wwPDB X-ray Structure Validation Summary Report (i)

Jun 24, 2024 – 10:26 AM EDT

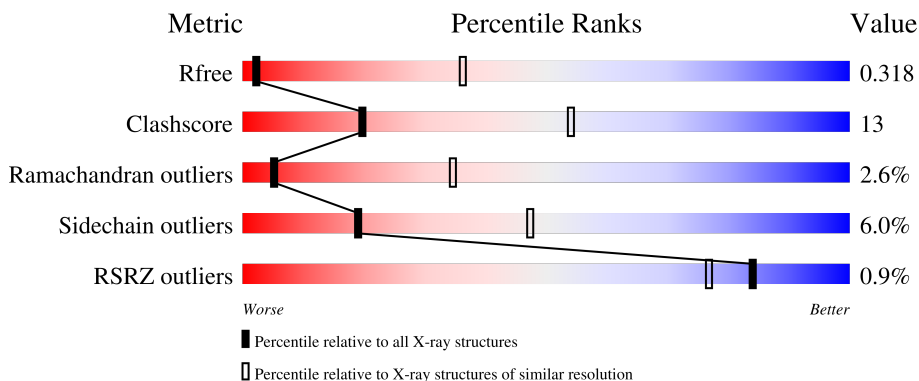|		
PDB ID	:	5T89
Title	:	Crystal structure of VEGF-A in complex with VEGFR-1 domains D1-6
Authors	:	Markovic-Mueller, S.; Stuttfeld, E.; Asthana, M.; Weinert, T.; Bliven, S.; Goldie, K.N.; Kisko, K.; Capitani, G.; Ballmer-Hofer, K.
Deposited on	:	2016-09-07
Resolution	:	4.00 Å(reported)

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 4.00 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	Percentile Ranks	Value
Rfree		0.318
Clashscore		13
Ramachandran outliers		2.6%
Sidechain outliers		6.0%
RSRZ outliers		0.9%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1087 (4.30-3.70)
Clashscore	141614	1148 (4.30-3.70)
Ramachandran outliers	138981	1108 (4.30-3.70)
Sidechain outliers	138945	1099 (4.30-3.70)
RSRZ outliers	127900	1028 (4.34-3.66)

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	V	131	63% 10% · 27%
1	W	131	65% 8% 27%
2	X	646	61% 27% · 8%
2	Y	646	59% 28% 5% 8%
3	A	2	100%

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Mol	Chain	Length	Quality of chain
3	B	2	

50% 50%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	B	2	-	-	-	X
4	NAG	X	705	-	-	-	X
4	NAG	Y	710	-	-	-	X
4	NAG	Y	711	-	-	-	X

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 11357 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 Vascular endothelial growth factor A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	V	96	Total	C	N	O	S	34	0	0
			779	489	131	146	13			
1	W	96	Total	C	N	O	S	0	0	0
			779	489	131	146	13			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
V	-9	GLY	-	expression tag	UNP P15692
V	-8	SER	-	expression tag	UNP P15692
V	-7	HIS	-	expression tag	UNP P15692
V	-6	HIS	-	expression tag	UNP P15692
V	-5	HIS	-	expression tag	UNP P15692
V	-4	HIS	-	expression tag	UNP P15692
V	-3	HIS	-	expression tag	UNP P15692
V	-2	HIS	-	expression tag	UNP P15692
V	-1	GLY	-	expression tag	UNP P15692
V	0	SER	-	expression tag	UNP P15692
V	115	ASN	LYS	conflict	UNP P15692
W	-9	GLY	-	expression tag	UNP P15692
W	-8	SER	-	expression tag	UNP P15692
W	-7	HIS	-	expression tag	UNP P15692
W	-6	HIS	-	expression tag	UNP P15692
W	-5	HIS	-	expression tag	UNP P15692
W	-4	HIS	-	expression tag	UNP P15692
W	-3	HIS	-	expression tag	UNP P15692
W	-2	HIS	-	expression tag	UNP P15692
W	-1	GLY	-	expression tag	UNP P15692
W	0	SER	-	expression tag	UNP P15692
W	115	ASN	LYS	conflict	UNP P15692

- Molecule 2 is a protein called Vascular endothelial growth factor receptor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	X	596	Total	C	N	O	S	183	0	0
			4734	3003	825	880	26			
2	Y	597	Total	C	N	O	S	0	0	0
			4743	3007	827	883	26			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	657	ASP	-	expression tag	UNP P17948
X	658	GLN	-	expression tag	UNP P17948
X	659	GLU	-	expression tag	UNP P17948
X	660	ALA	-	expression tag	UNP P17948
X	661	ILE	-	expression tag	UNP P17948
X	662	GLU	-	expression tag	UNP P17948
X	663	GLY	-	expression tag	UNP P17948
X	664	ARG	-	expression tag	UNP P17948
X	665	HIS	-	expression tag	UNP P17948
X	666	HIS	-	expression tag	UNP P17948
X	667	HIS	-	expression tag	UNP P17948
X	668	HIS	-	expression tag	UNP P17948
X	669	HIS	-	expression tag	UNP P17948
X	670	HIS	-	expression tag	UNP P17948
X	671	HIS	-	expression tag	UNP P17948
X	672	HIS	-	expression tag	UNP P17948
Y	657	ASP	-	expression tag	UNP P17948
Y	658	GLN	-	expression tag	UNP P17948
Y	659	GLU	-	expression tag	UNP P17948
Y	660	ALA	-	expression tag	UNP P17948
Y	661	ILE	-	expression tag	UNP P17948
Y	662	GLU	-	expression tag	UNP P17948
Y	663	GLY	-	expression tag	UNP P17948
Y	664	ARG	-	expression tag	UNP P17948
Y	665	HIS	-	expression tag	UNP P17948
Y	666	HIS	-	expression tag	UNP P17948
Y	667	HIS	-	expression tag	UNP P17948
Y	668	HIS	-	expression tag	UNP P17948
Y	669	HIS	-	expression tag	UNP P17948
Y	670	HIS	-	expression tag	UNP P17948
Y	671	HIS	-	expression tag	UNP P17948
Y	672	HIS	-	expression tag	UNP P17948

