Full wwPDB X-ray Structure Validation Report (i)

Dec 12, 2024 – 07:02 PM EST

PDB ID	:	7G73
Title	:	Crystal Structure of rat Autotaxin in complex with 6-(4-acetylpiperazin-1-yl)-3-[[1-[(3,4-dichlorophenyl)methyl]triazol-4-yl]methyl]quinazolin-4-one, i.e. SMILES c1(ccc2c(c1)C(=O)N(C=N2)CC1=CN(N=N1)Cc1ccc(c(c1)Cl)Cl)N1CCN(CC1)C(=O)C with IC50=0.0309414 microM
Authors	:	Stihle, M.; Benz, J.; Hunziker, D.; Martin-Rainer, E.; Rudolph, M.G.
Deposited on	:	2023-06-05
Resolution	:	1.52 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

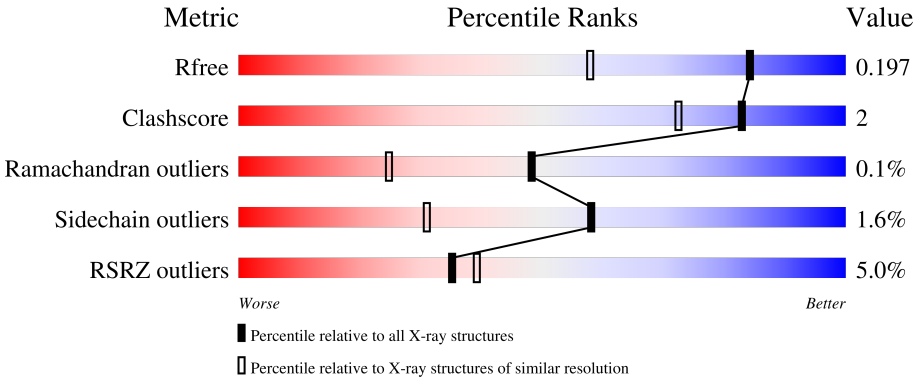
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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 1.52 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}	164625	5293 (1.54-1.50)
Clashscore	180529	5759 (1.54-1.50)
Ramachandran outliers	177936	5653 (1.54-1.50)
Sidechain outliers	177891	5650 (1.54-1.50)
RSRZ outliers	164620	5293 (1.54-1.50)

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 of 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 <=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	846	5% 89% 6% • 5%
2	B	9	100%

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 7581 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.

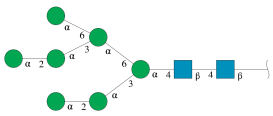
- Molecule 1 is a protein called Isoform 2 of Ectonucleotide pyrophosphatase/phosphodiesterase family member 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	806	6656	4223	1148	1231	54	0	26	0

There are 14 discrepancies between the modelled and reference sequences:

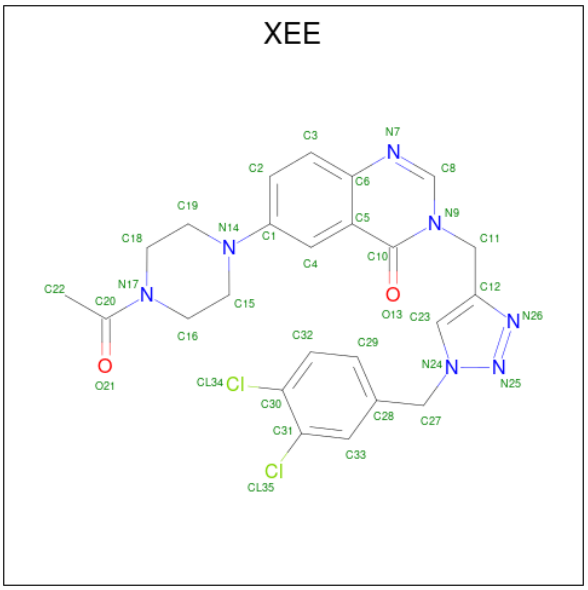
Chain	Residue	Modelled	Actual	Comment	Reference
A	53	ALA	ASN	engineered mutation	UNP Q64610
A	410	ALA	ASN	engineered mutation	UNP Q64610
A	591	THR	ARG	engineered mutation	UNP Q64610
A	863	GLY	-	expression tag	UNP Q64610
A	864	GLY	-	expression tag	UNP Q64610
A	865	ARG	-	expression tag	UNP Q64610
A	866	HIS	-	expression tag	UNP Q64610
A	867	HIS	-	expression tag	UNP Q64610
A	868	HIS	-	expression tag	UNP Q64610
A	869	HIS	-	expression tag	UNP Q64610
A	870	HIS	-	expression tag	UNP Q64610
A	871	HIS	-	expression tag	UNP Q64610
A	872	HIS	-	expression tag	UNP Q64610
A	873	HIS	-	expression tag	UNP Q64610

