



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2020 – 10:50 AM BST

PDB ID : 5LIA
Title : Crystal structure of murine autotaxin in complex with a small molecule inhibitor
Authors : Turnbull, A.P.; Shah, P.; Cheasty, A.; Raynham, T.; Pang, L.; Owen, P.
Deposited on : 2016-07-14
Resolution : 1.92 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

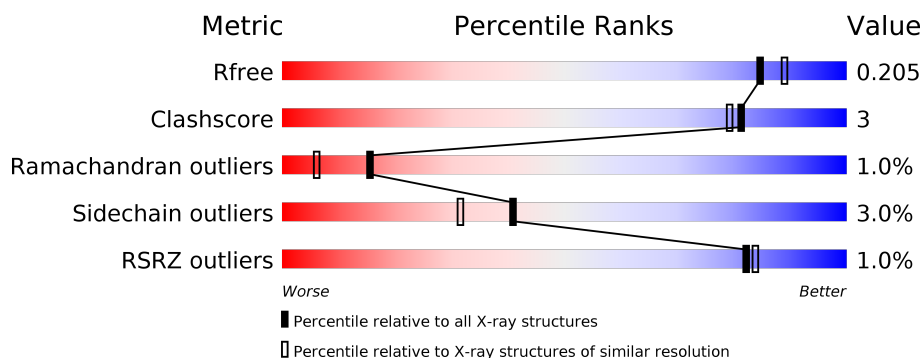
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.92 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	7937 (1.94-1.90)
Clashscore	141614	8644 (1.94-1.90)
Ramachandran outliers	138981	8530 (1.94-1.90)
Sidechain outliers	138945	8530 (1.94-1.90)
RSRZ outliers	127900	7793 (1.94-1.90)

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	838	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> % <div style="width: 86%; height: 10px; background-color: green;"></div> <div style="width: 9%; height: 10px; background-color: yellow;"></div> <div style="width: 5%; height: 10px; background-color: orange;"></div> <div style="width: 0%; height: 10px; background-color: grey;"></div> </div> <div style="display: flex; justify-content: space-between; align-items: center;"> 86% 9% • • </div> </div>
2	B	6	<div> <div style="width: 100%; height: 10px; background-color: yellow;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> 100% </div> </div>

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 6909 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	805	Total	C	N	O	S	0	2	0
			6339	4040	1075	1175	49			

There are 19 discrepancies between the modelled and reference sequences:

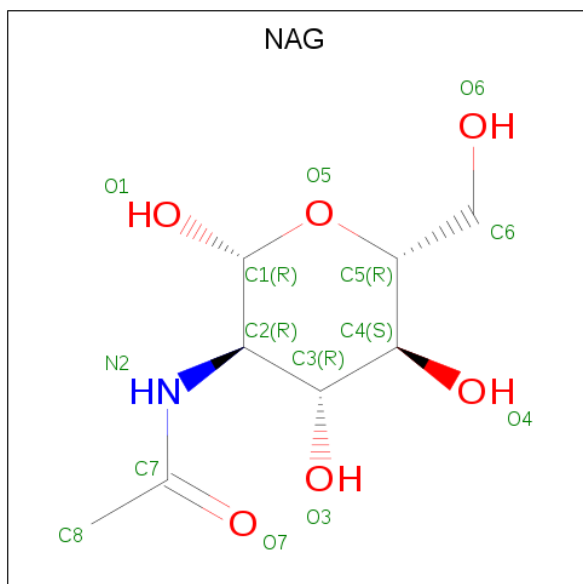
Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	LYS	deletion	UNP Q9R1E6
A	?	-	VAL	deletion	UNP Q9R1E6
A	?	-	GLU	deletion	UNP Q9R1E6
A	?	-	PRO	deletion	UNP Q9R1E6
A	859	SER	-	expression tag	UNP Q9R1E6
A	860	ARG	-	expression tag	UNP Q9R1E6
A	861	GLU	-	expression tag	UNP Q9R1E6
A	862	ASN	-	expression 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
A	867	GLY	-	expression tag	UNP Q9R1E6
A	868	HIS	-	expression tag	UNP Q9R1E6
A	869	HIS	-	expression tag	UNP Q9R1E6
A	870	HIS	-	expression tag	UNP Q9R1E6
A	871	HIS	-	expression tag	UNP Q9R1E6
A	872	HIS	-	expression tag	UNP Q9R1E6
A	873	HIS	-	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)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



