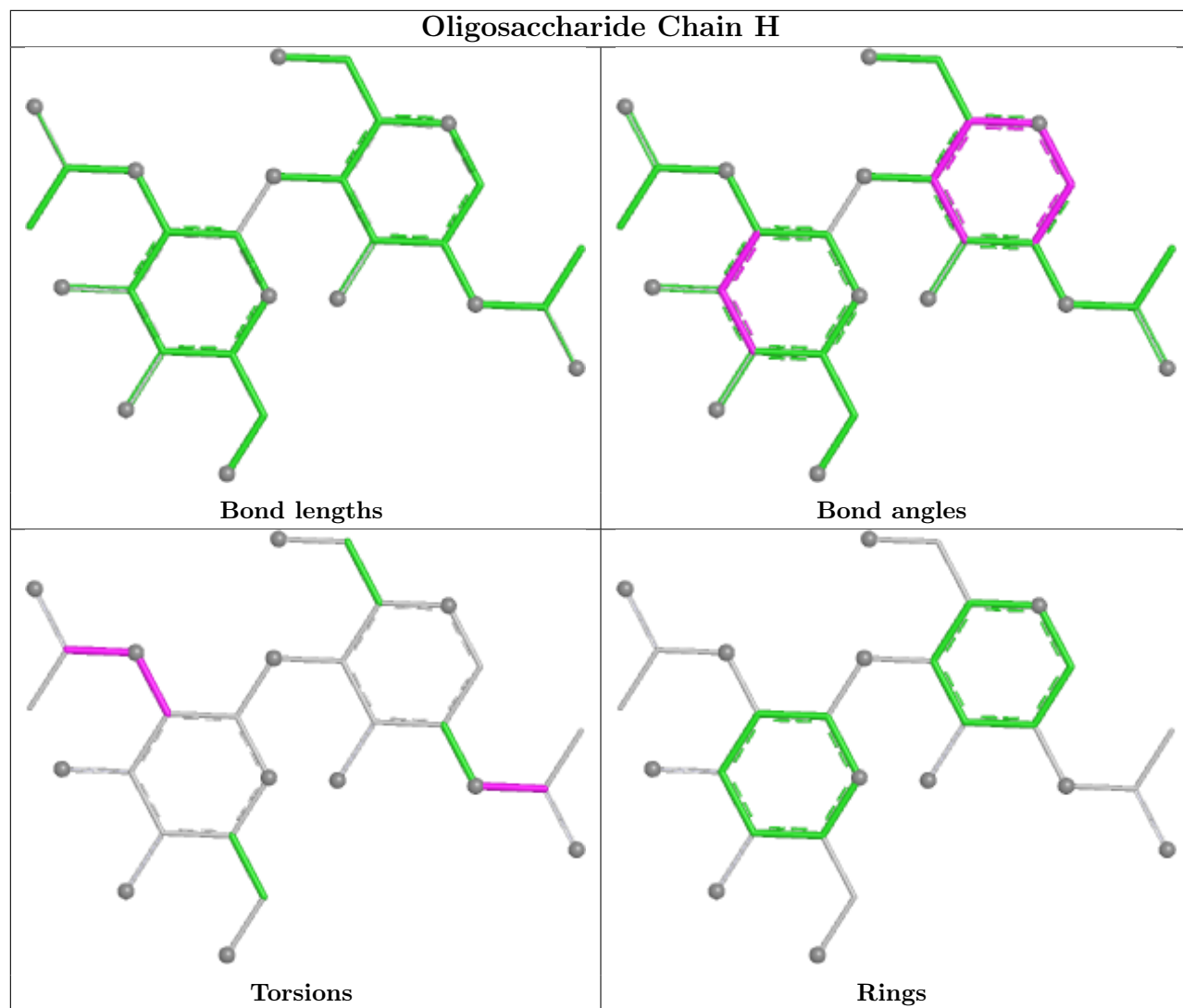
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	1	NAG	3	0
2	K	1	NAG	2	0
2	L	1	NAG	5	0
2	J	1	NAG	2	0

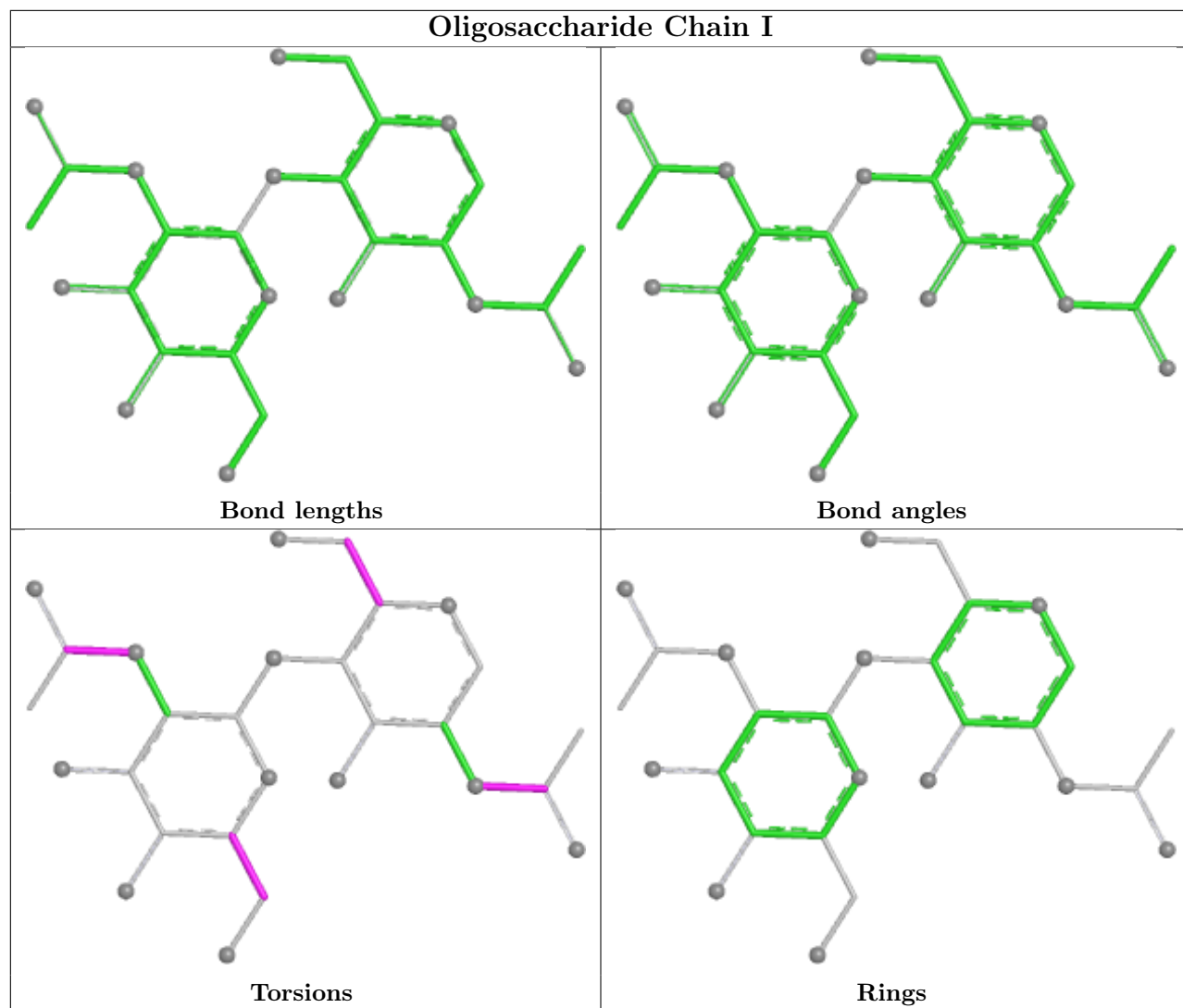
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

