



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 09:19 PM BST

PDB ID : 3WAV
Title : Crystal Structure of Autotaxin in Complex with Compound 10
Authors : Nishimasu, H.; Ishitani, R.; Nureki, O.
Deposited on : 2013-05-09
Resolution : 1.80 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

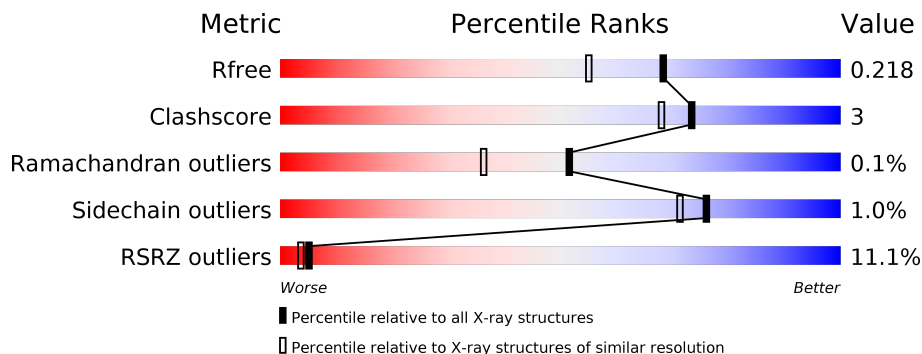
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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 style="display: flex; align-items: center;"> <div style="width: 11%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 88%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">11% 88% 8%</p>
2	B	2	<div style="width: 100%; height: 10px; background-color: yellow;"></div> <p style="text-align: center;">100%</p>
2	D	2	<div style="display: flex; align-items: center;"> <div style="width: 50%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 50%; height: 10px; background-color: orange;"></div> </div> <p style="text-align: center;">50% 50%</p>
3	C	6	<div style="display: flex; align-items: center;"> <div style="width: 50%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 50%; height: 10px; background-color: yellow;"></div> </div> <p style="text-align: center;">50% 50%</p>

2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 7096 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	801	6435	4088	1100	1197	50	0	3	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)-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	6	72	40	2	30	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

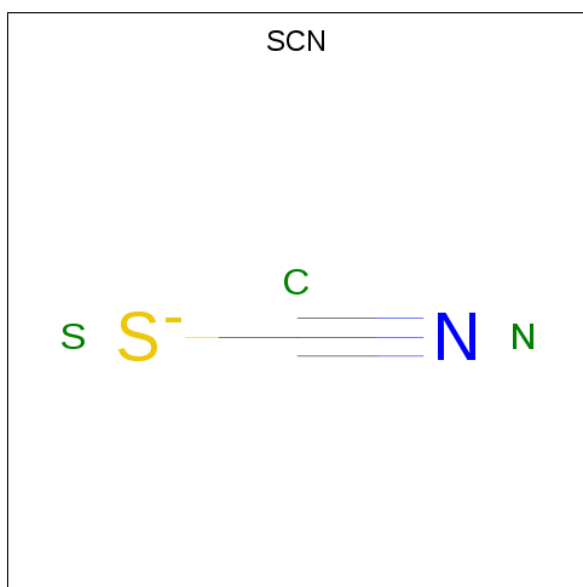
- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

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 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		

- 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			
9	A	1	Total	C	O		0	0
			4	2	2			

Continued on next page...

Continued from previous page...

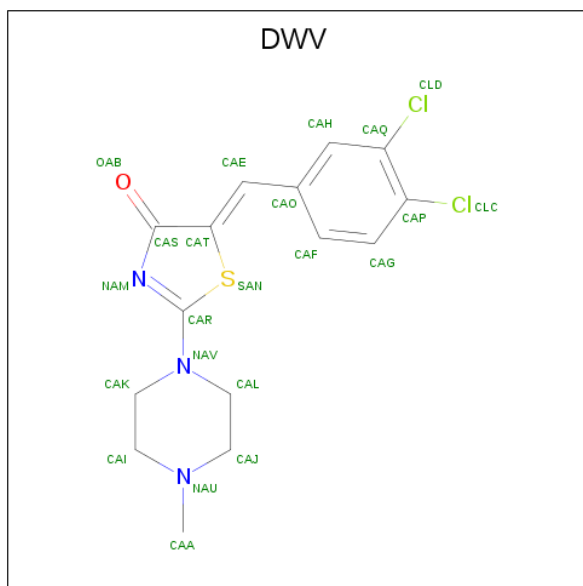
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			4	2	2		
9	A	1	Total	C	O	0	0
			4	2	2		
9	A	1	Total	C	O	0	0
			4	2	2		
9	A	1	Total	C	O	0	0
			4	2	2		
9	A	1	Total	C	O	0	0
			4	2	2		
9	A	1	Total	C	O	0	0
			4	2	2		
9	A	1	Total	C	O	0	0
			4	2	2		
9	A	1	Total	C	O	0	0
			4	2	2		
9	A	1	Total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

- Molecule 10 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 11 is (5Z)-5-(3,4-dichlorobenzylidene)-2-(4-methylpiperazin-1-yl)-1,3-thiazol-4(5H)-one (three-letter code: DWV) (formula: C₁₅H₁₅Cl₂N₃OS).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
11	A	1	Total	C	Cl	N	O	S	0	0
			22	15	2	3	1	1		

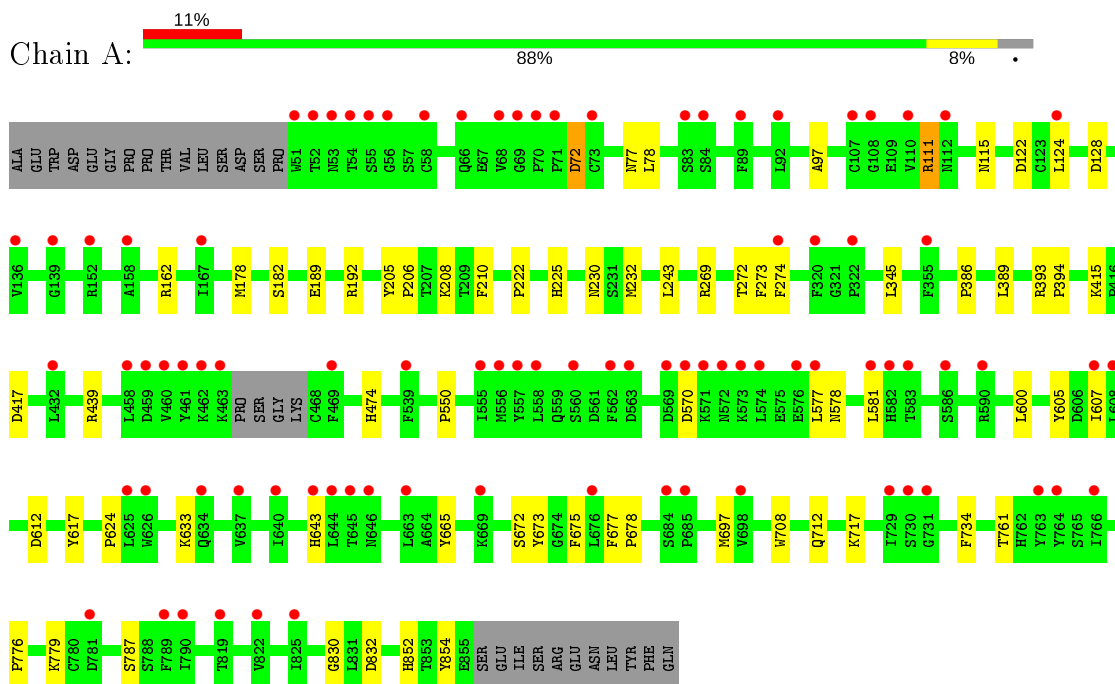
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	423	Total 423	O 423	0	0

