



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 12:47 PM BST

PDB ID : 3WAY
Title : Crystal Structure of Autotaxin in Complex with 4BoA
Authors : Nishimasu, H.; Ishitani, R.; Nureki, O.
Deposited on : 2013-05-09
Resolution : 1.75 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

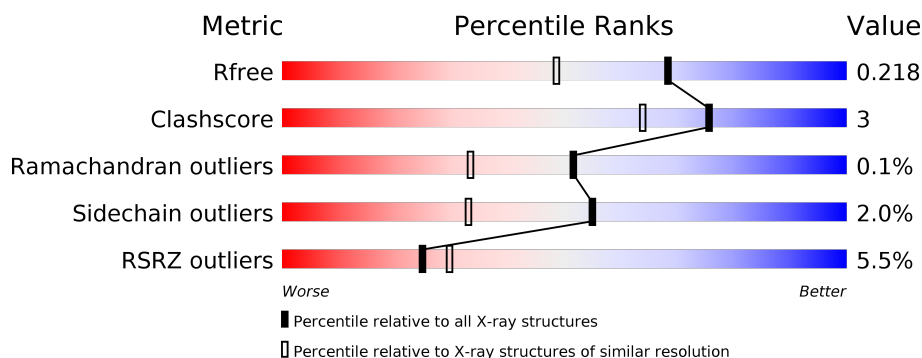
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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	3764 (1.76-1.72)
Clashscore	141614	3923 (1.76-1.72)
Ramachandran outliers	138981	3878 (1.76-1.72)
Sidechain outliers	138945	3878 (1.76-1.72)
RSRZ outliers	127900	3705 (1.76-1.72)

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	<div> <div>5%</div> <div>87%</div> <div>8%</div> <div>5%</div> </div>
2	B	2	<div> <div>50%</div> <div>50%</div> </div>
2	D	2	<div> <div>100%</div> </div>
3	C	6	<div> <div>17%</div> <div>83%</div> </div>

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 7011 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
1	A	787	Total	C	N	O	S	0	0	0
			6307	4008	1078	1173	48			

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
2	B	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			

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-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
3	C	6	Total	C	N	O	0	0	0
			72	40	2	30			

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

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

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

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

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

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

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

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

- Molecule 8 is THIOCYANATE ION (three-letter code: SCN) (formula: CNS).



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

- Molecule 9 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



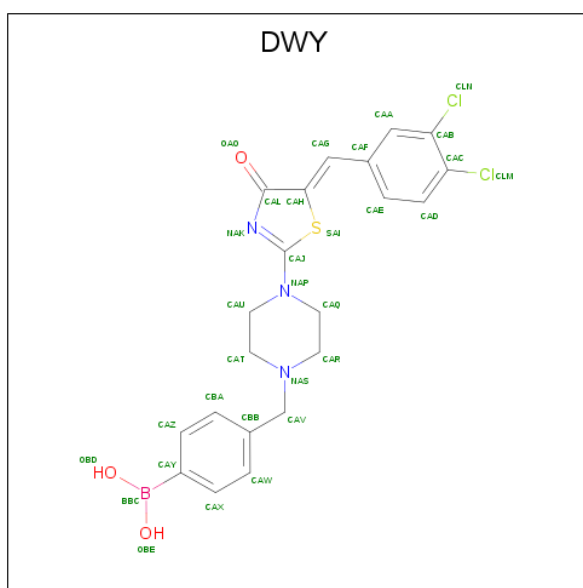
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			4	2	2		

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[illegible]

- Molecule 10 is [4-(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: DWY) (formula: $C_{21}H_{20}BCl_2N_3O_3S$).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
10	A	1	Total	B	C	Cl	N	O	S	0	1
			62	2	42	4	6	6	2		

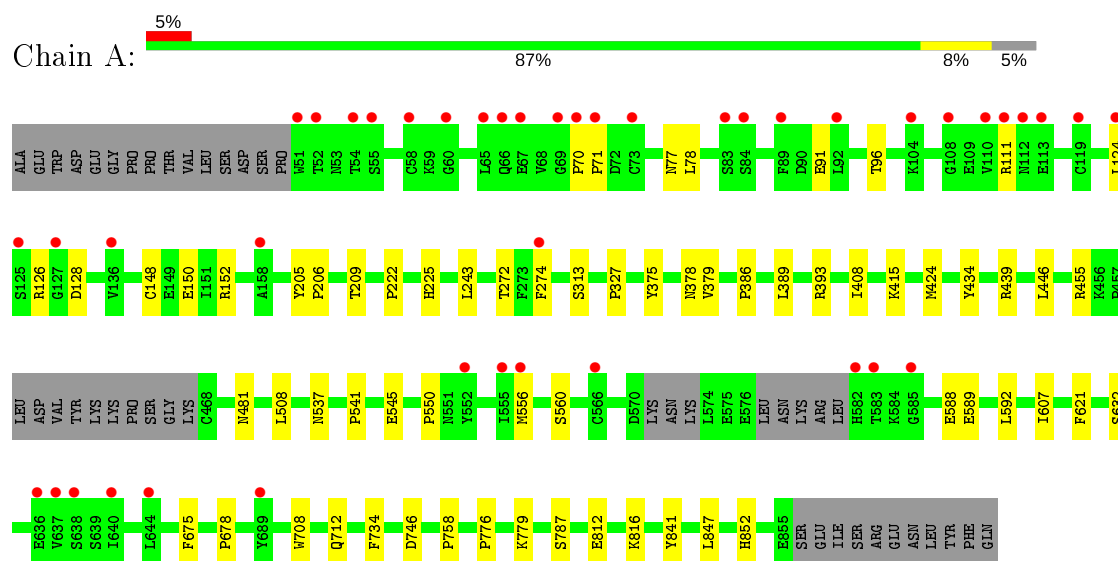
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	452	Total	O	0	0
			452	452		

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.

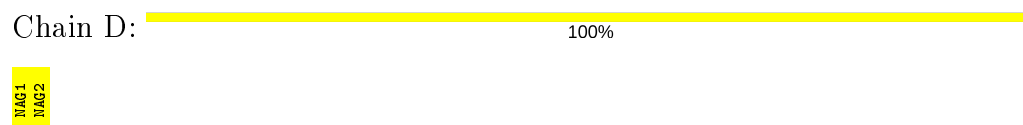
- Molecule 1: Ectonucleotide pyrophosphatase/phosphodiesterase family member 2



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



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



- Molecule 3: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



MAG1
MAG2
BM13
MAN4
MAN5
MAN6

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	61.56Å 94.52Å 75.24Å 90.00° 93.98° 90.00°	Depositor
Resolution (Å)	49.23 – 1.75 49.23 – 1.75	Depositor EDS
% Data completeness (in resolution range)	97.9 (49.23-1.75) 97.9 (49.23-1.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.12 (at 1.75Å)	Xtriage
Refinement program	PHENIX 1.7.2 _869	Depositor
R, R_{free}	0.181 , 0.221 0.178 , 0.218	Depositor DCC
R_{free} test set	4277 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	21.5	Xtriage
Anisotropy	0.173	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 46.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7011	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.48% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, BMA, NAG, NA, K, DWY, EDO, SCN, 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	0.72	0/6489	0.76	4/8817 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	393	ARG	NE-CZ-NH2	-6.88	116.86	120.30
1	A	393	ARG	NE-CZ-NH1	5.63	123.12	120.30
1	A	446	LEU	CA-CB-CG	5.21	127.29	115.30
1	A	148	CYS	CA-CB-SG	-5.10	104.82	114.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6307	0	5999	34	0
2	B	28	0	25	0	0
2	D	28	0	25	0	0
3	C	72	0	61	0	0
4	A	2	0	0	0	0
5	A	1	0	0	0	0
6	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	1	0	0	0	0
8	A	9	0	0	0	0
9	A	48	0	72	8	0
10	A	62	0	36	7	0
11	A	452	0	0	0	0
All	All	7011	0	6218	39	0

