



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 07:25 AM BST

PDB ID : 4V3E
Title : The CIDRa domain from IT4var07 PfEMP1 bound to endothelial protein C receptor
Authors : Lau, C.K.Y.; Turner, L.; Jespersen, J.S.; Lowe, E.D.; Petersen, B.; Wang, C.W.; Petersen, J.E.V.; Lusingu, J.; Theander, T.G.; Lavstsen, T.; Higgins, M.K.
Deposited on : 2014-10-17
Resolution : 2.90 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

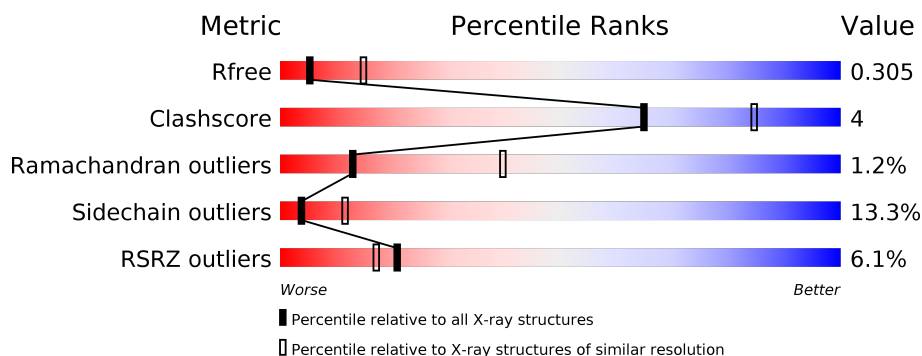
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	251	
2	B	171	
3	C	3	
4	D	2	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 3126 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.

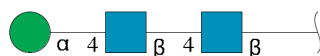
- Molecule 1 is a protein called IT4VAR07 CIDRA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	192	Total	C	N	O	S	0	0	0
			1614	1036	263	304	11			

- Molecule 2 is a protein called ENDOTHELIAL PROTEIN C RECEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	167	Total	C	N	O	S	0	0	0
			1367	873	243	247	4			

- 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.



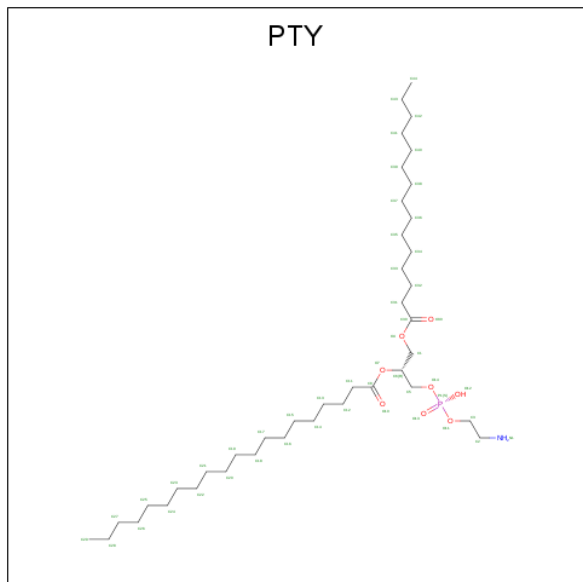
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	3	Total	C	N	O	0	0	0
			39	22	2	15			

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



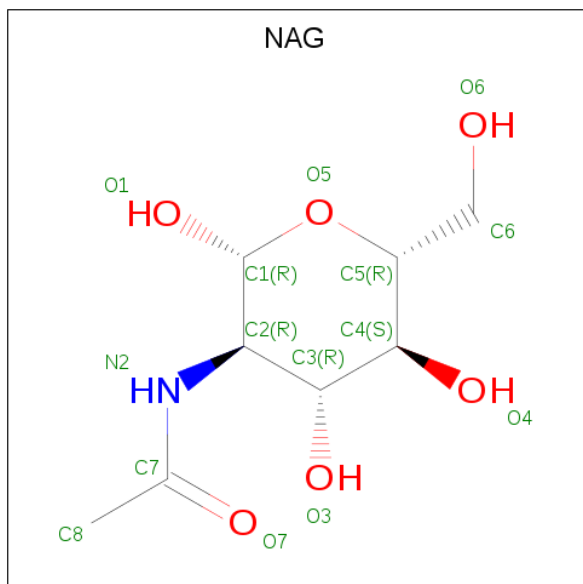
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is PHOSPHATIDYLETHANOLAMINE (three-letter code: PTY) (formula: $C_{40}H_{80}NO_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	50	0
			50	40	1	8	1		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	N	O	0	0
			14	8	1	5		

