wwPDB X-ray Structure Validation Summary Report (i)

Nov 7, 2023 – 01:08 pm GMT

PDB ID	:	7NZH
Title	:	Crystal structure of HLA-DR4 in complex with a citrullinated cilp peptide
Authors	:	Ge, C.; Holmdahl, R.
Deposited on	:	2021-03-24
Resolution	:	2.83 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 (i)) were used in the production of this report:

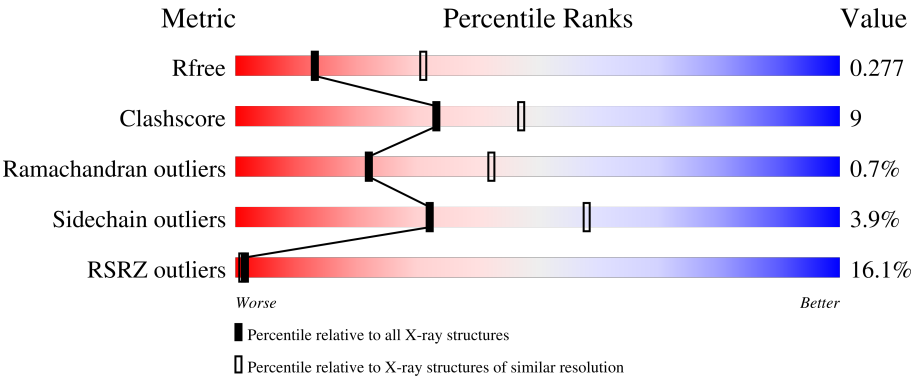
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.83 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	1031 (2.86-2.82)
Clashscore	141614	1078 (2.86-2.82)
Ramachandran outliers	138981	1050 (2.86-2.82)
Sidechain outliers	138945	1051 (2.86-2.82)
RSRZ outliers	127900	1019 (2.86-2.82)

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	AAA	180	6% 88% 12%
1	CCC	180	24% 78% 18%
2	BBB	189	2% 83% 17%
2	DDD	189	32% 74% 22%
3	EEE	14	7% 50% 29% 21%

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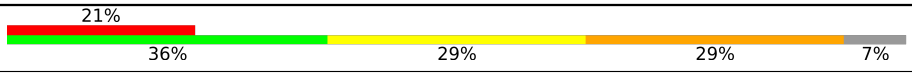
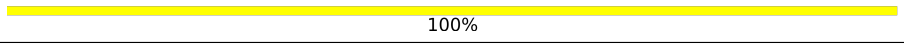
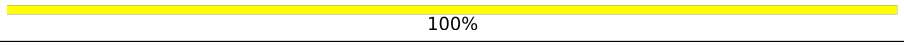
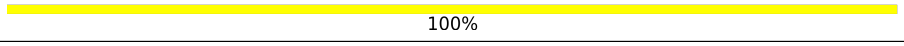
Mol	Chain	Length	Quality of chain
3	FFF	14	
4	AbA	2	
4	BaB	2	
4	CaC	2	

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
4	NAG	AbA	2	X	-	-	X
4	NAG	BaB	1	-	-	-	X
4	NAG	BaB	2	X	-	-	X
4	NAG	CaC	2	X	-	-	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 12529 atoms, of which 6135 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 HLA class II histocompatibility antigen, DR alpha chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	AAA	180	Total	C	H	N	O	S	36	0	0
			2909	960	1427	241	276	5			
1	CCC	177	Total	C	H	N	O	S	35	0	0
			2859	945	1403	237	269	5			

- Molecule 2 is a protein called HLA class II histocompatibility antigen, DR beta chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	BBB	189	Total	C	H	N	O	S	50	0	0
			3056	992	1487	278	294	5			
2	DDD	189	Total	C	H	N	O	S	49	0	0
			3057	992	1488	278	294	5			

- Molecule 3 is a protein called citrullinated cartilage intermediate layer protein (CILP) peptide 982-996.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	EEE	14	Total	C	H	N	O	3	0	0
			232	69	118	22	23			
3	FFF	13	Total	C	H	N	O	3	0	0
			220	65	114	21	20			

- 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	AbA	2	Total	C	H	N	O	5	0	0
			56	16	28	2	10			

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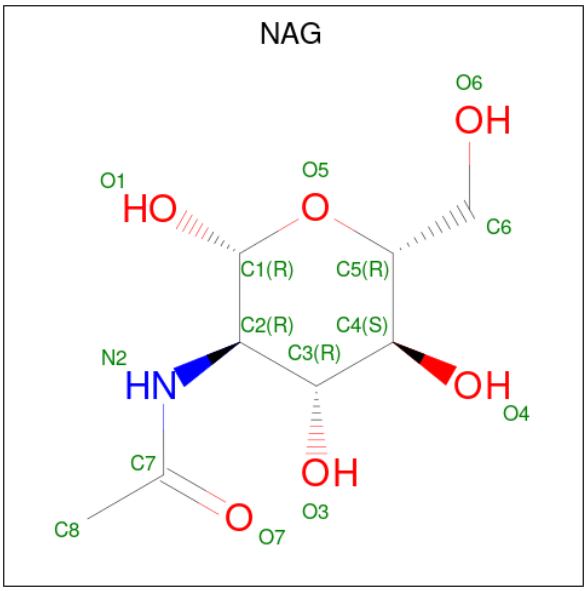
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	BaB	2	Total	C	H	N	O	5	0	0
			56	16	28	2	10			
4	CaC	2	Total	C	H	N	O	5	0	0
			56	16	28	2	10			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



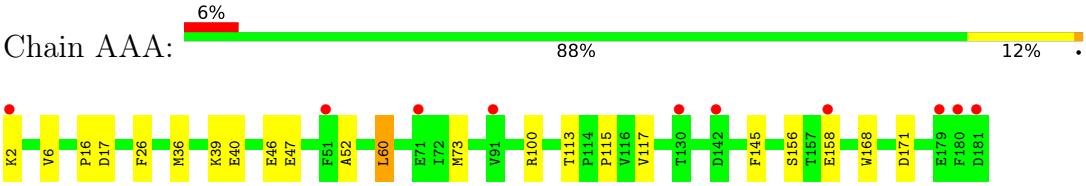
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	AAA	1	Total	C	H	N	O	3	0
			28	8	14	1	5		

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.

