



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:17 AM UTC

PDB ID : 8TTY / pdb_00008tty
Title : Crystal structure of monkey TLR7 ectodomain with compound 5
Authors : Critton, D.A.
Deposited on : 2023-08-15
Resolution : 2.10 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

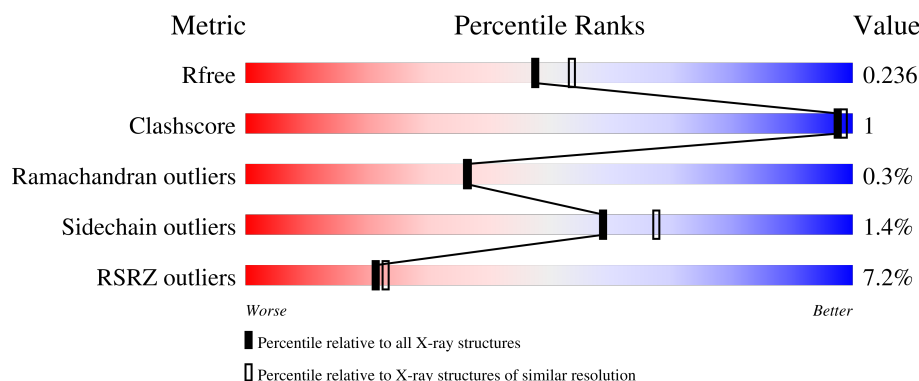
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	817	5% 90% 6%
1	B	817	9% 90% 6%
2	C	3	67% 33%
3	D	2	50% 50%
3	E	2	50% 50%

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Mol	Chain	Length	Quality of chain
3	F	2	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 25867 atoms, of which 12443 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.

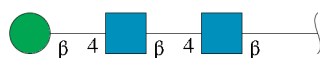
- Molecule 1 is a protein called Toll-like receptor 7.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	768	Total	C	H	N	O	S	6068	1	0
			12216	3945	6068	1031	1142	30			
1	B	768	Total	C	H	N	O	S	6022	0	0
			12150	3936	6022	1020	1142	30			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	ARG	-	expression tag	UNP G8E2R2
A	24	SER	-	expression tag	UNP G8E2R2
A	25	PRO	-	expression tag	UNP G8E2R2
A	26	TRP	-	expression tag	UNP G8E2R2
A	167	GLN	ASN	conflict	UNP G8E2R2
A	389	GLN	ASN	conflict	UNP G8E2R2
A	488	GLN	ASN	conflict	UNP G8E2R2
A	799	GLN	ASN	conflict	UNP G8E2R2
B	23	ARG	-	expression tag	UNP G8E2R2
B	24	SER	-	expression tag	UNP G8E2R2
B	25	PRO	-	expression tag	UNP G8E2R2
B	26	TRP	-	expression tag	UNP G8E2R2
B	167	GLN	ASN	conflict	UNP G8E2R2
B	389	GLN	ASN	conflict	UNP G8E2R2
B	488	GLN	ASN	conflict	UNP G8E2R2
B	799	GLN	ASN	conflict	UNP G8E2R2

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



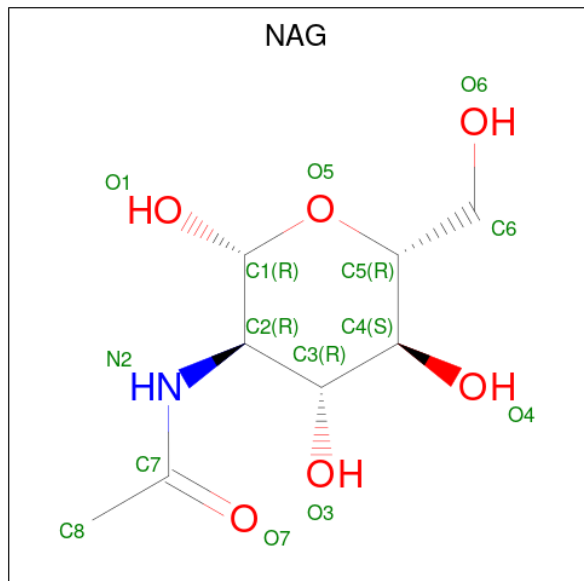
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	3	Total	C	H	N	O	34	0	0
			73	22	34	2	15			

- Molecule 3 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
3	D	2	Total	C	H	N	O	25	0	0
			53	16	25	2	10			
3	E	2	Total	C	H	N	O	25	0	0
			53	16	25	2	10			
3	F	2	Total	C	H	N	O	25	0	0
			53	16	25	2	10			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



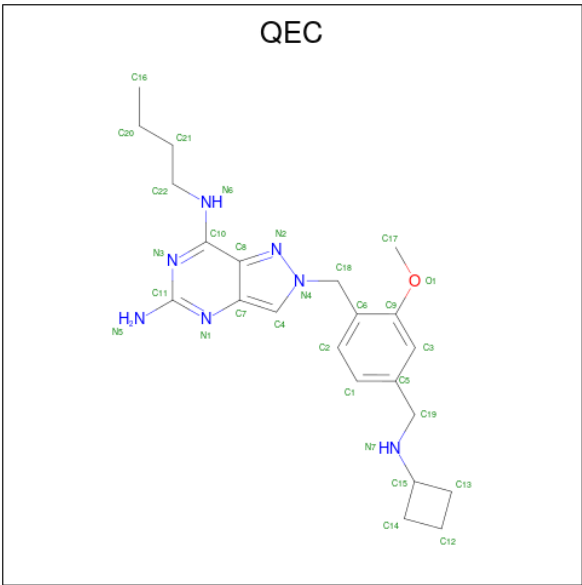
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	H	N	O	13	0
			27	8	13	1	5		
4	A	1	Total	C	H	N	O	13	0
			27	8	13	1	5		

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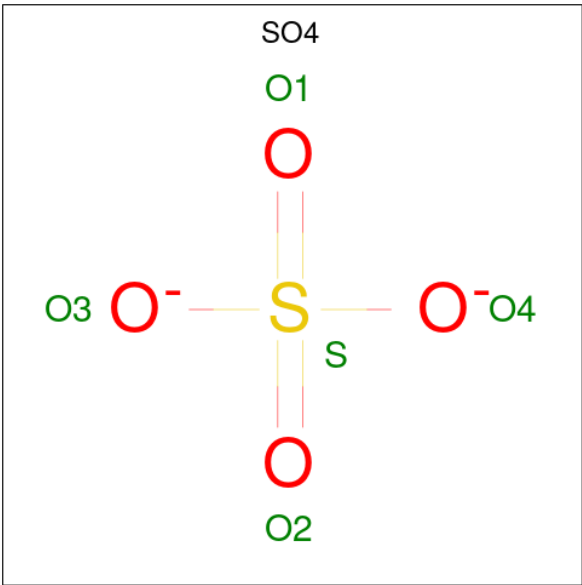
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	H	N	O	13	0
			27	8	13	1	5		
4	A	1	Total	C	H	N	O	13	0
			27	8	13	1	5		
4	A	1	Total	C	H	N	O	13	0
			27	8	13	1	5		
4	A	1	Total	C	H	N	O	13	0
			27	8	13	1	5		
4	A	1	Total	C	H	N	O	13	0
			27	8	13	1	5		
4	B	1	Total	C	H	N	O	13	0
			27	8	13	1	5		
4	B	1	Total	C	H	N	O	13	0
			27	8	13	1	5		
4	B	1	Total	C	H	N	O	13	0
			27	8	13	1	5		
4	B	1	Total	C	H	N	O	13	0
			27	8	13	1	5		
4	B	1	Total	C	H	N	O	13	0
			27	8	13	1	5		
4	B	1	Total	C	H	N	O	13	0
			27	8	13	1	5		

- Molecule 5 is N 7 -butyl-2-({4-[(cyclobutylamino)methyl]-2-methoxyphenyl}methyl)-2H-pyrazolo[4,3-d]pyrimidine-5,7-diamine (CCD ID: QEC) (formula: C₂₂H₃₁N₇O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	H	N	O	31	0
			61	22	31	7	1		
5	B	1	Total	C	H	N	O	31	0
			61	22	31	7	1		

