



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 09:53 PM UTC

PDB ID : 4PNZ / pdb_00004pnz
Title : Human dipeptidyl peptidase IV/CD26 in complex with the long-acting inhibitor Omarigliptin (MK-3102)
Authors : Scapin, G.; Yan, Y.
Deposited on : 2014-02-22
Resolution : 1.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

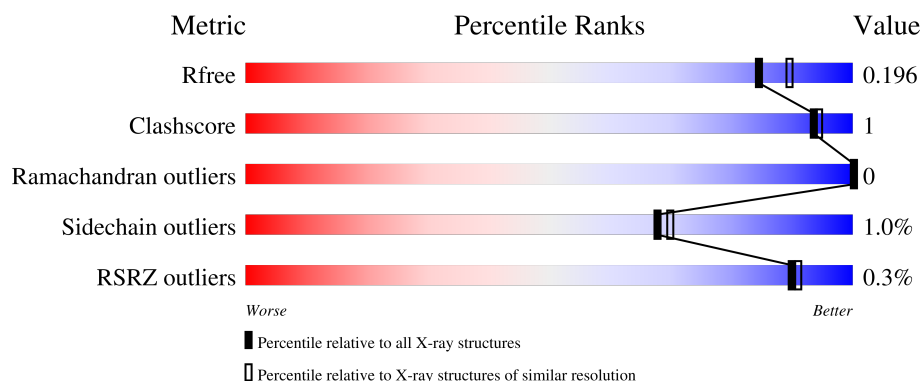
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	728	95%5%
1	B	728	95%5%
2	C	2	100%
2	D	2	50%50%
2	E	2	100%

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

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13862 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	728	Total	C	N	O	S	0	3	0
			5973	3833	983	1131	26			
1	B	727	Total	C	N	O	S	0	1	0
			5956	3822	980	1128	26			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	39	THR	SER	engineered mutation	UNP P27487
B	39	THR	SER	engineered mutation	UNP P27487

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

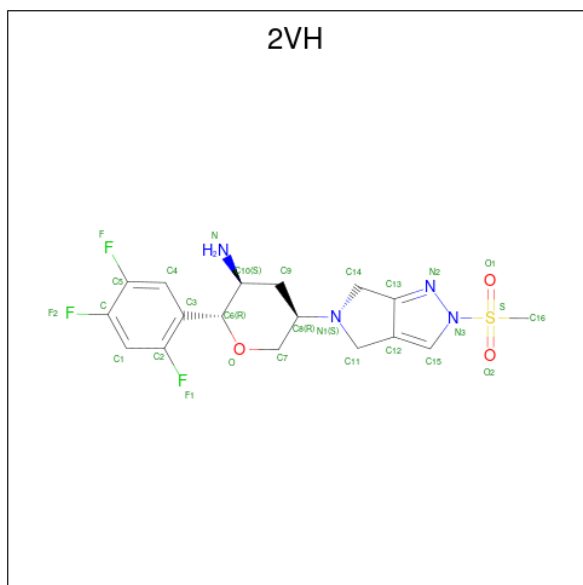


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	D	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	G	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		

- Molecule 4 is (2R,3S,5R)-5-[2-(methylsulfonyl)-2,6-dihydropyrrolo[3,4-c]pyrazol-5(4H)-yl]-2-(2,4,5-trifluorophenyl)tetrahydro-2H-pyran-3-amine (CCD ID: 2VH) (formula: C₁₇H₁₉F₃N₄O₃S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	F	N	O	S	0	0
			28	17	3	4	3	1		
4	B	1	Total	C	F	N	O	S	0	0
			28	17	3	4	3	1		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

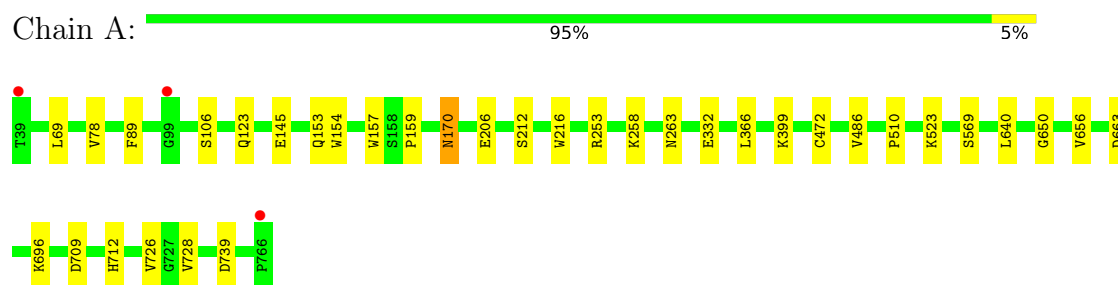
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	808	Total	O	0	0
			808	808		
6	B	816	Total	O	0	0
			816	816		

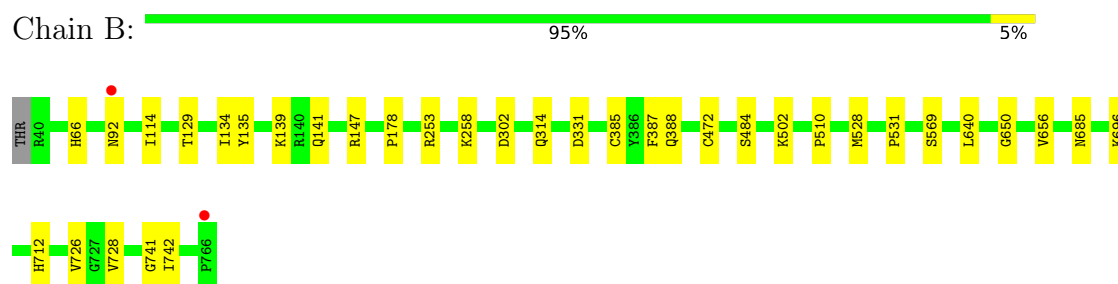
3 Residue-property plots [i](#)

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.

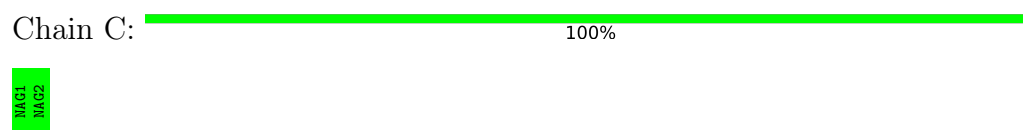
- Molecule 1: Dipeptidyl peptidase 4



- 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



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

Chain E:  100%

MAG1
MAG2

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

Chain F:  50%  50%

MAG1
MAG2

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

Chain G:  100%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	117.94Å 125.78Å 137.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.15 – 1.90 19.15 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (19.15-1.90) 99.6 (19.15-1.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.82 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.2.0019, BUSTER 2.11.5	Depositor
R, R_{free}	0.166 , 0.197 0.164 , 0.196	Depositor DCC
R_{free} test set	7998 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	22.7	Xtriage
Anisotropy	0.376	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 50.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	13862	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% 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: 2VH, NAG, NA

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	0.83	1/6156 (0.0%)	1.01	3/8373 (0.0%)
1	B	0.83	2/6132 (0.0%)	1.03	8/8340 (0.1%)
All	All	0.83	3/12288 (0.0%)	1.02	11/16713 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	123	GLN	CA-C	7.91	1.56	1.52
1	B	531	PRO	CA-C	7.01	1.55	1.51
1	B	528	MET	SD-CE	-5.03	1.67	1.79

