



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2026 – 01:10 PM UTC

PDB ID : 3G0D / pdb_00003g0d
Title : Crystal structure of dipeptidyl peptidase IV in complex with a pyrimidinedione inhibitor 2
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 : 2.39 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](#) ①) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

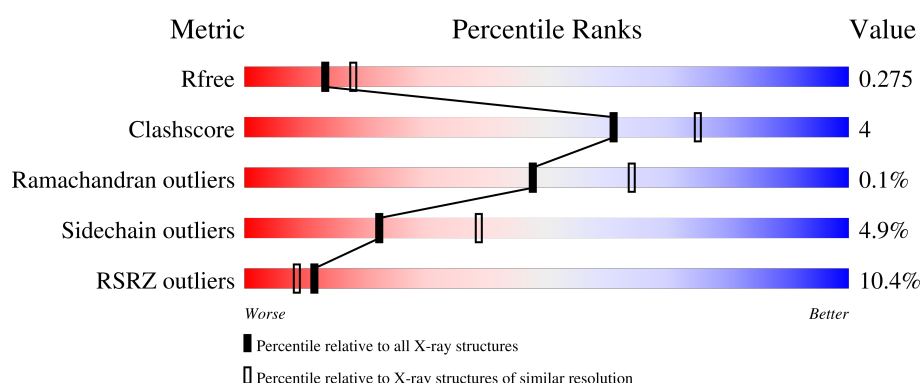
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.39 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.



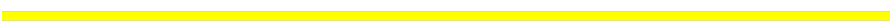
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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

Mol	Chain	Length	Quality of chain
1	A	740	7% 84% 12% ..
1	B	740	5% 84% 13% ..
1	C	740	9% 85% 11% ..
1	D	740	21% 85% 12% ..
2	E	2	100%

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

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
4	NAG	D	804	X	-	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 25530 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	723	Total	C	N	O	S	0	3	0
			5936	3813	977	1120	26			
1	B	728	Total	C	N	O	S	0	3	0
			5970	3833	985	1126	26			
1	C	723	Total	C	N	O	S	0	1	0
			5927	3808	975	1118	26			
1	D	723	Total	C	N	O	S	0	0	0
			5918	3800	973	1119	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.



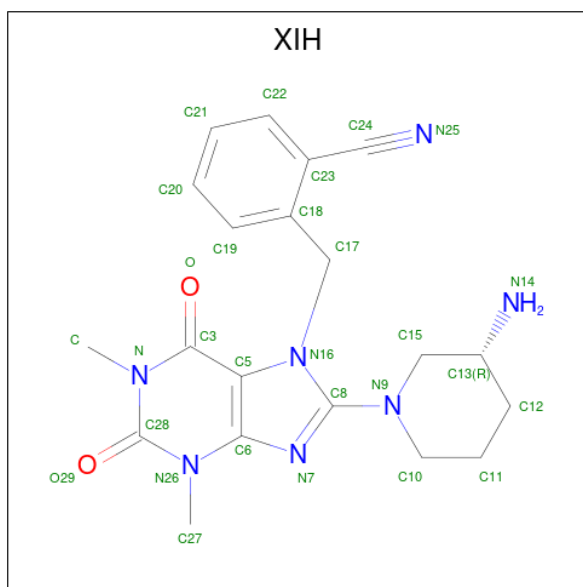
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	G	2	Total	C	N	O	0	0	0
			28	16	2	10			

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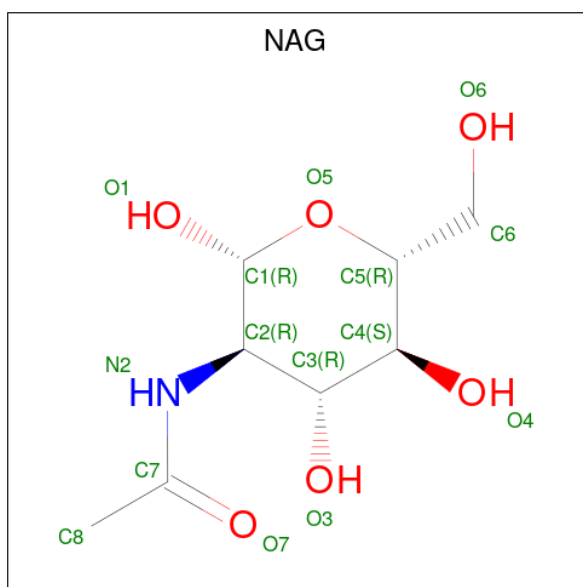
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	I	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is 2-({8-[(3R)-3-AMINOPIPERIDIN-1-YL]-1,3-DIMETHYL-2,6-DIOXO-1,2,3,6-TETRAHYDRO-7H-PURIN-7-YL}METHYL)BENZONITRILE (CCD ID: XIH) (formula: $C_{20}H_{23}N_7O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			29	20	7	2		
3	B	1	Total	C	N	O	0	0
			29	20	7	2		
3	C	1	Total	C	N	O	0	0
			29	20	7	2		
3	D	1	Total	C	N	O	0	0
			29	20	7	2		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

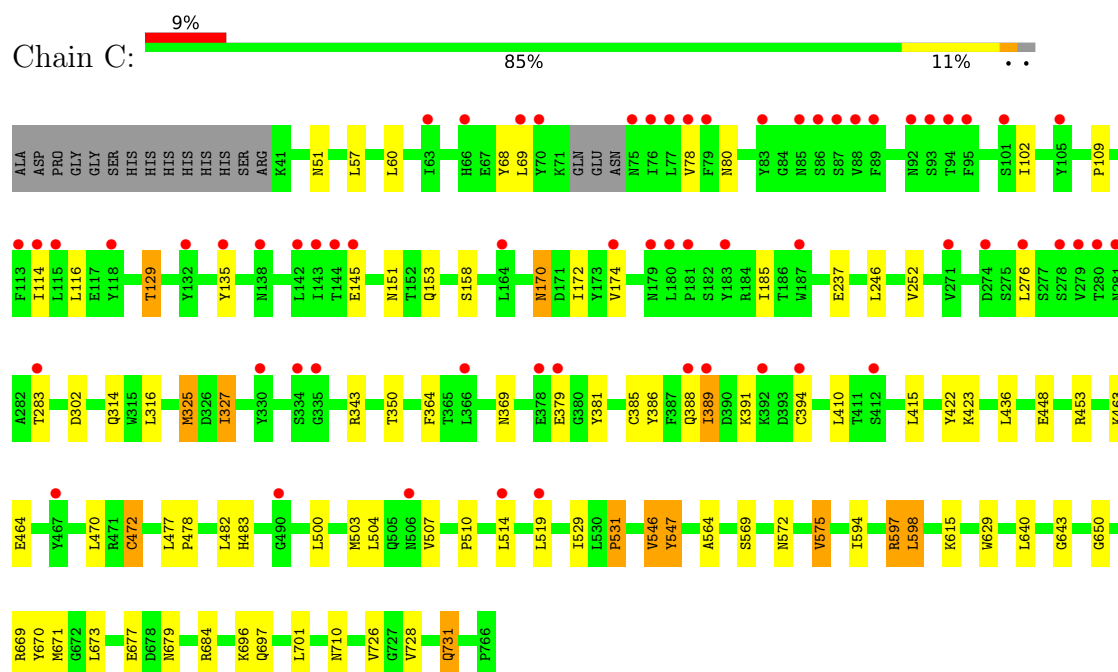
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	394	Total 394	O 394	0	0
5	B	370	Total 370	O 370	0	0
5	C	348	Total 348	O 348	0	0
5	D	215	Total 215	O 215	0	0

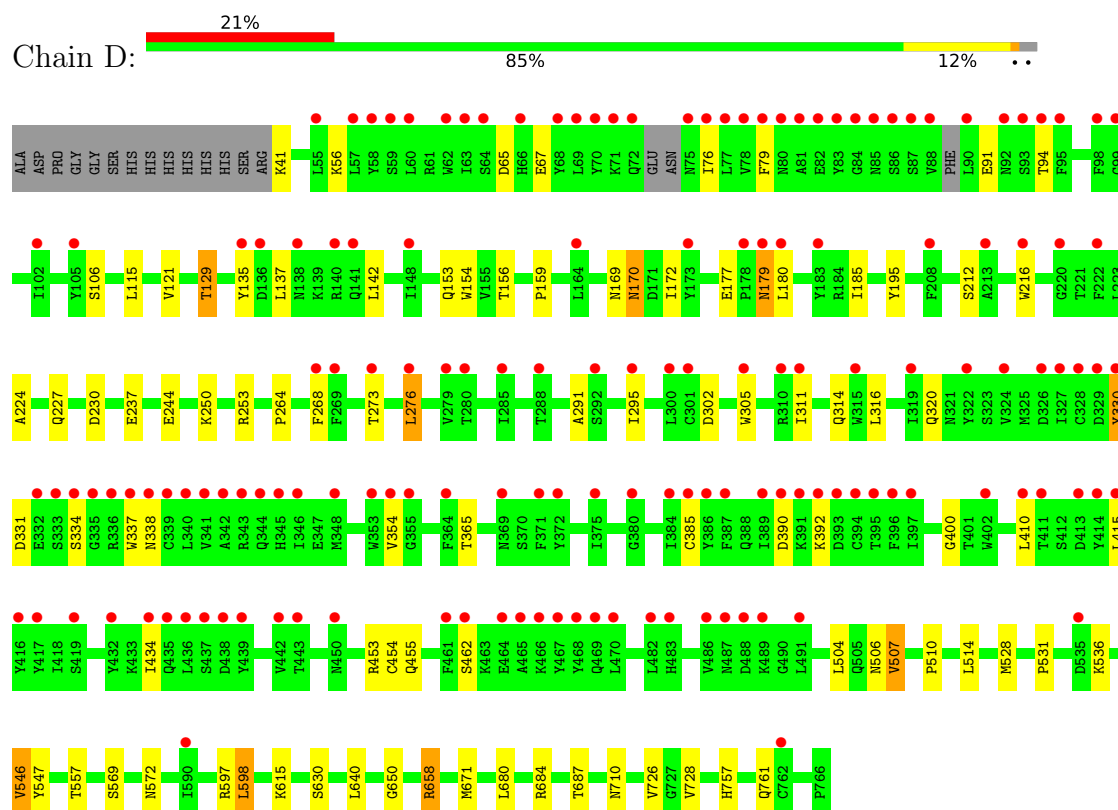
- Molecule 1: Dipeptidyl peptidase 4



- 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





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

Chain F:



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

Chain G:



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

Chain H:



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

Chain I:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	122.91Å 123.44Å 145.68Å 90.00° 114.69° 90.00°	Depositor
Resolution (Å)	50.00 – 2.39 50.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	95.2 (50.00-2.39) 95.2 (50.00-2.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.28 (at 2.39Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.187 , 0.239 0.232 , 0.275	Depositor DCC
R_{free} test set	7412 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	46.4	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 33.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.004 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	25530	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.29% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.53	0/6119	0.79	2/8321 (0.0%)
1	B	0.52	0/6155	0.80	4/8370 (0.0%)
1	C	0.53	1/6102 (0.0%)	0.80	1/8298 (0.0%)
1	D	0.56	2/6087 (0.0%)	0.79	7/8277 (0.1%)
All	All	0.54	3/24463 (0.0%)	0.80	14/33266 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	338	ASN	CG-OD1	13.24	1.48	1.23
1	D	338	ASN	C-O	9.07	1.34	1.24
1	C	531	PRO	CA-C	5.38	1.54	1.51

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	330	TYR	O-C-N	6.71	130.89	123.04
1	D	330	TYR	CA-C-O	-6.53	113.24	120.69
1	C	546	VAL	N-CA-C	6.21	117.72	108.46
1	A	630	SER	CB-CA-C	-6.09	108.95	117.23
1	D	546	VAL	N-CA-C	6.00	117.39	108.46

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5936	0	5655	60	0
1	B	5970	0	5678	56	0
1	C	5927	0	5650	45	0
1	D	5918	0	5641	39	0
2	E	28	0	25	0	0
2	F	28	0	25	0	0
2	G	28	0	25	0	0
2	H	28	0	25	0	0
2	I	28	0	25	0	0
3	A	29	0	23	0	0
3	B	29	0	23	1	0
3	C	29	0	23	1	0
3	D	29	0	23	0	0
4	A	56	0	52	0	0
4	B	56	0	52	0	0
4	C	56	0	52	0	0
4	D	28	0	26	0	0
5	A	394	0	0	2	0
5	B	370	0	0	2	0
5	C	348	0	0	1	0
5	D	215	0	0	1	0
All	All	25530	0	23023	200	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.

The worst 5 of 200 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:153:GLN:HE22	1:A:170:ASN:H	1.11	0.91
1:A:253:ARG:HH21	1:B:253:ARG:HH21	1.20	0.90
1:C:153:GLN:HE22	1:C:170:ASN:H	1.19	0.89
1:B:379:GLU:HG3	1:B:381:TYR:HD1	1.39	0.87
1:A:325:MET:HE3	1:A:327:ILE:HD11	1.54	0.86

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	722/740 (98%)	690 (96%)	32 (4%)	0	100	100
1	B	727/740 (98%)	702 (97%)	24 (3%)	1 (0%)	48	64
1	C	720/740 (97%)	692 (96%)	28 (4%)	0	100	100
1	D	717/740 (97%)	687 (96%)	29 (4%)	1 (0%)	48	64
All	All	2886/2960 (98%)	2771 (96%)	113 (4%)	2 (0%)	48	64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	463	LYS
1	D	390	ASP

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	651/662 (98%)	621 (95%)	30 (5%)	24	41
1	B	654/662 (99%)	621 (95%)	33 (5%)	22	38
1	C	649/662 (98%)	610 (94%)	39 (6%)	17	31
1	D	648/662 (98%)	622 (96%)	26 (4%)	28	47
All	All	2602/2648 (98%)	2474 (95%)	128 (5%)	22	39

5 of 128 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	453	ARG
1	D	514	LEU
1	B	436	LEU
1	B	415	LEU
1	D	536	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 55 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	112	GLN
1	C	572	ASN
1	D	731	GLN
1	D	455	GLN
1	C	123	GLN

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 ⓘ

10 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	0.67	0	17,19,21	1.09	1 (5%)
2	NAG	E	2	2	14,14,15	0.45	0	17,19,21	1.05	1 (5%)
2	NAG	F	1	1,2	14,14,15	0.50	0	17,19,21	1.24	2 (11%)
2	NAG	F	2	2	14,14,15	0.52	0	17,19,21	0.72	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	G	1	1,2	14,14,15	0.59	0	17,19,21	0.91	0
2	NAG	G	2	2	14,14,15	0.53	0	17,19,21	1.41	2 (11%)
2	NAG	H	1	1,2	14,14,15	0.62	0	17,19,21	1.05	1 (5%)
2	NAG	H	2	2	14,14,15	0.49	0	17,19,21	0.77	0
2	NAG	I	1	1,2	14,14,15	0.48	0	17,19,21	1.03	2 (11%)
2	NAG	I	2	2	14,14,15	0.48	0	17,19,21	1.01	1 (5%)

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

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

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	2	NAG	C1-O5-C5	4.74	118.54	112.19
2	E	2	NAG	C1-O5-C5	3.39	116.73	112.19
2	E	1	NAG	O5-C1-C2	-2.93	106.75	111.29
2	F	1	NAG	C1-O5-C5	2.76	115.89	112.19
2	I	2	NAG	C1-O5-C5	2.68	115.78	112.19

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	1	NAG	C8-C7-N2-C2

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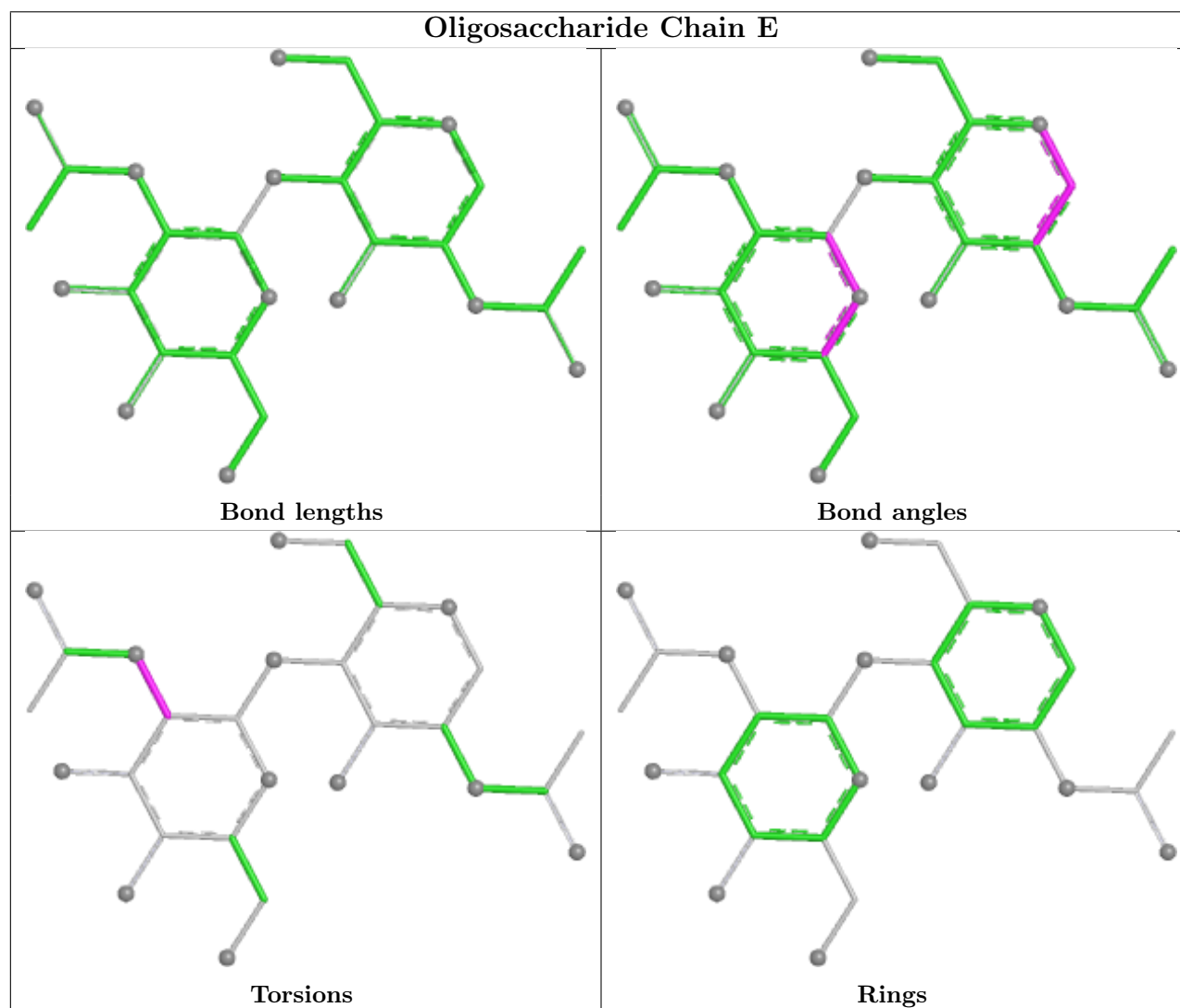
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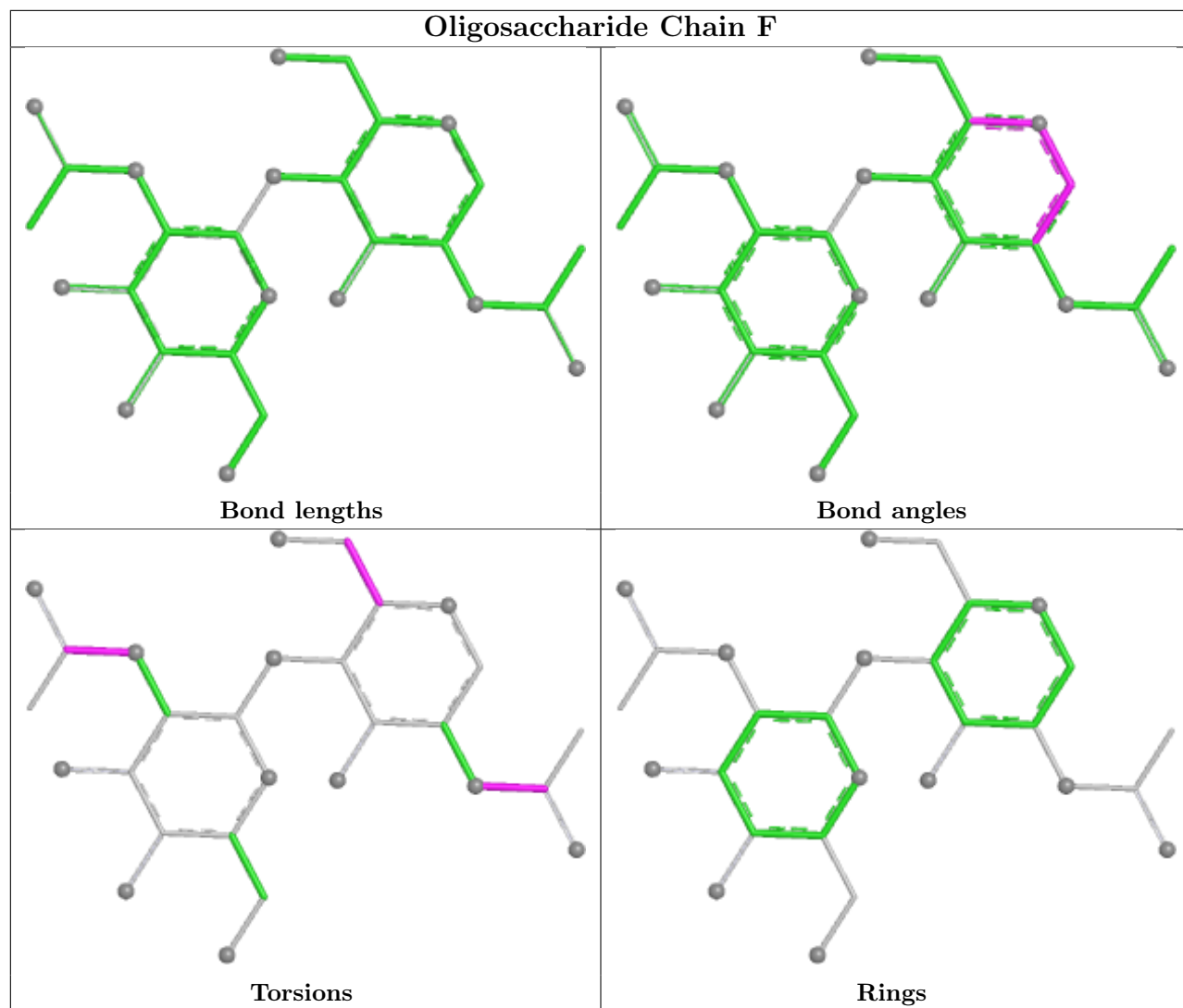
Mol	Chain	Res	Type	Atoms
2	F	1	NAG	O7-C7-N2-C2
2	F	2	NAG	C8-C7-N2-C2
2	F	2	NAG	O7-C7-N2-C2
2	H	2	NAG	C8-C7-N2-C2