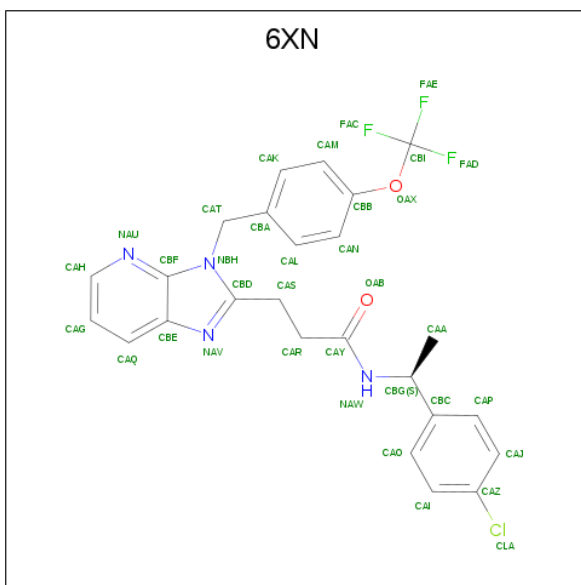
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is {N}-[(1 {S})-1-(4-chlorophenyl)ethyl]-3-[3-[[4-(trifluoromethoxy)phenyl]methyl]imidazo[4,5-b]pyridin-2-yl]propanamide (three-letter code: 6XN) (formula: $C_{25}H_{22}ClF_3N_4O_2$).

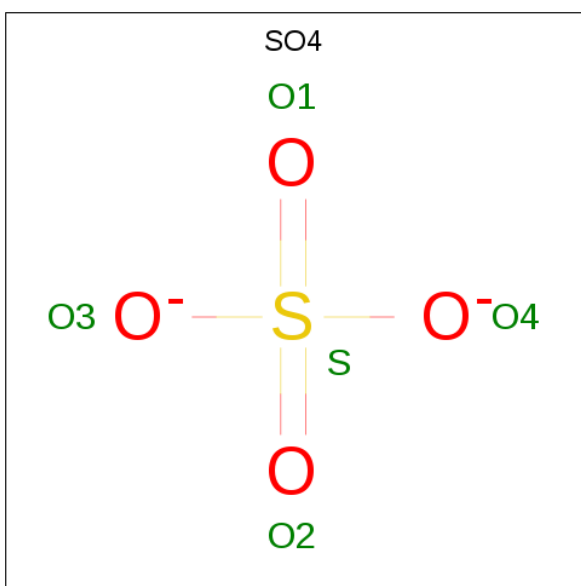


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	Cl	F	N	O	0	0
			35	25	1	3	4	2		

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

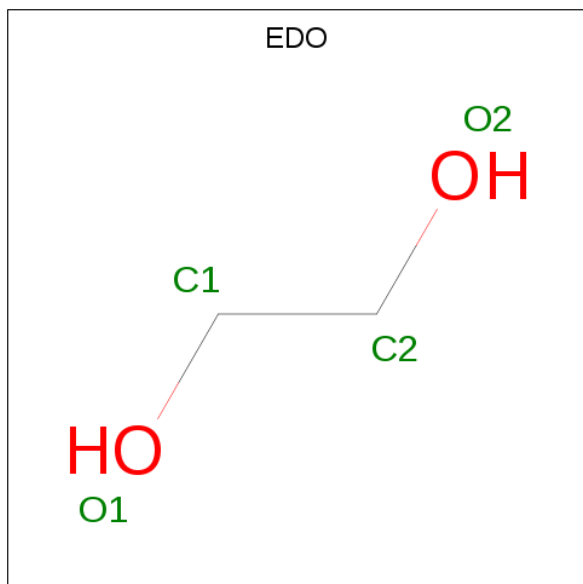
- Molecule 8 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 9 is POTASSIUM ION (three-letter code: K) (formula: K).