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	92	ASN	OD1-CG-ND2	-7.78	114.82	122.60
1	B	331	ASP	CA-C-N	5.83	128.90	120.38
1	B	331	ASP	C-N-CA	5.83	128.90	120.38
1	B	92	ASN	CA-CB-CG	5.46	118.06	112.60
1	B	388	GLN	N-CA-C	-5.44	100.83	109.96
1	B	92	ASN	CB-CG-ND2	5.23	124.24	116.40
1	A	656	VAL	N-CA-C	-5.17	102.91	109.58
1	B	387	PHE	CA-CB-CG	5.12	118.92	113.80
1	A	739	ASP	CA-CB-CG	5.12	117.72	112.60
1	B	656	VAL	N-CA-C	-5.11	102.26	109.21
1	A	486	VAL	N-CA-CB	5.09	116.16	110.51

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	5973	0	5683	17	0
1	B	5956	0	5663	16	0
2	C	28	0	25	0	0
2	D	28	0	25	0	0
2	E	28	0	25	0	0
2	F	28	0	25	0	0
2	G	28	0	25	0	0
3	A	1	0	0	0	0
4	A	28	0	19	0	0
4	B	28	0	19	0	0
5	A	42	0	39	0	0
5	B	70	0	65	2	0
6	A	808	0	0	0	0
6	B	816	0	0	4	0
All	All	13862	0	11613	33	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 1.

All (33) 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:78:VAL:HG23	1:A:89:PHE:HB2	1.69	0.75
1:A:253:ARG:HH21	1:B:253:ARG:HH21	1.35	0.73
1:B:696:LYS:HG3	1:B:728:VAL:HG22	1.75	0.67
1:B:258:LYS:NZ	1:B:712:HIS:HD2	1.93	0.66
1:A:69:LEU:HD23	1:A:78:VAL:HG22	1.78	0.66
1:B:129:THR:HG21	6:B:1224:HOH:O	2.01	0.59
1:A:258:LYS:NZ	1:A:712:HIS:HD2	2.01	0.59
1:A:640:LEU:HD11	1:A:650:GLY:HA3	1.85	0.59
1:A:69:LEU:CD2	1:A:78:VAL:HG22	2.34	0.57
1:B:129:THR:HG22	6:B:1215:HOH:O	2.04	0.56
1:B:114:ILE:HG23	1:B:135:TYR:HB3	1.90	0.54
1:A:696:LYS:HG3	1:A:728:VAL:HG22	1.89	0.54
1:B:258:LYS:HZ1	1:B:712:HIS:HD2	1.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:726:VAL:HG23	1:B:728:VAL:HG23	1.91	0.52
1:A:726:VAL:HG23	1:A:728:VAL:HG23	1.91	0.51
1:A:153:GLN:HE22	1:A:170:ASN:ND2	2.10	0.49
5:B:809:NAG:H83	6:B:1230:HOH:O	2.13	0.49
1:B:302:ASP:HB3	1:B:314:GLN:HB2	1.95	0.47
1:B:640:LEU:HD11	1:B:650:GLY:HA3	1.97	0.46
1:B:147:ARG:HE	5:B:804:NAG:H83	1.80	0.45
1:A:154:TRP:CE2	1:A:212[A]:SER:HB3	2.52	0.45
1:A:170:ASN:HD22	1:A:170:ASN:N	2.17	0.43
1:B:66:HIS:HB2	6:B:1501:HOH:O	2.19	0.43
1:B:139:LYS:HB3	1:B:141:GLN:HE21	1.83	0.43
1:A:106:SER:HG	1:A:157:TRP:CD1	2.38	0.42
1:A:159:PRO:HD3	1:A:216:TRP:HB3	2.01	0.42
1:A:258:LYS:HZ3	1:A:712:HIS:HD2	1.66	0.42
1:B:510:PRO:HD3	1:B:569:SER:HB2	2.01	0.42
1:A:206:GLU:OE2	1:A:663:ASP:OD2	2.39	0.41
1:A:510:PRO:HD3	1:A:569:SER:HB2	2.02	0.41
1:B:741:GLY:O	1:B:742:ILE:C	2.64	0.41
1:A:709:ASP:O	1:A:712:HIS:HE1	2.04	0.40
1:B:134:ILE:HD13	1:B:178:PRO:HB3	2.03	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	729/728 (100%)	706 (97%)	23 (3%)	0	100	100
1	B	726/728 (100%)	703 (97%)	23 (3%)	0	100	100
All	All	1455/1456 (100%)	1409 (97%)	46 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	655/653 (100%)	647 (99%)	8 (1%)	63	63
1	B	652/653 (100%)	647 (99%)	5 (1%)	73	75
All	All	1307/1306 (100%)	1294 (99%)	13 (1%)	68	70

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

Mol	Chain	Res	Type
1	A	145	GLU
1	A	170	ASN
1	A	263	ASN
1	A	332	GLU
1	A	366	LEU
1	A	399	LYS
1	A	472	CYS
1	A	523	LYS
1	B	385	CYS
1	B	472	CYS
1	B	484	SER
1	B	502	LYS
1	B	685	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	138	ASN
1	A	169	ASN
1	A	170	ASN
1	A	227	GLN
1	A	263	ASN
1	A	314	GLN
1	A	338	ASN
1	A	572	ASN
1	A	606	GLN

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Mol	Chain	Res	Type
1	A	685	ASN
1	A	694	ASN
1	A	712	HIS
1	A	731	GLN
1	B	72	GLN
1	B	141	GLN
1	B	169	ASN
1	B	338	ASN
1	B	345	HIS
1	B	388	GLN
1	B	430	ASN
1	B	533	HIS
1	B	606	GLN
1	B	694	ASN
1	B	712	HIS
1	B	761	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	C	1	1,2	14,14,15	0.28	0	17,19,21	0.84	0
2	NAG	C	2	2	14,14,15	0.29	0	17,19,21	0.53	0
2	NAG	D	1	1,2	14,14,15	0.32	0	17,19,21	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	D	2	2	14,14,15	0.33	0	17,19,21	0.81	1 (5%)
2	NAG	E	1	1,2	14,14,15	0.30	0	17,19,21	2.34	4 (23%)
2	NAG	E	2	2	14,14,15	0.38	0	17,19,21	1.44	2 (11%)
2	NAG	F	1	1,2	14,14,15	0.30	0	17,19,21	0.60	0
2	NAG	F	2	2	14,14,15	0.30	0	17,19,21	0.70	1 (5%)
2	NAG	G	1	1,2	14,14,15	0.35	0	17,19,21	0.69	0
2	NAG	G	2	2	14,14,15	0.30	0	17,19,21	0.49	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
2	NAG	C	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	NAG	D	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1
2	NAG	E	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	E	2	2	-	1/6/23/26	0/1/1/1
2	NAG	F	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	0/6/23/26	0/1/1/1
2	NAG	G	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1	NAG	C1-O5-C5	8.10	123.04	112.19
2	E	2	NAG	C1-O5-C5	5.05	118.95	112.19
2	E	1	NAG	O5-C1-C2	3.27	116.36	111.29
2	E	2	NAG	O5-C1-C2	2.63	115.36	111.29
2	F	2	NAG	C1-O5-C5	2.30	115.27	112.19
2	D	2	NAG	C1-C2-N2	2.23	113.95	110.43
2	E	1	NAG	O4-C4-C5	-2.14	104.05	109.32
2	E	1	NAG	C3-C4-C5	2.11	114.06	110.23

There are no chirality outliers.