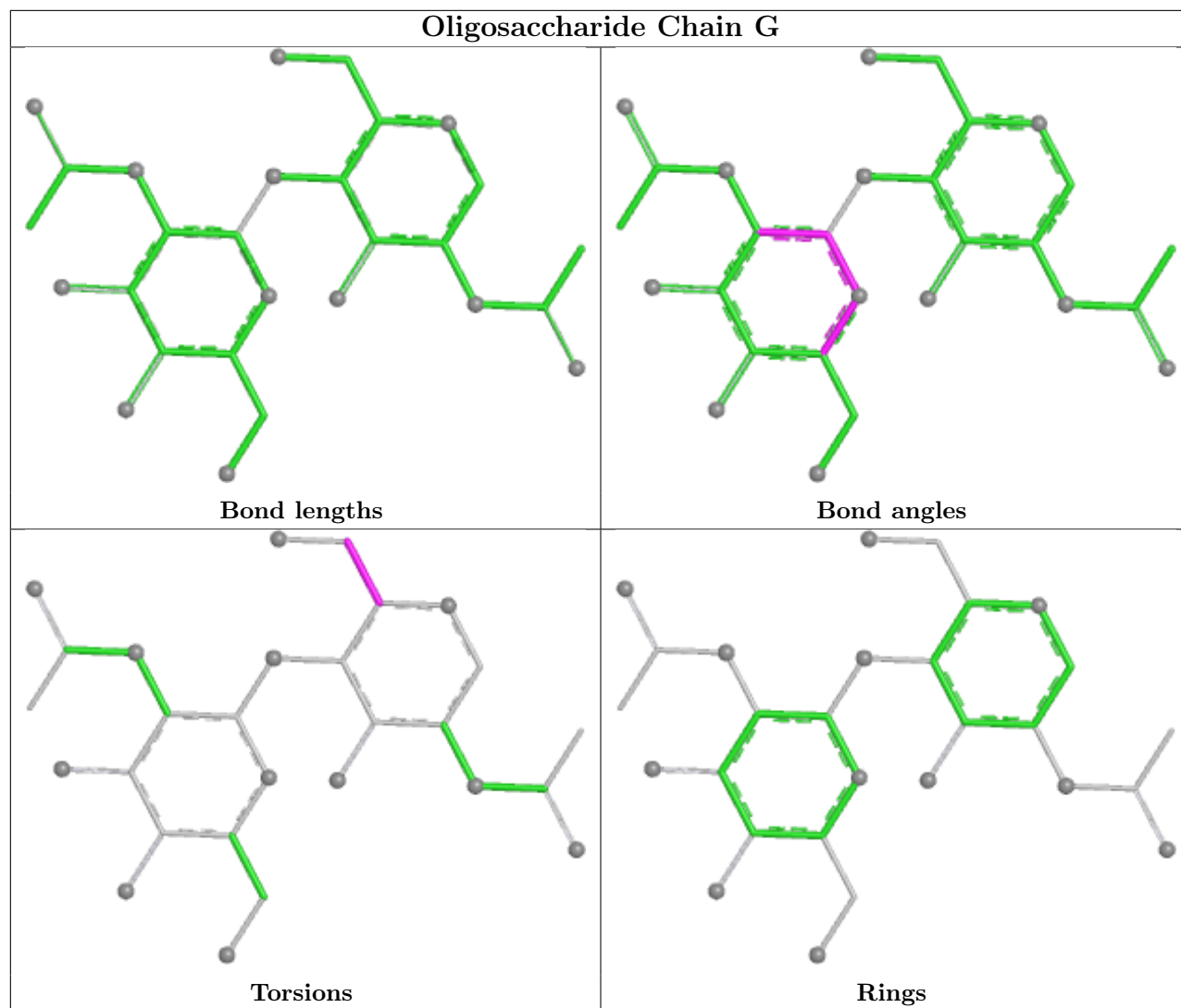
There are no ring outliers.

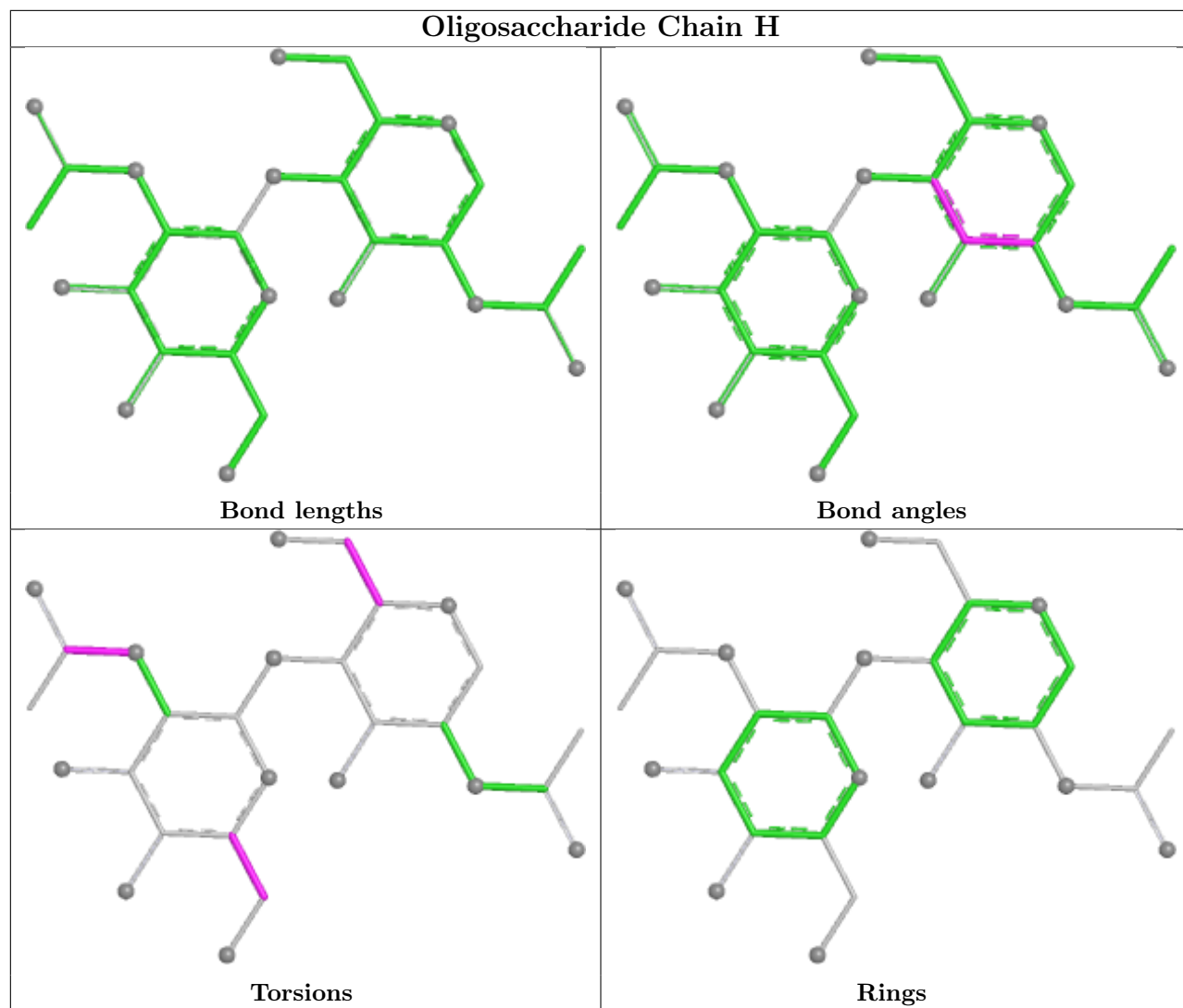
No monomer is involved in short contacts.