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



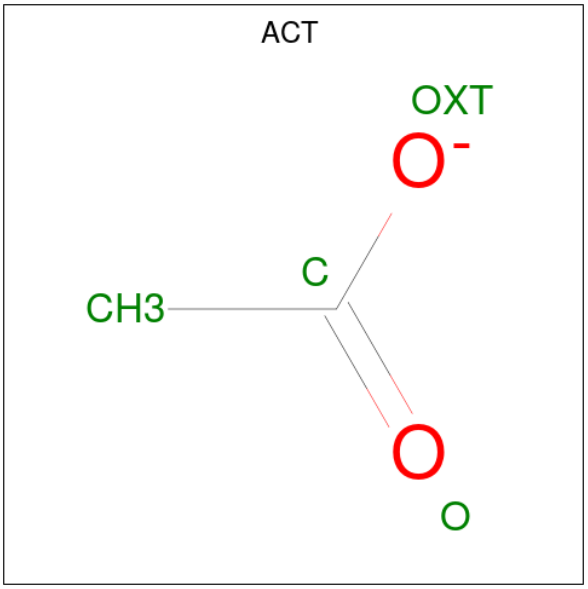
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	B	9	Total C N O 105 58 2 45	0	0	0

- Molecule 3 is 6-(4-acetylpiperazin-1-yl)-3-({1-[(3,4-dichlorophenyl)methyl]-1H-1,2,3-triazol-4-yl}methyl)quinazolin-4(3H)-one (three-letter code: XEE) (formula: $C_{24}H_{23}Cl_2N_7O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C Cl N O 35 24 2 7 2	0	0

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

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

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

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

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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	2	Total Ca 2 2	0	0

- Molecule 8 is POTASSIUM ION (three-letter code: K) (formula: K).

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

- Molecule 9 is water.

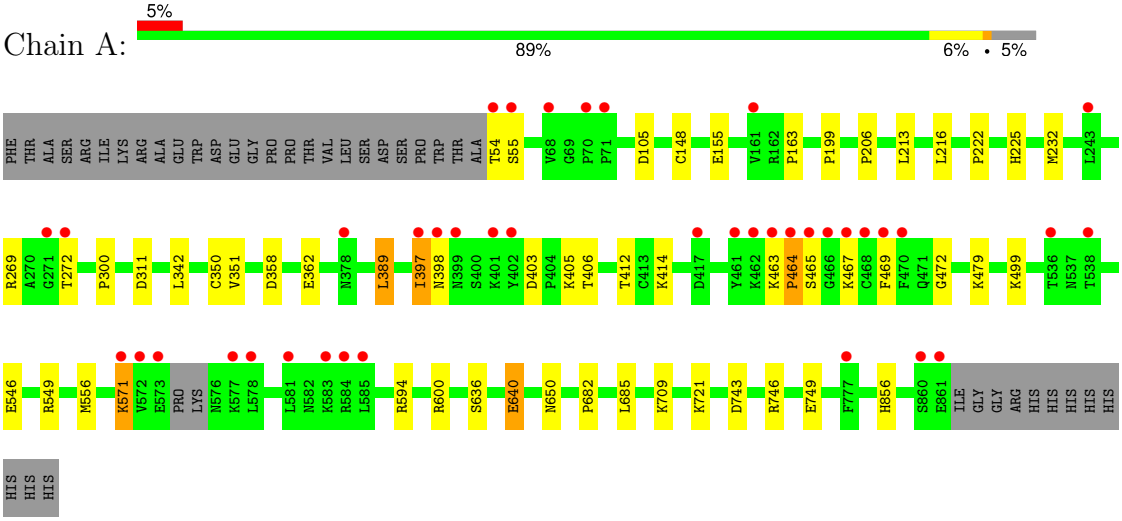
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	772	Total O 772 772	0	0

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.

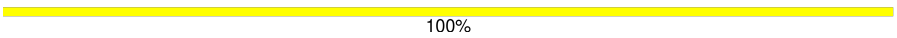
• Molecule 1: Isoform 2 of Ectonucleotide pyrophosphatase/phosphodiesterase family member 2

Chain A:



• Molecule 2: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]alpha-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 (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	84.22Å 91.86Å 120.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.02 – 1.52 49.02 – 1.52	Depositor EDS
% Data completeness (in resolution range)	98.7 (49.02-1.52) 93.7 (49.02-1.52)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.92 (at 1.52Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.167 , 0.195 0.170 , 0.197	Depositor DCC
R_{free} test set	7231 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	19.8	Xtriage
Anisotropy	0.325	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 33.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	7581	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, XEE, NA, CA, K, NAG, ACT, 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	0.75	1/6901 (0.0%)	0.86	5/9346 (0.1%)

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	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	546	GLU	CD-OE2	6.84	1.33	1.25