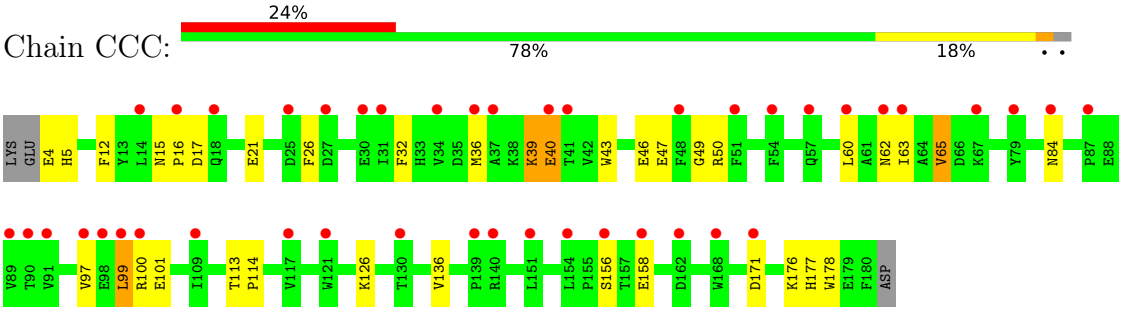
• Molecule 1: HLA class II histocompatibility antigen, DR alpha chain

Chain AAA:



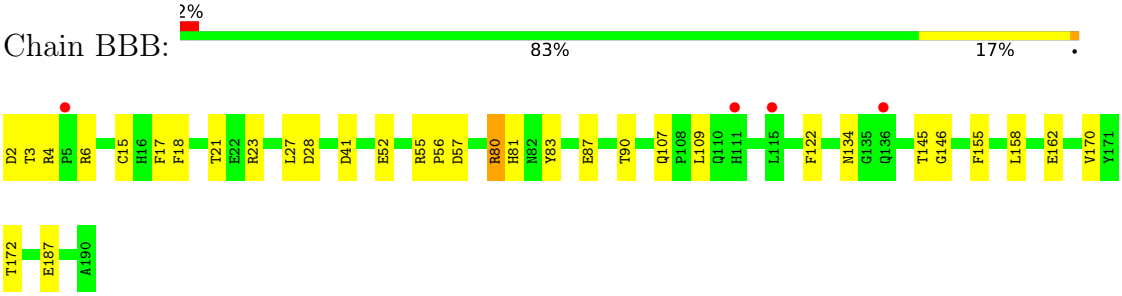
• Molecule 1: HLA class II histocompatibility antigen, DR alpha chain

Chain CCC:



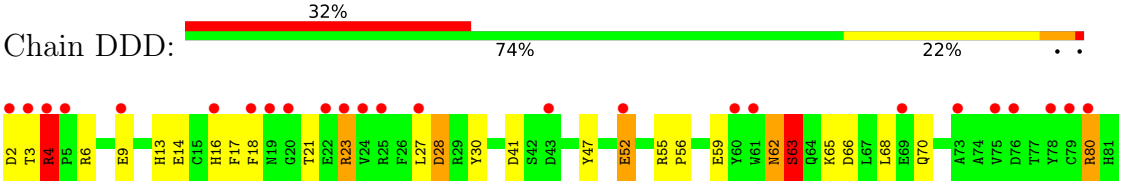
• Molecule 2: HLA class II histocompatibility antigen, DR beta chain

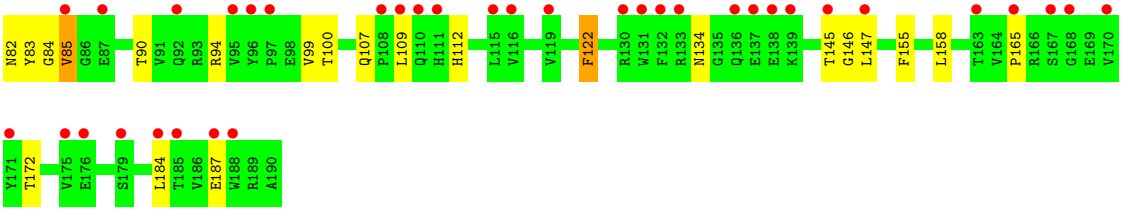
Chain BBB:



• Molecule 2: HLA class II histocompatibility antigen, DR beta chain

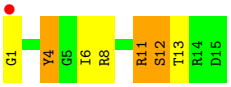
Chain DDD:





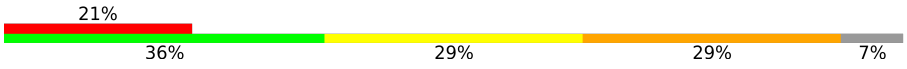
• Molecule 3: citrullinated cartilage intermediate layer protein (CILP) peptide 982-996

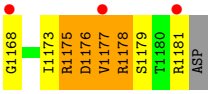
Chain EEE:



• Molecule 3: citrullinated cartilage intermediate layer protein (CILP) peptide 982-996

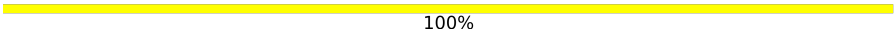
Chain FFF:





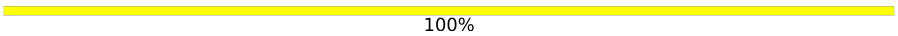
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain AbA:



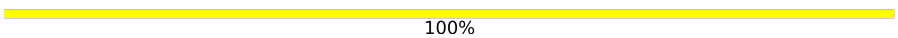
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain BaB:



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

Chain CaC:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	97.28Å 112.24Å 212.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.70 – 2.83 49.65 – 2.83	Depositor EDS
% Data completeness (in resolution range)	98.5 (49.70-2.83) 98.5 (49.65-2.83)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.02 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.244 , 0.283 0.244 , 0.277	Depositor DCC
R_{free} test set	1402 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	76.7	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 50.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	12529	wwPDB-VP
Average B, all atoms (Å^2)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.77% 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: NAG, CIR

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	AAA	0.78	4/1527 (0.3%)	0.81	0/2081
1	CCC	0.68	2/1501 (0.1%)	0.82	0/2047
2	BBB	0.70	2/1613 (0.1%)	0.94	5/2193 (0.2%)
2	DDD	0.75	1/1613 (0.1%)	1.05	8/2193 (0.4%)
3	EEE	1.48	2/90 (2.2%)	1.12	0/116
3	FFF	1.33	1/82 (1.2%)	0.87	0/105
All	All	0.76	12/6426 (0.2%)	0.91	13/8735 (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
2	BBB	0	1
2	DDD	0	3
3	EEE	0	2
3	FFF	0	4
All	All	0	10

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	DDD	4	ARG	CZ-NH1	13.27	1.50	1.33
1	CCC	40	GLU	CD-OE2	10.60	1.37	1.25
1	AAA	40	GLU	CD-OE2	9.47	1.36	1.25
1	AAA	40	GLU	CD-OE1	9.44	1.36	1.25
1	AAA	100	ARG	CG-CD	8.44	1.73	1.51

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	DDD	4	ARG	NE-CZ-NH1	-15.71	112.44	120.30
2	DDD	80	ARG	NE-CZ-NH2	15.62	128.11	120.30
2	BBB	80	ARG	NE-CZ-NH2	13.08	126.84	120.30
2	DDD	134	ASN	CB-CA-C	11.81	134.02	110.40
2	BBB	4	ARG	NE-CZ-NH2	-10.83	114.88	120.30

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	BBB	3	THR	Peptide
2	DDD	3	THR	Peptide
2	DDD	4	ARG	Sidechain
2	DDD	84	GLY	Peptide
3	EEE	6	ILE	Mainchain

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	AAA	1482	1427	1418	17	1
1	CCC	1456	1403	1396	31	0
2	BBB	1569	1487	1477	31	1
2	DDD	1569	1488	1478	45	0
3	EEE	114	118	107	3	0
3	FFF	106	114	100	5	0
4	AbA	28	28	25	0	0
4	BaB	28	28	25	0	0
4	CaC	28	28	25	0	0
5	AAA	14	14	13	1	0
All	All	6394	6135	6064	105	1

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 9.

The worst 5 of 105 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:BBB:21:THR:O	2:BBB:80:ARG:NH1	1.81	1.12
2:DDD:21:THR:O	2:DDD:80:ARG:NH1	1.80	1.12
2:DDD:82:ASN:O	2:DDD:85:VAL:O	1.77	1.01
1:CCC:156:SER:OG	1:CCC:158:GLU:HG2	1.79	0.81
1:CCC:36:MET:SD	1:CCC:63:ILE:CD1	2.70	0.80

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:158:GLU:OE1	2:BBB:87:GLU:OE2[8_545]	1.95	0.25

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	AAA	178/180 (99%)	176 (99%)	2 (1%)	0	100	100
1	CCC	175/180 (97%)	172 (98%)	3 (2%)	0	100	100
2	BBB	187/189 (99%)	182 (97%)	5 (3%)	0	100	100
2	DDD	187/189 (99%)	178 (95%)	7 (4%)	2 (1%)	14	30
3	EEE	10/14 (71%)	8 (80%)	1 (10%)	1 (10%)	0	0
3	FFF	9/14 (64%)	6 (67%)	1 (11%)	2 (22%)	0	0
All	All	746/766 (97%)	722 (97%)	19 (2%)	5 (1%)	22	42

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	EEE	12	SER
3	FFF	1176	ASP
3	FFF	1179	SER

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Mol	Chain	Res	Type
2	DDD	63	SER
2	DDD	85	VAL

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	AAA	165/165 (100%)	159 (96%)	6 (4%)	35 60
1	CCC	162/165 (98%)	152 (94%)	10 (6%)	18 35
2	BBB	171/171 (100%)	169 (99%)	2 (1%)	71 85
2	DDD	171/171 (100%)	163 (95%)	8 (5%)	26 50
3	EEE	10/10 (100%)	9 (90%)	1 (10%)	7 16
3	FFF	9/10 (90%)	9 (100%)	0	100 100
All	All	688/692 (99%)	661 (96%)	27 (4%)	32 58

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	CCC	99	LEU
1	CCC	176	LYS
2	DDD	70	GLN
1	CCC	171	ASP
2	DDD	23	ARG

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)