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a cetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	A	2	Total 28	C 16	N 2	O 10	0	0	0
3	B	2	Total 28	C 16	N 2	O 10	0	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).
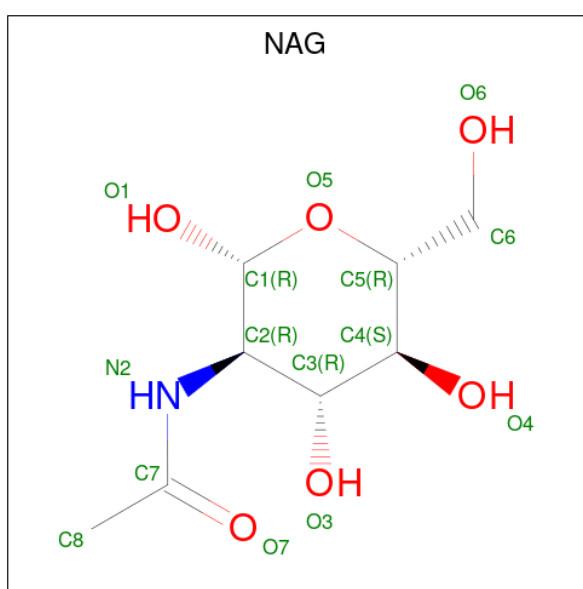
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	V	1	Total 14	C 8	N 1	O 5	0	0
4	W	1	Total 14	C 8	N 1	O 5	0	0
4	X	1	Total 14	C 8	N 1	O 5	0	0
4	X	1	Total 14	C 8	N 1	O 5	0	0
4	X	1	Total 14	C 8	N 1	O 5	0	0
4	X	1	Total 14	C 8	N 1	O 5	0	0
4	X	1	Total 14	C 8	N 1	O 5	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	X	1	Total	C	N	O	0	0
			14	8	1	5		
4	X	1	Total	C	N	O	0	0
			14	8	1	5		
4	X	1	Total	C	N	O	0	0
			14	8	1	5		
4	Y	1	Total	C	N	O	0	0
			14	8	1	5		
4	Y	1	Total	C	N	O	0	0
			14	8	1	5		
4	Y	1	Total	C	N	O	0	0
			14	8	1	5		
4	Y	1	Total	C	N	O	0	0
			14	8	1	5		
4	Y	1	Total	C	N	O	0	0
			14	8	1	5		
4	Y	1	Total	C	N	O	0	0
			14	8	1	5		
4	Y	1	Total	C	N	O	0	0
			14	8	1	5		
4	Y	1	Total	C	N	O	0	0
			14	8	1	5		
4	Y	1	Total	C	N	O	0	0
			14	8	1	5		

3 Residue-property plots ⓘ

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: Vascular endothelial growth factor A
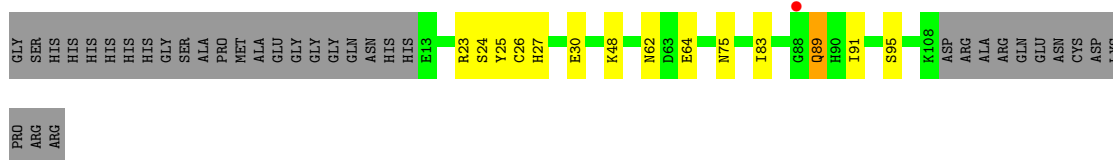
- Molecule 1: Vascular endothelial growth factor A