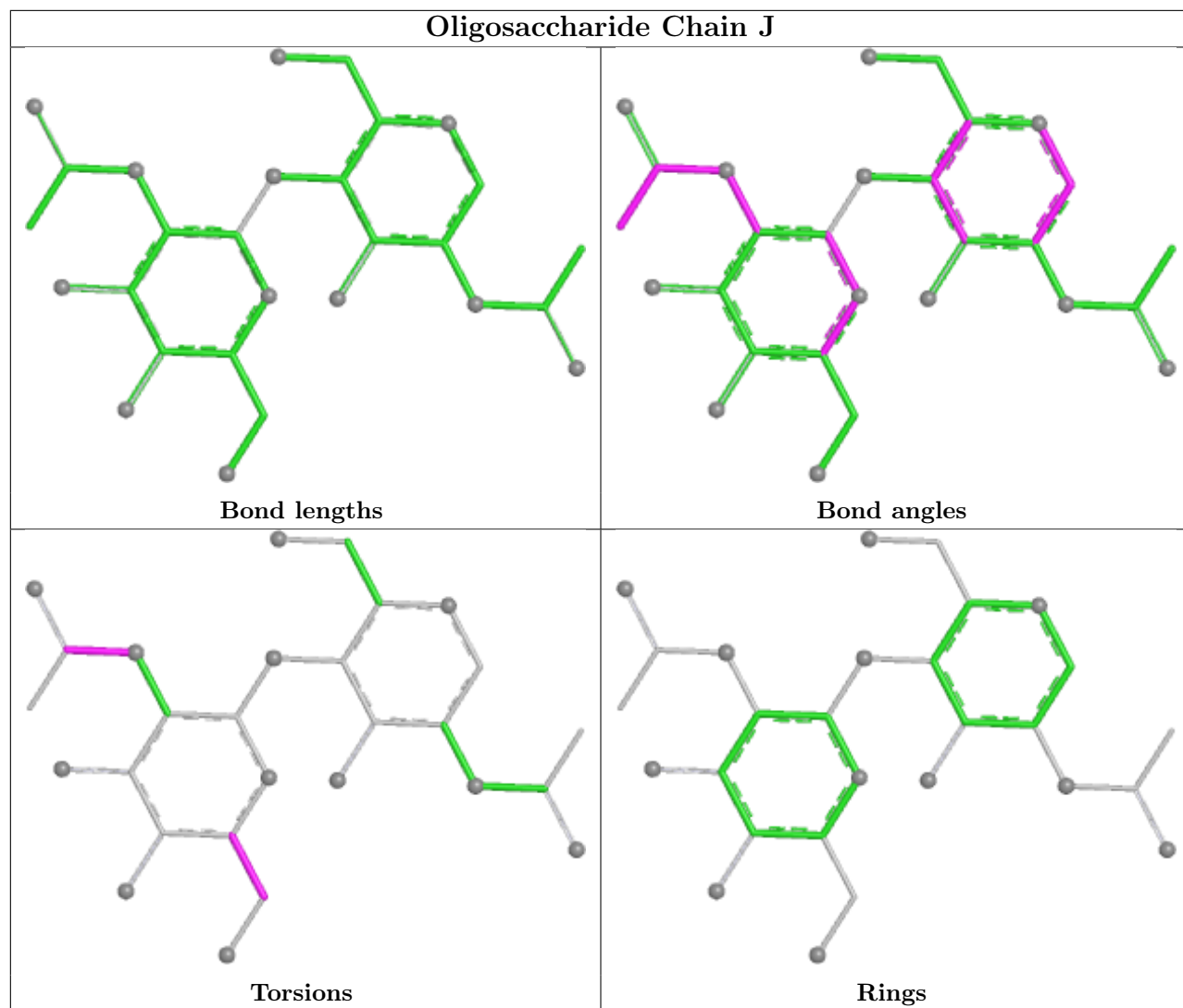


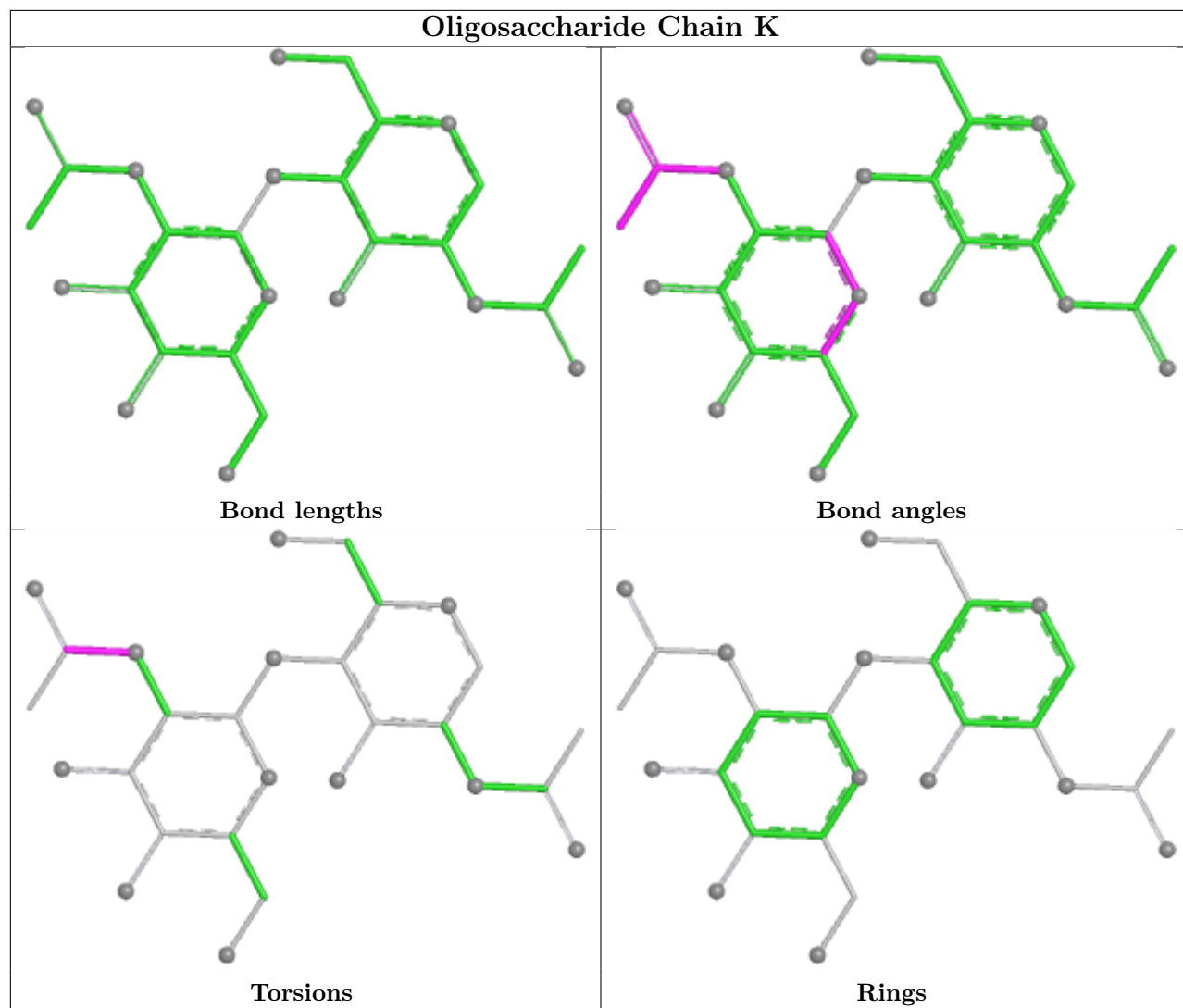


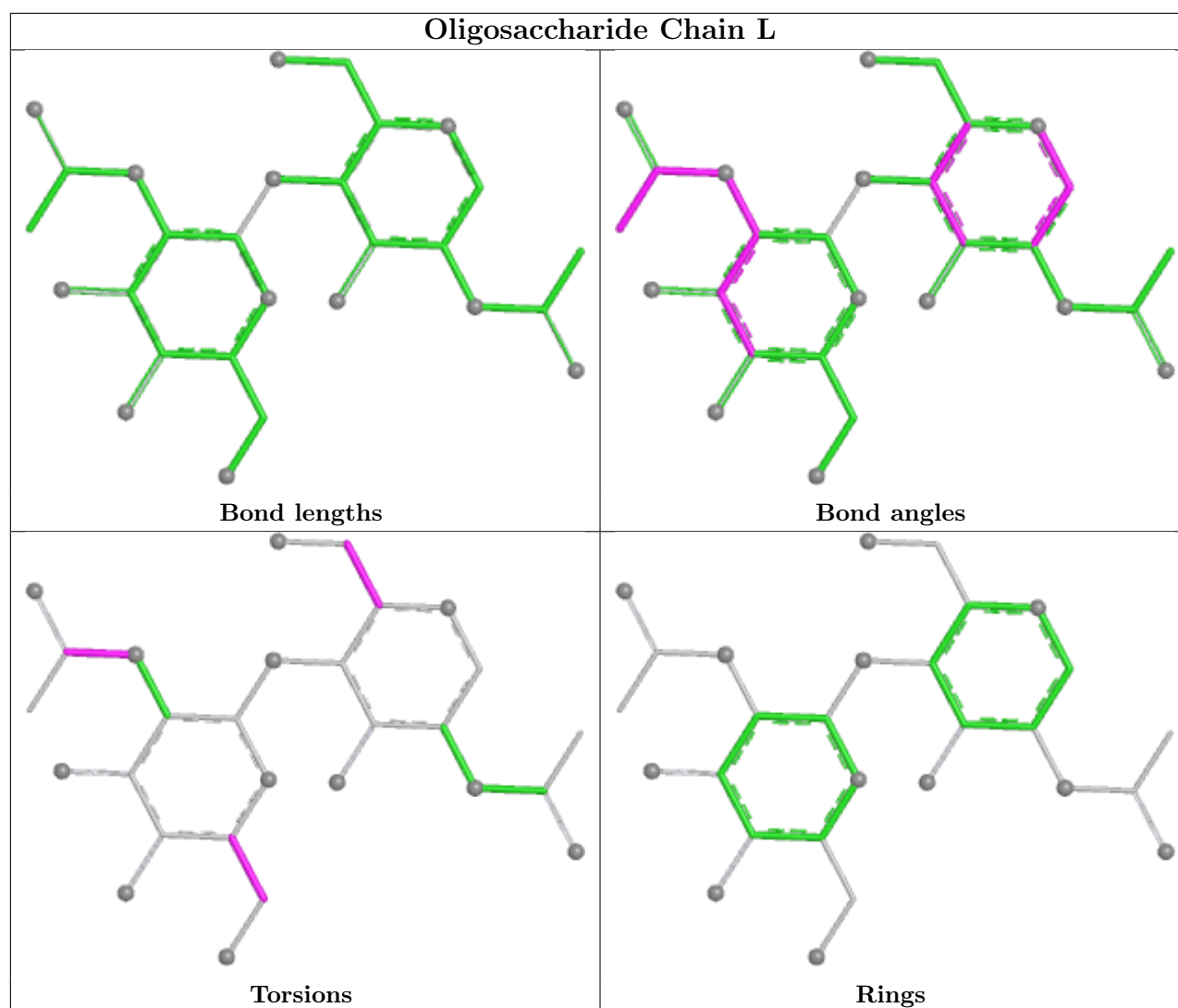












5.6 Ligand geometry [i](#)

21 ligands 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	$\# Z > 2$
3	NAG	A	804	-	14,14,15	0.47	0	17,19,21	0.80	0
4	T22	A	805	-	26,27,27	2.15	2 (7%)	31,38,38	2.64	7 (22%)
4	T22	D	806	-	26,27,27	2.15	2 (7%)	31,38,38	2.62	7 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	T22	B	805	-	26,27,27	2.15	2 (7%)	31,38,38	2.64	7 (22%)
3	NAG	C	801	-	14,14,15	0.57	0	17,19,21	1.29	2 (11%)
3	NAG	D	804	1	14,14,15	0.55	0	17,19,21	1.22	2 (11%)
3	NAG	B	804	-	14,14,15	0.54	0	17,19,21	1.19	1 (5%)
3	NAG	C	802	-	14,14,15	0.51	0	17,19,21	0.81	0
3	NAG	B	803	-	14,14,15	0.48	0	17,19,21	0.83	1 (5%)
3	NAG	B	801	-	14,14,15	0.46	0	17,19,21	0.99	1 (5%)
3	NAG	A	802	-	14,14,15	0.63	0	17,19,21	1.02	1 (5%)
4	T22	C	805	-	26,27,27	2.15	2 (7%)	31,38,38	2.63	7 (22%)
3	NAG	C	804	-	14,14,15	0.64	0	17,19,21	1.42	2 (11%)
3	NAG	C	803	1	14,14,15	0.58	0	17,19,21	1.00	1 (5%)
3	NAG	A	803	-	14,14,15	0.54	0	17,19,21	1.43	5 (29%)
3	NAG	A	801	-	14,14,15	0.51	0	17,19,21	0.65	0
3	NAG	D	803	1	14,14,15	0.77	0	17,19,21	1.36	2 (11%)
3	NAG	D	805	-	14,14,15	0.47	0	17,19,21	1.14	2 (11%)
3	NAG	D	801	1	14,14,15	1.16	1 (7%)	17,19,21	1.75	5 (29%)
3	NAG	D	802	-	14,14,15	0.60	0	17,19,21	1.28	2 (11%)
3	NAG	B	802	-	14,14,15	0.53	0	17,19,21	1.21	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	804	-	-	5/6/23/26	0/1/1/1
4	T22	A	805	-	-	1/10/20/20	0/3/3/3
4	T22	D	806	-	-	1/10/20/20	0/3/3/3
4	T22	B	805	-	-	1/10/20/20	0/3/3/3
3	NAG	C	801	-	-	3/6/23/26	0/1/1/1
3	NAG	D	804	1	1/1/5/7	4/6/23/26	0/1/1/1
3	NAG	B	804	-	-	0/6/23/26	0/1/1/1
3	NAG	C	802	-	-	4/6/23/26	0/1/1/1
3	NAG	B	803	-	-	4/6/23/26	0/1/1/1
