



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 30, 2022 – 12:28 am GMT

PDB ID : 6YXM
Title : Crystal structure of ACPA 1F2 in complex with CII-C-39-CIT
Authors : Ge, C.; Holmdahl, R.
Deposited on : 2020-05-03
Resolution : 2.85 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.31.3
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0267
CCP4 : 7.1.010 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

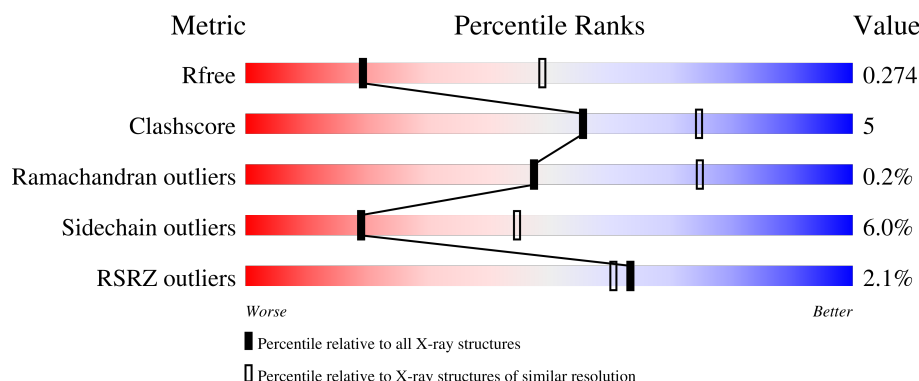
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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 $\leq 5\%$. 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	BBB	9	
2	HHH	222	
3	LLL	212	
4	A	4	

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	A	2	X	-	-	-
4	BMA	A	3	X	-	-	X

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 6589 atoms, of which 3218 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 CII-C-39-CIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	BBB	9	Total	C	H	N	O	2	0	0
			135	39	68	15	13			

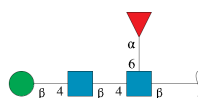
- Molecule 2 is a protein called ACPA 1F2 Fab fragment - heavy chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	HHH	213	Total	C	H	N	O	S	103	0	0
			3155	1019	1555	266	308	7			

- Molecule 3 is a protein called ACPA 1F2 Fab fragment - light chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	LLL	212	Total	C	H	N	O	S	105	0	0
			3163	1000	1545	276	336	6			

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	4	Total	C	H	N	O	10	0	0
			99	28	50	2	19			

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

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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	HHH	3	Total 3	Zn 3	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	BBB	2	Total 2	O 2	0	0
6	HHH	16	Total 16	O 16	0	0
6	LLL	15	Total 15	O 15	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.

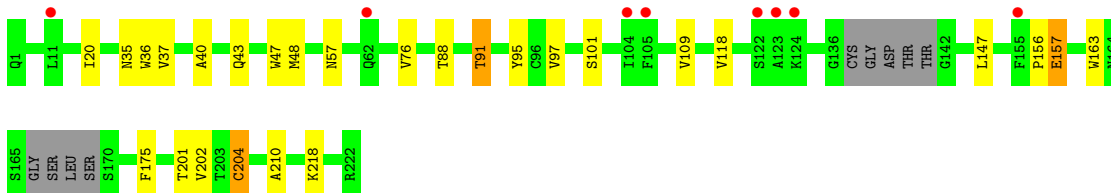
- Molecule 1: CII-C-39-CIT

Chain BBB: 




- Molecule 2: ACPA 1F2 Fab fragment - heavy chain

Chain HHH: 



- Molecule 3: ACPA 1F2 Fab fragment - light chain

Chain LLL: 



- Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain A: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	53.01Å 89.65Å 118.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.22 – 2.85 36.19 – 2.85	Depositor EDS
% Data completeness (in resolution range)	98.1 (36.22-2.85) 98.2 (36.19-2.85)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.10 (at 2.85Å)	Xtriage
Refinement program	REFMAC 5.8.0258, REFMAC 5.8.0258	Depositor
R, R_{free}	0.210 , 0.276 0.213 , 0.274	Depositor DCC
R_{free} test set	638 reflections (4.71%)	wwPDB-VP
Wilson B-factor (Å ²)	44.8	Xtriage
Anisotropy	0.173	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	6589	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.90% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CIR, FUC, ZN, BMA, 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	BBB	0.75	0/55	1.01	0/70
2	HHH	0.65	0/1645	0.76	0/2243
3	LLL	0.64	0/1655	0.76	0/2254
All	All	0.65	0/3355	0.77	0/4567