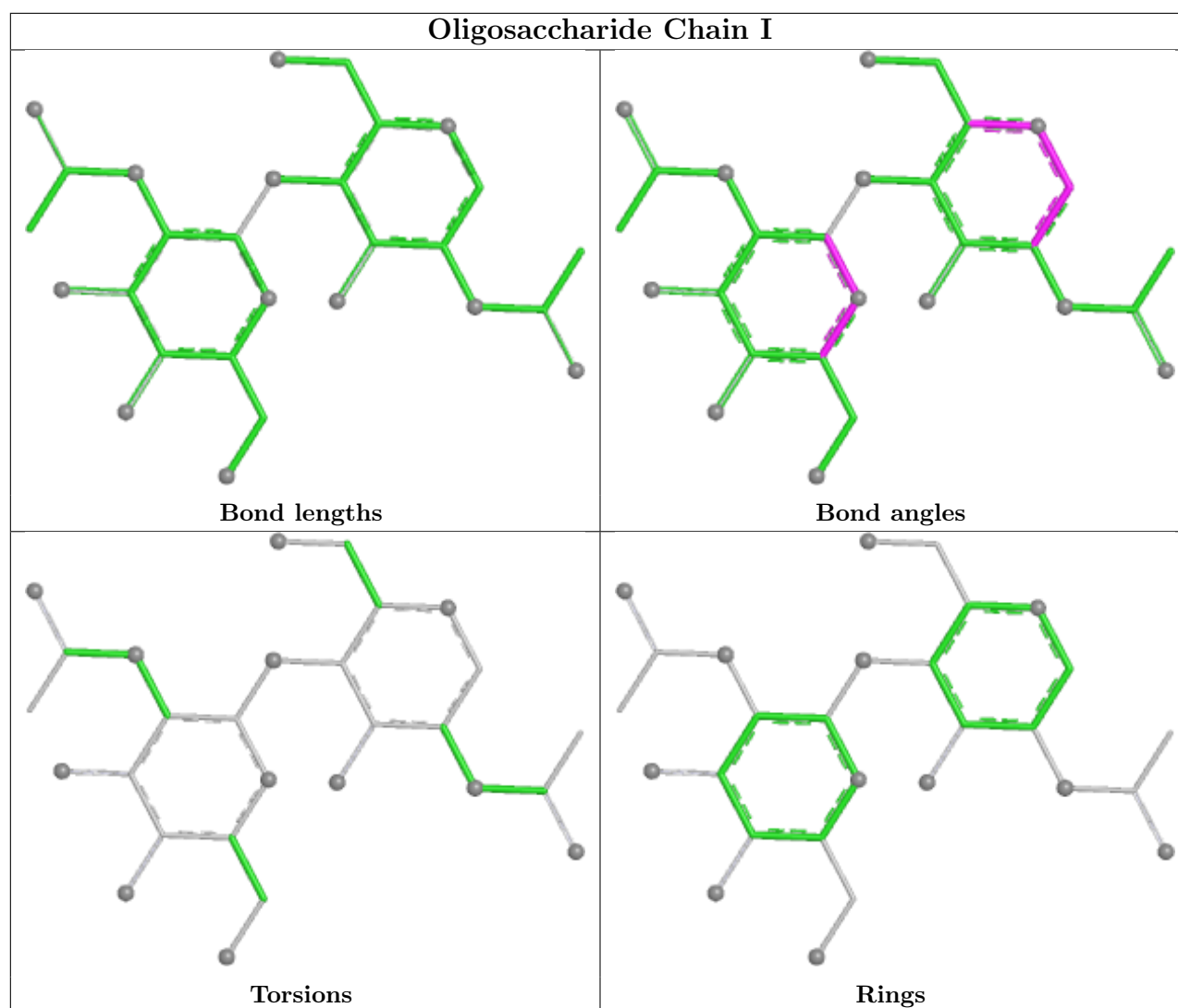
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

18 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	$\# Z > 2$
4	NAG	A	802	1	14,14,15	0.53	0	17,19,21	0.91	1 (5%)
3	XIH	B	800	-	31,32,32	2.12	3 (9%)	43,47,47	2.51	18 (41%)
4	NAG	B	803	1	14,14,15	0.62	0	17,19,21	0.96	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	C	801	1	14,14,15	0.64	0	17,19,21	1.03	1 (5%)
3	XIH	A	800	-	31,32,32	2.08	4 (12%)	43,47,47	2.56	20 (46%)
4	NAG	A	801	1	14,14,15	0.52	0	17,19,21	0.82	1 (5%)
4	NAG	B	801	1	14,14,15	0.71	0	17,19,21	1.55	3 (17%)
3	XIH	D	800	-	31,32,32	2.29	5 (16%)	43,47,47	2.41	15 (34%)
4	NAG	B	806	1	14,14,15	0.51	0	17,19,21	1.45	2 (11%)
4	NAG	C	805	1	14,14,15	0.64	0	17,19,21	1.10	1 (5%)
4	NAG	D	801	1	14,14,15	0.57	0	17,19,21	0.98	2 (11%)
3	XIH	C	800	-	31,32,32	2.27	4 (12%)	43,47,47	2.48	18 (41%)
4	NAG	C	802	1	14,14,15	0.61	0	17,19,21	0.99	1 (5%)
4	NAG	B	802	1	14,14,15	0.54	0	17,19,21	1.48	1 (5%)
4	NAG	C	806	1	14,14,15	0.53	0	17,19,21	0.96	0
4	NAG	A	808	1	14,14,15	0.56	0	17,19,21	1.13	1 (5%)
4	NAG	D	804	1	14,14,15	0.63	0	17,19,21	1.46	3 (17%)
4	NAG	A	803	1	14,14,15	0.53	0	17,19,21	0.85	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
4	NAG	A	802	1	-	0/6/23/26	0/1/1/1
3	XIH	B	800	-	-	3/10/20/20	0/4/4/4
4	NAG	B	803	1	-	0/6/23/26	0/1/1/1
4	NAG	C	801	1	-	0/6/23/26	0/1/1/1
3	XIH	A	800	-	-	4/10/20/20	0/4/4/4
4	NAG	A	801	1	-	2/6/23/26	0/1/1/1
4	NAG	B	801	1	-	4/6/23/26	0/1/1/1
3	XIH	D	800	-	-	4/10/20/20	0/4/4/4
4	NAG	B	806	1	-	4/6/23/26	0/1/1/1
4	NAG	C	805	1	-	2/6/23/26	0/1/1/1
4	NAG	D	801	1	-	2/6/23/26	0/1/1/1
3	XIH	C	800	-	-	3/10/20/20	0/4/4/4
4	NAG	C	802	1	-	2/6/23/26	0/1/1/1
4	NAG	B	802	1	-	0/6/23/26	0/1/1/1
4	NAG	C	806	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	808	1	-	2/6/23/26	0/1/1/1
4	NAG	D	804	1	1/1/5/7	4/6/23/26	0/1/1/1
4	NAG	A	803	1	-	2/6/23/26	0/1/1/1

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	800	XIH	C23-C24	-10.61	1.29	1.44
3	D	800	XIH	C23-C24	-10.58	1.29	1.44
3	B	800	XIH	C23-C24	-9.92	1.30	1.44
3	A	800	XIH	C23-C24	-9.60	1.30	1.44
3	D	800	XIH	C5-C6	3.31	1.47	1.37

The worst 5 of 89 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	800	XIH	C18-C17-N16	6.24	120.68	113.14
3	A	800	XIH	N9-C8-N7	-6.06	116.03	124.93
3	B	800	XIH	C10-N9-C15	6.00	124.64	113.07
3	D	800	XIH	N9-C8-N7	-5.96	116.18	124.93
3	A	800	XIH	C10-N9-C15	5.90	124.45	113.07

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	D	804	NAG	C1

5 of 40 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	800	XIH	N7-C8-N9-C15
3	A	800	XIH	N16-C8-N9-C15
3	B	800	XIH	N7-C8-N9-C15
3	B	800	XIH	N16-C8-N9-C15
3	C	800	XIH	N7-C8-N9-C15

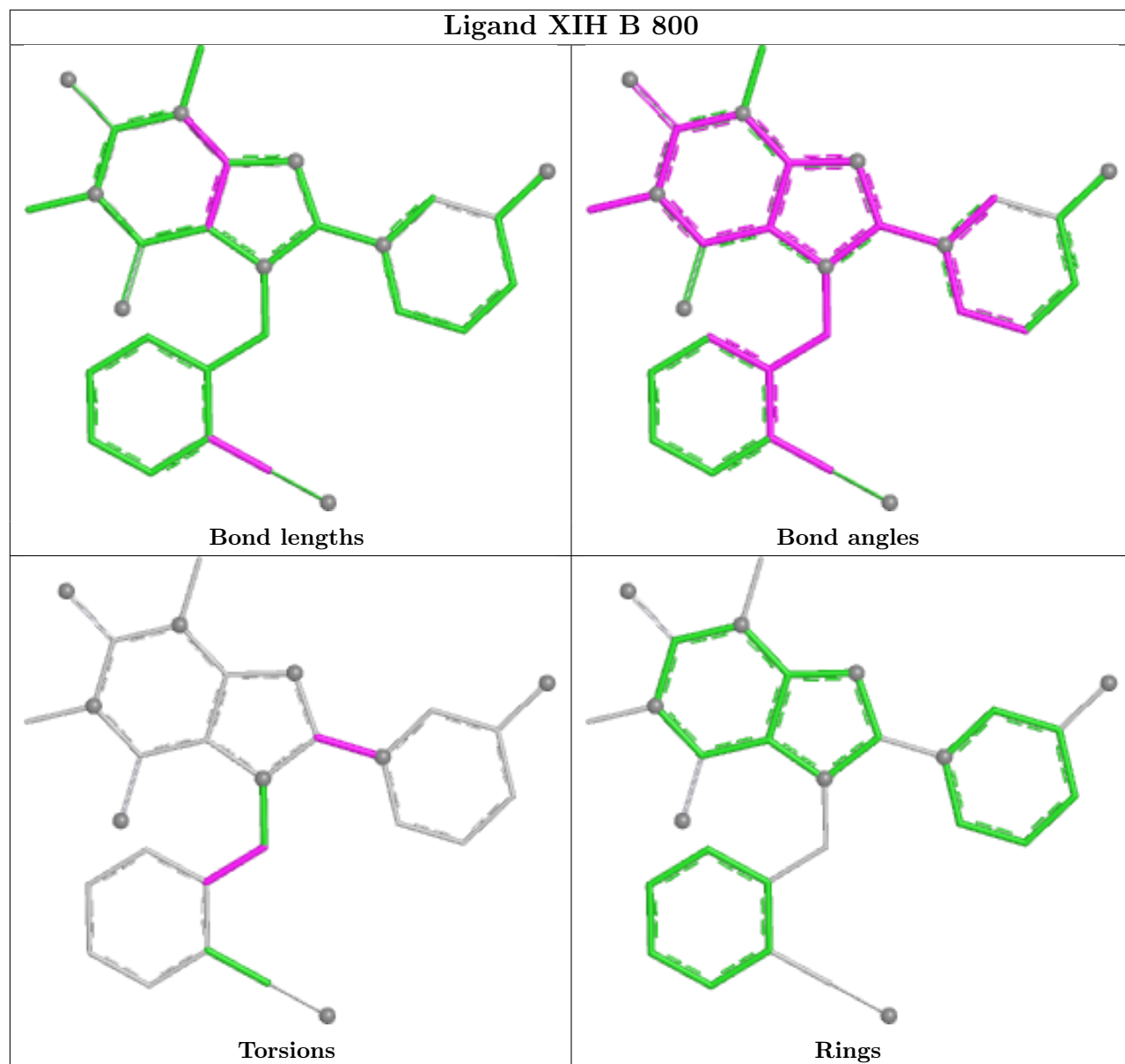
There are no ring outliers.

