

wwPDB X-ray Structure Validation Summary Report (i)

Aug 7, 2023 – 05:18 AM EDT

PDB ID	:	1NAM
Title	:	MURINE ALLOREACTIVE SCFV TCR-PEPTIDE-MHC CLASS I
		MOLECULE COMPLEX
Authors	:	Reiser, JB.; Darnault, C.; Gregoire, C.; Mosser, T.; Mazza, G.; Kearnay, A.;
		van der Merwe, P.A.; Fontecilla-Camps, J.C.; Housset, D.; Malissen, B.
Deposited on		
Resolution	:	2.70 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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:

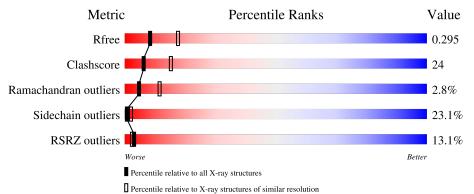
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY\;DIFFRACTION$

The reported resolution of this entry is 2.70 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$		
R_{free}	130704	2808 (2.70-2.70)		
Clashscore	141614	3122 (2.70-2.70)		
Ramachandran outliers	138981	3069 (2.70-2.70)		
Sidechain outliers	138945	3069 (2.70-2.70)		
RSRZ outliers	127900	2737 (2.70-2.70)		

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	Qua	lity of chai	n		
1	А	116	50%		25%	150/	
1	A	110	.%		25%	15%	•
2	В	113	58%		34%	7%	•
	тт	075	11%				
3	Н	275	56%		34%	10%)
4	Р	8	62%		38%		-
			49%				
5	L	100	30%	46%		23%	•



Continued from previous page...

Mol	Chain	Length	Quality	of chain
6	С	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
6	NAG	С	1	Х	-	-	-
6	NAG	С	2	Х	-	-	-



2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 5091 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 BM3.3 T Cell Receptor alpha-Chain.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	А	116	Total 908	C 579	N 145	0 179	${ m S}{ m 5}$	0	0	0

• Molecule 2 is a protein called BM3.3 T Cell Receptor beta-Chain.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
2	В	113	Total 917	C 580	N 166	0 166	${ m S}{ m 5}$	0	0	0

• Molecule 3 is a protein called H-2 class I histocompatibility antigen, K-B alpha chain precursor.

Mol	Chain	Residues		Ate	oms			ZeroOcc	AltConf	Trace
3	Н	275	Total 2240	C 1413	N 394	0 424	S 9	0	0	0

• Molecule 4 is a protein called Nucleocapsid.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	Р	8	Total 68	С 44	N 12	O 12	0	0	0

• Molecule 5 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
5	L	100	Total 829	C 529	N 139	0 153	S 8	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	0	MET	-	cloning artifact	UNP P01887



• Molecule 6 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
6	С	2	Total C N O 28 16 2 10	0	0	0

• Molecule 7 is water.

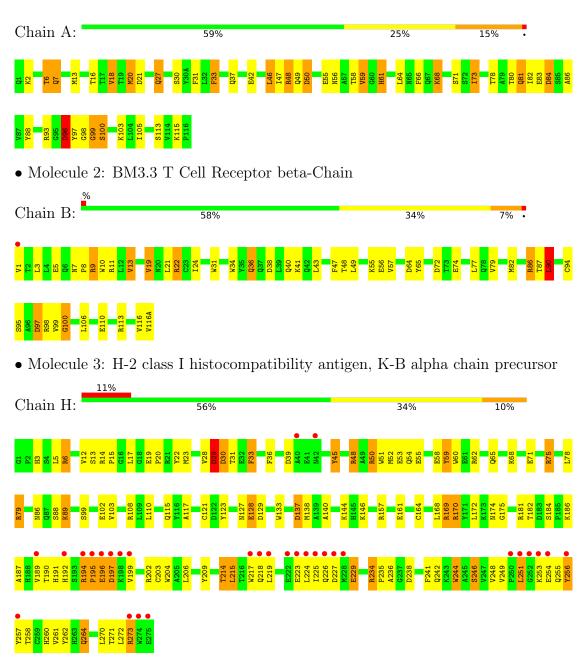
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	А	25	TotalO2525	0	0
7	В	32	$\begin{array}{cc} \text{Total} & \text{O} \\ 32 & 32 \end{array}$	0	0
7	Н	35	Total O 35 35	0	0
7	Р	2	Total O 2 2	0	0
7	L	7	Total O 7 7	0	0





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: BM3.3 T Cell Receptor alpha-Chain