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	148[A]	CYS	CA-CB-SG	9.17	130.50	114.00
1	A	148[B]	CYS	CA-CB-SG	9.17	130.50	114.00
1	A	311	ASP	CB-CG-OD2	5.32	123.09	118.30
1	A	743	ASP	CB-CG-OD1	5.18	122.96	118.30
1	A	358	ASP	CB-CG-OD2	-5.10	113.71	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	54	THR	Peptide

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Mol	Chain	Res	Type	Group
1	A	746[A]	ARG	Sidechain
1	A	746[B]	ARG	Sidechain

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	6656	0	6480	31	0
2	B	105	0	88	0	0
3	A	35	0	0	0	0
4	A	8	0	6	0	0
5	A	1	0	0	0	0
6	A	1	0	0	0	0
7	A	2	0	0	0	0
8	A	1	0	0	0	0
9	A	772	0	0	10	0
All	All	7581	0	6574	31	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 2.

All (31) 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:556[A]:MET:SD	9:A:1370:HOH:O	2.40	0.76
1:A:199:PRO:HG3	1:A:499[B]:LYS:HE3	1.71	0.71
1:A:709:LYS:HE3	9:A:1601:HOH:O	1.90	0.71
1:A:463:LYS:HA	1:A:464:PRO:O	1.93	0.69
1:A:594:ARG:HH22	1:A:636:SER:HB3	1.59	0.66
1:A:594:ARG:NH2	1:A:636:SER:HB3	2.15	0.62
1:A:222:PRO:HA	1:A:225:HIS:CE1	2.38	0.59
1:A:650:ASN:O	9:A:1001:HOH:O	2.17	0.57
1:A:269[A]:ARG:NH1	9:A:1008:HOH:O	2.37	0.54
1:A:600:ARG:NE	9:A:1005:HOH:O	2.26	0.54
1:A:479:LYS:NZ	9:A:1014:HOH:O	2.42	0.53
1:A:571:LYS:NZ	9:A:1015:HOH:O	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269[A]:ARG:HB3	1:A:300:PRO:HA	1.91	0.51
1:A:397:ILE:HG13	1:A:398:ASN:N	2.26	0.50
1:A:206:PRO:HB3	1:A:389[B]:LEU:HD23	1.92	0.50
1:A:199:PRO:HG3	1:A:499[B]:LYS:CE	2.40	0.50
1:A:342:LEU:HD13	1:A:351:VAL:HG21	1.95	0.49
1:A:403:ASP:OD2	1:A:406:THR:HG23	2.12	0.48
1:A:163:PRO:HB3	1:A:350:CYS:O	2.13	0.48
1:A:636:SER:O	1:A:721[A]:LYS:NZ	2.46	0.48
1:A:269[B]:ARG:HB3	1:A:300:PRO:HA	1.94	0.48
1:A:397:ILE:HG13	1:A:398:ASN:H	1.78	0.48
1:A:213:LEU:HD23	1:A:216:LEU:HD12	1.97	0.47
1:A:397:ILE:HD13	9:A:1397:HOH:O	2.14	0.47
1:A:640:GLU:HG2	9:A:1619:HOH:O	2.13	0.47
1:A:467:LYS:HB3	1:A:469:PHE:CE2	2.51	0.46
1:A:155:GLU:O	1:A:350:CYS:HB2	2.18	0.43
1:A:682:PRO:HG3	1:A:685:LEU:HD12	2.01	0.43
1:A:412:THR:O	1:A:414:LYS:HE3	2.19	0.42
1:A:549:ARG:HD2	9:A:1281:HOH:O	2.19	0.42
1:A:362:GLU:O	1:A:472:GLY:HA2	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	829/846 (98%)	805 (97%)	23 (3%)	1 (0%)	48 25

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	464	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	757/765 (99%)	744 (98%)	13 (2%)	56 28

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	SER
1	A	105	ASP
1	A	232	MET
1	A	272	THR
1	A	389[A]	LEU
1	A	389[B]	LEU
1	A	397	ILE
1	A	405	LYS
1	A	465	SER
1	A	571	LYS
1	A	640	GLU
1	A	749	GLU
1	A	856	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

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	2,1	14,14,15	0.79	0	17,19,21	0.92	1 (5%)
2	NAG	B	2	2	14,14,15	0.60	0	17,19,21	0.95	1 (5%)
2	MAN	B	3	2	11,11,12	1.65	2 (18%)	15,15,17	1.40	2 (13%)
2	MAN	B	4	2	11,11,12	1.37	2 (18%)	15,15,17	1.12	0
2	MAN	B	5	2	11,11,12	1.40	1 (9%)	15,15,17	0.95	1 (6%)
2	MAN	B	6	2	11,11,12	1.27	1 (9%)	15,15,17	1.37	2 (13%)
2	MAN	B	7	2	11,11,12	1.88	5 (45%)	15,15,17	1.08	1 (6%)
2	MAN	B	8	2	11,11,12	1.90	4 (36%)	15,15,17	0.89	0
2	MAN	B	9	2	11,11,12	1.87	4 (36%)	15,15,17	0.97	2 (13%)