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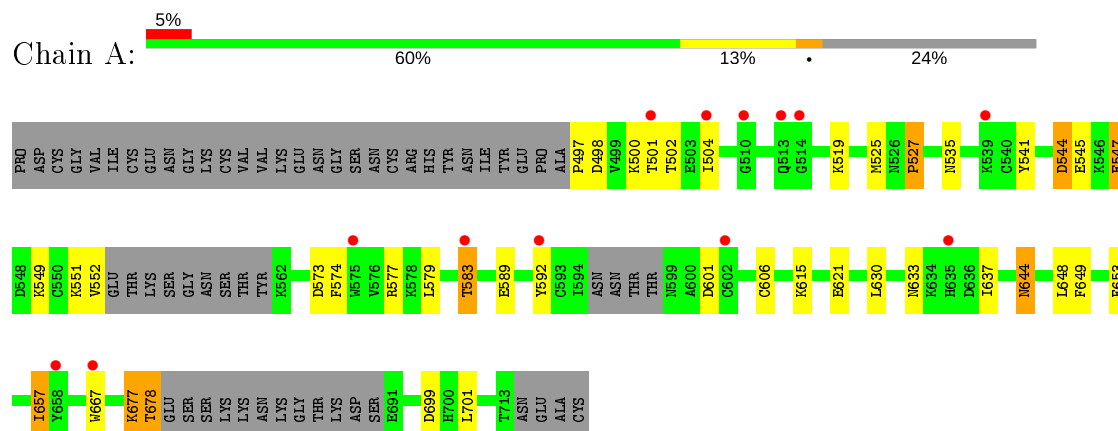
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	N	O	0	0
			14	8	1	5		

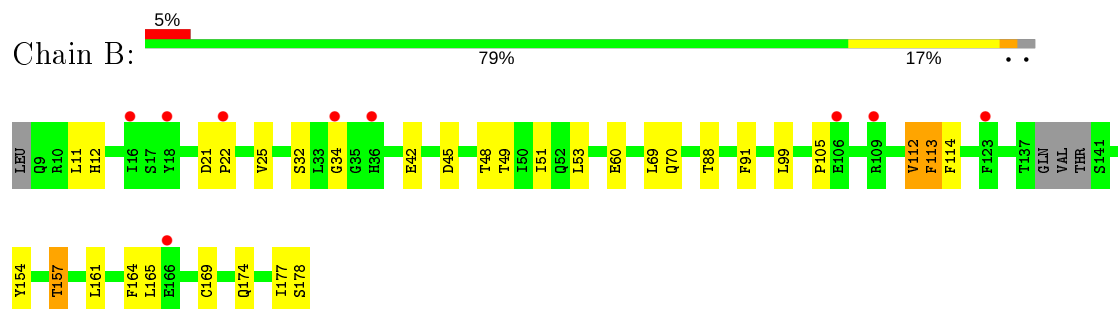
3 Residue-property plots [i](#)

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: IT4VAR07 CIDRA



- Molecule 2: ENDOTHELIAL PROTEIN C RECEPTOR



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



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



MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	56.02Å 56.02Å 250.50Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	83.50 – 2.90 48.51 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (83.50-2.90) 99.8 (48.51-2.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 2.91Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.247 , 0.276 0.259 , 0.305	Depositor DCC
R_{free} test set	520 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å ²)	103.0	Xtriage
Anisotropy	0.413	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 97.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.047 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3126	wwPDB-VP
Average B, all atoms (Å ²)	122.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.49% 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: NAG, PTY, 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	0.55	0/1646	0.80	2/2208 (0.1%)
2	B	0.54	0/1404	0.74	0/1909
All	All	0.55	0/3050	0.77	2/4117 (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
1	A	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	678	THR	N-CA-C	-7.24	91.45	111.00
1	A	677	LYS	N-CA-C	7.08	130.12	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	497	PRO	Peptide

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	1614	0	1578	13	0
2	B	1367	0	1315	12	0
3	C	39	0	34	0	0
4	D	28	0	25	0	0
5	B	50	0	79	0	0
6	B	28	0	26	0	0
All	All	3126	0	3057	25	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 (25) 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:579:LEU:O	1:A:583:THR:HG23	1.63	0.95
1:A:644:ASN:H	1:A:644:ASN:HD22	1.34	0.76
1:A:527:PRO:HB3	1:A:615:LYS:HD3	1.69	0.72
1:A:653:PHE:O	1:A:657:ILE:HB	1.94	0.68
1:A:677:LYS:HE3	1:A:699:ASP:HB3	1.76	0.67
2:B:112:VAL:HG21	2:B:165:LEU:HB3	1.79	0.63
2:B:22:PRO:HG3	2:B:91:PHE:CE2	2.35	0.62
2:B:112:VAL:CG2	2:B:165:LEU:HB3	2.33	0.59
2:B:161:LEU:O	2:B:165:LEU:HD23	2.05	0.57
1:A:649:PHE:HA	1:A:667:TRP:CZ2	2.42	0.55
2:B:154:TYR:HB2	2:B:157:THR:HG22	1.91	0.53
1:A:644:ASN:H	1:A:644:ASN:ND2	2.05	0.51
1:A:573:ASP:OD1	1:A:577:ARG:NH1	2.44	0.51
2:B:174:GLN:O	2:B:178:SER:HB3	2.13	0.49
2:B:25:VAL:CG1	2:B:45:ASP:HB3	2.42	0.49
2:B:25:VAL:HG12	2:B:45:ASP:HB3	1.96	0.46
1:A:544:ASP:HB2	1:A:547:GLU:H	1.81	0.46
1:A:501:THR:HG22	1:A:541:TYR:HD1	1.81	0.45
1:A:501:THR:HG22	1:A:541:TYR:CD1	2.53	0.44
1:A:583:THR:HB	1:A:701:LEU:HD21	1.99	0.43
2:B:21:ASP:HB2	2:B:22:PRO:CD	2.49	0.42
1:A:649:PHE:HA	1:A:667:TRP:HZ2	1.81	0.41
2:B:164:PHE:HD2	2:B:165:LEU:HD22	1.85	0.41
2:B:113:PHE:CD1	2:B:113:PHE:N	2.89	0.40
2:B:165:LEU:O	2:B:169:CYS:HB3	2.20	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	184/251 (73%)	172 (94%)	11 (6%)	1 (0%)	29	61
2	B	163/171 (95%)	151 (93%)	9 (6%)	3 (2%)	8	29
All	All	347/422 (82%)	323 (93%)	20 (6%)	4 (1%)	13	40