2 monomers are involved in 2 short contacts:

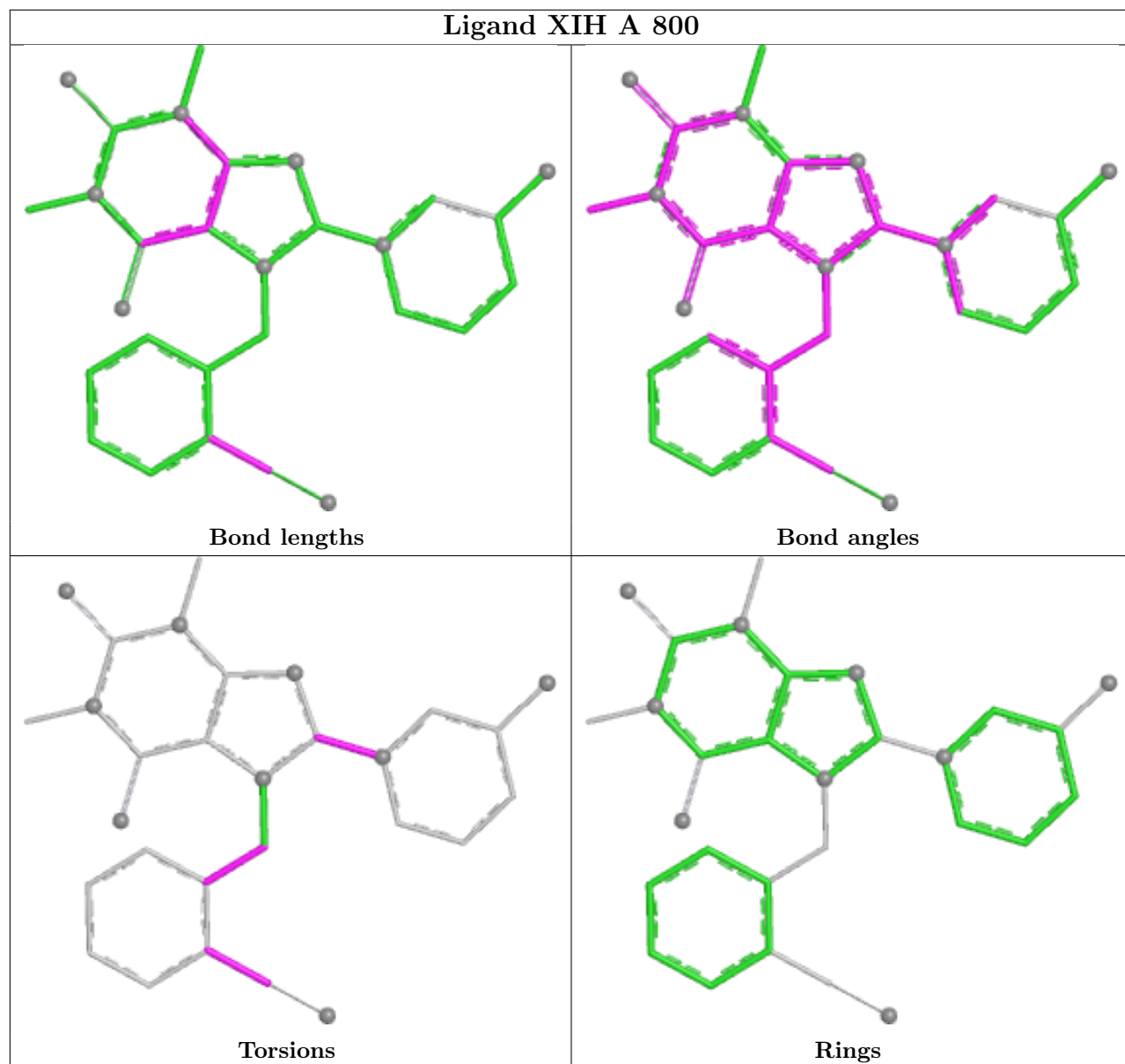
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	800	XIH	1	0
3	C	800	XIH	1	0

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.