4 non-standard protein/DNA/RNA residues 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	CIR	EEE	8	3	9,10,11	3.91	4 (44%)	6,11,13	3.11	4 (66%)
3	CIR	FFF	1178	3	9,10,11	1.96	2 (22%)	6,11,13	2.91	4 (66%)
3	CIR	FFF	1175	3	9,10,11	0.69	0	6,11,13	1.25	1 (16%)
3	CIR	EEE	11	3	9,10,11	0.93	0	6,11,13	2.45	3 (50%)

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	CIR	EEE	8	3	-	2/8/9/11	-
3	CIR	FFF	1178	3	-	3/8/9/11	-
3	CIR	FFF	1175	3	-	3/8/9/11	-
3	CIR	EEE	11	3	-	3/8/9/11	-

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	EEE	8	CIR	C7-N6	9.30	1.46	1.34
3	EEE	8	CIR	O7-C7	5.78	1.33	1.24
3	FFF	1178	CIR	C3-CA	5.30	1.60	1.53
3	EEE	8	CIR	C3-CA	2.64	1.57	1.53
3	EEE	8	CIR	O-C	2.42	1.29	1.19

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	EEE	8	CIR	O7-C7-N6	6.02	126.21	121.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	FFF	1178	CIR	N8-C7-N6	4.37	121.47	116.85
3	EEE	11	CIR	N8-C7-N6	4.17	121.25	116.85
3	FFF	1178	CIR	O7-C7-N6	-3.95	118.81	121.74
3	FFF	1178	CIR	C5-N6-C7	3.34	126.70	122.73

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	FFF	1175	CIR	C4-C3-CA-C
3	FFF	1175	CIR	C4-C3-CA-N
3	EEE	8	CIR	C3-C4-C5-N6
3	FFF	1175	CIR	C3-C4-C5-N6
3	EEE	11	CIR	O7-C7-N6-C5

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

6 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	AbA	1	1,4	14,14,15	1.31	2 (14%)	17,19,21	1.81	4 (23%)
4	NAG	AbA	2	4	14,14,15	3.81	5 (35%)	17,19,21	2.68	6 (35%)
4	NAG	BaB	1	4,2	14,14,15	1.55	1 (7%)	17,19,21	1.45	3 (17%)
4	NAG	BaB	2	4	14,14,15	1.54	3 (21%)	17,19,21	1.59	4 (23%)
4	NAG	CaC	1	1,4	14,14,15	0.70	0	17,19,21	1.13	2 (11%)
4	NAG	CaC	2	4	14,14,15	0.97	0	17,19,21	0.97	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
4	NAG	AbA	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	AbA	2	4	1/1/7/7	2/6/23/26	0/1/1/1
4	NAG	BaB	1	4,2	-	2/6/23/26	0/1/1/1
4	NAG	BaB	2	4	1/1/7/7	2/6/23/26	0/1/1/1
4	NAG	CaC	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	CaC	2	4	1/1/7/7	3/6/23/26	0/1/1/1

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	AbA	2	NAG	C7-N2	10.00	1.68	1.34
4	AbA	2	NAG	O7-C7	-7.76	1.05	1.23
4	BaB	1	NAG	O7-C7	4.94	1.34	1.23
4	AbA	2	NAG	C8-C7	-4.65	1.40	1.50
4	AbA	1	NAG	O6-C6	3.38	1.56	1.42

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	AbA	2	NAG	C2-N2-C7	6.48	132.13	122.90
4	AbA	2	NAG	O7-C7-N2	-5.65	111.57	121.95
4	AbA	1	NAG	C2-N2-C7	4.36	129.11	122.90
4	AbA	2	NAG	O7-C7-C8	4.13	129.73	122.06
4	BaB	2	NAG	C4-C3-C2	3.43	116.05	111.02

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	AbA	2	NAG	C1
4	BaB	2	NAG	C1
4	CaC	2	NAG	C1

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	AbA	2	NAG	C1-C2-N2-C7
4	CaC	2	NAG	O5-C5-C6-O6
4	CaC	1	NAG	O5-C5-C6-O6

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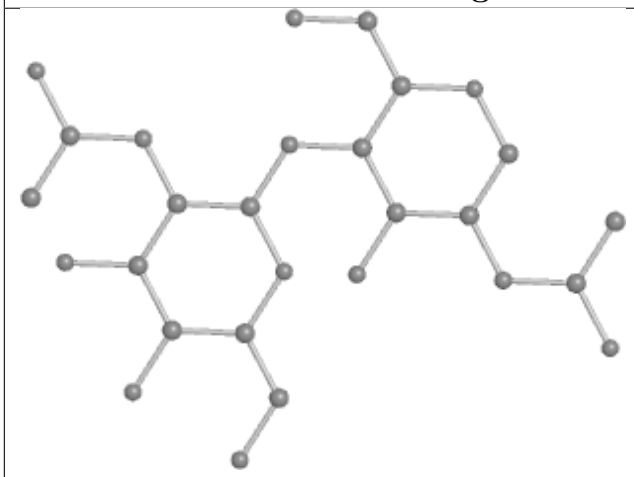
Mol	Chain	Res	Type	Atoms
4	CaC	2	NAG	C4-C5-C6-O6
4	BaB	1	NAG	C4-C5-C6-O6

There are no ring outliers.