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	527	PRO
2	B	34	GLY
2	B	105	PRO
2	B	88	THR

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	183/235 (78%)	156 (85%)	27 (15%)	3	9
2	B	149/153 (97%)	132 (89%)	17 (11%)	5	17
All	All	332/388 (86%)	288 (87%)	44 (13%)	4	11

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	498	ASP
1	A	500	LYS
1	A	502	THR
1	A	504	ILE
1	A	519	LYS
1	A	525	MET
1	A	535	ASN
1	A	544	ASP
1	A	545	GLU
1	A	547	GLU
1	A	549	LYS
1	A	551	LYS
1	A	552	VAL
1	A	574	PHE
1	A	583	THR
1	A	589	GLU
1	A	592	TYR
1	A	601	ASP
1	A	606	CYS
1	A	621	GLU
1	A	630	LEU
1	A	633	ASN
1	A	637	ILE
1	A	644	ASN
1	A	648	LEU
1	A	657	ILE
1	A	678	THR
2	B	11	LEU
2	B	12	HIS
2	B	32	SER
2	B	42	GLU
2	B	48	THR
2	B	49	THR
2	B	51	ILE
2	B	53	LEU
2	B	60	GLU
2	B	69	LEU
2	B	70	GLN
2	B	99	LEU
2	B	112	VAL
2	B	113	PHE
2	B	114	PHE
2	B	157	THR

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Mol	Chain	Res	Type
2	B	177	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	505	ASN
1	A	534	ASN
1	A	607	ASN
1	A	644	ASN
2	B	171	GLN

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 ⓘ

5 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	C	1	3,2	14,14,15	0.36	0	17,19,21	0.70	0
3	NAG	C	2	3	14,14,15	0.38	0	17,19,21	1.90	3 (17%)
3	MAN	C	3	3	11,11,12	0.52	0	15,15,17	1.07	2 (13%)
4	NAG	D	1	2,4	14,14,15	0.47	0	17,19,21	1.89	2 (11%)
4	NAG	D	2	4	14,14,15	0.38	0	17,19,21	1.99	3 (17%)

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	C	1	3,2	-	1/6/23/26	0/1/1/1
3	NAG	C	2	3	-	2/6/23/26	0/1/1/1
3	MAN	C	3	3	-	0/2/19/22	0/1/1/1
4	NAG	D	1	2,4	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	2	NAG	O5-C1-C2	6.79	122.01	111.29
3	C	2	NAG	C1-O5-C5	6.18	120.57	112.19
4	D	1	NAG	C1-O5-C5	5.38	119.49	112.19
4	D	1	NAG	O5-C1-C2	4.37	118.19	111.29
4	D	2	NAG	C1-O5-C5	3.54	116.99	112.19
3	C	2	NAG	O5-C1-C2	3.36	116.59	111.29
3	C	3	MAN	C1-C2-C3	3.18	113.57	109.67
3	C	2	NAG	O4-C4-C3	2.47	116.05	110.35
4	D	2	NAG	C1-C2-N2	-2.19	106.75	110.49
3	C	3	MAN	C1-O5-C5	2.17	115.13	112.19

There are no chirality outliers.