- Molecule 2: Vascular endothelial growth factor receptor 1
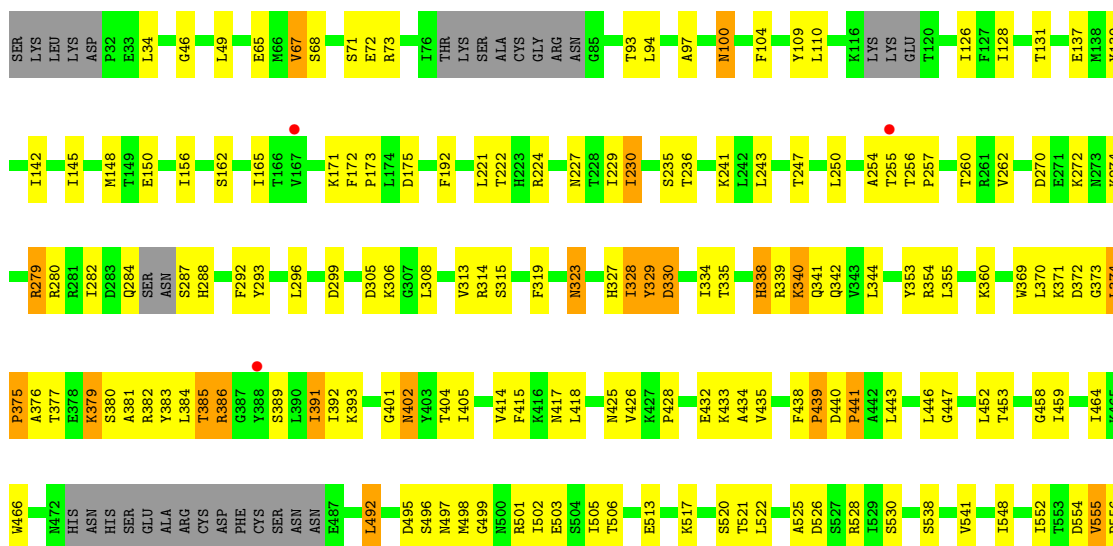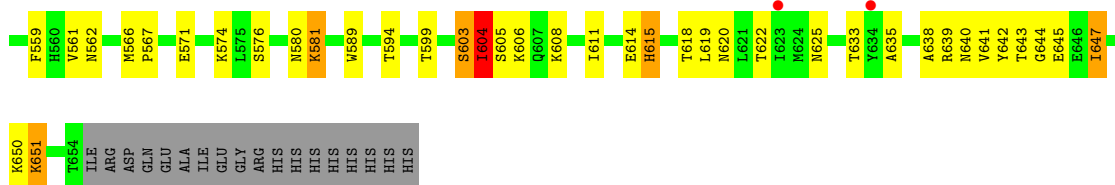
F559 H560 V561 N562 M566 P567 E571 K574 L575 S576 N580 K581 W589 T594 T599 S603 I604 S605 K606 Q607 K608 I611 E614 H615 T618 L619 N620 L621 I622 I623 M624 N625 T633 Y634 A635 A638 R639 N640 V641 Y642 T643 G644 E645 E646 I647

K650 K651 T654 ILE ARG ASP GLN GLU ALA ILE GLU GLY ARG HIS HIS HIS HIS HIS HIS

• Molecule 2: Vascular endothelial growth factor receptor 1

Chain Y:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-gluc opyranose

Chain A:

NAG1 NAG2

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-gluc opyranose

Chain B:

NAG1 NAG2
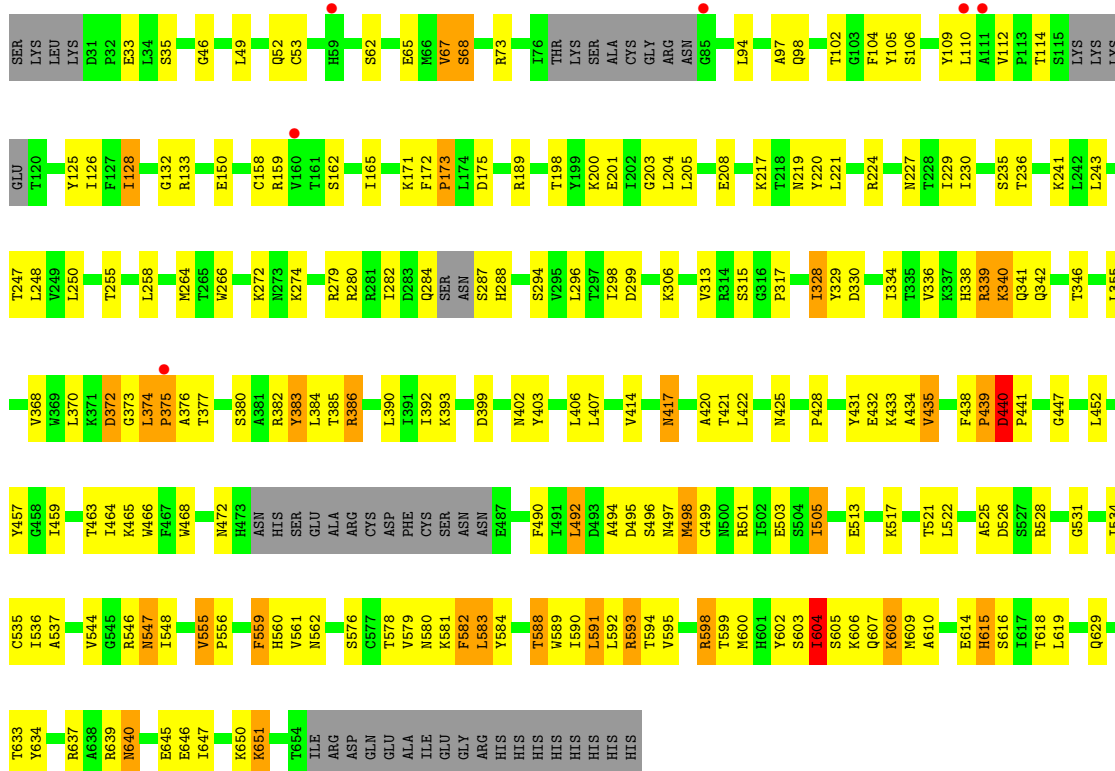
4   Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	166.71Å 123.09Å 167.37Å 90.00° 109.56° 90.00°	Depositor
Resolution (Å)	19.99 – 4.00 49.25 – 4.00	Depositor EDS
% Data completeness (in resolution range)	99.5 (19.99-4.00) 99.6 (49.25-4.00)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.89 (at 4.00Å)	Xtriage
Refinement program	PHENIX dev_2420	Depositor
R, R_{free}	0.285 , 0.315 0.293 , 0.318	Depositor DCC
R_{free} test set	810 reflections (3.00%)	wwPDB-VP
Wilson B-factor (Å^2)	138.9	Xtriage
Anisotropy	0.519	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 159.7	EDS
L-test for twinning[2]	$< |L| > = 0.43, < L^2 > = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	11357	wwPDB-VP
Average B, all atoms (Å^2)	219.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.02% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG

