



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 10:24 PM BST

PDB ID : 6LEH
Title : Crystal structure of Autotaxin in complex with an inhibitor
Authors : Nishimasu, H.; Osamu, N.
Deposited on : 2019-11-25
Resolution : 2.00 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

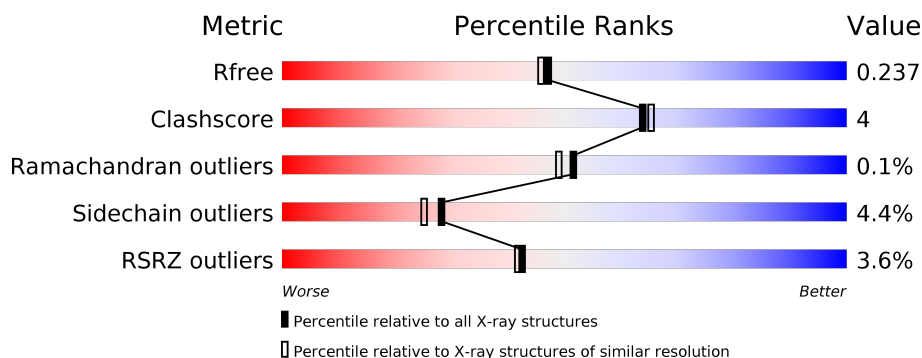
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	835	<div> <div>3%</div> <div>83%</div> <div>10%</div> <div>6%</div> </div>
2	B	6	<div> <div>17%</div> <div>83%</div> </div>
3	C	3	<div> <div>100%</div> </div>

2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 6712 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.

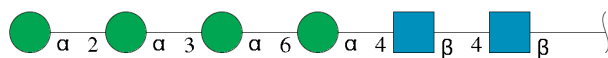
- Molecule 1 is a protein called Ectonucleotide pyrophosphatase/phosphodiesterase family member 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	783	6264	3978	1072	1166	48	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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 alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-alpha-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			
2	B	6	72	40	2	30	0	0	0

- Molecule 3 is an oligosaccharide called alpha-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	3	Total	C	N	O	0	0	0
			39	22	2	15			

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

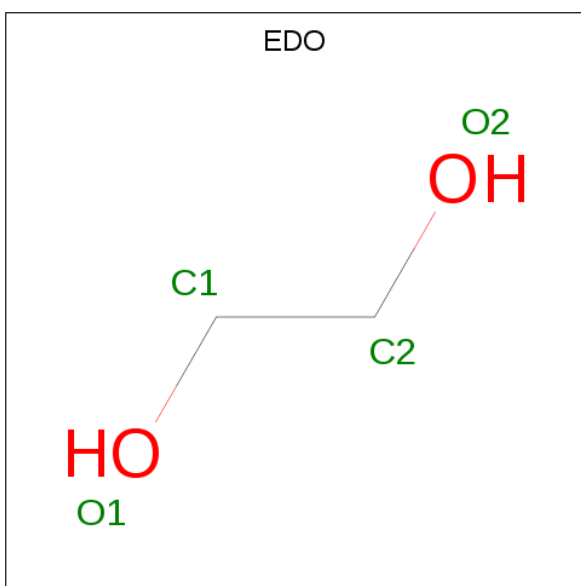


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 9 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

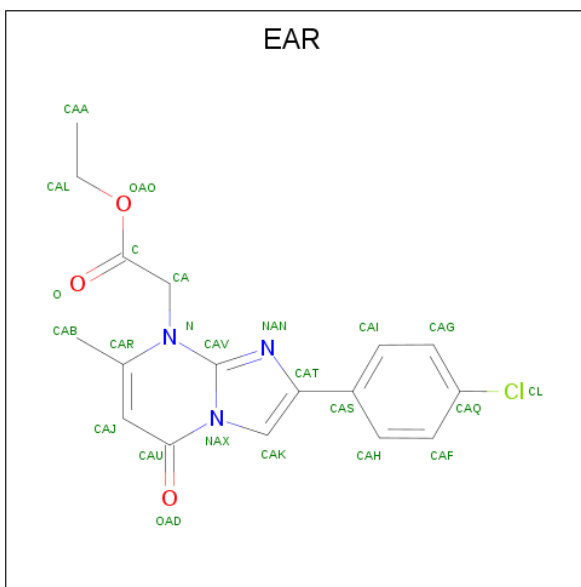
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	2	Total	Cl	0	0
			2	2		

- 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
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

- Molecule 11 is ethyl 2-[2-(4-chlorophenyl)-7-methyl-5-oxidanylidene-imidazo[1,2-a]pyrimidin-8-yl]ethanoate (three-letter code: EAR) (formula: C₁₇H₁₆ClN₃O₃) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	A	1	Total	C	Cl	N	O	0	0
			24	17	1	3	3		