3	NAG	A	802	-	-	3/6/23/26	0/1/1/1
3	NAG	B	801	-	-	4/6/23/26	0/1/1/1
4	T22	C	805	-	-	1/10/20/20	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	C	804	-	-	2/6/23/26	0/1/1/1
3	NAG	C	803	1	-	2/6/23/26	0/1/1/1
3	NAG	A	803	-	-	4/6/23/26	0/1/1/1
3	NAG	A	801	-	-	2/6/23/26	0/1/1/1
3	NAG	D	803	1	-	2/6/23/26	0/1/1/1
3	NAG	D	805	-	-	2/6/23/26	0/1/1/1
3	NAG	D	801	1	-	3/6/23/26	0/1/1/1
3	NAG	D	802	-	-	3/6/23/26	0/1/1/1
3	NAG	B	802	-	-	4/6/23/26	0/1/1/1

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	805	T22	C22-C23	-9.24	1.31	1.44
4	A	805	T22	C22-C23	-9.24	1.31	1.44
4	D	806	T22	C22-C23	-9.23	1.31	1.44
4	C	805	T22	C22-C23	-9.22	1.31	1.44
3	D	801	NAG	O5-C1	-3.90	1.37	1.43

The worst 5 of 56 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	805	T22	C5-C6-N7	-8.93	114.68	125.28
4	A	805	T22	C5-C6-N7	-8.93	114.69	125.28
4	C	805	T22	C5-C6-N7	-8.91	114.71	125.28
4	D	806	T22	C5-C6-N7	-8.89	114.73	125.28
4	C	805	T22	C5-C3-N2	5.48	120.50	115.36

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	D	804	NAG	C1

5 of 55 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	801	NAG	C8-C7-N2-C2
3	A	801	NAG	O7-C7-N2-C2
3	A	802	NAG	C8-C7-N2-C2
3	A	802	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
3	A	803	NAG	C1-C2-N2-C7

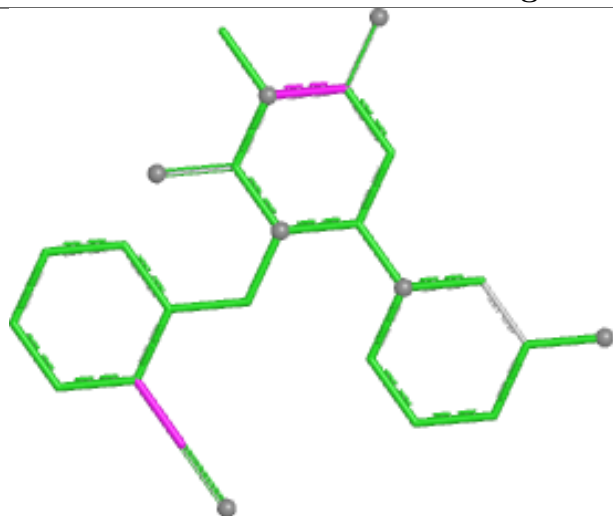
There are no ring outliers.

16 monomers are involved in 20 short contacts:

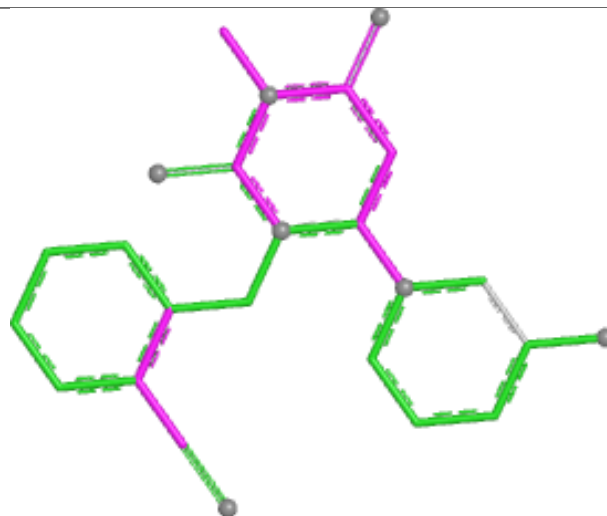
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	805	T22	1	0
4	D	806	T22	1	0
4	B	805	T22	1	0
3	C	801	NAG	1	0
3	D	804	NAG	1	0
3	B	804	NAG	2	0
3	C	802	NAG	1	0
3	B	803	NAG	1	0
3	B	801	NAG	1	0
4	C	805	T22	1	0
3	C	804	NAG	1	0
3	A	803	NAG	3	0
3	A	801	NAG	1	0
3	D	805	NAG	2	0
3	D	802	NAG	1	0
3	B	802	NAG	1	0