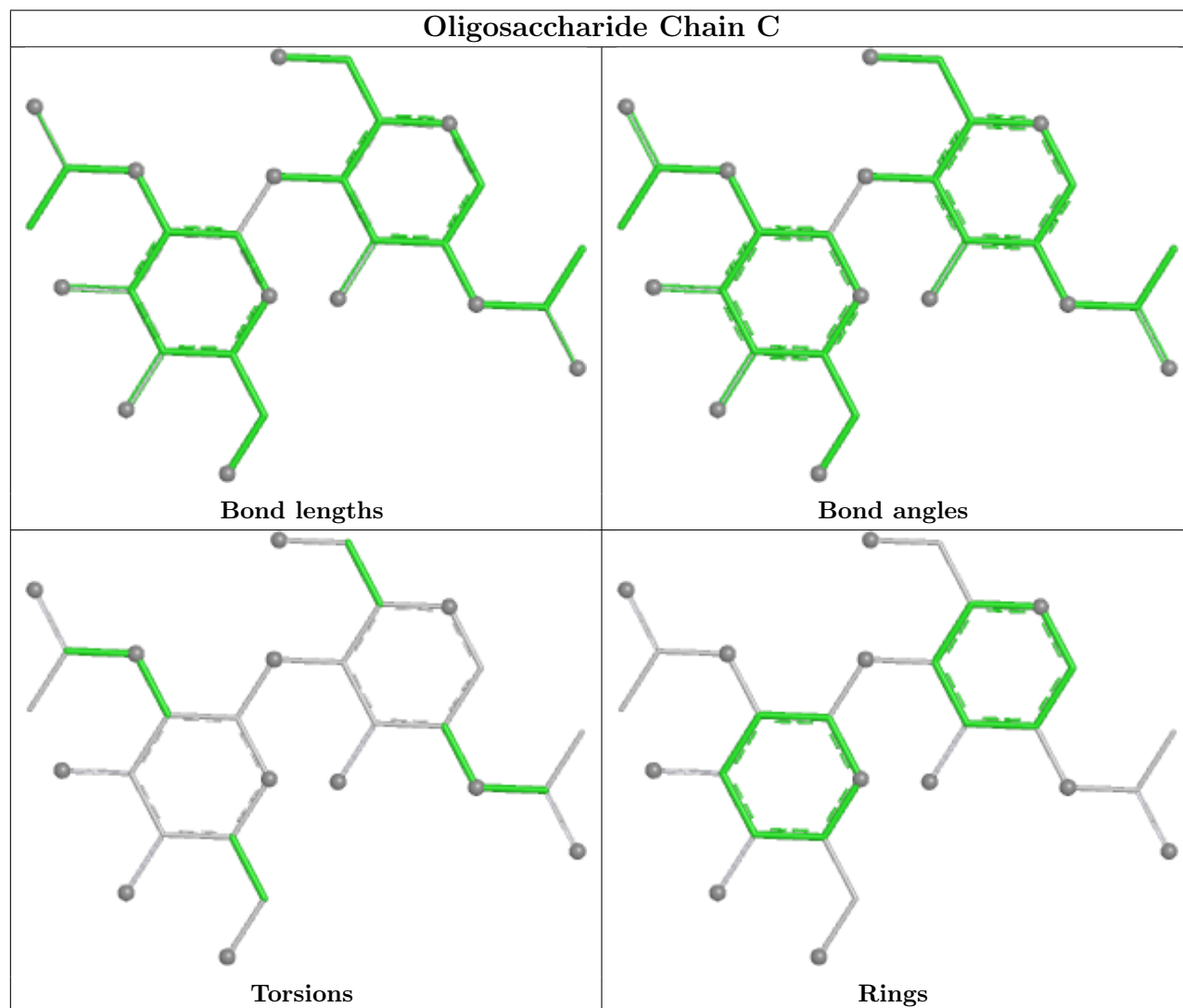
All (2) torsion outliers are listed below:

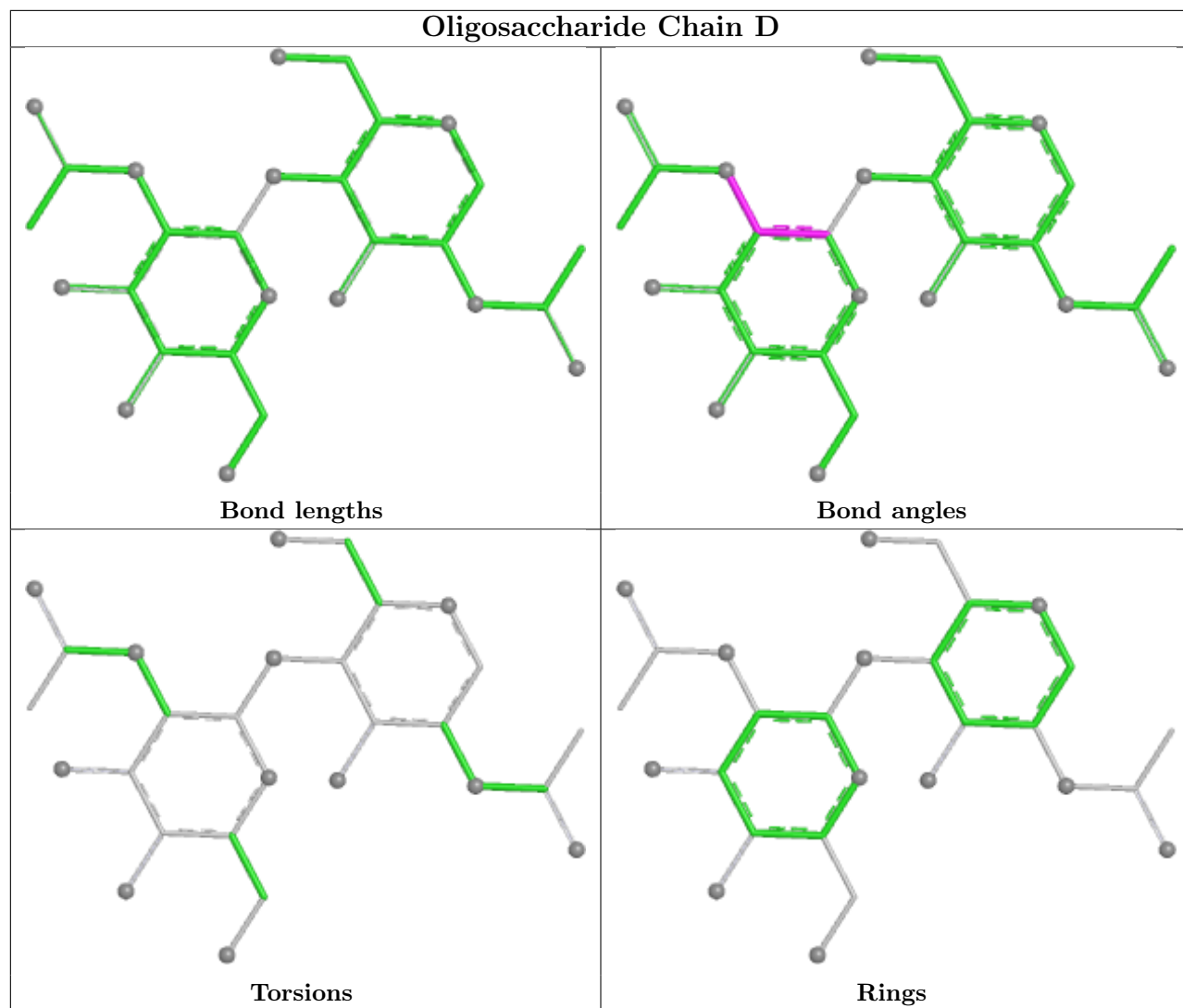
Mol	Chain	Res	Type	Atoms
2	E	1	NAG	O5-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6