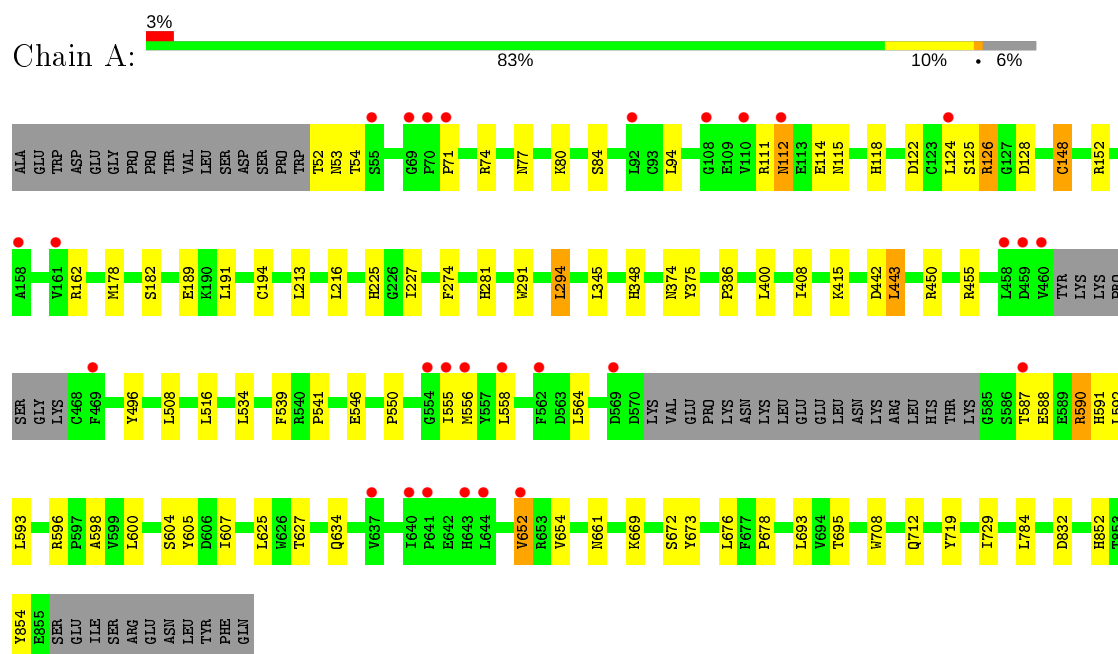
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	233	Total	O	0	0
			233	233		

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.

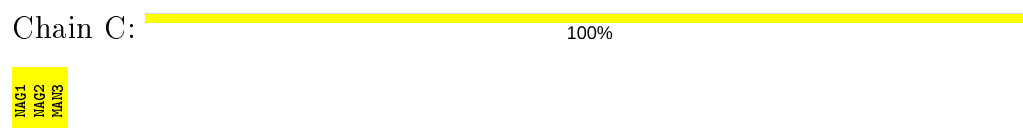
- Molecule 1: Ectonucleotide pyrophosphatase/phosphodiesterase family member 2



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



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



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 94.14Å 75.56Å 90.00° 93.92° 90.00°	Depositor
Resolution (Å)	47.07 – 2.00 47.07 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.07-2.00) 99.9 (47.07-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.14 _3260	Depositor
R, R_{free}	0.189 , 0.237 0.189 , 0.237	Depositor DCC
R_{free} test set	2807 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	35.1	Xtriage
Anisotropy	0.303	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 50.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6712	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.55% 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, NAG, CL, NA, K, EDO, SO4, EAR, 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	0.39	0/6444	0.56	0/8758

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	6264	0	5960	53	0
2	B	72	0	61	0	0
3	C	39	0	34	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	2	0	0	0	0
10	A	68	0	102	4	0
11	A	24	0	0	0	0
12	A	233	0	0	3	0
All	All	6712	0	6157	53	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 4.

