



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 02:11 PM BST

PDB ID : 6F33
Title : Crystal structure of ectonucleotide phosphodiesterase/pyrophosphatase-3 (NPP3) in complex with AMPNPP
Authors : Dohler, C.; Zebisch, M.; Strater, N.
Deposited on : 2017-11-27
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

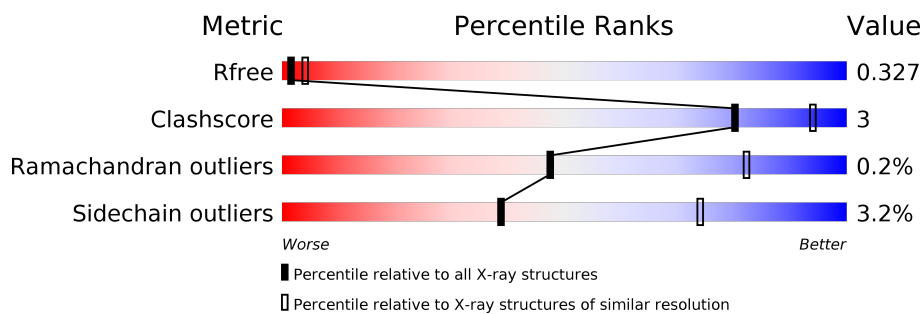
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	749	
1	B	749	
2	C	2	
2	D	2	
2	E	2	
2	F	2	
2	G	2	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11831 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 Ectonucleotide pyrophosphatase/phosphodiesterase family member 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	719	Total	C	N	O	S	0	0	0
			5788	3707	974	1074	33			
1	B	720	Total	C	N	O	S	0	0	0
			5793	3710	975	1075	33			

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	136	ALA	-	expression tag	UNP P97675
A	137	GLU	-	expression tag	UNP P97675
A	138	THR	-	expression tag	UNP P97675
A	139	GLY	-	expression tag	UNP P97675
A	201	VAL	MET	variant	UNP P97675
A	206	ALA	THR	conflict	UNP P97675
A	596	ASN	SER	variant	UNP P97675
A	597	ARG	GLY	variant	UNP P97675
A	876	GLY	-	expression tag	UNP P97675
A	877	THR	-	expression tag	UNP P97675
A	878	LYS	-	expression tag	UNP P97675
A	879	HIS	-	expression tag	UNP P97675
A	880	HIS	-	expression tag	UNP P97675
A	881	HIS	-	expression tag	UNP P97675
A	882	HIS	-	expression tag	UNP P97675
A	883	HIS	-	expression tag	UNP P97675
A	884	HIS	-	expression tag	UNP P97675
B	136	ALA	-	expression tag	UNP P97675
B	137	GLU	-	expression tag	UNP P97675
B	138	THR	-	expression tag	UNP P97675
B	139	GLY	-	expression tag	UNP P97675
B	201	VAL	MET	variant	UNP P97675
B	206	ALA	THR	conflict	UNP P97675
B	596	ASN	SER	variant	UNP P97675

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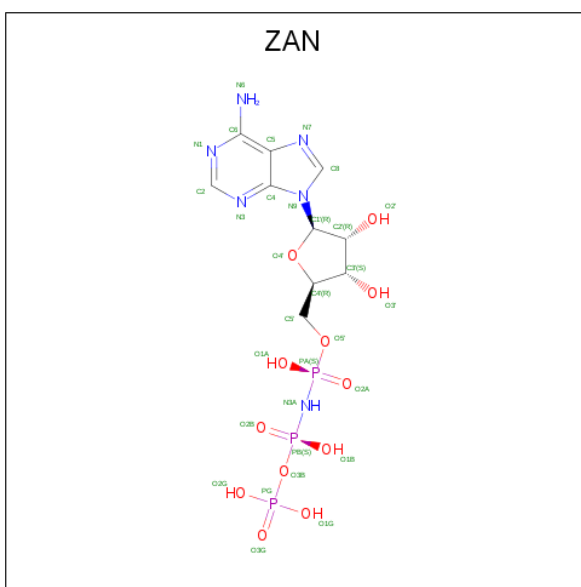
Chain	Residue	Modelled	Actual	Comment	Reference
B	597	ARG	GLY	variant	UNP P97675
B	876	GLY	-	expression tag	UNP P97675
B	877	THR	-	expression tag	UNP P97675
B	878	LYS	-	expression tag	UNP P97675
B	879	HIS	-	expression tag	UNP P97675
B	880	HIS	-	expression tag	UNP P97675
B	881	HIS	-	expression tag	UNP P97675
B	882	HIS	-	expression tag	UNP P97675
B	883	HIS	-	expression tag	UNP P97675
B	884	HIS	-	expression tag	UNP P97675

- 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 5'-O-[(S)-hydroxy{[(S)-hydroxy(phosphonooxy)phosphoryl]amino}phosphoryl]adenosine (three-letter code: ZAN) (formula: C₁₀H₁₇N₆O₁₂P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 31	C 10	N 6	O 12	P 3	0	0
3	B	1	Total 31	C 10	N 6	O 12	P 3	0	0

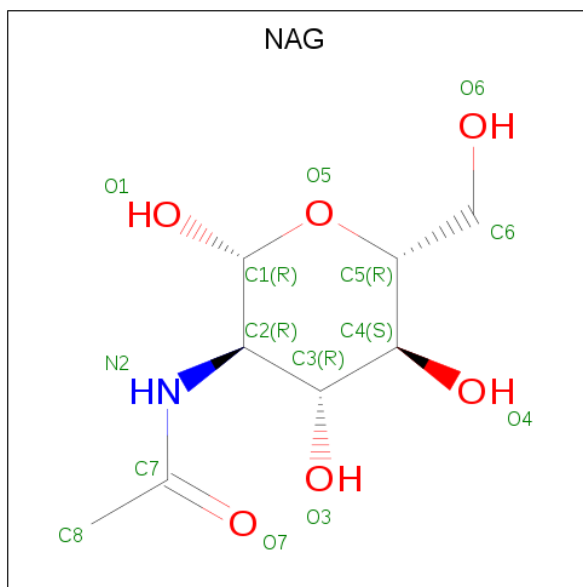
- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	2	Total Zn 2 2	0	0
4	A	2	Total Zn 2 2	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Ca 1 1	0	0
5	A	1	Total Ca 1 1	0	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $\text{C}_8\text{H}_{15}\text{NO}_6$).

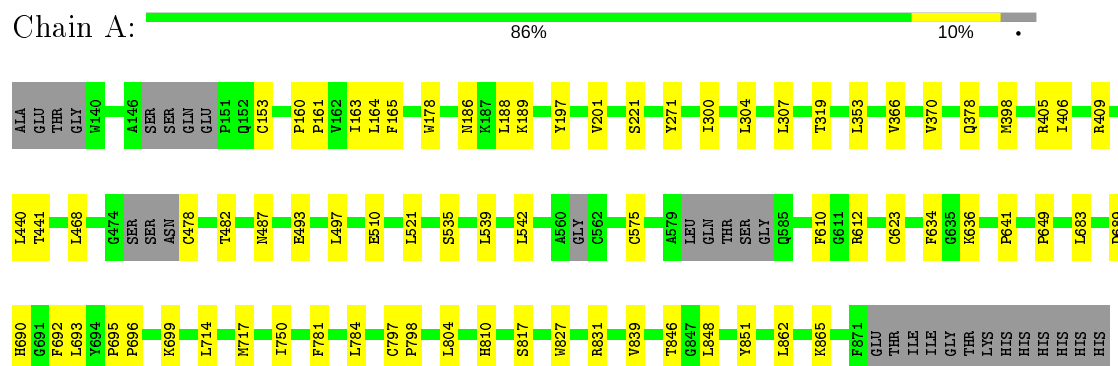


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	B	1	Total	C	N	O	0	0
			14	8	1	5		
6	B	1	Total	C	N	O	0	0
			14	8	1	5		