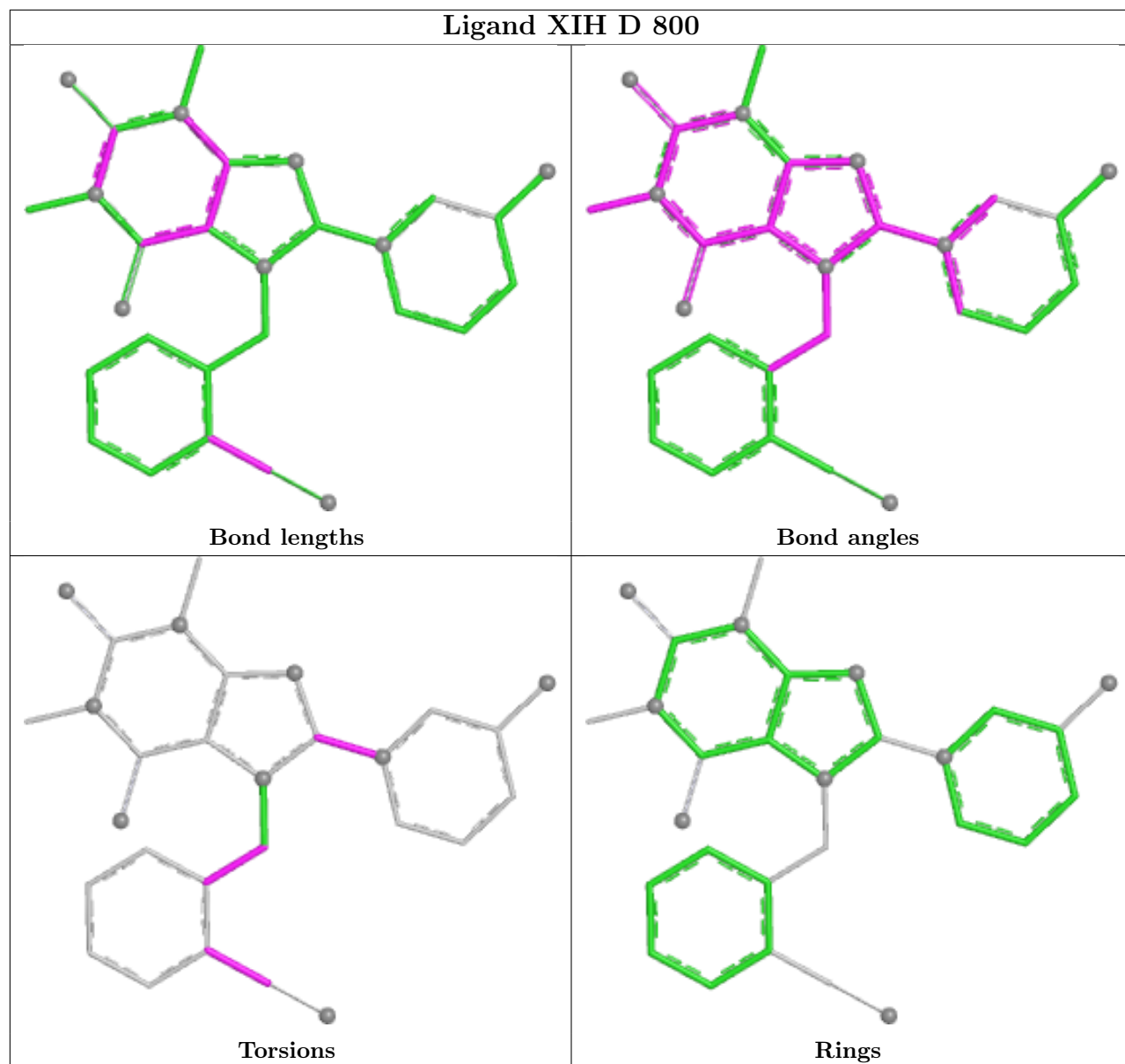
Ligand XIH B 800

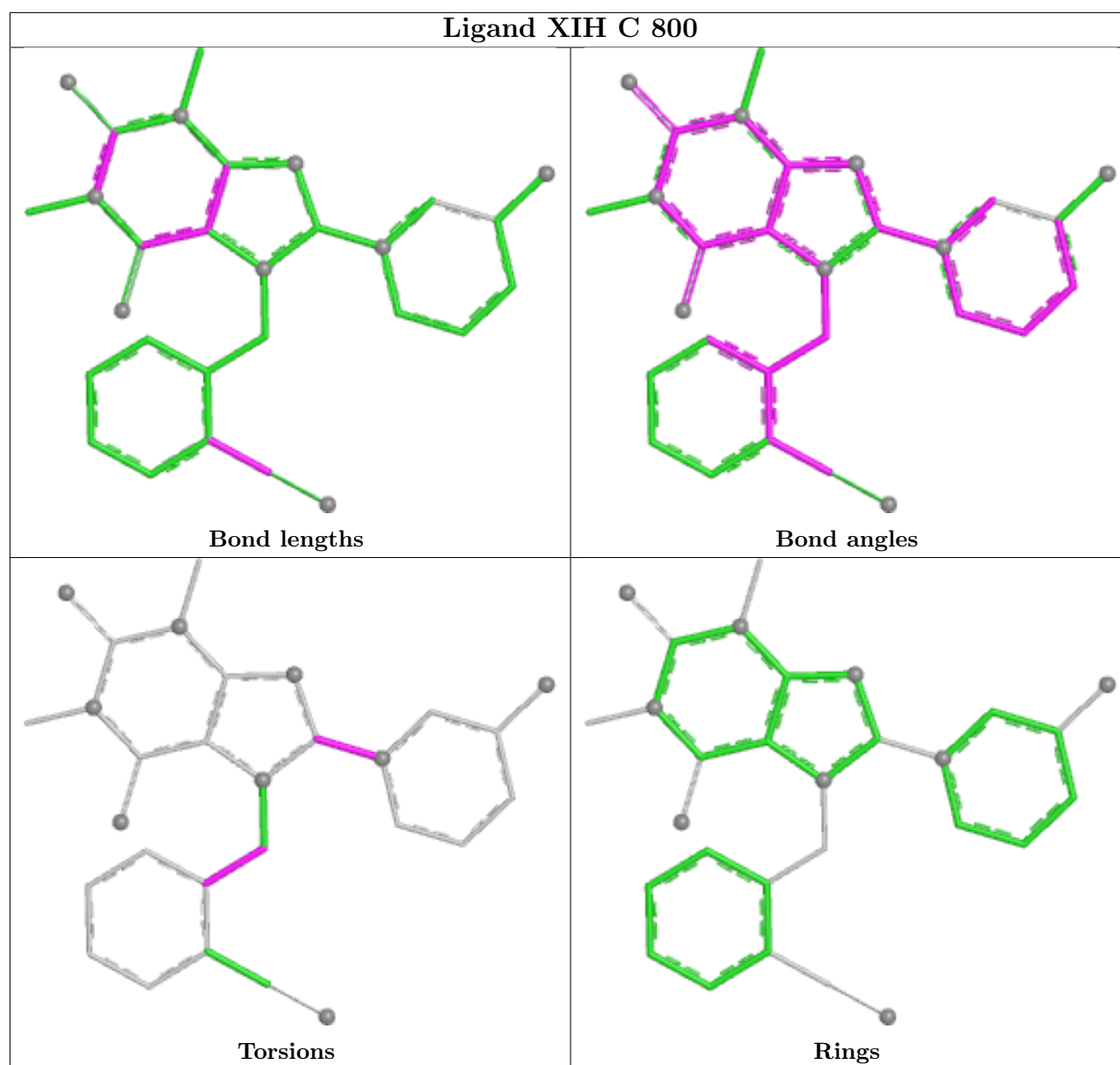


Ligand XIX A 800



Ligand XIX D 800





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](#)

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	723/740 (97%)	0.72	49 (6%)	23 20	31, 48, 74, 104	3 (0%)
1	B	728/740 (98%)	0.74	35 (4%)	35 32	30, 49, 72, 93	3 (0%)
1	C	723/740 (97%)	0.80	63 (8%)	16 13	29, 49, 73, 93	1 (0%)
1	D	723/740 (97%)	1.24	154 (21%)	2 2	38, 54, 82, 118	0
All	All	2897/2960 (97%)	0.88	301 (10%)	11 9	29, 50, 76, 118	7 (0%)

The worst 5 of 301 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	81	ALA	6.5
1	D	90	LEU	5.9
1	D	88	VAL	5.3
1	D	322	TYR	4.9
1	D	337	TRP	4.9

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.

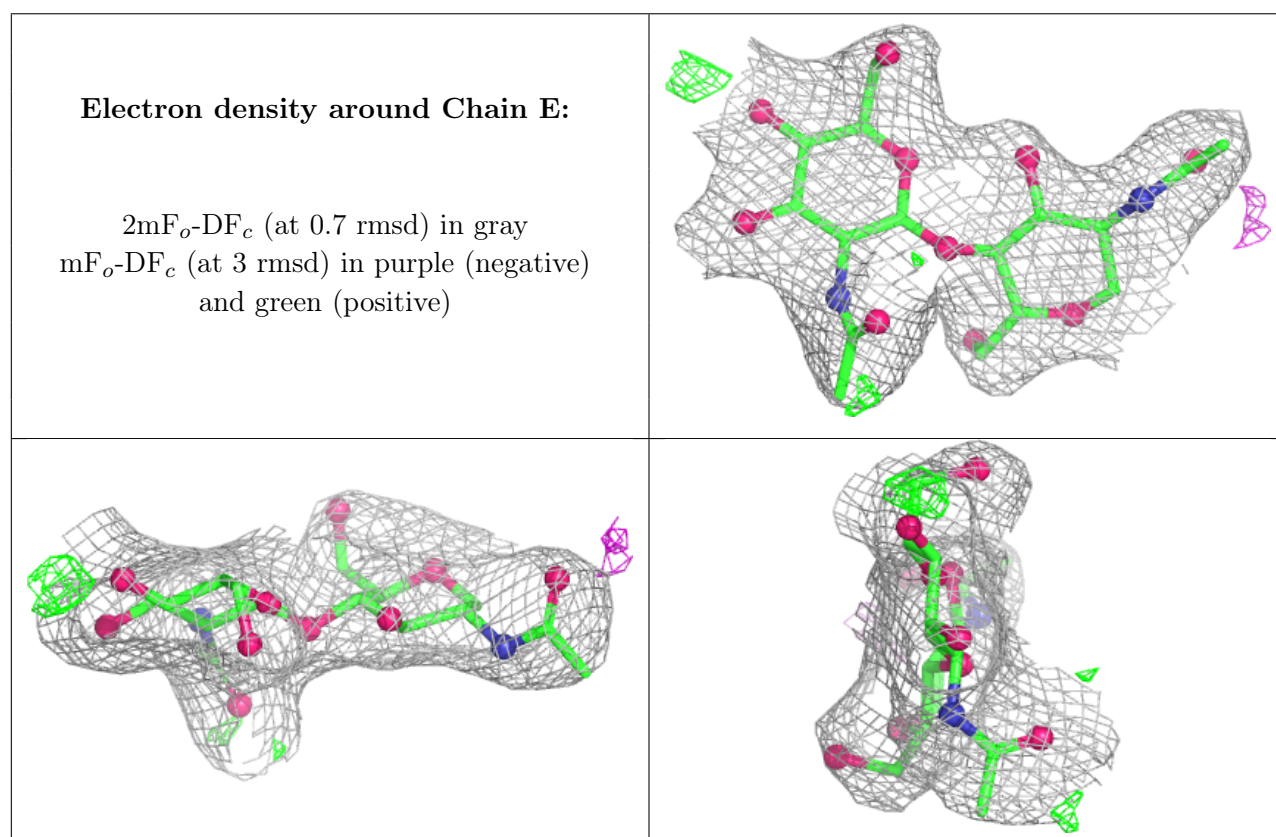
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	F	1	14/15	0.63	0.17	80,84,85,87	0
2	NAG	G	2	14/15	0.65	0.13	77,79,80,80	0

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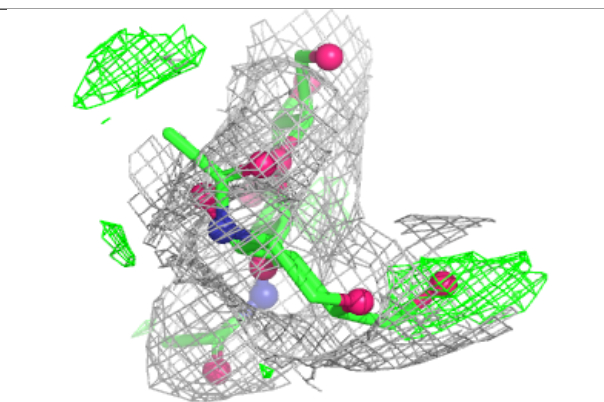
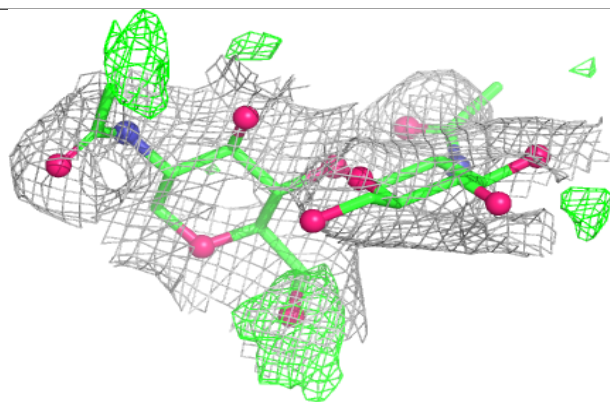
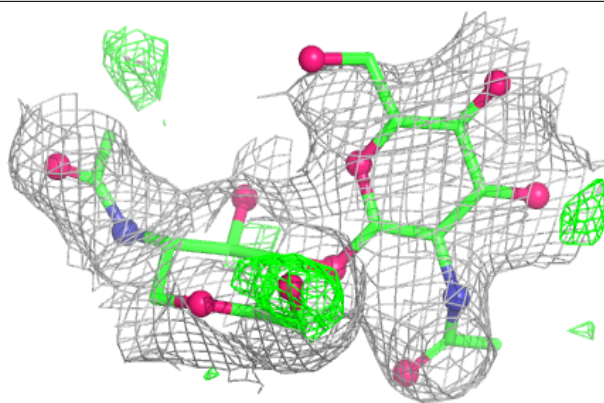
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	F	2	14/15	0.71	0.15	90,91,92,92	0
2	NAG	H	2	14/15	0.81	0.12	73,75,77,77	0
2	NAG	E	2	14/15	0.82	0.11	67,68,69,69	0
2	NAG	H	1	14/15	0.85	0.12	60,63,66,70	0
2	NAG	I	2	14/15	0.85	0.11	73,75,76,77	0
2	NAG	E	1	14/15	0.88	0.12	56,59,62,65	0
2	NAG	I	1	14/15	0.88	0.12	60,63,65,69	0
2	NAG	G	1	14/15	0.88	0.11	62,65,69,73	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.