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

All (39) 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)
10:A:931[B]:DWY:BBC	10:A:931[B]:DWY:CAY	1.77	1.56
10:A:931[A]:DWY:CAY	10:A:931[A]:DWY:BBC	1.85	1.54
1:A:209:THR:OG1	10:A:931[A]:DWY:BBC	1.84	1.24
1:A:209:THR:OG1	10:A:931[B]:DWY:BBC	1.97	1.11
10:A:931[A]:DWY:CAX	10:A:931[A]:DWY:BBC	2.68	0.71
1:A:111:ARG:NH2	1:A:128:ASP:OD2	2.21	0.70
10:A:931[B]:DWY:BBC	10:A:931[B]:DWY:CAX	2.65	0.66
1:A:439:ARG:CZ	9:A:929:EDO:H21	2.28	0.63
1:A:787:SER:HB3	9:A:930:EDO:H11	1.88	0.56
1:A:758:PRO:HD3	9:A:925:EDO:H22	1.88	0.55
1:A:389:LEU:N	1:A:389:LEU:HD23	2.23	0.54
1:A:588:GLU:HG3	1:A:592:LEU:HD23	1.92	0.52
1:A:150:GLU:OE1	1:A:152:ARG:NH1	2.43	0.52
1:A:78:LEU:HD21	1:A:274:PHE:HB2	1.92	0.52
1:A:222:PRO:HA	1:A:225:HIS:CE1	2.48	0.49
1:A:734:PHE:CD1	9:A:921:EDO:H11	2.48	0.48
1:A:847:LEU:HD12	9:A:926:EDO:H11	1.95	0.48
1:A:708:TRP:CD1	9:A:920:EDO:H11	2.48	0.48
1:A:205:TYR:CD1	1:A:206:PRO:HA	2.49	0.47
1:A:111:ARG:HH22	1:A:128:ASP:CG	2.13	0.47
1:A:78:LEU:HD23	1:A:272:THR:HG21	1.96	0.47
1:A:70:PRO:HA	1:A:71:PRO:HA	1.74	0.46
1:A:243:LEU:HA	1:A:243:LEU:HD23	1.71	0.45
1:A:550:PRO:HB2	1:A:607:ILE:HG12	1.99	0.45
1:A:678:PRO:HB3	1:A:712:GLN:HB3	1.99	0.45
1:A:776:PRO:HG3	1:A:779:LYS:HD2	1.99	0.45
1:A:379:VAL:HB	1:A:455:ARG:HG2	2.00	0.44
1:A:415:LYS:HB2	1:A:415:LYS:HE3	1.70	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:SER:CB	1:A:327:PRO:HG3	2.50	0.42
1:A:812:GLU:O	1:A:816:LYS:HG3	2.19	0.42
1:A:206:PRO:HD3	1:A:434:TYR:CE1	2.55	0.42
1:A:126:ARG:HE	1:A:126:ARG:HB3	1.63	0.42
1:A:541:PRO:HG2	1:A:841:TYR:CD2	2.55	0.42
1:A:375:TYR:OH	1:A:415:LYS:HE2	2.20	0.41
1:A:408:ILE:HD11	1:A:424:MET:SD	2.59	0.41
1:A:77:ASN:HD21	1:A:272:THR:HB	1.85	0.41
1:A:621:PHE:CD1	9:A:925:EDO:H12	2.56	0.41
1:A:675:PHE:HB2	9:A:920:EDO:H22	2.02	0.40
10:A:931[B]:DWY:BBC	10:A:931[B]:DWY:CAZ	2.77	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	779/831 (94%)	754 (97%)	24 (3%)	1 (0%)	51 33

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	702/756 (93%)	688 (98%)	14 (2%)	55 33

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	91	GLU
1	A	96	THR
1	A	124	LEU
1	A	378	ASN
1	A	481	ASN
1	A	508	LEU
1	A	537	ASN
1	A	545	GLU
1	A	556	MET
1	A	560	SER
1	A	589	GLU
1	A	632	SER
1	A	746	ASP
1	A	852	HIS

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	537	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](#)

10 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	B	1	1,2	14,14,15	0.53	0	17,19,21	0.90	0
2	NAG	B	2	2	14,14,15	0.67	0	17,19,21	1.04	2 (11%)
3	NAG	C	1	1,3	14,14,15	0.81	0	17,19,21	1.04	0
3	NAG	C	2	3	14,14,15	0.59	0	17,19,21	1.20	2 (11%)
3	BMA	C	3	3	11,11,12	0.76	0	15,15,17	1.22	2 (13%)
3	MAN	C	4	3	11,11,12	0.64	0	15,15,17	1.24	2 (13%)
3	MAN	C	5	3	11,11,12	0.58	0	15,15,17	1.29	3 (20%)
3	MAN	C	6	3	11,11,12	0.58	0	15,15,17	1.25	2 (13%)
2	NAG	D	1	1,2	14,14,15	0.77	0	17,19,21	1.49	2 (11%)
2	NAG	D	2	2	14,14,15	0.44	0	17,19,21	2.54	3 (17%)

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	-	0/6/23/26	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	-	0/2/19/22	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
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 (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2	NAG	C1-O5-C5	9.08	124.50	112.19
2	D	1	NAG	O5-C1-C2	-4.15	104.73	111.29
2	D	2	NAG	O5-C1-C2	3.67	117.09	111.29
3	C	6	MAN	O2-C2-C3	-3.14	103.85	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	4	MAN	O2-C2-C1	2.69	114.66	109.15
3	C	3	BMA	C1-O5-C5	-2.55	108.74	112.19
3	C	2	NAG	O7-C7-C8	-2.51	117.39	122.06
3	C	3	BMA	O5-C1-C2	-2.51	106.90	110.77
3	C	4	MAN	O5-C5-C6	2.48	111.09	107.20
3	C	6	MAN	C1-O5-C5	2.48	115.55	112.19
3	C	2	NAG	C1-O5-C5	-2.39	108.96	112.19
3	C	5	MAN	O5-C5-C6	2.37	110.92	107.20
3	C	5	MAN	O5-C1-C2	-2.34	107.15	110.77
2	B	2	NAG	C1-O5-C5	2.33	115.36	112.19
3	C	5	MAN	O3-C3-C4	-2.27	105.11	110.35
2	D	1	NAG	C1-C2-N2	-2.22	106.70	110.49
2	D	2	NAG	O5-C5-C4	2.14	116.04	110.83
2	B	2	NAG	O5-C1-C2	2.11	114.61	111.29

There are no chirality outliers.