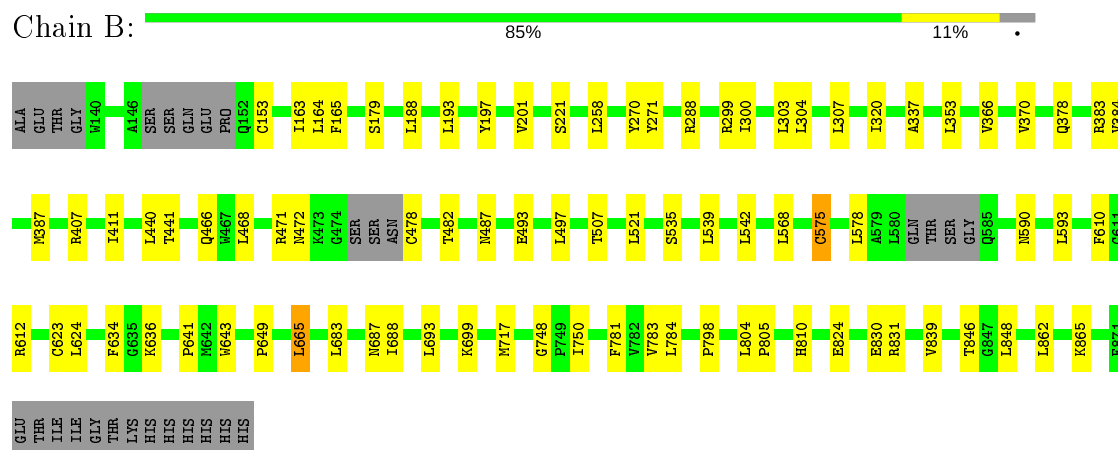
3 Residue-property plots

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: Ectonucleotide pyrophosphatase/phosphodiesterase family member 3



- Molecule 1: Ectonucleotide pyrophosphatase/phosphodiesterase family member 3



- 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 D:  50% 50%


MAC1
MAC2

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

Chain E:  50% 50%

MAC1
MAC2

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

Chain F:  100%

MAC1
MAC2

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

Chain G:  50% 50%

MAC1
MAC2

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	74.49Å 126.94Å 112.25Å 90.00° 96.75° 90.00°	Depositor
Resolution (Å)	47.26 – 3.00 47.26 – 3.00	Depositor EDS
% Data completeness (in resolution range)	97.4 (47.26-3.00) 97.4 (47.26-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 3.01Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.245 , 0.268 0.295 , 0.327	Depositor DCC
R_{free} test set	809 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å ²)	61.5	Xtriage
Anisotropy	0.441	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 32.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	11831	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.22% 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: ZAN, ZN, CA, 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	0.37	0/5960	0.55	0/8111
1	B	0.37	0/5965	0.55	0/8119
All	All	0.37	0/11925	0.55	0/16230

There are no bond length outliers.

There are no bond angle outliers.

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	5788	0	5577	31	0
1	B	5793	0	5582	32	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	31	0	16	0	0
3	B	31	0	15	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	14	0	13	0	0
6	B	28	0	26	0	0
All	All	11831	0	11354	62	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (62) 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:164:LEU:HB3	1:A:319:THR:HG22	1.87	0.56
1:A:690:HIS:HB2	1:A:714:LEU:HD22	1.88	0.54
1:B:384:VAL:HG22	1:B:468:LEU:HB2	1.89	0.54
1:A:817:SER:HB3	1:A:831:ARG:HG3	1.90	0.53
1:B:624:LEU:HD11	1:B:643:TRP:CZ2	2.44	0.52
1:B:299:ARG:HB3	1:B:320:ILE:HD11	1.94	0.50
1:B:539:LEU:HG	1:B:542:LEU:HD13	1.95	0.49
1:B:370:VAL:HG13	1:B:497:LEU:HB2	1.94	0.48
1:B:634:PHE:HA	1:B:641:PRO:HA	1.95	0.48
1:A:539:LEU:HG	1:A:542:LEU:HD13	1.95	0.48
1:A:641:PRO:HG2	1:A:693:LEU:HD12	1.94	0.48
1:B:784:LEU:HD12	1:B:804:LEU:HD23	1.96	0.48
1:A:370:VAL:HG13	1:A:497:LEU:HB2	1.95	0.48
1:B:649:PRO:HD3	1:B:699:LYS:HD3	1.96	0.48
1:A:784:LEU:HD12	1:A:804:LEU:HD23	1.96	0.47
1:A:634:PHE:HA	1:A:641:PRO:HA	1.95	0.47
1:B:468:LEU:HD21	1:B:482:THR:HG21	1.97	0.47
1:B:717:MET:HA	1:B:810:HIS:NE2	2.29	0.47
1:A:468:LEU:HD21	1:A:482:THR:HG21	1.97	0.47
1:B:383:ARG:HH11	1:B:466:GLN:HB3	1.80	0.47
1:A:164:LEU:HD13	1:A:521:LEU:HD21	1.97	0.47
1:B:197:TYR:HB2	1:B:493:GLU:HB3	1.97	0.47
1:A:649:PRO:HD3	1:A:699:LYS:HD3	1.97	0.47
1:A:186:ASN:HA	1:A:189:LYS:HG2	1.96	0.46
1:B:164:LEU:HD13	1:B:521:LEU:HD21	1.97	0.46
1:A:717:MET:HA	1:A:810:HIS:NE2	2.29	0.46
1:B:783:VAL:HG22	1:B:805:PRO:HB3	1.97	0.46
1:B:201:VAL:HA	1:B:487:ASN:HD22	1.80	0.46
1:A:535:SER:HB3	1:A:862:LEU:HD22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:387:MET:HB2	1:B:471:ARG:HA	1.98	0.45
1:A:201:VAL:HA	1:A:487:ASN:HD22	1.80	0.45
1:B:623:CYS:HB3	1:B:636:LYS:HE3	1.99	0.45
1:A:197:TYR:HB2	1:A:493:GLU:HB3	1.97	0.45
1:B:624:LEU:HD11	1:B:643:TRP:HZ2	1.81	0.45
1:B:535:SER:HB3	1:B:862:LEU:HD22	1.98	0.45
1:A:163:ILE:HD12	1:A:366:VAL:HG11	1.98	0.45
1:B:407:ARG:HH12	1:B:411:ILE:HD13	1.82	0.44
1:B:270:TYR:CD2	1:B:288:ARG:HG3	2.53	0.43
1:A:623:CYS:HB3	1:A:636:LYS:HE3	2.01	0.43
1:A:817:SER:HB3	1:A:831:ARG:CG	2.48	0.43
1:B:300:ILE:HD12	1:B:353:LEU:HB2	2.00	0.43
1:A:817:SER:HB2	1:A:827:TRP:HB2	2.01	0.43
1:B:304:LEU:HA	1:B:307:LEU:HD12	2.02	0.42
1:B:163:ILE:HD12	1:B:366:VAL:HG11	2.00	0.42
1:B:590:ASN:HA	1:B:593:LEU:HD12	2.01	0.42
1:B:846:THR:HB	1:B:848:LEU:HD12	2.00	0.42
1:A:300:ILE:HD12	1:A:353:LEU:HB2	2.01	0.42
1:A:178:TRP:HA	1:B:337:ALA:HB2	2.01	0.42
1:A:846:THR:HB	1:A:848:LEU:HD12	2.01	0.42
1:A:398:MET:HG3	1:A:406:ILE:HG13	2.02	0.42
1:B:575:CYS:SG	1:B:665:LEU:HB3	2.59	0.41
1:B:693:LEU:HD21	1:B:748:GLY:HA2	2.02	0.41
1:A:160:PRO:HA	1:A:161:PRO:HD3	1.95	0.41
1:B:193:LEU:HD12	1:B:507:THR:HB	2.03	0.41
1:B:750:ILE:HD11	1:B:781:PHE:HB3	2.03	0.41
1:A:797:CYS:HA	1:A:798:PRO:HD3	1.93	0.41
1:A:839:VAL:HB	1:A:865:LYS:HA	2.02	0.41
1:A:839:VAL:HG11	1:A:851:TYR:HE2	1.86	0.41
1:A:750:ILE:HD11	1:A:781:PHE:HB3	2.03	0.40
1:A:695:PRO:HA	1:A:696:PRO:HD3	2.02	0.40
1:B:839:VAL:HB	1:B:865:LYS:HA	2.02	0.40
1:A:304:LEU:HA	1:A:307:LEU:HD12	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	709/749 (95%)	664 (94%)	44 (6%)	1 (0%)	51	85
1	B	712/749 (95%)	660 (93%)	50 (7%)	2 (0%)	41	76
All	All	1421/1498 (95%)	1324 (93%)	94 (7%)	3 (0%)	47	82