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	435	Total	O	0	0
			435	435		
7	B	319	Total	O	0	0
			319	319		



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	98.86Å 139.89Å 149.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	102.21 – 2.10 102.21 – 2.10	Depositor EDS
% Data completeness (in resolution range)	80.1 (102.21-2.10) 80.1 (102.21-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.26 (at 2.10Å)	Xtriage
Refinement program	BUSTER 2.11.7 (20-MAY-2020)	Depositor
R, R_{free}	0.205 , 0.238 0.204 , 0.236	Depositor DCC
R_{free} test set	4728 reflections (3.90%)	wwPDB-VP
Wilson B-factor (Å ²)	51.2	Xtriage
Anisotropy	0.014	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 48.8	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	0.95	EDS
Total number of atoms	25867	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.75% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, SO4, QEC, BMA

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	0.75	2/6279 (0.0%)	0.96	5/8532 (0.1%)
1	B	0.73	0/6259	0.96	3/8509 (0.0%)
All	All	0.74	2/12538 (0.0%)	0.96	8/17041 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	602	MET	SD-CE	-5.30	1.66	1.79
1	A	792	VAL	CA-CB	5.17	1.60	1.54

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	679	ASN	CA-CB-CG	8.07	120.67	112.60
1	B	649	LEU	N-CA-C	-7.48	99.16	109.71
1	A	649	LEU	N-CA-C	-7.42	99.25	109.71
1	A	679	ASN	OD1-CG-ND2	-5.92	116.68	122.60
1	A	280	GLN	CG-CD-NE2	5.66	124.89	116.40
1	A	767	PHE	CA-CB-CG	5.40	119.20	113.80
1	A	394	HIS	N-CA-C	5.23	116.98	111.28
1	B	770	ASN	CA-CB-CG	5.00	117.60	112.60

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	6148	6068	6059	9	0
1	B	6128	6022	6013	12	0
2	C	39	34	34	0	0
3	D	28	25	25	0	0
3	E	28	25	25	0	0
3	F	28	25	25	0	0
4	A	98	91	91	2	0
4	B	98	91	91	0	0
5	A	30	31	0	0	0
5	B	30	31	0	0	0
6	B	15	0	0	1	0
7	A	435	0	0	0	0
7	B	319	0	0	1	0
All	All	13424	12443	12363	20	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 (20) 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:206:LEU:O	1:A:226:THR:HG23	2.02	0.60
1:B:206:LEU:O	1:B:226:THR:HG23	2.02	0.60
1:B:767:PHE:HB3	1:B:772:LEU:HD11	1.84	0.58
1:B:510:SER:OG	1:B:536:SER:O	2.22	0.57
1:A:510:SER:OG	1:A:536:SER:O	2.22	0.57
1:A:679:ASN:HB3	4:A:907:NAG:O5	2.08	0.53
1:B:588:MET:HE3	6:B:911:SO4:O4	2.10	0.52
1:A:299:SER:HA	1:A:323:GLN:O	2.11	0.50
1:B:299:SER:HA	1:B:323:GLN:O	2.12	0.50
1:B:378:ARG:HD2	1:B:403:ASP:OD2	2.12	0.50
1:B:725:LEU:O	1:B:748:GLN:HG2	2.12	0.49
1:B:787:CYS:HB3	1:B:828:LEU:HD21	1.97	0.47
1:B:108:LYS:HD2	1:B:108:LYS:N	2.31	0.46
1:A:787:CYS:HB3	1:A:828:LEU:HD21	1.98	0.45
1:A:108:LYS:HD2	1:A:108:LYS:N	2.31	0.45
1:A:593:LYS:HB3	4:A:902:NAG:H81	2.00	0.43
1:A:767:PHE:HB3	1:A:772:LEU:HD11	2.00	0.42
1:A:186:ARG:HD3	1:B:637:ASP:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:587:HIS:HD2	7:B:1073:HOH:O	2.02	0.41
1:B:433:ILE:H	1:B:503:ASN:ND2	2.18	0.41

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	763/817 (93%)	718 (94%)	43 (6%)	2 (0%)	36	36
1	B	762/817 (93%)	714 (94%)	46 (6%)	2 (0%)	36	36
All	All	1525/1634 (93%)	1432 (94%)	89 (6%)	4 (0%)	36	36

All (4) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains [i](#)

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

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	697/768 (91%)	687 (99%)	10 (1%)	59 67
1	B	691/768 (90%)	681 (99%)	10 (1%)	59 67
All	All	1388/1536 (90%)	1368 (99%)	20 (1%)	59 67

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	LEU
1	A	202	ASN
1	A	213	ASP
1	A	470	LYS
1	A	613	SER
1	A	614	ARG
1	A	627	ARG
1	A	698	LEU
1	A	792	VAL
1	A	825	VAL
1	B	202	ASN
1	B	213	ASP
1	B	613	SER
1	B	614	ARG
1	B	627	ARG
1	B	679	ASN
1	B	698	LEU
1	B	717	ARG
1	B	792	VAL
1	B	825	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	275	ASN
1	A	337	HIS
1	A	389	GLN
1	A	398	ASN
1	A	419	GLN
1	A	503	ASN
1	A	515	HIS

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Mol	Chain	Res	Type
1	A	587	HIS
1	A	594	ASN
1	A	734	GLN
1	A	800	HIS
1	B	76	HIS
1	B	275	ASN
1	B	337	HIS
1	B	398	ASN
1	B	503	ASN
1	B	581	GLN
1	B	594	ASN
1	B	820	HIS
1	B	823	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 ⓘ

9 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	0.72	0
2	NAG	C	2	2	14,14,15	0.26	0	17,19,21	0.63	1 (5%)
2	BMA	C	3	2	11,11,12	0.22	0	15,15,17	0.35	0
3	NAG	D	1	1,3	14,14,15	0.25	0	17,19,21	0.74	1 (5%)
3	NAG	D	2	3	14,14,15	0.28	0	17,19,21	0.63	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	E	1	1,3	14,14,15	0.27	0	17,19,21	0.74	0
3	NAG	E	2	3	14,14,15	0.25	0	17,19,21	0.64	1 (5%)
3	NAG	F	1	1,3	14,14,15	0.27	0	17,19,21	0.77	1 (5%)
3	NAG	F	2	3	14,14,15	0.28	0	17,19,21	0.57	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	BMA	C	3	2	-	0/2/19/22	0/1/1/1
3	NAG	D	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1
3	NAG	E	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	0/6/23/26	0/1/1/1
3	NAG	F	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	1	NAG	O5-C1-C2	-2.37	107.63	111.29
3	E	2	NAG	C1-O5-C5	2.20	115.13	112.19
2	C	2	NAG	C1-O5-C5	2.16	115.08	112.19
3	D	1	NAG	O5-C1-C2	-2.10	108.04	111.29