All (53) 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:225:HIS:HD2	1:A:227:ILE:H	1.26	0.81
1:A:600:LEU:HD11	1:A:832:ASP:HB2	1.72	0.70
1:A:225:HIS:CD2	1:A:227:ILE:H	2.10	0.68
1:A:678:PRO:HB3	1:A:712:GLN:HB3	1.76	0.68
1:A:111:ARG:NH1	1:A:122:ASP:OD2	2.26	0.67
1:A:111:ARG:HH12	1:A:126:ARG:HD3	1.60	0.66
1:A:118:HIS:HD2	1:A:128:ASP:HB3	1.63	0.64
1:A:555:ILE:HG23	1:A:652:VAL:HG13	1.81	0.62
1:A:784:LEU:HD21	10:A:934:EDO:H21	1.80	0.62
1:A:450:ARG:NH1	12:A:1001:HOH:O	2.25	0.60
1:A:348:HIS:CD2	1:A:348:HIS:H	2.21	0.58
1:A:442:ASP:HB2	10:A:926:EDO:H12	1.87	0.56
1:A:281:HIS:ND1	12:A:1002:HOH:O	2.34	0.54
1:A:291:TRP:HA	1:A:294:LEU:HD22	1.90	0.54
1:A:148:CYS:HB2	1:A:194:CYS:SG	2.48	0.53
1:A:408:ILE:HG12	1:A:443:LEU:HD21	1.91	0.53
1:A:546:GLU:HG2	1:A:598:ALA:HB1	1.90	0.52
1:A:112:ASN:HB3	1:A:115:ASN:ND2	2.25	0.52
1:A:719:TYR:CD1	10:A:933:EDO:H22	2.44	0.52
1:A:852:HIS:HD2	1:A:854:TYR:CZ	2.28	0.51
1:A:550:PRO:HB2	1:A:607:ILE:HG12	1.93	0.50
1:A:112:ASN:ND2	1:A:114:GLU:H	2.09	0.50
1:A:654:VAL:HG21	1:A:695:THR:HG21	1.94	0.50
1:A:53:ASN:HA	1:A:71:PRO:O	2.12	0.49
1:A:672:SER:OG	1:A:673:TYR:N	2.46	0.48
1:A:539:PHE:O	1:A:541:PRO:HD3	2.14	0.48
1:A:374:ASN:ND2	12:A:1013:HOH:O	2.46	0.47
1:A:148:CYS:SG	1:A:496:TYR:HE2	2.38	0.46
1:A:587:THR:HG23	1:A:591:HIS:HD2	1.80	0.46
1:A:588:GLU:HG3	1:A:592:LEU:HD23	1.97	0.46
1:A:415:LYS:HB3	1:A:415:LYS:HE2	1.78	0.45
1:A:77:ASN:HB3	1:A:274:PHE:O	2.16	0.45
1:A:111:ARG:NH1	1:A:126:ARG:HD3	2.30	0.44
1:A:627:THR:O	1:A:729:ILE:HA	2.19	0.43
1:A:590:ARG:HG3	1:A:590:ARG:O	2.19	0.43
1:A:182:SER:HB2	1:A:189:GLU:HG2	2.00	0.42
1:A:564:LEU:HB3	1:A:661:ASN:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:HIS:H	1:A:348:HIS:HD2	1.65	0.42
1:A:508:LEU:HD23	1:A:508:LEU:HA	1.92	0.42
1:A:550:PRO:HB3	1:A:605:TYR:CE1	2.54	0.42
1:A:587:THR:HG23	1:A:591:HIS:CD2	2.55	0.42
1:A:118:HIS:CD2	1:A:128:ASP:HB3	2.50	0.42
1:A:375:TYR:OH	1:A:415:LYS:HD3	2.20	0.42
1:A:550:PRO:HB3	1:A:605:TYR:CZ	2.54	0.42
1:A:676:LEU:HA	1:A:676:LEU:HD23	1.77	0.42
1:A:555:ILE:HG23	1:A:652:VAL:CG1	2.50	0.41
1:A:213:LEU:HA	1:A:213:LEU:HD23	1.87	0.41
1:A:592:LEU:HD21	1:A:596:ARG:HB3	2.03	0.41
1:A:546:GLU:OE1	1:A:596:ARG:NH2	2.54	0.41
1:A:712:GLN:HG3	10:A:921:EDO:O2	2.21	0.40
1:A:74:ARG:HD3	1:A:84:SER:OG	2.21	0.40
1:A:112:ASN:HD22	1:A:112:ASN:C	2.25	0.40
1:A:708:TRP:O	1:A:712:GLN:HG2	2.21	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	777/835 (93%)	751 (97%)	25 (3%)	1 (0%)	51 49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	386	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	697/760 (92%)	666 (96%)	31 (4%)	28	25

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	THR
1	A	54	THR
1	A	80	LYS
1	A	94	LEU
1	A	112	ASN
1	A	124	LEU
1	A	125	SER
1	A	126	ARG
1	A	148	CYS
1	A	152	ARG
1	A	162	ARG
1	A	178	MET
1	A	191	LEU
1	A	216	LEU
1	A	294	LEU
1	A	345	LEU
1	A	400	LEU
1	A	443	LEU
1	A	455	ARG
1	A	516	LEU
1	A	534	LEU
1	A	556	MET
1	A	558	LEU
1	A	590	ARG
1	A	593	LEU
1	A	604	SER
1	A	625	LEU
1	A	634	GLN
1	A	652	VAL
1	A	669	LYS

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Mol	Chain	Res	Type
1	A	693	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	ASN
1	A	118	HIS
1	A	134	GLN
1	A	225	HIS
1	A	257	GLN
1	A	337	GLN
1	A	348	HIS
1	A	374	ASN
1	A	481	ASN
1	A	667	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

9 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	B	1	1,2	14,14,15	0.24	0	17,19,21	0.82	0
2	NAG	B	2	2	14,14,15	0.86	1 (7%)	17,19,21	0.86	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MAN	B	3	2	11,11,12	0.92	0	15,15,17	1.07	1 (6%)
2	MAN	B	4	2	11,11,12	1.33	1 (9%)	15,15,17	1.35	1 (6%)
2	MAN	B	5	2	11,11,12	1.08	0	15,15,17	1.20	2 (13%)
2	MAN	B	6	2	11,11,12	0.82	0	15,15,17	1.35	2 (13%)
3	NAG	C	1	1,3	14,14,15	0.66	1 (7%)	17,19,21	0.50	0
3	NAG	C	2	3	14,14,15	0.72	0	17,19,21	1.56	3 (17%)
3	MAN	C	3	3	11,11,12	1.28	1 (9%)	15,15,17	1.46	3 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	2	2	-	0/6/23/26	0/1/1/1
2	MAN	B	3	2	-	0/2/19/22	1/1/1/1
2	MAN	B	4	2	-	0/2/19/22	0/1/1/1
2	MAN	B	5	2	-	0/2/19/22	0/1/1/1
2	MAN	B	6	2	-	0/2/19/22	0/1/1/1
3	NAG	C	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	2/6/23/26	0/1/1/1
3	MAN	C	3	3	-	1/2/19/22	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	3	MAN	O5-C5	3.22	1.50	1.43
2	B	2	NAG	O5-C1	-3.07	1.38	1.43
2	B	4	MAN	C1-C2	2.87	1.58	1.52
3	C	1	NAG	O5-C1	-2.29	1.40	1.43