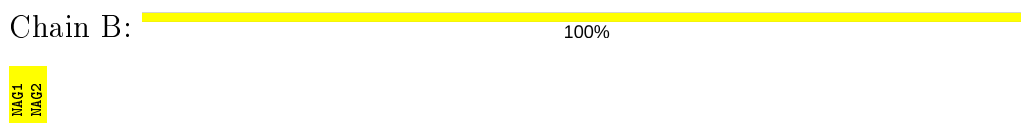
3 Residue-property plots [\(i\)](#)

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



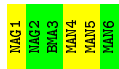
- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- 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-acetam

ido-2-deoxy-beta-D-glucopyranose

Chain C:  50% 50%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	61.51Å 94.02Å 75.45Å 90.00° 94.52° 90.00°	Depositor
Resolution (Å)	33.24 – 1.80 33.25 – 1.80	Depositor EDS
% Data completeness (in resolution range)	97.1 (33.24-1.80) 97.1 (33.25-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.07 (at 1.79Å)	Xtrriage
Refinement program	PHENIX 1.7.2_869	Depositor
R, R_{free}	0.188 , 0.223 0.183 , 0.218	Depositor DCC
R_{free} test set	3882 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	25.6	Xtrriage
Anisotropy	0.128	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 49.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7096	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.68% 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, DWV, NAG, NA, K, 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	0.38	0/6629	0.54	0/9007

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	6435	0	6134	42	0
2	B	28	0	25	0	0
2	D	28	0	25	1	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
7	A	1	0	0	0	0
8	A	6	0	0	0	0
9	A	72	0	108	6	0
10	A	5	0	0	0	0
11	A	22	0	15	1	0
12	A	423	0	0	1	0
All	All	7096	0	6368	43	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 (43) 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:675:PHE:H	9:A:920:EDO:H11	1.55	0.72
1:A:678:PRO:HB3	1:A:712:GLN:HB3	1.80	0.63
1:A:633:LYS:O	1:A:717:LYS:NZ	2.31	0.63
1:A:178:MET:HE2	1:A:192:ARG:HD3	1.82	0.62
1:A:78:LEU:HD21	1:A:274:PHE:HB2	1.80	0.62
1:A:111:ARG:NH1	1:A:122:ASP:OD1	2.36	0.58
1:A:570:ASP:HB2	1:A:643:HIS:CD2	2.38	0.57
1:A:222:PRO:HA	1:A:225:HIS:CE1	2.41	0.56
1:A:570:ASP:HB2	1:A:643:HIS:HD2	1.70	0.55
1:A:550:PRO:HB2	1:A:607:ILE:HG12	1.91	0.52
1:A:612:ASP:HB3	1:A:677:PHE:CZ	2.44	0.52
1:A:761:THR:HA	9:A:923:EDO:H12	1.92	0.52
1:A:230:ASN:HB3	1:A:243:LEU:HG	1.91	0.51
1:A:210:PHE:CE1	1:A:243:LEU:HD23	2.46	0.50
1:A:439:ARG:CZ	9:A:932:EDO:H21	2.43	0.48
1:A:617:TYR:HA	1:A:624:PRO:HA	1.95	0.48
1:A:600:LEU:HD11	1:A:832:ASP:HB2	1.96	0.48
1:A:97:ALA:HB3	1:A:115:ASN:HA	1.96	0.47
1:A:111:ARG:NH2	1:A:128:ASP:OD1	2.48	0.47
12:A:1320:HOH:O	2:D:2:NAG:H2	2.16	0.46
1:A:550:PRO:HB3	1:A:605:TYR:CZ	2.50	0.46
1:A:208:LYS:HE2	1:A:474:HIS:O	2.16	0.46
1:A:852:HIS:HD2	1:A:854:TYR:CZ	2.34	0.45
1:A:210:PHE:HE1	1:A:243:LEU:HD23	1.82	0.44
1:A:393:ARG:HB2	1:A:394:PRO:HD2	2.00	0.44
1:A:830:GLY:HA2	9:A:928:EDO:H21	1.99	0.43
1:A:578:ASN:HB3	1:A:581:LEU:HB2	2.00	0.43
1:A:734:PHE:CD1	9:A:921:EDO:H11	2.53	0.43
1:A:417:ASP:N	1:A:417:ASP:OD1	2.52	0.42
1:A:77:ASN:HD21	1:A:272:THR:HB	1.85	0.42
1:A:708:TRP:O	1:A:712:GLN:HG2	2.19	0.42
1:A:665:TYR:HE2	1:A:697:MET:HE3	1.85	0.42
1:A:72:ASP:OD1	1:A:72:ASP:N	2.53	0.42
1:A:550:PRO:HB3	1:A:605:TYR:CE2	2.55	0.41
1:A:206:PRO:HB3	1:A:389:LEU:HD13	2.03	0.41
1:A:124:LEU:HD12	1:A:124:LEU:HA	1.95	0.41
1:A:672:SER:OG	1:A:673:TYR:N	2.53	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:776:PRO:HG2	1:A:779:LYS:HB2	2.02	0.41
1:A:182:SER:HB3	1:A:189:GLU:HG2	2.02	0.40
1:A:205:TYR:CD1	1:A:206:PRO:HA	2.56	0.40
1:A:415:LYS:HB3	1:A:415:LYS:HE2	1.94	0.40
1:A:787:SER:HB3	9:A:933:EDO:H11	2.03	0.40
1:A:273:PHE:O	11:A:937:DWV:H13	2.22	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	800/831 (96%)	775 (97%)	24 (3%)	1 (0%)	51 36