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	271	TYR
1	A	271	TYR
1	B	798	PRO

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	643/668 (96%)	626 (97%)	17 (3%)	46	78
1	B	643/668 (96%)	619 (96%)	24 (4%)	34	70
All	All	1286/1336 (96%)	1245 (97%)	41 (3%)	39	74

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	153	CYS
1	A	165	PHE
1	A	188	LEU

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Mol	Chain	Res	Type
1	A	221	SER
1	A	378	GLN
1	A	405	ARG
1	A	409	ARG
1	A	440	LEU
1	A	441	THR
1	A	478	CYS
1	A	510	GLU
1	A	575	CYS
1	A	610	PHE
1	A	612	ARG
1	A	683	LEU
1	A	689	ASP
1	A	692	PHE
1	B	153	CYS
1	B	165	PHE
1	B	179	SER
1	B	188	LEU
1	B	221	SER
1	B	258	LEU
1	B	303	LEU
1	B	378	GLN
1	B	440	LEU
1	B	441	THR
1	B	472	ASN
1	B	478	CYS
1	B	568	LEU
1	B	575	CYS
1	B	578	LEU
1	B	610	PHE
1	B	612	ARG
1	B	665	LEU
1	B	683	LEU
1	B	687	ASN
1	B	688	ILE
1	B	824	GLU
1	B	830	GLU
1	B	831	ARG

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

Mol	Chain	Res	Type
1	A	526	HIS

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	0.29	0	17,19,21	0.91	1 (5%)
2	NAG	C	2	2	14,14,15	0.29	0	17,19,21	0.72	1 (5%)
2	NAG	D	1	1,2	14,14,15	0.30	0	17,19,21	0.51	0
2	NAG	D	2	2	14,14,15	0.29	0	17,19,21	0.67	1 (5%)
2	NAG	E	1	1,2	14,14,15	0.30	0	17,19,21	0.90	1 (5%)
2	NAG	E	2	2	14,14,15	0.30	0	17,19,21	0.68	0
2	NAG	F	1	1,2	14,14,15	0.28	0	17,19,21	0.89	1 (5%)
2	NAG	F	2	2	14,14,15	0.30	0	17,19,21	0.75	1 (5%)
2	NAG	G	1	1,2	14,14,15	0.30	0	17,19,21	0.75	1 (5%)
2	NAG	G	2	2	14,14,15	0.29	0	17,19,21	0.55	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	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	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 (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	NAG	O5-C1-C2	-3.04	106.48	111.29
2	F	1	NAG	O5-C1-C2	-3.01	106.53	111.29
2	E	1	NAG	O5-C1-C2	-2.81	106.85	111.29
2	F	2	NAG	C1-O5-C5	2.53	115.62	112.19
2	C	2	NAG	C1-O5-C5	2.50	115.58	112.19
2	G	1	NAG	O5-C1-C2	-2.28	107.69	111.29
2	D	2	NAG	C1-O5-C5	2.03	114.94	112.19

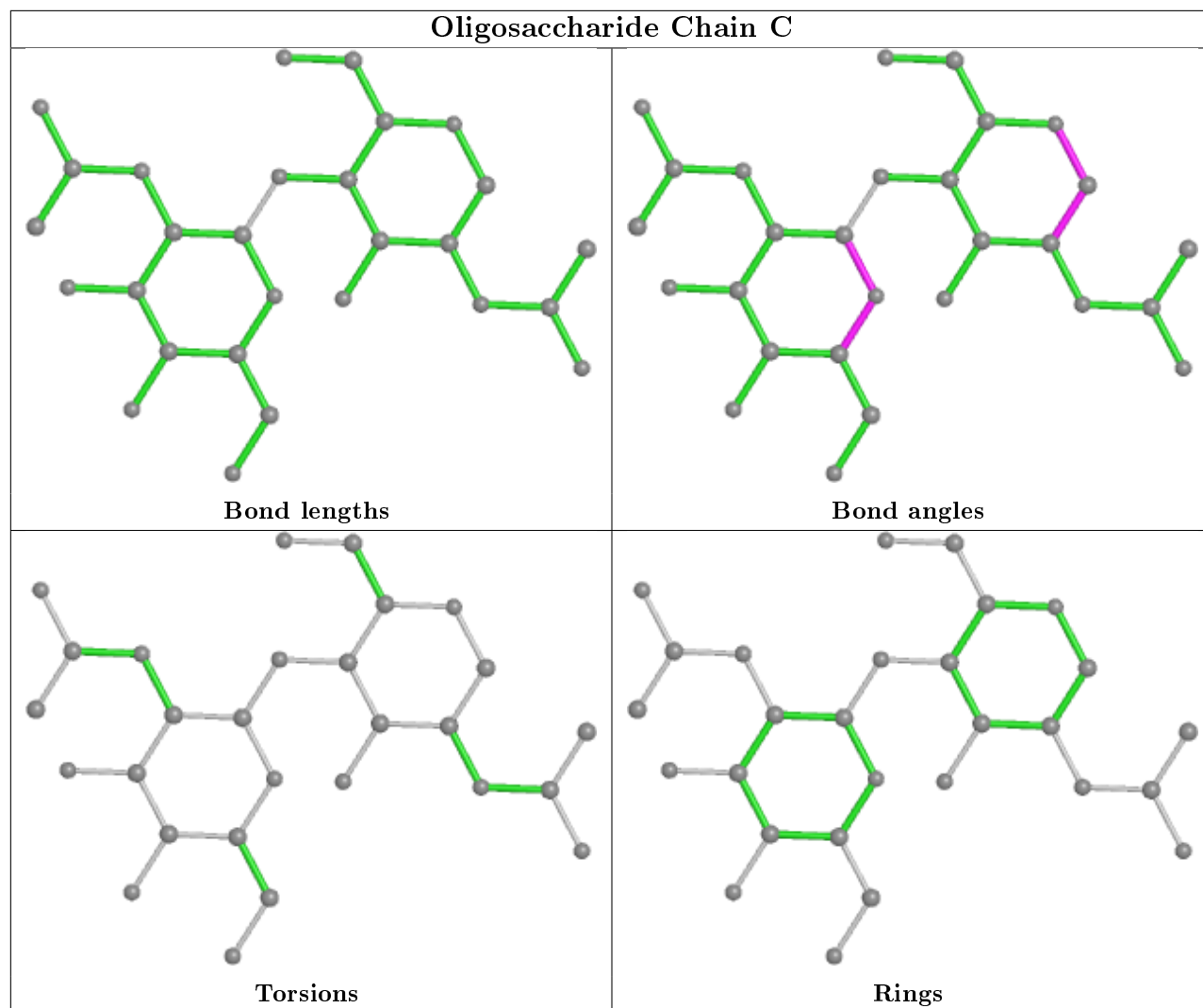
There are no chirality outliers.