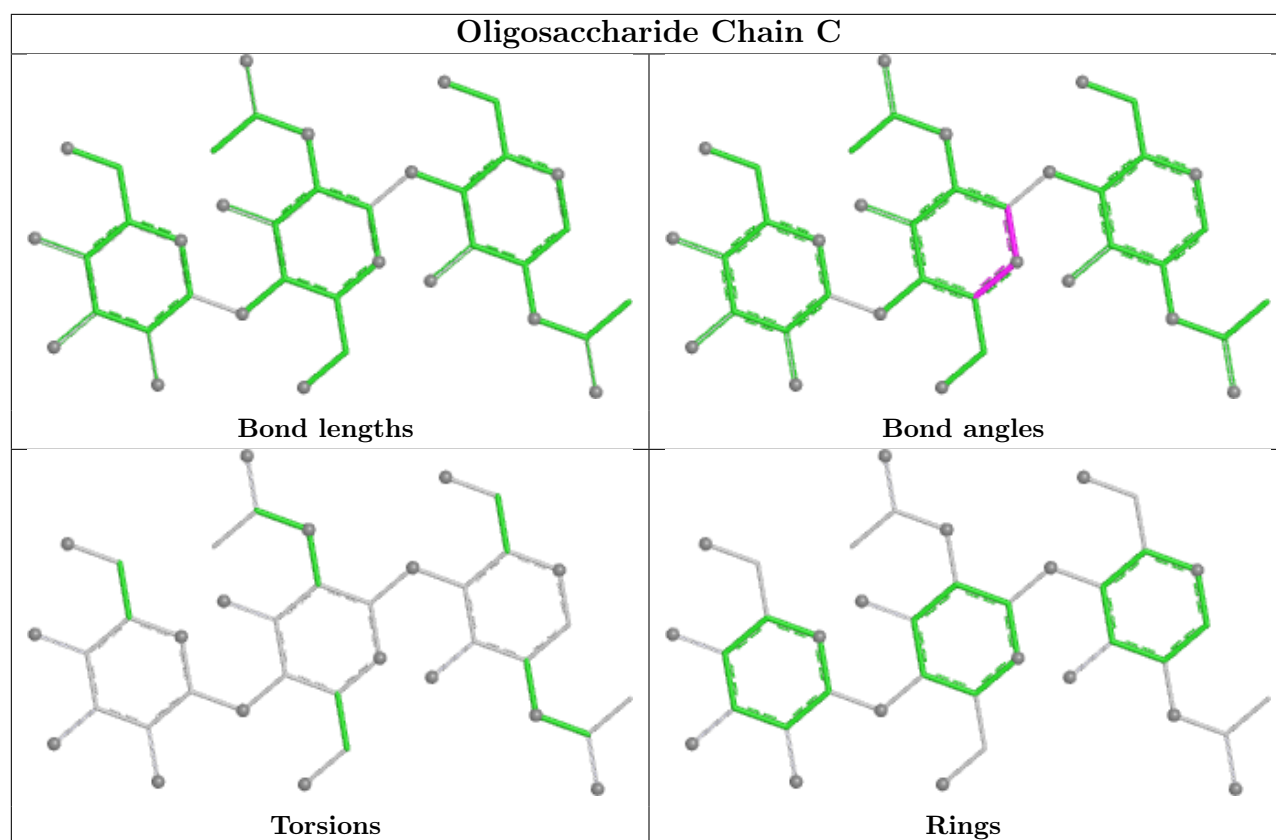
There are no chirality outliers.

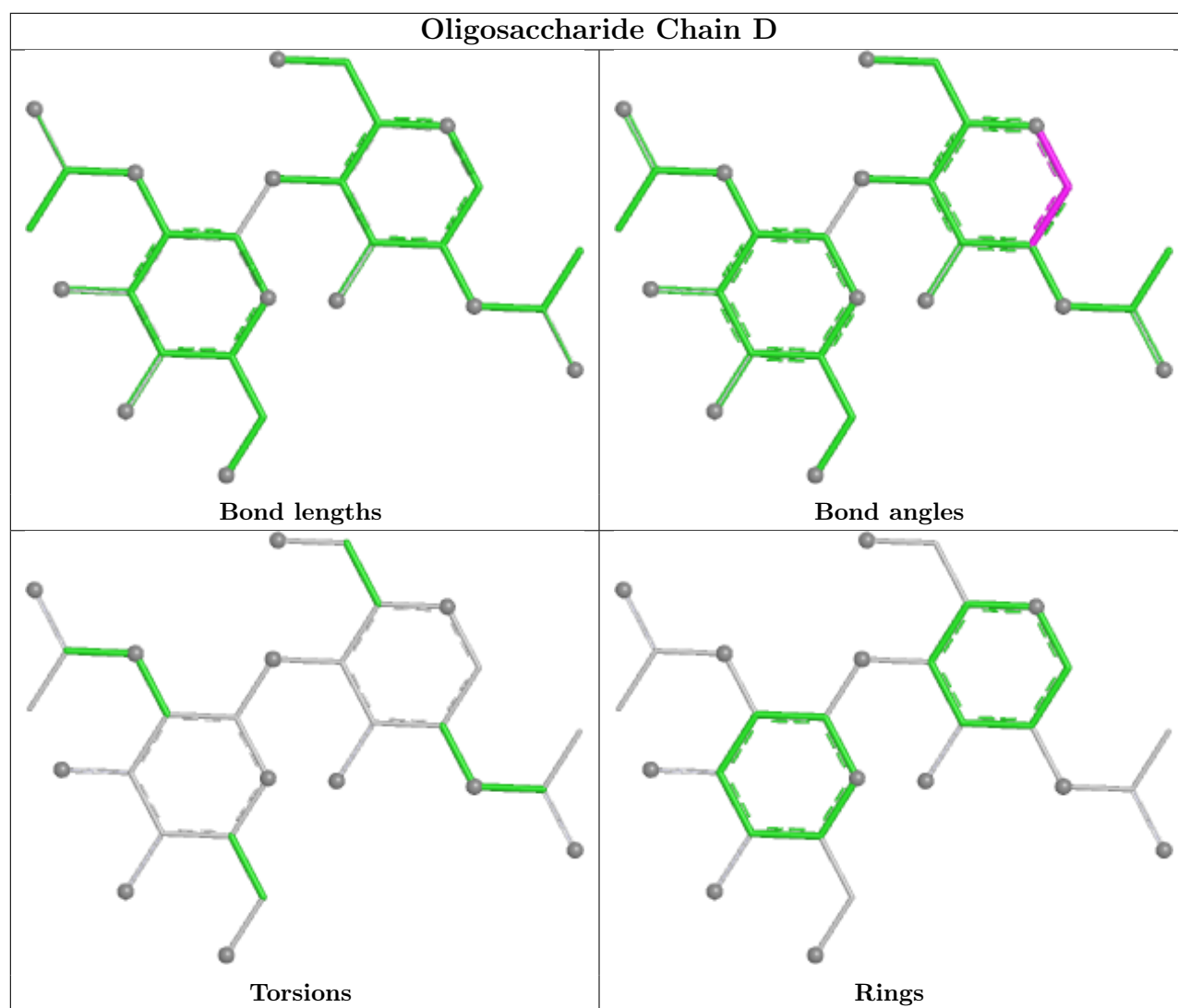
There are no torsion outliers.

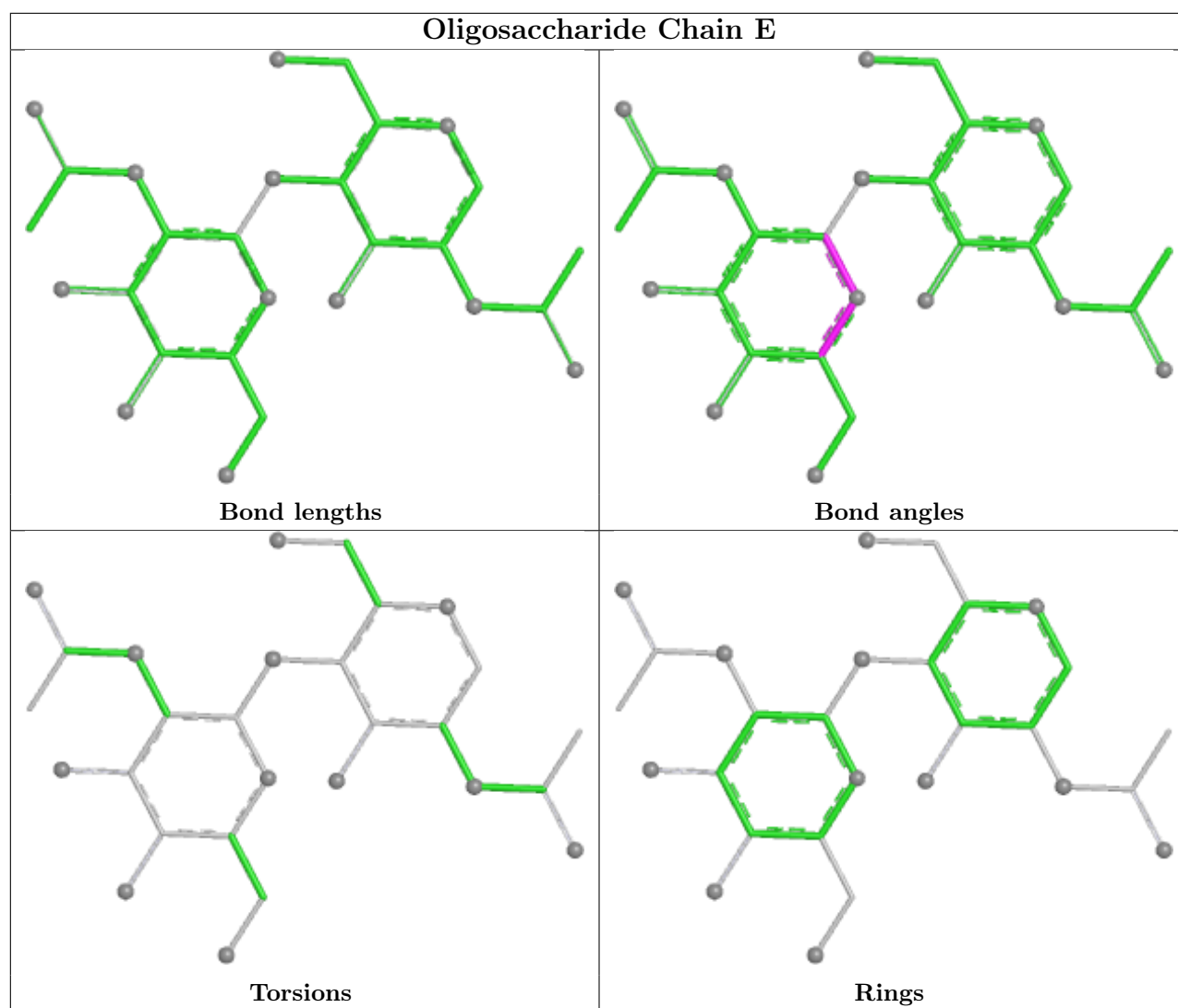
There are no ring outliers.

