



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 21, 2020 – 04:54 AM BST

PDB ID : 5ZSG
Title : Crystal structure of monkey TLR7 in complex with gardiquimod
Authors : Zhang, Z.; Ohto, U.; Shimizu, T.
Deposited on : 2018-04-28
Resolution : 2.30 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 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

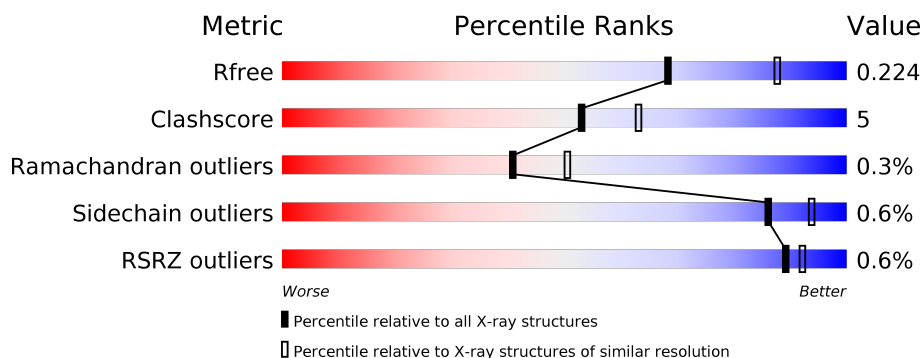
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 $\leq 5\%$. 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	823	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 13%, green 80%, grey 6%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 80% 13% 6% </div> </div>
1	B	823	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 85%, yellow 9%, grey 6%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 85% 9% 6% </div> </div>
2	C	2	<div> <div style="width: 100%; height: 10px; background: yellow;"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 100% </div> </div>
2	D	2	<div> <div style="width: 100%; height: 10px; background: green;"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 100% </div> </div>
2	E	2	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 50%, yellow 50%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 50% 50% </div> </div>
2	F	2	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 50%, orange 50%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 50% 50% </div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13527 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 Toll-like receptor 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	772	Total	C	N	O	S	0	1	0
			6258	4010	1066	1152	30			
1	A	772	Total	C	N	O	S	0	1	0
			6258	4010	1066	1152	30			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	23	ARG	-	expression tag	UNP G7NS93
B	24	SER	-	expression tag	UNP G7NS93
B	25	PRO	-	expression tag	UNP G7NS93
B	26	TRP	-	expression tag	UNP G7NS93
B	167	GLN	ASN	engineered mutation	UNP G7NS93
B	389	GLN	ASN	engineered mutation	UNP G7NS93
B	440	LEU	SER	see sequence details	UNP G7NS93
B	441	VAL	GLU	see sequence details	UNP G7NS93
B	442	PRO	VAL	see sequence details	UNP G7NS93
B	443	ARG	GLY	see sequence details	UNP G7NS93
B	444	GLY	PHE	see sequence details	UNP G7NS93
B	445	SER	CYS	see sequence details	UNP G7NS93
B	488	GLN	ASN	engineered mutation	UNP G7NS93
B	799	GLN	ASN	engineered mutation	UNP G7NS93
B	840	GLU	-	expression tag	UNP G7NS93
B	841	PHE	-	expression tag	UNP G7NS93
B	842	LEU	-	expression tag	UNP G7NS93
B	843	VAL	-	expression tag	UNP G7NS93
B	844	PRO	-	expression tag	UNP G7NS93
B	845	ARG	-	expression tag	UNP G7NS93
A	23	ARG	-	expression tag	UNP G7NS93
A	24	SER	-	expression tag	UNP G7NS93
A	25	PRO	-	expression tag	UNP G7NS93
A	26	TRP	-	expression tag	UNP G7NS93
A	167	GLN	ASN	engineered mutation	UNP G7NS93

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Chain	Residue	Modelled	Actual	Comment	Reference
A	389	GLN	ASN	engineered mutation	UNP G7NS93
A	440	LEU	SER	see sequence details	UNP G7NS93
A	441	VAL	GLU	see sequence details	UNP G7NS93
A	442	PRO	VAL	see sequence details	UNP G7NS93
A	443	ARG	GLY	see sequence details	UNP G7NS93
A	444	GLY	PHE	see sequence details	UNP G7NS93
A	445	SER	CYS	see sequence details	UNP G7NS93
A	488	GLN	ASN	engineered mutation	UNP G7NS93
A	799	GLN	ASN	engineered mutation	UNP G7NS93
A	840	GLU	-	expression tag	UNP G7NS93
A	841	PHE	-	expression tag	UNP G7NS93
A	842	LEU	-	expression tag	UNP G7NS93
A	843	VAL	-	expression tag	UNP G7NS93
A	844	PRO	-	expression tag	UNP G7NS93
A	845	ARG	-	expression tag	UNP G7NS93

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



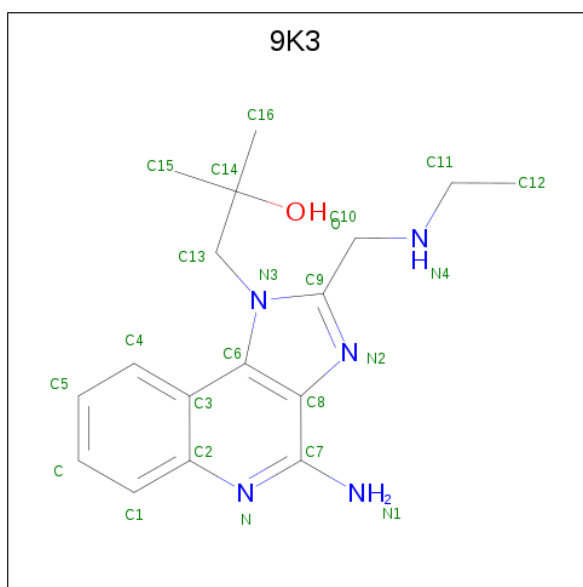
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	D	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	F	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 4 is 1-{4-amino-2-[(ethylamino)methyl]-1H-imidazo[4,5-c]quinolin-1-yl}-2-methylpropan-2-ol (three-letter code: 9K3) (formula: C₁₇H₂₃N₅O) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			23	17	5	1		
4	A	1	Total	C	N	O	0	0
			23	17	5	1		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		

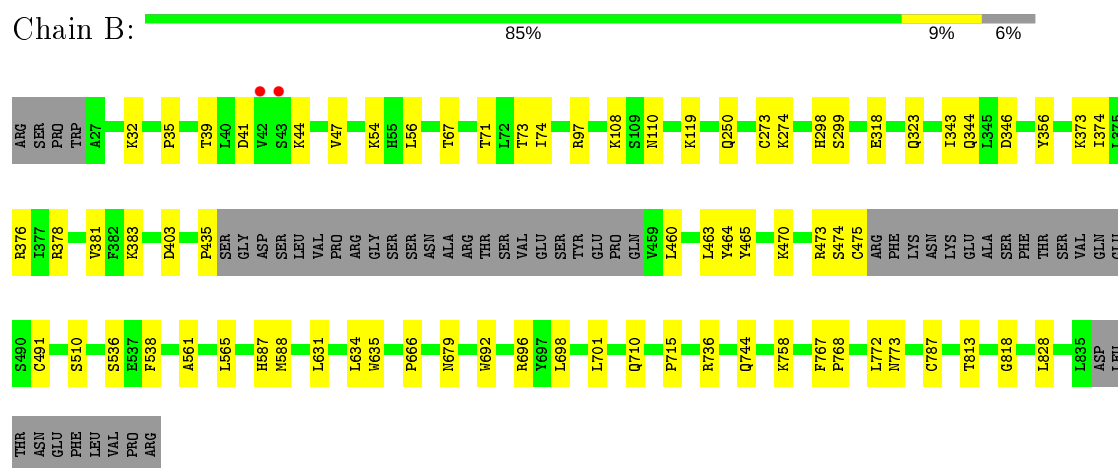
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	396	Total	O	0	0
			396	396		
6	A	263	Total	O	0	0
			263	263		