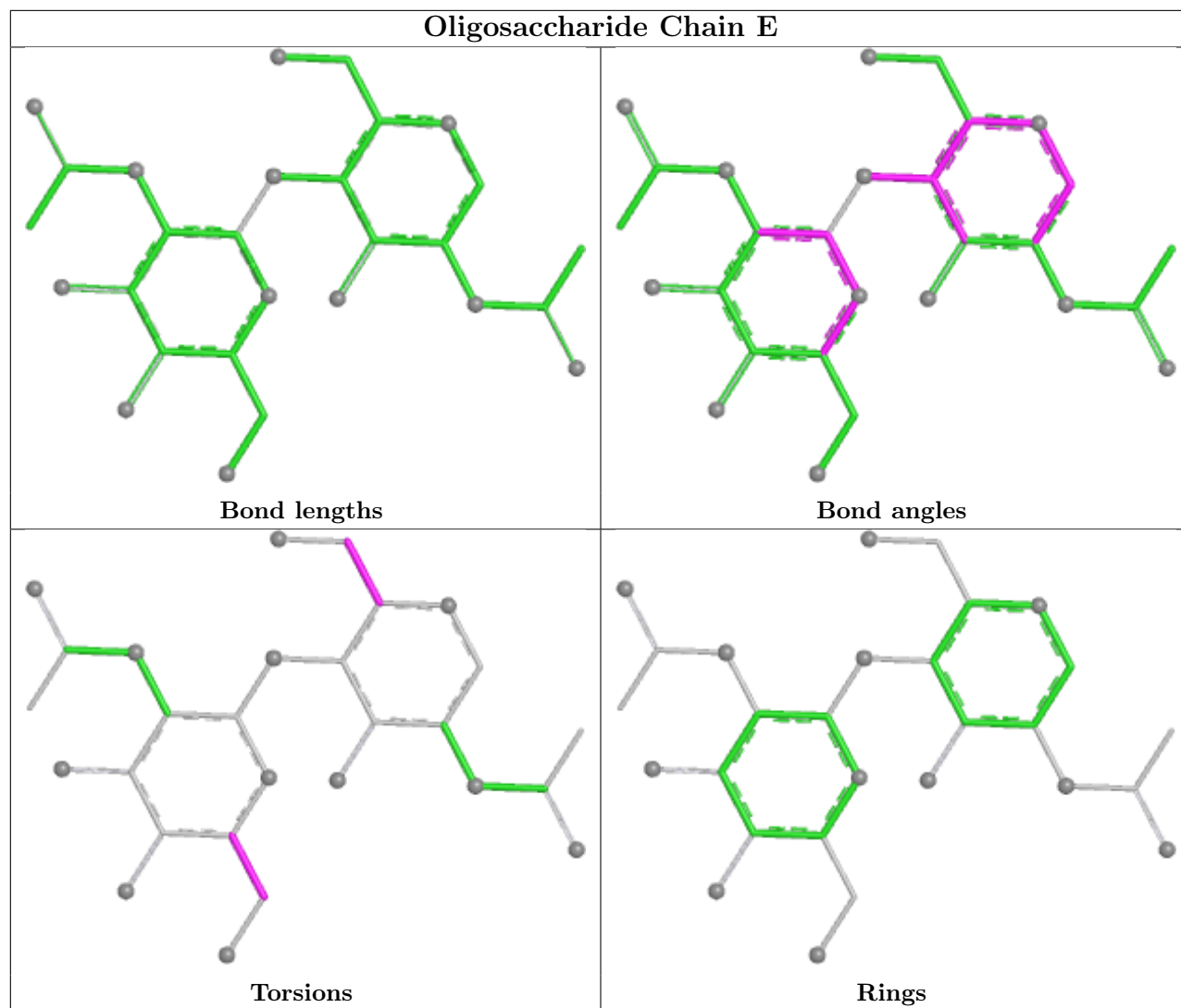
There are no ring outliers.

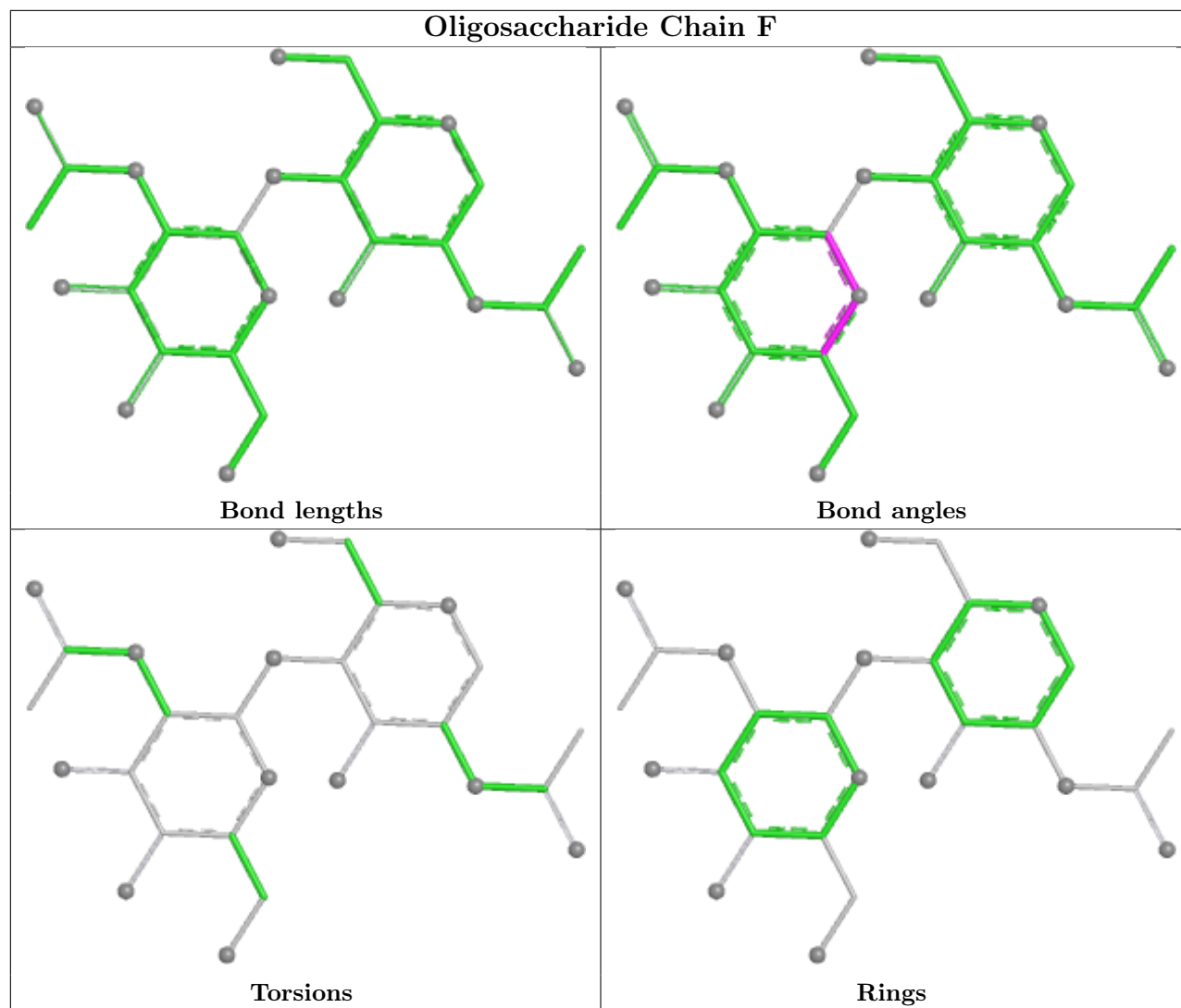
No monomer is involved in short contacts.