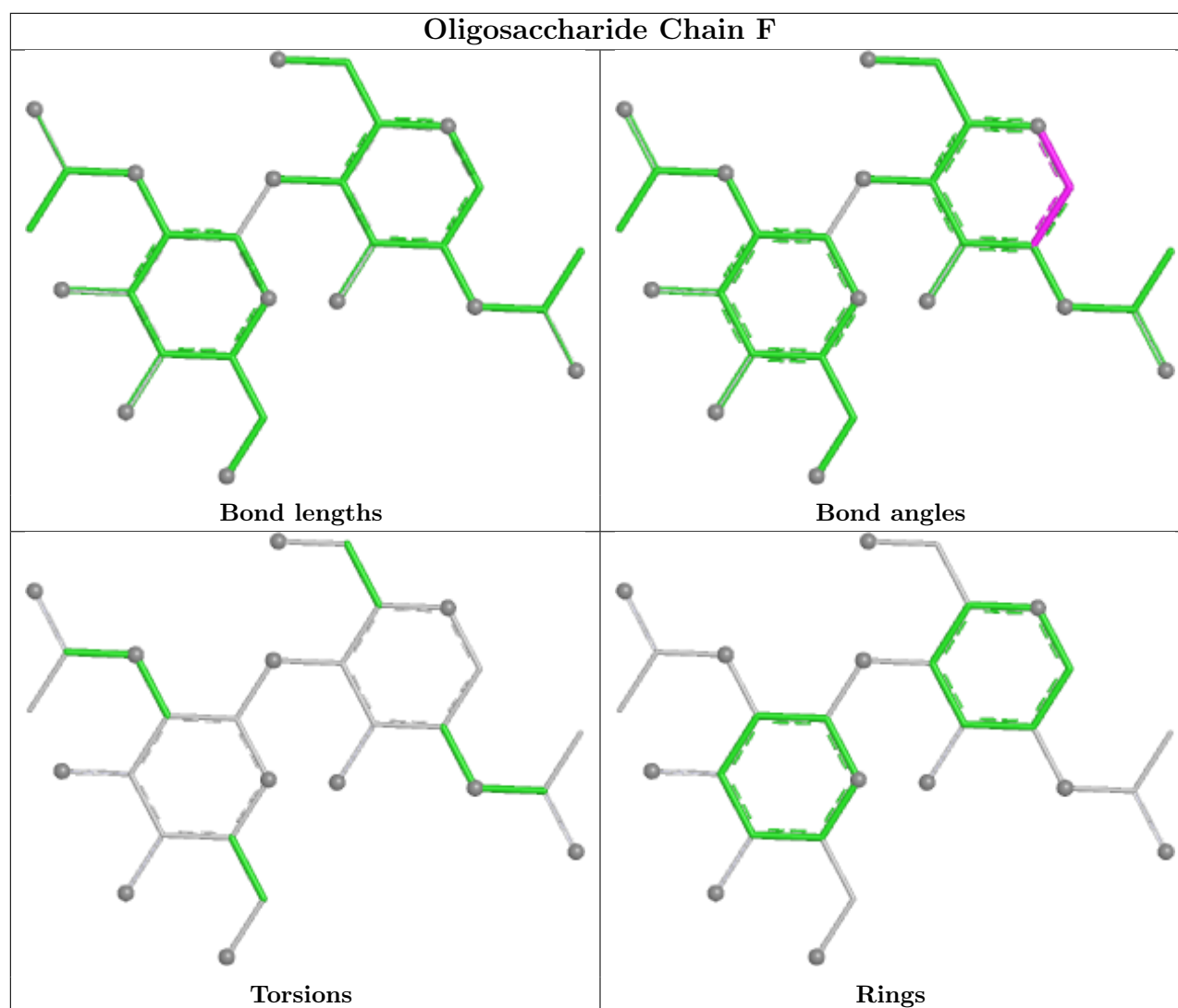
No monomer is involved in short contacts.

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](#)

19 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	B	901	1	14,14,15	0.29	0	17,19,21	0.88	2 (11%)
4	NAG	A	902	1	14,14,15	0.31	0	17,19,21	0.89	1 (5%)
5	QEC	A	908	-	32,33,33	1.10	3 (9%)	37,45,45	0.94	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	A	901	1	14,14,15	0.29	0	17,19,21	0.87	2 (11%)
6	SO4	B	909	-	4,4,4	0.26	0	6,6,6	0.10	0
6	SO4	B	910	-	4,4,4	0.28	0	6,6,6	0.08	0
4	NAG	A	903	1	14,14,15	0.28	0	17,19,21	0.54	0
4	NAG	B	902	1	14,14,15	0.30	0	17,19,21	0.68	0
6	SO4	B	911	-	4,4,4	0.27	0	6,6,6	0.10	0
4	NAG	B	904	1	14,14,15	0.33	0	17,19,21	0.69	1 (5%)
5	QEC	B	908	-	32,33,33	1.05	3 (9%)	37,45,45	1.02	1 (2%)
4	NAG	B	906	1	14,14,15	0.29	0	17,19,21	0.97	1 (5%)
4	NAG	A	904	1	14,14,15	0.32	0	17,19,21	0.48	0
4	NAG	A	906	1	14,14,15	0.36	0	17,19,21	0.85	1 (5%)
4	NAG	B	903	1	14,14,15	0.27	0	17,19,21	1.02	1 (5%)
4	NAG	B	905	1	14,14,15	0.39	0	17,19,21	0.89	1 (5%)
4	NAG	A	905	1	14,14,15	0.28	0	17,19,21	0.56	0
4	NAG	B	907	1	14,14,15	0.36	0	17,19,21	0.95	1 (5%)
4	NAG	A	907	1	14,14,15	0.44	0	17,19,21	0.53	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	901	1	-	0/6/23/26	0/1/1/1
4	NAG	B	902	1	-	0/6/23/26	0/1/1/1
4	NAG	A	902	1	-	0/6/23/26	0/1/1/1
4	NAG	A	904	1	-	2/6/23/26	0/1/1/1
4	NAG	A	906	1	-	0/6/23/26	0/1/1/1
4	NAG	B	903	1	-	0/6/23/26	0/1/1/1
4	NAG	B	906	1	-	0/6/23/26	0/1/1/1
4	NAG	B	907	1	-	0/6/23/26	0/1/1/1
4	NAG	B	904	1	-	0/6/23/26	0/1/1/1
5	QEC	B	908	-	-	4/14/22/22	0/4/4/4
4	NAG	B	905	1	-	0/6/23/26	0/1/1/1
5	QEC	A	908	-	-	4/14/22/22	0/4/4/4
4	NAG	A	901	1	-	0/6/23/26	0/1/1/1
4	NAG	A	905	1	-	0/6/23/26	0/1/1/1
4	NAG	A	903	1	-	0/6/23/26	0/1/1/1
4	NAG	A	907	1	-	0/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	908	QEC	C4-C7	4.77	1.47	1.39
5	B	908	QEC	C4-C7	4.28	1.47	1.39
5	A	908	QEC	C10-C8	-2.29	1.41	1.44
5	B	908	QEC	C8-N2	2.19	1.36	1.33
5	B	908	QEC	C10-C8	-2.13	1.41	1.44
5	A	908	QEC	C8-N2	2.04	1.35	1.33