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	BBB	67	68	62	7	0
2	HHH	1600	1555	1547	17	0
3	LLL	1618	1545	1541	14	1
4	A	49	50	43	0	0
5	BBB	1	0	0	0	1
5	HHH	3	0	0	0	0
6	BBB	2	0	0	1	0
6	HHH	16	0	0	0	0
6	LLL	15	0	0	0	0
All	All	3371	3218	3193	33	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 5.

The worst 5 of 33 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:HHH:88:THR:O	2:HHH:91:THR:HG23	1.89	0.72
3:LLL:154:VAL:O	3:LLL:157:THR:HG23	2.01	0.60
2:HHH:20:ILE:HD11	2:HHH:118:VAL:HG21	1.83	0.60
2:HHH:201:THR:HG23	2:HHH:218:LYS:HE3	1.89	0.55
2:HHH:36:TRP:HB3	2:HHH:48:MET:CE	2.37	0.54

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)
3:LLL:192:HIS:HD2	5:BBB:701:ZN:ZN[3_655]	1.60	0.00

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	BBB	4/9 (44%)	3 (75%)	0	1 (25%)	0	0
2	HHH	207/222 (93%)	194 (94%)	13 (6%)	0	100	100
3	LLL	210/212 (99%)	204 (97%)	6 (3%)	0	100	100
All	All	421/443 (95%)	401 (95%)	19 (4%)	1 (0%)	47	75

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	BBB	604	ARG

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	BBB	5/5 (100%)	4 (80%)	1 (20%)	1	3
2	HHH	178/186 (96%)	170 (96%)	8 (4%)	27	57
3	LLL	186/186 (100%)	173 (93%)	13 (7%)	15	37
All	All	369/377 (98%)	347 (94%)	22 (6%)	19	45

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	LLL	118	SER
3	LLL	157	THR
3	LLL	148	VAL
3	LLL	163	MET
2	HHH	109	VAL

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](#)

1 non-standard protein/DNA/RNA residue 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
1	CIR	BBB	601	1	9,10,11	1.14	1 (11%)	6,11,13	2.51	2 (33%)

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
1	CIR	BBB	601	1	-	6/8/9/11	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	BBB	601	CIR	O7-C7	-2.10	1.21	1.24

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BBB	601	CIR	N8-C7-N6	4.63	121.73	116.85
1	BBB	601	CIR	O7-C7-N8	-3.19	117.74	123.22

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	BBB	601	CIR	C1-C2-C3-C4
1	BBB	601	CIR	N2-C2-C3-C4
1	BBB	601	CIR	O7-C7-N6-C5
1	BBB	601	CIR	N8-C7-N6-C5
1	BBB	601	CIR	C2-C3-C4-C5

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	BBB	601	CIR	1	0

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	$\# Z > 2$
4	NAG	A	1	4,2	14,14,15	0.33	0	17,19,21	0.94	0
4	NAG	A	2	4	14,14,15	0.28	0	17,19,21	1.09	2 (11%)
4	BMA	A	3	4	11,11,12	0.62	0	15,15,17	1.41	1 (6%)
4	FUC	A	4	4	10,10,11	0.28	0	14,14,16	0.84	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
4	NAG	A	1	4,2	-	0/6/23/26	0/1/1/1
4	NAG	A	2	4	1/1/7/7	2/6/23/26	0/1/1/1
4	BMA	A	3	4	1/1/5/5	2/2/19/22	0/1/1/1
4	FUC	A	4	4	-	-	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	3	BMA	C1-C2-C3	4.28	114.93	109.67
4	A	2	NAG	C4-C3-C2	-2.53	107.31	111.02
4	A	2	NAG	C1-O5-C5	2.46	115.52	112.19

