



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 05:19 PM BST

PDB ID : 3WAW
Title : Crystal Structure of Autotaxin in Complex with 2BoA
Authors : Nishimasu, H.; Ishitani, R.; Nureki, O.
Deposited on : 2013-05-09
Resolution : 1.95 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

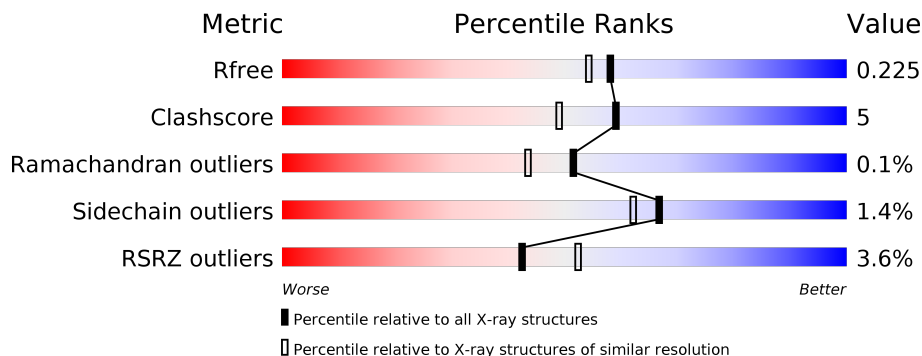
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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	831	
2	B	2	
2	D	2	
3	C	7	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	DWW	A	937	-	-	X	-

2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 6867 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 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	779	6249	3972	1069	1160	48	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

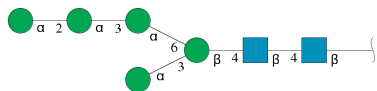
Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	LYS	SEE REMARK 999	UNP Q9R1E6
A	?	-	VAL	SEE REMARK 999	UNP Q9R1E6
A	?	-	GLU	SEE REMARK 999	UNP Q9R1E6
A	?	-	PRO	SEE REMARK 999	UNP Q9R1E6
A	859	SER	-	expression tag	UNP Q9R1E6
A	860	ARG	-	expression tag	UNP Q9R1E6
A	861	GLU	-	expression tag	UNP Q9R1E6
A	862	ASN	-	expression tag	UNP Q9R1E6
A	863	LEU	-	expression tag	UNP Q9R1E6
A	864	TYR	-	expression tag	UNP Q9R1E6
A	865	PHE	-	expression tag	UNP Q9R1E6
A	866	GLN	-	expression tag	UNP Q9R1E6

- 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
			Total	C	N	O			
2	B	2	28	16	2	10	0	0	0
2	D	2	28	16	2	10	0	0	0

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]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
			Total	C	N	O			
3	C	7	83	46	2	35	0	0	0

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

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

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

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

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 7 is POTASSIUM ION (three-letter code: K) (formula: K).

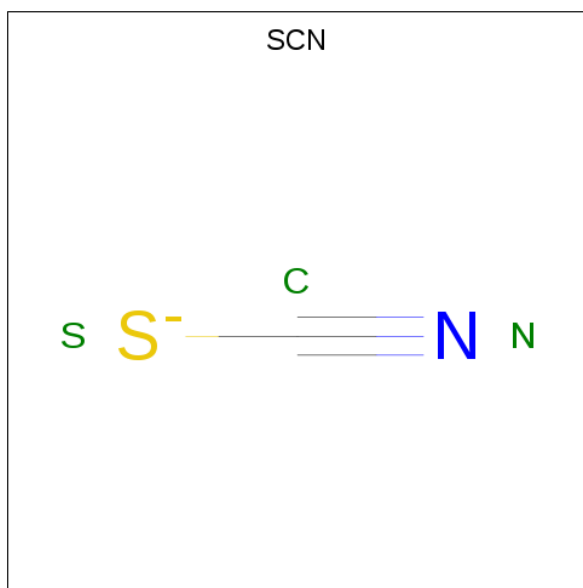
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	K		
7	A	1	1	1	0	0

- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



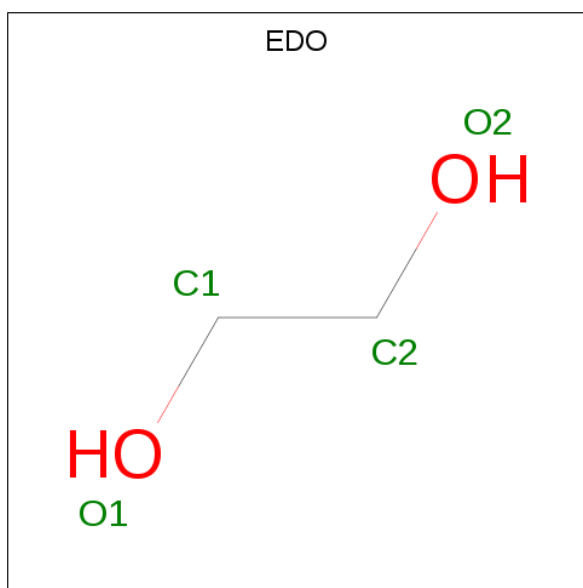
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 9 is THIOCYANATE ION (three-letter code: SCN) (formula: CNS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	N	S	0	0
			3	1	1	1		
9	A	1	Total	C	N	S	0	0
			3	1	1	1		
9	A	1	Total	C	N	S	0	0
			3	1	1	1		