• Molecule	4: Nucleocapsid			
Chain P:	Chain P: 62%			38%
R1 V4 L8				
• Molecule	5: Beta-2-microg	lobulin		
Chain L:	49%			000/
Ullalli L.	30%	4	16%	23% •
M0 11 Q2 17 17 Q8 V9 Y10	S11 R12 H13 P14 P15 E16 C18 C18 C18 C18 C18 C18 C18 C18 C18 C123 C123	N24 C25 Y26 V27 T28 T28 H31 P32 P33 P33 P33 T35	E36 137 038 038 038 038 038 038 048 643 643 643 1466 1466	r4/ K488 852 852 852 853 853 853 853 853 853 853 853 853 853
E69 F70 P72 T73 E74 E74 T75 D76	T777 Y78 A79 C80 C80 C80 K83 K83 K83 S86 S86 S86 S86 S86 S86 S86 S86 S86 S86	P90 K91 T92 V93 V94 N95 D96 R97 R97 D98 M99		

• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:	50%	50%
NAC2 NAC2		



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants	101.86Å 101.86Å 201.36Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.00 - 2.70	Depositor
Resolution (A)	33.78 - 2.70	EDS
% Data completeness	96.5 (12.00-2.70)	Depositor
(in resolution range)	96.7(33.78-2.70)	EDS
R _{merge}	(Not available)	Depositor
R _{sym}	0.08	Depositor
$< I/\sigma(I) > 1$	$2.60 (at 2.68 \text{\AA})$	Xtriage
Refinement program	REFMAC	Depositor
D D.	0.230 , 0.298	Depositor
R, R_{free}	0.233 , 0.295	DCC
R_{free} test set	2998 reflections (10.09%)	wwPDB-VP
Wilson B-factor $(Å^2)$	42.3	Xtriage
Anisotropy	0.526	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.31, 49.3	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	0.91	EDS
Total number of atoms	5091	wwPDB-VP
Average B, all atoms $(Å^2)$	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.87% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

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	
IVIOI	Ullalli	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.54	0/925	0.81	3/1249~(0.2%)
2	В	0.60	0/936	0.88	4/1271~(0.3%)
3	Н	0.43	0/2301	0.71	7/3125~(0.2%)
4	Р	0.56	0/69	0.67	0/90
5	L	0.39	0/855	0.72	6/1158~(0.5%)
All	All	0.48	0/5086	0.77	20/6893~(0.3%)

There are no bond length outliers.

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
1	А	50	ASP	CB-CG-OD2	6.64	124.28	118.30
2	В	64	ASP	CB-CG-OD2	6.36	124.02	118.30
2	В	72	ASP	CB-CG-OD2	6.09	123.78	118.30
3	Н	238	ASP	CB-CG-OD2	5.77	123.49	118.30
3	Н	197	ASP	CB-CG-OD2	5.60	123.34	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	908	0	899	44	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	В	917	0	923	40	0
3	Н	2240	0	2131	105	0
4	Р	68	0	67	3	0
5	L	829	0	805	59	0
6	С	28	0	25	2	0
7	А	25	0	0	10	0
7	В	32	0	0	5	0
7	Н	35	0	0	3	0
7	L	7	0	0	0	0
7	Р	2	0	0	1	0
All	All	5091	0	4850	239	0

Continued from previous page...

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 24.

The worst 5 of 239 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:48:ARG:HG3	1:A:48:ARG:HH11	1.09	1.10
3:H:128:GLU:CD	3:H:128:GLU:H	1.50	1.03
5:L:17:ASN:H	5:L:17:ASN:ND2	1.54	0.96
1:A:100:SER:HB2	1:A:103:LYS:HE3	1.46	0.95
3:H:235:PRO:O	5:L:10:TYR:OH	1.84	0.95

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	А	114/116~(98%)	98~(86%)	12 (10%)	4 (4%)	3 8	
2	В	$111/113 \ (98\%)$	108 (97%)	2(2%)	1 (1%)	17 40	



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	Н	273/275~(99%)	241 (88%)	29 (11%)	3~(1%)	14	34
4	Р	6/8~(75%)	5 (83%)	1 (17%)	0	100	100
5	L	98/100~(98%)	73 (74%)	16 (16%)	9~(9%)	1	0
All	All	602/612~(98%)	525 (87%)	60 (10%)	17 (3%)	5	11

Continued from previous page...

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	96	ASP
1	А	100	SER
3	Н	195	PRO
5	L	41	LYS
5	L	95	TRP

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	А	102/102~(100%)	77~(76%)	25~(24%)	0 2
2	В	101/101~(100%)	81 (80%)	20 (20%)	1 3
3	Н	233/233~(100%)	183~(78%)	50 (22%)	1 3
4	Р	6/6~(100%)	5 (83%)	1 (17%)	2 5
5	L	95/95~(100%)	67~(70%)	28 (30%)	0 1
All	All	537/537~(100%)	413 (77%)	124 (23%)	1 2

5 of 124 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	Н	75	ARG
5	L	70	PHE
3	Н	194	ARG
5	L	67	HIS
5	L	91	LYS



Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
5	L	17	ASN
5	L	2	GLN
3	Н	115	GLN
3	Н	264	GLN
3	Н	72	GLN

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)

2 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).