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	718/756 (95%)	711 (99%)	7 (1%)	76 71

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	ASP
1	A	111	ARG
1	A	162	ARG
1	A	232	MET
1	A	269	ARG
1	A	345	LEU
1	A	577	LEU

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	643	HIS

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	0.50	0	17,19,21	0.95	1 (5%)
2	NAG	B	2	2	14,14,15	0.58	0	17,19,21	0.93	1 (5%)
3	NAG	C	1	1,3	14,14,15	0.59	0	17,19,21	1.40	1 (5%)
3	NAG	C	2	3	14,14,15	0.59	0	17,19,21	0.71	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BMA	C	3	3	11,11,12	0.66	0	15,15,17	0.69	0
3	MAN	C	4	3	11,11,12	0.53	0	15,15,17	1.02	1 (6%)
3	MAN	C	5	3	11,11,12	0.59	0	15,15,17	0.84	1 (6%)
3	MAN	C	6	3	11,11,12	0.60	0	15,15,17	0.87	0
2	NAG	D	1	1,2	14,14,15	0.63	0	17,19,21	0.95	0
2	NAG	D	2	2	14,14,15	0.58	0	17,19,21	1.85	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	-	2/6/23/26	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	-	1/2/19/22	0/1/1/1
3	MAN	C	4	3	-	0/2/19/22	0/1/1/1
3	MAN	C	5	3	-	2/2/19/22	0/1/1/1
3	MAN	C	6	3	-	1/2/19/22	0/1/1/1
2	NAG	D	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2	NAG	C1-O5-C5	6.74	121.32	112.19
3	C	1	NAG	O5-C1-C2	-4.41	104.32	111.29
2	B	1	NAG	C1-O5-C5	2.93	116.16	112.19
3	C	4	MAN	O5-C5-C6	2.68	111.40	107.20
2	D	2	NAG	O5-C1-C2	2.52	115.26	111.29
2	B	2	NAG	C1-O5-C5	2.11	115.05	112.19
3	C	5	MAN	O5-C5-C6	2.00	110.34	107.20

There are no chirality outliers.

All (12) torsion outliers are listed below:

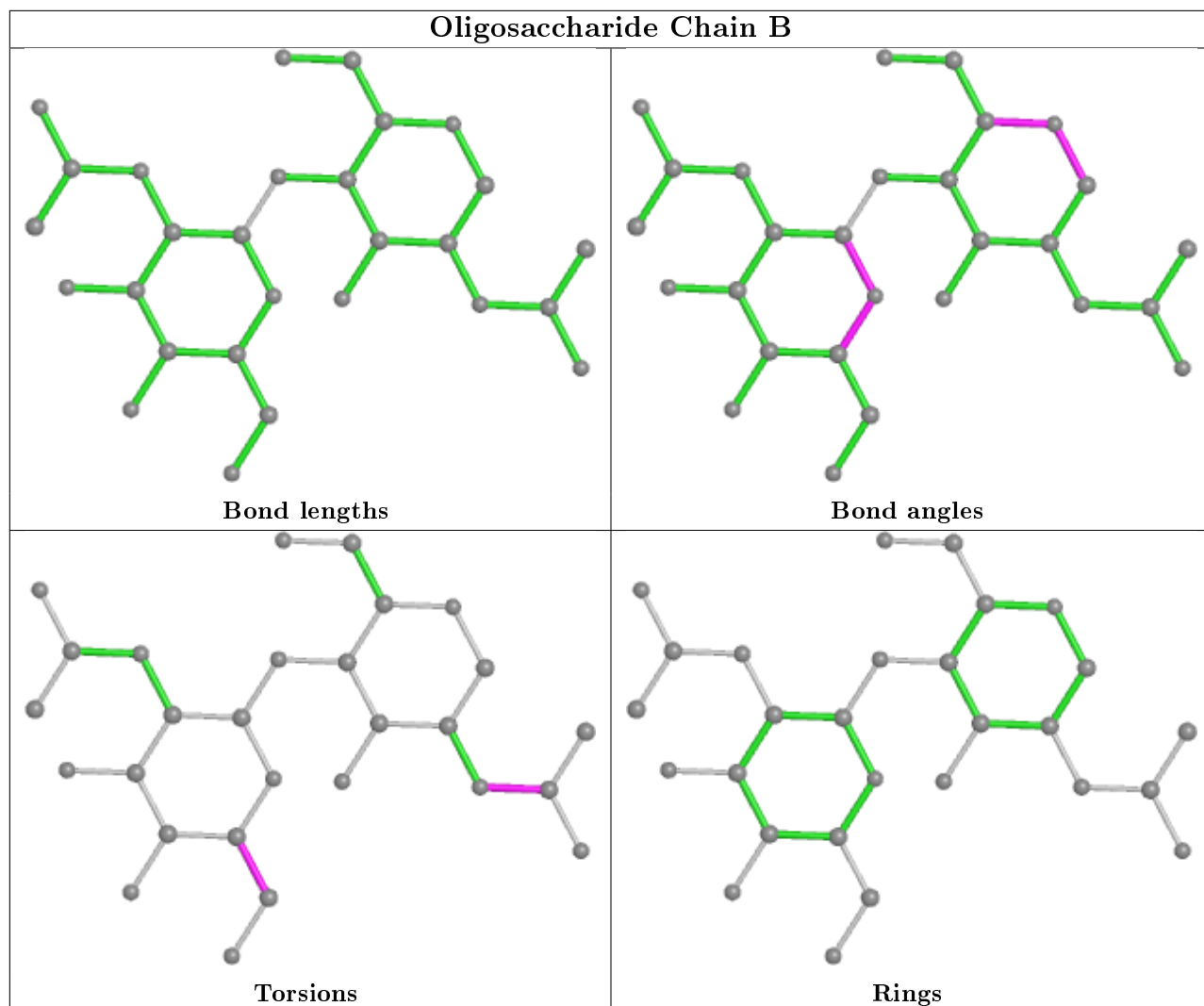
Mol	Chain	Res	Type	Atoms
2	B	1	NAG	C8-C7-N2-C2
2	B	1	NAG	O7-C7-N2-C2
2	D	2	NAG	O5-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
3	C	5	MAN	C4-C5-C6-O6
3	C	5	MAN	O5-C5-C6-O6
2	D	2	NAG	C8-C7-N2-C2
3	C	3	BMA	O5-C5-C6-O6
2	D	2	NAG	O7-C7-N2-C2
2	B	2	NAG	C4-C5-C6-O6
2	B	2	NAG	O5-C5-C6-O6
3	C	6	MAN	C4-C5-C6-O6