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2	NAG	C1-O5-C5	4.46	118.23	112.19
2	B	4	MAN	C1-O5-C5	3.89	117.46	112.19
3	C	3	MAN	C1-O5-C5	3.31	116.68	112.19
2	B	6	MAN	C1-O5-C5	3.27	116.62	112.19
2	B	5	MAN	O2-C2-C3	-3.07	104.00	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	NAG	O4-C4-C5	-3.05	101.72	109.30
2	B	6	MAN	O2-C2-C3	-2.88	104.36	110.14
3	C	3	MAN	C1-C2-C3	-2.72	106.33	109.67
3	C	2	NAG	O4-C4-C5	2.53	115.57	109.30
2	B	3	MAN	C1-O5-C5	2.39	115.43	112.19
3	C	2	NAG	O4-C4-C3	2.38	115.85	110.35
3	C	3	MAN	O2-C2-C3	-2.25	105.63	110.14
2	B	5	MAN	C1-O5-C5	2.16	115.11	112.19

There are no chirality outliers.

All (3) torsion outliers are listed below:

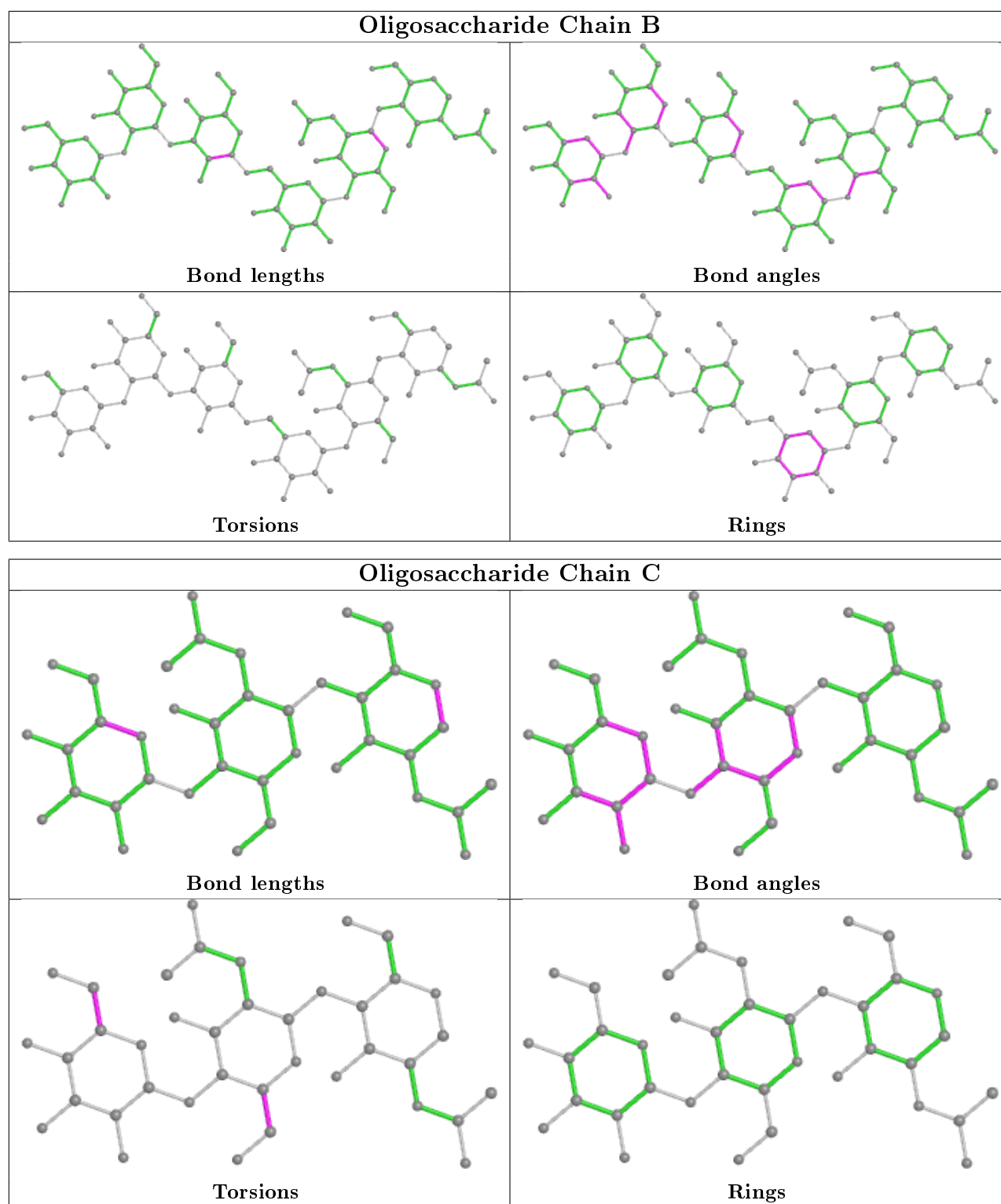
Mol	Chain	Res	Type	Atoms
3	C	2	NAG	O5-C5-C6-O6
3	C	2	NAG	C4-C5-C6-O6
3	C	3	MAN	C4-C5-C6-O6