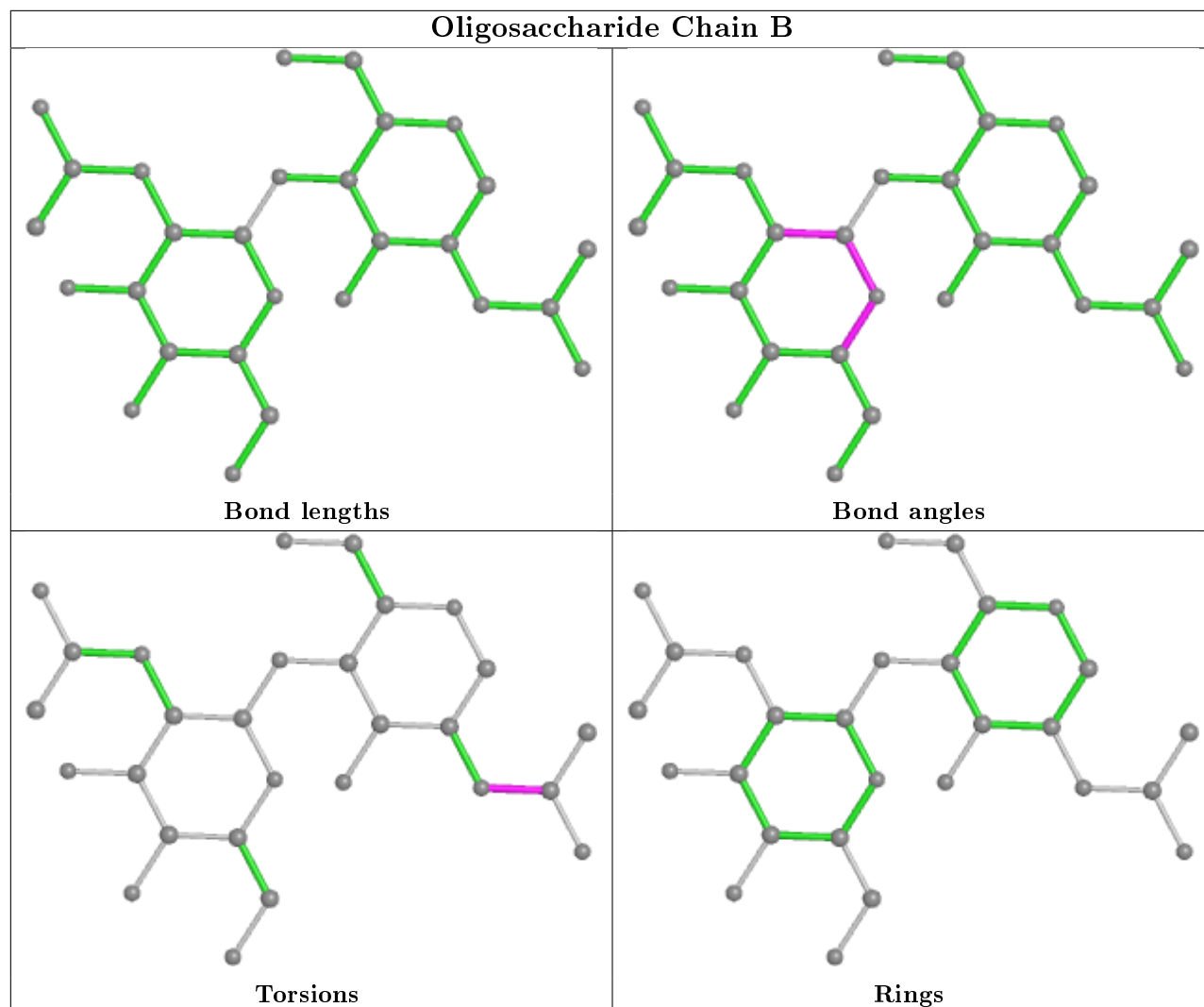
All (2) torsion outliers are listed below:

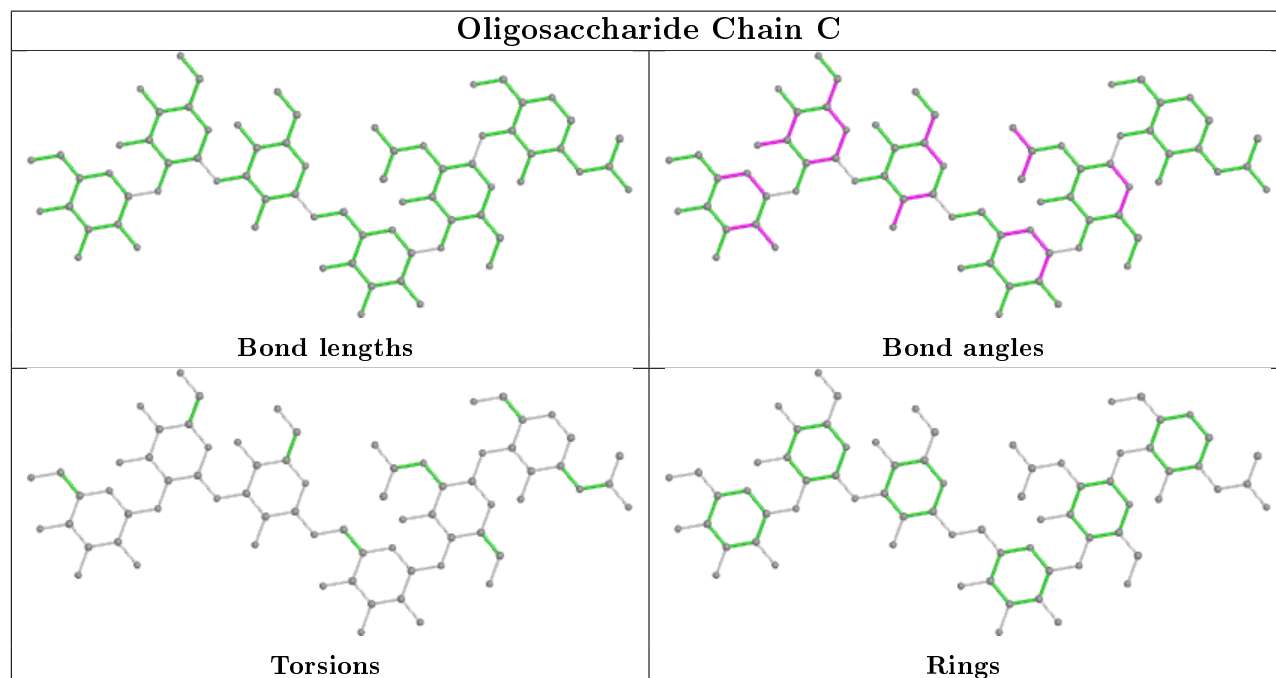
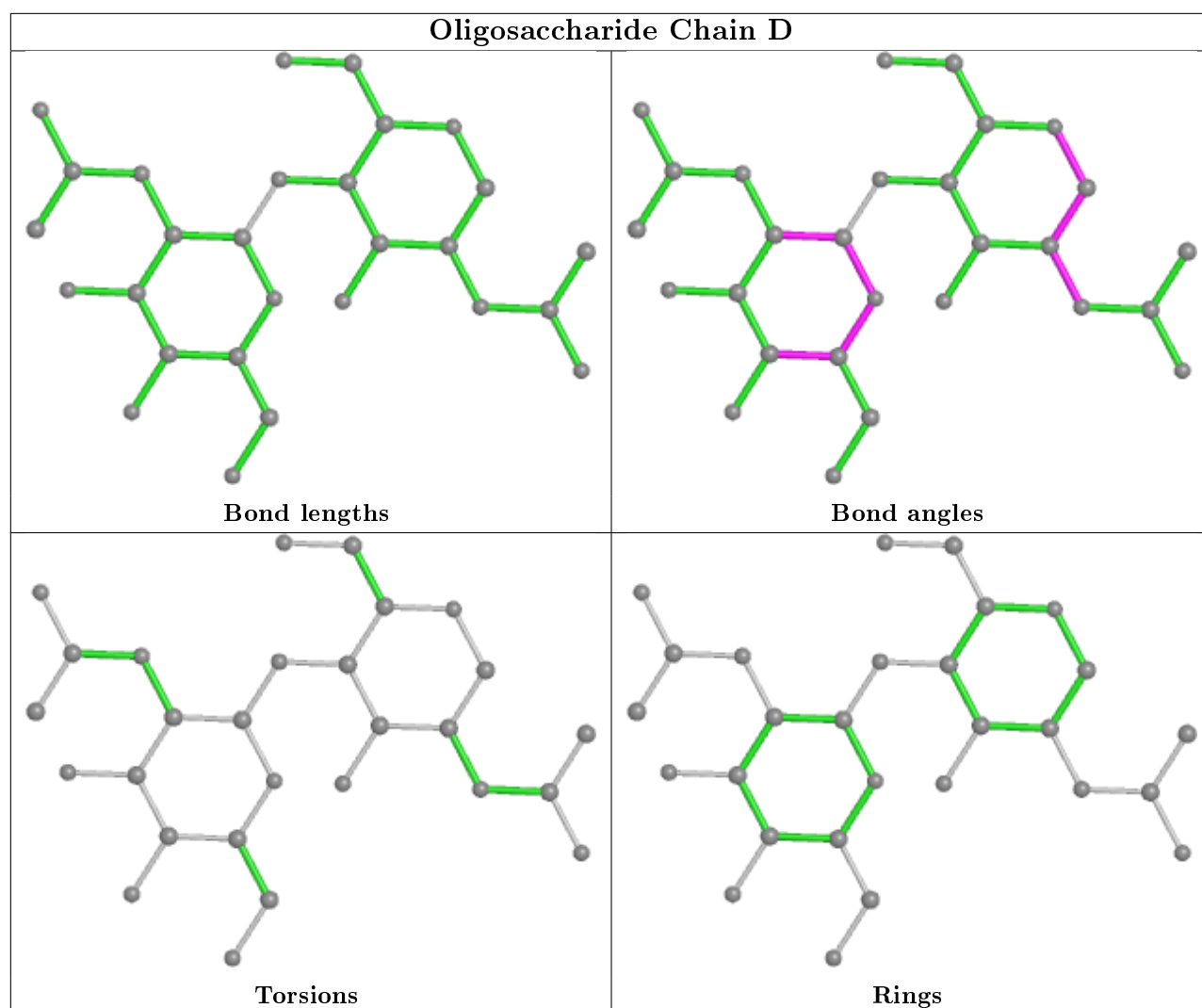
Mol	Chain	Res	Type	Atoms
2	B	1	NAG	C8-C7-N2-C2
2	B	1	NAG	O7-C7-N2-C2

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

Of 22 ligands modelled in this entry, 5 are monoatomic - leaving 17 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
9	EDO	A	930	-	3,3,3	0.74	0	2,2,2	0.30	0
9	EDO	A	925	-	3,3,3	0.41	0	2,2,2	0.49	0
10	DWY	A	931[B]	4	34,34,34	3.82	7 (20%)	48,48,48	2.42	18 (37%)
9	EDO	A	929	-	3,3,3	0.48	0	2,2,2	0.50	0
10	DWY	A	931[A]	4	34,34,34	4.07	9 (26%)	48,48,48	2.72	18 (37%)
9	EDO	A	920	-	3,3,3	0.22	0	2,2,2	0.89	0
8	SCN	A	916	-	1,2,2	0.88	0	0,1,1	0.00	-
8	SCN	A	917	-	1,2,2	0.87	0	0,1,1	0.00	-
9	EDO	A	924	-	3,3,3	0.61	0	2,2,2	0.35	0
8	SCN	A	918	-	1,2,2	1.02	0	0,1,1	0.00	-
9	EDO	A	928	-	3,3,3	0.70	0	2,2,2	0.09	0
9	EDO	A	922	-	3,3,3	0.69	0	2,2,2	0.39	0
9	EDO	A	927	-	3,3,3	0.52	0	2,2,2	0.20	0
9	EDO	A	919	-	3,3,3	0.98	0	2,2,2	1.16	0
9	EDO	A	926	-	3,3,3	0.47	0	2,2,2	0.23	0
9	EDO	A	923	-	3,3,3	0.46	0	2,2,2	0.52	0
9	EDO	A	921	-	3,3,3	0.54	0	2,2,2	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
9	EDO	A	930	-	-	1/1/1/1	-
9	EDO	A	925	-	-	1/1/1/1	-
10	DWY	A	931[B]	4	-	2/16/38/38	0/4/4/4
9	EDO	A	929	-	-	1/1/1/1	-
10	DWY	A	931[A]	4	-	2/16/38/38	0/4/4/4
9	EDO	A	920	-	-	1/1/1/1	-
9	EDO	A	924	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	EDO	A	923	-	-	0/1/1/1	-
9	EDO	A	928	-	-	1/1/1/1	-
9	EDO	A	922	-	-	0/1/1/1	-
9	EDO	A	927	-	-	0/1/1/1	-
9	EDO	A	919	-	-	0/1/1/1	-
9	EDO	A	926	-	-	0/1/1/1	-
9	EDO	A	921	-	-	0/1/1/1	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	931[A]	DWY	BBC-CAY	13.91	1.85	1.57
10	A	931[A]	DWY	BBC-OB	11.40	1.55	1.36
10	A	931[B]	DWY	CAL-CAH	-10.99	1.35	1.50
10	A	931[B]	DWY	BBC-OB	10.04	1.53	1.36
10	A	931[B]	DWY	BBC-CAY	9.96	1.77	1.57
10	A	931[A]	DWY	CAL-CAH	-9.69	1.36	1.50
10	A	931[B]	DWY	BBC-OB	9.18	1.52	1.36
10	A	931[A]	DWY	BBC-OB	8.80	1.51	1.36
10	A	931[B]	DWY	CAV-CBB	-6.08	1.40	1.51
10	A	931[B]	DWY	CAJ-SAI	-5.70	1.62	1.75
10	A	931[A]	DWY	CAV-CBB	-5.00	1.42	1.51
10	A	931[B]	DWY	CAF-CAG	-3.00	1.41	1.46
10	A	931[A]	DWY	CAC-CLM	2.88	1.80	1.73
10	A	931[A]	DWY	CAJ-SAI	-2.77	1.68	1.75
10	A	931[A]	DWY	CAF-CAG	-2.14	1.42	1.46
10	A	931[A]	DWY	CAH-SAI	2.11	1.78	1.73