- Molecule 10 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



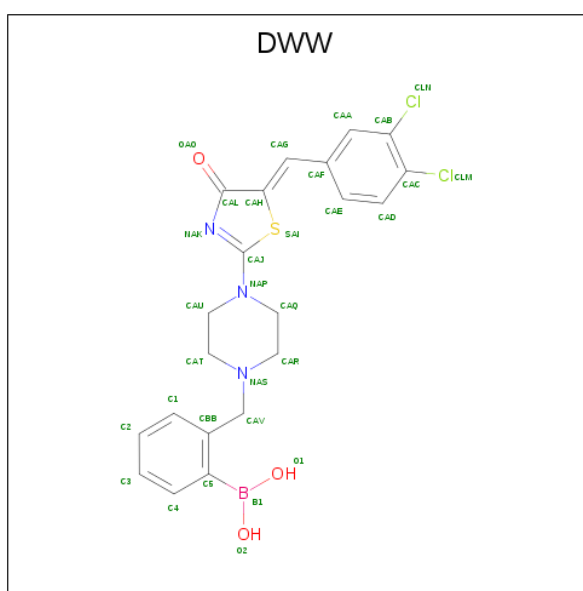
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total C O 4 2 2	0	0
10	A	1	Total C O 4 2 2	0	0
10	A	1	Total C O 4 2 2	0	0
10	A	1	Total C O 4 2 2	0	0
10	A	1	Total C O 4 2 2	0	0
10	A	1	Total C O 4 2 2	0	0
10	A	1	Total C O 4 2 2	0	0
10	A	1	Total C O 4 2 2	0	0
10	A	1	Total C O 4 2 2	0	0
10	A	1	Total C O 4 2 2	0	0
10	A	1	Total C O 4 2 2	0	0
10	A	1	Total C O 4 2 2	0	0
10	A	1	Total C O 4 2 2	0	0
10	A	1	Total C O 4 2 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			4	2	2		
10	A	1	Total	C	O	0	0
			4	2	2		
10	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 11 is [2-({4-[(5Z)-5-(3,4-dichlorobenzylidene)-4-oxo-4,5-dihydro-1,3-thiazol-2-yl]piperazin-1-yl}methyl)phenyl]boronic acid (three-letter code: DWW) (formula: C₂₁H₂₀BCl₂N₃O₃S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
11	A	1	Total	C	Cl	N	O	S	0	0
			23	16	2	3	1	1		

- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	373	Total	O	0	0
			373	373		



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	61.65Å 94.26Å 75.36Å 90.00° 94.73° 90.00°	Depositor
Resolution (Å)	47.13 – 1.95 47.13 – 1.95	Depositor EDS
% Data completeness (in resolution range)	98.0 (47.13-1.95) 98.0 (47.13-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.24 (at 1.95Å)	Xtrriage
Refinement program	PHENIX 1.7.2_869	Depositor
R, R_{free}	0.192 , 0.231 0.189 , 0.225	Depositor DCC
R_{free} test set	3081 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	29.0	Xtrriage
Anisotropy	0.152	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 47.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6867	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.35% 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: ZN, BMA, DWW, NA, K, NAG, EDO, SCN, SO4, CA, MAN

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	0.34	0/6431	0.52	0/8741

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 [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	6249	0	5947	46	0
2	B	28	0	25	0	0
2	D	28	0	25	0	0
3	C	83	0	70	0	0
4	A	2	0	0	0	0
5	A	1	0	0	0	0
6	A	1	0	0	0	0
7	A	1	0	0	0	0
8	A	5	0	0	0	0
9	A	9	0	0	0	0
10	A	64	0	96	6	0
11	A	23	0	14	15	0
12	A	373	0	0	1	0
All	All	6867	0	6177	60	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 5.

All (60) 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)
11:A:937:DWW:NAS	11:A:937:DWW:CAU	2.08	1.16
11:A:937:DWW:NAP	11:A:937:DWW:CAT	2.07	1.15
11:A:937:DWW:NAP	11:A:937:DWW:CAR	2.13	1.11
11:A:937:DWW:NAS	11:A:937:DWW:CAQ	2.13	1.10
11:A:937:DWW:H14	11:A:937:DWW:CAR	1.47	0.99
11:A:937:DWW:H8	11:A:937:DWW:CAU	1.47	0.98
11:A:937:DWW:H9	11:A:937:DWW:CAT	1.47	0.97
11:A:937:DWW:H10	11:A:937:DWW:CAT	1.47	0.97
11:A:937:DWW:CAQ	11:A:937:DWW:H11	1.47	0.96
11:A:937:DWW:H13	11:A:937:DWW:CAR	1.47	0.96
11:A:937:DWW:CAQ	11:A:937:DWW:H12	1.47	0.96
11:A:937:DWW:CAU	11:A:937:DWW:H7	1.47	0.96
11:A:937:DWW:CAQ	11:A:937:DWW:CAR	0.84	0.84
11:A:937:DWW:CAT	11:A:937:DWW:CAU	0.83	0.83
1:A:639:SER:O	1:A:688:LYS:NZ	2.21	0.74
1:A:78:LEU:HD21	1:A:274:PHE:HB2	1.74	0.70
1:A:600:LEU:HD11	1:A:832:ASP:HB2	1.74	0.70
1:A:77:ASN:HD21	1:A:272:THR:HB	1.58	0.67
1:A:649:ARG:NH1	1:A:689:TYR:O	2.29	0.66
1:A:678:PRO:HB3	1:A:712:GLN:HB3	1.81	0.63
1:A:178:MET:HE2	1:A:192:ARG:HD3	1.80	0.62
1:A:150:GLU:OE1	1:A:152:ARG:NH1	2.34	0.61
1:A:210:PHE:HE2	1:A:243:LEU:HD23	1.66	0.60
1:A:550:PRO:HB2	1:A:607:ILE:HG12	1.86	0.57
1:A:112:ASN:HD21	1:A:114:GLU:HB3	1.69	0.57
1:A:222:PRO:HA	1:A:225:HIS:CE1	2.40	0.56
1:A:682:SER:OG	1:A:688:LYS:HG2	2.06	0.56
1:A:758:PRO:HD3	10:A:930:EDO:H22	1.88	0.56
1:A:633:LYS:O	1:A:717:LYS:NZ	2.40	0.55
1:A:550:PRO:HB3	1:A:605:TYR:CE2	2.42	0.55
1:A:210:PHE:CE2	1:A:243:LEU:HD23	2.44	0.52
1:A:274:PHE:CE1	11:A:937:DWW:H25	2.46	0.51
1:A:852:HIS:HD2	1:A:854:TYR:CZ	2.29	0.51
1:A:151:ILE:HD12	10:A:922:EDO:H21	1.92	0.51
1:A:98:ARG:HD3	1:A:115:ASN:OD1	2.11	0.50
1:A:745:GLU:OE2	10:A:930:EDO:O1	2.26	0.50
1:A:80:LYS:NZ	12:A:1348:HOH:O	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:734:PHE:CD1	10:A:924:EDO:H11	2.48	0.49
1:A:612:ASP:OD2	1:A:687:ALA:HB1	2.13	0.49
1:A:685:PRO:O	1:A:689:TYR:HD1	1.96	0.48
1:A:558:LEU:HD12	1:A:561:ASP:OD2	2.14	0.48
1:A:761:THR:HA	10:A:926:EDO:H12	1.96	0.47
1:A:230:ASN:HB3	1:A:243:LEU:HG	1.95	0.47
1:A:685:PRO:HA	1:A:688:LYS:HG3	1.96	0.47
1:A:417:ASP:OD1	1:A:417:ASP:N	2.50	0.45
1:A:543:LEU:HD12	1:A:544:PRO:HD2	1.98	0.44
1:A:206:PRO:HD3	1:A:434:TYR:CE1	2.52	0.44
1:A:98:ARG:HH21	1:A:106:ARG:HG2	1.82	0.44
1:A:72:ASP:OD1	1:A:72:ASP:N	2.50	0.43
1:A:617:TYR:HA	1:A:624:PRO:HA	2.00	0.43
1:A:65:LEU:HD21	1:A:291:TRP:CE2	2.54	0.42
1:A:343:LYS:HA	1:A:348:HIS:ND1	2.35	0.42
1:A:388:THR:OG1	1:A:475:GLY:HA3	2.20	0.42
1:A:736:TYR:OH	1:A:750:GLN:HB3	2.19	0.42
1:A:162:ARG:NH2	1:A:301:SER:OG	2.52	0.42
1:A:539:PHE:O	1:A:541:PRO:HD3	2.20	0.41
1:A:393:ARG:HB2	1:A:394:PRO:HD2	2.02	0.41
1:A:715:LEU:HA	1:A:715:LEU:HD23	1.88	0.41
1:A:415:LYS:HB2	1:A:415:LYS:HE3	1.77	0.41
1:A:823:ARG:CZ	10:A:921:EDO:H11	2.50	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	773/831 (93%)	746 (96%)	26 (3%)	1 (0%)	51 43