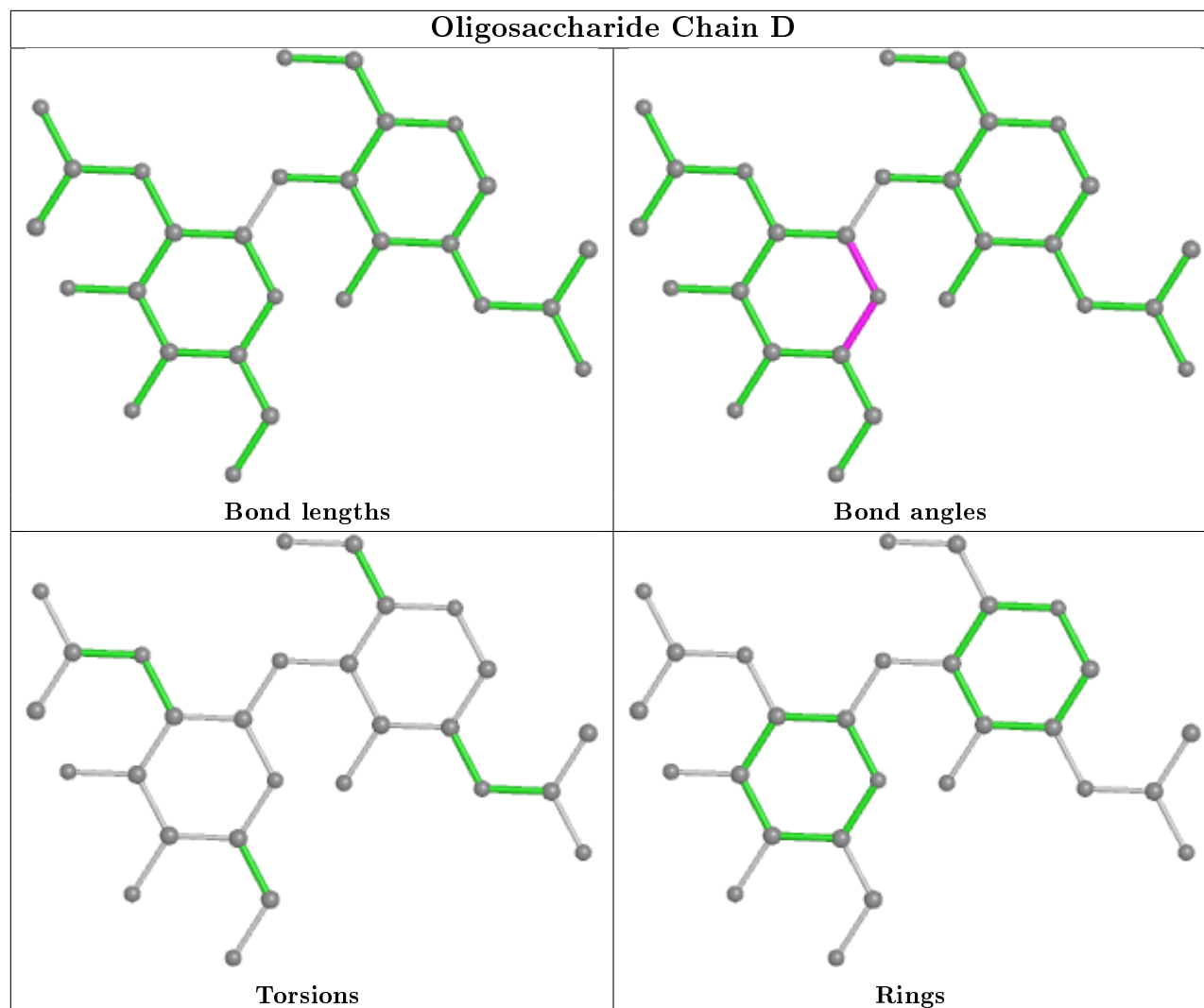
There are no torsion outliers.

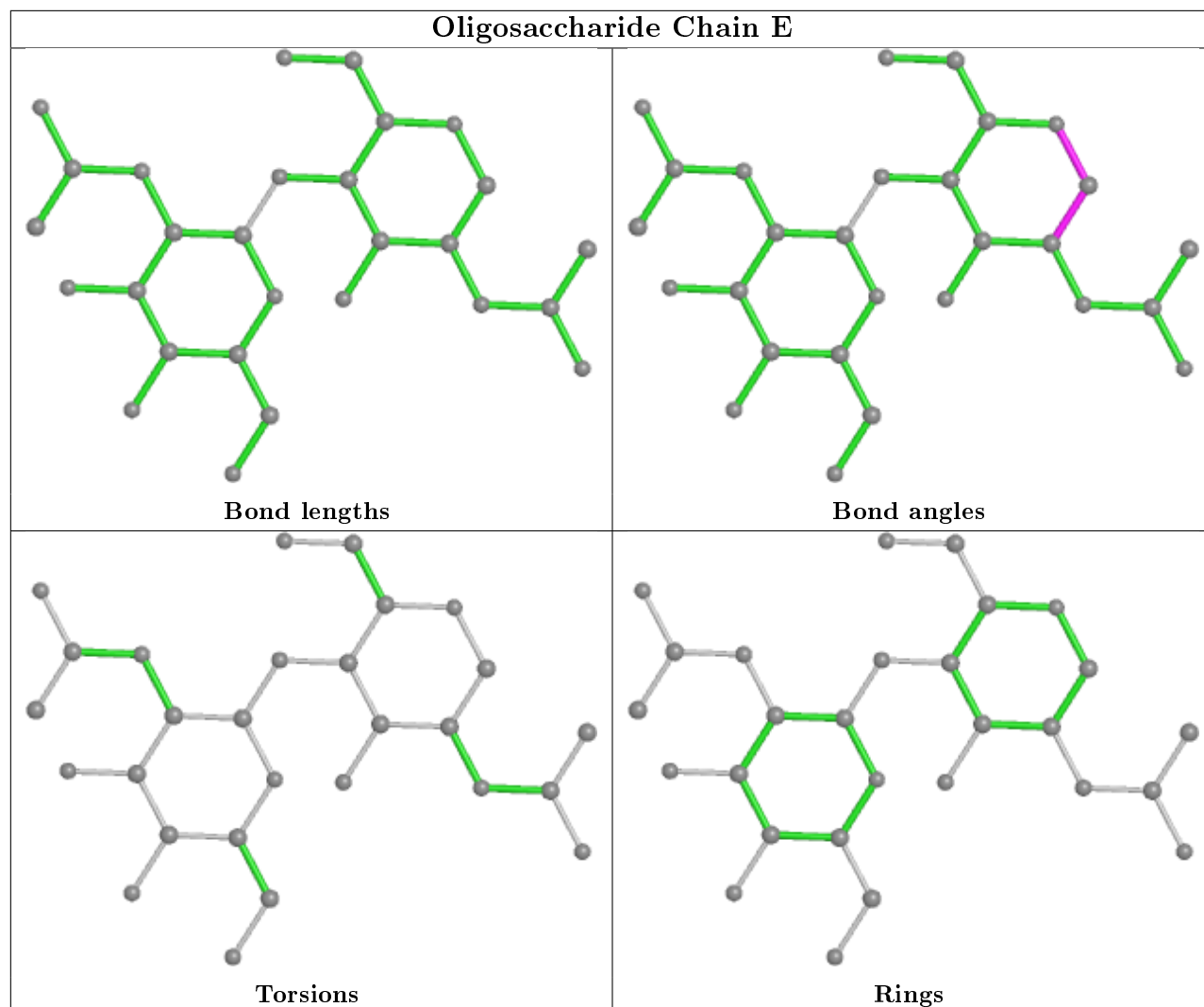
There are no ring outliers.