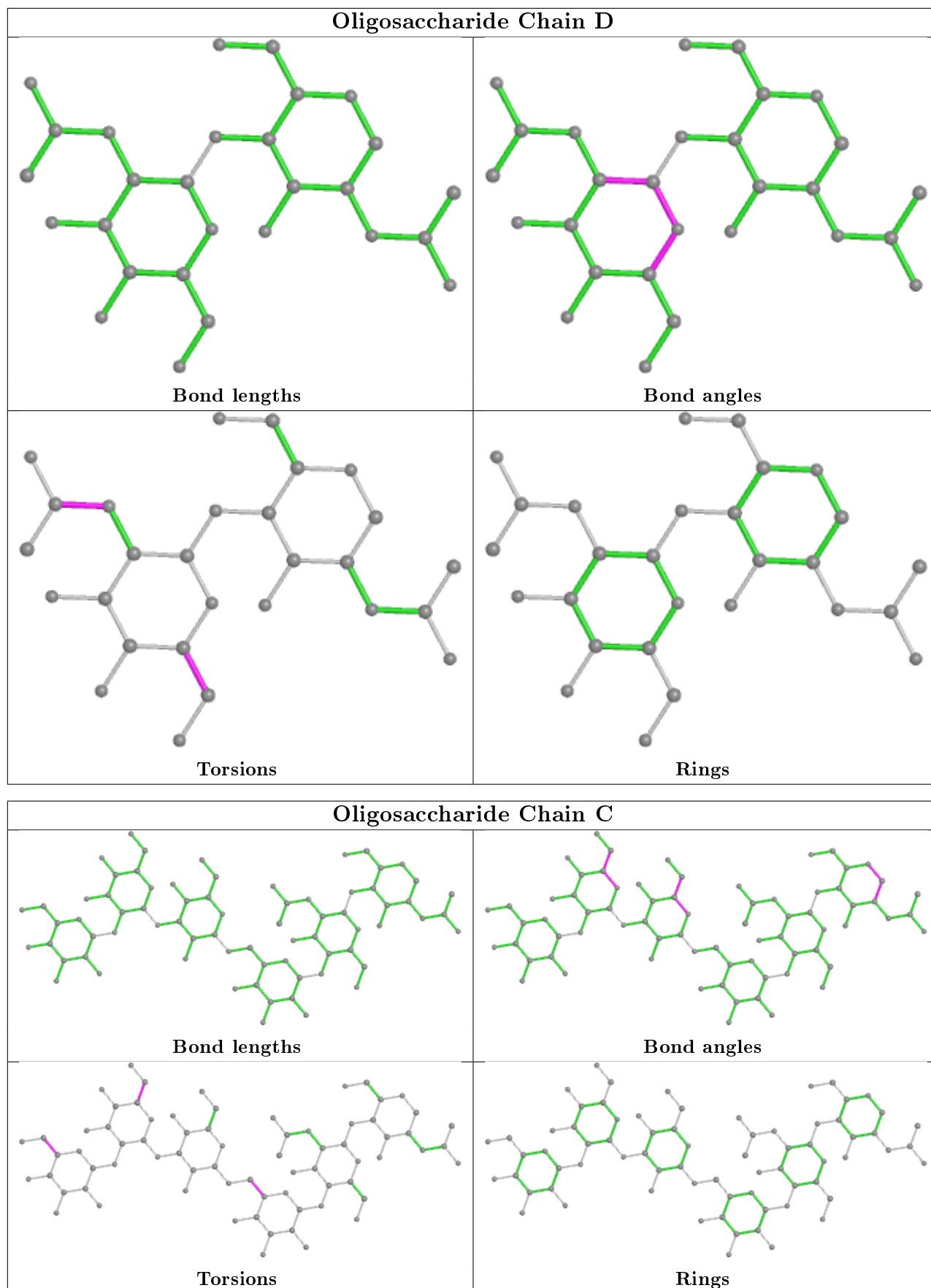
There are no ring outliers.

1 monomer is involved in 1 short contact:

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

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





5.6 Ligand geometry [i](#)

Of 27 ligands modelled in this entry, 5 are monoatomic - leaving 22 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	931	-	3,3,3	0.45	0	2,2,2	0.27	0
9	EDO	A	926	-	3,3,3	0.45	0	2,2,2	0.26	0
9	EDO	A	930	-	3,3,3	0.55	0	2,2,2	0.24	0
9	EDO	A	929	-	3,3,3	0.47	0	2,2,2	0.39	0
9	EDO	A	933	-	3,3,3	0.50	0	2,2,2	0.28	0
9	EDO	A	921	-	3,3,3	0.51	0	2,2,2	0.42	0
9	EDO	A	924	-	3,3,3	0.49	0	2,2,2	0.52	0
9	EDO	A	932	-	3,3,3	0.41	0	2,2,2	0.39	0
9	EDO	A	928	-	3,3,3	0.48	0	2,2,2	0.30	0
9	EDO	A	934	-	3,3,3	0.48	0	2,2,2	0.59	0
9	EDO	A	918	-	3,3,3	0.50	0	2,2,2	0.39	0
9	EDO	A	919	-	3,3,3	0.57	0	2,2,2	0.12	0
9	EDO	A	922	-	3,3,3	0.57	0	2,2,2	0.12	0
10	SO4	A	936	4	4,4,4	0.28	0	6,6,6	0.41	0
9	EDO	A	935	-	3,3,3	0.49	0	2,2,2	0.28	0
9	EDO	A	923	-	3,3,3	0.45	0	2,2,2	0.47	0
9	EDO	A	920	-	3,3,3	0.28	0	2,2,2	0.53	0
8	SCN	A	916	-	1,2,2	0.90	0	0,1,1	0.00	-
9	EDO	A	925	-	3,3,3	0.47	0	2,2,2	0.13	0
8	SCN	A	917	-	1,2,2	1.04	0	0,1,1	0.00	-
9	EDO	A	927	-	3,3,3	0.47	0	2,2,2	0.42	0
11	DWV	A	937	-	24,24,24	4.75	12 (50%)	34,34,34	3.51	13 (38%)