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

- 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

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

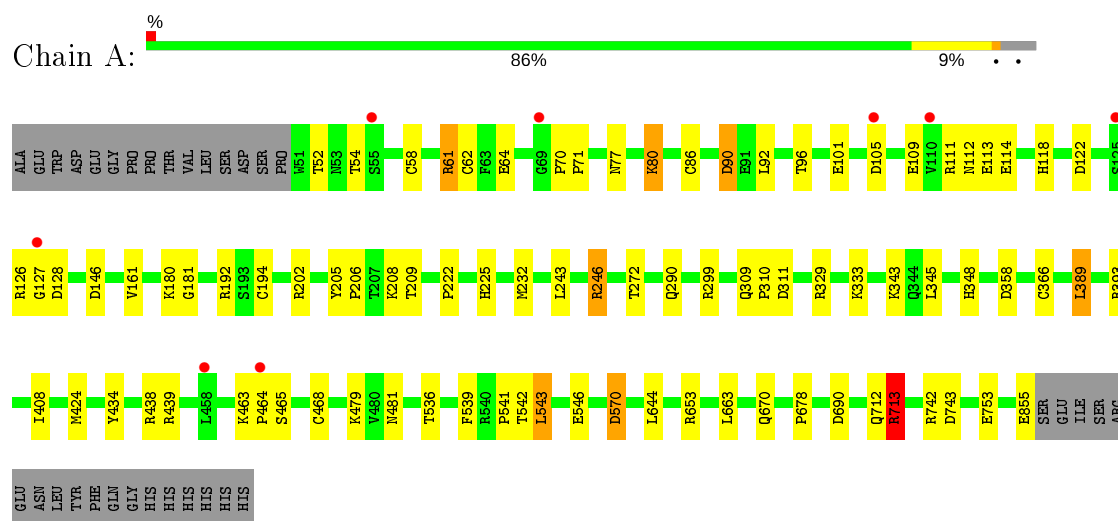
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	427	Total	O	0	0
			427	427		

3 Residue-property plots [i](#)

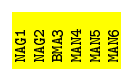
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	61.16Å 61.58Å 66.14Å 85.77° 72.68° 80.21°	Depositor
Resolution (Å)	50.00 – 1.92 60.66 – 1.92	Depositor EDS
% Data completeness (in resolution range)	97.2 (50.00-1.92) 97.2 (60.66-1.92)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.34 (at 1.92Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.160 , 0.201 0.169 , 0.205	Depositor DCC
R_{free} test set	3411 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	27.3	Xtriage
Anisotropy	0.256	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 46.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	6909	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.97% 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, EDO, 6XN, 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	0.96	3/6531 (0.0%)	0.98	24/8896 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	546	GLU	CD-OE2	7.61	1.34	1.25
1	A	439	ARG	CZ-NH1	-5.79	1.25	1.33
1	A	290	GLN	CG-CD	5.14	1.62	1.51

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	713	ARG	NE-CZ-NH1	9.64	125.12	120.30
1	A	246	ARG	NE-CZ-NH1	8.26	124.43	120.30
1	A	194[A]	CYS	CA-CB-SG	-8.03	99.55	114.00
1	A	194[B]	CYS	CA-CB-SG	-8.03	99.55	114.00
1	A	202	ARG	NE-CZ-NH2	-7.28	116.66	120.30
1	A	743	ASP	CB-CG-OD2	-7.09	111.92	118.30
1	A	202	ARG	NE-CZ-NH1	6.75	123.67	120.30
1	A	299	ARG	NE-CZ-NH1	6.67	123.63	120.30
1	A	653	ARG	NE-CZ-NH2	-6.49	117.06	120.30
1	A	311	ASP	CB-CG-OD2	6.39	124.05	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	439	ARG	NE-CZ-NH1	6.39	123.50	120.30
1	A	192	ARG	CG-CD-NE	-6.26	98.64	111.80
1	A	543	LEU	CA-CB-CG	6.23	129.64	115.30
1	A	438	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	A	713	ARG	NE-CZ-NH2	-5.95	117.33	120.30
1	A	208	LYS	CD-CE-NZ	-5.71	98.57	111.70
1	A	77	ASN	CB-CA-C	-5.39	99.61	110.40
1	A	299	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	A	61	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	A	742	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	A	393	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	A	743	ASP	CB-CG-OD1	5.10	122.89	118.30
1	A	690	ASP	CB-CG-OD1	5.05	122.85	118.30
1	A	246	ARG	NE-CZ-NH2	-5.02	117.79	120.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	180	LYS	Peptide
1	A	205	TYR	Mainchain,Peptide
1	A	309	GLN	Mainchain,Peptide
1	A	70	PRO	Peptide