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	3	MAN	C1-C2-C3-C4-C5-O5

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, 7 are monoatomic - leaving 19 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	931	-	3,3,3	0.51	0	2,2,2	0.37	0
10	EDO	A	924	-	3,3,3	0.43	0	2,2,2	0.73	0
10	EDO	A	928	-	3,3,3	0.45	0	2,2,2	0.41	0
10	EDO	A	932	-	3,3,3	0.43	0	2,2,2	0.50	0
10	EDO	A	919	-	3,3,3	0.60	0	2,2,2	0.55	0
10	EDO	A	927	-	3,3,3	0.49	0	2,2,2	0.33	0
10	EDO	A	930	-	3,3,3	0.49	0	2,2,2	0.36	0
10	EDO	A	925	-	3,3,3	0.70	0	2,2,2	0.35	0
11	EAR	A	935	-	21,26,26	1.68	3 (14%)	25,37,37	1.29	4 (16%)
10	EDO	A	922	-	3,3,3	0.43	0	2,2,2	0.76	0
10	EDO	A	929	-	3,3,3	0.49	0	2,2,2	0.30	0
10	EDO	A	923	-	3,3,3	0.57	0	2,2,2	0.25	0
10	EDO	A	926	-	3,3,3	0.43	0	2,2,2	0.43	0
10	EDO	A	933	-	3,3,3	0.40	0	2,2,2	0.52	0
8	SO4	A	915	4	4,4,4	0.29	0	6,6,6	0.56	0
10	EDO	A	934	-	3,3,3	0.44	0	2,2,2	0.36	0
10	EDO	A	921	-	3,3,3	0.34	0	2,2,2	0.87	0
10	EDO	A	920	-	3,3,3	0.57	0	2,2,2	0.19	0
10	EDO	A	918	-	3,3,3	0.53	0	2,2,2	0.30	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	931	-	-	1/1/1/1	-
10	EDO	A	924	-	-	1/1/1/1	-
10	EDO	A	928	-	-	1/1/1/1	-
10	EDO	A	932	-	-	1/1/1/1	-
10	EDO	A	919	-	-	1/1/1/1	-
10	EDO	A	927	-	-	0/1/1/1	-
10	EDO	A	930	-	-	0/1/1/1	-
10	EDO	A	925	-	-	0/1/1/1	-
11	EAR	A	935	-	-	2/11/11/11	0/3/3/3
10	EDO	A	922	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	EDO	A	929	-	-	0/1/1/1	-
10	EDO	A	923	-	-	0/1/1/1	-
10	EDO	A	926	-	-	1/1/1/1	-
10	EDO	A	933	-	-	0/1/1/1	-
10	EDO	A	934	-	-	0/1/1/1	-
10	EDO	A	921	-	-	1/1/1/1	-
10	EDO	A	920	-	-	0/1/1/1	-
10	EDO	A	918	-	-	0/1/1/1	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	935	EAR	CAS-CAT	-5.48	1.40	1.48
11	A	935	EAR	CAV-NAN	-3.48	1.30	1.35
11	A	935	EAR	CAR-N	2.05	1.39	1.36

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	935	EAR	OAO-C-CA	3.41	118.21	109.29
11	A	935	EAR	OAO-CAL-CAA	2.29	116.84	108.42
11	A	935	EAR	CAI-CAS-CAT	-2.27	117.70	121.28
11	A	935	EAR	CAT-NAN-CAV	2.19	109.29	104.28

There are no chirality outliers.

All (10) torsion outliers are listed below:

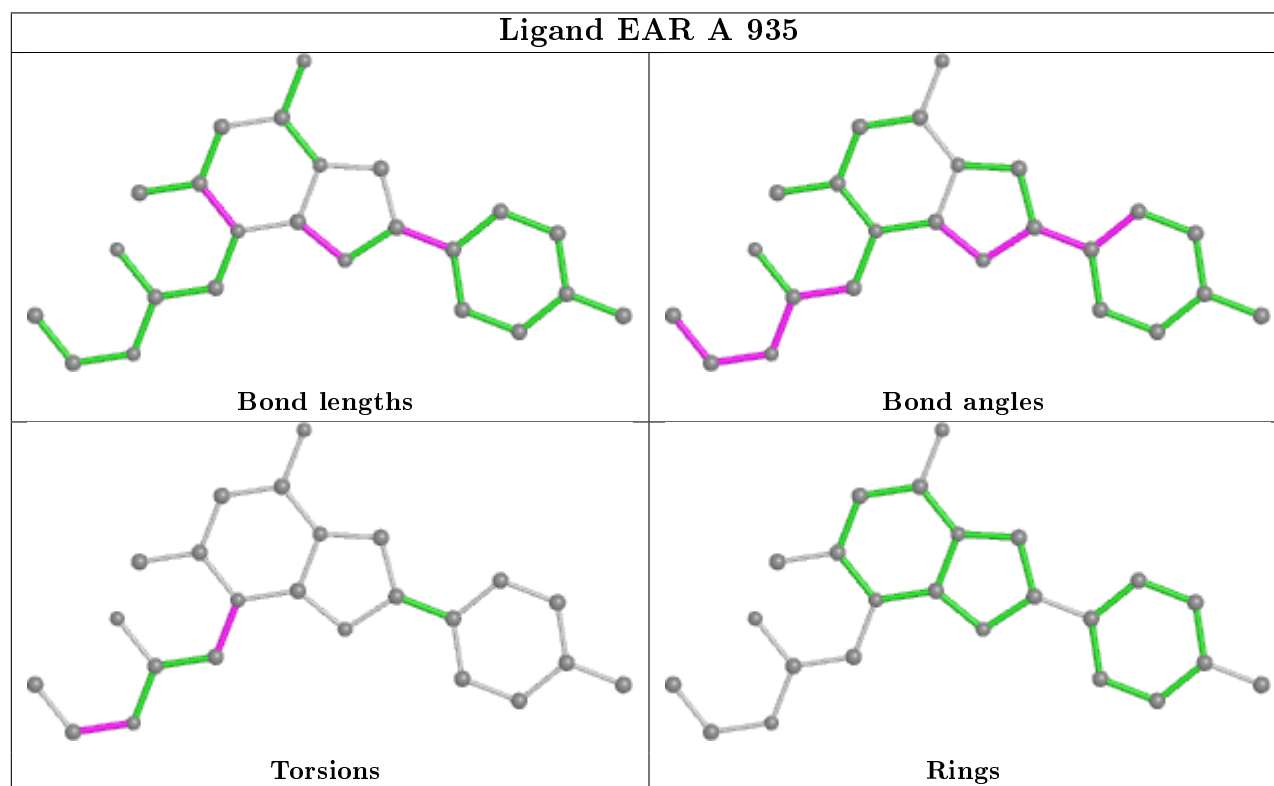
Mol	Chain	Res	Type	Atoms
11	A	935	EAR	C-CA-N-CAR
10	A	931	EDO	O1-C1-C2-O2
10	A	926	EDO	O1-C1-C2-O2
11	A	935	EAR	CAA-CAL-OAO-C
10	A	924	EDO	O1-C1-C2-O2
10	A	921	EDO	O1-C1-C2-O2
10	A	932	EDO	O1-C1-C2-O2
10	A	919	EDO	O1-C1-C2-O2
10	A	928	EDO	O1-C1-C2-O2
10	A	922	EDO	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	926	EDO	1	0
10	A	933	EDO	1	0
10	A	934	EDO	1	0
10	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

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	783/835 (93%)	0.17	28 (3%) 42 42	21, 39, 63, 80	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	460	VAL	5.9
1	A	70	PRO	4.7
1	A	556	MET	4.2
1	A	110	VAL	3.8
1	A	569	ASP	3.7
1	A	640	ILE	3.3
1	A	652	VAL	3.2
1	A	562	PHE	3.1
1	A	558	LEU	3.1
1	A	554	GLY	3.1
1	A	158	ALA	3.0
1	A	71	PRO	2.8
1	A	112	ASN	2.7
1	A	108	GLY	2.7
1	A	637	VAL	2.7
1	A	643	HIS	2.7
1	A	124	LEU	2.7
1	A	644	LEU	2.7
1	A	469	PHE	2.6
1	A	459	ASP	2.6
1	A	458	LEU	2.6
1	A	555	ILE	2.5
1	A	69	GLY	2.4
1	A	161	VAL	2.4
1	A	587	THR	2.4
1	A	55	SER	2.2
1	A	92	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	641	PRO	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](#)

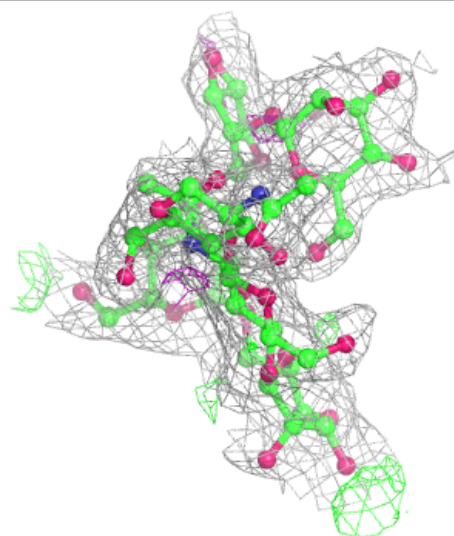
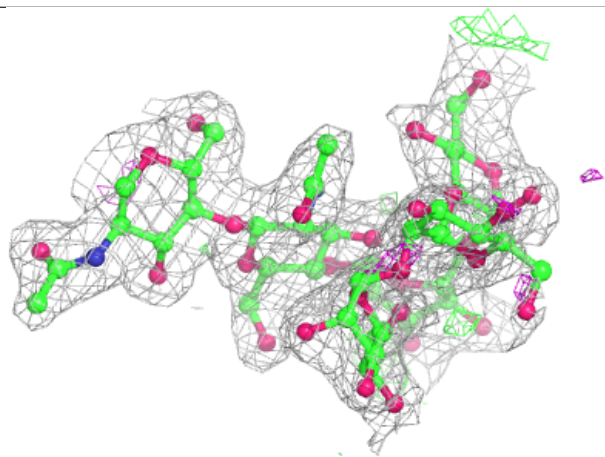
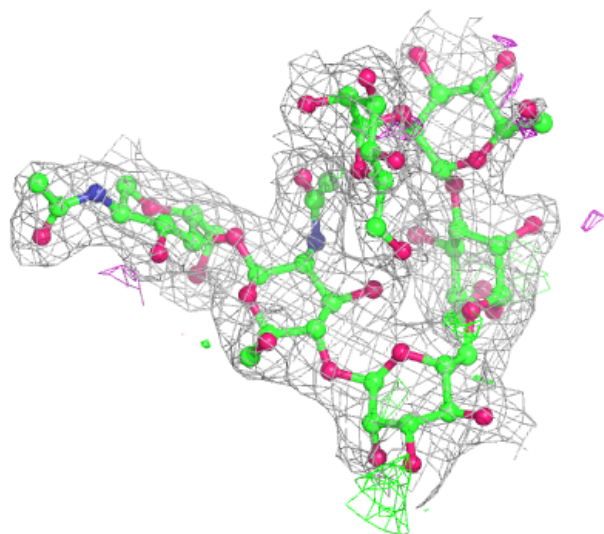
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