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	2,1	-	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
2	MAN	B	7	2	-	2/2/19/22	0/1/1/1
2	MAN	B	8	2	-	2/2/19/22	0/1/1/1
2	MAN	B	9	2	-	0/2/19/22	0/1/1/1

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	9	MAN	C2-C3	4.26	1.59	1.52
2	B	8	MAN	C2-C3	3.80	1.58	1.52
2	B	3	MAN	C2-C3	3.64	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	7	MAN	O5-C5	3.34	1.49	1.43
2	B	3	MAN	O5-C5	3.20	1.49	1.43
2	B	8	MAN	O5-C5	2.97	1.49	1.43
2	B	7	MAN	C4-C5	2.79	1.59	1.53
2	B	4	MAN	O5-C5	2.65	1.48	1.43
2	B	5	MAN	O5-C5	2.60	1.48	1.43
2	B	8	MAN	C1-C2	2.58	1.58	1.52
2	B	4	MAN	C2-C3	2.53	1.56	1.52
2	B	9	MAN	O5-C5	2.38	1.48	1.43
2	B	6	MAN	O2-C2	2.20	1.48	1.43
2	B	9	MAN	C1-C2	2.19	1.57	1.52
2	B	8	MAN	C4-C3	2.18	1.58	1.52
2	B	7	MAN	C4-C3	2.16	1.58	1.52
2	B	9	MAN	C4-C3	2.14	1.57	1.52
2	B	7	MAN	C2-C3	2.09	1.55	1.52
2	B	7	MAN	C6-C5	2.03	1.58	1.51

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	6	MAN	C1-O5-C5	4.01	117.56	112.19
2	B	3	MAN	C1-O5-C5	3.48	116.85	112.19
2	B	5	MAN	O2-C2-C3	-3.08	103.76	110.15
2	B	6	MAN	O2-C2-C3	-2.91	104.12	110.15
2	B	7	MAN	C1-O5-C5	2.48	115.51	112.19
2	B	3	MAN	O6-C6-C5	-2.25	103.68	111.33
2	B	2	NAG	O4-C4-C5	-2.21	103.89	109.32
2	B	9	MAN	O3-C3-C2	2.21	114.56	110.05
2	B	9	MAN	C1-O5-C5	2.15	115.06	112.19
2	B	1	NAG	O4-C4-C5	-2.04	104.31	109.32

There are no chirality outliers.

All (4) torsion outliers are listed below:

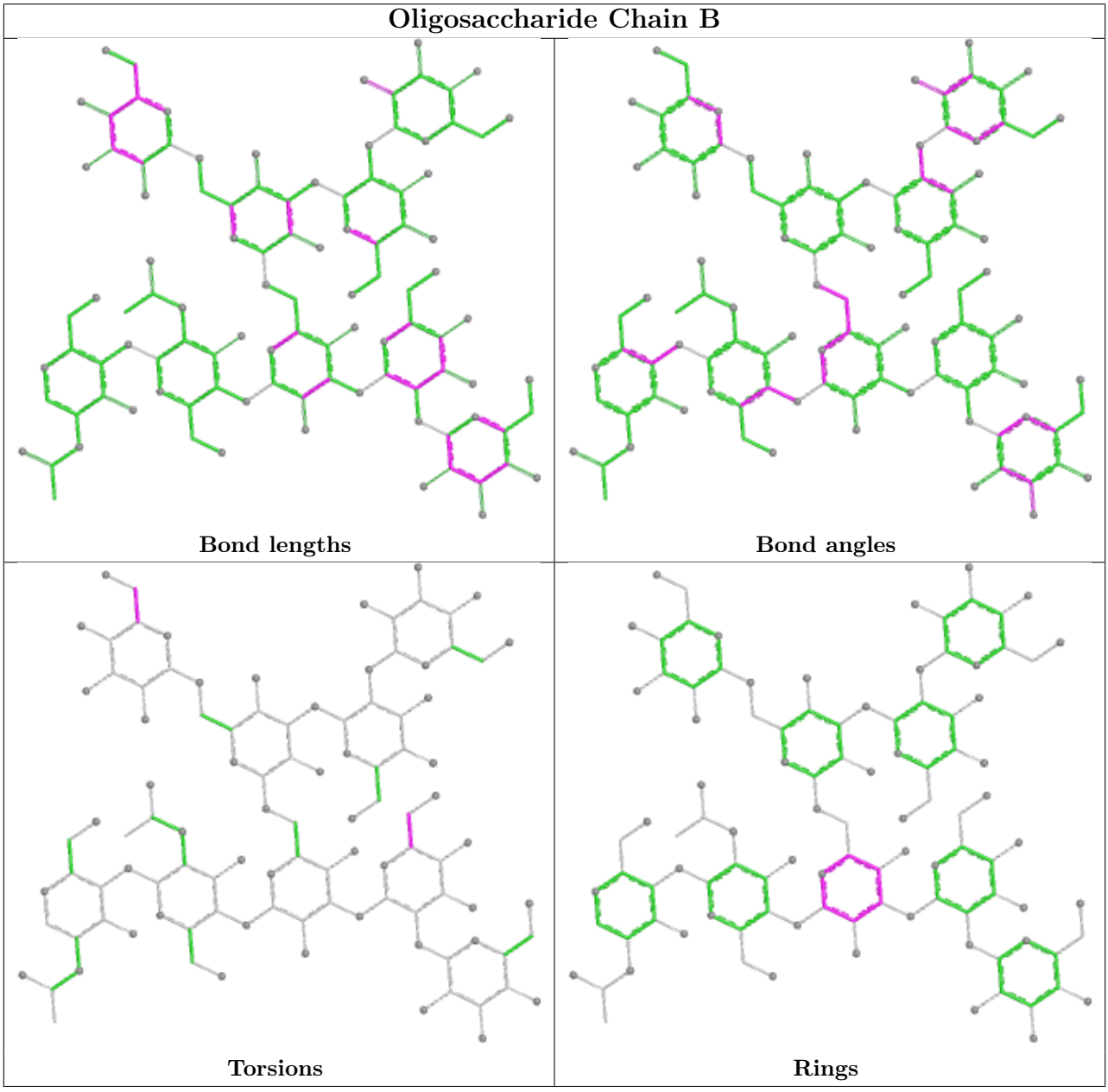
Mol	Chain	Res	Type	Atoms
2	B	7	MAN	O5-C5-C6-O6
2	B	7	MAN	C4-C5-C6-O6
2	B	8	MAN	O5-C5-C6-O6
2	B	8	MAN	C4-C5-C6-O6