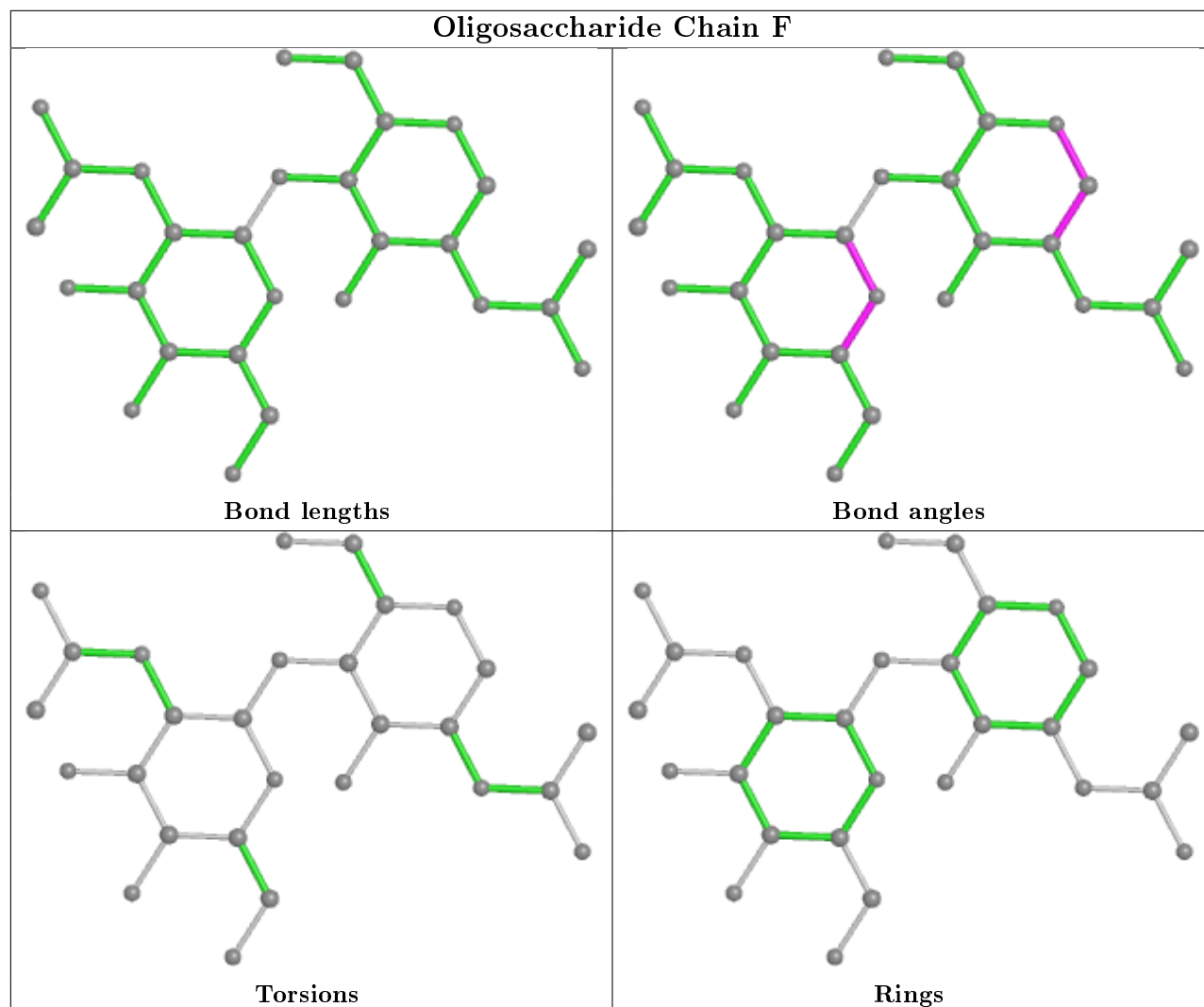
No monomer is involved in short contacts.

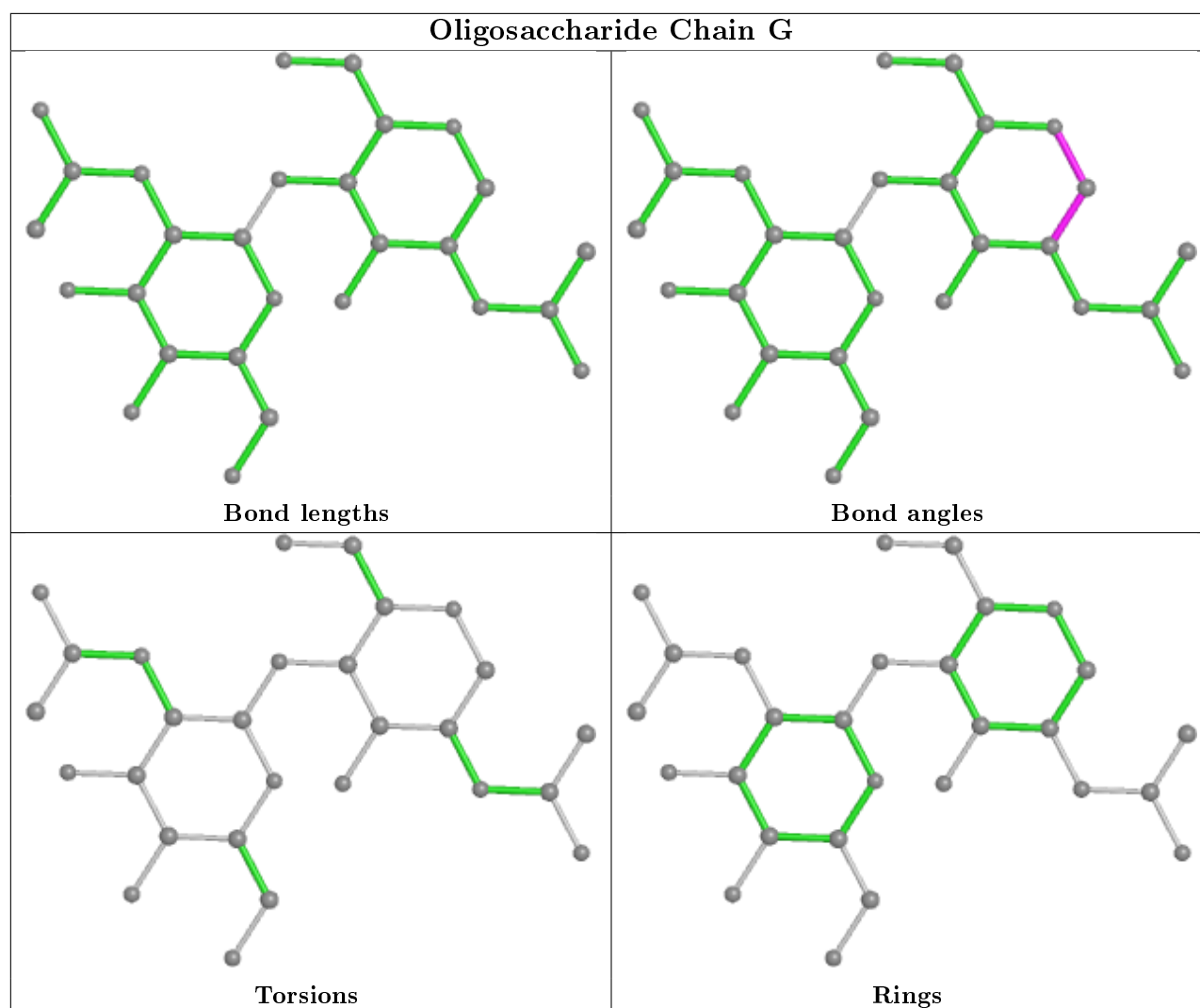
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 6 are monoatomic - leaving 5 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	$\# Z > 2$
6	NAG	B	1009	1	14,14,15	0.30	0	17,19,21	0.56	0
3	ZAN	A	1001	4	29,33,33	1.78	2 (6%)	34,52,52	0.96	3 (8%)
3	ZAN	B	1001	4	29,33,33	1.73	2 (6%)	34,52,52	0.90	3 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	B	1010	1	14,14,15	0.31	0	17,19,21	0.44	0
6	NAG	A	1007	1	14,14,15	0.30	0	17,19,21	0.74	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
6	NAG	B	1009	1	-	1/6/23/26	0/1/1/1
3	ZAN	A	1001	4	-	10/15/38/38	0/3/3/3
3	ZAN	B	1001	4	-	5/15/38/38	0/3/3/3
6	NAG	B	1010	1	-	1/6/23/26	0/1/1/1
6	NAG	A	1007	1	-	1/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1001	ZAN	PB-O2B	8.02	1.58	1.46
3	B	1001	ZAN	PB-O2B	7.84	1.58	1.46
3	B	1001	ZAN	PB-O1B	-4.03	1.45	1.56
3	A	1001	ZAN	PB-O1B	-4.03	1.45	1.56