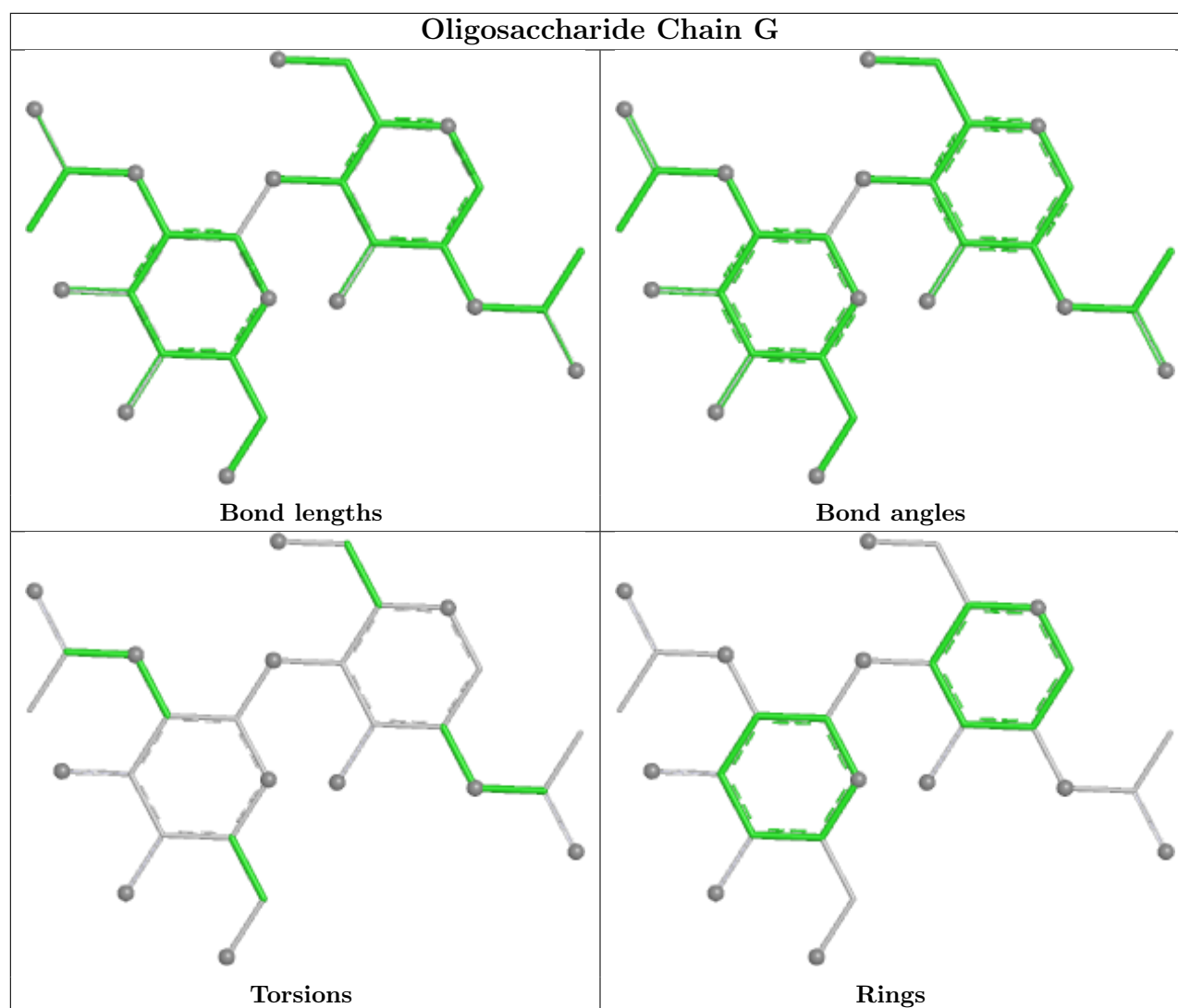
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 1 is monoatomic - leaving 10 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	$\# Z > 2$
5	NAG	A	809	1	14,14,15	0.35	0	17,19,21	0.58	0
5	NAG	A	804	1	14,14,15	0.32	0	17,19,21	0.71	1 (5%)
5	NAG	B	809	1	14,14,15	0.27	0	17,19,21	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	B	802	1	14,14,15	0.33	0	17,19,21	0.84	1 (5%)
4	2VH	B	801	-	30,31,31	1.33	4 (13%)	30,48,48	1.17	1 (3%)
5	NAG	A	803	1	14,14,15	0.31	0	17,19,21	0.94	1 (5%)
4	2VH	A	802	-	30,31,31	1.48	4 (13%)	30,48,48	1.07	1 (3%)
5	NAG	B	803	1	14,14,15	0.41	0	17,19,21	2.06	4 (23%)
5	NAG	B	810	1	14,14,15	0.33	0	17,19,21	0.90	1 (5%)
5	NAG	B	804	1	14,14,15	0.33	0	17,19,21	0.84	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
5	NAG	A	809	1	-	0/6/23/26	0/1/1/1
5	NAG	A	804	1	-	0/6/23/26	0/1/1/1
5	NAG	B	809	1	-	2/6/23/26	0/1/1/1
5	NAG	B	802	1	-	0/6/23/26	0/1/1/1
4	2VH	B	801	-	-	3/13/35/35	0/4/4/4
5	NAG	A	803	1	-	1/6/23/26	0/1/1/1
4	2VH	A	802	-	-	3/13/35/35	0/4/4/4
5	NAG	B	803	1	-	1/6/23/26	0/1/1/1
5	NAG	B	810	1	-	0/6/23/26	0/1/1/1
5	NAG	B	804	1	-	0/6/23/26	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	802	2VH	C14-C13	-4.76	1.46	1.51
4	B	801	2VH	C14-C13	-4.11	1.46	1.51
4	A	802	2VH	C11-N1	3.85	1.60	1.47
4	B	801	2VH	C11-C12	-3.67	1.45	1.50
4	A	802	2VH	C11-C12	-3.50	1.45	1.50
4	B	801	2VH	C11-N1	3.29	1.58	1.47
4	A	802	2VH	C14-N1	2.58	1.55	1.47
4	B	801	2VH	C14-N1	2.44	1.55	1.47

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	803	NAG	C1-O5-C5	6.95	121.50	112.19
4	B	801	2VH	C15-N3-N2	-5.64	110.15	112.59
4	A	802	2VH	C15-N3-N2	-4.78	110.52	112.59
5	B	804	NAG	C1-O5-C5	3.17	116.44	112.19
5	B	803	NAG	C1-C2-N2	2.95	115.09	110.43
5	B	810	NAG	C1-O5-C5	2.69	115.80	112.19
5	B	802	NAG	C1-O5-C5	2.58	115.64	112.19
5	B	803	NAG	C2-N2-C7	2.49	126.23	122.90
5	A	804	NAG	C1-O5-C5	2.48	115.51	112.19
5	B	803	NAG	O5-C1-C2	2.47	115.12	111.29
5	A	803	NAG	C1-O5-C5	2.08	114.98	112.19