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: Toll-like receptor 7



• Molecule 1: Toll-like receptor 7



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

Chain C:  100%

NAG1
NAG2

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

Chain D:  100%

NAG1
NAG2

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

Chain E:  50% 50%

NAG1
NAG2

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

Chain F:  50% 50%

NAG1
NAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	99.34Å 140.18Å 151.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.20 – 2.30 47.20 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.20-2.30) 100.0 (47.20-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.94 (at 2.29Å)	Xtriage
Refinement program	PHENIX (1.11.1 _2575: ???)	Depositor
R, R_{free}	0.186 , 0.224 0.186 , 0.224	Depositor DCC
R_{free} test set	4671 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	39.6	Xtriage
Anisotropy	0.158	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 42.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13527	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% 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: 9K3, NAG, SO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.49	6/6389 (0.1%)	0.74	13/8657 (0.2%)
1	B	0.46	1/6389 (0.0%)	0.65	1/8657 (0.0%)
All	All	0.48	7/12778 (0.1%)	0.69	14/17314 (0.1%)

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	723	ARG	CG-CD	9.51	1.75	1.51
1	A	723	ARG	CZ-NH2	6.56	1.41	1.33
1	A	748	GLN	CD-NE2	6.35	1.48	1.32
1	A	44	LYS	CE-NZ	-6.29	1.33	1.49
1	A	723	ARG	CB-CG	6.18	1.69	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	723	ARG	NE-CZ-NH2	15.11	127.86	120.30
1	A	723	ARG	NE-CZ-NH1	-13.71	113.45	120.30
1	A	723	ARG	CG-CD-NE	10.17	133.16	111.80
1	A	723	ARG	CB-CG-CD	9.31	135.82	111.60
1	A	493	LYS	CG-CD-CE	-8.05	87.76	111.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6258	0	6302	84	1
1	B	6258	0	6301	51	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	1	0
3	A	70	0	65	5	0
3	B	84	0	78	4	1
4	A	23	0	0	0	0
4	B	23	0	0	0	0
5	A	15	0	0	1	0
5	B	25	0	0	1	0
6	A	263	0	0	22	0
6	B	396	0	0	18	0
All	All	13527	0	12846	139	1

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 5.

The worst 5 of 139 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:723:ARG:CD	1:A:723:ARG:CG	1.75	1.63
1:B:473:ARG:NH1	6:B:1103:HOH:O	1.96	0.98
1:A:284:ASN:OD1	6:A:1101:HOH:O	1.81	0.97
1:A:432:LYS:NZ	6:A:1104:HOH:O	1.98	0.92
1:B:32:LYS:NZ	6:B:1106:HOH:O	2.07	0.87

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:770:ASN:ND2	3:B:1005:NAG:O7[3_554]	2.15	0.05

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	767/823 (93%)	720 (94%)	45 (6%)	2 (0%)	41	50
1	B	767/823 (93%)	724 (94%)	41 (5%)	2 (0%)	41	50
All	All	1534/1646 (93%)	1444 (94%)	86 (6%)	4 (0%)	41	50

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	818	GLY
1	A	818	GLY
1	B	381	VAL
1	A	381	VAL

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	726/774 (94%)	721 (99%)	5 (1%)	84	92
1	B	726/774 (94%)	722 (99%)	4 (1%)	86	94
All	All	1452/1548 (94%)	1443 (99%)	9 (1%)	86	94

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	108	LYS
1	A	770	ASN

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Mol	Chain	Res	Type
1	A	493	LYS
1	B	474	SER
1	A	370	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	394	HIS
1	A	732	ASN
1	A	250	GLN
1	B	280	GLN
1	A	252	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 ⓘ

8 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	0.34	0	17,19,21	0.66	1 (5%)
2	NAG	C	2	2	14,14,15	0.53	0	17,19,21	0.74	1 (5%)
2	NAG	D	1	1,2	14,14,15	0.35	0	17,19,21	0.46	0
2	NAG	D	2	2	14,14,15	0.41	0	17,19,21	0.69	0
2	NAG	E	1	1,2	14,14,15	0.51	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	E	2	2	14,14,15	0.94	2 (14%)	17,19,21	0.64	0
2	NAG	F	1	1,2	14,14,15	0.26	0	17,19,21	0.59	0
2	NAG	F	2	2	14,14,15	0.31	0	17,19,21	0.93	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	C	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
2	NAG	D	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	1/6/23/26	0/1/1/1
2	NAG	E	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
2	NAG	F	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	2	NAG	C1-C2	2.58	1.56	1.52
2	E	2	NAG	O5-C1	-2.14	1.40	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	2	NAG	C1-O5-C5	2.83	116.02	112.19
2	C	2	NAG	C1-O5-C5	2.22	115.20	112.19
2	C	1	NAG	C1-O5-C5	2.06	114.98	112.19

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	2	NAG	C4-C5-C6-O6
2	F	2	NAG	O5-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6

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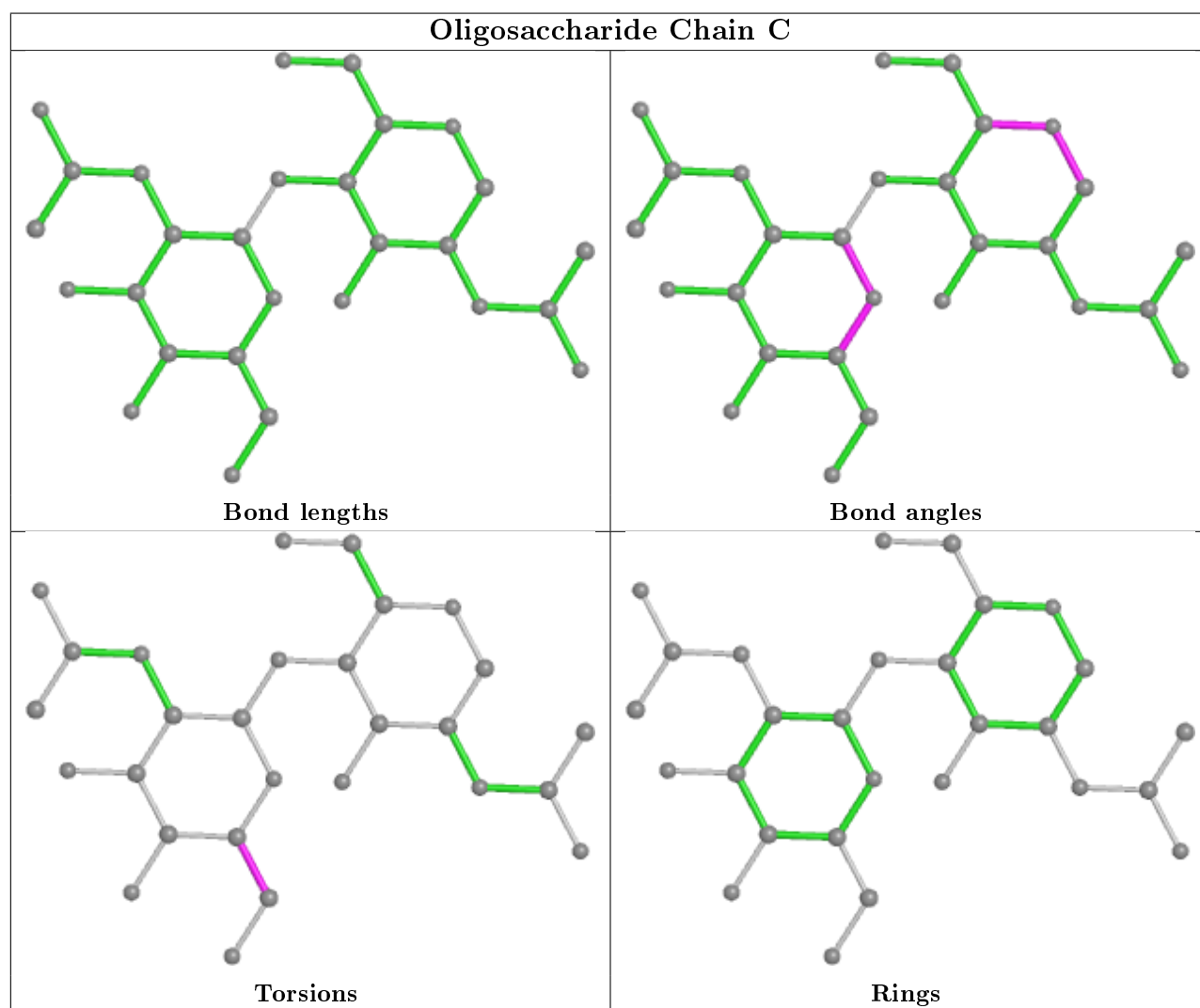
Mol	Chain	Res	Type	Atoms
2	F	1	NAG	C4-C5-C6-O6