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 8 ligands modelled in this entry, 5 are monoatomic - leaving 3 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	$\#\|Z\| > 2$
4	ACT	A	902	-	3,3,3	1.97	1 (33%)	3,3,3	1.05	0
3	XEE	A	901	-	38,39,39	1.58	7 (18%)	51,56,56	2.93	19 (37%)
4	ACT	A	903	-	3,3,3	1.54	1 (33%)	3,3,3	1.57	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
3	XEE	A	901	-	-	2/16/26/26	0/5/5/5

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	901	XEE	C23-C12	4.02	1.42	1.36
3	A	901	XEE	C15-N14	3.21	1.52	1.46
3	A	901	XEE	C27-N24	3.11	1.52	1.47
4	A	902	ACT	CH3-C	2.77	1.60	1.49
3	A	901	XEE	C33-C28	2.73	1.43	1.39
3	A	901	XEE	C5-C10	-2.51	1.42	1.47
3	A	901	XEE	C12-N26	2.31	1.37	1.34
3	A	901	XEE	C3-C2	-2.30	1.35	1.38
4	A	903	ACT	CH3-C	2.16	1.57	1.49

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	901	XEE	N9-C8-N7	-9.68	118.25	126.31
3	A	901	XEE	C31-C33-C28	-7.35	115.70	120.46
3	A	901	XEE	C5-C10-N9	7.19	118.03	113.76
3	A	901	XEE	C6-N7-C8	6.13	122.92	116.69
3	A	901	XEE	C19-N14-C1	-5.08	104.27	118.11
3	A	901	XEE	C29-C28-C33	4.81	125.18	118.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	901	XEE	C23-C12-N26	-4.35	104.86	111.27
3	A	901	XEE	C6-C5-C10	-3.53	116.41	119.54
3	A	901	XEE	C32-C30-C31	3.44	126.09	120.00
3	A	901	XEE	C28-C27-N24	-3.19	107.34	111.94
3	A	901	XEE	N26-N25-N24	-2.82	105.12	107.22
3	A	901	XEE	C15-C16-N17	-2.77	104.91	110.42
3	A	901	XEE	C12-C11-N9	-2.72	108.72	112.75
3	A	901	XEE	C29-C32-C30	-2.47	116.57	119.98
3	A	901	XEE	C27-C28-C33	-2.44	115.48	120.23
3	A	901	XEE	C16-C15-N14	-2.39	105.76	110.78
3	A	901	XEE	C32-C29-C28	-2.29	117.98	121.00
3	A	901	XEE	C11-N9-C10	2.29	120.18	117.84
3	A	901	XEE	C18-N17-C16	-2.26	108.08	112.68

There are no chirality outliers.