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	921	-	-	0/1/1/1	-
9	EDO	A	922	-	-	0/1/1/1	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	EDO	A	931	-	-	1/1/1/1	-
9	EDO	A	930	-	-	0/1/1/1	-
9	EDO	A	935	-	-	0/1/1/1	-
9	EDO	A	926	-	-	0/1/1/1	-
9	EDO	A	925	-	-	0/1/1/1	-
9	EDO	A	928	-	-	0/1/1/1	-
9	EDO	A	923	-	-	0/1/1/1	-
9	EDO	A	929	-	-	0/1/1/1	-
9	EDO	A	919	-	-	0/1/1/1	-
9	EDO	A	934	-	-	1/1/1/1	-
9	EDO	A	918	-	-	0/1/1/1	-
9	EDO	A	920	-	-	0/1/1/1	-
9	EDO	A	932	-	-	0/1/1/1	-
9	EDO	A	924	-	-	0/1/1/1	-
11	DWV	A	937	-	-	2/8/30/30	0/3/3/3
9	EDO	A	933	-	-	0/1/1/1	-
9	EDO	A	927	-	-	1/1/1/1	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	937	DWV	CAE-CAT	18.51	1.55	1.34
11	A	937	DWV	OAB-CAS	9.49	1.39	1.23
11	A	937	DWV	CAO-CAE	4.47	1.55	1.46
11	A	937	DWV	CAR-NAV	3.99	1.44	1.34
11	A	937	DWV	CAS-CAT	-3.71	1.45	1.50
11	A	937	DWV	CAH-CAO	3.56	1.45	1.39
11	A	937	DWV	CAH-CAQ	-2.99	1.33	1.38
11	A	937	DWV	CAR-NAM	2.47	1.37	1.31
11	A	937	DWV	CAF-CAG	-2.26	1.34	1.38
11	A	937	DWV	CAL-NAV	-2.18	1.43	1.47
11	A	937	DWV	CAA-NAU	-2.18	1.41	1.46
11	A	937	DWV	CAG-CAP	2.14	1.43	1.38

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	937	DWV	CAO-CAE-CAT	-8.76	118.96	130.94
11	A	937	DWV	CAS-CAT-SAN	-8.72	104.31	109.12
11	A	937	DWV	SAN-CAR-NAV	7.17	129.63	120.36
11	A	937	DWV	SAN-CAR-NAM	-6.88	106.46	116.31
11	A	937	DWV	CAA-NAU-CAI	5.80	119.34	110.66

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	937	DWV	CAA-NAU-CAJ	5.33	118.63	110.66
11	A	937	DWV	CAR-SAN-CAT	5.30	98.02	90.75
11	A	937	DWV	CAT-CAS-NAM	4.19	115.75	113.56
11	A	937	DWV	CAL-NAV-CAK	4.13	120.57	112.62
11	A	937	DWV	CAE-CAT-SAN	3.03	133.10	129.22
11	A	937	DWV	CAI-CAK-NAV	2.59	115.98	110.44
11	A	937	DWV	CAR-NAM-CAS	2.51	115.46	110.64
11	A	937	DWV	CAK-NAV-CAR	-2.06	116.89	122.03

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	A	937	DWV	CAT-CAE-CAO-CAH
11	A	937	DWV	CAT-CAE-CAO-CAF
9	A	927	EDO	O1-C1-C2-O2
9	A	931	EDO	O1-C1-C2-O2
9	A	934	EDO	O1-C1-C2-O2

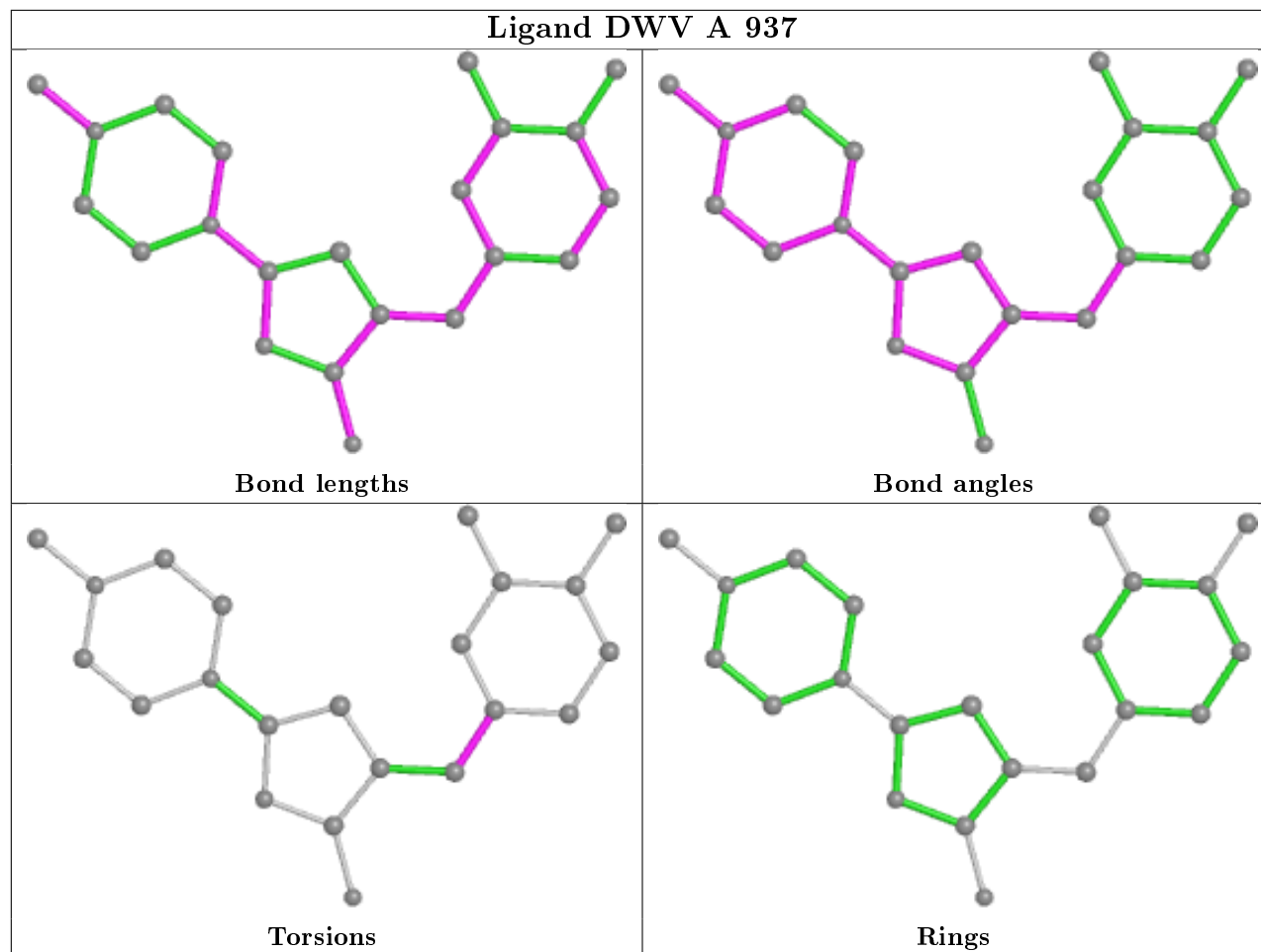
There are no ring outliers.