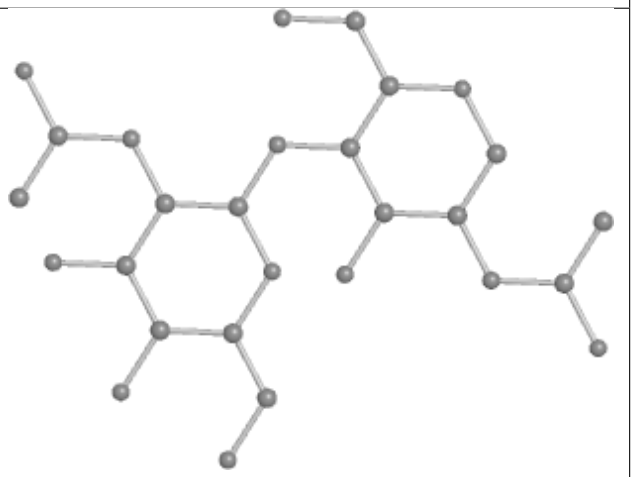
No monomer is involved in short contacts.

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

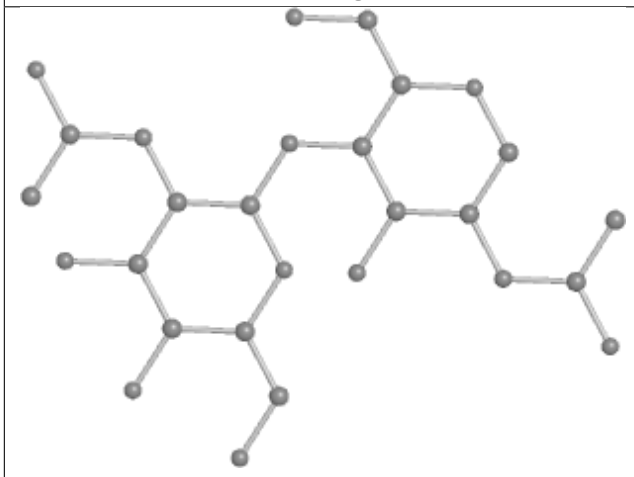
Oligosaccharide Chain AbA



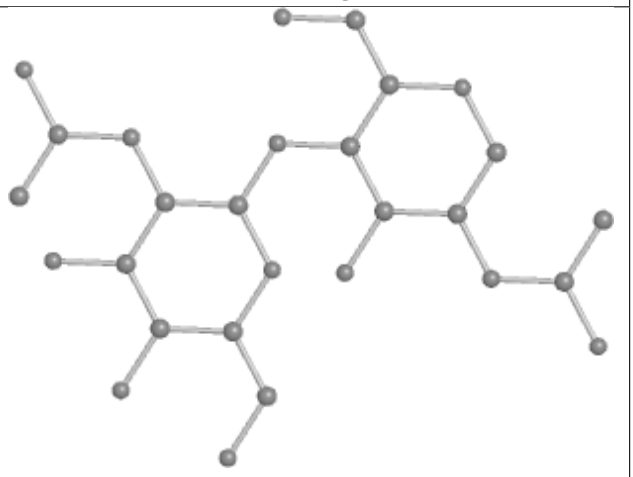
Bond lengths



Bond angles

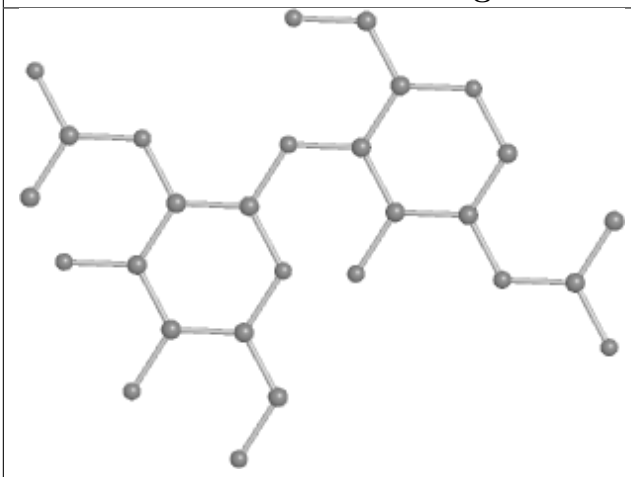


Torsions

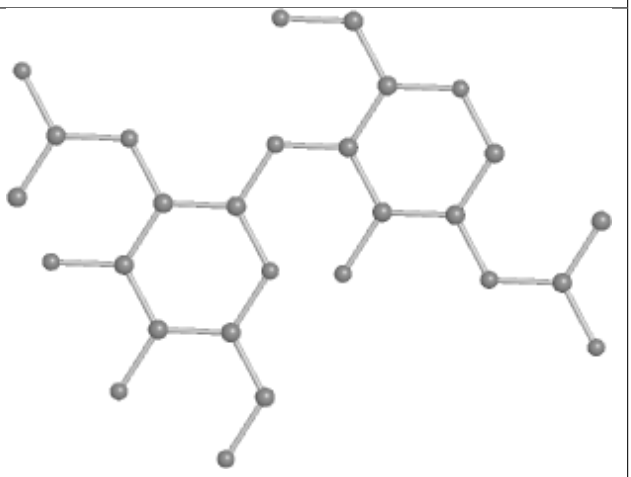


Rings

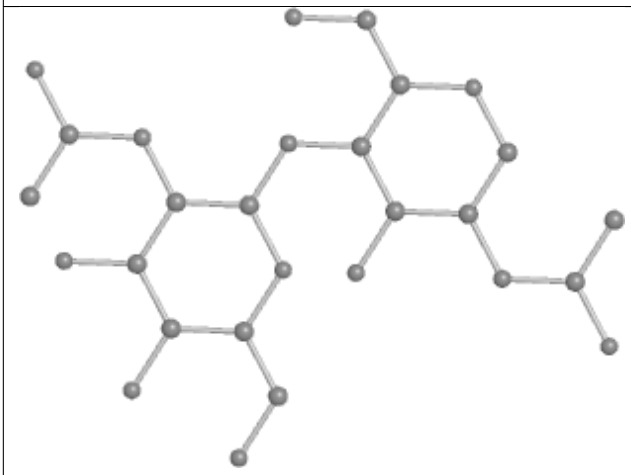
Oligosaccharide Chain BaB