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	931[A]	DWY	BBC-CAY-CAX	-7.03	111.74	121.56
10	A	931[A]	DWY	CAH-CAL-NAK	6.62	117.03	113.56
10	A	931[A]	DWY	CAL-CAH-SAI	-6.46	105.55	109.12
10	A	931[A]	DWY	CAZ-CAY-CAX	6.26	123.88	116.88
10	A	931[B]	DWY	CAL-CAH-SAI	-6.14	105.73	109.12
10	A	931[B]	DWY	CAF-CAG-CAH	-5.94	122.81	130.94
10	A	931[B]	DWY	CAZ-CAY-CAX	5.77	123.34	116.88
10	A	931[B]	DWY	BBC-CAY-CAX	-5.29	114.18	121.56
10	A	931[A]	DWY	CAW-CAX-CAY	-4.97	117.15	121.81
10	A	931[B]	DWY	CAW-CAX-CAY	-4.67	117.44	121.81
10	A	931[A]	DWY	SAI-CAJ-NAP	4.22	125.81	120.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	931[B]	DWY	CAH-CAL-NAK	4.15	115.73	113.56
10	A	931[A]	DWY	CAV-CBB-CAW	-4.02	113.22	120.77
10	A	931[B]	DWY	CAV-CBB-CAW	-3.74	113.74	120.77
10	A	931[A]	DWY	CBA-CAZ-CAY	-3.65	118.39	121.81
10	A	931[B]	DWY	CBA-CAZ-CAY	-3.37	118.65	121.81
10	A	931[B]	DWY	SAI-CAJ-NAK	-3.35	111.52	116.31
10	A	931[A]	DWY	SAI-CAJ-NAK	-3.28	111.62	116.31
10	A	931[A]	DWY	CAR-NAS-CAT	-3.08	101.90	108.83
10	A	931[A]	DWY	CAQ-CAR-NAS	2.91	116.61	110.64
10	A	931[A]	DWY	CAE-CAF-CAG	-2.85	111.50	121.22
10	A	931[A]	DWY	OAQ-CAL-NAK	-2.72	118.86	124.36
10	A	931[A]	DWY	CAZ-CBA-CBB	-2.62	117.42	121.03
10	A	931[B]	DWY	CAR-NAS-CAT	-2.60	102.97	108.83
10	A	931[B]	DWY	SAI-CAJ-NAP	2.59	123.71	120.36
10	A	931[A]	DWY	CAG-CAH-CAL	2.37	124.67	122.31
10	A	931[A]	DWY	CAF-CAG-CAH	-2.32	127.76	130.94
10	A	931[B]	DWY	CAJ-SAI-CAH	2.30	93.90	90.75
10	A	931[A]	DWY	CBA-CBB-CAW	2.29	121.76	118.17
10	A	931[A]	DWY	CAV-CBB-CBA	2.24	124.98	120.77
10	A	931[B]	DWY	CAZ-CBA-CBB	-2.22	117.97	121.03
10	A	931[B]	DWY	CAV-CBB-CBA	2.19	124.89	120.77
10	A	931[B]	DWY	OBD-BBC-CAY	-2.08	113.74	119.95
10	A	931[B]	DWY	CAQ-CAR-NAS	2.06	114.88	110.64
10	A	931[B]	DWY	OBE-BBC-CAY	-2.06	113.79	119.95
10	A	931[B]	DWY	CBA-CBB-CAW	2.04	121.37	118.17

There are no chirality outliers.

All (9) torsion outliers are listed below:

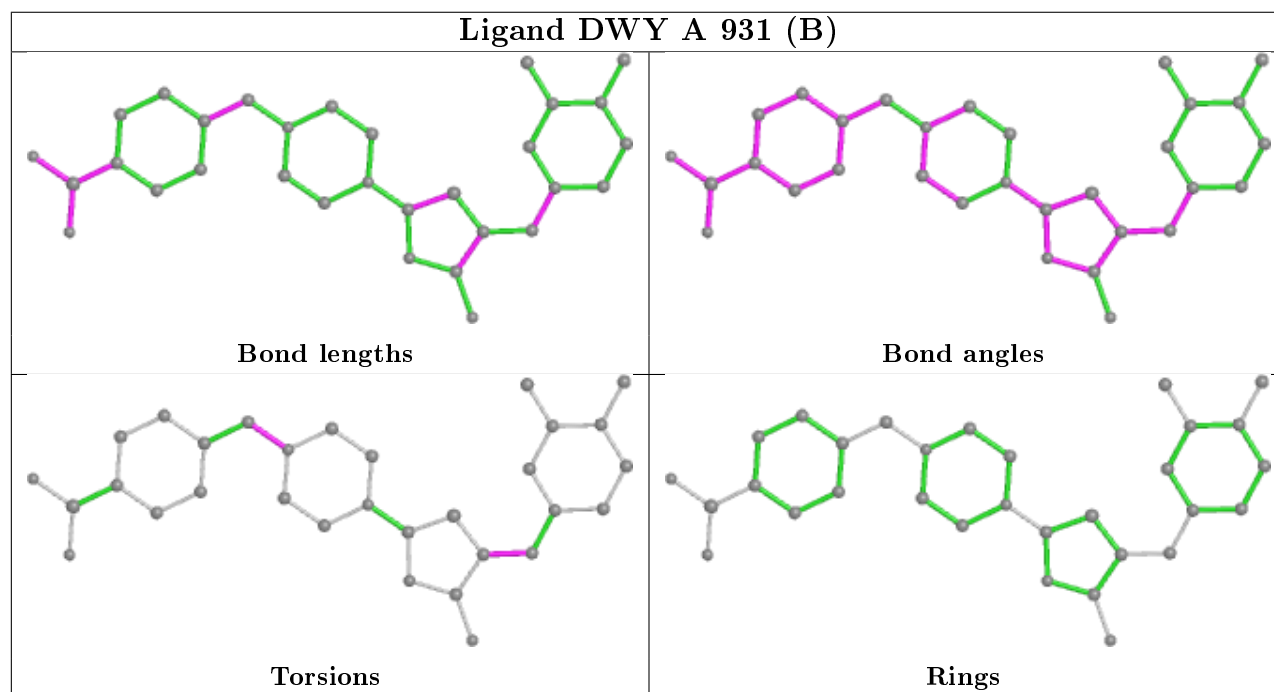
Mol	Chain	Res	Type	Atoms
10	A	931[A]	DWY	CAF-CAG-CAH-SAI
10	A	931[B]	DWY	CAF-CAG-CAH-SAI
9	A	925	EDO	O1-C1-C2-O2
10	A	931[A]	DWY	CBB-CAV-NAS-CAR
10	A	931[B]	DWY	CBB-CAV-NAS-CAR
9	A	920	EDO	O1-C1-C2-O2
9	A	930	EDO	O1-C1-C2-O2
9	A	929	EDO	O1-C1-C2-O2
9	A	928	EDO	O1-C1-C2-O2