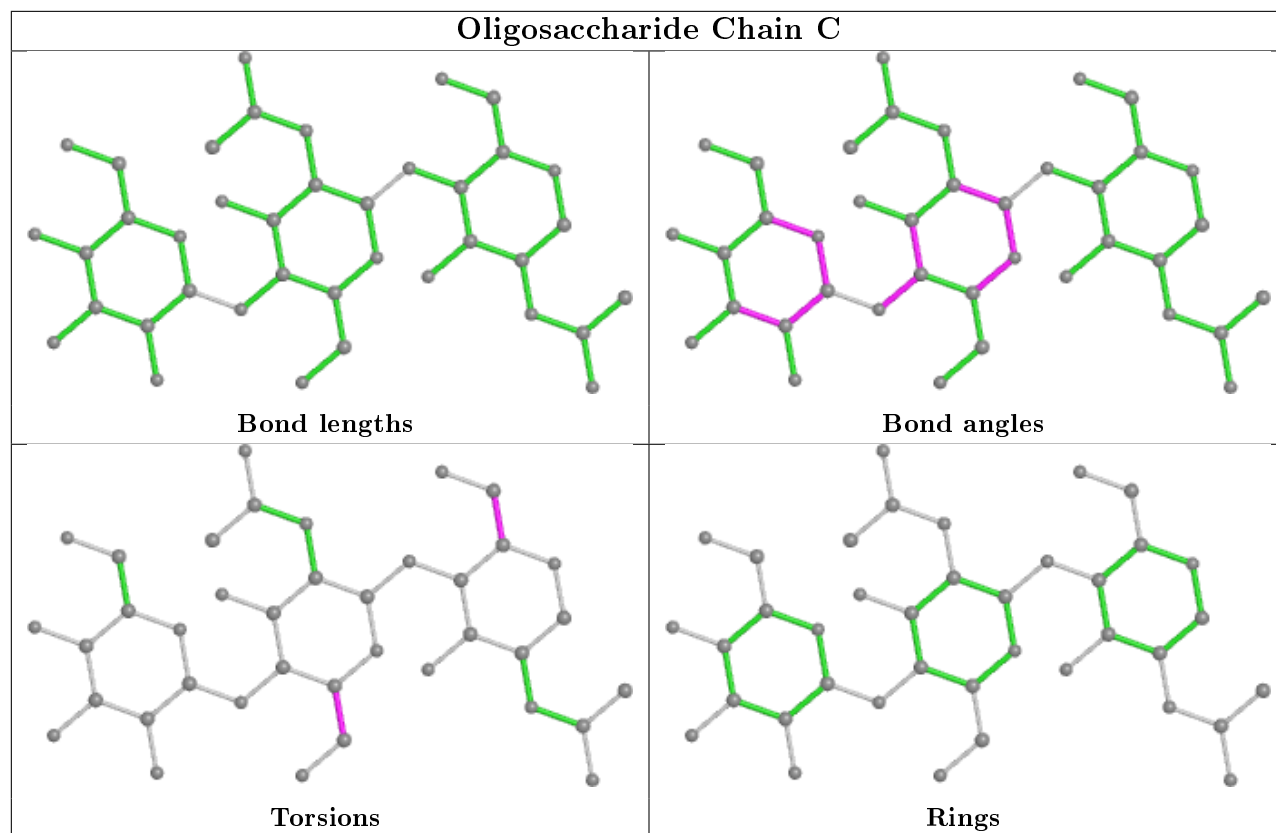
All (3) torsion outliers are listed below:

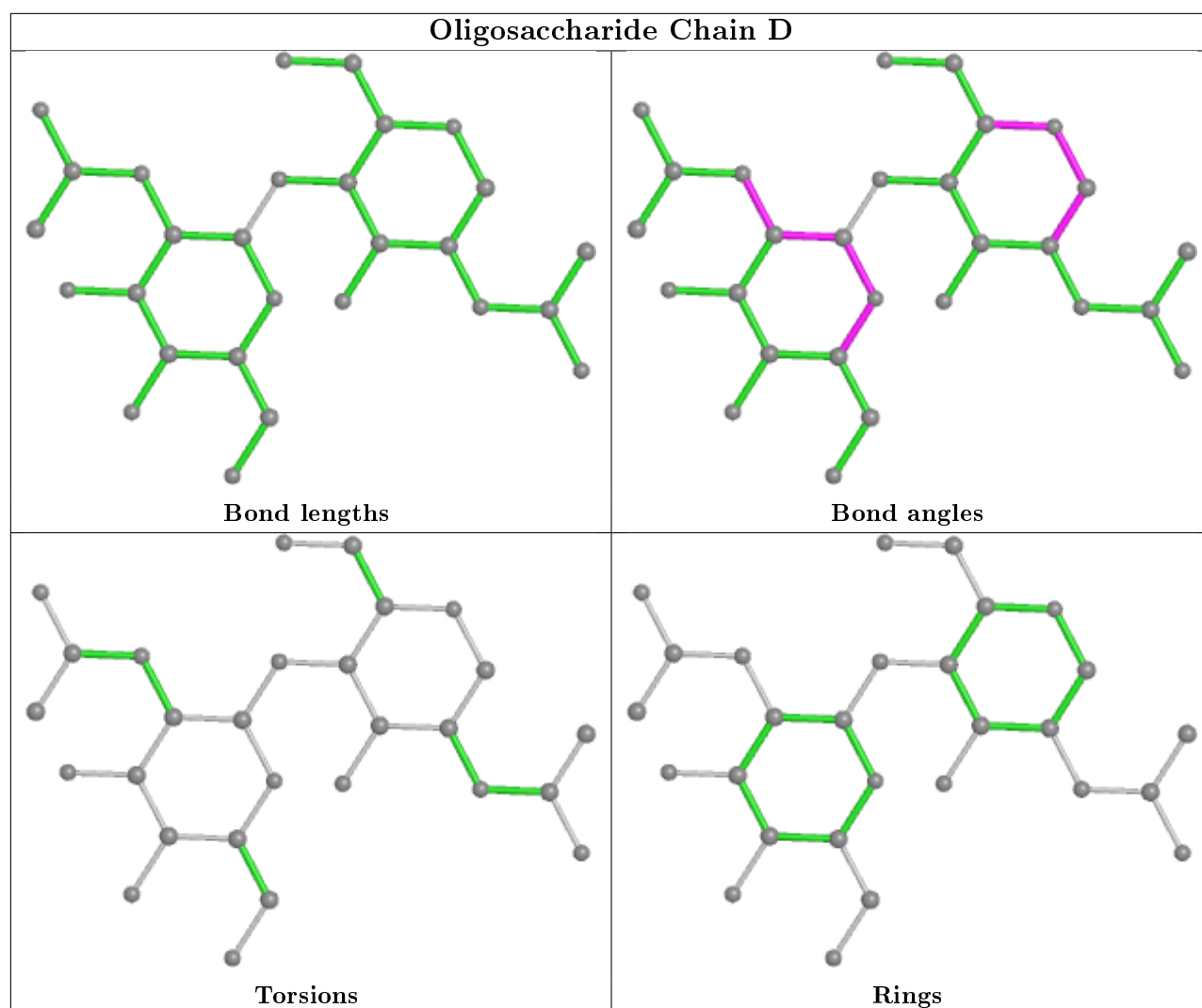
Mol	Chain	Res	Type	Atoms
3	C	2	NAG	C4-C5-C6-O6
3	C	1	NAG	O5-C5-C6-O6
3	C	2	NAG	O5-C5-C6-O6

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](#)

3 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	$\# Z > 2$
6	NAG	B	201	2	14,14,15	0.39	0	17,19,21	1.22	2 (11%)
5	PTY	B	200	-	49,49,49	0.35	0	52,54,54	0.61	2 (3%)
6	NAG	B	206	2	14,14,15	0.34	0	17,19,21	0.91	1 (5%)

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
6	NAG	B	201	2	-	2/6/23/26	0/1/1/1
5	PTY	B	200	-	-	28/53/53/53	-
6	NAG	B	206	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	201	NAG	C1-O5-C5	3.78	117.31	112.19
6	B	206	NAG	C1-O5-C5	3.25	116.59	112.19
6	B	201	NAG	C1-C2-N2	2.45	114.67	110.49
5	B	200	PTY	O14-P1-O13	-2.32	99.99	109.07
5	B	200	PTY	O11-P1-O13	-2.14	100.71	109.07

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	200	PTY	N1-C2-C3-O11
5	B	200	PTY	C3-O11-P1-O13
6	B	201	NAG	O5-C5-C6-O6
5	B	200	PTY	C31-C30-O4-C1
5	B	200	PTY	C11-C8-O7-C6
6	B	201	NAG	C4-C5-C6-O6
5	B	200	PTY	O10-C8-O7-C6
5	B	200	PTY	O30-C30-O4-C1
5	B	200	PTY	C8-C11-C12-C13
5	B	200	PTY	C30-C31-C32-C33
5	B	200	PTY	C35-C36-C37-C38
5	B	200	PTY	C23-C24-C25-C26
5	B	200	PTY	C11-C12-C13-C14
5	B	200	PTY	C32-C33-C34-C35
5	B	200	PTY	C34-C35-C36-C37
5	B	200	PTY	C36-C37-C38-C39
5	B	200	PTY	C13-C14-C15-C16
5	B	200	PTY	C22-C23-C24-C25
5	B	200	PTY	C25-C26-C27-C28