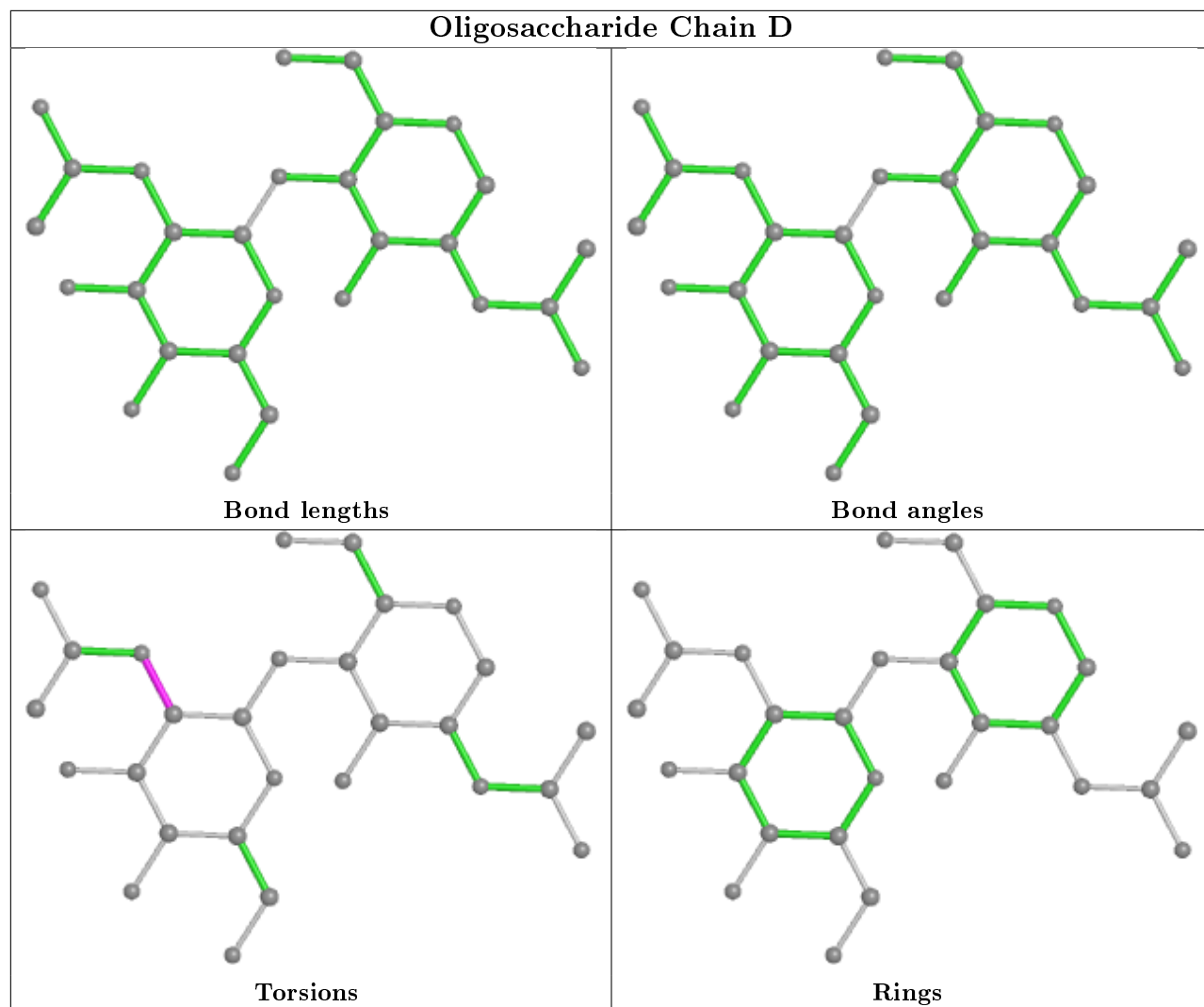
There are no ring outliers.