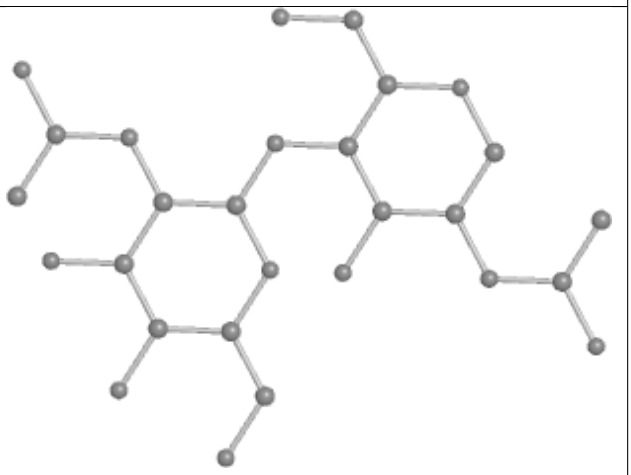
Bond lengths



Bond angles

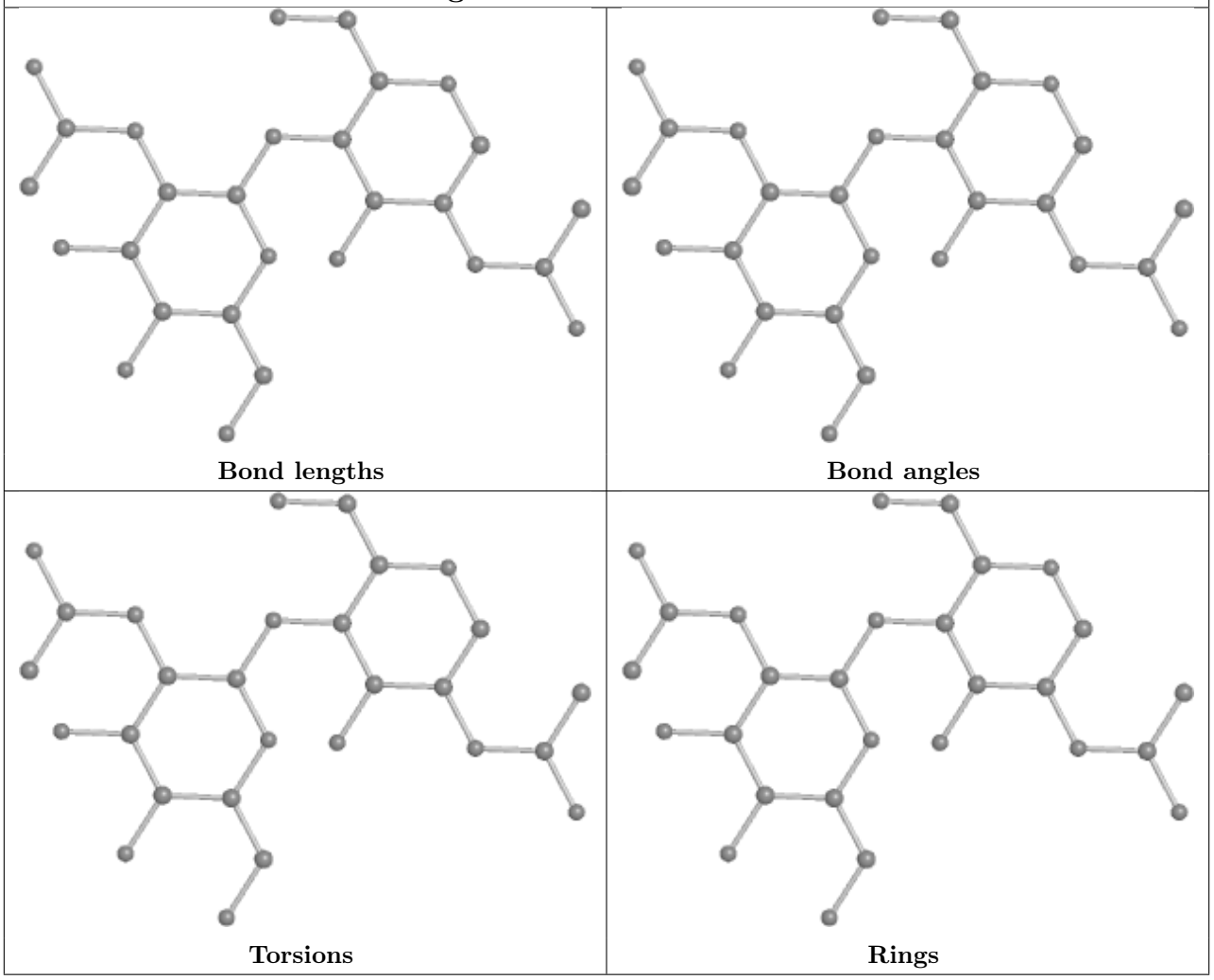


Torsions



Rings

Oligosaccharide Chain CaC



5.6 Ligand geometry (i)

1 ligand is 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	$\#\|Z\| > 2$
5	NAG	AAA	201	1	14,14,15	1.27	1 (7%)	17,19,21	1.70	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
5	NAG	AAA	201	1	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	AAA	201	NAG	O7-C7	-3.05	1.16	1.23