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	V	0.27	0/797	0.43	0/1073
1	W	0.26	0/797	0.42	0/1073
2	X	0.27	0/4825	0.49	1/6531 (0.0%)
2	Y	0.27	0/4835	0.49	0/6547
All	All	0.27	0/11254	0.48	1/15224 (0.0%)

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
2	Y	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	X	603	SER	C-N-CA	5.55	135.57	121.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	Y	372	ASP	Peptide
2	Y	440	ASP	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	V	779	0	744	13	0
1	W	779	0	744	14	0
2	X	4734	0	4815	131	0
2	Y	4743	0	4811	143	0
3	A	28	0	25	0	0
3	B	28	0	25	1	0
4	V	14	0	13	0	0
4	W	14	0	13	3	0
4	X	112	0	104	3	0
4	Y	126	0	117	2	0
All	All	11357	0	11411	284	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 13.

The worst 5 of 284 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)
2:Y:241:LYS:NZ	2:Y:330:ASP:OD2	2.08	0.86
2:Y:150:GLU:OE1	2:Y:224:ARG:NH1	2.12	0.81
2:Y:562:ASN:HB3	2:Y:576:SER:HB3	1.64	0.78
1:V:23:ARG:NH2	1:W:30:GLU:OE2	2.18	0.77
2:X:603:SER:HB3	2:X:604:ILE:O	1.87	0.75

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	V	94/131 (72%)	90 (96%)	3 (3%)	1 (1%)	14	51
1	W	94/131 (72%)	90 (96%)	4 (4%)	0	100	100
2	X	586/646 (91%)	474 (81%)	96 (16%)	16 (3%)	5	34
2	Y	587/646 (91%)	483 (82%)	85 (14%)	19 (3%)	4	31
All	All	1361/1554 (88%)	1137 (84%)	188 (14%)	36 (3%)	5	34

5 of 36 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	X	67	VAL
2	X	581	LYS
2	X	604	ILE
2	Y	68	SER
2	Y	604	ILE

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	V	91/118 (77%)	90 (99%)	1 (1%)	73	85
1	W	91/118 (77%)	91 (100%)	0	100	100
2	X	537/582 (92%)	503 (94%)	34 (6%)	18	46
2	Y	538/582 (92%)	497 (92%)	41 (8%)	13	40
All	All	1257/1400 (90%)	1181 (94%)	76 (6%)	19	47

5 of 76 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	Y	555	VAL
2	Y	645	GLU
2	Y	561	VAL
2	Y	598	ARG

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Mol	Chain	Res	Type
2	Y	651	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
2	Y	580	ASN
2	Y	425	ASN
2	Y	284	GLN
2	X	425	ASN
2	Y	338	HIS

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 ⓘ

4 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	$\#|Z| > 2$
3	NAG	A	1	2,3	14,14,15	0.55	0	17,19,21	0.49	0
3	NAG	A	2	3	14,14,15	0.28	0	17,19,21	0.56	0
3	NAG	B	1	2,3	14,14,15	0.77	1 (7%)	17,19,21	1.20	1 (5%)
3	NAG	B	2	3	14,14,15	0.50	0	17,19,21	0.48	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	NAG	A	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	A	2	3	-	3/6/23/26	0/1/1/1
3	NAG	B	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	B	2	3	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1	NAG	O5-C1	2.72	1.48	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1	NAG	C1-O5-C5	4.77	118.65	112.19

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2	NAG	C4-C5-C6-O6
3	B	1	NAG	C4-C5-C6-O6
3	A	2	NAG	O5-C5-C6-O6
3	A	1	NAG	O5-C5-C6-O6
3	B	1	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2	NAG	1	0
3	B	1	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.