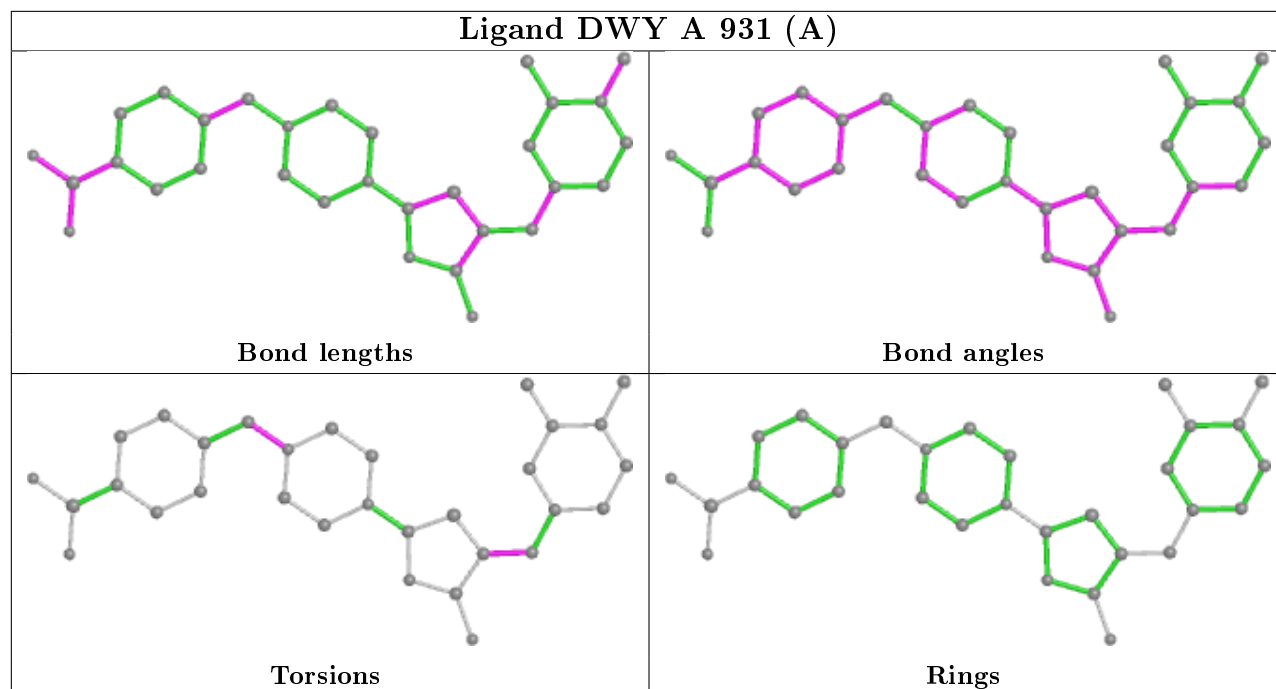
There are no ring outliers.

8 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	930	EDO	1	0
9	A	925	EDO	2	0
10	A	931[B]	DWY	4	0
9	A	929	EDO	1	0
10	A	931[A]	DWY	3	0
9	A	920	EDO	2	0
9	A	926	EDO	1	0
9	A	921	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	787/831 (94%)	0.23	43 (5%) 25 30	12, 26, 56, 96	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	110	VAL	6.2
1	A	51	TRP	6.0
1	A	70	PRO	5.4
1	A	55	SER	4.9
1	A	583	THR	4.6
1	A	58	CYS	4.5
1	A	66	GLN	4.3
1	A	124	LEU	4.1
1	A	644	LEU	4.1
1	A	71	PRO	3.9
1	A	54	THR	3.8
1	A	69	GLY	3.8
1	A	640	ILE	3.7
1	A	52	THR	3.4
1	A	112	ASN	3.3
1	A	582	HIS	3.1
1	A	637	VAL	3.0
1	A	83	SER	3.0
1	A	111	ARG	2.9
1	A	636	GLU	2.7
1	A	89	PHE	2.7
1	A	555	ILE	2.6
1	A	108	GLY	2.5
1	A	556	MET	2.5
1	A	158	ALA	2.5
1	A	92	LEU	2.5
1	A	60	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	136	VAL	2.4
1	A	67	GLU	2.4
1	A	127	GLY	2.4
1	A	566	CYS	2.4
1	A	585	GLY	2.4
1	A	113	GLU	2.3
1	A	104	LYS	2.3
1	A	274	PHE	2.2
1	A	638	SER	2.2
1	A	119	CYS	2.1
1	A	125	SER	2.1
1	A	73	CYS	2.1
1	A	65	LEU	2.1
1	A	84	SER	2.1
1	A	552	TYR	2.0
1	A	689	TYR	2.0