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	386	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	696/756 (92%)	686 (99%)	10 (1%)	67 62

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	ASP
1	A	114	GLU
1	A	124	LEU
1	A	153	VAL
1	A	232	MET
1	A	269	ARG
1	A	345	LEU
1	A	558	LEU
1	A	590	ARG
1	A	649	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	112	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates i

11 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	B	1	1,2	14,14,15	0.52	0	17,19,21	1.09	1 (5%)
2	NAG	B	2	2	14,14,15	0.55	0	17,19,21	0.86	0
3	NAG	C	1	1,3	14,14,15	0.55	0	17,19,21	1.13	2 (11%)
3	NAG	C	2	3	14,14,15	0.65	0	17,19,21	0.71	0
3	BMA	C	3	3	11,11,12	0.67	0	15,15,17	1.00	0
3	MAN	C	4	3	11,11,12	0.66	0	15,15,17	1.06	1 (6%)
3	MAN	C	5	3	11,11,12	0.55	0	15,15,17	0.90	1 (6%)
3	MAN	C	6	3	11,11,12	0.60	0	15,15,17	0.79	0
3	MAN	C	7	3	11,11,12	0.73	0	15,15,17	0.91	1 (6%)
2	NAG	D	1	1,2	14,14,15	0.48	0	17,19,21	1.02	1 (5%)
2	NAG	D	2	2	14,14,15	0.41	0	17,19,21	1.71	2 (11%)

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	B	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	B	2	2	-	3/6/23/26	0/1/1/1
3	NAG	C	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	0/6/23/26	0/1/1/1
3	BMA	C	3	3	-	2/2/19/22	0/1/1/1
3	MAN	C	4	3	-	0/2/19/22	0/1/1/1
3	MAN	C	5	3	-	0/2/19/22	0/1/1/1
3	MAN	C	6	3	-	0/2/19/22	0/1/1/1
3	MAN	C	7	3	-	2/2/19/22	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

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2	NAG	C1-O5-C5	5.90	120.18	112.19
2	B	1	NAG	C1-O5-C5	3.52	116.97	112.19
3	C	4	MAN	O5-C5-C6	2.92	111.78	107.20
2	D	2	NAG	O5-C5-C6	2.66	111.38	107.20
3	C	1	NAG	O5-C1-C2	-2.49	107.36	111.29
2	D	1	NAG	C1-O5-C5	2.35	115.38	112.19
3	C	7	MAN	C1-C2-C3	2.24	112.42	109.67
3	C	1	NAG	O4-C4-C3	-2.20	105.27	110.35
3	C	5	MAN	O5-C1-C2	-2.04	107.63	110.77

There are no chirality outliers.

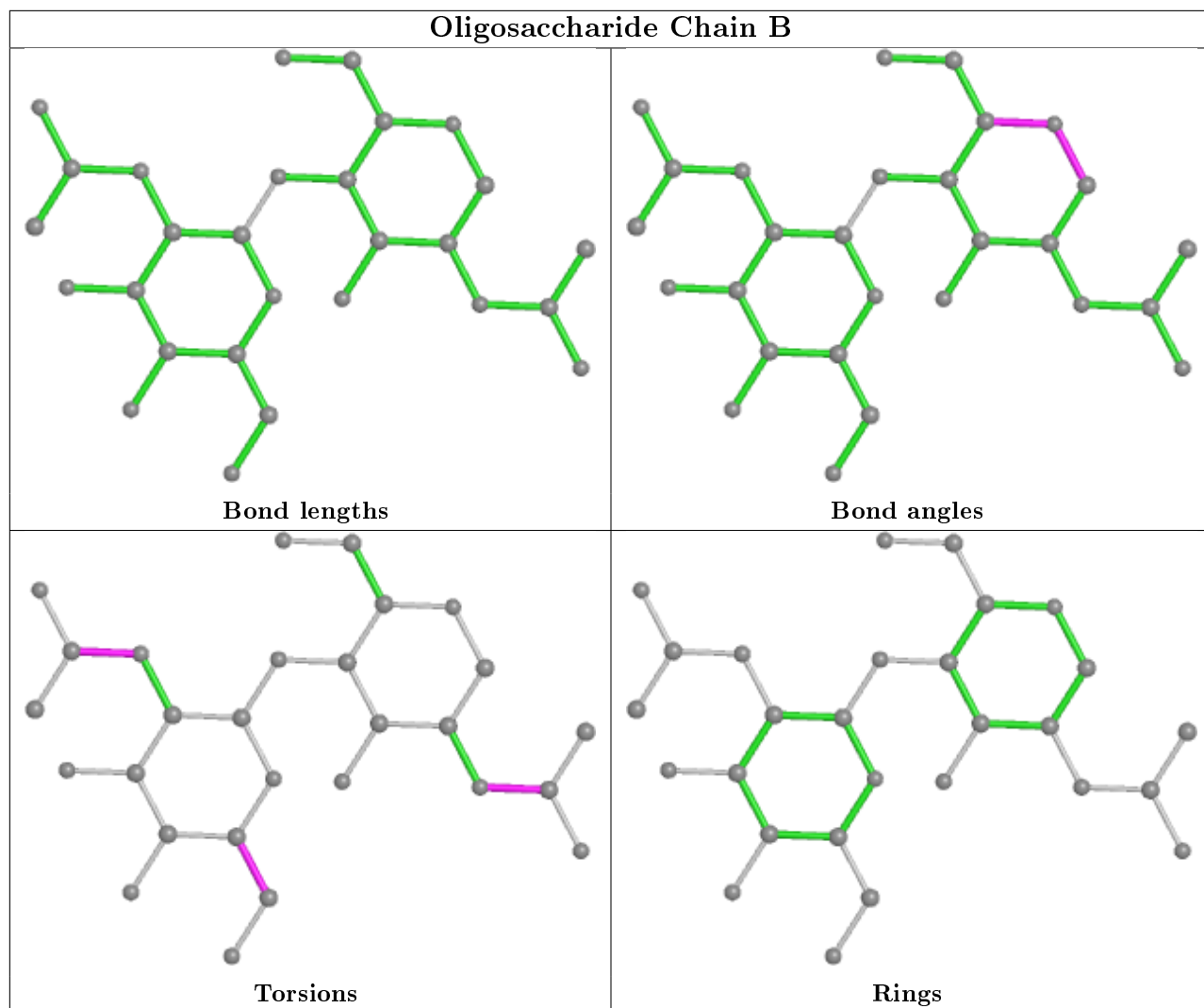
All (9) torsion outliers are listed below:

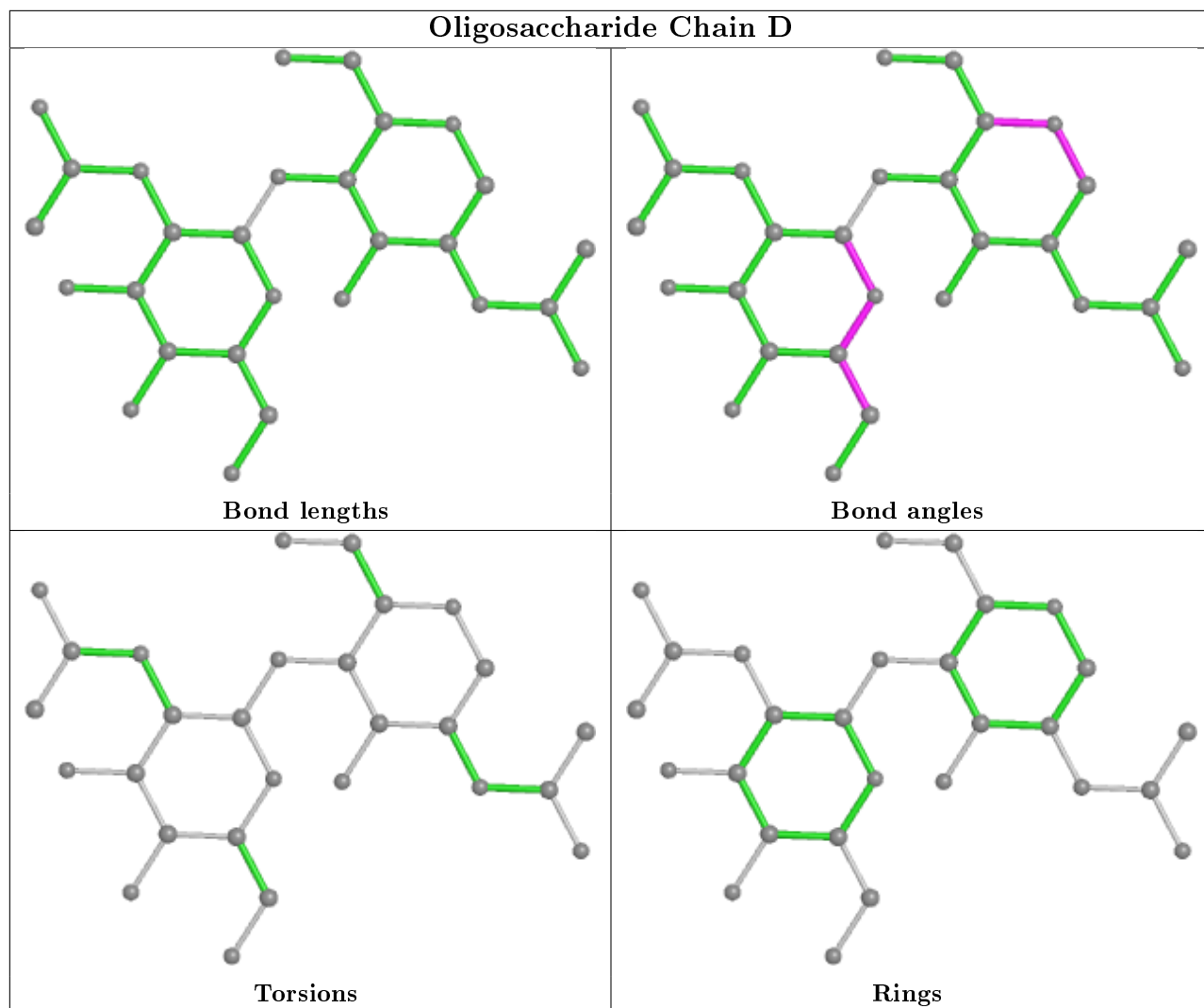
Mol	Chain	Res	Type	Atoms
2	B	1	NAG	C8-C7-N2-C2
2	B	1	NAG	O7-C7-N2-C2
3	C	3	BMA	O5-C5-C6-O6
3	C	7	MAN	O5-C5-C6-O6
3	C	3	BMA	C4-C5-C6-O6
3	C	7	MAN	C4-C5-C6-O6
2	B	2	NAG	C8-C7-N2-C2
2	B	2	NAG	C4-C5-C6-O6
2	B	2	NAG	O7-C7-N2-C2