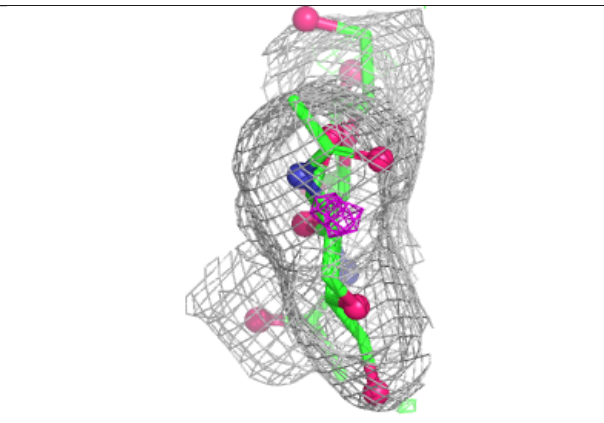
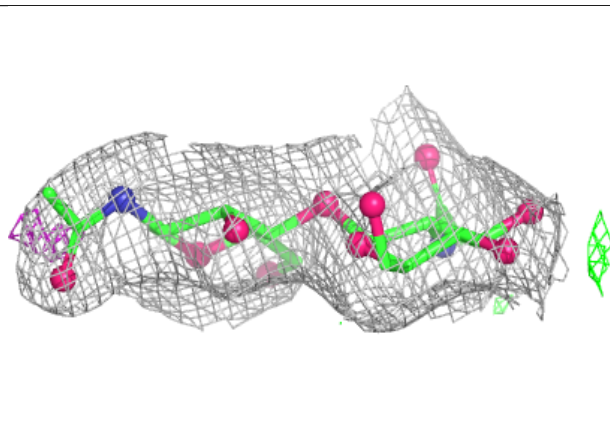
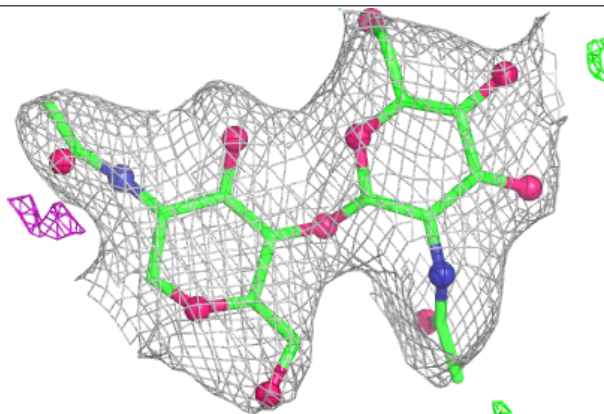


Electron density around Chain F:

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

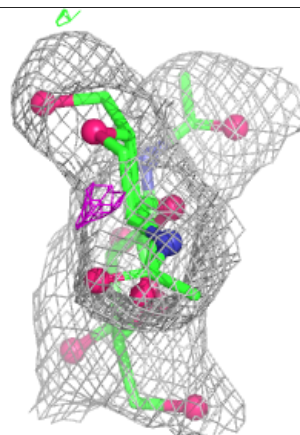
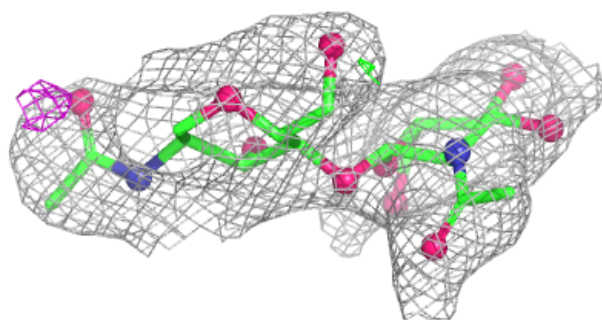
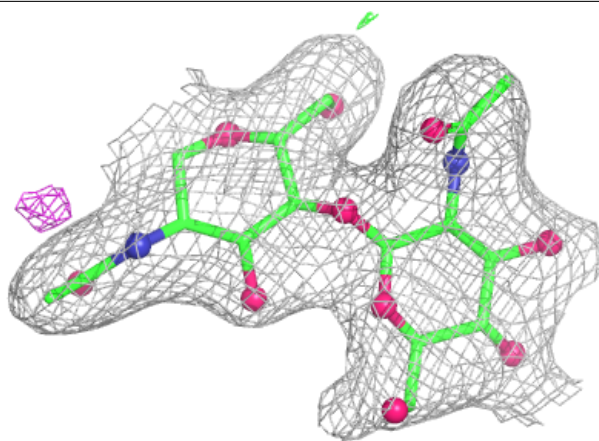
**Electron density around Chain G:**

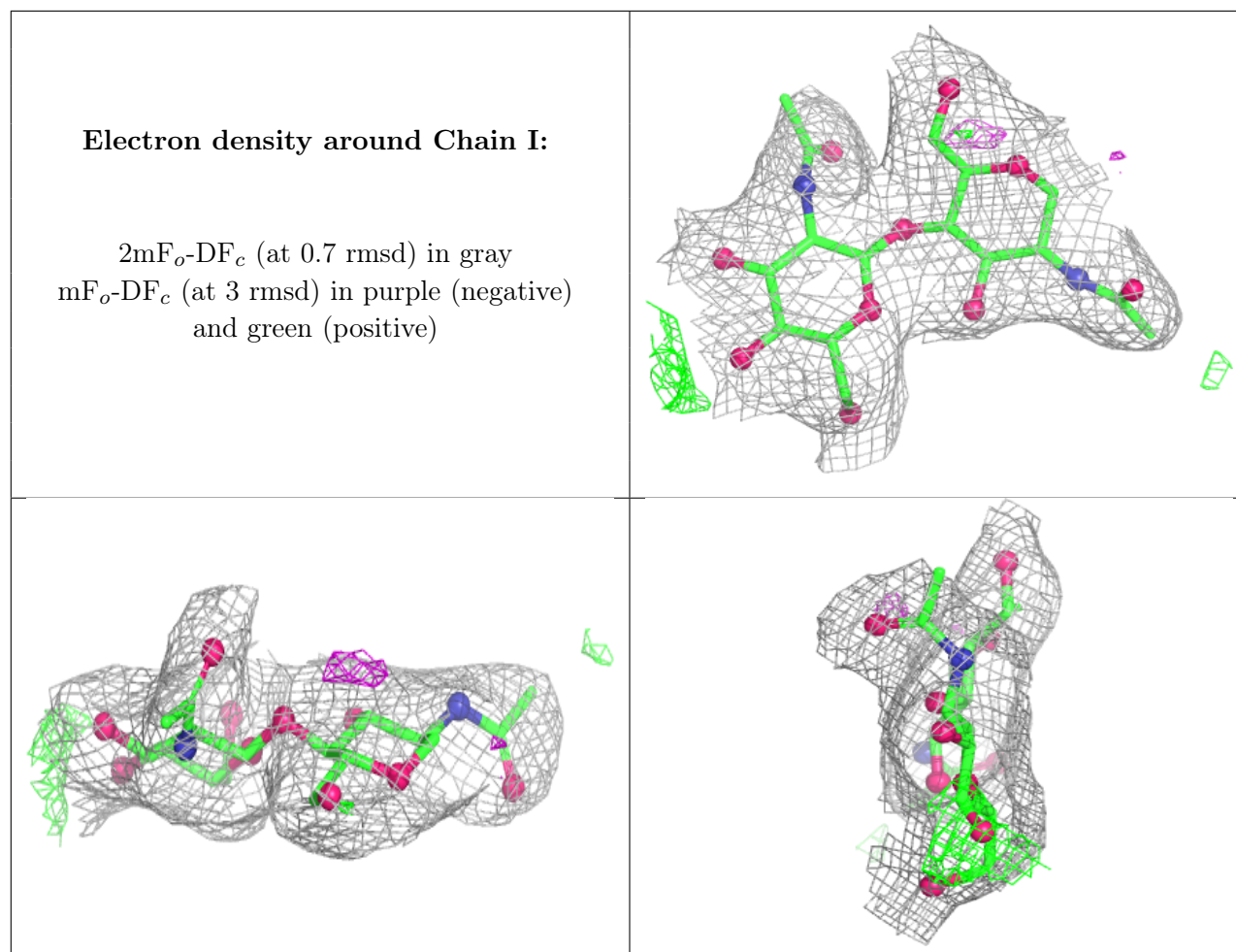
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	A	801	14/15	0.52	0.17	95,95,96,96	0
4	NAG	A	802	14/15	0.52	0.17	75,78,79,79	0
4	NAG	D	804	14/15	0.54	0.17	81,83,85,85	0
4	NAG	B	801	14/15	0.58	0.18	79,80,81,81	0
4	NAG	C	805	14/15	0.68	0.15	78,81,82,82	0
4	NAG	B	806	14/15	0.70	0.15	69,71,74,74	0
4	NAG	A	803	14/15	0.71	0.14	69,72,76,77	0
4	NAG	D	801	14/15	0.73	0.14	65,67,68,69	0
4	NAG	C	801	14/15	0.74	0.14	60,60,61,62	0
4	NAG	C	806	14/15	0.78	0.15	68,73,74,74	0
4	NAG	B	802	14/15	0.79	0.12	67,68,69,70	0