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	802	2VH	N2-N3-S-O2
4	A	802	2VH	C15-N3-S-O2
4	A	802	2VH	C15-N3-S-C16
4	B	801	2VH	N2-N3-S-O2
4	B	801	2VH	C15-N3-S-O2
4	B	801	2VH	C15-N3-S-C16
5	B	809	NAG	C8-C7-N2-C2
5	B	809	NAG	O7-C7-N2-C2
5	B	803	NAG	C3-C2-N2-C7
5	A	803	NAG	C4-C5-C6-O6

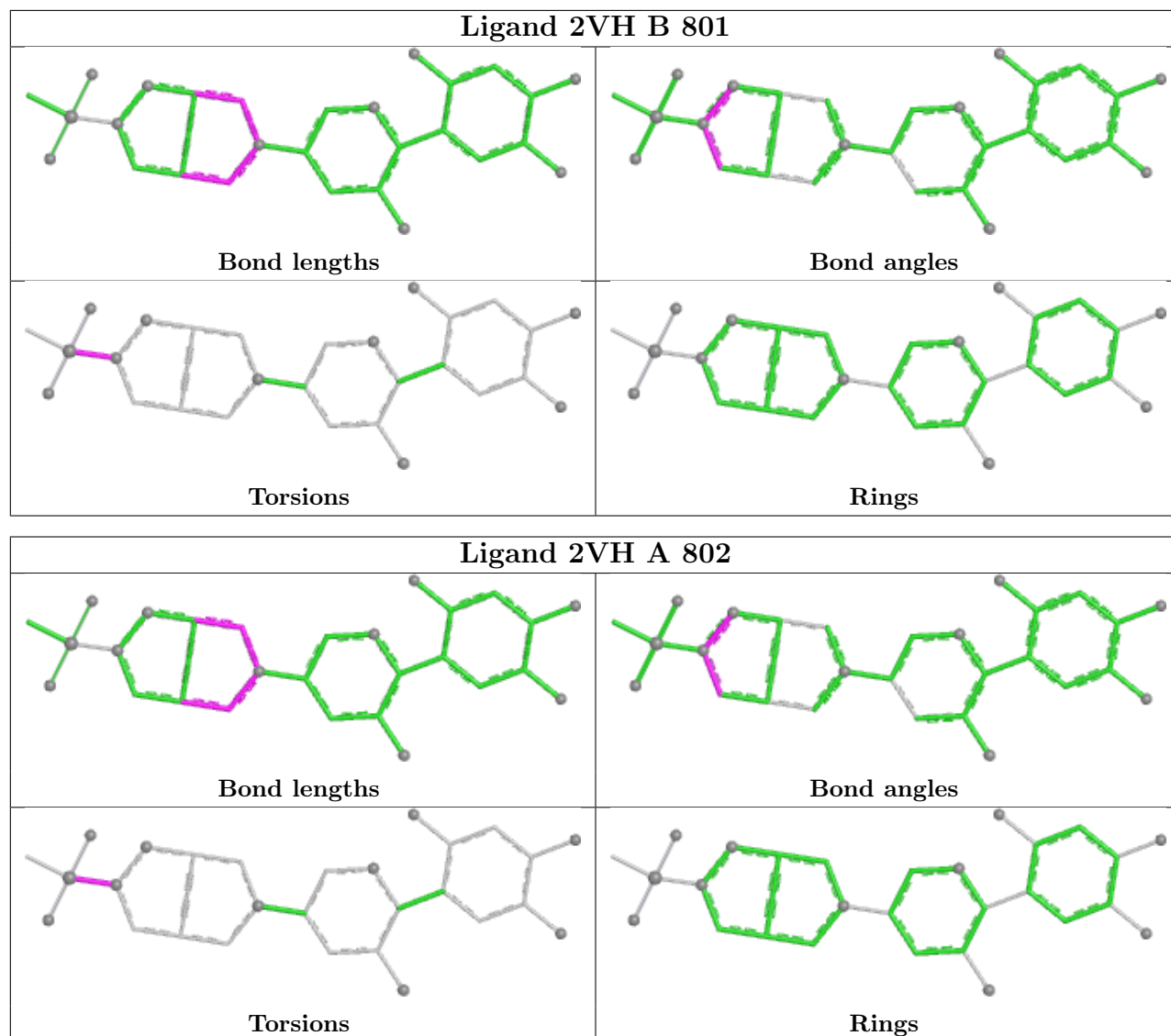
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	809	NAG	1	0
5	B	804	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.



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	728/728 (100%)	-0.37	3 (0%) 88 90	14, 23, 51, 71	3 (0%)
1	B	727/728 (99%)	-0.35	2 (0%) 90 91	14, 24, 49, 74	1 (0%)
All	All	1455/1456 (99%)	-0.36	5 (0%) 90 91	14, 24, 50, 74	4 (0%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	39	THR	3.0
1	B	92	ASN	3.0
1	B	766	PRO	2.6
1	A	99	GLY	2.2
1	A	766	PRO	2.1

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.

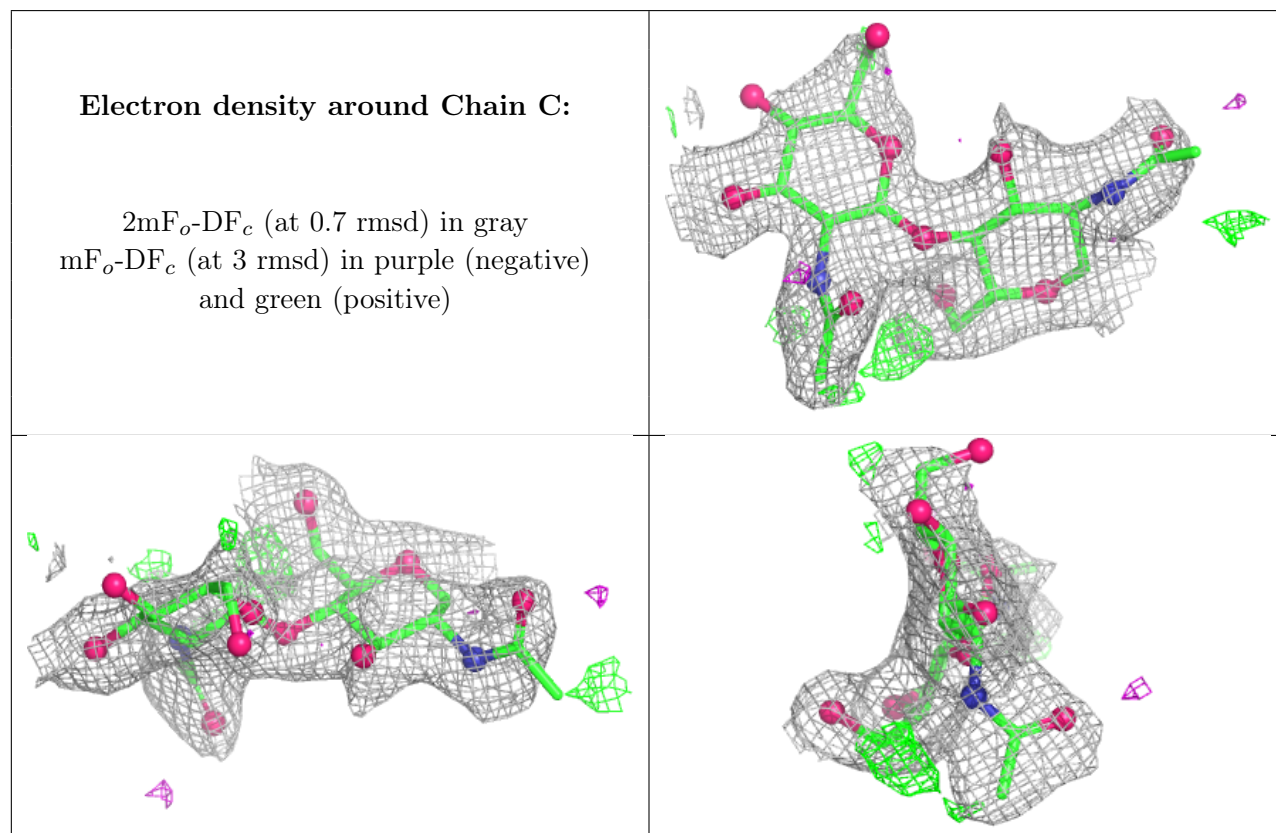
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	E	2	14/15	0.54	0.17	72,76,85,86	0
2	NAG	C	2	14/15	0.63	0.15	60,64,70,71	0
2	NAG	D	2	14/15	0.71	0.14	53,61,67,69	0
2	NAG	G	2	14/15	0.78	0.11	45,50,54,55	0