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	908	QEC	C6-C18-N4	-4.44	106.06	112.27
4	B	903	NAG	O5-C1-C2	-4.07	105.00	111.29
5	A	908	QEC	C6-C18-N4	-3.97	106.71	112.27
4	B	906	NAG	O5-C1-C2	-3.66	105.62	111.29
4	A	902	NAG	O5-C1-C2	-2.89	106.81	111.29
4	B	905	NAG	C1-O5-C5	2.71	115.82	112.19
4	A	906	NAG	C1-O5-C5	2.62	115.70	112.19
4	B	907	NAG	O5-C1-C2	-2.61	107.25	111.29
4	B	901	NAG	O5-C1-C2	-2.26	107.79	111.29
4	A	901	NAG	O5-C1-C2	-2.24	107.82	111.29
4	B	901	NAG	C1-O5-C5	2.15	115.07	112.19
4	A	901	NAG	C1-O5-C5	2.09	114.98	112.19
4	B	904	NAG	O5-C1-C2	-2.07	108.09	111.29

There are no chirality outliers.

All (10) torsion outliers are listed below:

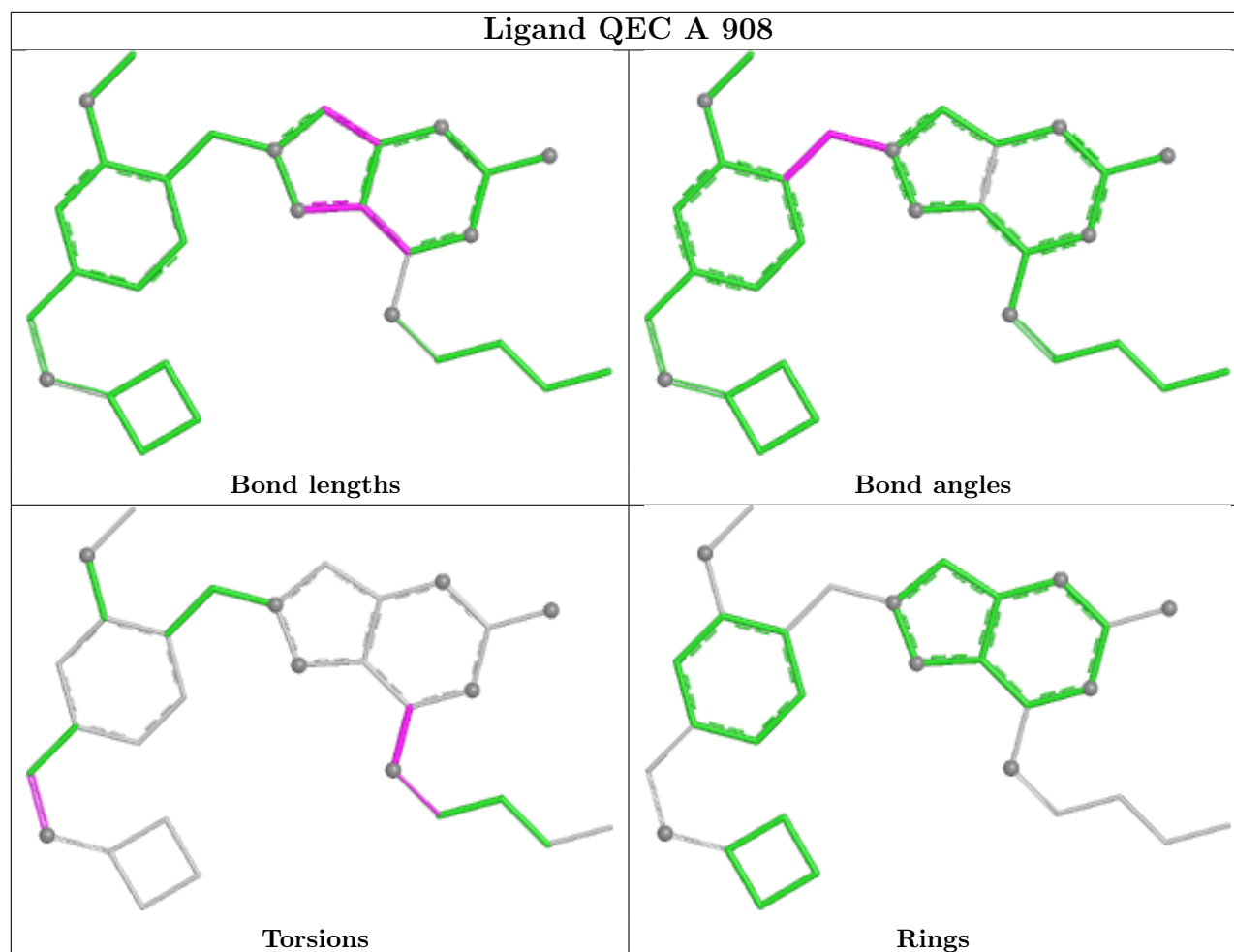
Mol	Chain	Res	Type	Atoms
5	A	908	QEC	C8-C10-N6-C22
5	B	908	QEC	C8-C10-N6-C22
5	A	908	QEC	C5-C19-N7-C15
5	B	908	QEC	C5-C19-N7-C15
5	A	908	QEC	N3-C10-N6-C22
5	B	908	QEC	N3-C10-N6-C22
5	A	908	QEC	C21-C22-N6-C10
4	A	904	NAG	C4-C5-C6-O6
5	B	908	QEC	C21-C22-N6-C10
4	A	904	NAG	O5-C5-C6-O6