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

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

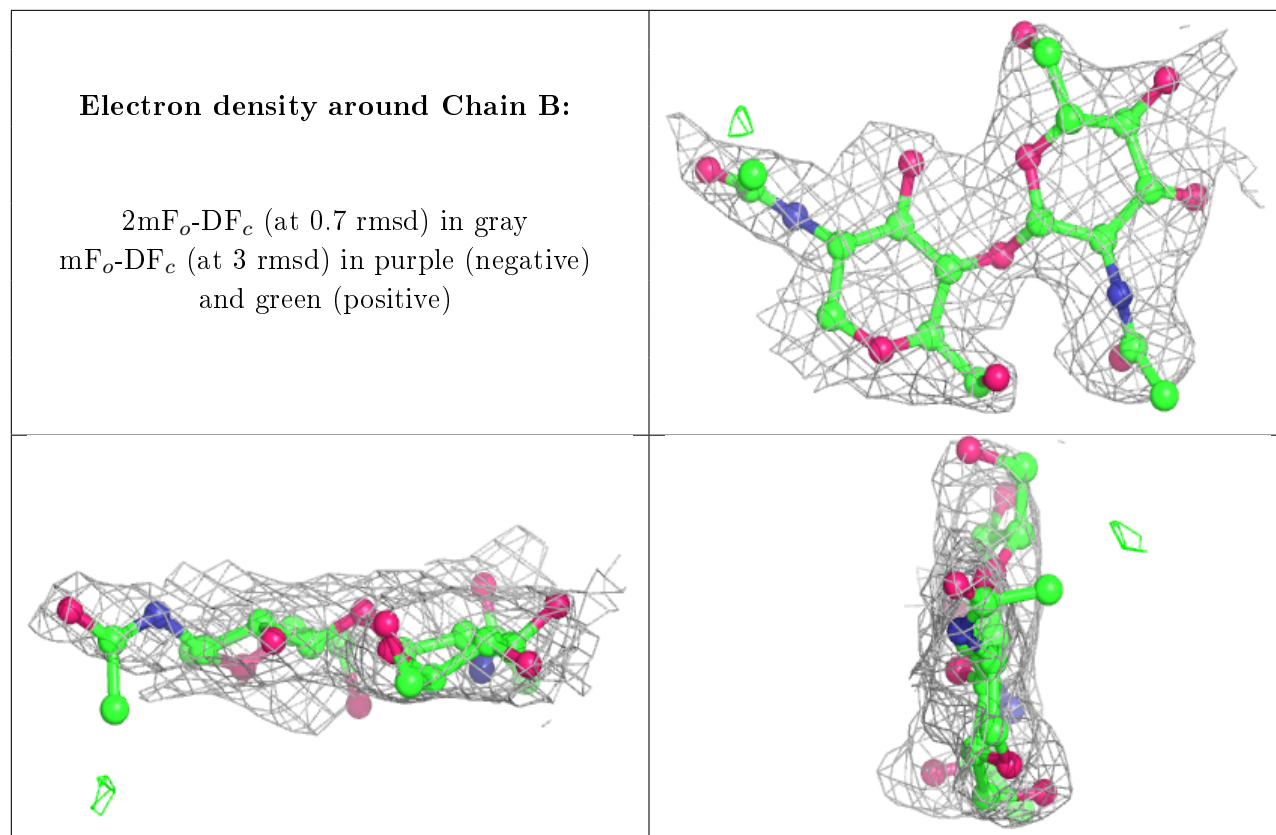
6.3 Carbohydrates ⓘ

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	BMA	C	3	11/12	0.80	0.14	37,42,50,51	0
2	NAG	B	1	14/15	0.81	0.29	75,80,82,84	0
2	NAG	D	2	14/15	0.81	0.18	45,55,62,63	0
3	MAN	C	4	11/12	0.88	0.13	34,38,42,43	0
2	NAG	B	2	14/15	0.89	0.15	73,82,84,84	0
2	NAG	D	1	14/15	0.93	0.09	22,26,38,43	0
3	MAN	C	5	11/12	0.93	0.17	29,36,43,52	0
3	NAG	C	2	14/15	0.95	0.08	22,29,35,39	0
3	MAN	C	6	11/12	0.95	0.11	22,32,36,38	0
3	NAG	C	1	14/15	0.97	0.10	13,18,21,25	0

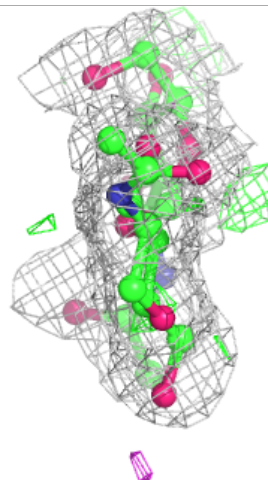
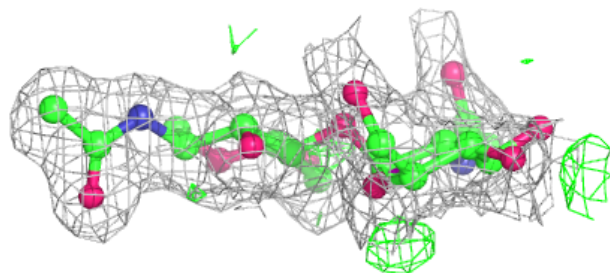
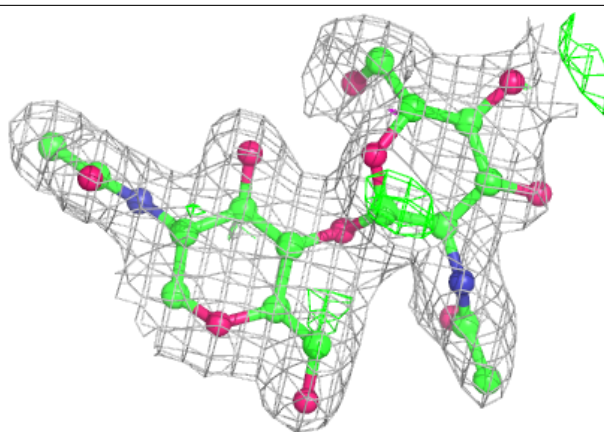
The following is a graphical depiction of the model fit to experimental electron density for oligosac-

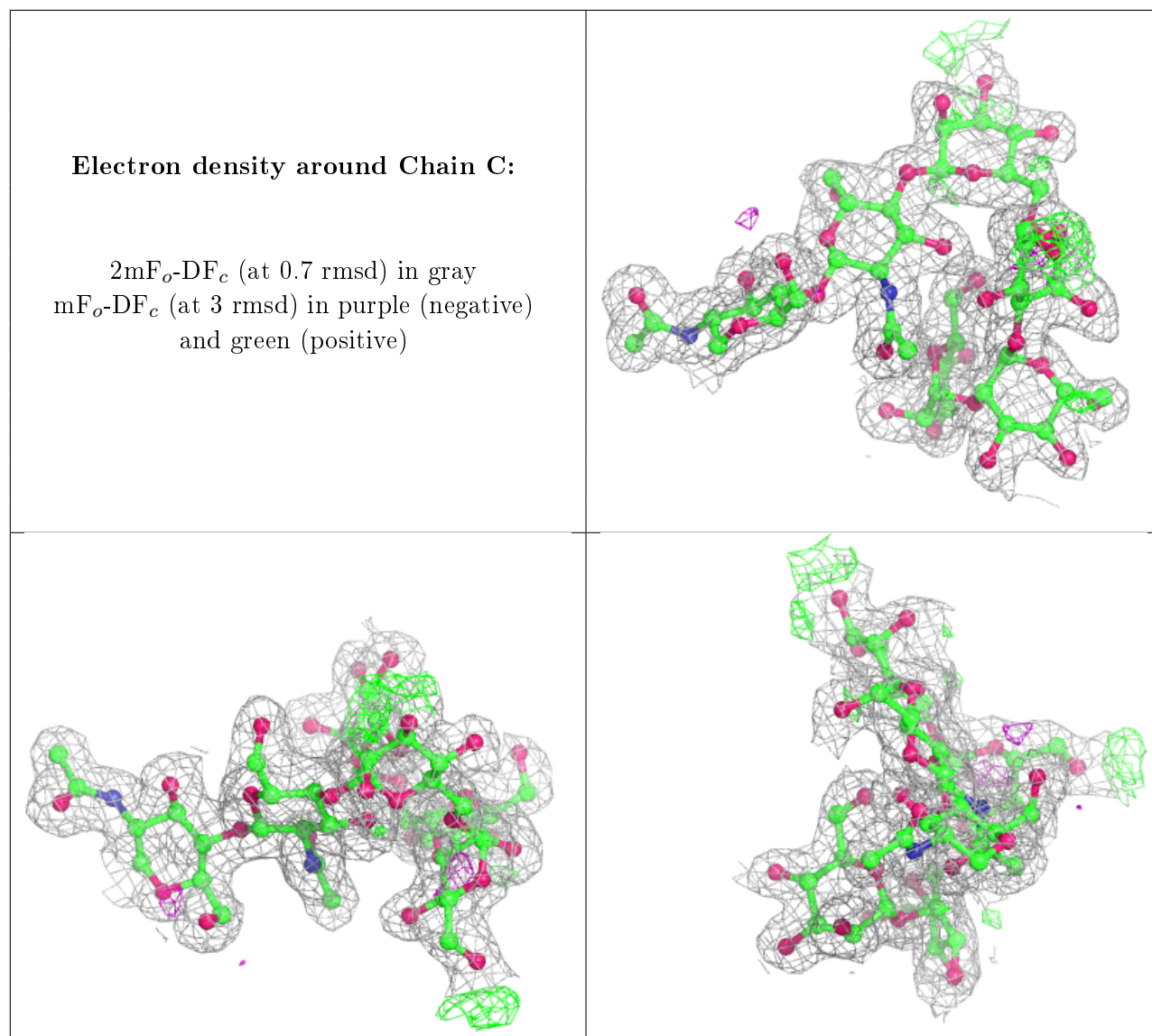
charide. Each fit is shown from different orientation to approximate a three-dimensional view.