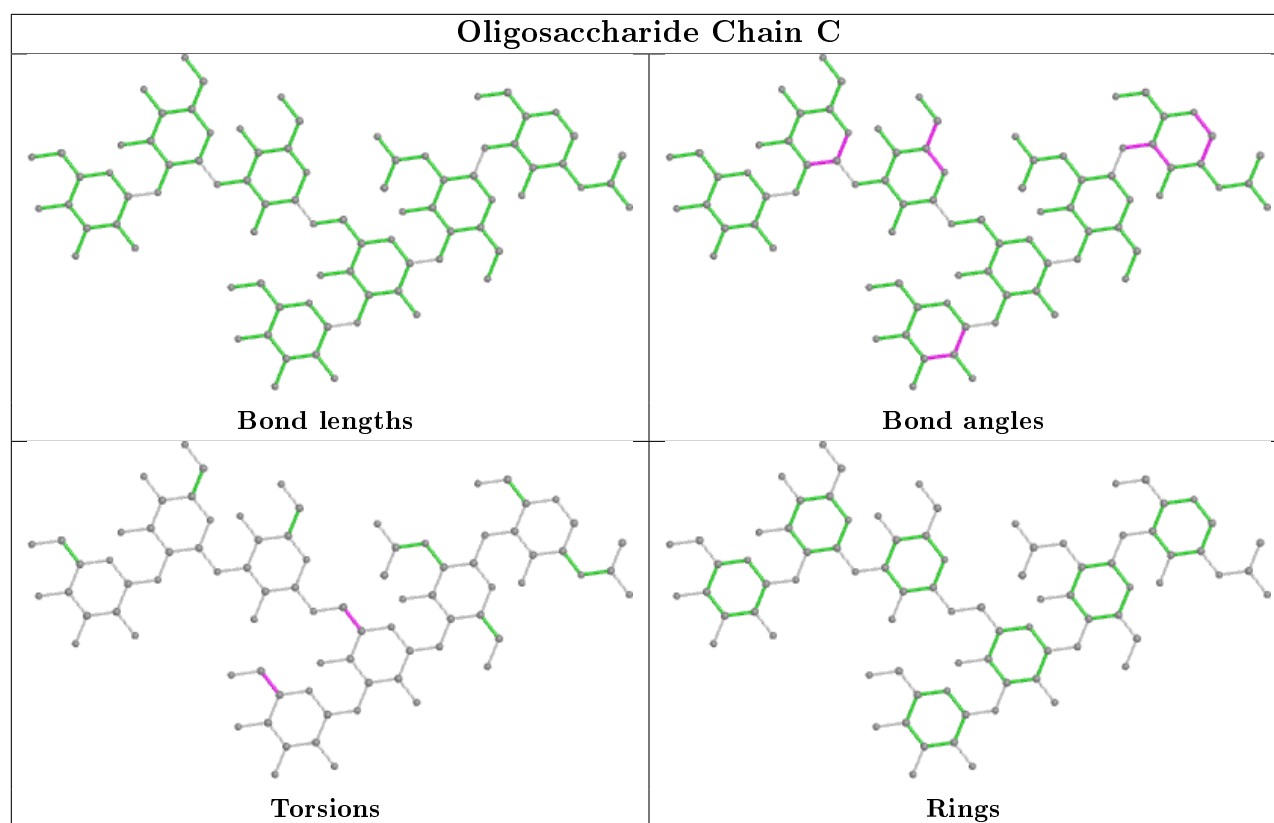
There are no ring outliers.

No monomer is involved in short contacts.

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







5.6 Ligand geometry [i](#)

Of 26 ligands modelled in this entry, 5 are monoatomic - leaving 21 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	$\# Z > 2$
10	EDO	A	925	-	3,3,3	0.50	0	2,2,2	0.30	0
10	EDO	A	936	-	3,3,3	0.42	0	2,2,2	0.50	0
10	EDO	A	924	-	3,3,3	0.48	0	2,2,2	0.40	0
10	EDO	A	932	-	3,3,3	0.49	0	2,2,2	0.41	0
9	SCN	A	920	-	1,2,2	1.01	0	0,1,1	0.00	-
10	EDO	A	933	-	3,3,3	0.49	0	2,2,2	0.33	0
8	SO4	A	917	4	4,4,4	0.26	0	6,6,6	0.35	0
10	EDO	A	929	-	3,3,3	0.50	0	2,2,2	0.33	0
10	EDO	A	923	-	3,3,3	0.39	0	2,2,2	0.50	0
10	EDO	A	934	-	3,3,3	0.51	0	2,2,2	0.26	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	EDO	A	928	-	3,3,3	0.48	0	2,2,2	0.31	0
10	EDO	A	931	-	3,3,3	0.53	0	2,2,2	0.28	0
10	EDO	A	930	-	3,3,3	0.43	0	2,2,2	0.43	0
9	SCN	A	918	-	1,2,2	0.91	0	0,1,1	0.00	-
10	EDO	A	927	-	3,3,3	0.50	0	2,2,2	0.37	0
11	DWW	A	937	-	25,25,34	6.87	13 (52%)	35,35,48	3.11	14 (40%)
10	EDO	A	926	-	3,3,3	0.43	0	2,2,2	0.57	0
10	EDO	A	921	-	3,3,3	0.46	0	2,2,2	0.46	0
9	SCN	A	919	-	1,2,2	0.96	0	0,1,1	0.00	-
10	EDO	A	922	-	3,3,3	0.61	0	2,2,2	0.14	0
10	EDO	A	935	-	3,3,3	0.44	0	2,2,2	0.40	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
10	EDO	A	925	-	-	0/1/1/1	-
10	EDO	A	936	-	-	0/1/1/1	-
10	EDO	A	924	-	-	0/1/1/1	-
10	EDO	A	932	-	-	0/1/1/1	-
10	EDO	A	933	-	-	0/1/1/1	-
10	EDO	A	929	-	-	1/1/1/1	-
10	EDO	A	923	-	-	0/1/1/1	-
10	EDO	A	934	-	-	0/1/1/1	-
10	EDO	A	928	-	-	0/1/1/1	-
10	EDO	A	931	-	-	1/1/1/1	-
10	EDO	A	930	-	-	0/1/1/1	-
10	EDO	A	935	-	-	0/1/1/1	-
10	EDO	A	927	-	-	1/1/1/1	-
10	EDO	A	926	-	-	0/1/1/1	-
10	EDO	A	921	-	-	1/1/1/1	-
11	DWW	A	937	-	-	3/10/32/38	0/3/3/4
10	EDO	A	922	-	-	0/1/1/1	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	937	DWW	CAU-CAT	-17.83	0.83	1.51
11	A	937	DWW	CAQ-CAR	-17.52	0.84	1.51
11	A	937	DWW	CAG-CAH	13.76	1.49	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	937	DWW	OAO-CAL	8.69	1.38	1.23
11	A	937	DWW	CAQ-NAP	8.41	1.62	1.47
11	A	937	DWW	CAU-NAP	7.94	1.61	1.47
11	A	937	DWW	CAL-CAH	-7.31	1.40	1.50
11	A	937	DWW	CAR-NAS	5.48	1.62	1.46
11	A	937	DWW	CAT-NAS	5.24	1.61	1.46
11	A	937	DWW	CAJ-NAP	4.49	1.45	1.34
11	A	937	DWW	CAJ-SAI	-2.32	1.69	1.75
11	A	937	DWW	CBB-CAV	-2.31	1.36	1.49
11	A	937	DWW	CAJ-NAK	2.17	1.36	1.31