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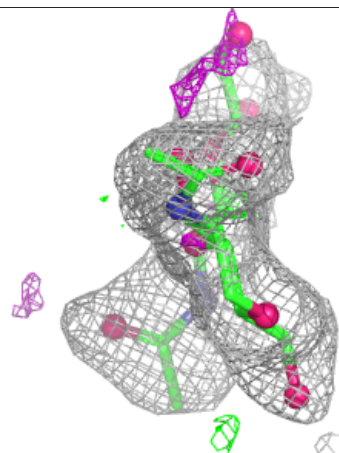
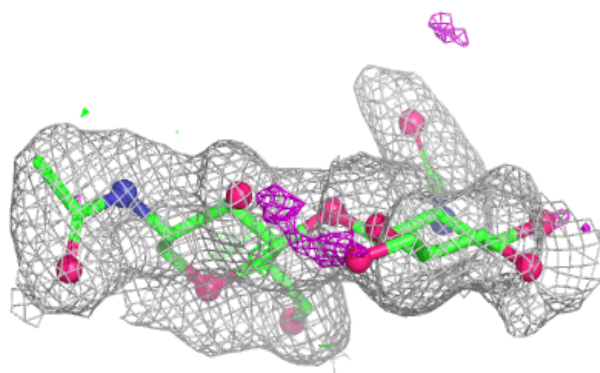
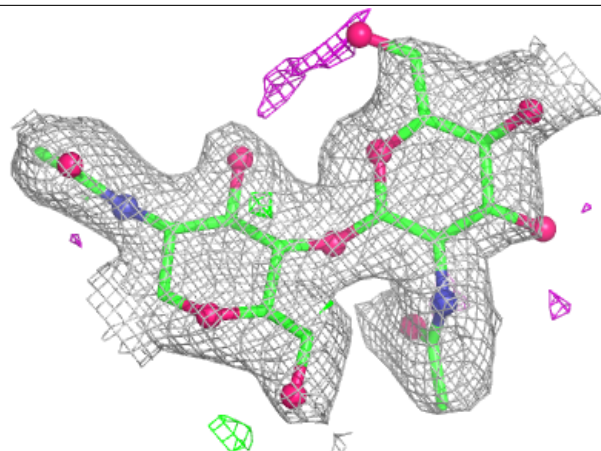
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	E	1	14/15	0.80	0.12	44,51,60,65	0
2	NAG	F	2	14/15	0.84	0.11	43,52,57,60	0
2	NAG	C	1	14/15	0.84	0.12	39,49,62,62	0
2	NAG	G	1	14/15	0.91	0.08	24,30,39,40	0
2	NAG	D	1	14/15	0.91	0.08	29,39,48,50	0
2	NAG	F	1	14/15	0.92	0.08	32,39,50,51	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.

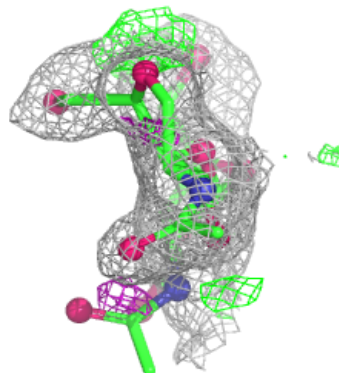
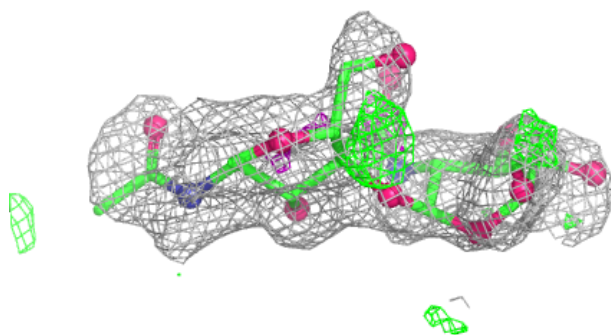
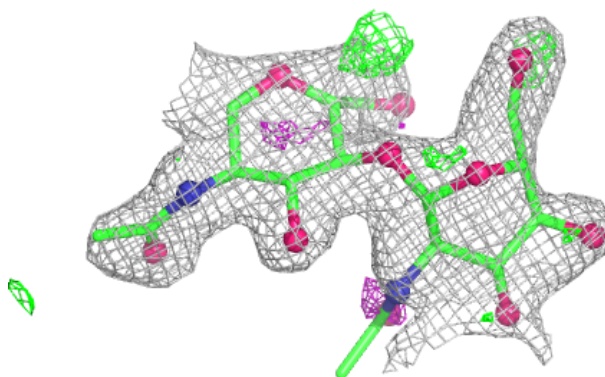


Electron density around Chain D:

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

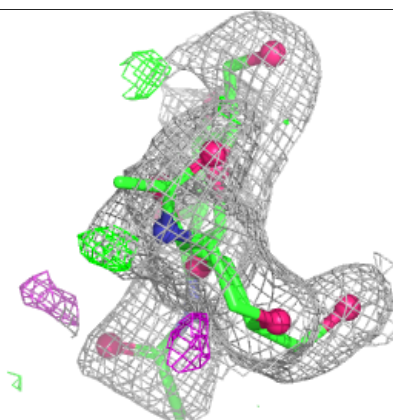
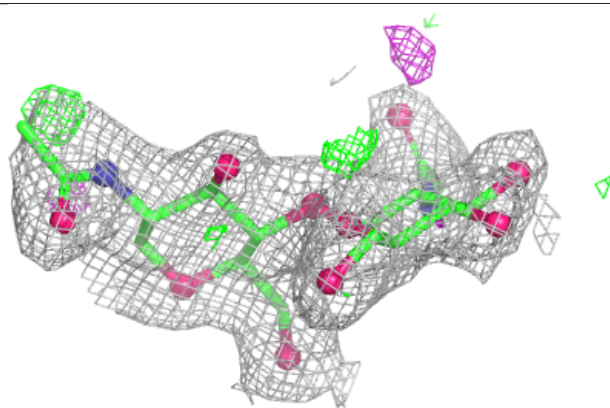
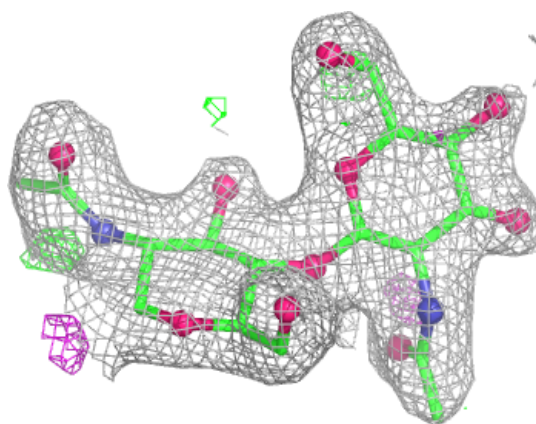
**Electron density around Chain E:**