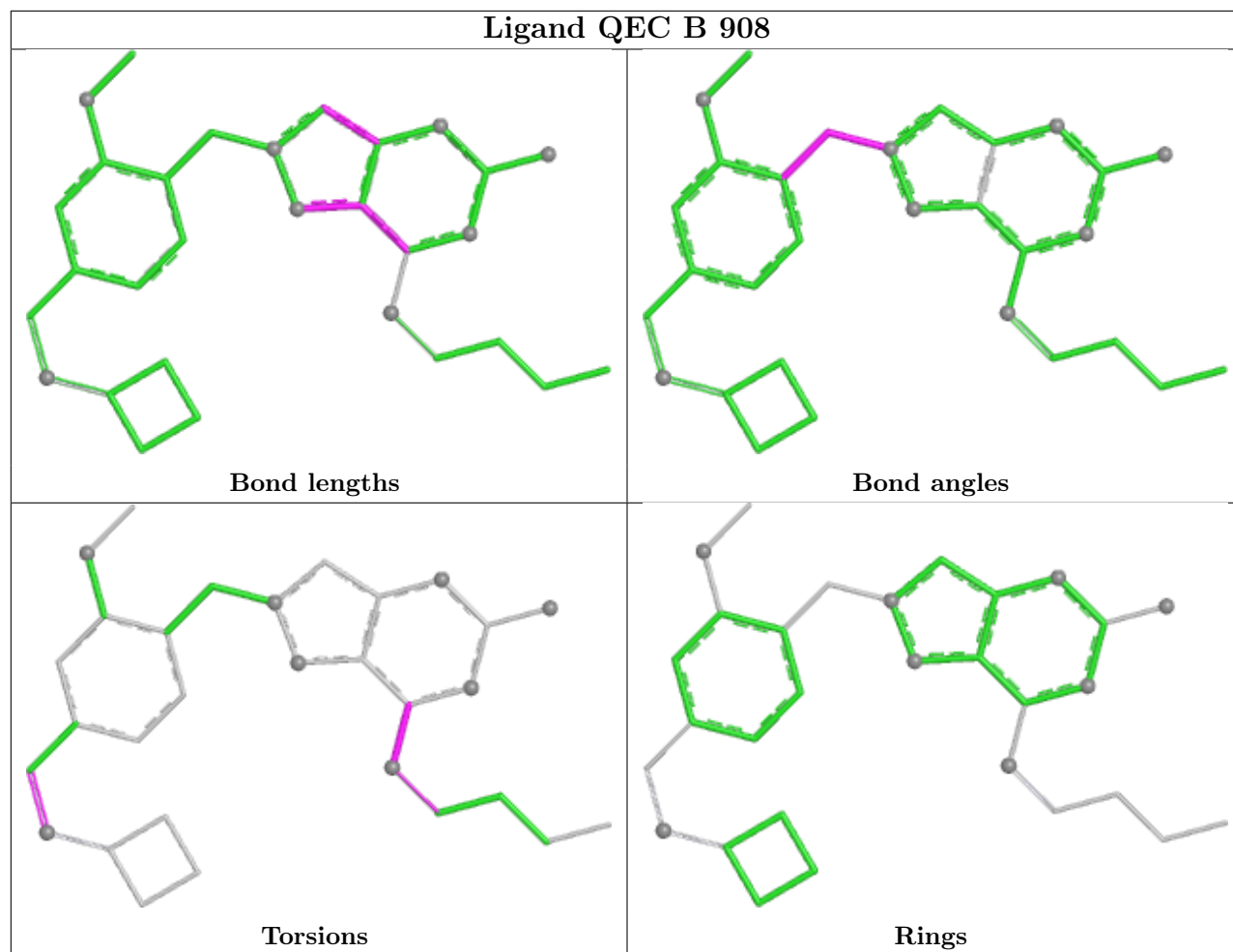
There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	902	NAG	1	0
6	B	911	SO4	1	0
4	A	907	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

6.1 Protein, DNA and RNA chains

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	768/817 (94%)	0.54	38 (4%)	35 37	14, 27, 40, 61	1 (0%)
1	B	768/817 (94%)	0.84	72 (9%)	14 14	19, 32, 46, 72	0
All	All	1536/1634 (94%)	0.69	110 (7%)	21 23	14, 29, 44, 72	1 (0%)

All (110) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	313	ILE	4.4
1	A	109	SER	4.2
1	A	435	PRO	4.0
1	B	105	LEU	3.9
1	B	275	ASN	3.8
1	B	29	TRP	3.8
1	B	809	ALA	3.8
1	B	42	VAL	3.7
1	A	809	ALA	3.7
1	B	582	SER	3.6
1	B	435	PRO	3.5
1	B	238	ALA	3.5
1	A	27	ALA	3.4
1	B	474	SER	3.4
1	A	551	ASN	3.4
1	A	40	LEU	3.2
1	B	40	LEU	3.2
1	B	43	SER	3.2
1	A	105	LEU	3.1
1	B	835	LEU	3.1
1	B	826	ILE	3.1
1	A	810	THR	3.0
1	A	506	PHE	3.0
1	B	475	CYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	65	THR	3.0
1	B	44	LYS	3.0
1	A	607	ASP	3.0
1	A	526	GLY	2.9
1	B	360	MET	2.9
1	A	466	PHE	2.9
1	B	464	TYR	2.9
1	A	42	VAL	2.9
1	B	33	THR	2.8
1	B	772	LEU	2.8
1	B	808	LEU	2.8
1	B	226	THR	2.8
1	B	276	ASN	2.8
1	A	388	PHE	2.8
1	B	650	LEU	2.8
1	B	591	PHE	2.7
1	A	276	ASN	2.7
1	A	313	ILE	2.7
1	B	112	CYS	2.7
1	A	819	ALA	2.7
1	A	807	TYR	2.7
1	A	101	VAL	2.7
1	A	106	GLY	2.6
1	B	530	SER	2.6
1	B	794	PHE	2.5
1	B	85	PHE	2.5
1	B	670	PHE	2.5
1	B	584	GLY	2.5
1	B	825	VAL	2.5
1	B	466	PHE	2.5
1	B	88	LEU	2.5
1	B	830	LEU	2.5
1	B	39	THR	2.4
1	A	507	PHE	2.4
1	B	285	ALA	2.4
1	B	246	ASN	2.4
1	B	388	PHE	2.4
1	B	417	PHE	2.4
1	A	89	VAL	2.4
1	A	475	CYS	2.4
1	B	665	LEU	2.4
1	A	473	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	420	PHE	2.3
1	B	513	PHE	2.3
1	B	767	PHE	2.3
1	A	582	SER	2.3
1	B	38	VAL	2.3
1	B	248	LEU	2.3
1	B	691	ILE	2.3
1	B	676	ASN	2.3
1	A	74	ILE	2.3
1	A	581	GLN	2.2
1	B	771	VAL	2.2
1	B	27	ALA	2.2
1	B	463	LEU	2.2
1	A	835	LEU	2.2
1	B	344	GLN	2.2
1	B	114	ARG	2.2
1	A	812	VAL	2.2
1	B	222	VAL	2.2
1	A	88	LEU	2.2
1	A	528	LEU	2.2
1	A	77	ILE	2.1
1	B	669	VAL	2.1
1	B	327	ALA	2.1
1	B	710	GLN	2.1
1	B	664	PHE	2.1
1	A	825	VAL	2.1
1	B	90	HIS	2.1
1	A	43	SER	2.1
1	B	116	LEU	2.1
1	A	118	ILE	2.1
1	B	690	PHE	2.1
1	B	780	LEU	2.1
1	B	789	CYS	2.1
1	A	468	TYR	2.1
1	B	832	THR	2.1
1	B	667	SER	2.1
1	B	745	ASP	2.0
1	B	818	GLY	2.0
1	A	513	PHE	2.0
1	B	803	VAL	2.0
1	B	45	ASN	2.0
1	A	808	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	760	GLN	2.0
1	B	820	HIS	2.0

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](#)

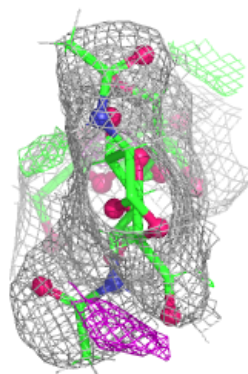
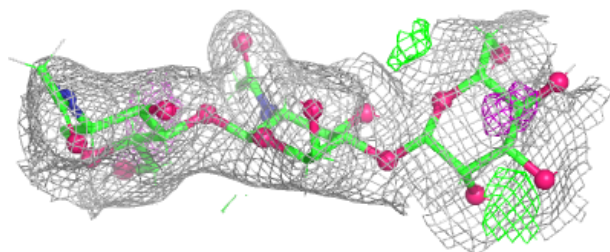
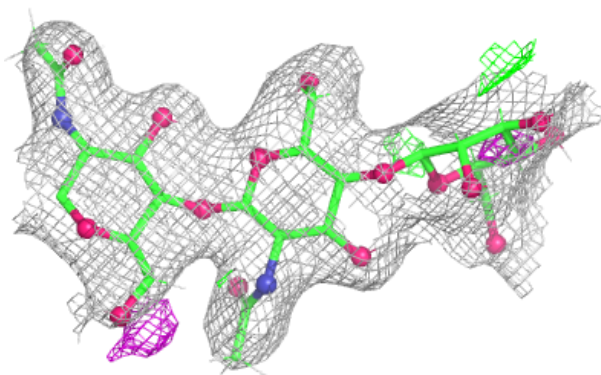
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists 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	BMA	C	3	11/12	0.60	0.13	88,91,119,120	10
3	NAG	D	2	14/15	0.64	0.14	84,86,103,104	13
3	NAG	F	2	14/15	0.66	0.13	96,98,127,128	13
2	NAG	C	2	14/15	0.84	0.10	78,83,105,106	12
3	NAG	E	2	14/15	0.87	0.09	73,76,95,96	13
3	NAG	F	1	14/15	0.89	0.12	89,92,118,118	12
3	NAG	D	1	14/15	0.91	0.10	75,78,92,93	12
2	NAG	C	1	14/15	0.91	0.11	66,71,88,89	12
3	NAG	E	1	14/15	0.91	0.10	65,69,85,85	12