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

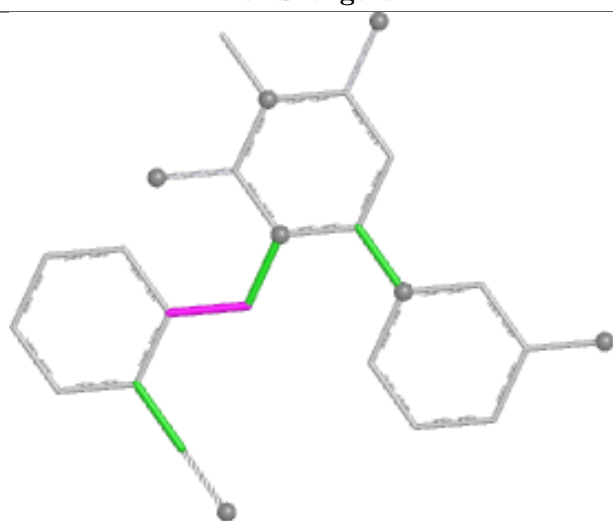
Ligand T22 A 805



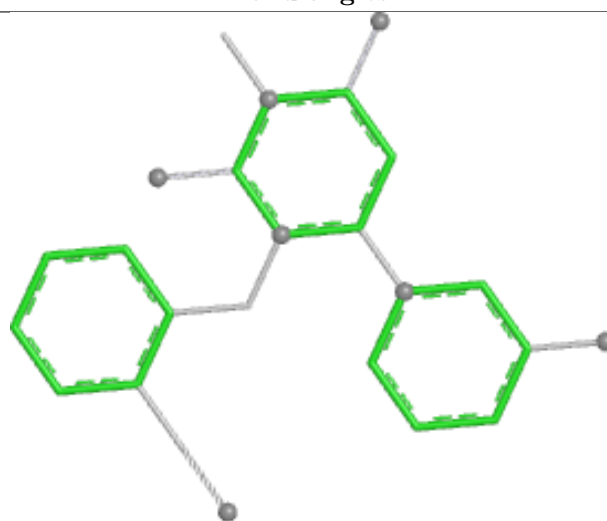
Bond lengths



Bond angles

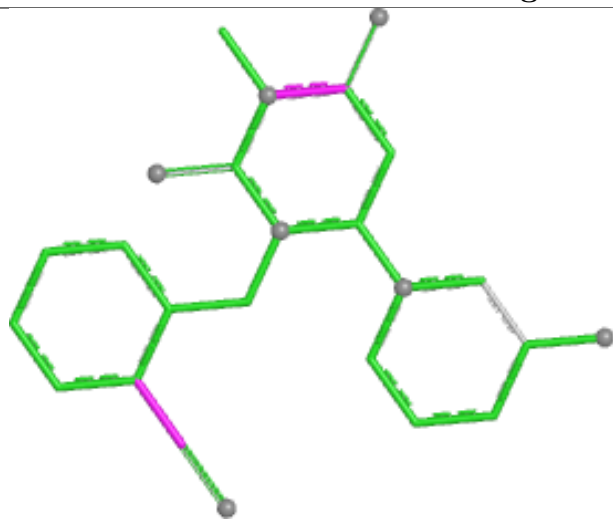


Torsions

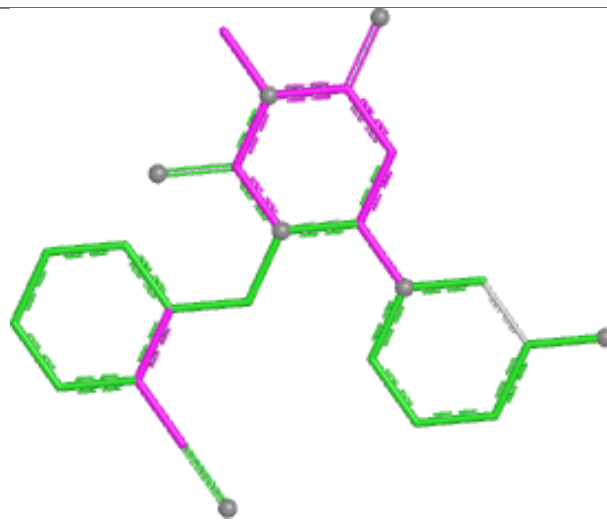


Rings

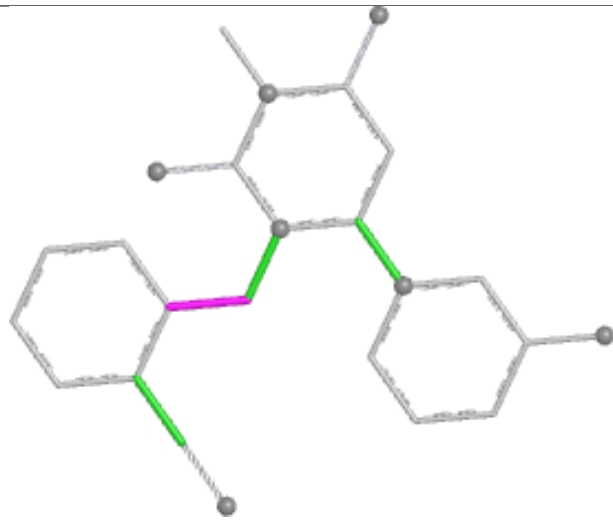
Ligand T22 D 806



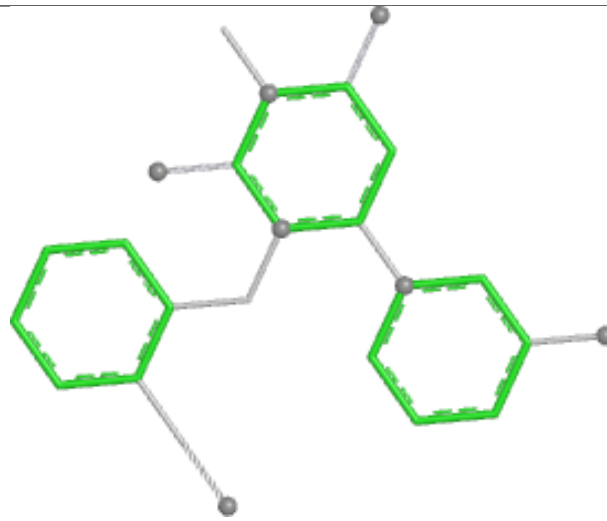
Bond lengths



Bond angles

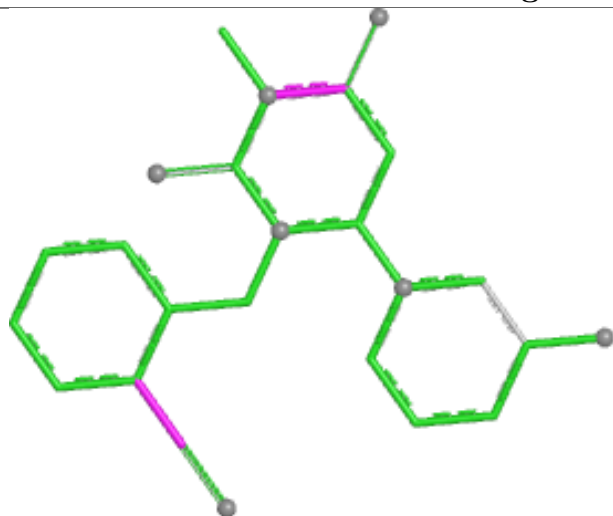


Torsions

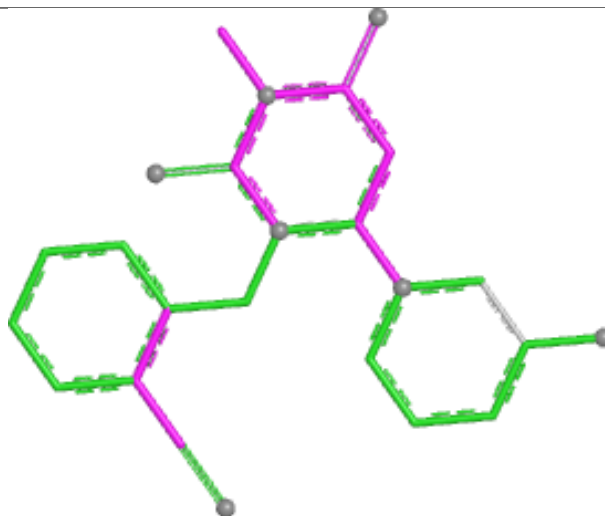


Rings

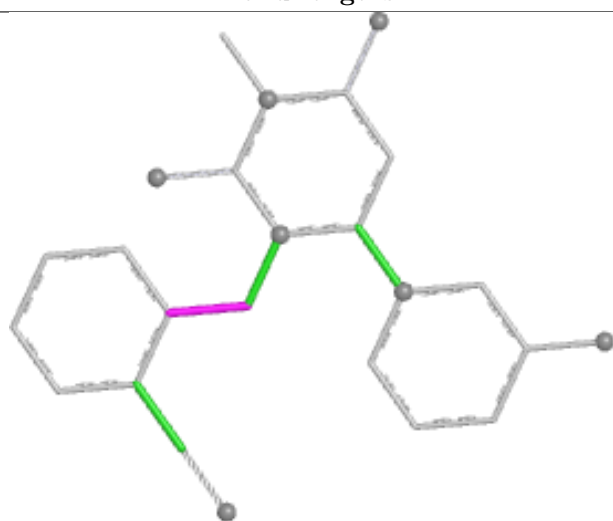
Ligand T22 B 805



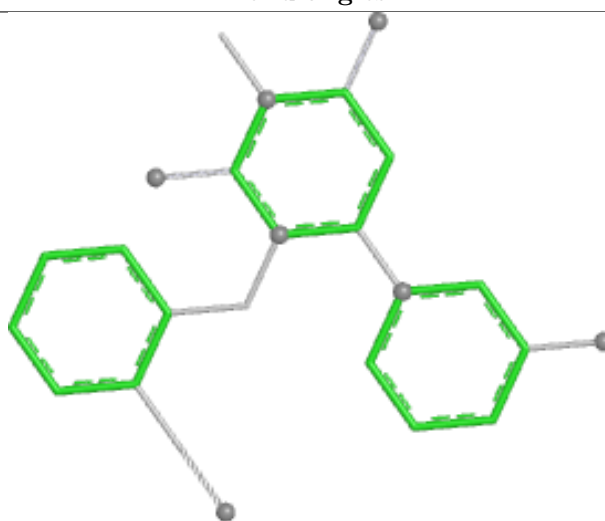
Bond lengths



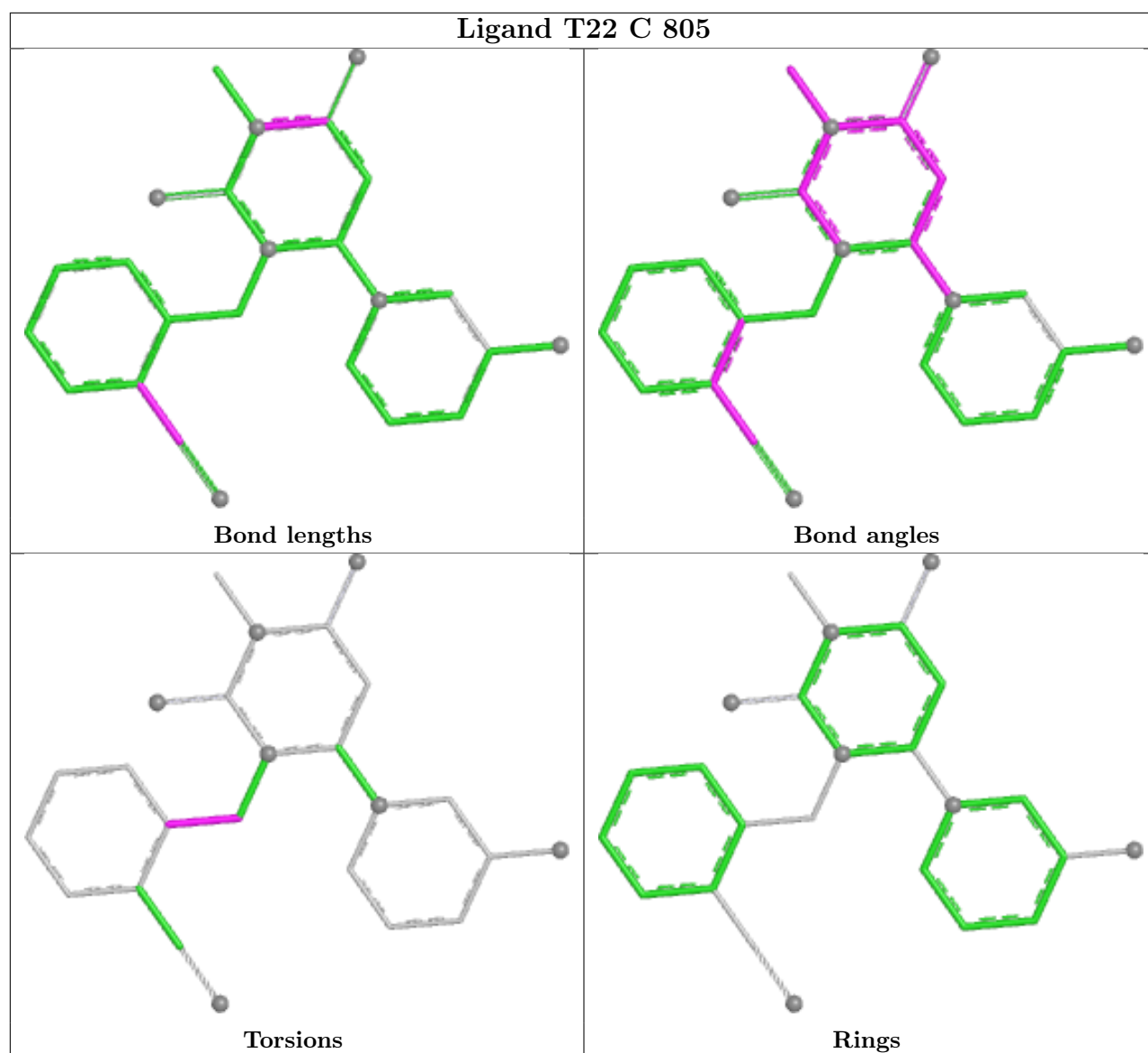
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

Warning: The R factor obtained from EDS is 0.2673, which does not match the depositor's R factor of 0.20675. Please interpret the results in this section carefully.

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	727/740 (98%)	0.71	38 (5%) 34 34	41, 50, 64, 77	0
1	B	733/740 (99%)	0.73	33 (4%) 39 38	38, 50, 64, 77	0
1	C	726/740 (98%)	1.31	142 (19%) 4 3	44, 51, 73, 88	0
1	D	727/740 (98%)	0.77	36 (4%) 35 35	43, 50, 66, 79	0
All	All	2913/2960 (98%)	0.88	249 (8%) 18 18	38, 50, 67, 88	0