7 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	933	EDO	1	0
9	A	921	EDO	1	0
9	A	932	EDO	1	0
9	A	928	EDO	1	0
9	A	923	EDO	1	0
9	A	920	EDO	1	0
11	A	937	DWV	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	801/831 (96%)	0.61	89 (11%) 5 4	15, 33, 60, 81	0

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	460	VAL	7.3
1	A	461	TYR	7.2
1	A	70	PRO	6.7
1	A	51	TRP	6.5
1	A	574	LEU	6.2
1	A	71	PRO	5.6
1	A	55	SER	5.2
1	A	110	VAL	5.0
1	A	69	GLY	4.5
1	A	320	PHE	4.4
1	A	685	PRO	4.4
1	A	583	THR	4.4
1	A	569	ASP	4.2
1	A	469	PHE	4.1
1	A	572	ASN	4.1
1	A	66	GLN	4.0
1	A	52	THR	3.9
1	A	83	SER	3.9
1	A	676	LEU	3.8
1	A	637	VAL	3.7
1	A	54	THR	3.7
1	A	644	LEU	3.4
1	A	764	TYR	3.4
1	A	555	ILE	3.3
1	A	729	ILE	3.3
1	A	68	VAL	3.3
1	A	108	GLY	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	167	ILE	3.3
1	A	124	LEU	3.3
1	A	766	ILE	3.3
1	A	577	LEU	3.2
1	A	463	LYS	3.2
1	A	663	LEU	3.2
1	A	560	SER	3.1
1	A	556	MET	3.0
1	A	84	SER	3.0
1	A	669	LYS	3.0
1	A	73	CYS	3.0
1	A	731	GLY	3.0
1	A	571	LYS	2.9
1	A	562	PHE	2.9
1	A	136	VAL	2.9
1	A	581	LEU	2.9
1	A	58	CYS	2.8
1	A	539	PHE	2.8
1	A	626	TRP	2.8
1	A	573	LYS	2.8
1	A	789	PHE	2.7
1	A	645	THR	2.7
1	A	790	ILE	2.7
1	A	825	ILE	2.7
1	A	112	ASN	2.7
1	A	152	ARG	2.6
1	A	56	GLY	2.5
1	A	590	ARG	2.5
1	A	89	PHE	2.5
1	A	570	ASP	2.5
1	A	53	ASN	2.5
1	A	730	SER	2.5
1	A	563	ASP	2.5
1	A	557	TYR	2.5
1	A	625	LEU	2.5
1	A	763	TYR	2.4
1	A	158	ALA	2.4
1	A	684	SER	2.4
1	A	634	GLN	2.4
1	A	640	ILE	2.4
1	A	92	LEU	2.4
1	A	139	GLY	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	646	ASN	2.4
1	A	582	HIS	2.4
1	A	608	LEU	2.3
1	A	822	VAL	2.3
1	A	322	PRO	2.3
1	A	274	PHE	2.3
1	A	643	HIS	2.2
1	A	458	LEU	2.2
1	A	558	LEU	2.2
1	A	462	LYS	2.2
1	A	107	CYS	2.2
1	A	698	VAL	2.1
1	A	432	LEU	2.1
1	A	607	ILE	2.1
1	A	355	PHE	2.1
1	A	576	GLU	2.1
1	A	781	ASP	2.0
1	A	586	SER	2.0
1	A	459	ASP	2.0
1	A	819	THR	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.

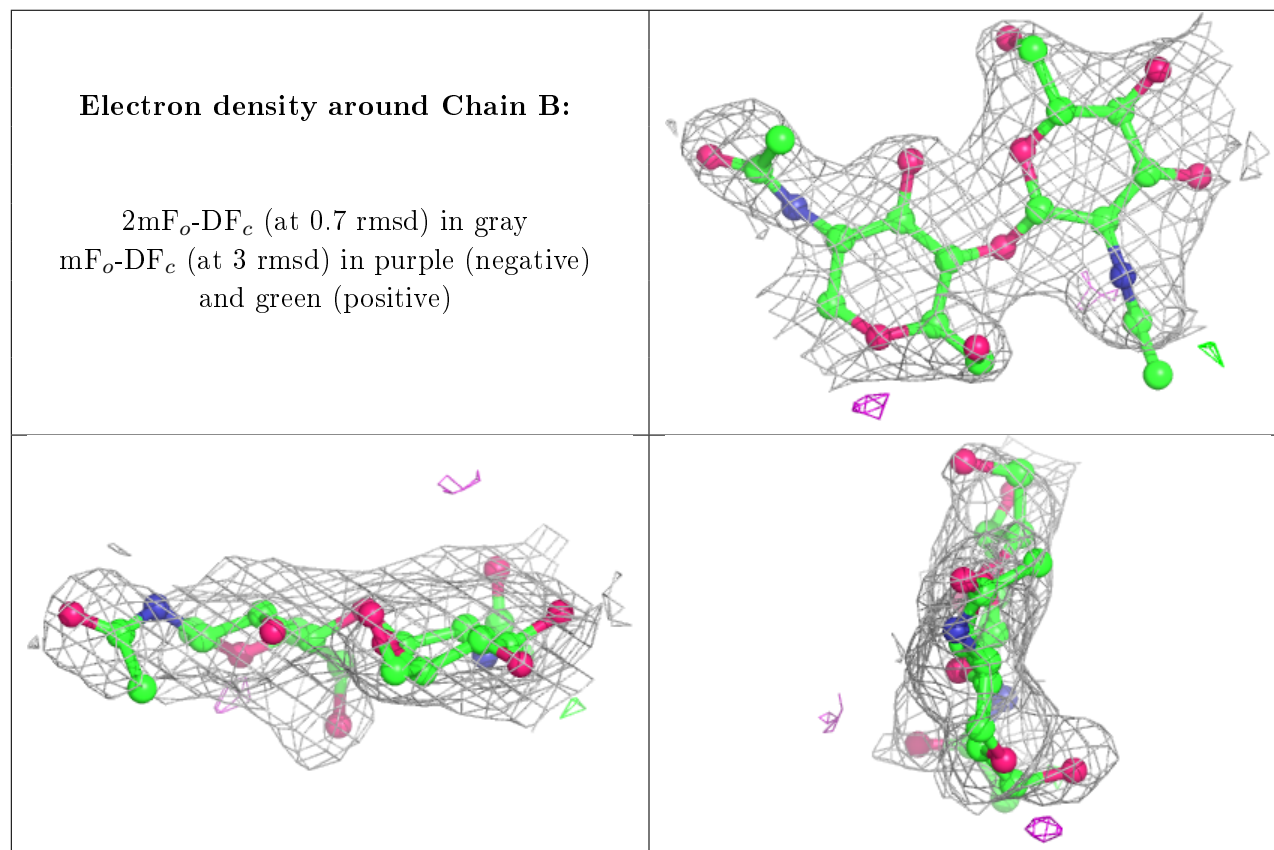
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	B	1	14/15	0.84	0.29	64,68,71,72	0
2	NAG	D	2	14/15	0.86	0.25	47,59,63,64	0
3	BMA	C	3	11/12	0.87	0.18	41,48,54,55	0
2	NAG	B	2	14/15	0.89	0.23	68,74,78,79	0
3	MAN	C	4	11/12	0.91	0.22	37,41,49,50	0
3	MAN	C	5	11/12	0.91	0.28	37,42,50,55	0
2	NAG	D	1	14/15	0.93	0.09	26,34,41,46	0
3	MAN	C	6	11/12	0.94	0.17	27,35,39,40	0