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	937	DWW	CAF-CAG-CAH	-8.69	119.05	130.94
11	A	937	DWW	CAR-NAS-CAV	7.67	132.12	110.84
11	A	937	DWW	SAI-CAJ-NAK	-5.87	107.91	116.31
11	A	937	DWW	CAU-NAP-CAJ	5.61	136.06	122.03
11	A	937	DWW	CAL-CAH-SAI	-4.95	106.39	109.12
11	A	937	DWW	CAJ-SAI-CAH	4.25	96.57	90.75
11	A	937	DWW	CAQ-NAP-CAJ	-4.19	111.55	122.03
11	A	937	DWW	SAI-CAJ-NAP	4.07	125.62	120.36
11	A	937	DWW	OAO-CAL-CAH	-3.39	120.49	122.51
11	A	937	DWW	CAQ-CAR-NAS	2.81	116.42	110.64
11	A	937	DWW	CAR-CAQ-NAP	2.77	116.38	110.44
11	A	937	DWW	NAP-CAJ-NAK	2.25	126.45	123.25
11	A	937	DWW	CAH-CAL-NAK	2.02	114.62	113.56
11	A	937	DWW	CAJ-NAK-CAL	2.02	114.52	110.64

There are no chirality outliers.

All (7) torsion outliers are listed below:

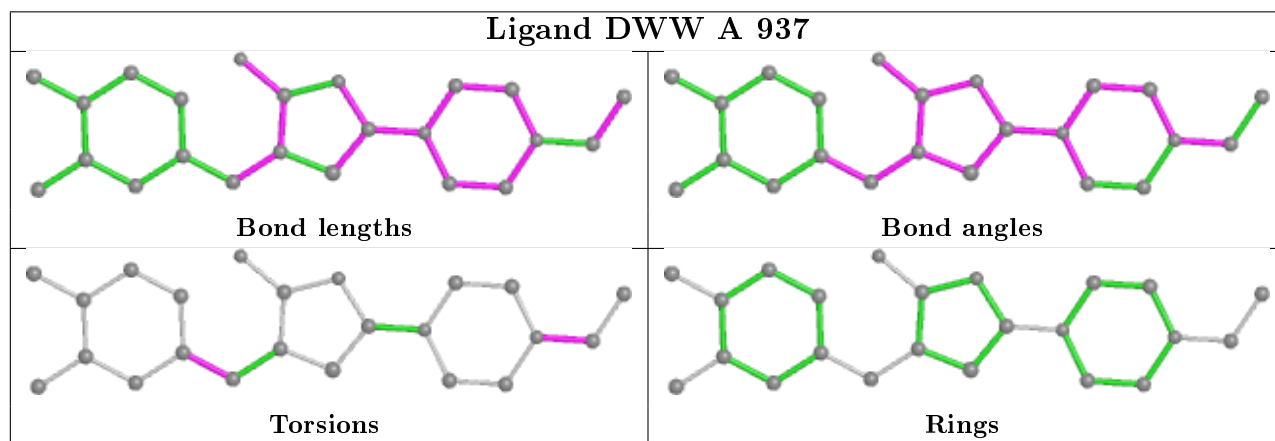
Mol	Chain	Res	Type	Atoms
11	A	937	DWW	CBB-CAV-NAS-CAR
10	A	929	EDO	O1-C1-C2-O2
11	A	937	DWW	CAA-CAF-CAG-CAH
11	A	937	DWW	CAE-CAF-CAG-CAH
10	A	931	EDO	O1-C1-C2-O2
10	A	921	EDO	O1-C1-C2-O2
10	A	927	EDO	O1-C1-C2-O2

There are no ring outliers.

6 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	924	EDO	1	0
10	A	930	EDO	2	0
11	A	937	DWW	15	0
10	A	926	EDO	1	0
10	A	921	EDO	1	0
10	A	922	EDO	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	779/831 (93%)	0.12	28 (3%) 42 52	17, 36, 65, 77	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	51	TRP	5.2
1	A	644	LEU	4.8
1	A	640	ILE	4.6
1	A	637	VAL	4.1
1	A	554	GLY	4.0
1	A	652	VAL	3.8
1	A	71	PRO	3.7
1	A	125	SER	3.7
1	A	110	VAL	3.7
1	A	556	MET	3.6
1	A	469	PHE	3.4
1	A	641	PRO	3.4
1	A	55	SER	3.0
1	A	679	PRO	3.0
1	A	70	PRO	2.9
1	A	689	TYR	2.6
1	A	634	GLN	2.6
1	A	274	PHE	2.6
1	A	587	THR	2.5
1	A	691	ALA	2.5
1	A	83	SER	2.5
1	A	126	ARG	2.4
1	A	158	ALA	2.3
1	A	684	SER	2.2
1	A	108	GLY	2.1
1	A	643	HIS	2.1
1	A	562	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	112	ASN	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