The worst 5 of 249 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	90	LEU	5.3
1	C	244	GLU	4.8
1	C	247	GLN	4.5
1	C	241	TYR	4.4
1	C	322	TYR	4.3

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

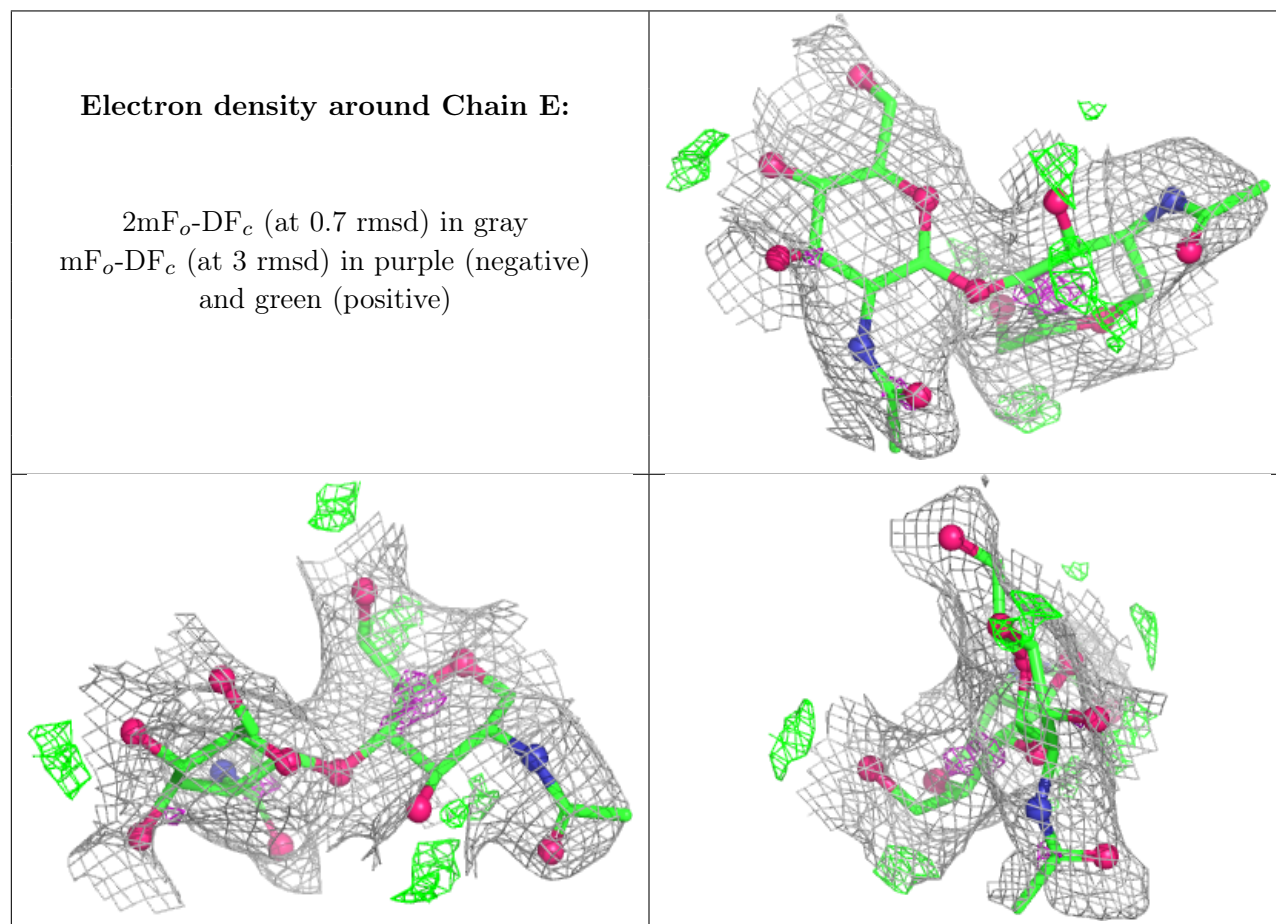
There are no non-standard protein/DNA/RNA residues in this entry.

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.

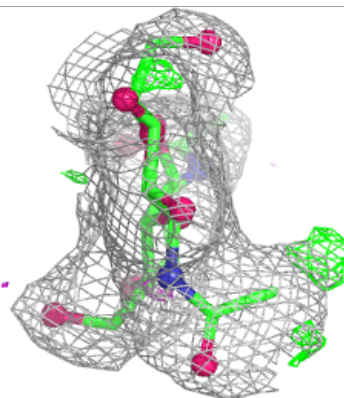
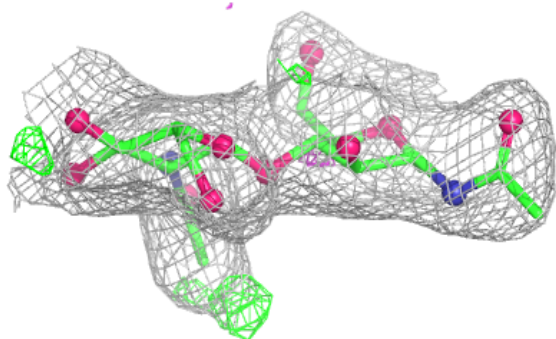
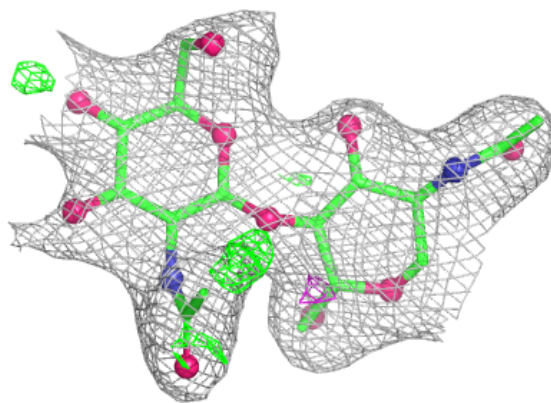
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NAG	G	1	14/15	0.46	0.21	97,101,102,102	0
2	NAG	E	2	14/15	0.49	0.17	88,91,91,91	0
2	NAG	H	2	14/15	0.49	0.20	106,107,108,108	0
2	NAG	J	2	14/15	0.51	0.18	81,85,86,87	0
2	NAG	I	2	14/15	0.59	0.18	117,119,119,119	0
2	NAG	I	1	14/15	0.61	0.18	116,118,119,119	0
2	NAG	G	2	14/15	0.62	0.17	102,103,103,103	0
2	NAG	E	1	14/15	0.63	0.17	73,78,81,85	0
2	NAG	L	2	14/15	0.63	0.17	80,85,87,87	0
2	NAG	K	2	14/15	0.67	0.16	64,65,66,67	0
2	NAG	F	2	14/15	0.69	0.14	71,71,74,74	0
2	NAG	J	1	14/15	0.81	0.14	69,76,79,82	0
2	NAG	H	1	14/15	0.82	0.15	99,102,103,105	0
2	NAG	K	1	14/15	0.84	0.12	54,58,60,62	0
2	NAG	L	1	14/15	0.87	0.12	74,77,79,81	0
2	NAG	F	1	14/15	0.89	0.10	61,66,68,69	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.