Oligosaccharide Chain A

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain B

Bond lengths

Bond angles

Torsions

Rings
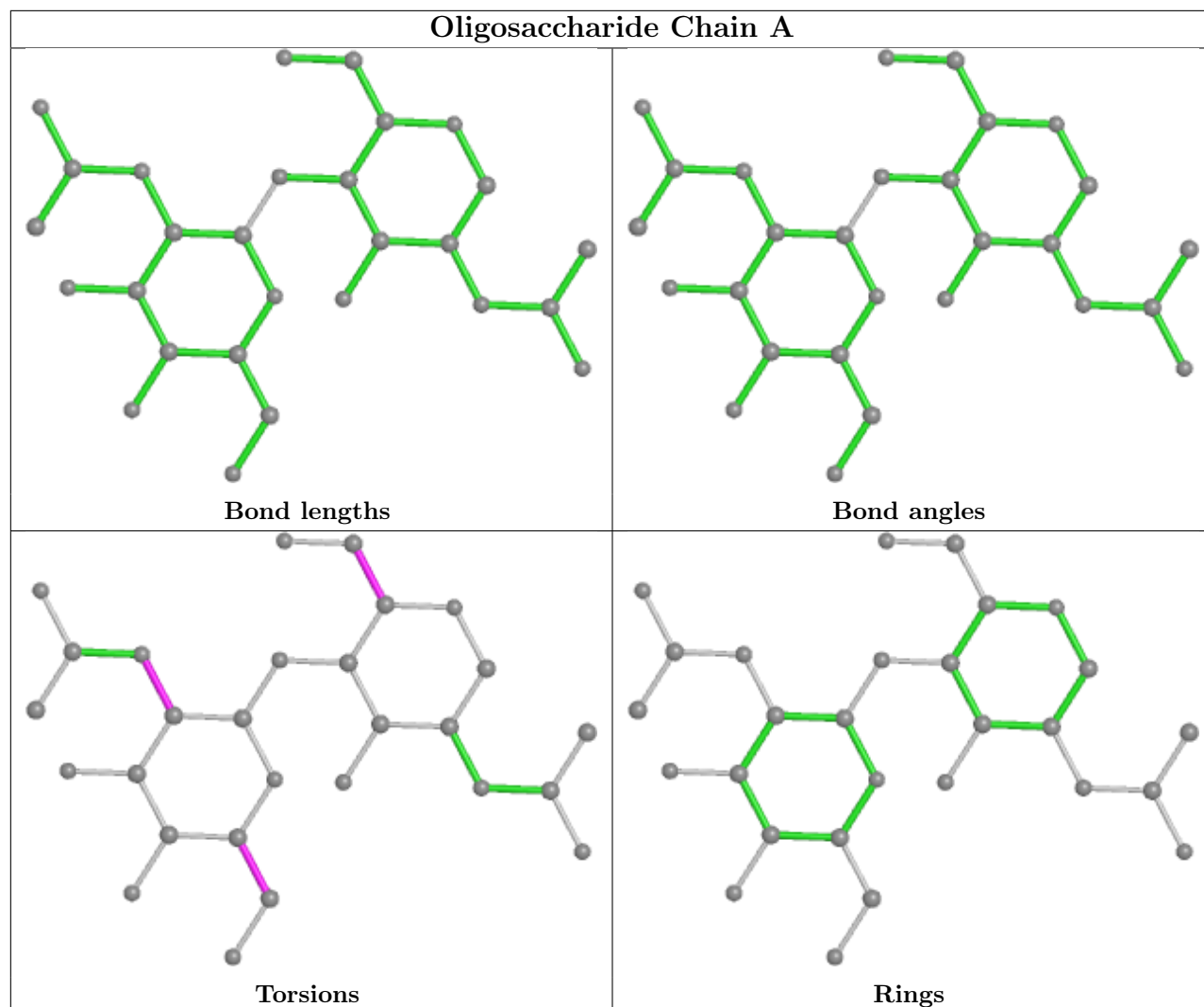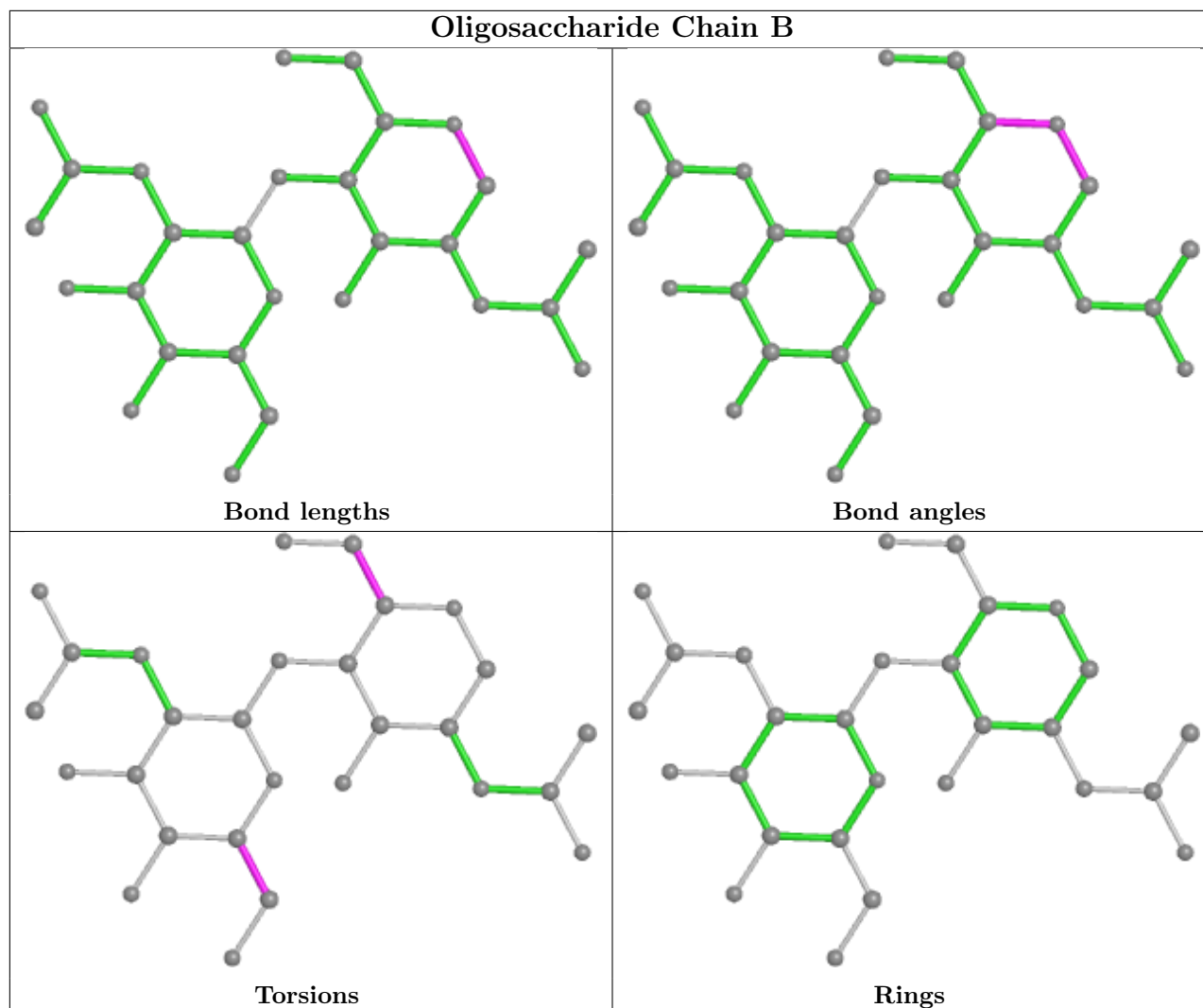
5.6 Ligand geometry (i)