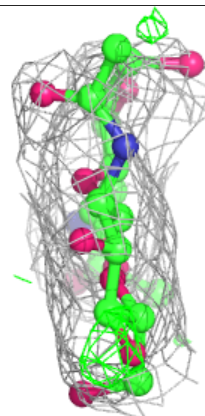
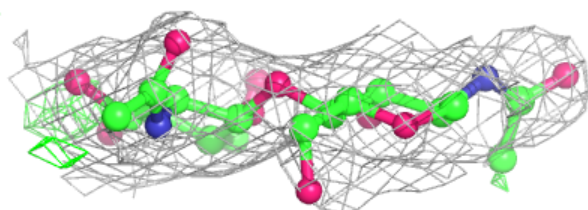
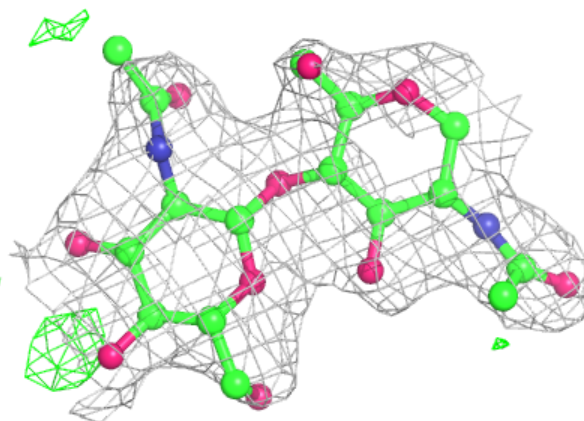
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MAN	C	7	11/12	0.79	0.13	74,76,81,82	0
2	NAG	D	2	14/15	0.84	0.14	51,60,64,65	0
2	NAG	B	2	14/15	0.84	0.16	74,81,85,86	0
2	NAG	B	1	14/15	0.88	0.21	68,73,76,81	0
3	BMA	C	3	11/12	0.90	0.09	50,57,65,72	0
3	MAN	C	4	11/12	0.91	0.09	46,50,53,54	0
3	MAN	C	6	11/12	0.92	0.09	31,41,45,49	0
2	NAG	D	1	14/15	0.95	0.09	30,37,48,49	0
3	MAN	C	5	11/12	0.95	0.14	40,46,55,62	0
3	NAG	C	2	14/15	0.96	0.09	28,36,45,47	0
3	NAG	C	1	14/15	0.98	0.10	16,24,30,31	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.

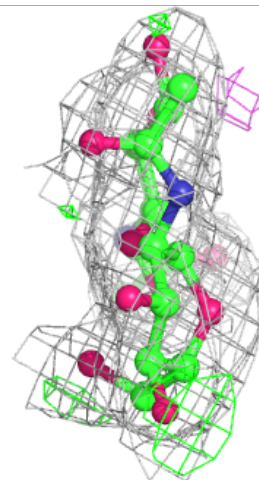
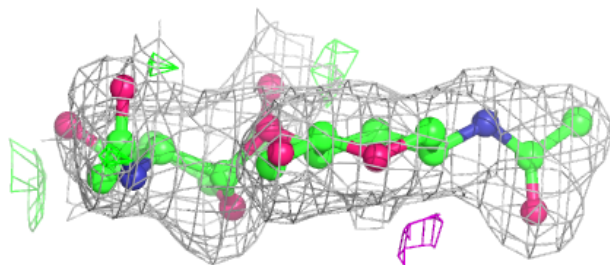
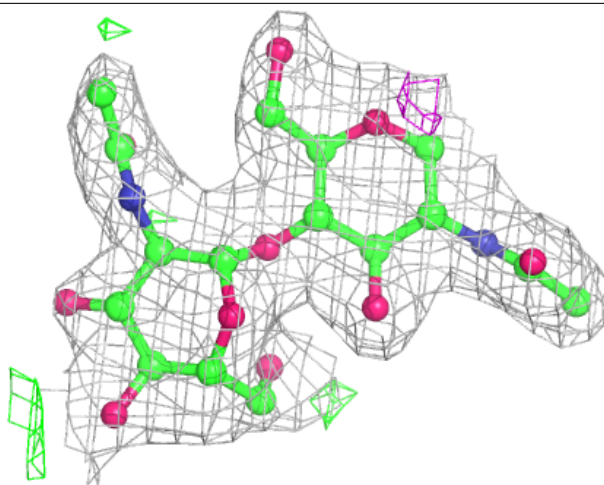
Electron density around Chain B:

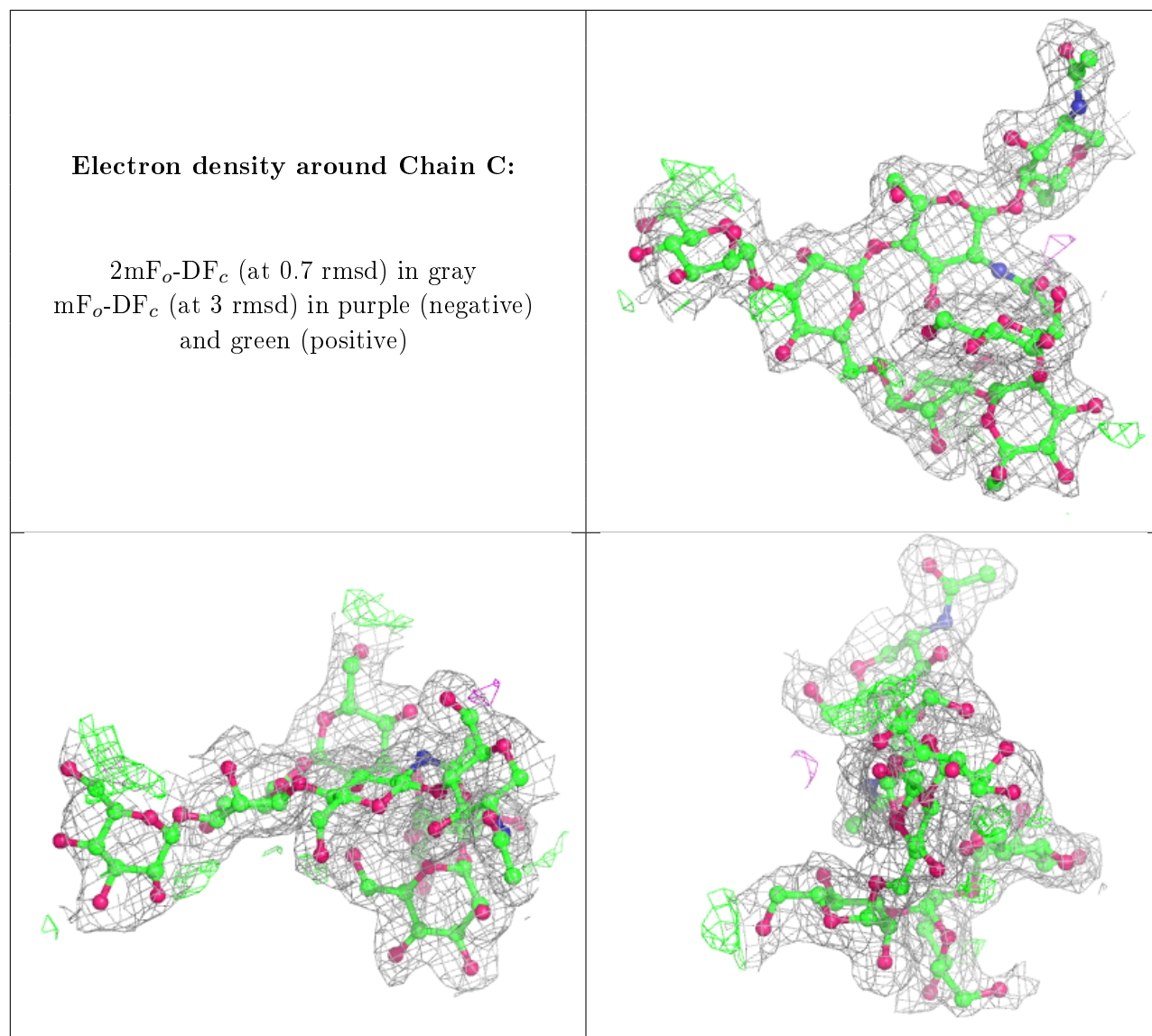
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.4 Ligands [i](#)