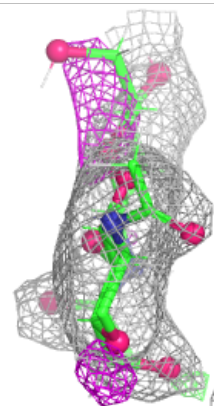
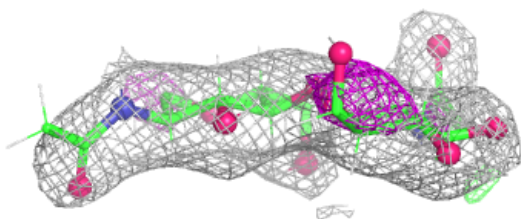
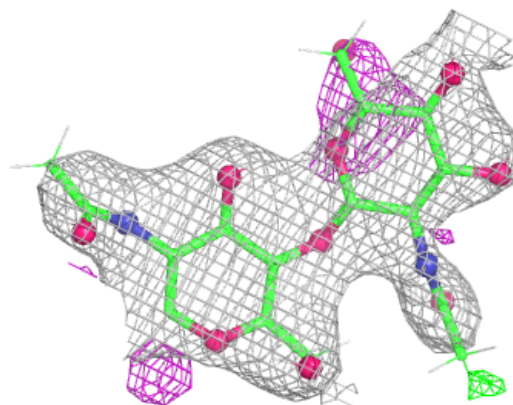
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain C:

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

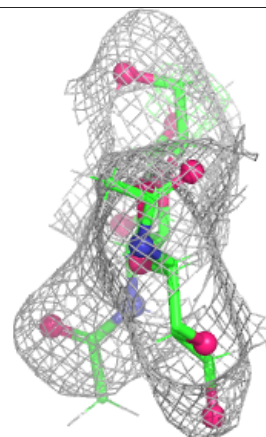
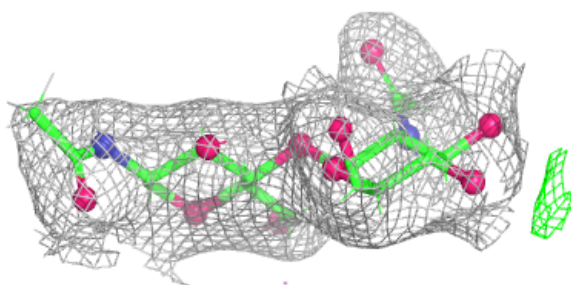
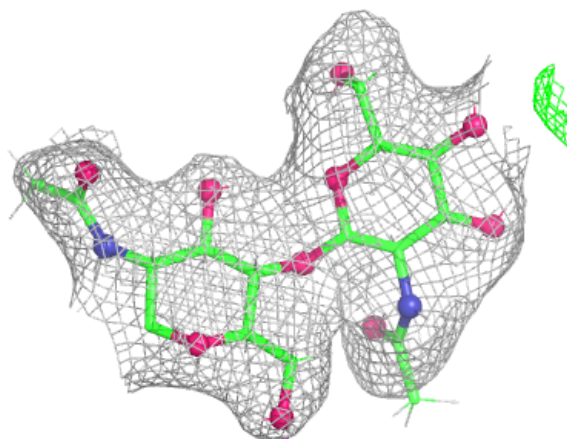
**Electron density around Chain D:**

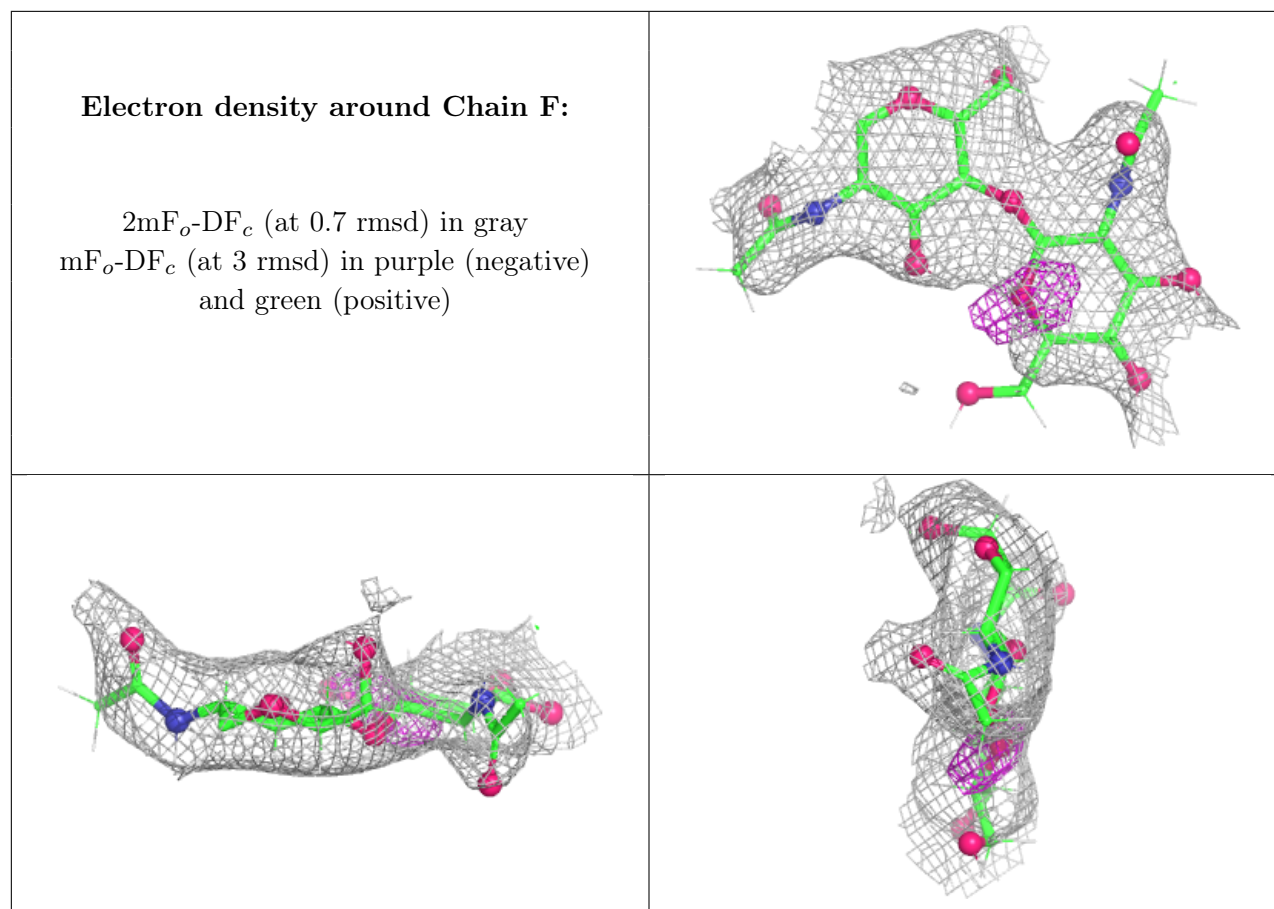
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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 ⓘ