19 ligands 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	$\#|Z| > 2$
4	NAG	W	201	1	14,14,15	0.26	0	17,19,21	0.39	0
4	NAG	Y	709	2	14,14,15	0.20	0	17,19,21	0.32	0
4	NAG	X	703	2	14,14,15	0.94	1 (7%)	17,19,21	1.25	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
4	NAG	X	707	2	14,14,15	0.43	0	17,19,21	0.41	0
4	NAG	V	201	1	14,14,15	0.48	0	17,19,21	0.66	0
4	NAG	Y	701	2	14,14,15	0.86	1 (7%)	17,19,21	1.32	1 (5%)
4	NAG	Y	711	-	14,14,15	0.25	0	17,19,21	0.39	0
4	NAG	X	704	2	14,14,15	0.24	0	17,19,21	0.42	0
4	NAG	X	710	-	14,14,15	0.24	0	17,19,21	0.42	0
4	NAG	X	705	2	14,14,15	0.35	0	17,19,21	1.26	2 (11%)
4	NAG	X	709	2	14,14,15	0.46	0	17,19,21	0.62	0
4	NAG	Y	708	2	14,14,15	0.25	0	17,19,21	0.44	0
4	NAG	Y	707	2	14,14,15	0.34	0	17,19,21	0.32	0
4	NAG	Y	710	2	14,14,15	0.26	0	17,19,21	0.44	0
4	NAG	Y	705	2	14,14,15	0.22	0	17,19,21	0.47	0
4	NAG	X	708	2	14,14,15	0.19	0	17,19,21	0.46	0
4	NAG	Y	702	2	14,14,15	0.21	0	17,19,21	0.43	0
4	NAG	Y	706	2	14,14,15	0.23	0	17,19,21	0.55	0
4	NAG	X	706	2	14,14,15	1.37	2 (14%)	17,19,21	1.74	4 (23%)

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
4	NAG	W	201	1	-	2/6/23/26	0/1/1/1
4	NAG	Y	709	2	-	2/6/23/26	0/1/1/1
4	NAG	X	703	2	-	1/6/23/26	0/1/1/1
4	NAG	X	707	2	-	2/6/23/26	0/1/1/1
4	NAG	V	201	1	-	2/6/23/26	0/1/1/1
4	NAG	Y	701	2	-	2/6/23/26	0/1/1/1
4	NAG	Y	711	-	-	4/6/23/26	0/1/1/1
4	NAG	X	704	2	-	2/6/23/26	0/1/1/1
4	NAG	X	710	-	-	2/6/23/26	0/1/1/1
4	NAG	X	705	2	-	5/6/23/26	0/1/1/1
4	NAG	X	709	2	-	3/6/23/26	0/1/1/1
4	NAG	Y	708	2	-	2/6/23/26	0/1/1/1
4	NAG	Y	707	2	-	2/6/23/26	0/1/1/1
4	NAG	Y	710	2	-	2/6/23/26	0/1/1/1
4	NAG	Y	705	2	-	0/6/23/26	0/1/1/1
4	NAG	X	708	2	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	Y	702	2	-	2/6/23/26	0/1/1/1
4	NAG	Y	706	2	-	3/6/23/26	0/1/1/1
4	NAG	X	706	2	-	4/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	X	706	NAG	O5-C1	-3.80	1.37	1.43
4	X	703	NAG	O5-C1	3.40	1.49	1.43
4	Y	701	NAG	O5-C1	3.08	1.48	1.43
4	X	706	NAG	C1-C2	2.72	1.56	1.52

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	X	703	NAG	C1-O5-C5	4.90	118.83	112.19
4	Y	701	NAG	C1-O5-C5	4.88	118.81	112.19
4	X	706	NAG	C2-N2-C7	4.44	129.22	122.90
4	X	705	NAG	C2-N2-C7	4.35	129.09	122.90
4	X	706	NAG	C4-C3-C2	3.89	116.72	111.02

There are no chirality outliers.