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	6339	0	5905	33	0
2	B	72	0	61	0	0
3	A	14	0	13	0	0
4	A	35	0	0	0	0
5	A	2	0	0	1	0
6	A	5	0	0	0	0
7	A	1	0	0	0	0
8	A	1	0	0	0	0
9	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	A	12	0	18	0	0
11	A	427	0	0	3	0
All	All	6909	0	5997	33	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 (33) 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:118:HIS:HD2	1:A:128:ASP:CB	1.81	0.92
1:A:118:HIS:CD2	1:A:128:ASP:CB	2.69	0.74
1:A:209:THR:OG1	5:A:909:ZN:ZN	1.35	0.74
1:A:61:ARG:HD2	1:A:64:GLU:OE2	1.93	0.68
1:A:539:PHE:O	1:A:541:PRO:HD3	1.98	0.64
1:A:146:ASP:OD2	1:A:343:LYS:NZ	2.31	0.61
1:A:62:CYS:SG	1:A:92:LEU:HD22	2.41	0.60
1:A:348:HIS:CD2	1:A:348:HIS:H	2.19	0.59
1:A:243:LEU:HD12	11:A:1124:HOH:O	2.01	0.59
1:A:209:THR:OG1	1:A:358:ASP:OD2	2.10	0.58
1:A:479:LYS:O	1:A:855:GLU:HG3	2.03	0.58
1:A:408:ILE:HD11	1:A:424:MET:SD	2.44	0.58
1:A:570:ASP:HB3	1:A:644:LEU:HD21	1.86	0.57
1:A:80:LYS:NZ	1:A:90:ASP:OD2	2.40	0.54
1:A:463:LYS:HB3	1:A:464:PRO:HD2	1.91	0.53
1:A:112:ASN:OD1	1:A:113:GLU:N	2.42	0.52
1:A:112:ASN:OD1	1:A:112:ASN:C	2.48	0.52
1:A:112:ASN:OD1	1:A:114:GLU:N	2.45	0.50
1:A:92:LEU:O	1:A:92:LEU:HD23	2.12	0.50
1:A:329:ARG:NH1	11:A:1008:HOH:O	2.42	0.49
1:A:366:CYS:SG	1:A:468:CYS:HB3	2.54	0.47
1:A:222:PRO:HA	1:A:225:HIS:CE1	2.50	0.47
1:A:105:ASP:N	1:A:105:ASP:OD1	2.48	0.46
1:A:348:HIS:HE1	11:A:1394:HOH:O	1.98	0.46
1:A:678:PRO:HB3	1:A:712:GLN:HB3	1.96	0.46
1:A:713:ARG:HH11	1:A:713:ARG:HG2	1.80	0.46
1:A:58:CYS:O	1:A:61:ARG:HB2	2.17	0.44
1:A:101:GLU:OE2	1:A:333:LYS:CE	2.65	0.44
1:A:570:ASP:CB	1:A:644:LEU:HD21	2.48	0.43
1:A:206:PRO:HB3	1:A:389:LEU:HD13	2.02	0.41
1:A:206:PRO:HD3	1:A:434:TYR:CE1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:ASP:OD1	1:A:122:ASP:C	2.60	0.40
1:A:58:CYS:SG	1:A:86:CYS:HB2	2.61	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	805/838 (96%)	755 (94%)	42 (5%)	8 (1%)	15 6

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	109	GLU
1	A	465	SER
1	A	71	PRO
1	A	126	ARG
1	A	181	GLY
1	A	111	ARG
1	A	127	GLY
1	A	310	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	677/762 (89%)	657 (97%)	20 (3%)	41	31

All (20) 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	90	ASP
1	A	96	THR
1	A	161	VAL
1	A	232	MET
1	A	246	ARG
1	A	272	THR
1	A	345	LEU
1	A	389	LEU
1	A	481	ASN
1	A	536	THR
1	A	542	THR
1	A	543	LEU
1	A	570	ASP
1	A	663	LEU
1	A	670	GLN
1	A	713	ARG
1	A	753	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	118	HIS
1	A	337	GLN
1	A	348	HIS
1	A	374	ASN
1	A	670	GLN
1	A	802	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 ⓘ

6 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	0.90	0	17,19,21	1.79	4 (23%)
2	NAG	B	2	2	14,14,15	1.09	1 (7%)	17,19,21	1.71	4 (23%)
2	BMA	B	3	2	11,11,12	0.82	0	15,15,17	1.38	3 (20%)
2	MAN	B	4	2	11,11,12	0.72	0	15,15,17	1.91	4 (26%)
2	MAN	B	5	2	11,11,12	1.10	1 (9%)	15,15,17	2.04	4 (26%)
2	MAN	B	6	2	11,11,12	1.09	0	15,15,17	1.35	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	BMA	B	3	2	-	0/2/19/22	0/1/1/1
2	MAN	B	4	2	-	0/2/19/22	0/1/1/1
2	MAN	B	5	2	-	1/2/19/22	0/1/1/1
2	MAN	B	6	2	-	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	5	MAN	C2-C3	3.13	1.57	1.52
2	B	2	NAG	O5-C1	-2.70	1.39	1.43