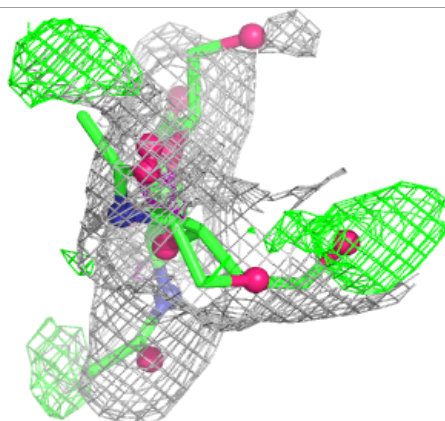
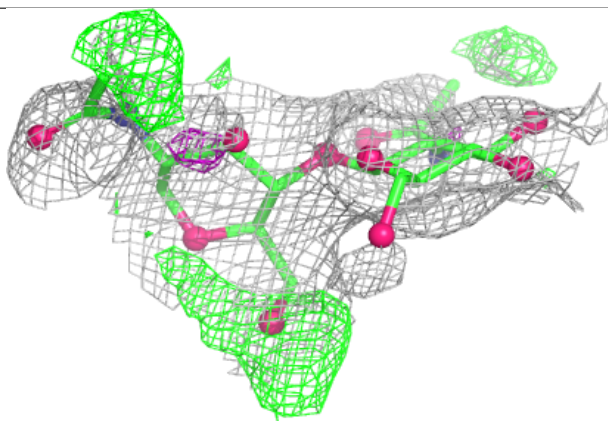
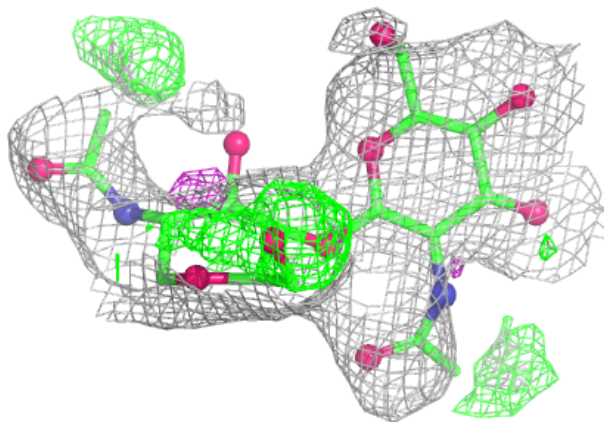


Electron density around Chain F:

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

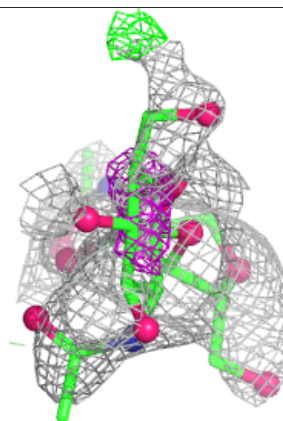
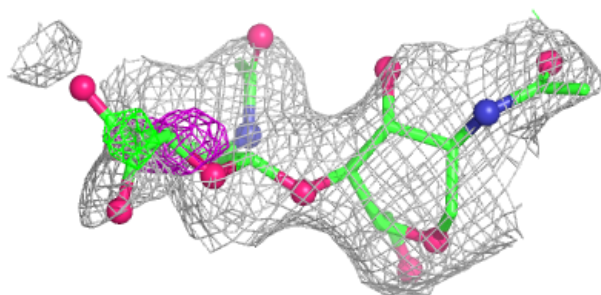
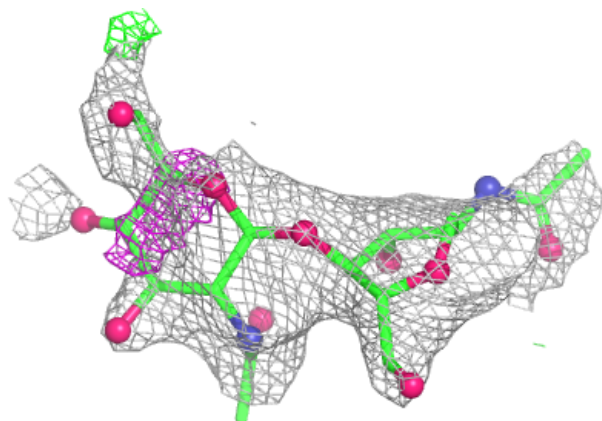
**Electron density around Chain G:**

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



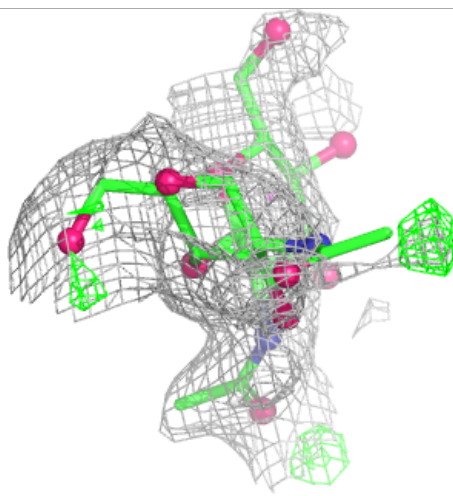
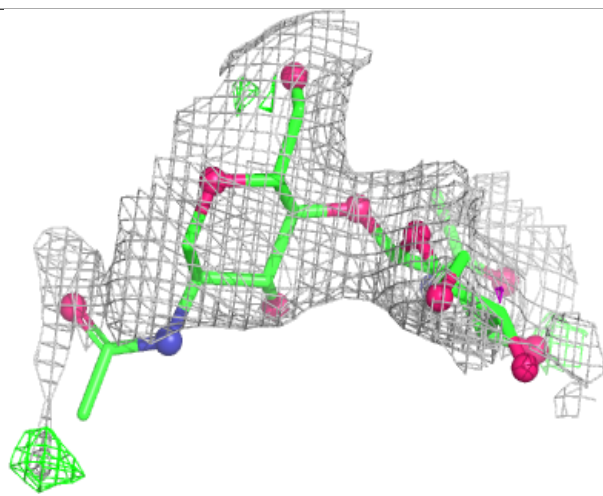
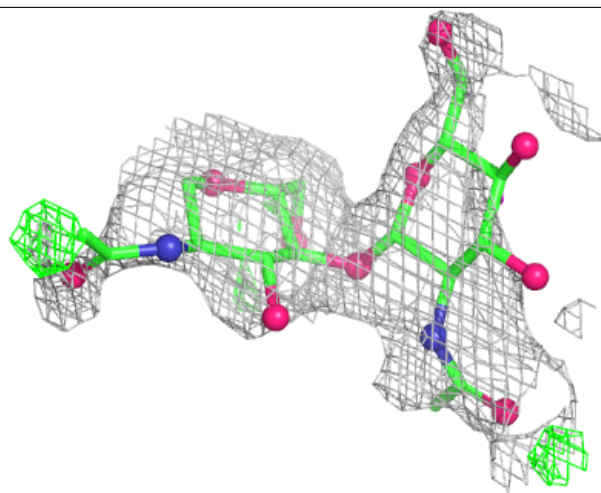
Electron density around Chain H:

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



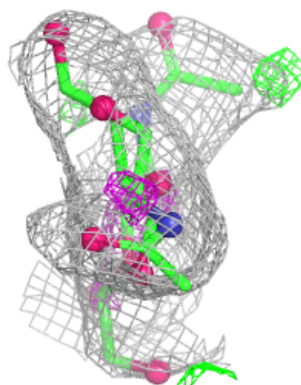
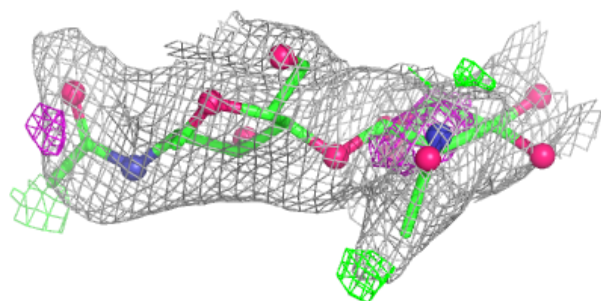
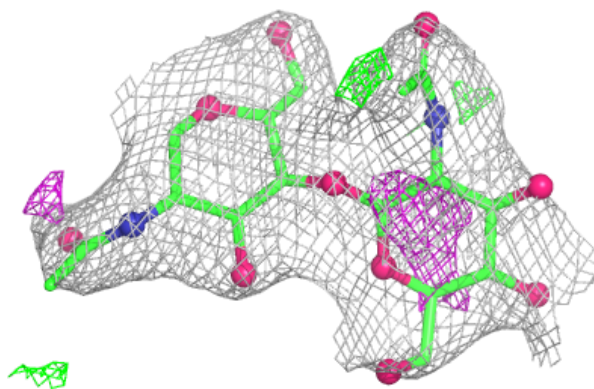
Electron density around Chain I:

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



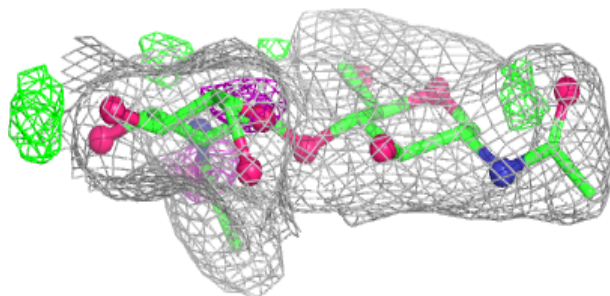
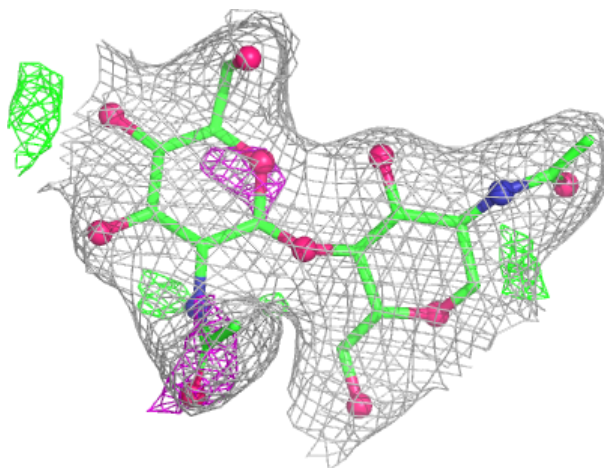
Electron density around Chain J:

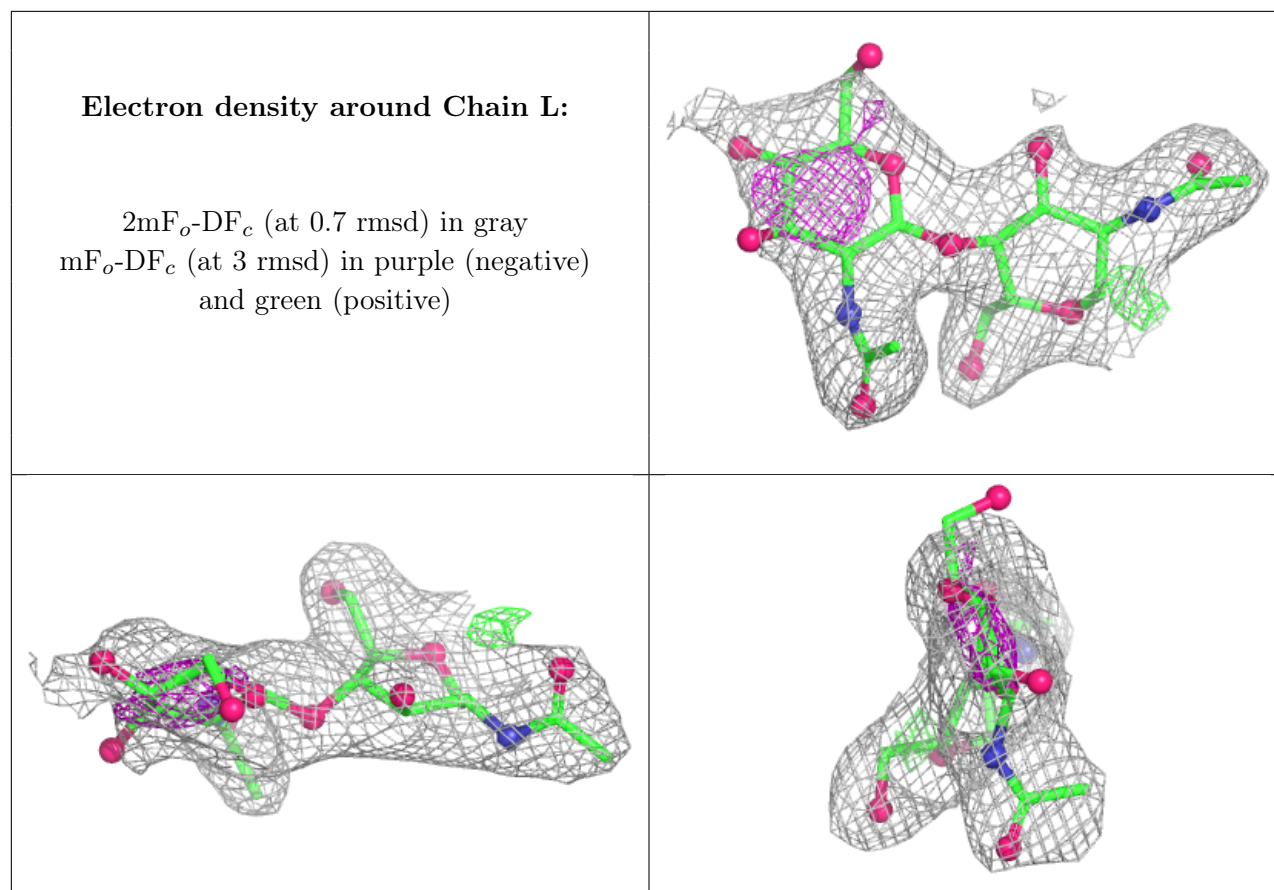
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain K:

$2mF_o-DF_c$ (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
3	NAG	A	804	14/15	0.40	0.19	111,112,114,114	0
3	NAG	A	803	14/15	0.48	0.21	71,75,77,78	0
3	NAG	D	805	14/15	0.51	0.18	91,93,94,94	0
3	NAG	C	804	14/15	0.54	0.20	89,91,92,92	0
3	NAG	A	802	14/15	0.60	0.22	97,98,99,99	0
3	NAG	D	803	14/15	0.62	0.17	70,74,75,76	0
3	NAG	C	801	14/15	0.62	0.19	88,90,90,90	0
3	NAG	D	802	14/15	0.63	0.17	84,85,86,86	0
3	NAG	B	804	14/15	0.64	0.19	90,92,92,92	0
3	NAG	A	801	14/15	0.66	0.17	94,97,97,98	0
3	NAG	D	804	14/15	0.67	0.18	73,75,80,80	0
3	NAG	D	801	14/15	0.67	0.16	66,69,70,71	0
3	NAG	B	801	14/15	0.69	0.16	84,86,86,87	0

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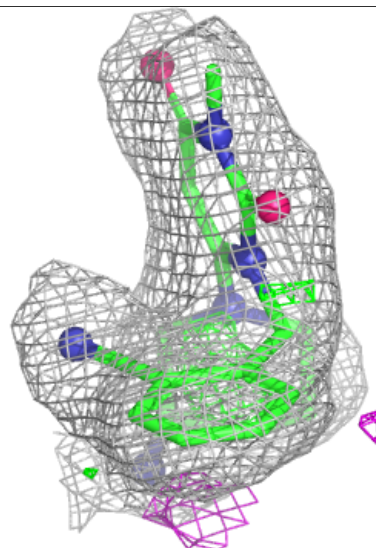
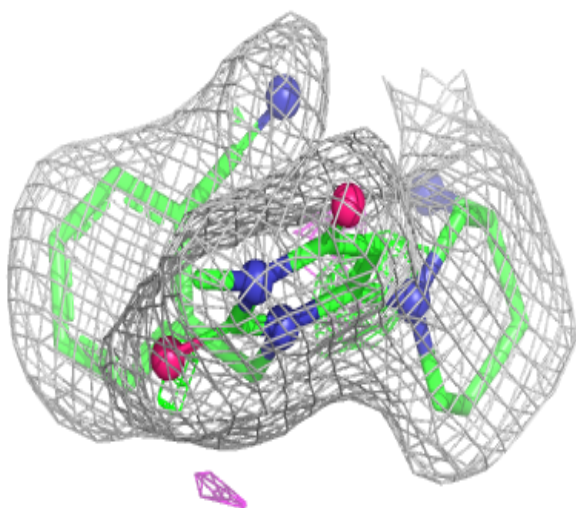
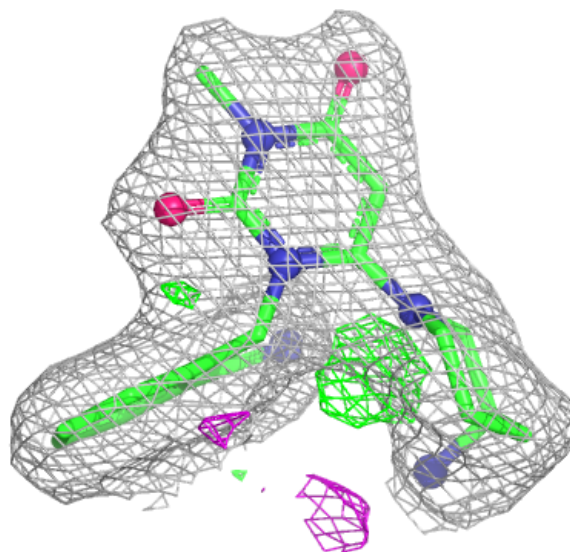
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NAG	C	803	14/15	0.69	0.17	71,75,78,78	0
3	NAG	B	802	14/15	0.71	0.17	88,89,90,90	0
3	NAG	C	802	14/15	0.72	0.16	92,95,96,96	0
3	NAG	B	803	14/15	0.74	0.15	93,94,95,96	0
4	T22	B	805	25/25	0.93	0.11	48,50,51,52	0
4	T22	D	806	25/25	0.93	0.10	48,50,51,52	0
4	T22	C	805	25/25	0.94	0.10	48,50,51,52	0
4	T22	A	805	25/25	0.95	0.09	48,50,51,52	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.