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

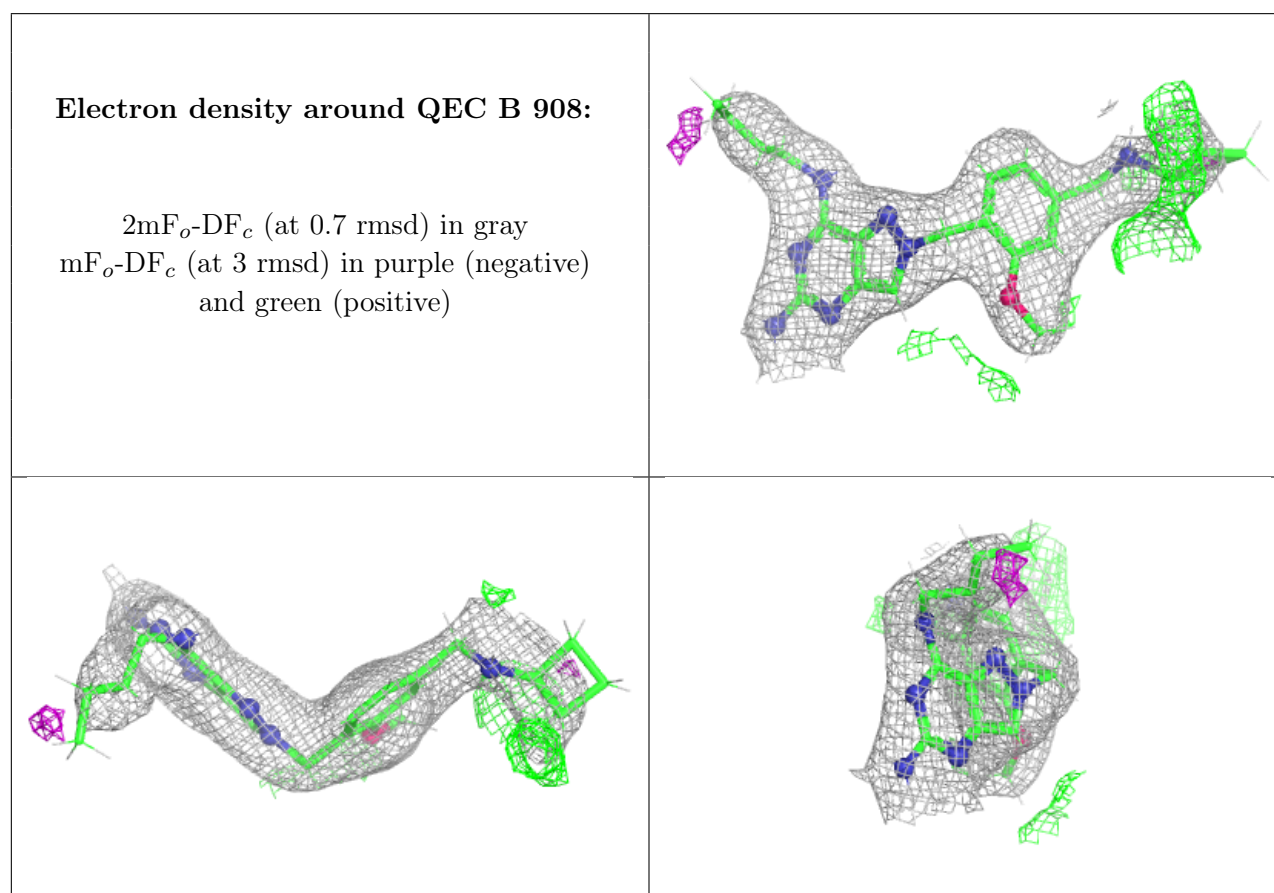
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	B	907	14/15	0.35	0.18	99,102,141,143	13
4	NAG	B	906	14/15	0.60	0.15	85,88,111,112	13
6	SO4	B	910	5/5	0.67	0.15	156,156,156,156	0
4	NAG	B	905	14/15	0.69	0.14	93,95,132,133	13
4	NAG	A	907	14/15	0.73	0.15	75,77,84,85	13
4	NAG	A	906	14/15	0.76	0.13	75,77,103,103	13
4	NAG	B	903	14/15	0.78	0.10	84,86,119,120	13
4	NAG	A	905	14/15	0.81	0.10	75,78,106,108	13
6	SO4	B	909	5/5	0.85	0.14	155,155,155,155	0
4	NAG	B	902	14/15	0.85	0.11	73,75,103,104	13
6	SO4	B	911	5/5	0.86	0.12	157,157,157,157	0
5	QEC	B	908	30/30	0.87	0.14	52,63,84,85	31
4	NAG	A	903	14/15	0.87	0.10	63,66,78,80	13

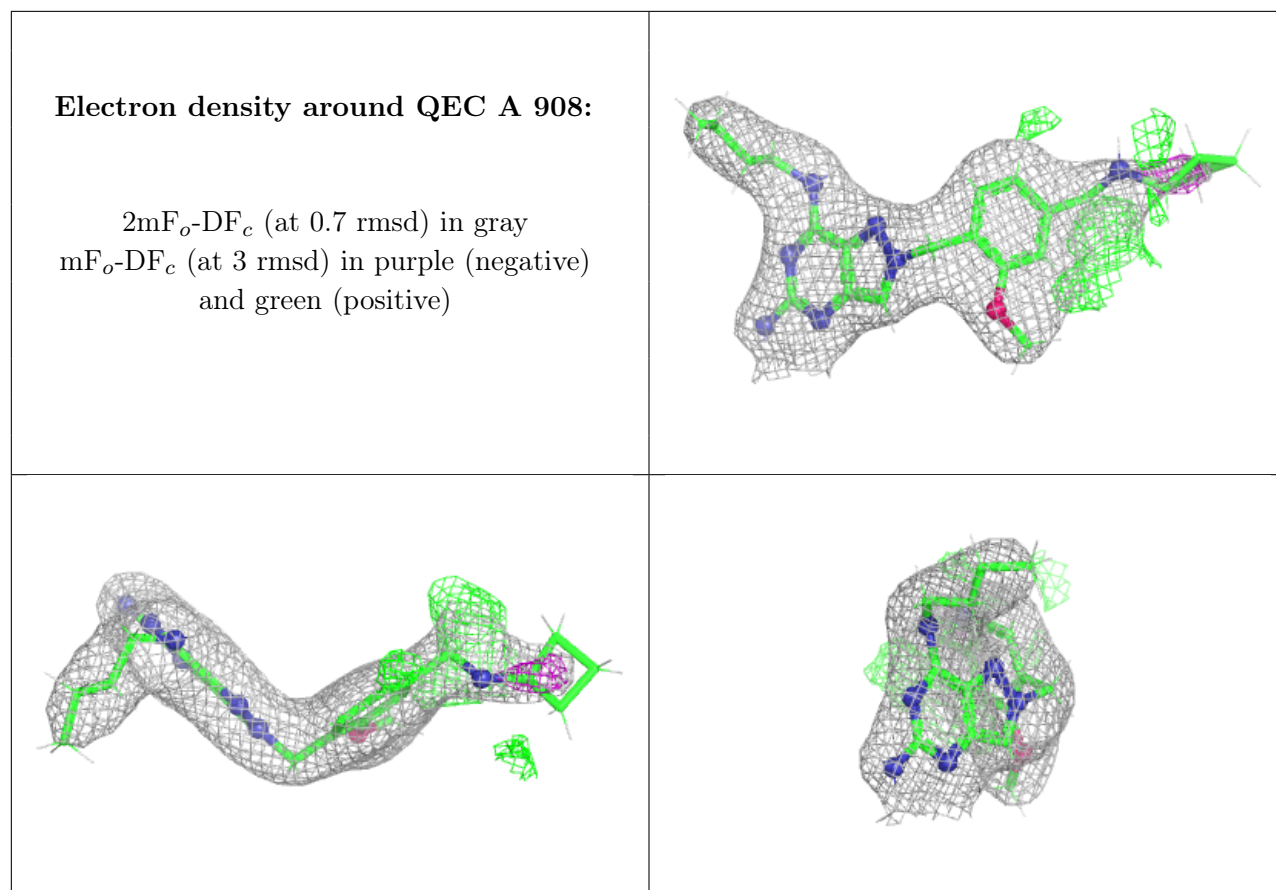
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	B	904	14/15	0.88	0.09	80,81,117,119	13
4	NAG	A	902	14/15	0.88	0.09	64,67,86,88	13
4	NAG	A	904	14/15	0.90	0.09	69,71,97,99	13
5	QEC	A	908	30/30	0.91	0.13	55,67,85,85	31
4	NAG	A	901	14/15	0.92	0.08	48,53,59,61	13
4	NAG	B	901	14/15	0.94	0.08	56,59,67,68	13

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.





6.5 Other polymers [i](#)

There are no such residues in this entry.