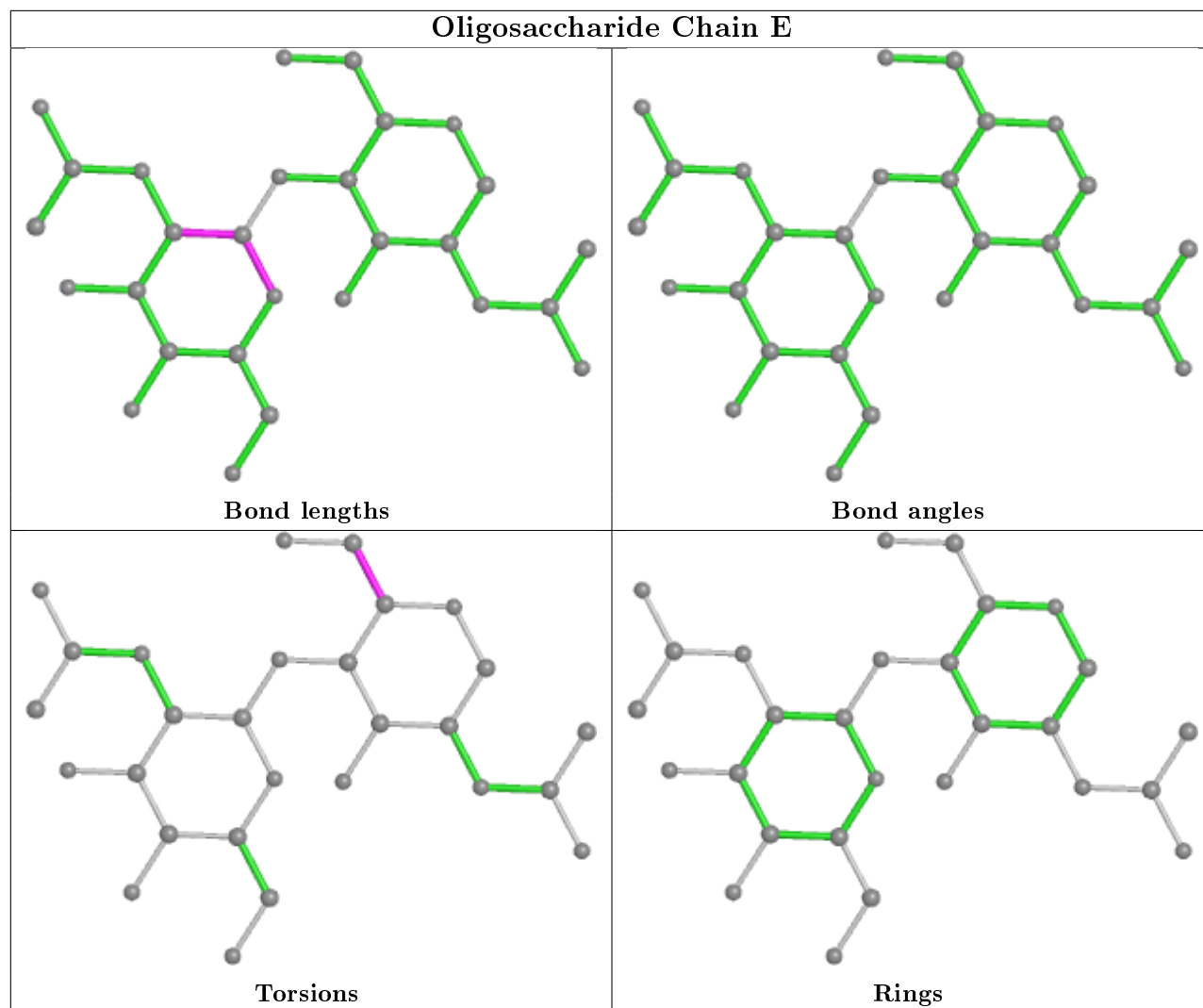
1 monomer is involved in 1 short contact:

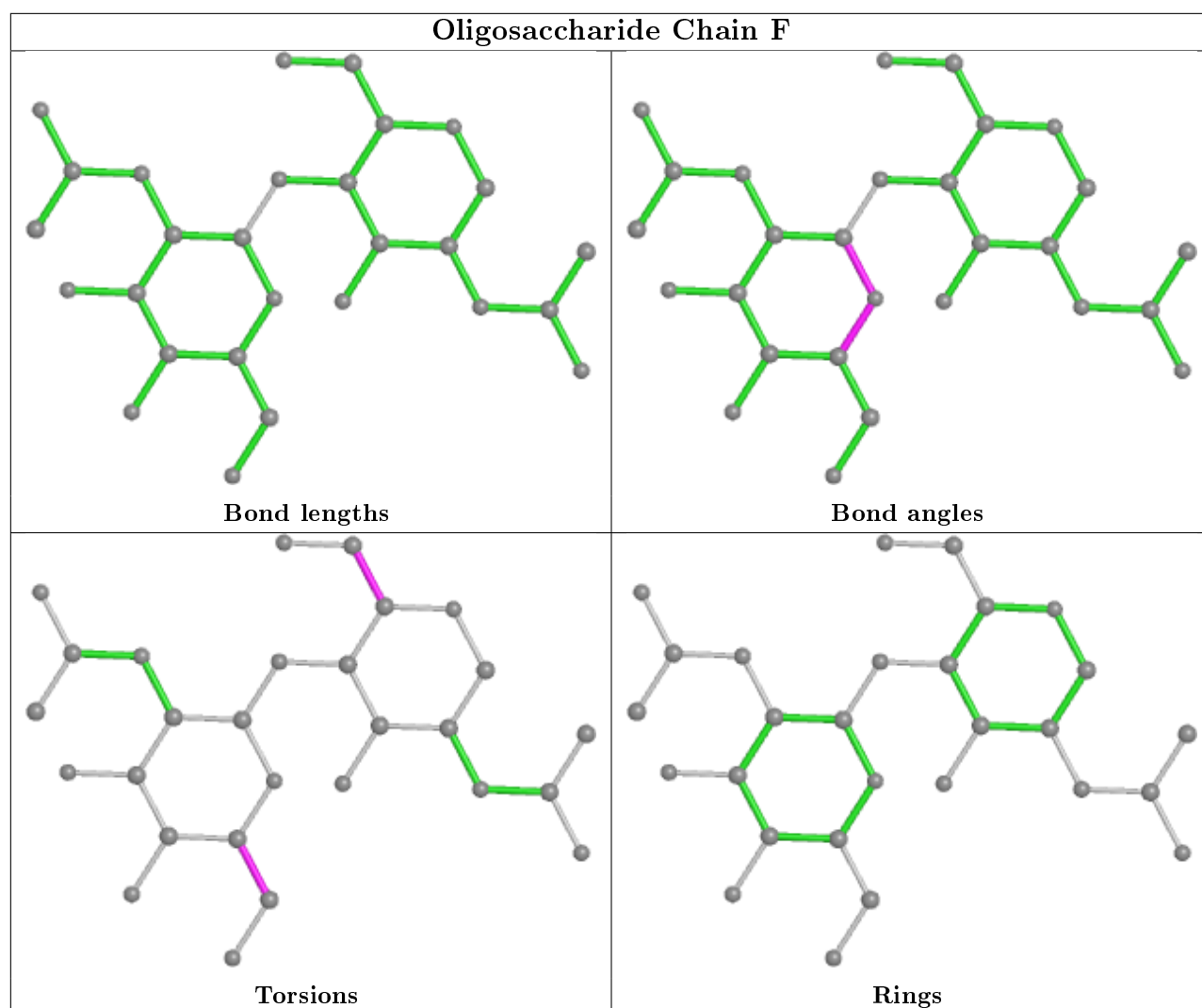
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	2	NAG	1	0

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









5.6 Ligand geometry ⓘ

21 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	SO4	B	1013	-	4,4,4	0.21	0	6,6,6	0.26	0
5	SO4	A	1013	-	4,4,4	0.23	0	6,6,6	0.23	0
3	NAG	A	1008	1	14,14,15	0.65	1 (7%)	17,19,21	0.69	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	B	1001	1	14,14,15	0.56	0	17,19,21	0.61	0
3	NAG	A	1001	1	14,14,15	0.41	0	17,19,21	0.59	0
5	SO4	B	1016	-	4,4,4	0.17	0	6,6,6	0.14	0
5	SO4	A	1011	-	4,4,4	0.20	0	6,6,6	0.48	0
3	NAG	B	1010	1	14,14,15	0.30	0	17,19,21	0.33	0
3	NAG	B	1009	1	14,14,15	0.83	1 (7%)	17,19,21	0.57	0
3	NAG	A	1009	1	14,14,15	0.82	1 (7%)	17,19,21	0.81	0
5	SO4	B	1015	-	4,4,4	0.21	0	6,6,6	0.19	0
5	SO4	B	1012	-	4,4,4	0.18	0	6,6,6	0.43	0
3	NAG	A	1004	1	14,14,15	0.49	0	17,19,21	2.17	3 (17%)
5	SO4	A	1012	-	4,4,4	0.14	0	6,6,6	0.24	0
3	NAG	B	1005	1	14,14,15	0.56	0	17,19,21	0.44	0
3	NAG	B	1008	1	14,14,15	0.48	0	17,19,21	0.78	1 (5%)
4	9K3	B	1011	-	20,25,25	1.39	1 (5%)	25,37,37	1.50	7 (28%)
3	NAG	A	1007	1	14,14,15	1.00	1 (7%)	17,19,21	1.17	3 (17%)
5	SO4	B	1014	-	4,4,4	0.17	0	6,6,6	0.18	0
3	NAG	B	1002	1	14,14,15	0.40	0	17,19,21	0.46	0
4	9K3	A	1010	-	20,25,25	1.38	2 (10%)	25,37,37	1.56	5 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	1001	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1001	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1010	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1009	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1009	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1008	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1004	1	-	6/6/23/26	0/1/1/1
3	NAG	B	1005	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1008	1	-	2/6/23/26	0/1/1/1
4	9K3	B	1011	-	-	1/5/9/9	0/3/3/3
3	NAG	A	1007	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1002	1	-	2/6/23/26	0/1/1/1
4	9K3	A	1010	-	-	0/5/9/9	0/3/3/3