All (2) torsion outliers are listed below:

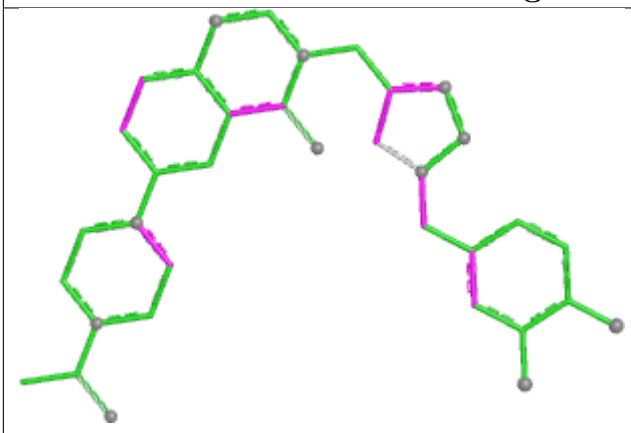
Mol	Chain	Res	Type	Atoms
3	A	901	XEE	N9-C11-C12-C23
3	A	901	XEE	N9-C11-C12-N26

There are no ring outliers.

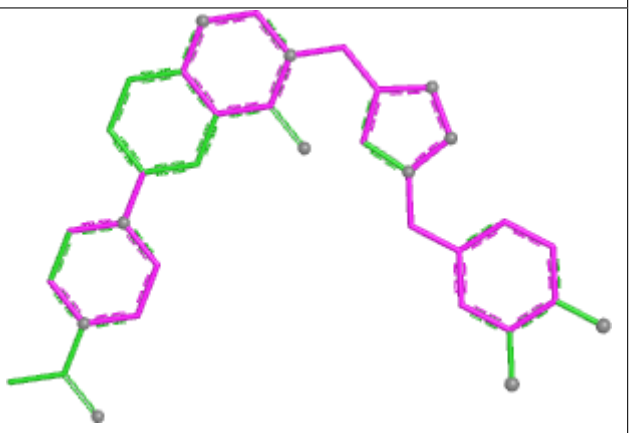
No monomer is involved in short contacts.

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 then 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.

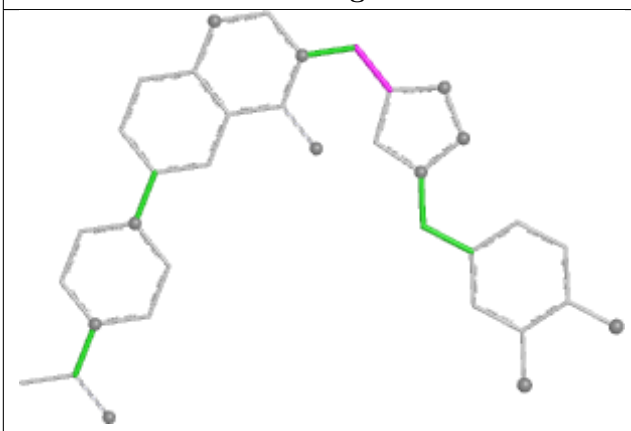
Ligand XEE A 901



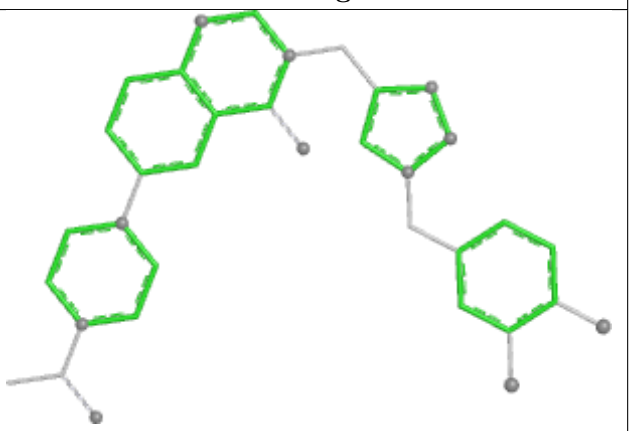
Bond lengths



Bond angles



Torsions



Rings

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, 95^{th} 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	806/846 (95%)	0.07	40 (4%) 35 39	9, 25, 61, 110	26 (3%)

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	397	ILE	6.3
1	A	578	LEU	6.1
1	A	572	VAL	5.8
1	A	469	PHE	5.8
1	A	464	PRO	5.7
1	A	468	CYS	5.2
1	A	463	LYS	4.6
1	A	272	THR	4.6
1	A	71	PRO	4.5
1	A	54	THR	4.5
1	A	465	SER	4.4
1	A	581	LEU	4.4
1	A	467	LYS	3.2
1	A	243	LEU	2.9
1	A	577	LYS	2.8
1	A	462	LYS	2.8
1	A	573	GLU	2.7
1	A	271	GLY	2.7
1	A	461	TYR	2.5
1	A	68	VAL	2.5
1	A	70	PRO	2.5
1	A	536	THR	2.4
1	A	470	PHE	2.4
1	A	860	SER	2.4
1	A	399	ASN	2.3
1	A	538	THR	2.3
1	A	466	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	585	LEU	2.2
1	A	55	SER	2.2
1	A	571	LYS	2.2
1	A	583	LYS	2.2
1	A	417	ASP	2.2
1	A	861	GLU	2.2
1	A	161	VAL	2.1
1	A	398	ASN	2.1
1	A	777	PHE	2.1
1	A	378	ASN	2.1
1	A	584	ARG	2.0
1	A	401	LYS	2.0
1	A	402	TYR	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)