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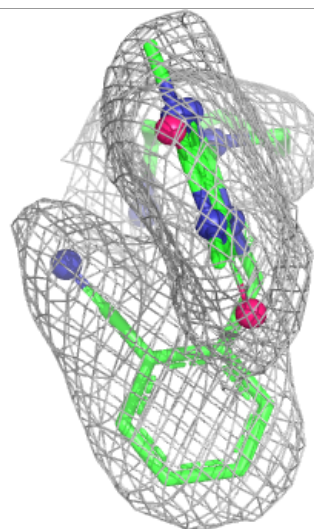
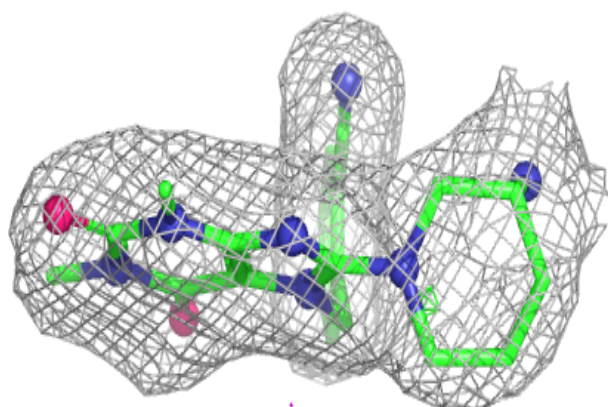
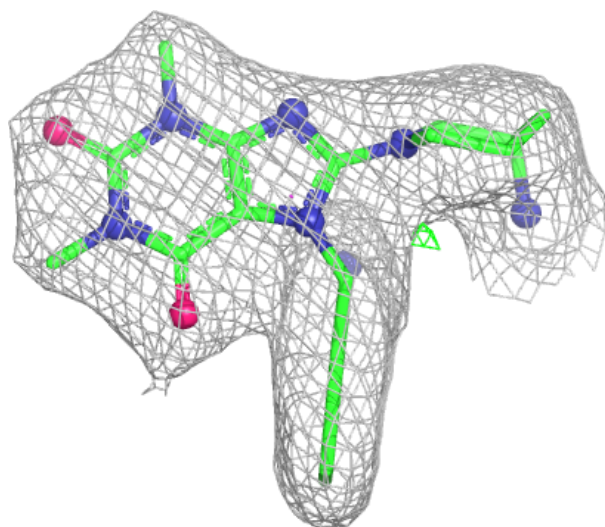
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	B	803	14/15	0.79	0.13	64,67,70,71	0
4	NAG	C	802	14/15	0.83	0.12	70,72,75,75	0
4	NAG	A	808	14/15	0.88	0.10	62,66,68,68	0
3	XIH	D	800	29/29	0.95	0.09	40,42,43,45	0
3	XIH	B	800	29/29	0.95	0.10	35,39,40,41	0
3	XIH	C	800	29/29	0.95	0.09	35,37,38,39	0
3	XIH	A	800	29/29	0.96	0.10	38,43,44,44	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.

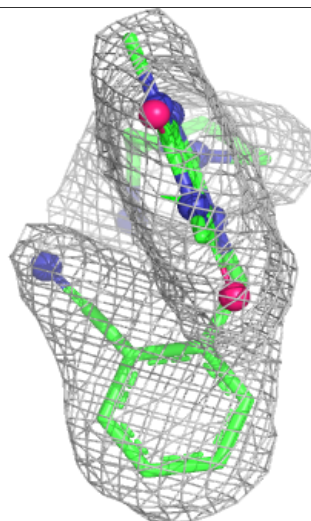
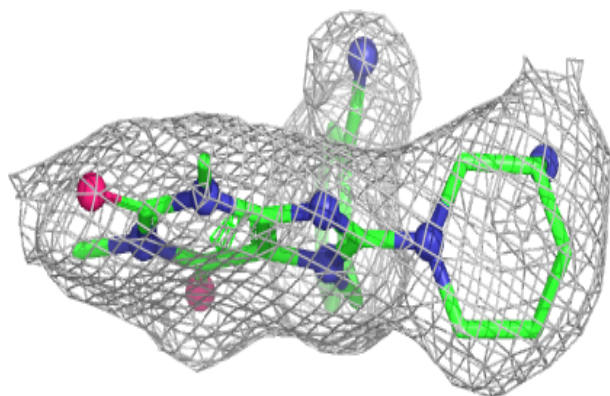
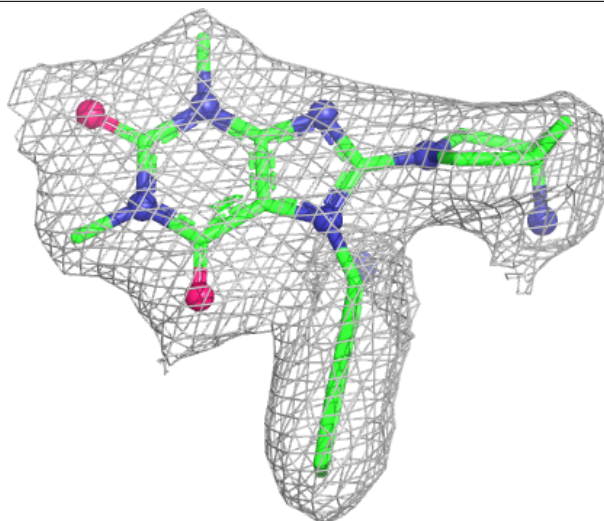
Electron density around XIH D 800:

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



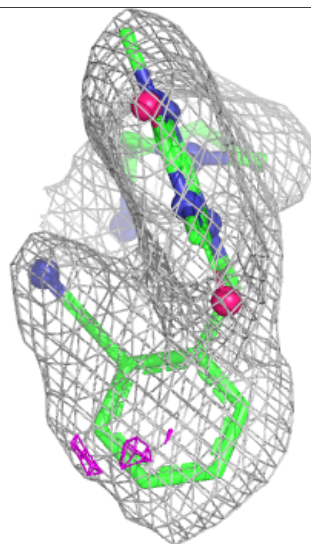
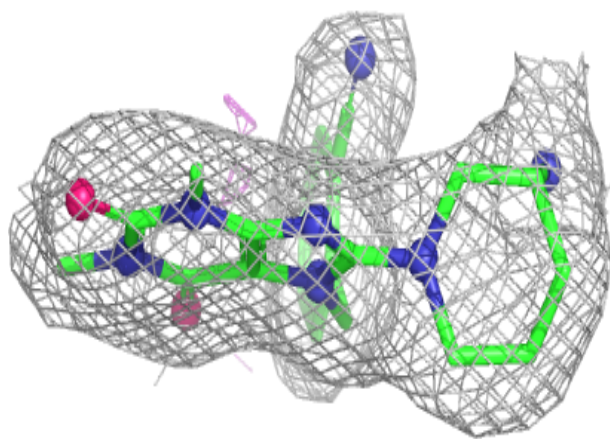
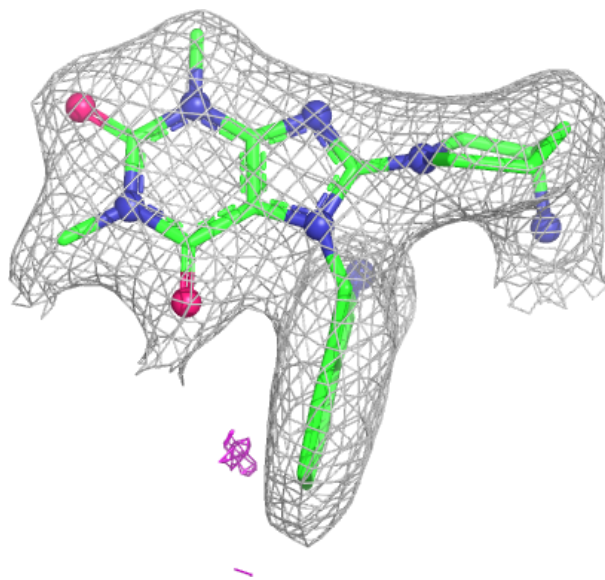
Electron density around XIH B 800:

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



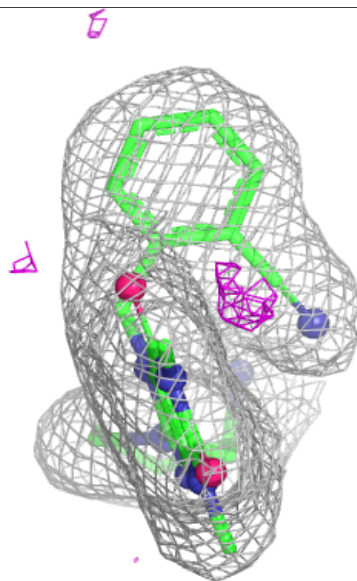
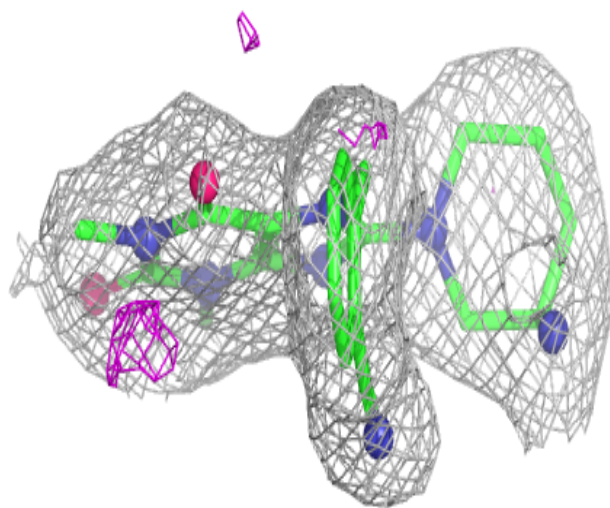
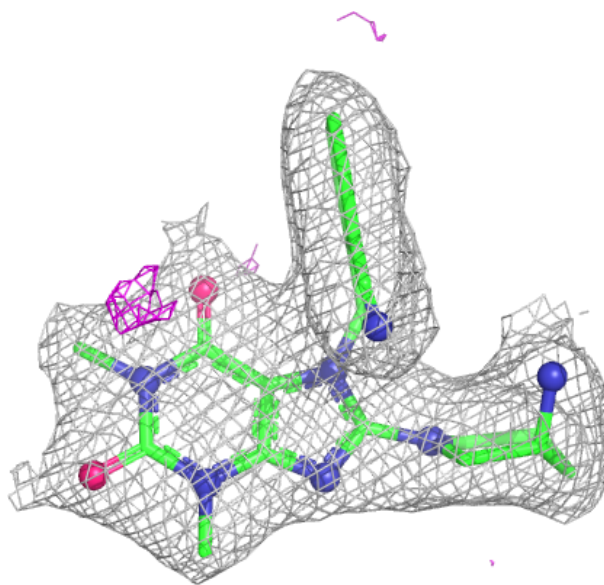
Electron density around XIH C 800:

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



Electron density around XIH A 800:

$2mF_o-DF_c$ (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.