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1011	9K3	C3-C2	4.87	1.50	1.41
4	A	1010	9K3	C13-C14	3.84	1.58	1.54
4	A	1010	9K3	C3-C2	3.66	1.48	1.41
3	A	1007	NAG	O5-C1	-3.33	1.38	1.43
3	A	1009	NAG	O5-C1	-2.57	1.39	1.43

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1004	NAG	C2-N2-C7	7.33	133.34	122.90
4	B	1011	9K3	C15-C14-C13	3.67	119.45	110.13
4	A	1010	9K3	C8-C7-N	-3.55	118.68	121.01
3	A	1004	NAG	O3-C3-C4	-3.51	102.23	110.35
4	A	1010	9K3	C6-C3-C2	-3.41	117.06	119.65

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1004	NAG	C1-C2-N2-C7
4	B	1011	9K3	C9-C10-N4-C11
3	B	1008	NAG	O5-C5-C6-O6
3	A	1007	NAG	O5-C5-C6-O6
3	B	1002	NAG	O5-C5-C6-O6

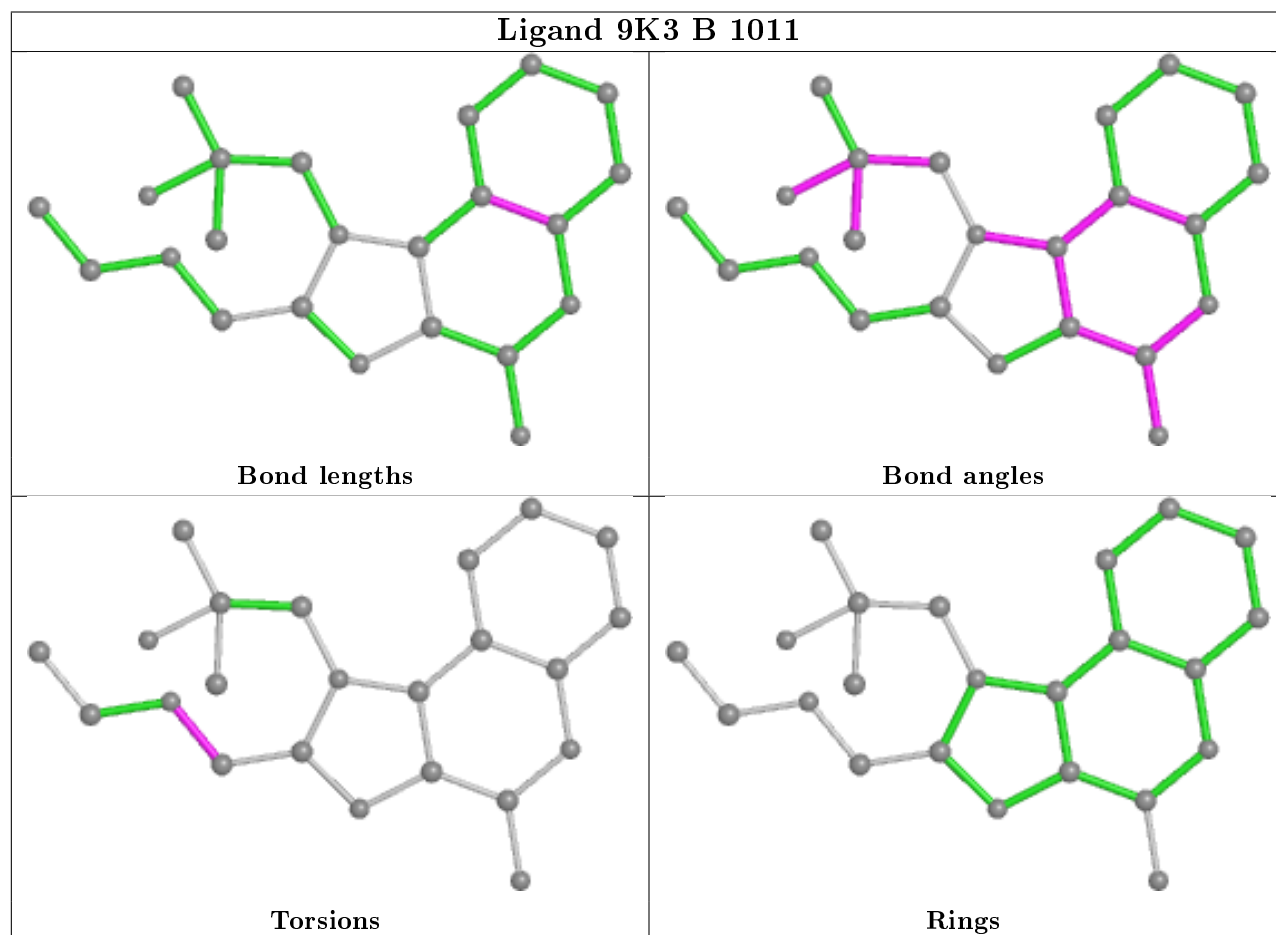
There are no ring outliers.