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1001	ZAN	O2B-PB-N3A	-2.73	107.75	111.77
6	A	1007	NAG	C1-O5-C5	2.61	115.72	112.19
3	B	1001	ZAN	O2B-PB-N3A	-2.57	107.98	111.77
3	B	1001	ZAN	O1B-PB-O3B	2.41	112.70	104.64
3	A	1001	ZAN	C5-C6-N6	2.23	123.73	120.35
3	B	1001	ZAN	C5-C6-N6	2.20	123.70	120.35
3	A	1001	ZAN	O1B-PB-O3B	2.17	111.87	104.64

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1001	ZAN	PB-N3A-PA-O2A
3	A	1001	ZAN	PB-N3A-PA-O5'

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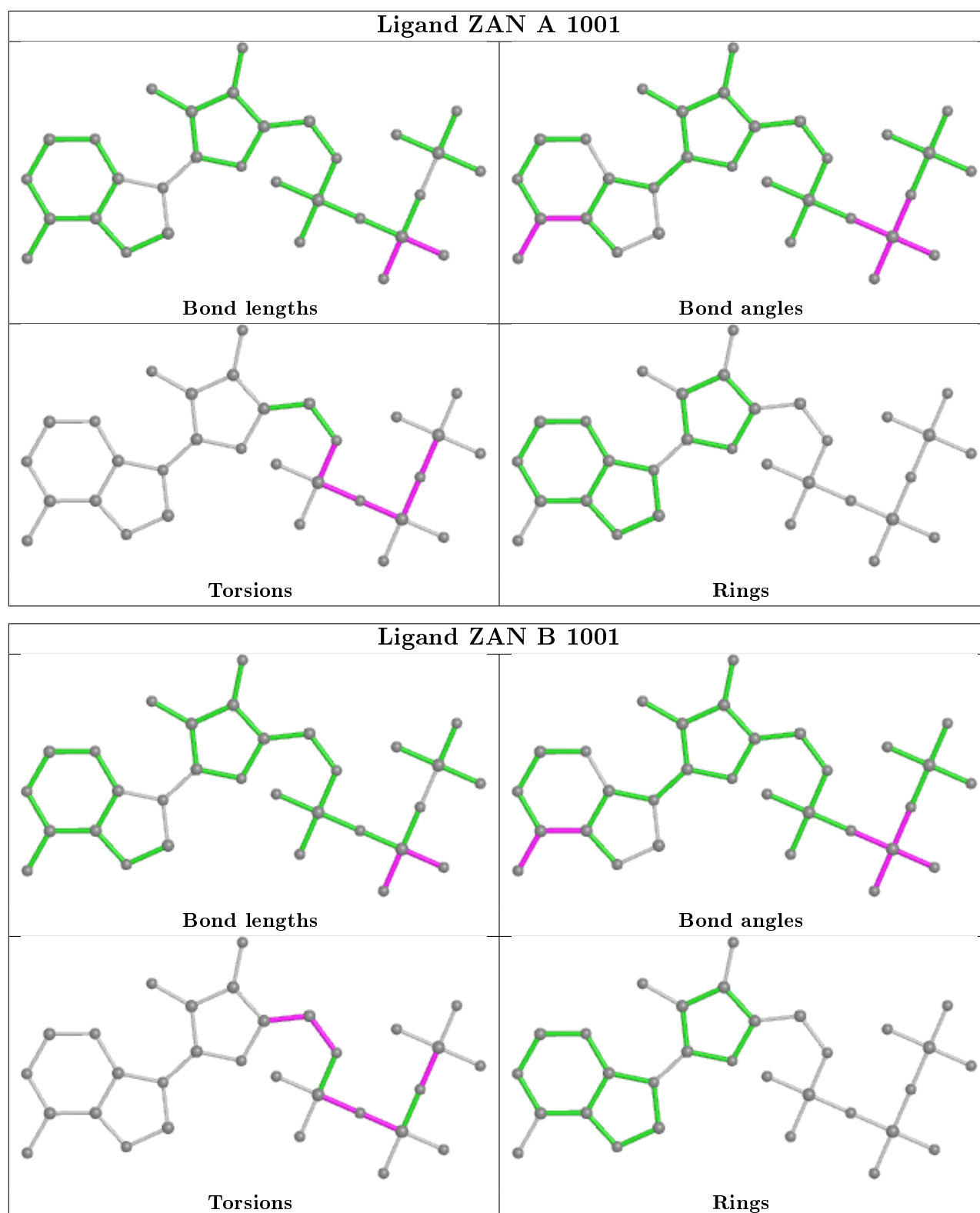
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Mol	Chain	Res	Type	Atoms
3	A	1001	ZAN	C5'-O5'-PA-O1A
3	A	1001	ZAN	PA-N3A-PB-O2B
3	A	1001	ZAN	PG-O3B-PB-O1B
3	A	1001	ZAN	PG-O3B-PB-O2B
3	A	1001	ZAN	PB-O3B-PG-O1G
3	B	1001	ZAN	PB-N3A-PA-O2A
3	B	1001	ZAN	PA-N3A-PB-O2B
3	B	1001	ZAN	PB-O3B-PG-O2G
6	B	1010	NAG	O5-C5-C6-O6
6	B	1009	NAG	O5-C5-C6-O6
6	A	1007	NAG	O5-C5-C6-O6
3	A	1001	ZAN	PB-O3B-PG-O3G
3	A	1001	ZAN	C5'-O5'-PA-O2A
3	B	1001	ZAN	C4'-C5'-O5'-PA
3	B	1001	ZAN	O4'-C4'-C5'-O5'
3	A	1001	ZAN	C5'-O5'-PA-N3A

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 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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