Continued on next page...

Continued from previous page...

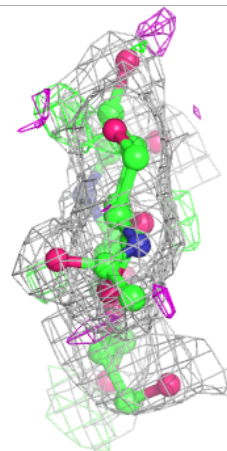
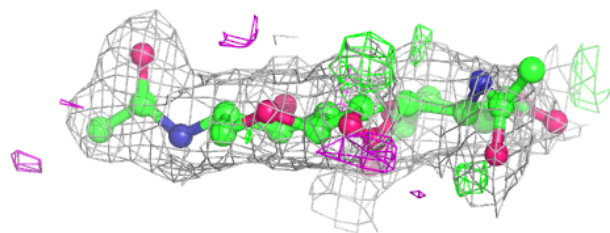
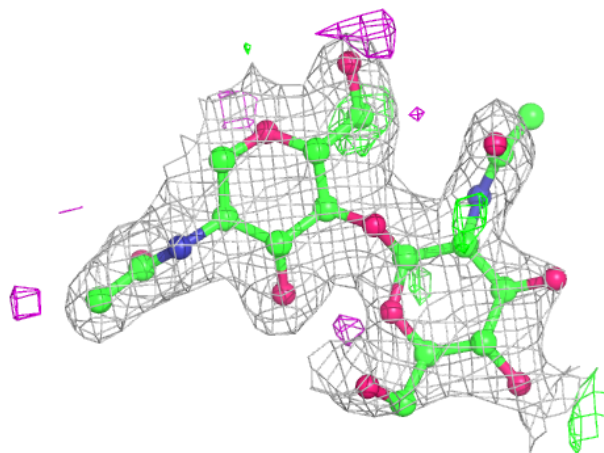
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NAG	C	2	14/15	0.96	0.07	25,32,39,44	0
3	NAG	C	1	14/15	0.97	0.07	18,21,26,27	0

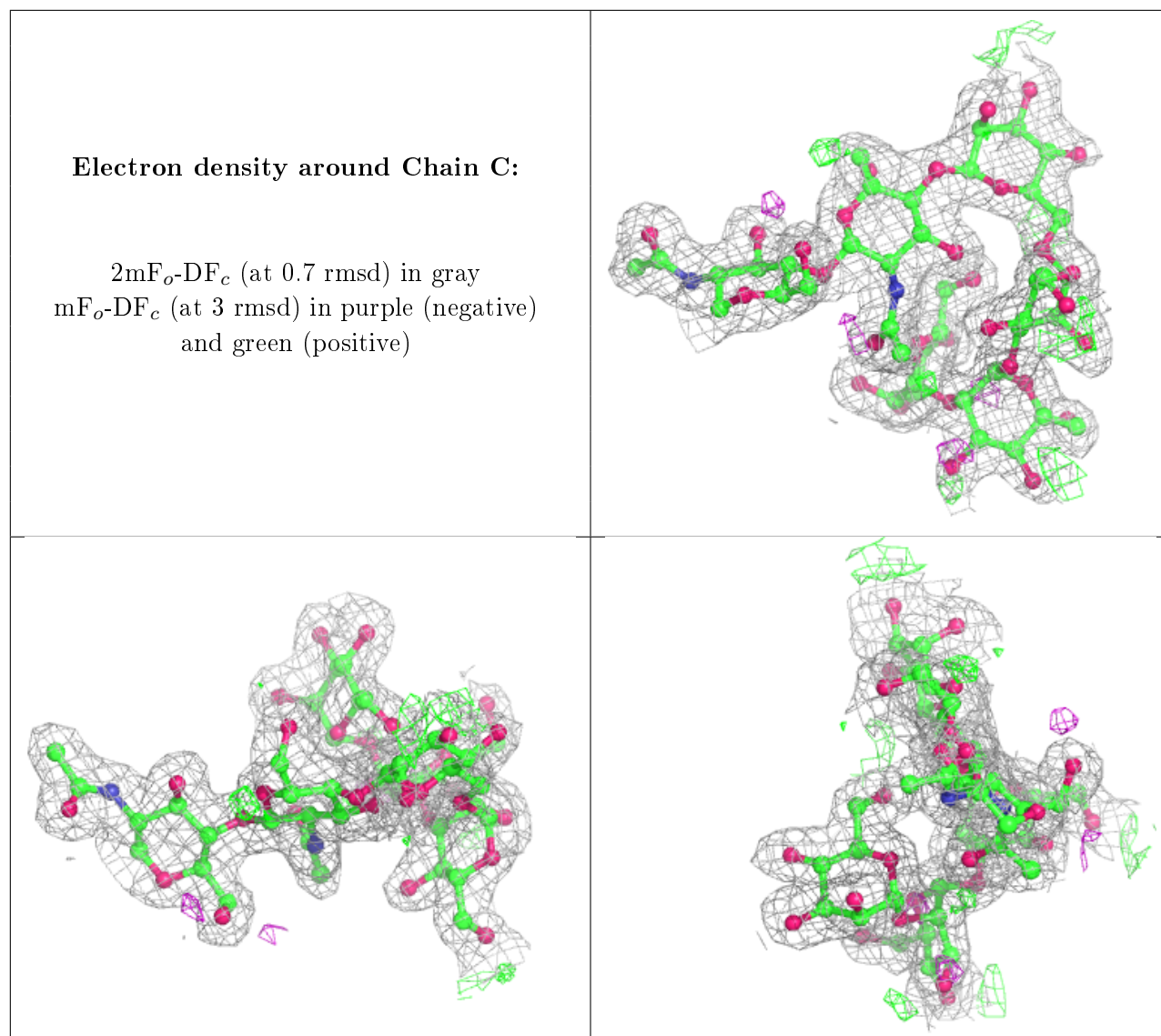
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



Electron density around Chain D:

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





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.