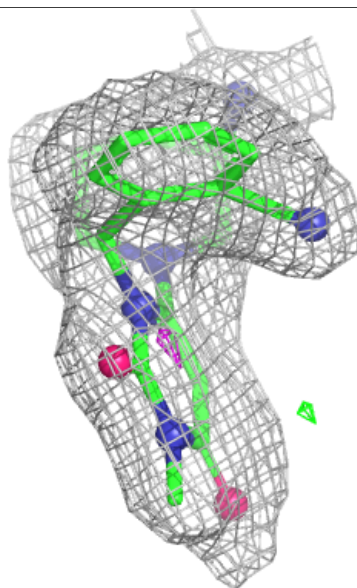
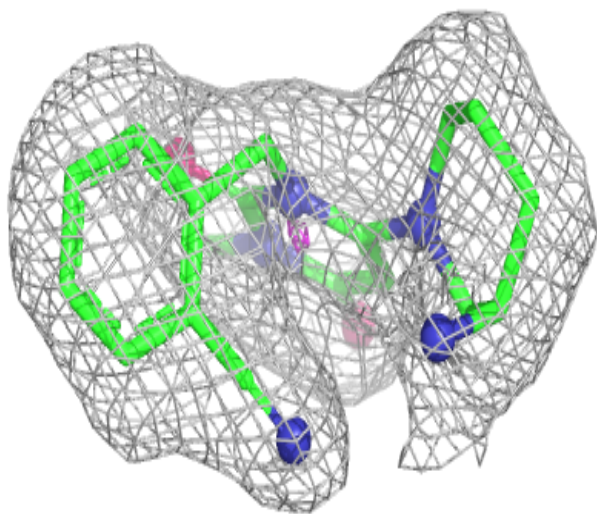
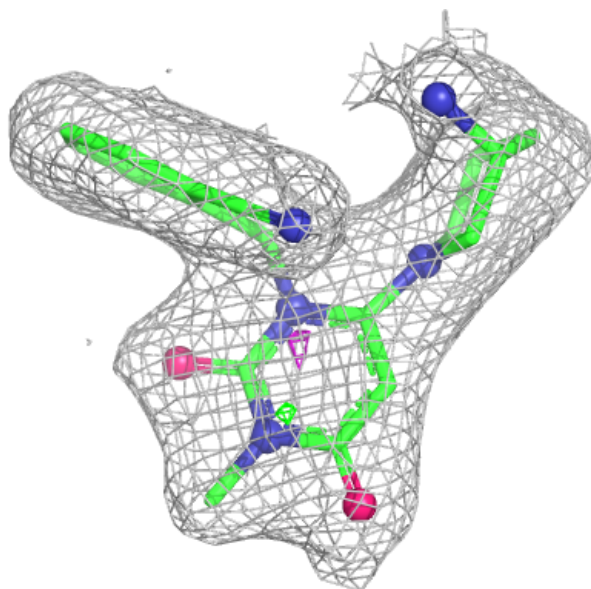
Electron density around T22 B 805:

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



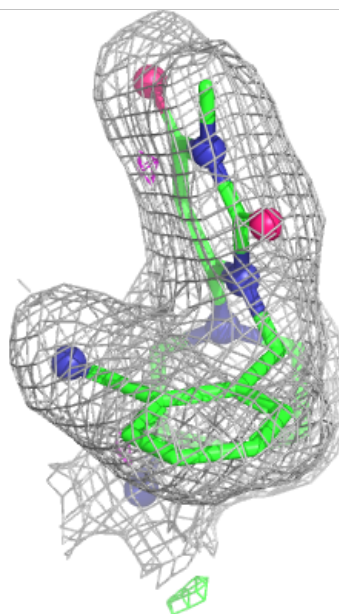
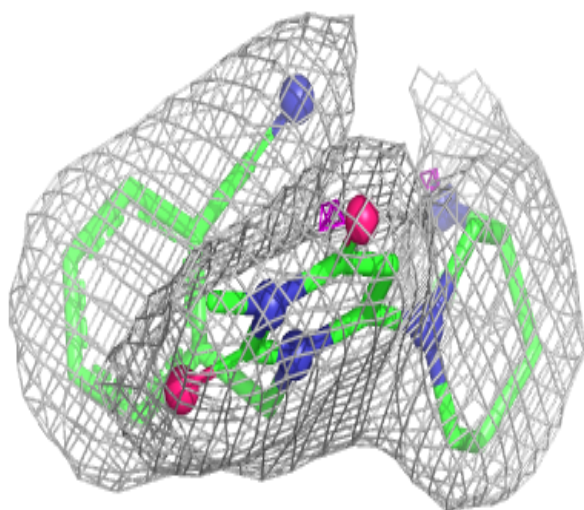
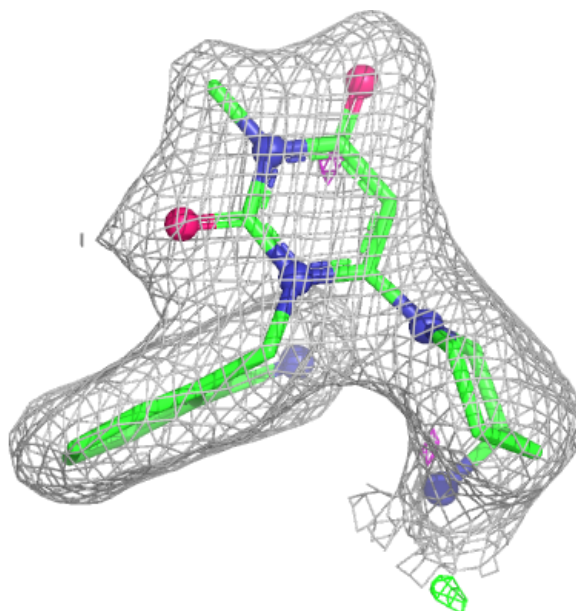
Electron density around T22 D 806:

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



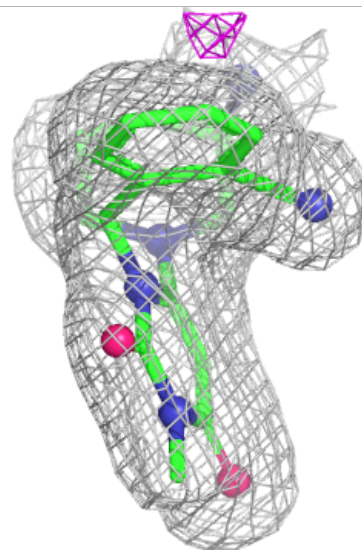
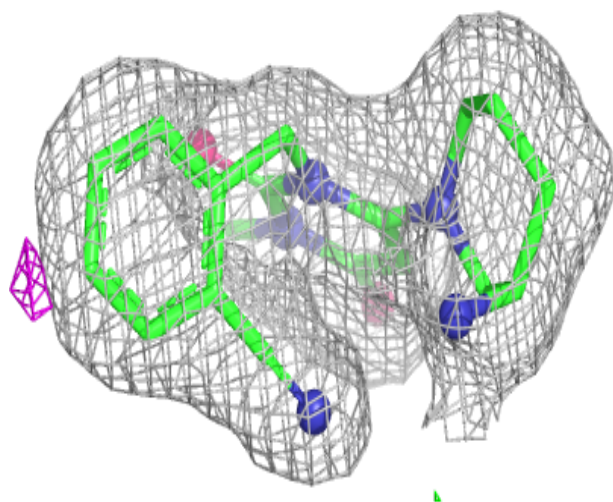
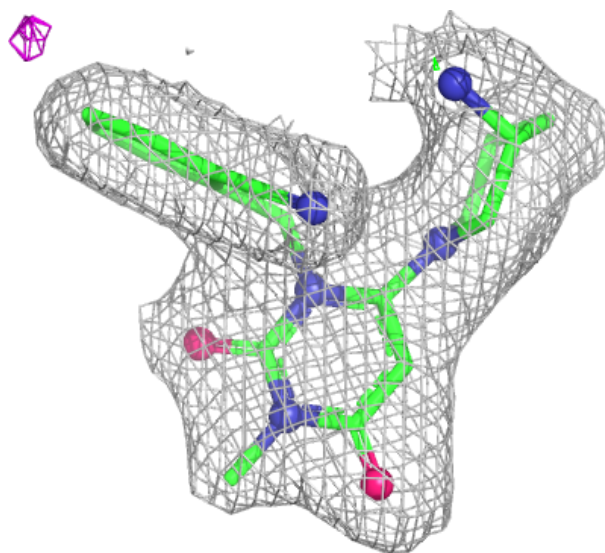
Electron density around T22 C 805:

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



Electron density around T22 A 805:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.