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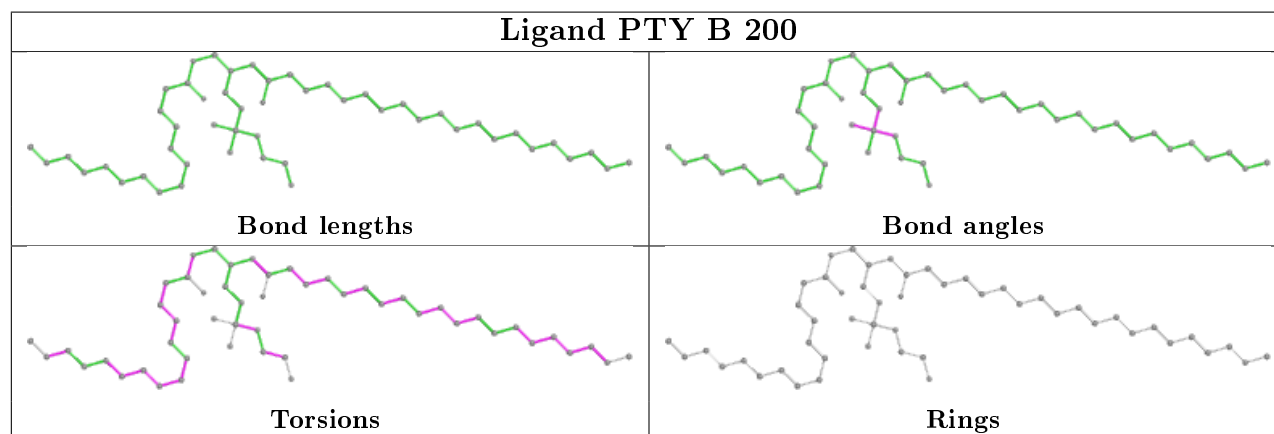
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Mol	Chain	Res	Type	Atoms
5	B	200	PTY	C17-C18-C19-C20
5	B	200	PTY	C15-C16-C17-C18
5	B	200	PTY	C38-C39-C40-C41
5	B	200	PTY	C24-C25-C26-C27
5	B	200	PTY	C37-C38-C39-C40
5	B	200	PTY	C41-C42-C43-C44
5	B	200	PTY	C18-C19-C20-C21
5	B	200	PTY	C26-C27-C28-C29
5	B	200	PTY	C19-C20-C21-C22
5	B	200	PTY	C3-O11-P1-O14
5	B	200	PTY	C31-C32-C33-C34

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 ⓘ

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	192/251 (76%)	0.49	13 (6%) 17 13	74, 126, 184, 207	0
2	B	167/171 (97%)	0.51	9 (5%) 25 22	69, 119, 155, 180	0
All	All	359/422 (85%)	0.50	22 (6%) 21 17	69, 123, 173, 207	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	513	GLN	8.4
2	B	106	GLU	6.2
1	A	514	GLY	4.6
1	A	602	CYS	4.4
1	A	592	TYR	3.9
2	B	18	TYR	3.9
1	A	635	HIS	3.6
2	B	36	HIS	3.3
1	A	510	GLY	3.0
1	A	667	TRP	2.7
1	A	504	ILE	2.6
1	A	658	TYR	2.6
1	A	583	THR	2.6
2	B	34	GLY	2.5
2	B	16	ILE	2.5
1	A	539	LYS	2.5
1	A	575	TRP	2.4
2	B	22	PRO	2.4
2	B	109	ARG	2.3
1	A	501	THR	2.2
2	B	123	PHE	2.1
2	B	166	GLU	2.0

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

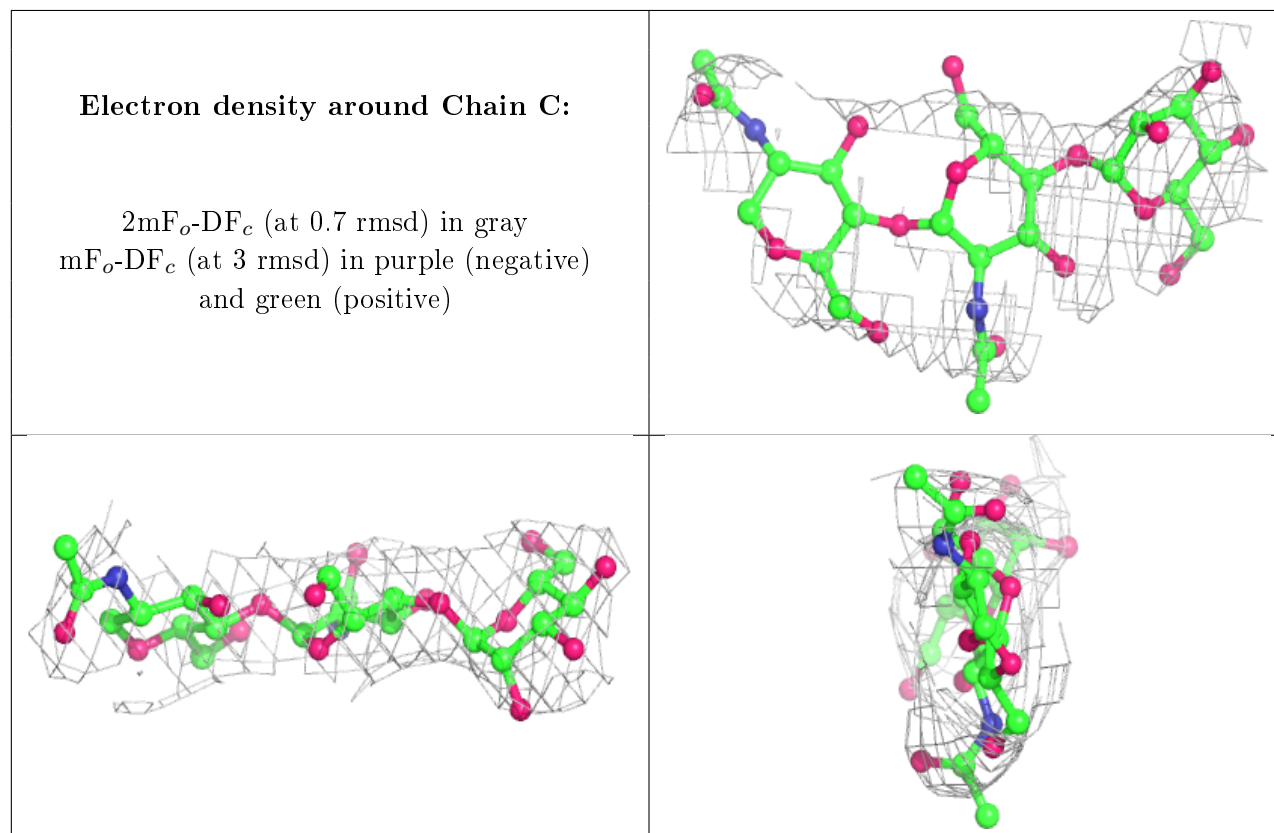
There are no non-standard protein/DNA/RNA residues in this entry.