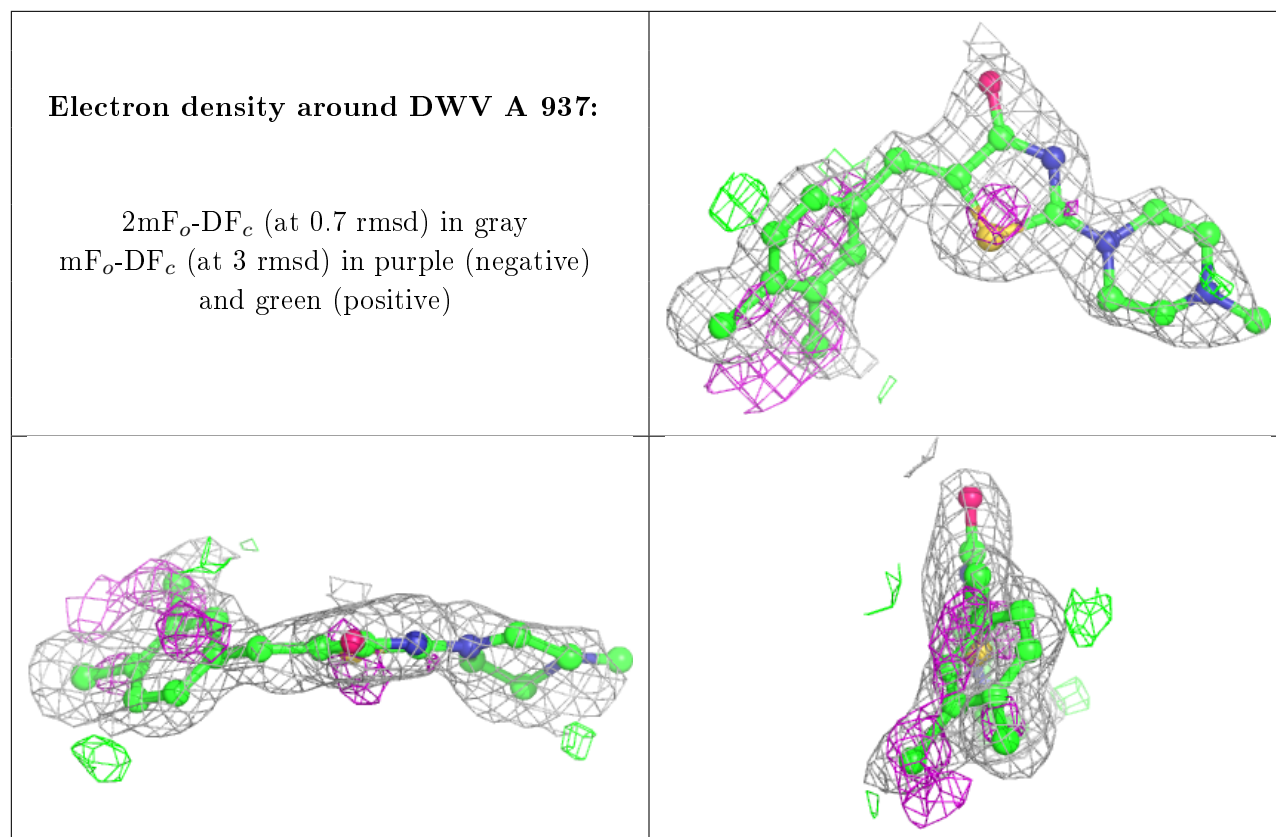
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	EDO	A	920	4/4	0.85	0.19	35,39,40,41	0
9	EDO	A	928	4/4	0.88	0.15	38,41,43,47	0
8	SCN	A	917	3/3	0.88	0.20	33,33,41,44	0
11	DWV	A	937	22/22	0.88	0.14	31,45,53,64	0
9	EDO	A	935	4/4	0.89	0.18	35,39,47,47	0
9	EDO	A	929	4/4	0.91	0.08	40,42,43,49	0
7	K	A	915	1/1	0.91	0.06	47,47,47,47	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
9	EDO	A	925	4/4	0.93	0.17	24,32,34,35	0
9	EDO	A	922	4/4	0.93	0.10	30,31,32,38	0
9	EDO	A	921	4/4	0.93	0.14	31,35,37,39	0
9	EDO	A	926	4/4	0.93	0.11	40,44,47,58	0
9	EDO	A	924	4/4	0.94	0.10	30,30,32,37	0
9	EDO	A	933	4/4	0.94	0.09	36,38,39,51	0
9	EDO	A	923	4/4	0.94	0.18	34,37,41,46	0
9	EDO	A	919	4/4	0.94	0.12	30,35,37,41	0
9	EDO	A	934	4/4	0.95	0.09	34,34,41,43	0
9	EDO	A	932	4/4	0.95	0.19	29,32,36,47	0
10	SO4	A	936	5/5	0.96	0.09	23,32,37,40	0
9	EDO	A	931	4/4	0.96	0.07	27,29,31,38	0
9	EDO	A	927	4/4	0.96	0.11	29,31,36,46	0
9	EDO	A	918	4/4	0.96	0.10	33,33,34,41	0
8	SCN	A	916	3/3	0.98	0.10	32,32,46,61	0
6	NA	A	914	1/1	0.98	0.06	30,30,30,30	0
9	EDO	A	930	4/4	0.98	0.15	23,24,24,26	0
5	CA	A	913	1/1	0.99	0.07	27,27,27,27	0
4	ZN	A	911	1/1	0.99	0.09	24,24,24,24	0
4	ZN	A	912	1/1	1.00	0.10	18,18,18,18	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.