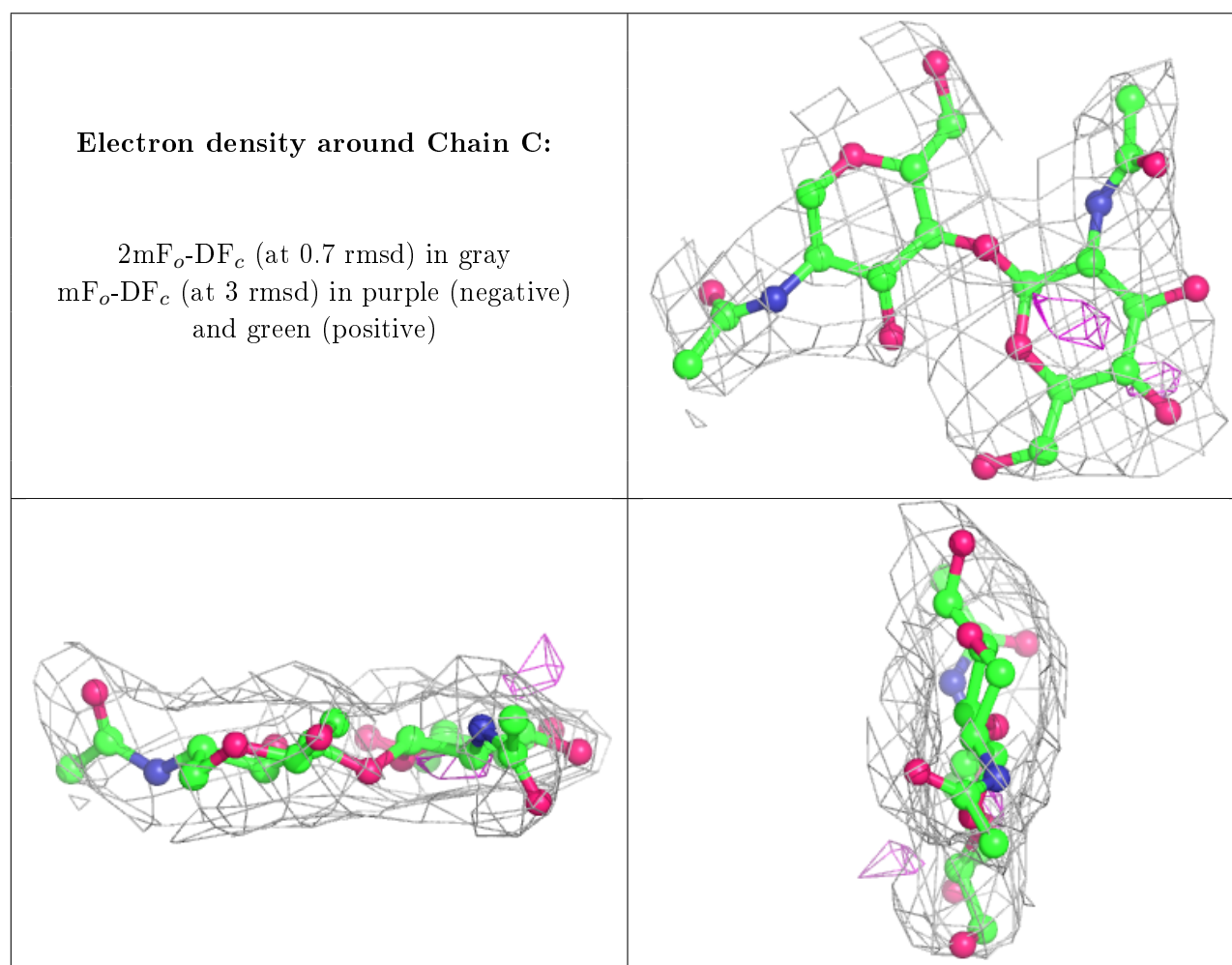
6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates ⓘ

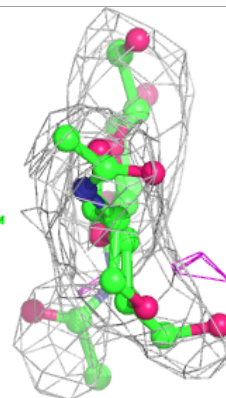
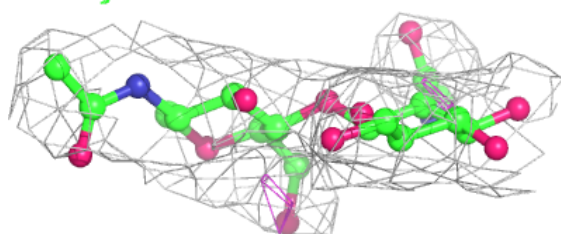
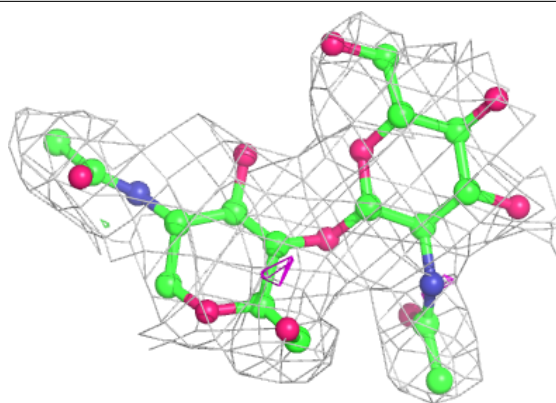
Unable to reproduce the depositors R factor - this section is therefore empty.

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.

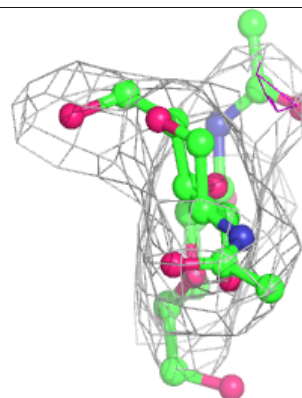
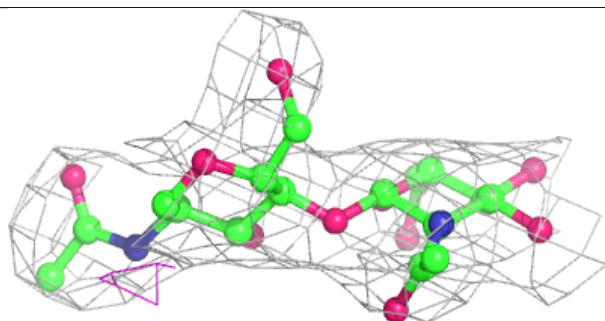
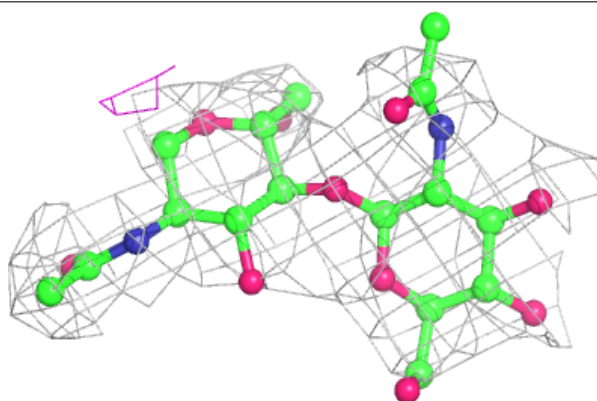


Electron density around Chain D:

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

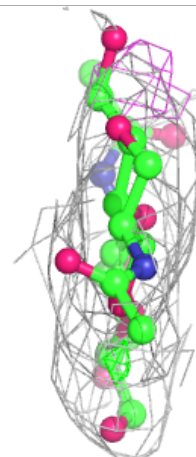
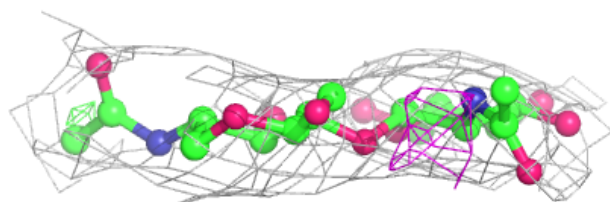
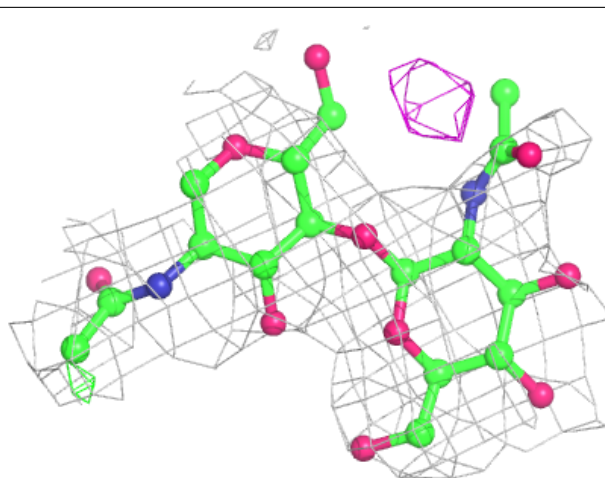
**Electron density around Chain E:**