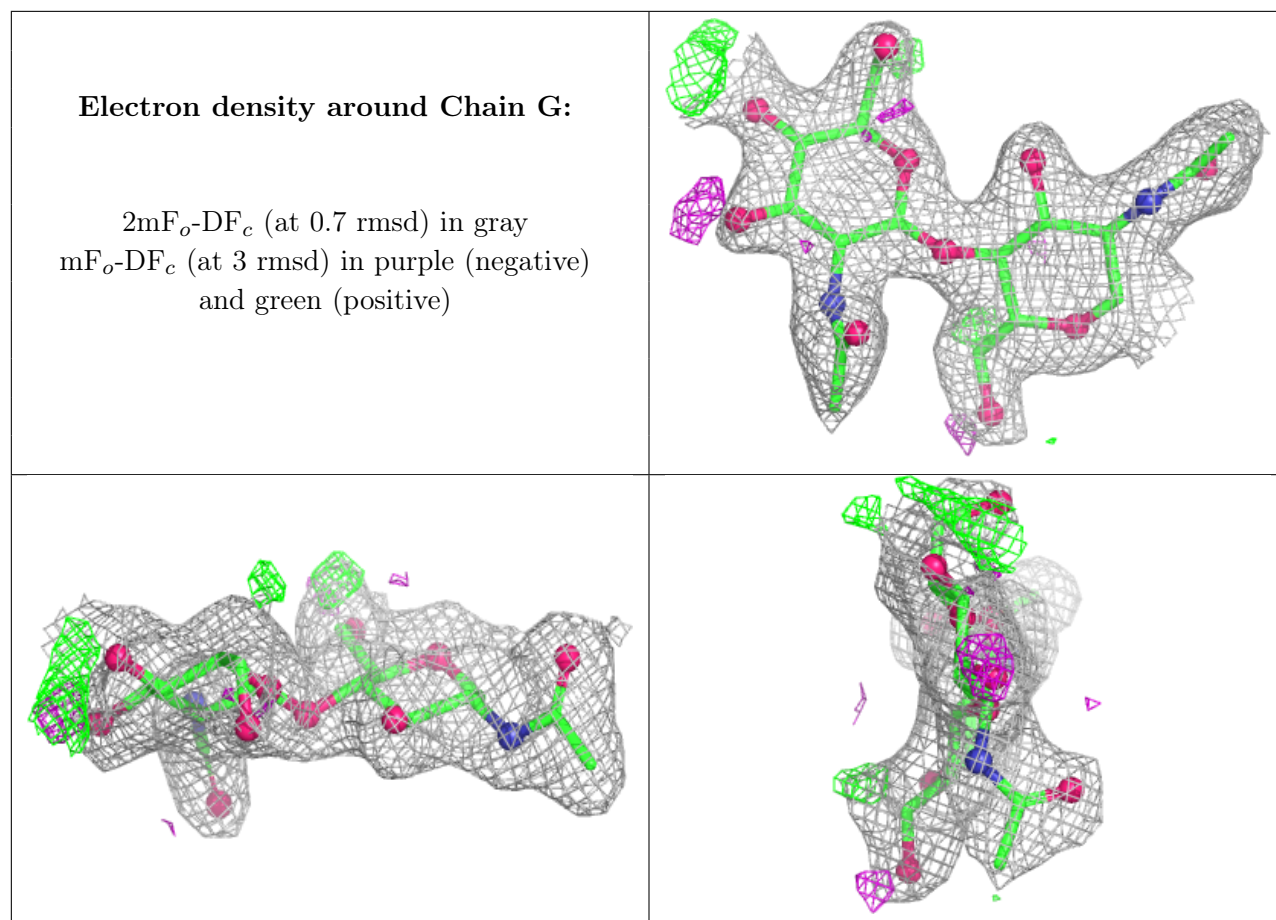
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain F:

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





6.4 Ligands [i](#)

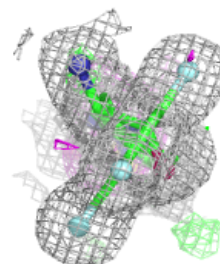
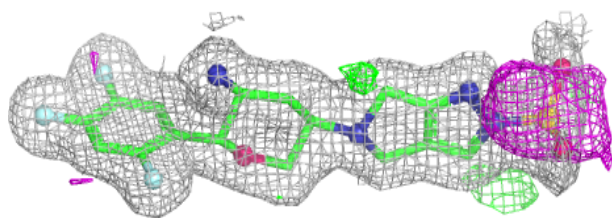
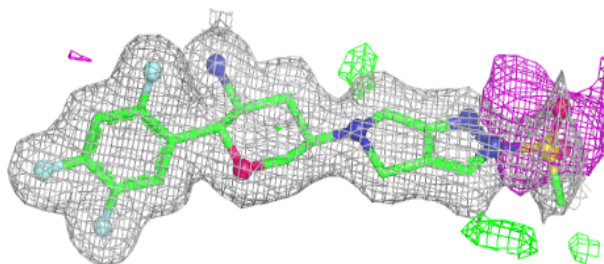
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	NAG	B	803	14/15	0.42	0.19	96,98,99,100	0
5	NAG	B	804	14/15	0.73	0.12	57,67,73,73	0
5	NAG	B	810	14/15	0.73	0.14	36,44,49,50	0
5	NAG	A	804	14/15	0.80	0.10	51,54,60,61	0
5	NAG	A	803	14/15	0.81	0.10	35,47,59,62	0
5	NAG	B	802	14/15	0.84	0.09	45,57,65,68	0
5	NAG	A	809	14/15	0.86	0.11	44,52,57,57	0
5	NAG	B	809	14/15	0.89	0.10	21,30,42,42	0
4	2VH	A	802	28/28	0.91	0.09	16,21,56,57	0
4	2VH	B	801	28/28	0.92	0.09	17,21,53,55	0
3	NA	A	801	1/1	0.98	0.06	24,24,24,24	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.

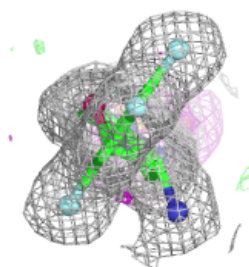
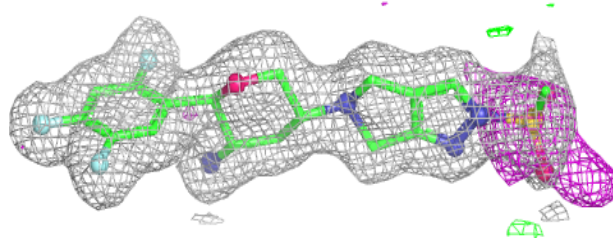
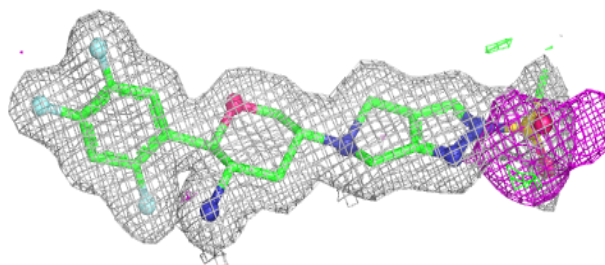
Electron density around 2VH A 802:

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



Electron density around 2VH B 801:

$2mF_o - DF_c$ (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.