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	4	MAN	O5-C5-C6	4.61	114.43	107.20
2	B	2	NAG	O4-C4-C3	-4.08	100.93	110.35
2	B	5	MAN	O3-C3-C2	3.90	117.46	109.99
2	B	1	NAG	O5-C1-C2	-3.88	105.17	111.29
2	B	1	NAG	C1-O5-C5	3.72	117.24	112.19
2	B	4	MAN	O3-C3-C2	3.70	117.08	109.99
2	B	5	MAN	O6-C6-C5	-3.70	98.61	111.29
2	B	2	NAG	O7-C7-C8	-3.00	116.48	122.06
2	B	4	MAN	C1-O5-C5	2.79	115.97	112.19
2	B	5	MAN	C1-C2-C3	2.73	113.02	109.67
2	B	5	MAN	C1-O5-C5	2.66	115.80	112.19
2	B	6	MAN	O5-C1-C2	2.63	114.84	110.77
2	B	6	MAN	O3-C3-C4	2.58	116.32	110.35
2	B	3	BMA	C1-C2-C3	2.56	112.81	109.67
2	B	3	BMA	O2-C2-C1	-2.40	104.24	109.15
2	B	1	NAG	O4-C4-C5	-2.36	103.44	109.30
2	B	2	NAG	C8-C7-N2	2.27	119.94	116.10
2	B	6	MAN	O2-C2-C3	-2.10	105.92	110.14
2	B	3	BMA	O6-C6-C5	-2.08	104.14	111.29
2	B	4	MAN	O2-C2-C1	-2.07	104.92	109.15
2	B	2	NAG	C1-O5-C5	2.05	114.97	112.19
2	B	1	NAG	C2-N2-C7	-2.01	120.03	122.90

There are no chirality outliers.

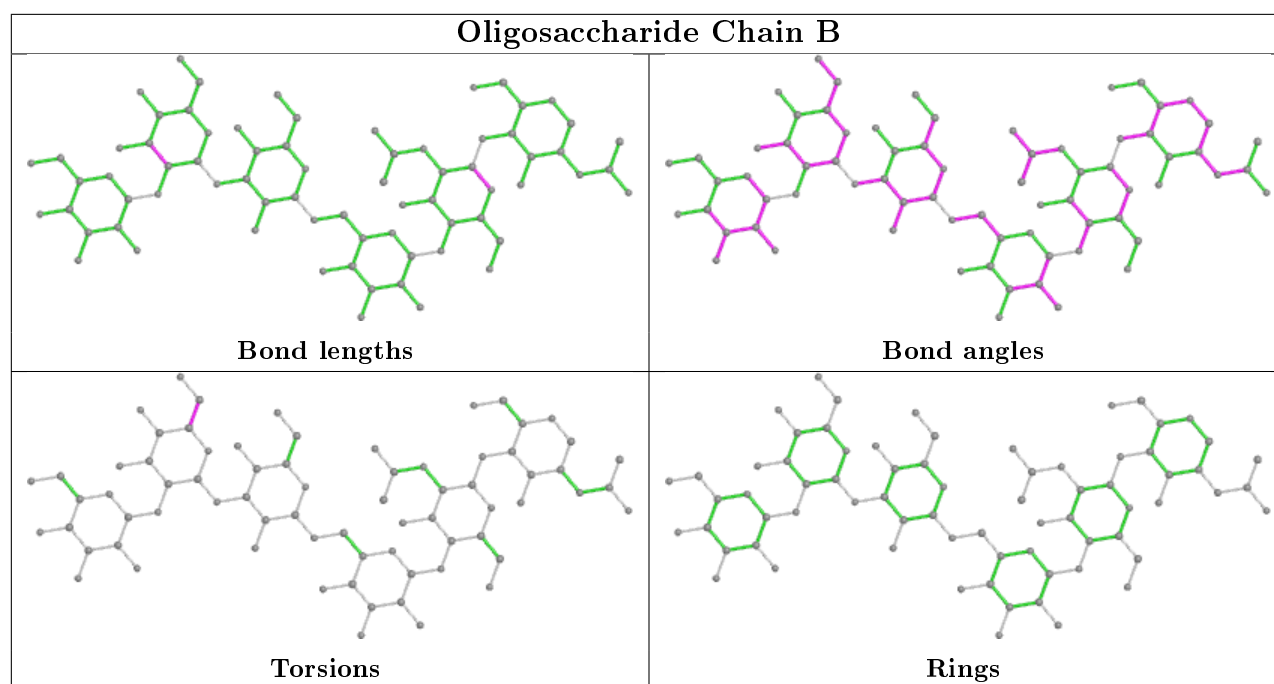
All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	5	MAN	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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