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)





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
9	EDO	A	919	4/4	0.87	0.14	24,29,32,35	0
8	SCN	A	918	3/3	0.88	0.12	21,21,22,36	0
7	K	A	915	1/1	0.90	0.07	45,45,45,45	0
9	EDO	A	930	4/4	0.90	0.15	29,34,36,43	0
9	EDO	A	924	4/4	0.92	0.12	26,28,29,37	0
9	EDO	A	920	4/4	0.92	0.13	25,27,29,38	0

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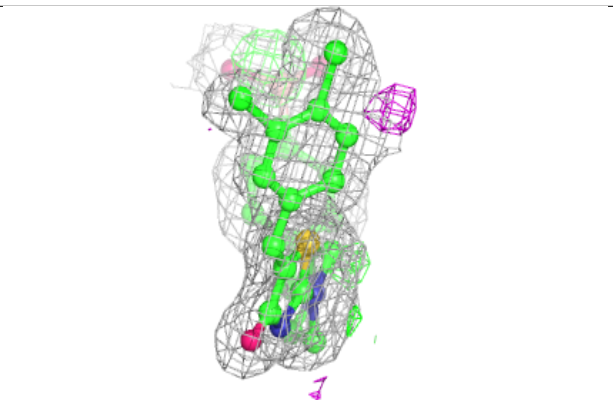
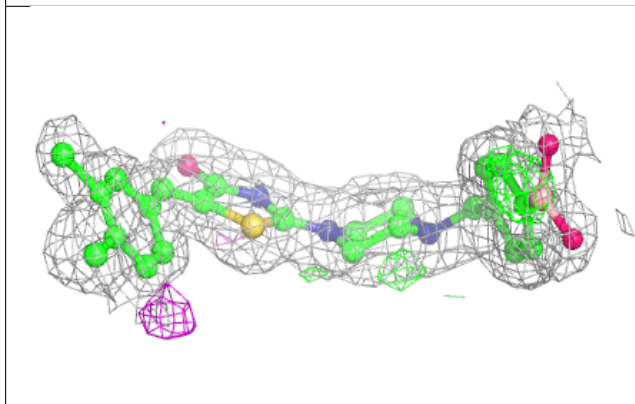
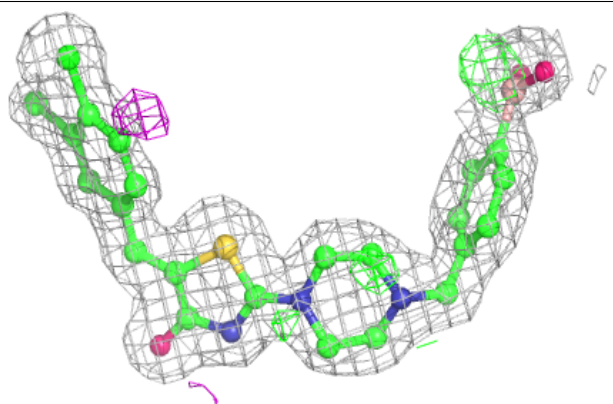
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
9	EDO	A	921	4/4	0.93	0.12	27,29,29,31	0
9	EDO	A	929	4/4	0.93	0.16	27,28,31,41	0
9	EDO	A	925	4/4	0.94	0.10	33,35,36,43	0
10	DWY	A	931[B]	31/31	0.94	0.11	16,23,28,33	31
9	EDO	A	923	4/4	0.94	0.20	26,29,32,41	0
10	DWY	A	931[A]	31/31	0.94	0.11	15,23,32,36	31
9	EDO	A	928	4/4	0.95	0.09	24,26,26,33	0
8	SCN	A	916	3/3	0.96	0.31	41,41,48,58	0
9	EDO	A	926	4/4	0.96	0.09	23,26,37,38	0
9	EDO	A	922	4/4	0.96	0.09	29,30,31,36	0
9	EDO	A	927	4/4	0.97	0.08	16,19,19,22	0
8	SCN	A	917	3/3	0.98	0.14	27,27,37,57	0
5	CA	A	913	1/1	0.99	0.07	22,22,22,22	0
4	ZN	A	911	1/1	1.00	0.10	16,16,16,16	0
4	ZN	A	912	1/1	1.00	0.10	16,16,16,16	0
6	NA	A	914	1/1	1.00	0.04	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.

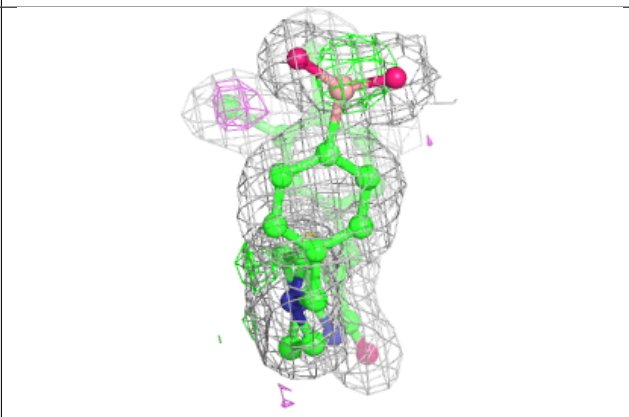
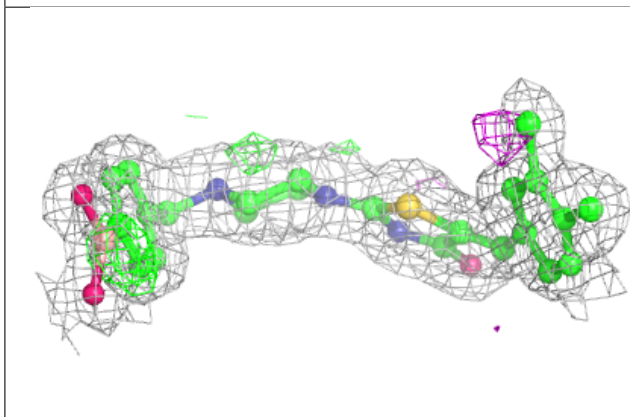
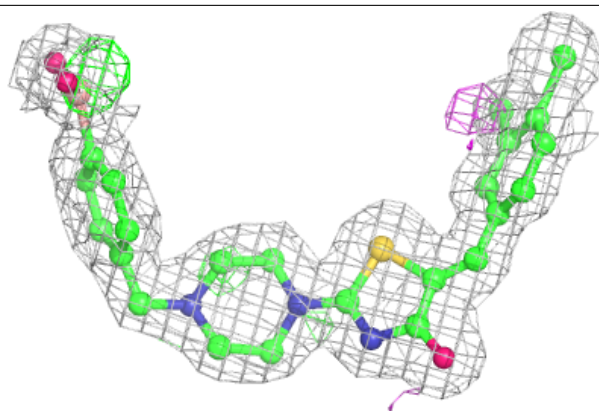
Electron density around DWY A 931 (B):

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 DWY A 931 (A):

$2mF_o-DF_c$ (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.