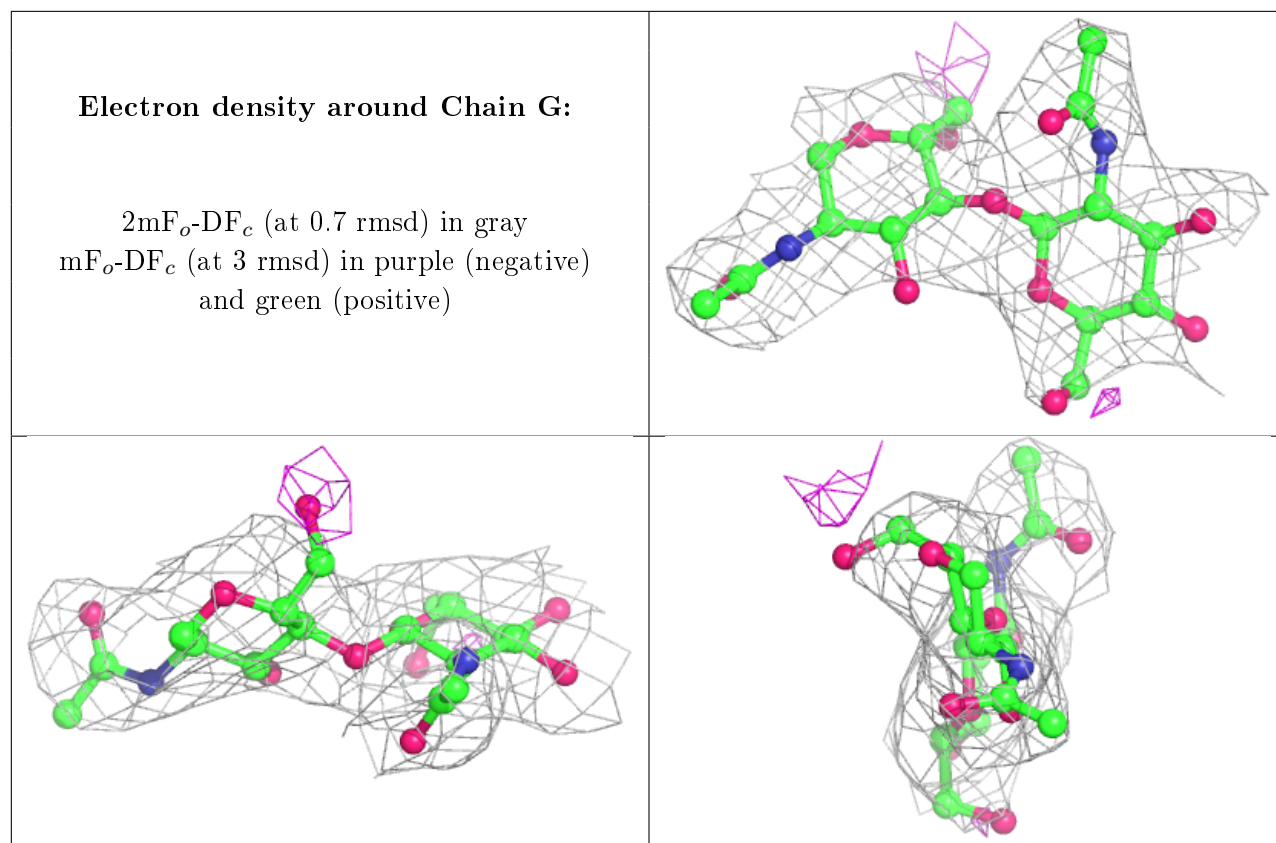
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





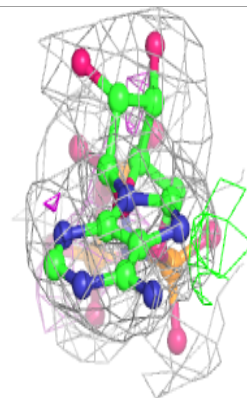
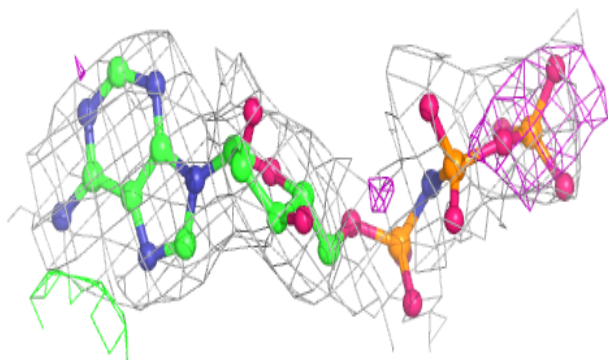
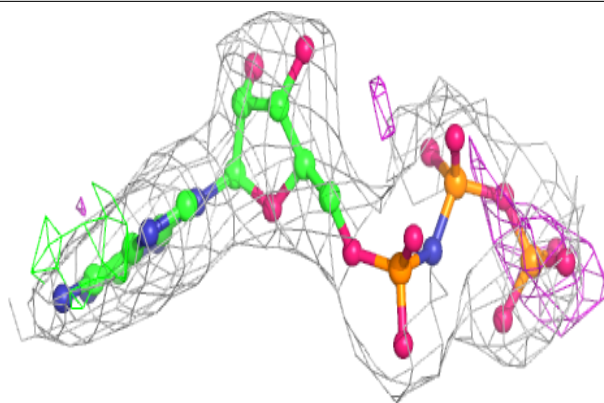
6.4 Ligands [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

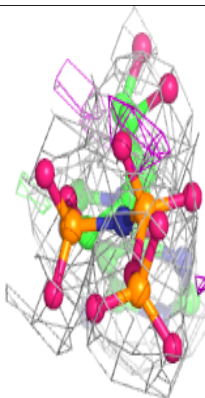
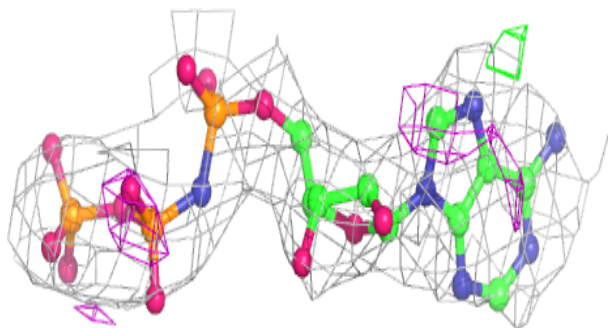
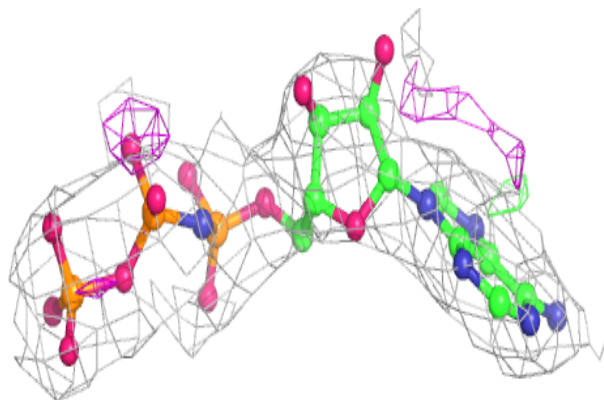
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around ZAN A 1001:

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

**Electron density around ZAN B 1001:**

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



6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.