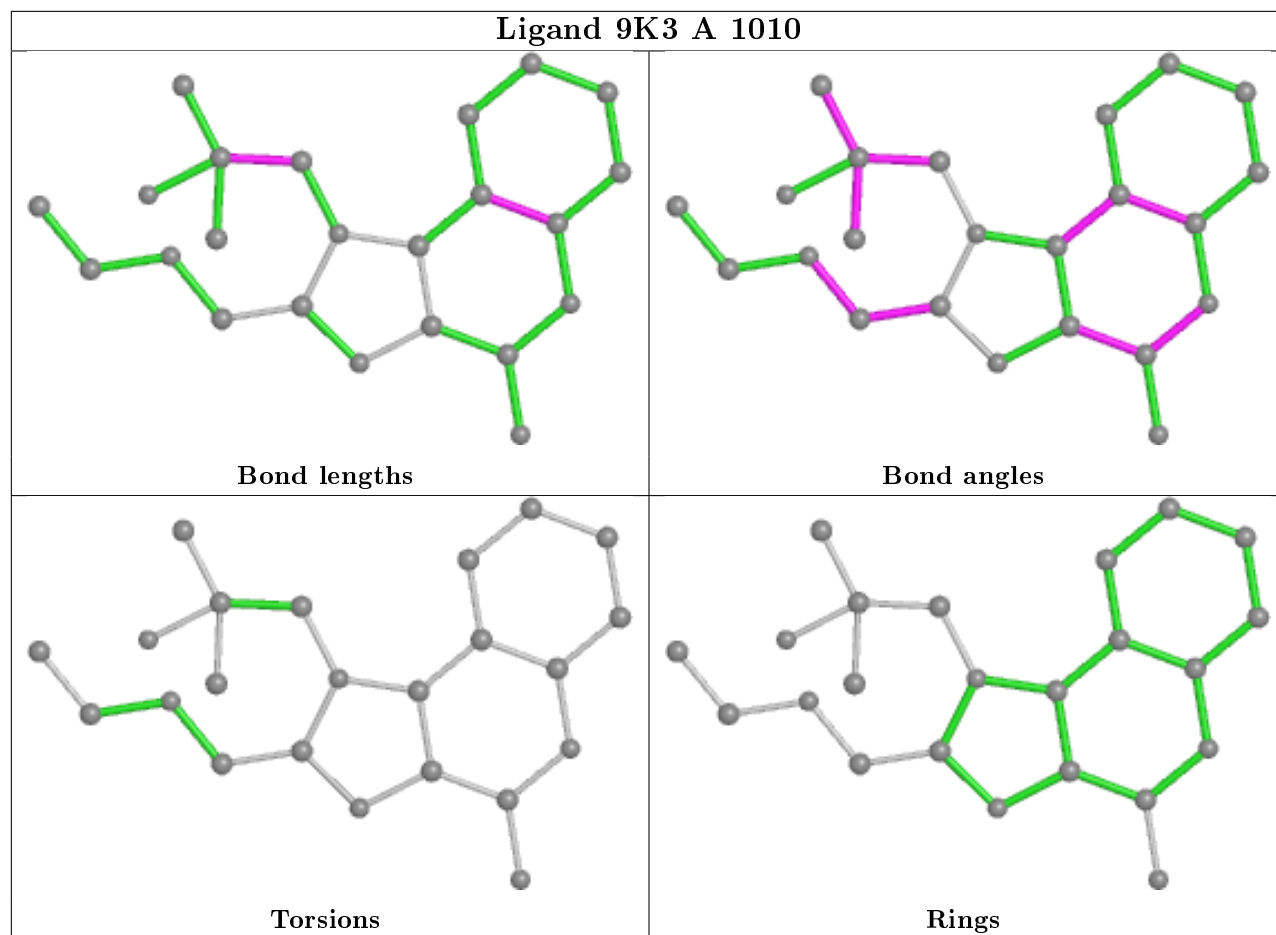
8 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1013	SO4	1	0
3	B	1001	NAG	1	0
3	A	1001	NAG	1	0
5	B	1016	SO4	1	0
3	B	1009	NAG	2	0
3	A	1004	NAG	4	0
3	B	1005	NAG	0	1
3	B	1008	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	772/823 (93%)	0.01	8 (1%) 82 86	30, 46, 65, 91	0
1	B	772/823 (93%)	-0.13	2 (0%) 94 96	24, 38, 57, 81	0
All	All	1544/1646 (93%)	-0.06	10 (0%) 89 92	24, 42, 62, 91	0

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	723	ARG	4.6
1	A	748	GLN	4.3
1	A	774	ASN	2.7
1	A	776	LYS	2.6
1	A	388	PHE	2.5

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.

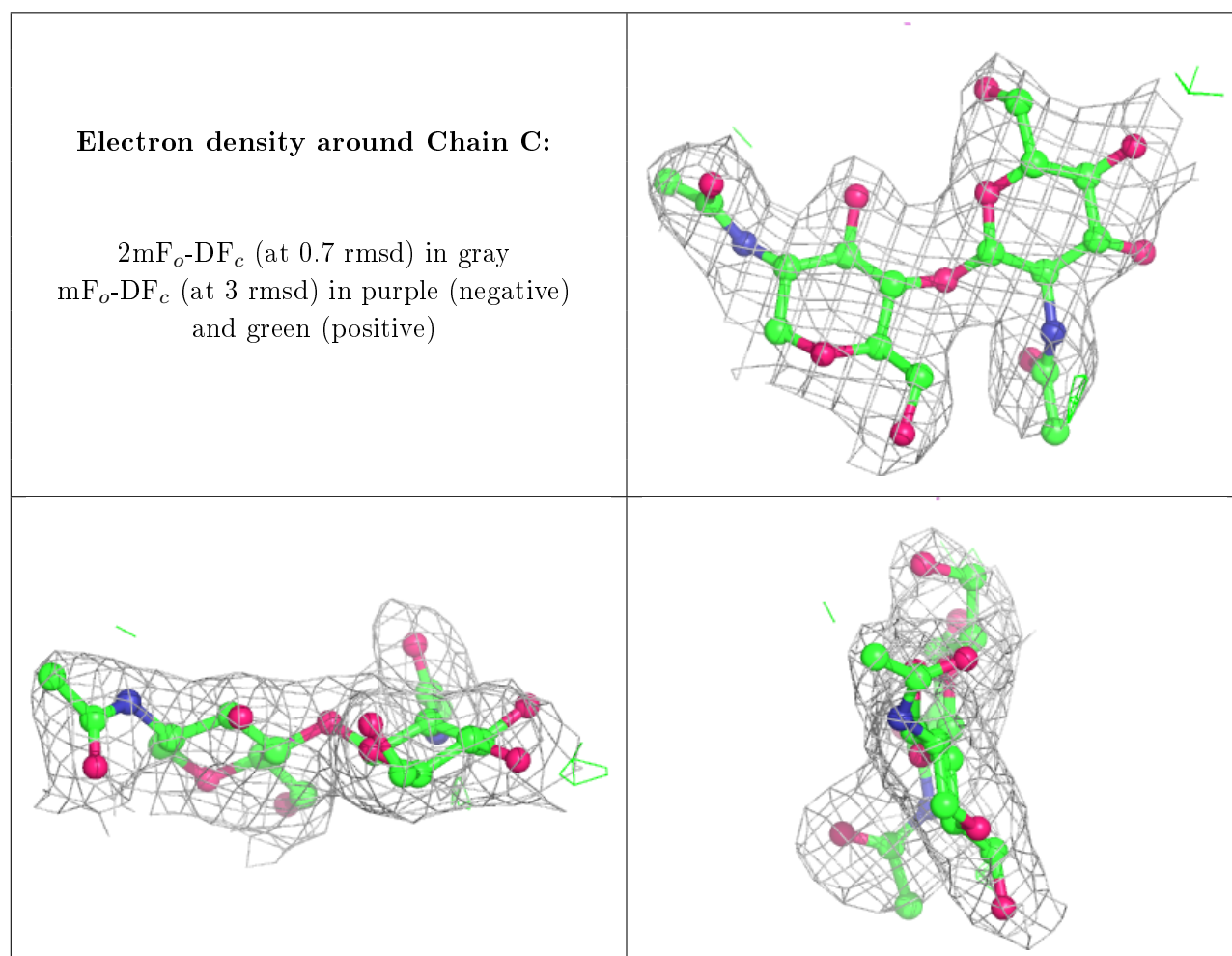
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	C	2	14/15	0.89	0.14	52,57,62,66	0
2	NAG	E	2	14/15	0.89	0.13	59,64,71,72	0
2	NAG	F	2	14/15	0.89	0.21	63,70,76,82	0
2	NAG	D	2	14/15	0.90	0.23	64,68,72,73	0
2	NAG	F	1	14/15	0.92	0.10	47,53,58,63	0