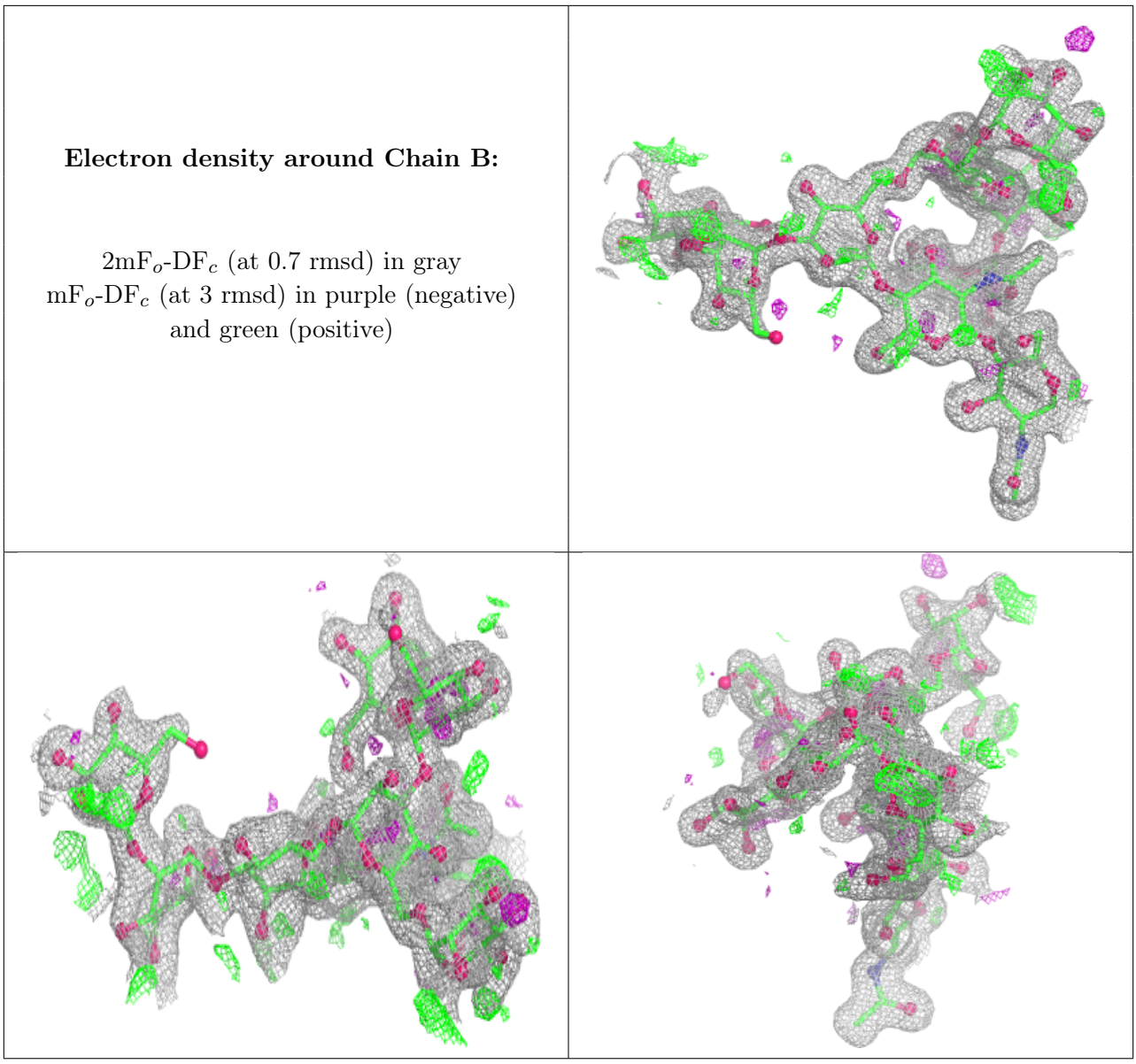
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	MAN	B	7	11/12	0.64	0.15	46,66,71,74	0
2	MAN	B	8	11/12	0.67	0.15	71,75,77,77	0
2	MAN	B	9	11/12	0.71	0.14	41,68,77,78	0
2	MAN	B	3	11/12	0.76	0.13	50,55,65,66	0
2	MAN	B	5	11/12	0.88	0.12	31,47,57,64	0
2	MAN	B	4	11/12	0.90	0.10	38,52,55,61	0
2	NAG	B	2	14/15	0.91	0.09	24,28,39,50	0
2	MAN	B	6	11/12	0.93	0.12	26,37,49,52	0
2	NAG	B	1	14/15	0.98	0.06	15,17,21,23	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