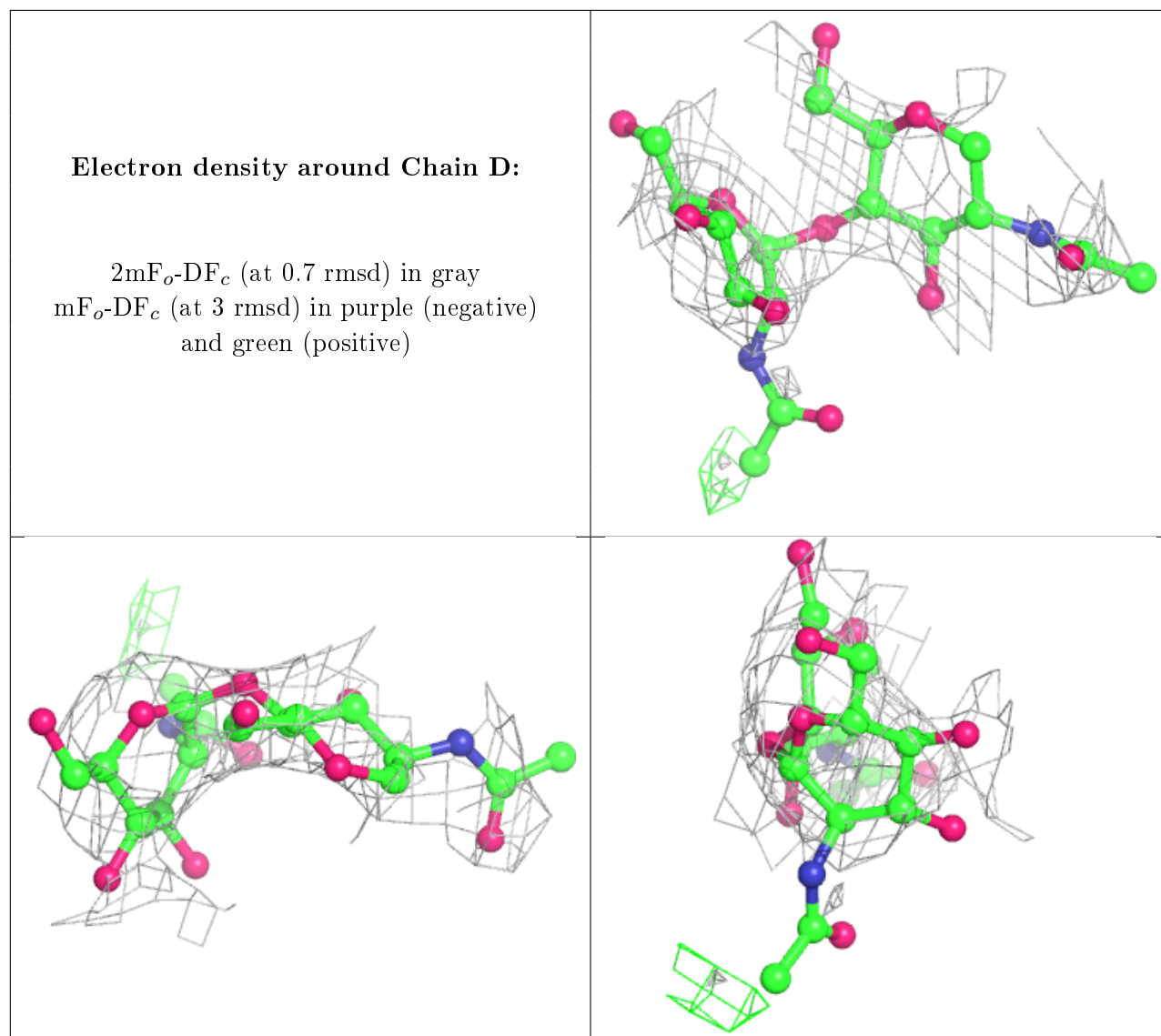
6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	NAG	D	2	14/15	0.62	0.31	193,200,205,207	0
4	NAG	D	1	14/15	0.68	0.29	187,195,201,204	0
3	MAN	C	3	11/12	0.83	0.19	199,202,205,205	0
3	NAG	C	2	14/15	0.92	0.14	171,180,189,196	0
3	NAG	C	1	14/15	0.93	0.14	123,139,151,161	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.