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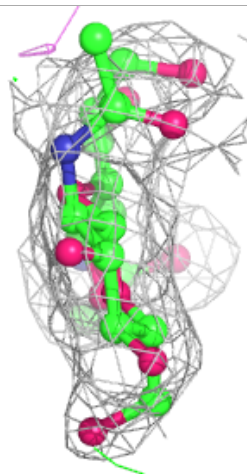
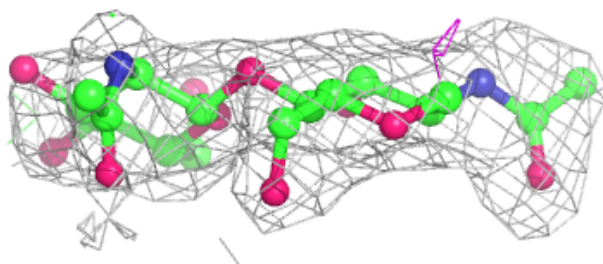
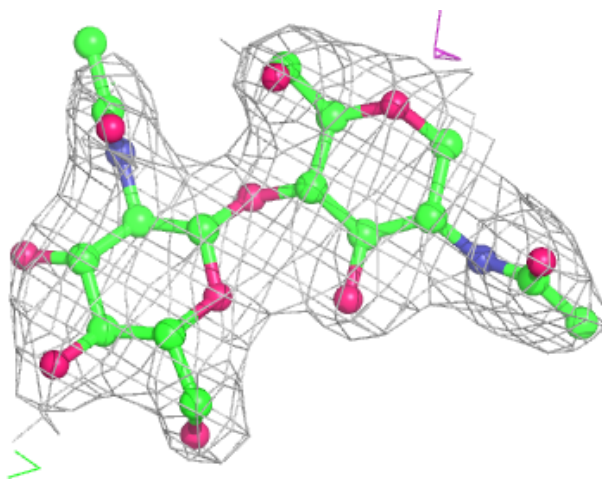
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NAG	D	1	14/15	0.94	0.12	43,50,54,64	0
2	NAG	E	1	14/15	0.96	0.10	35,47,52,53	0
2	NAG	C	1	14/15	0.97	0.11	37,45,51,53	0

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.



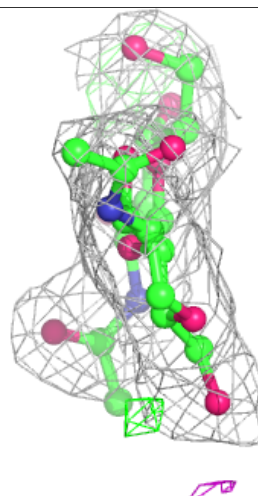
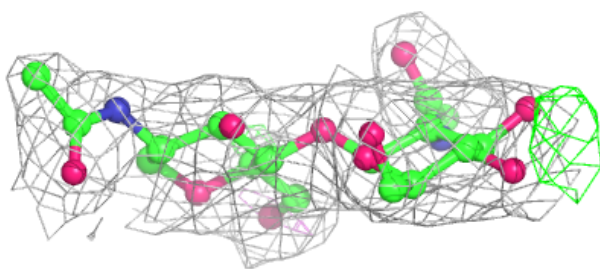
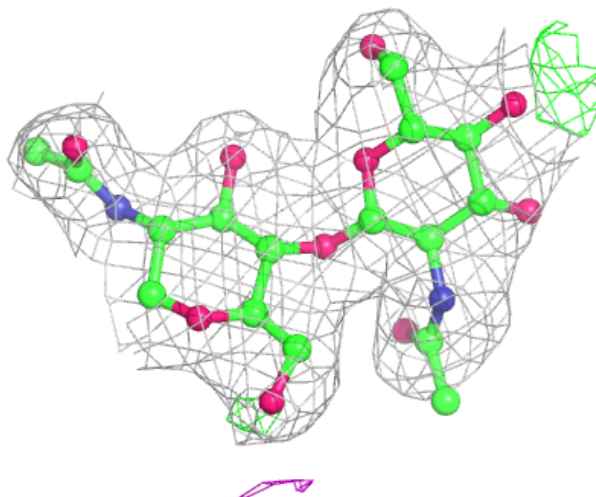
Electron density around Chain D:

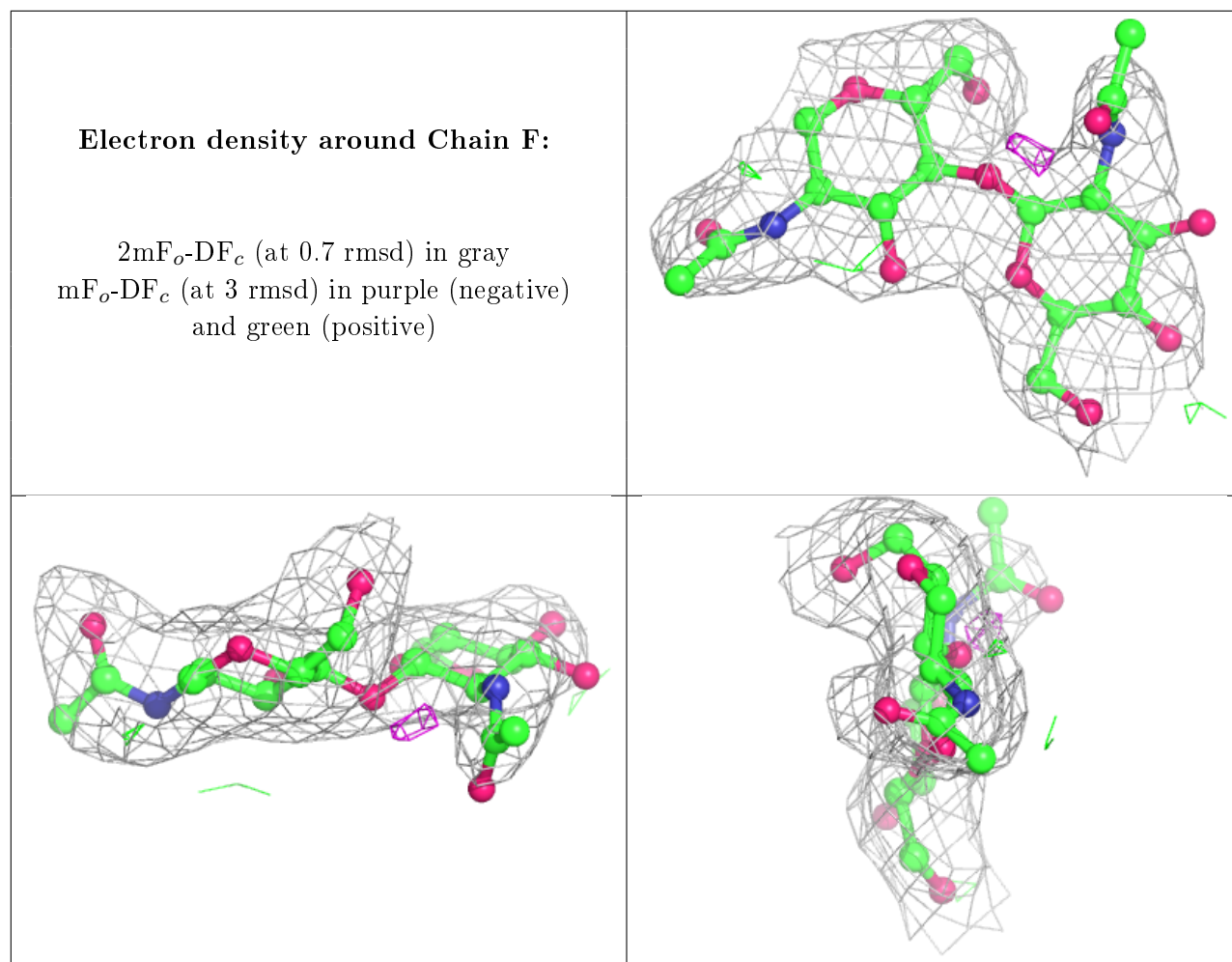
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