5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 5 are monoatomic - leaving 6 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	915	-	3,3,3	0.51	0	2,2,2	0.41	0
6	SO4	A	911	5	4,4,4	0.97	0	6,6,6	0.70	0
3	NAG	A	901	1	14,14,15	1.00	1 (7%)	17,19,21	1.66	3 (17%)
4	6XN	A	908	-	36,38,38	1.94	8 (22%)	44,54,54	1.09	3 (6%)
10	EDO	A	917	-	3,3,3	1.06	0	2,2,2	0.47	0
10	EDO	A	916	-	3,3,3	0.40	0	2,2,2	0.27	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	915	-	-	0/1/1/1	-
3	NAG	A	901	1	-	0/6/23/26	0/1/1/1
10	EDO	A	917	-	-	0/1/1/1	-
4	6XN	A	908	-	-	1/22/22/22	0/4/4/4
10	EDO	A	916	-	-	0/1/1/1	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	908	6XN	CAQ-CBE	-5.50	1.32	1.41
4	A	908	6XN	CAT-NBH	4.65	1.57	1.48
4	A	908	6XN	CAT-CBA	-4.60	1.40	1.51
4	A	908	6XN	CAH-NAU	2.93	1.38	1.32
3	A	901	NAG	C1-C2	2.91	1.56	1.52
4	A	908	6XN	CBC-CBG	-2.78	1.44	1.52
4	A	908	6XN	CAG-CAQ	2.54	1.42	1.36
4	A	908	6XN	CBE-CBF	-2.36	1.34	1.40
4	A	908	6XN	CAZ-CLA	-2.15	1.69	1.74

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	901	NAG	O5-C1-C2	-4.36	104.40	111.29
4	A	908	6XN	CAP-CAJ-CAZ	3.01	122.42	119.24
3	A	901	NAG	O4-C4-C5	2.68	115.94	109.30
3	A	901	NAG	C3-C4-C5	2.38	114.48	110.24
4	A	908	6XN	CAG-CAH-NAU	-2.32	120.38	123.94
4	A	908	6XN	CBG-NAW-CAY	-2.02	120.02	122.90

There are no chirality outliers.

All (1) torsion outliers are listed below:

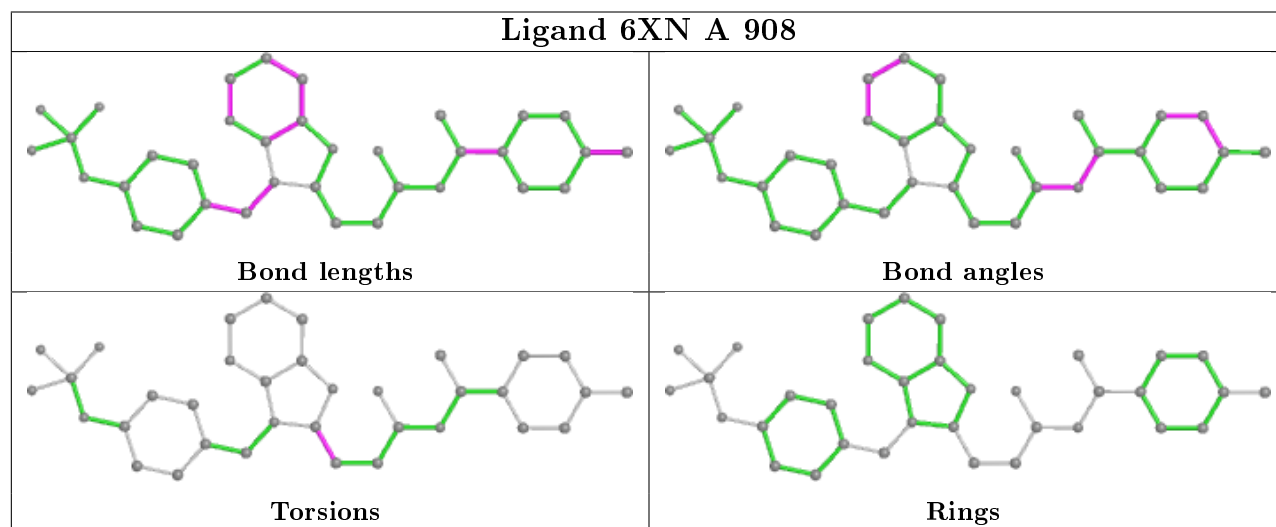
Mol	Chain	Res	Type	Atoms
4	A	908	6XN	CAR-CAS-CBD-NBH