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

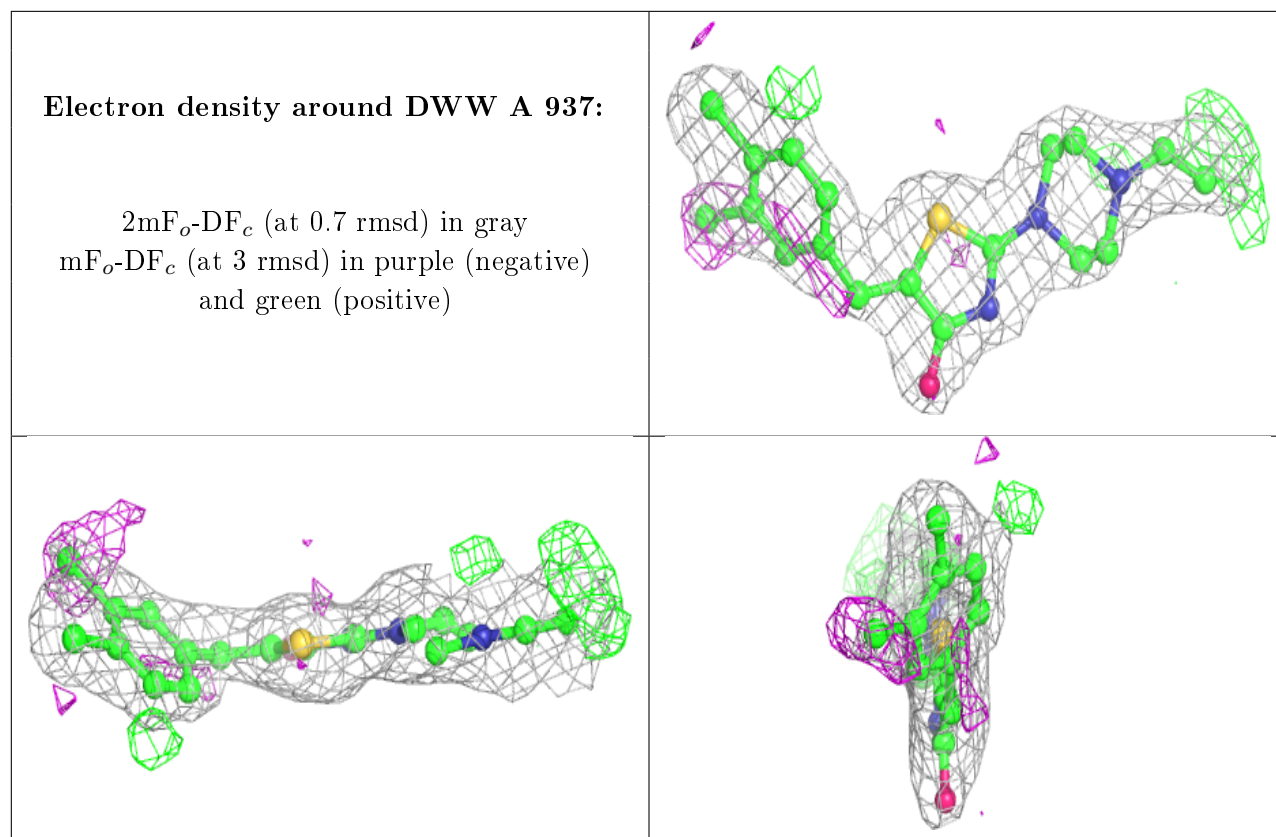
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
11	DWW	A	937	23/31	0.86	0.16	38,48,59,72	0
10	EDO	A	929	4/4	0.86	0.15	34,39,40,46	0
10	EDO	A	923	4/4	0.88	0.14	38,38,41,53	0
10	EDO	A	922	4/4	0.89	0.13	35,36,39,42	0
10	EDO	A	926	4/4	0.89	0.23	32,36,42,46	0
9	SCN	A	918	3/3	0.89	0.12	47,47,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
10	EDO	A	924	4/4	0.91	0.20	35,36,40,41	0
10	EDO	A	930	4/4	0.92	0.16	45,46,46,54	0
10	EDO	A	933	4/4	0.92	0.12	38,41,50,52	0
10	EDO	A	931	4/4	0.93	0.12	31,37,41,43	0
7	K	A	916	1/1	0.93	0.06	65,65,65,65	0
9	SCN	A	920	3/3	0.93	0.14	33,33,42,49	0
10	EDO	A	925	4/4	0.94	0.13	39,40,41,44	0
10	EDO	A	927	4/4	0.94	0.12	33,33,34,38	0
10	EDO	A	936	4/4	0.95	0.12	31,33,34,50	0
10	EDO	A	921	4/4	0.95	0.15	31,34,38,41	0
10	EDO	A	928	4/4	0.95	0.15	29,34,36,37	0
10	EDO	A	932	4/4	0.96	0.12	37,41,47,54	0
6	NA	A	915	1/1	0.97	0.05	30,30,30,30	0
8	SO4	A	917	5/5	0.97	0.09	27,28,33,36	0
9	SCN	A	919	3/3	0.98	0.16	32,32,47,66	0
10	EDO	A	935	4/4	0.98	0.07	29,31,33,38	0
10	EDO	A	934	4/4	0.99	0.06	25,26,26,30	0
4	ZN	A	912	1/1	0.99	0.11	25,25,25,25	0
5	CA	A	914	1/1	0.99	0.08	29,29,29,29	0
4	ZN	A	913	1/1	1.00	0.12	20,20,20,20	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.