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(\AA^2)	Q<0.9
5	SO4	B	1015	5/5	0.83	0.20	69,70,93,94	0
3	NAG	B	1008	14/15	0.86	0.15	45,56,63,71	0
3	NAG	A	1004	14/15	0.88	0.14	57,67,73,75	0
3	NAG	B	1005	14/15	0.88	0.15	56,61,72,78	0
3	NAG	A	1008	14/15	0.88	0.17	55,65,68,70	0
3	NAG	A	1009	14/15	0.90	0.14	67,74,78,79	0
5	SO4	B	1012	5/5	0.90	0.19	49,58,71,81	0
5	SO4	B	1016	5/5	0.91	0.17	72,79,80,94	0
5	SO4	B	1013	5/5	0.91	0.24	64,74,83,92	0
5	SO4	B	1014	5/5	0.91	0.21	63,78,84,93	0

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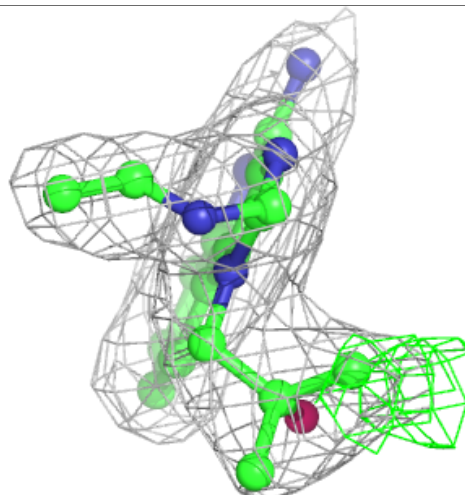
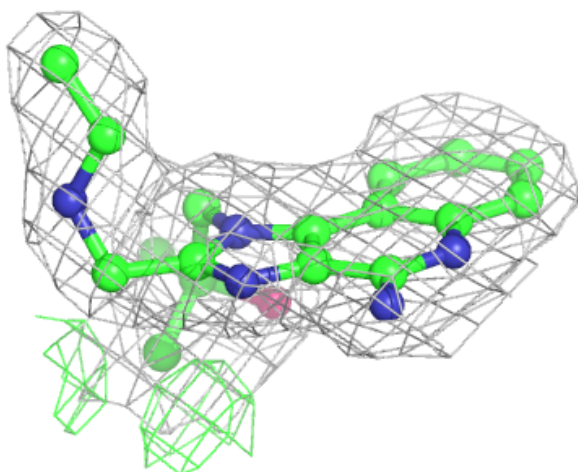
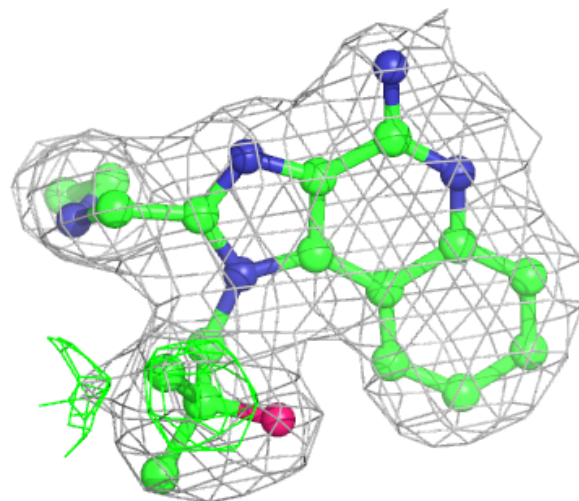
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	SO4	A	1013	5/5	0.92	0.16	67,68,85,89	0
3	NAG	B	1010	14/15	0.92	0.09	58,65,71,72	0
3	NAG	A	1007	14/15	0.93	0.26	57,68,72,77	0
5	SO4	A	1012	5/5	0.93	0.12	59,68,81,82	0
3	NAG	B	1009	14/15	0.94	0.11	44,47,52,54	0
3	NAG	A	1001	14/15	0.94	0.14	40,47,50,53	0
3	NAG	B	1002	14/15	0.94	0.13	50,56,61,61	0
4	9K3	B	1011	23/23	0.96	0.16	33,39,43,47	0
3	NAG	B	1001	14/15	0.96	0.13	29,34,40,43	0
4	9K3	A	1010	23/23	0.96	0.19	33,39,43,44	0
5	SO4	A	1011	5/5	0.97	0.12	52,54,59,60	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.

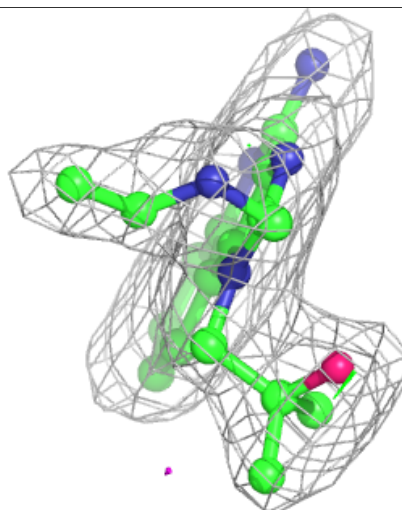
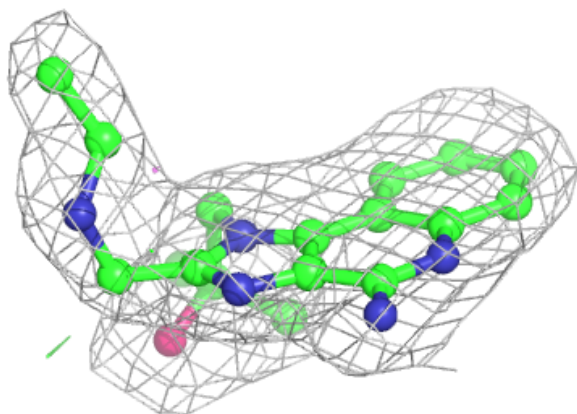
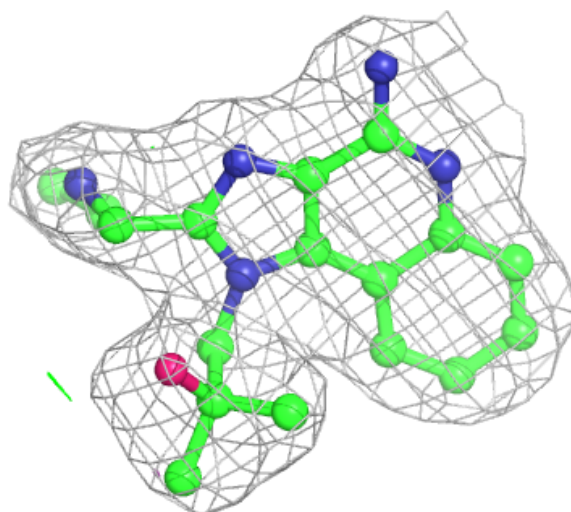
Electron density around 9K3 B 1011:

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 9K3 A 1010:

$2mF_o-DF_c$ (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.