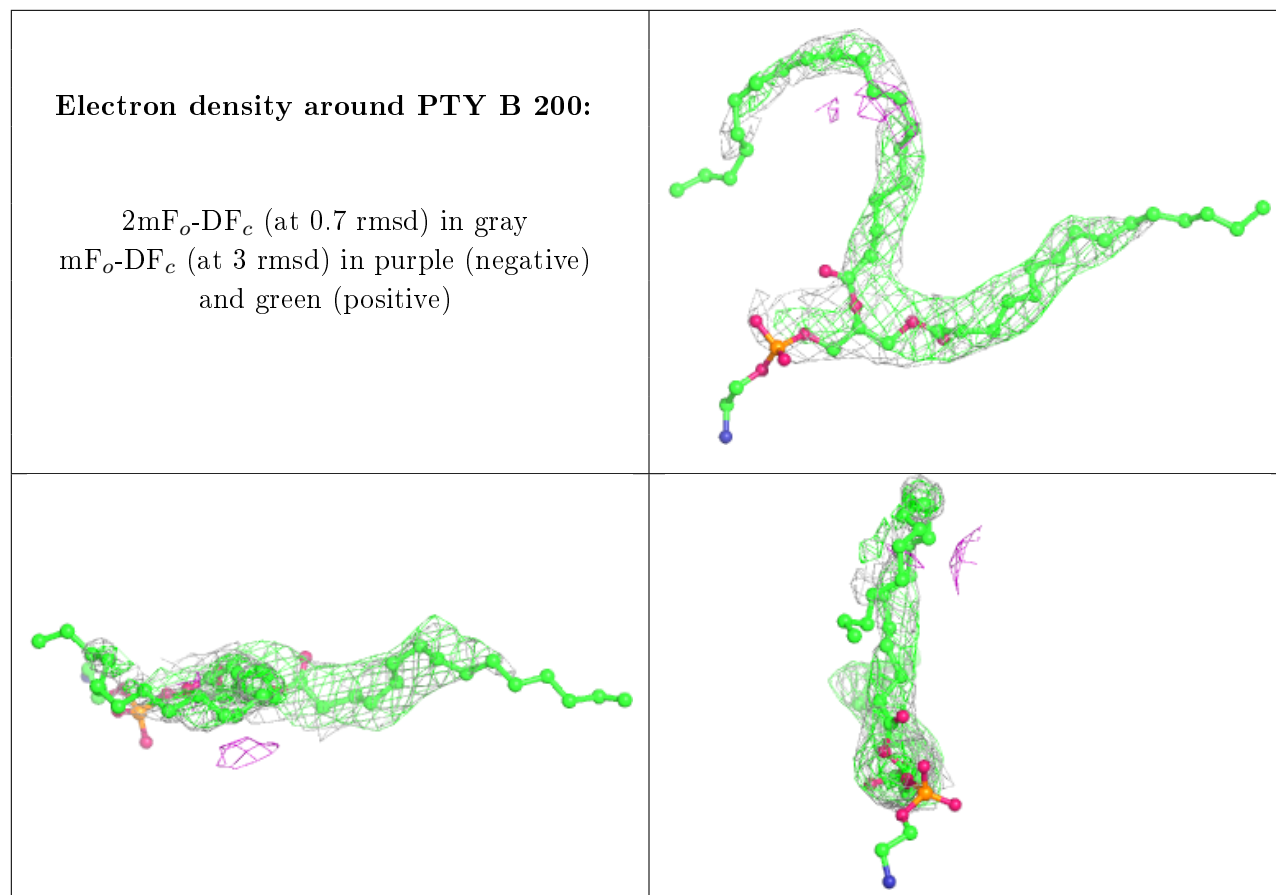
6.4 Ligands [i](#)

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
6	NAG	B	206	14/15	0.43	0.28	169,175,190,193	0
5	PTY	B	200	50/50	-	-	18,20,31,36	50
6	NAG	B	201	14/15	0.81	0.19	125,128,129,129	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.