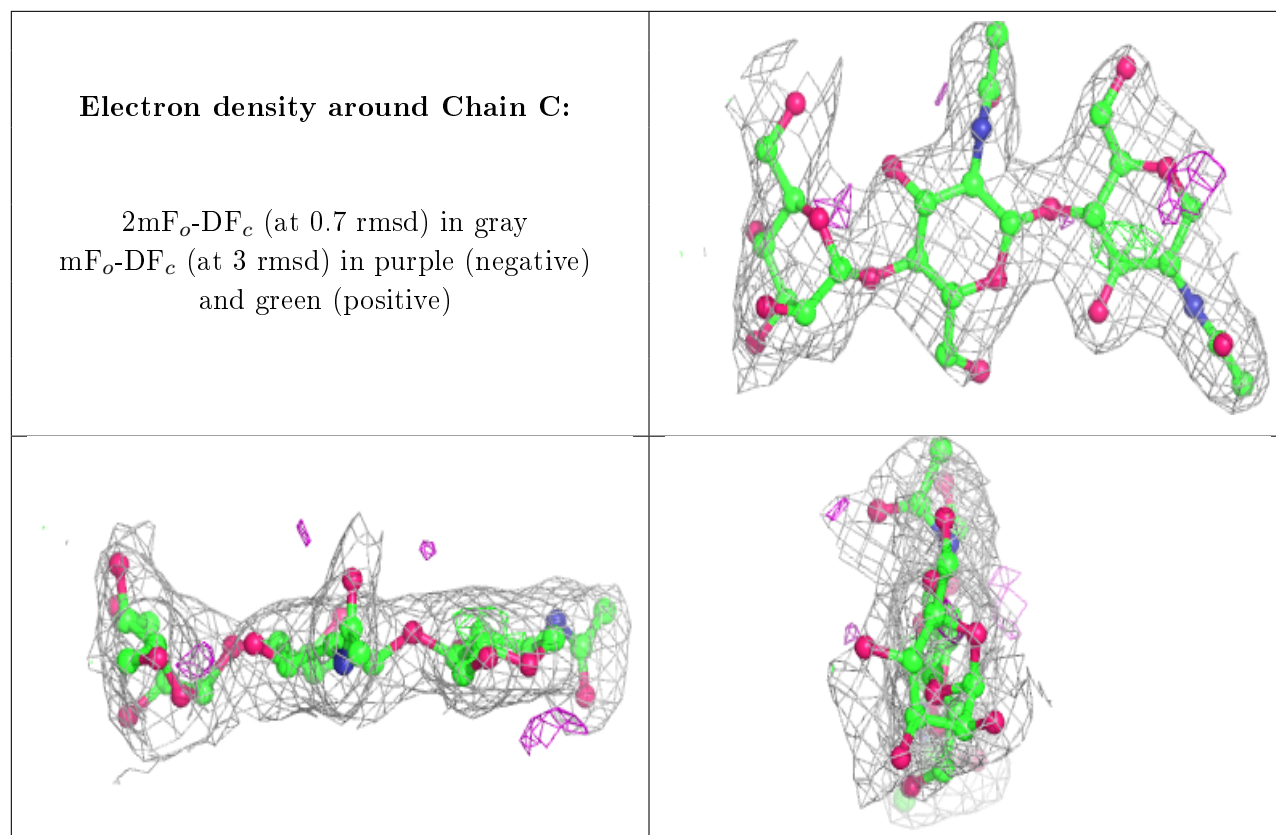
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MAN	C	3	11/12	0.59	0.21	73,80,82,83	0
3	NAG	C	2	14/15	0.80	0.19	57,64,72,76	0
2	MAN	B	3	11/12	0.83	0.11	57,58,66,66	0
2	MAN	B	4	11/12	0.85	0.12	51,55,58,58	0
2	MAN	B	5	11/12	0.85	0.24	46,51,56,57	0
2	MAN	B	6	11/12	0.93	0.12	37,44,51,55	0
2	NAG	B	2	14/15	0.95	0.09	37,44,50,55	0
3	NAG	C	1	14/15	0.96	0.12	33,38,52,53	0
2	NAG	B	1	14/15	0.98	0.12	27,31,33,36	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)