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 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	805/838 (96%)	-0.22	8 (0%) 82 84	17, 33, 67, 83	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	110	VAL	6.1
1	A	464	PRO	4.7
1	A	125	SER	3.3
1	A	55	SER	2.8
1	A	127	GLY	2.6
1	A	69	GLY	2.4
1	A	458	LEU	2.4
1	A	105	ASP	2.2

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

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

6.3 Carbohydrates [i](#)

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

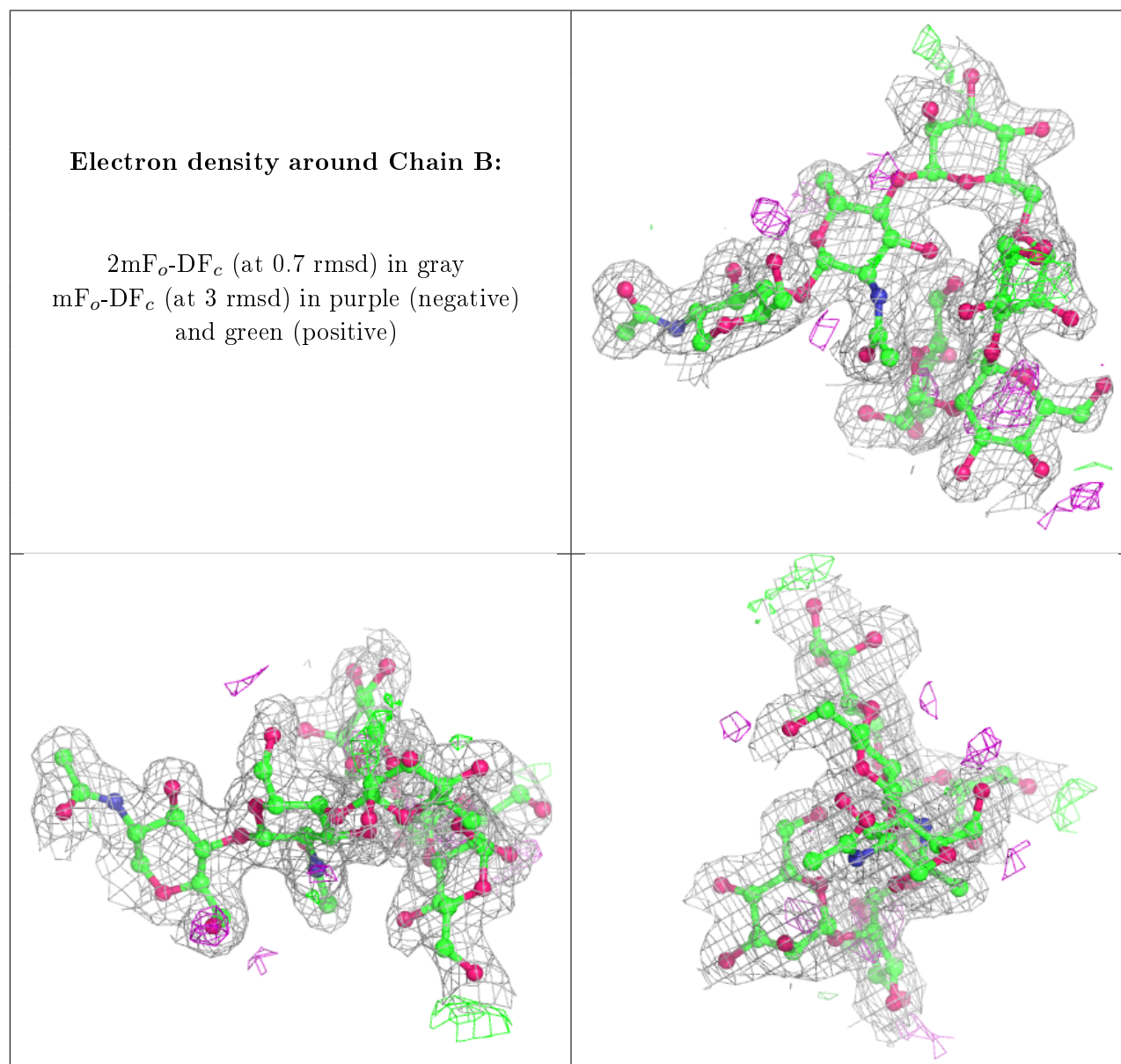
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	BMA	B	3	11/12	0.87	0.15	41,45,51,56	0
2	MAN	B	4	11/12	0.88	0.17	43,47,48,49	0
2	MAN	B	5	11/12	0.90	0.25	41,45,49,52	0
2	MAN	B	6	11/12	0.92	0.12	28,38,42,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NAG	B	2	14/15	0.94	0.09	27,32,41,44	0
2	NAG	B	1	14/15	0.98	0.07	19,21,24,24	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.