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	AAA	201	NAG	C1-O5-C5	4.67	118.52	112.19
5	AAA	201	NAG	C4-C3-C2	-2.51	107.34	111.02
5	AAA	201	NAG	O4-C4-C5	2.27	114.92	109.30
5	AAA	201	NAG	O5-C5-C6	-2.00	104.07	107.20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	AAA	201	NAG	1	0

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	AAA	180/180 (100%)	0.79	10 (5%) 24 17	47, 67, 94, 171	0
1	CCC	177/180 (98%)	1.32	43 (24%) 0 0	85, 115, 151, 163	0
2	BBB	189/189 (100%)	0.68	4 (2%) 63 58	49, 73, 106, 133	3 (1%)
2	DDD	189/189 (100%)	1.55	61 (32%) 0 0	82, 116, 142, 150	1 (0%)
3	EEE	12/14 (85%)	0.88	1 (8%) 11 6	56, 68, 109, 114	0
3	FFF	11/14 (78%)	0.93	3 (27%) 0 0	108, 116, 125, 131	0
All	All	758/766 (98%)	1.08	122 (16%) 1 1	47, 96, 141, 171	4 (0%)

The worst 5 of 122 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	181	ASP	6.3
1	CCC	97	VAL	6.2
2	DDD	138	GLU	5.4
1	CCC	60	LEU	4.7
2	DDD	179	SER	4.6

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

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
3	CIR	FFF	1175	11/12	0.79	0.26	111,126,138,141	0
3	CIR	FFF	1178	11/12	0.84	0.25	108,119,133,134	0
3	CIR	EEE	8	11/12	0.85	0.26	67,81,91,94	0
3	CIR	EEE	11	11/12	0.88	0.32	70,84,110,115	0

6.3 Carbohydrates (i)

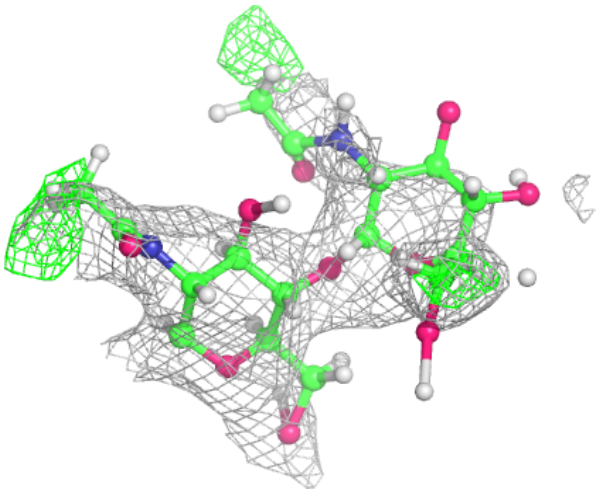
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

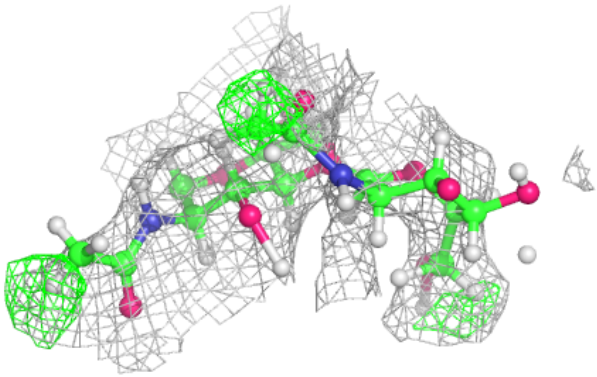
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAG	AbA	2	14/15	0.53	0.49	30,162,170,174	3
4	NAG	CaC	2	14/15	0.64	0.34	30,162,171,172	3
4	NAG	AbA	1	14/15	0.65	0.32	30,139,145,151	2
4	NAG	BaB	2	14/15	0.68	0.64	30,188,193,196	3
4	NAG	BaB	1	14/15	0.71	0.41	30,160,172,176	2
4	NAG	CaC	1	14/15	0.79	0.28	30,128,143,148	2

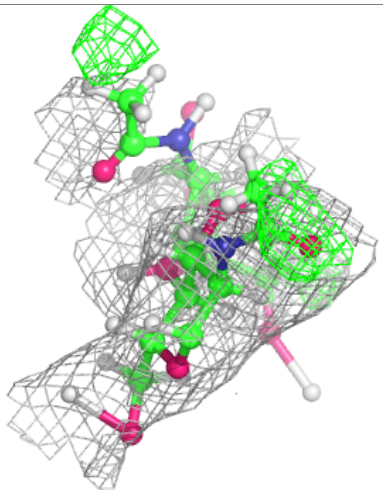
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain AbA:

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

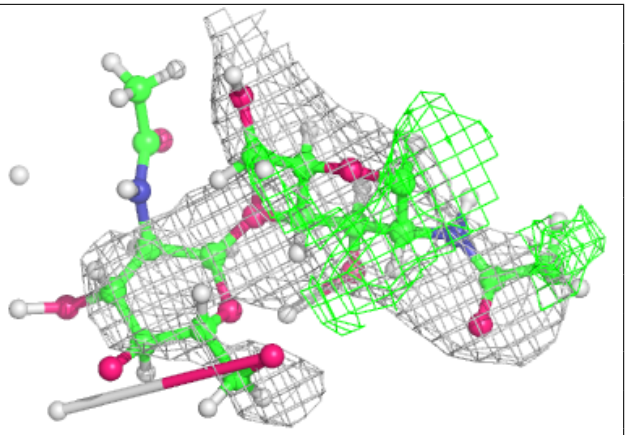


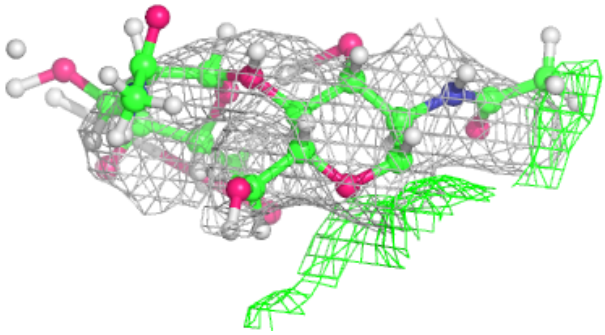


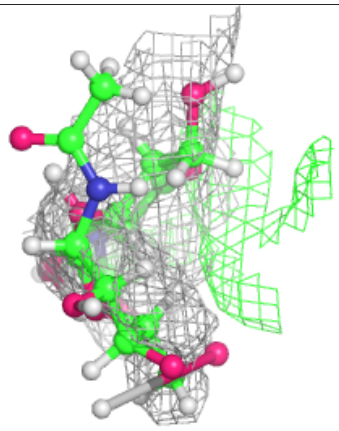


Electron density around Chain BaB:

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

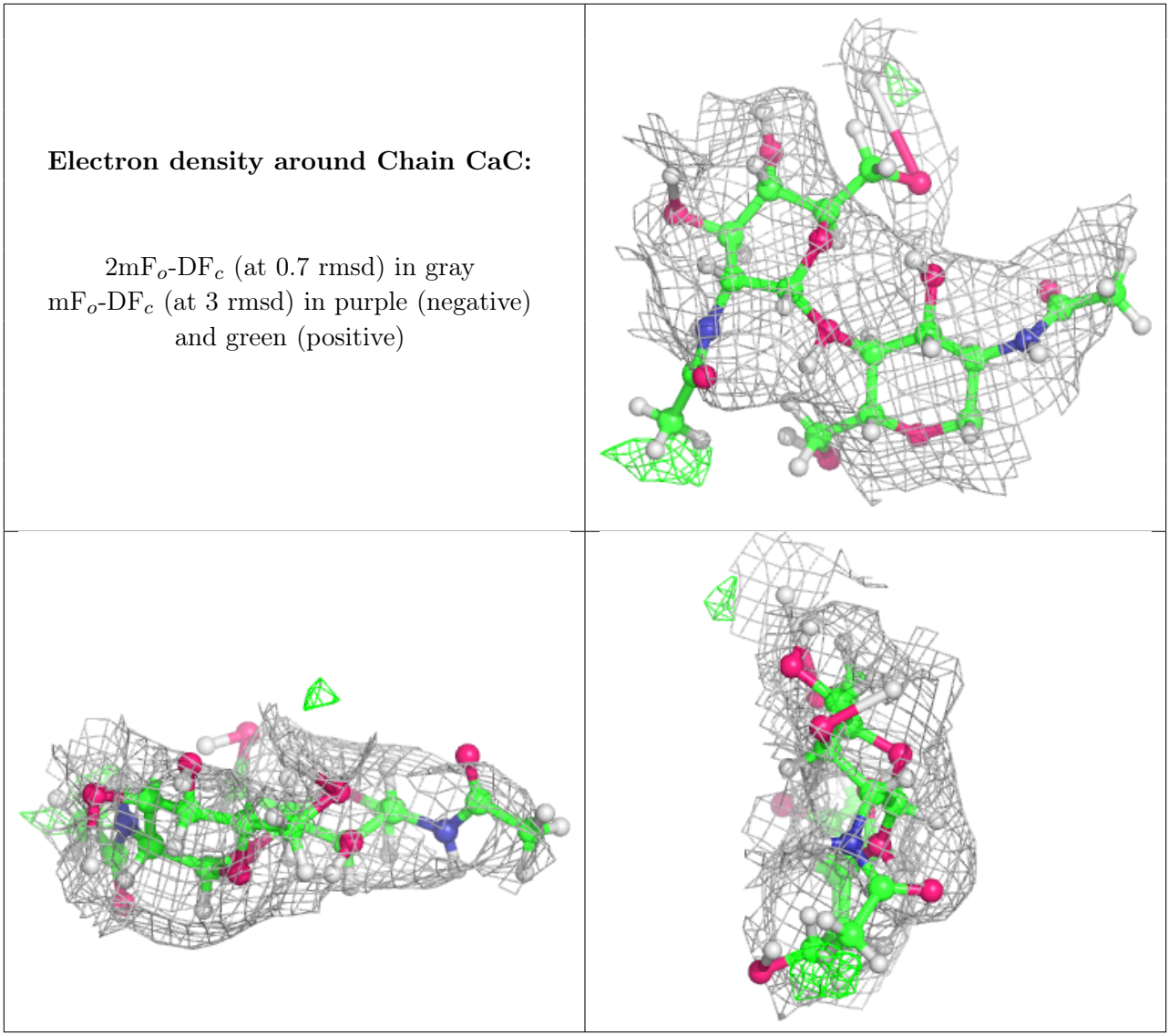






Electron density around Chain CaC:

$2mF_o$-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
5	NAG	AAA	201	14/15	0.76	0.38	30,94,108,111	3

6.5 Other polymers

There are no such residues in this entry.