6.4 Ligands [i](#)

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

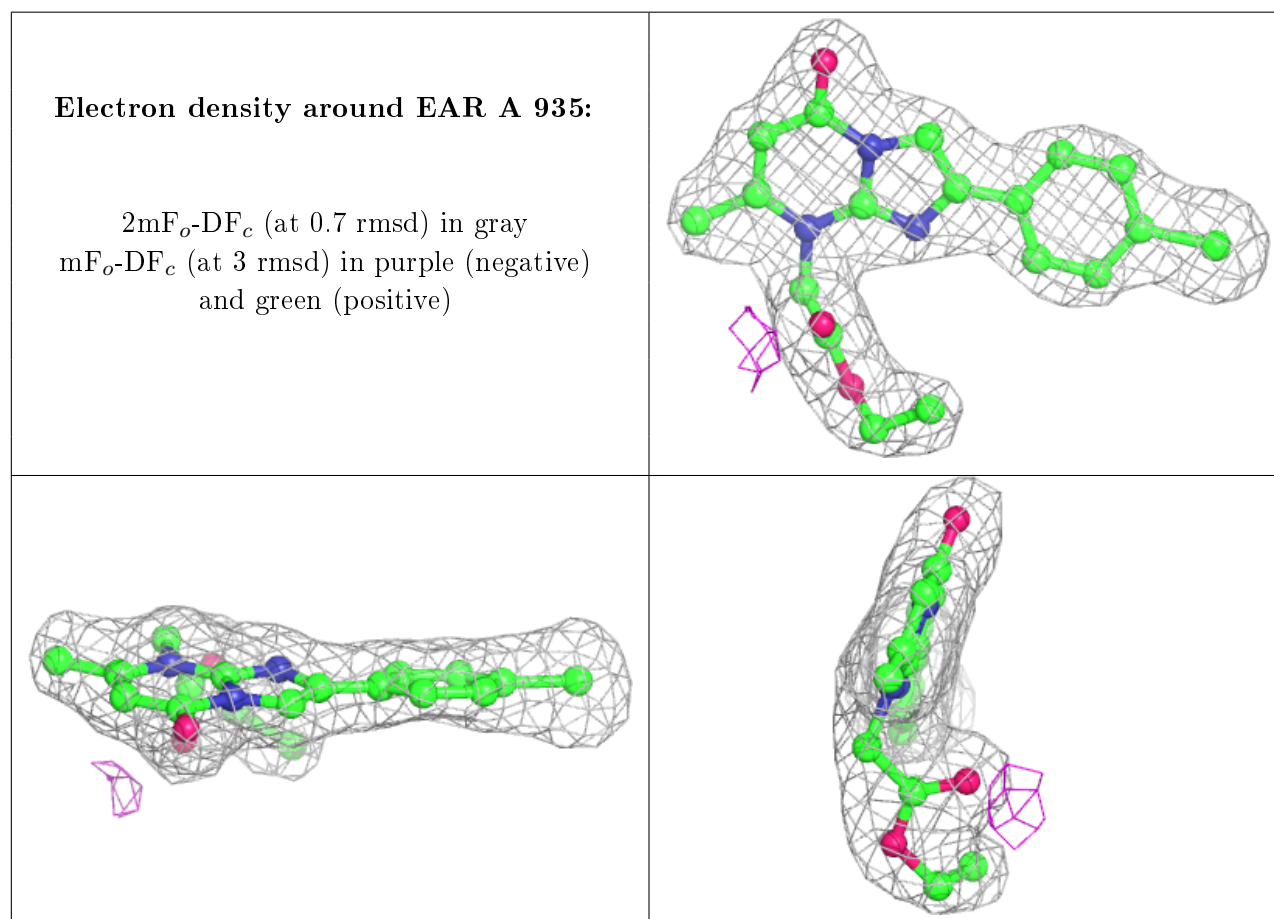
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
10	EDO	A	925	4/4	0.79	0.17	39,40,45,46	0
10	EDO	A	933	4/4	0.80	0.16	44,48,48,49	0
10	EDO	A	924	4/4	0.85	0.30	41,43,50,54	0
10	EDO	A	926	4/4	0.88	0.32	35,42,42,49	0
10	EDO	A	919	4/4	0.89	0.19	38,41,41,43	0
10	EDO	A	929	4/4	0.89	0.12	38,40,45,49	0
10	EDO	A	931	4/4	0.90	0.20	44,44,47,53	0
10	EDO	A	932	4/4	0.92	0.11	41,43,49,49	0
10	EDO	A	927	4/4	0.92	0.32	49,53,57,64	0
9	CL	A	917	1/1	0.92	0.13	49,49,49,49	0
7	K	A	914	1/1	0.93	0.07	48,48,48,48	0
10	EDO	A	921	4/4	0.94	0.21	45,48,48,51	0
10	EDO	A	934	4/4	0.94	0.10	45,48,51,52	0
10	EDO	A	928	4/4	0.95	0.20	39,42,43,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
10	EDO	A	923	4/4	0.95	0.10	40,42,42,44	0
6	NA	A	913	1/1	0.95	0.06	36,36,36,36	0
10	EDO	A	930	4/4	0.95	0.17	46,49,51,54	0
10	EDO	A	920	4/4	0.96	0.18	36,39,41,44	0
10	EDO	A	922	4/4	0.96	0.11	35,36,39,40	0
10	EDO	A	918	4/4	0.97	0.10	28,31,32,33	0
11	EAR	A	935	24/24	0.97	0.10	25,30,33,37	0
4	ZN	A	910	1/1	0.98	0.17	32,32,32,32	0
8	SO4	A	915	5/5	0.98	0.10	29,33,38,38	0
9	CL	A	916	1/1	0.98	0.06	47,47,47,47	0
5	CA	A	912	1/1	0.99	0.12	34,34,34,34	0
4	ZN	A	911	1/1	1.00	0.13	24,24,24,24	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.