5 of 44 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	Y	707	NAG	C4-C5-C6-O6
4	X	704	NAG	C4-C5-C6-O6
4	X	708	NAG	C4-C5-C6-O6
4	X	709	NAG	C4-C5-C6-O6
4	X	710	NAG	O5-C5-C6-O6

There are no ring outliers.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	W	201	NAG	3	0
4	X	707	NAG	1	0
4	Y	701	NAG	1	0
4	X	705	NAG	1	0
4	X	709	NAG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	Y	707	NAG	1	0

5.7 Other polymers ⓘ

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(Å²)	Q<0.9
1	V	92/131 (70%)	-0.17	1 (1%)	80	72	168, 217, 251, 273	0
1	W	96/131 (73%)	-0.21	0	100	100	152, 226, 254, 268	0
2	X	571/646 (88%)	-0.13	5 (0%)	84	77	139, 233, 290, 338	0
2	Y	597/646 (92%)	-0.15	6 (1%)	82	74	122, 211, 273, 352	0
All	All	1356/1554 (87%)	-0.15	12 (0%)	84	77	122, 221, 281, 352	0

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	V	88	GLY	3.6
2	Y	59	HIS	2.8
2	Y	85	GLY	2.8
2	X	167	VAL	2.6
2	Y	110	LEU	2.3

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

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

6.3 Carbohydrates ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.
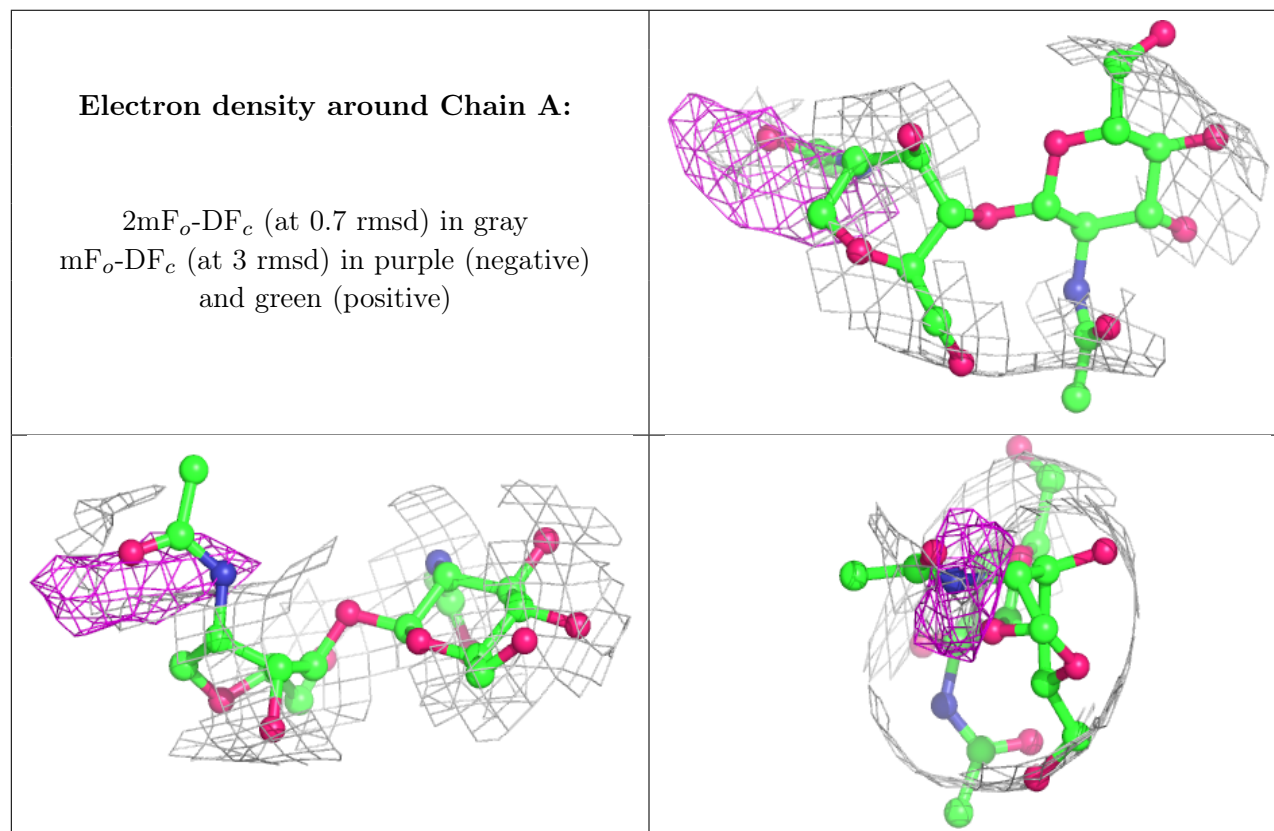
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å²)	Q<0.9
3	NAG	B	2	14/15	0.46	0.66	332,332,332,332	0
3	NAG	A	1	14/15	0.77	0.28	266,266,266,266	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	B	1	14/15	0.86	0.49	328,328,328,328	0
3	NAG	A	2	14/15	0.88	0.15	272,272,272,272	0