Mal	Trune	Chain	Dec	Tinle	Bo	ond leng	ths	B	ond ang	les
Mol	Type	Chain	Res	Link	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
6	NAG	С	1	6,1	14,14,15	0.52	0	17,19,21	1.25	2 (11%)
6	NAG	С	2	6	$14,\!14,\!15$	0.45	0	17,19,21	0.89	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
6	NAG	С	1	6,1	1/1/5/7	2/6/23/26	0/1/1/1
6	NAG	С	2	6	1/1/5/7	4/6/23/26	0/1/1/1



There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
6	С	1	NAG	C1-O5-C5	2.47	115.54	112.19
6	С	1	NAG	O5-C1-C2	-2.24	107.76	111.29

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	С	1	NAG	C1
6	С	2	NAG	C1

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	С	1	NAG	C8-C7-N2-C2
6	С	1	NAG	O7-C7-N2-C2
6	С	2	NAG	C8-C7-N2-C2
6	С	2	NAG	O7-C7-N2-C2
6	С	2	NAG	O5-C5-C6-O6

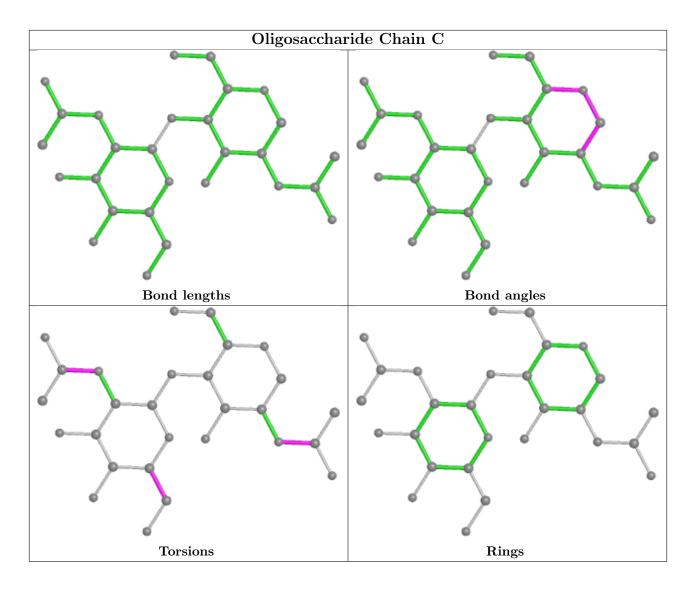
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mo	Chair	n Res	Type	Clashes	Symm-Clashes
6	C	1	NAG	2	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.





5.6 Ligand geometry (i)

There are no ligands in this entry.

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, 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	$\langle RSRZ \rangle$	#RSRZ>2	$\mathbf{OWAB}(\mathbf{\AA}^2)$	$\mathbf{Q} \! < \! 0.9$
1	А	116/116~(100%)	-0.02	0 100 100	18, 39, 59, 61	0
2	В	113/113 (100%)	-0.12	1 (0%) 84 85	16, 28, 44, 62	0
3	Н	275/275~(100%)	0.69	30 (10%) 5 4	16, 55, 122, 135	1 (0%)
4	Р	8/8 (100%)	0.57	0 100 100	28, 32, 40, 54	0
5	L	100/100~(100%)	2.34	49 (49%) 0 0	29, 98, 125, 129	0
All	All	612/612~(100%)	0.68	80 (13%) 3 2	16, 45, 121, 135	1 (0%)

The worst 5 of 80 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	L	77	THR	10.9
5	L	79	ALA	10.0
3	Н	195	PRO	9.2
5	L	97	ARG	8.3
5	L	68	THR	8.3

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.

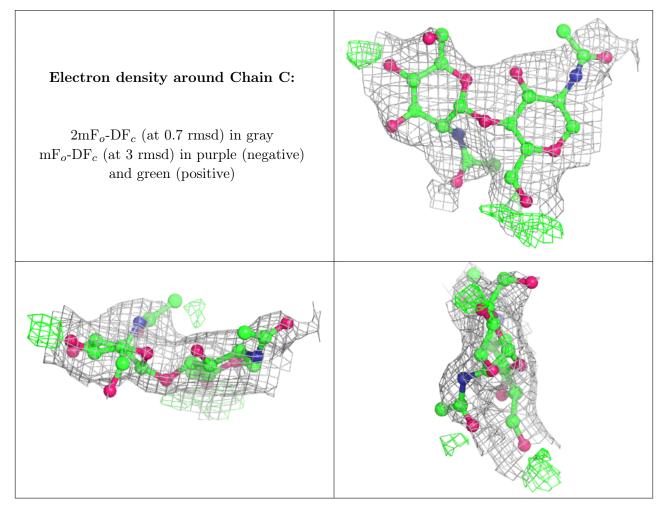
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q<0.9
6	NAG	С	2	14/15	0.85	0.31	74,77,79,81	0



Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
6	NAG	С	1	14/15	0.86	0.20	58,63,68,70	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.