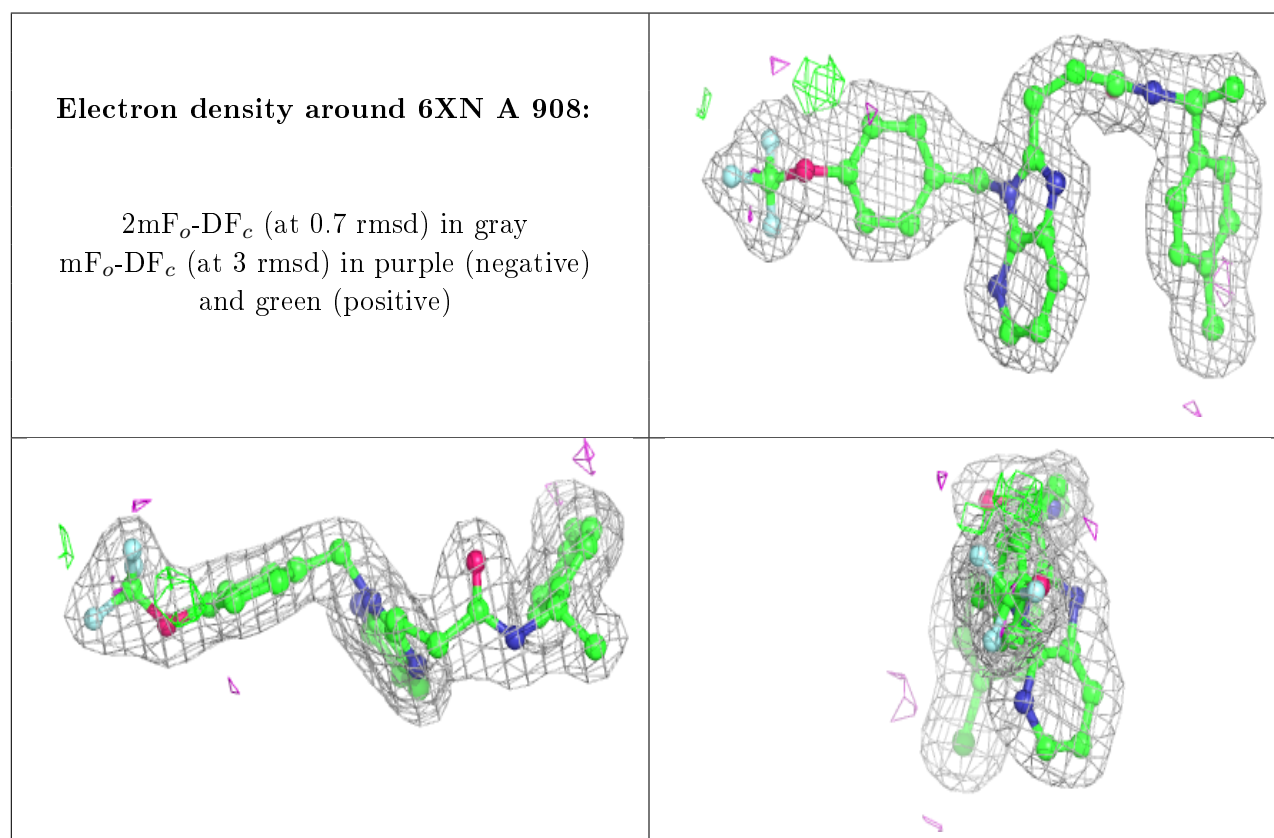


6.4 Ligands ⓘ

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(\AA^2)	Q<0.9
10	EDO	A	917	4/4	0.87	0.17	47,55,57,57	0
3	NAG	A	901	14/15	0.88	0.13	44,50,61,64	0
10	EDO	A	916	4/4	0.95	0.10	33,36,40,45	0
4	6XN	A	908	35/35	0.96	0.08	20,25,39,41	0
9	K	A	914	1/1	0.97	0.07	40,40,40,40	0
10	EDO	A	915	4/4	0.98	0.10	24,25,26,26	0
6	SO4	A	911	5/5	0.98	0.07	24,26,32,33	0
8	NA	A	913	1/1	0.99	0.12	28,28,28,28	0
5	ZN	A	909	1/1	0.99	0.08	31,31,31,31	0
5	ZN	A	910	1/1	1.00	0.11	21,21,21,21	0
7	CA	A	912	1/1	1.00	0.12	23,23,23,23	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 ⓘ

There are no such residues in this entry.