The following is a graphical depiction of the model fit to experimental electron density for oligosac-charide. Each fit is shown from different orientation to approximate a three-dimensional view.
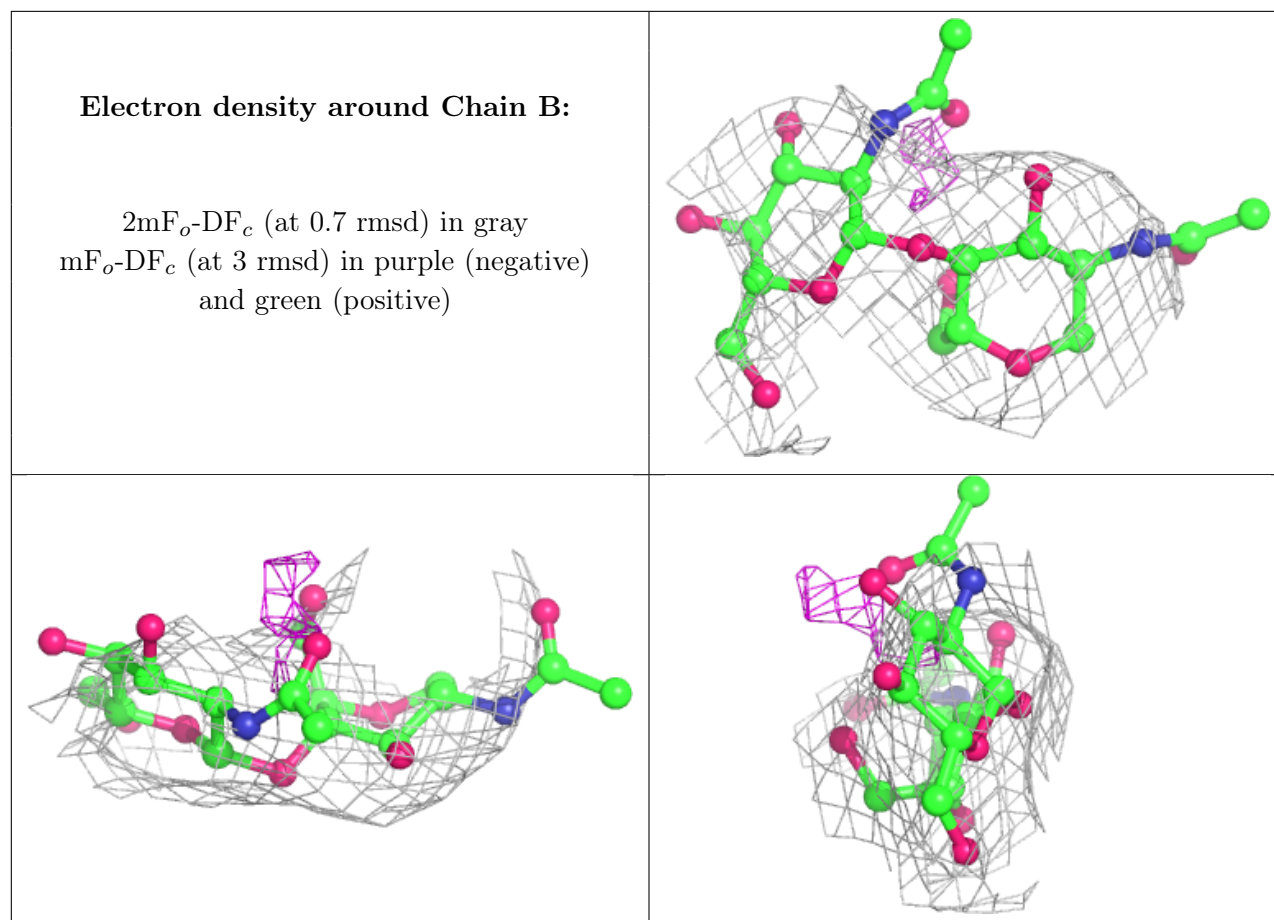
Electron density around Chain A:

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

Electron density around Chain B:

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

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
4	NAG	X	705	14/15	0.52	0.51	293,293,293,293	0
4	NAG	X	704	14/15	0.65	0.32	283,283,283,283	0
4	NAG	X	703	14/15	0.66	0.23	322,322,322,322	0
4	NAG	Y	711	14/15	0.66	0.80	247,247,247,247	0
4	NAG	X	706	14/15	0.67	0.20	284,284,284,284	0
4	NAG	Y	708	14/15	0.69	0.26	280,280,280,280	0
4	NAG	X	707	14/15	0.69	0.16	297,297,297,297	0
4	NAG	X	708	14/15	0.70	0.24	265,265,265,265	0
4	NAG	Y	710	14/15	0.74	0.41	289,289,289,289	0
4	NAG	X	710	14/15	0.75	0.14	273,273,273,273	0
4	NAG	Y	707	14/15	0.76	0.31	241,241,241,241	0
4	NAG	Y	701	14/15	0.76	0.30	240,240,240,240	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAG	W	201	14/15	0.78	0.28	248,248,248,248	0
4	NAG	Y	702	14/15	0.78	0.22	296,296,296,296	0
4	NAG	Y	709	14/15	0.80	0.32	273,273,273,273	0
4	NAG	Y	705	14/15	0.81	0.37	255,255,255,255	0
4	NAG	V	201	14/15	0.83	0.24	262,262,262,262	0
4	NAG	Y	706	14/15	0.85	0.42	243,243,243,243	0
4	NAG	X	709	14/15	0.86	0.40	280,280,280,280	0

6.5 Other polymers ⓘ

There are no such residues in this entry.