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, 95^{th} 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
4	ACT	A	903	4/4	0.85	0.14	43,47,47,50	0
3	XEE	A	901	35/35	0.94	0.08	20,24,30,38	0
4	ACT	A	902	4/4	0.95	0.08	22,28,33,35	0
7	CA	A	907	1/1	0.96	0.20	41,41,41,41	0
8	K	A	908	1/1	0.96	0.07	27,27,27,27	0

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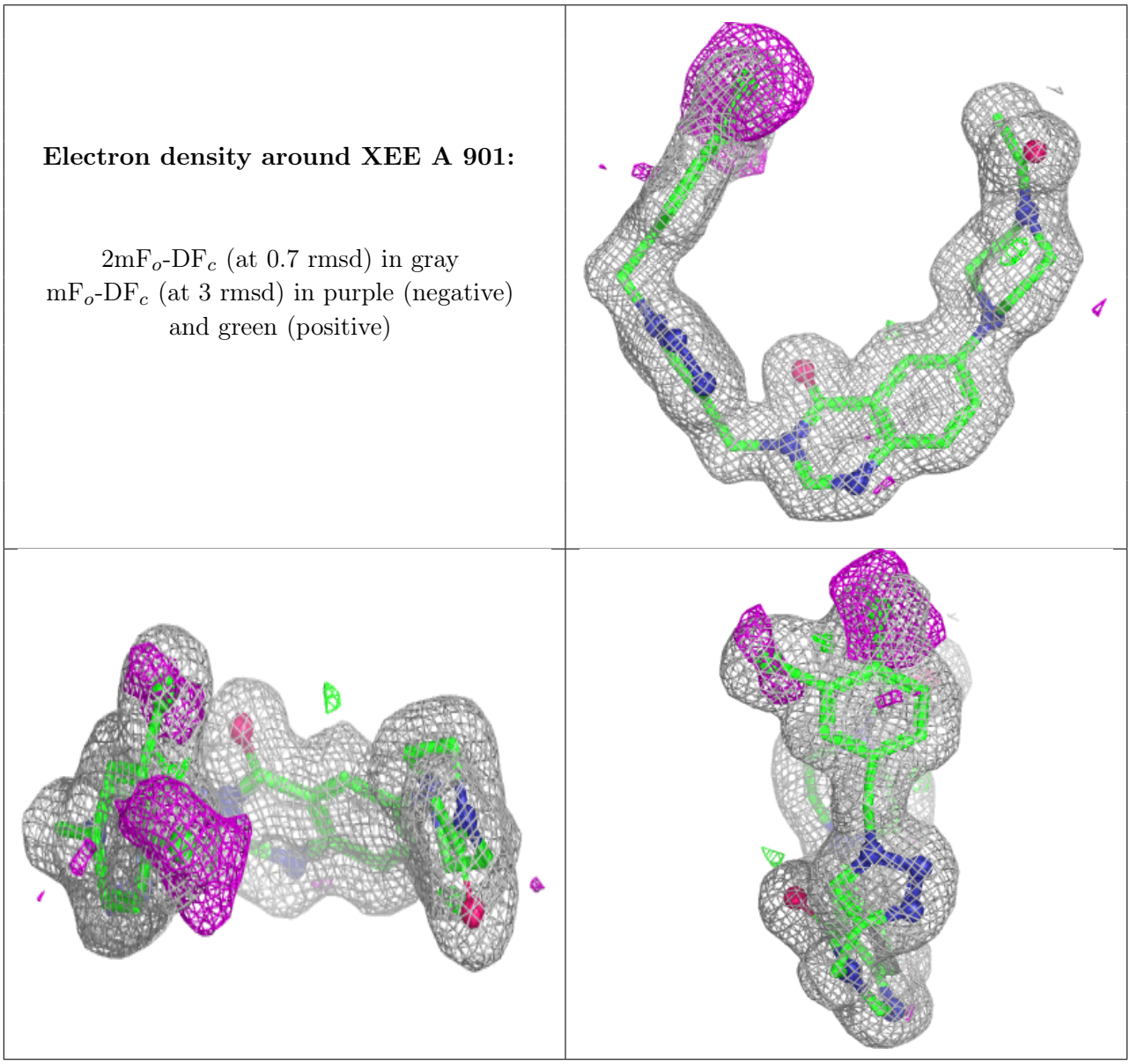
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	NA	A	905	1/1	0.97	0.08	27,27,27,27	0
5	ZN	A	904	1/1	0.99	0.03	20,20,20,20	0
7	CA	A	906	1/1	1.00	0.02	18,18,18,18	0

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.

Electron density around XEE A 901:

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



6.5 Other polymers

There are no such residues in this entry.