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	2	NAG	C1
4	A	3	BMA	C1

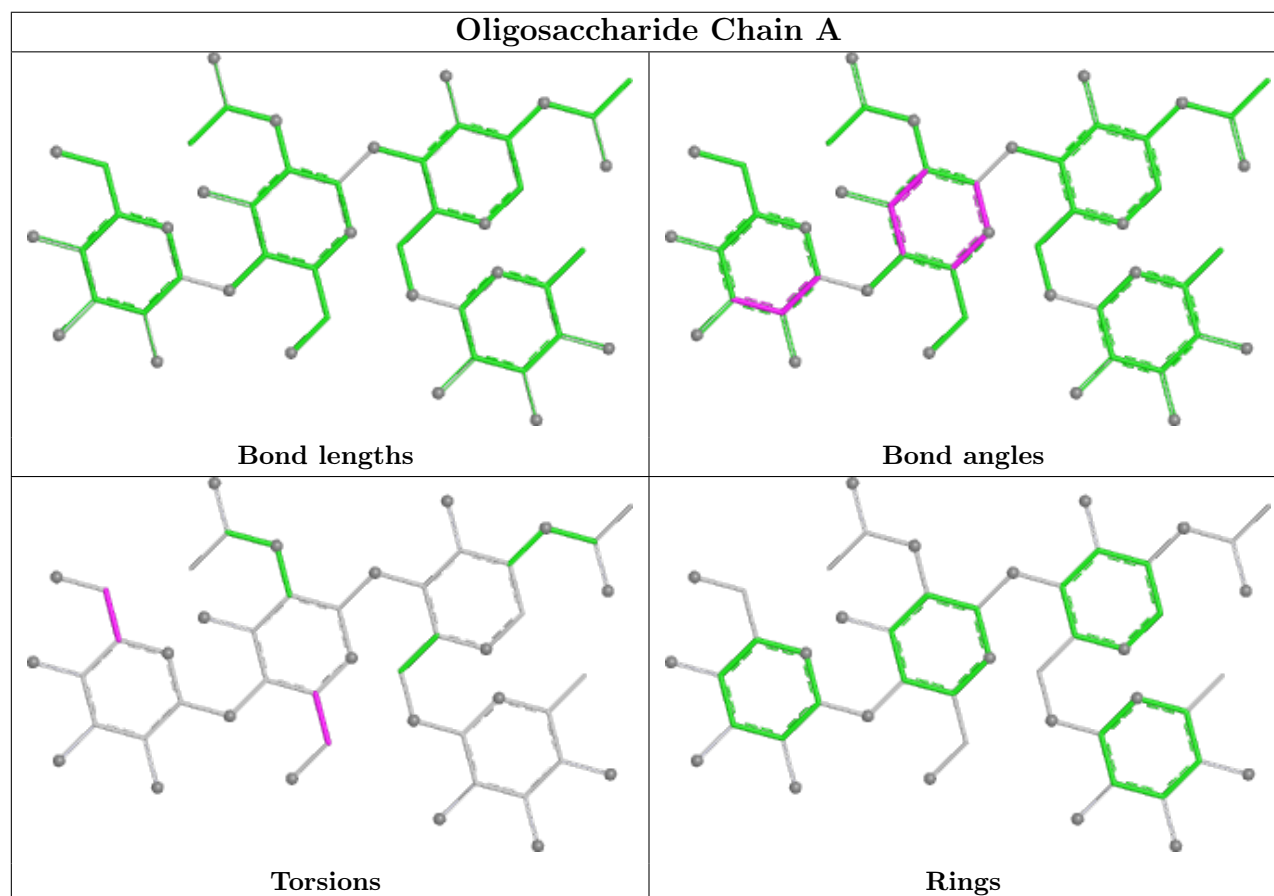
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	3	BMA	O5-C5-C6-O6
4	A	3	BMA	C4-C5-C6-O6
4	A	2	NAG	C4-C5-C6-O6
4	A	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](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 [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, 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	BBB	8/9 (88%)	0.94	1 (12%) 3 2	43, 46, 55, 55	0
2	HHH	213/222 (95%)	0.29	8 (3%) 40 35	30, 45, 60, 70	0
3	LLL	212/212 (100%)	0.16	0 100 100	29, 38, 50, 56	0
All	All	433/443 (97%)	0.24	9 (2%) 63 60	29, 41, 57, 70	0

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	HHH	104	ILE	4.2
2	HHH	122	SER	4.0
2	HHH	123	ALA	2.9
2	HHH	124	LYS	2.8
2	HHH	11	LEU	2.7

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

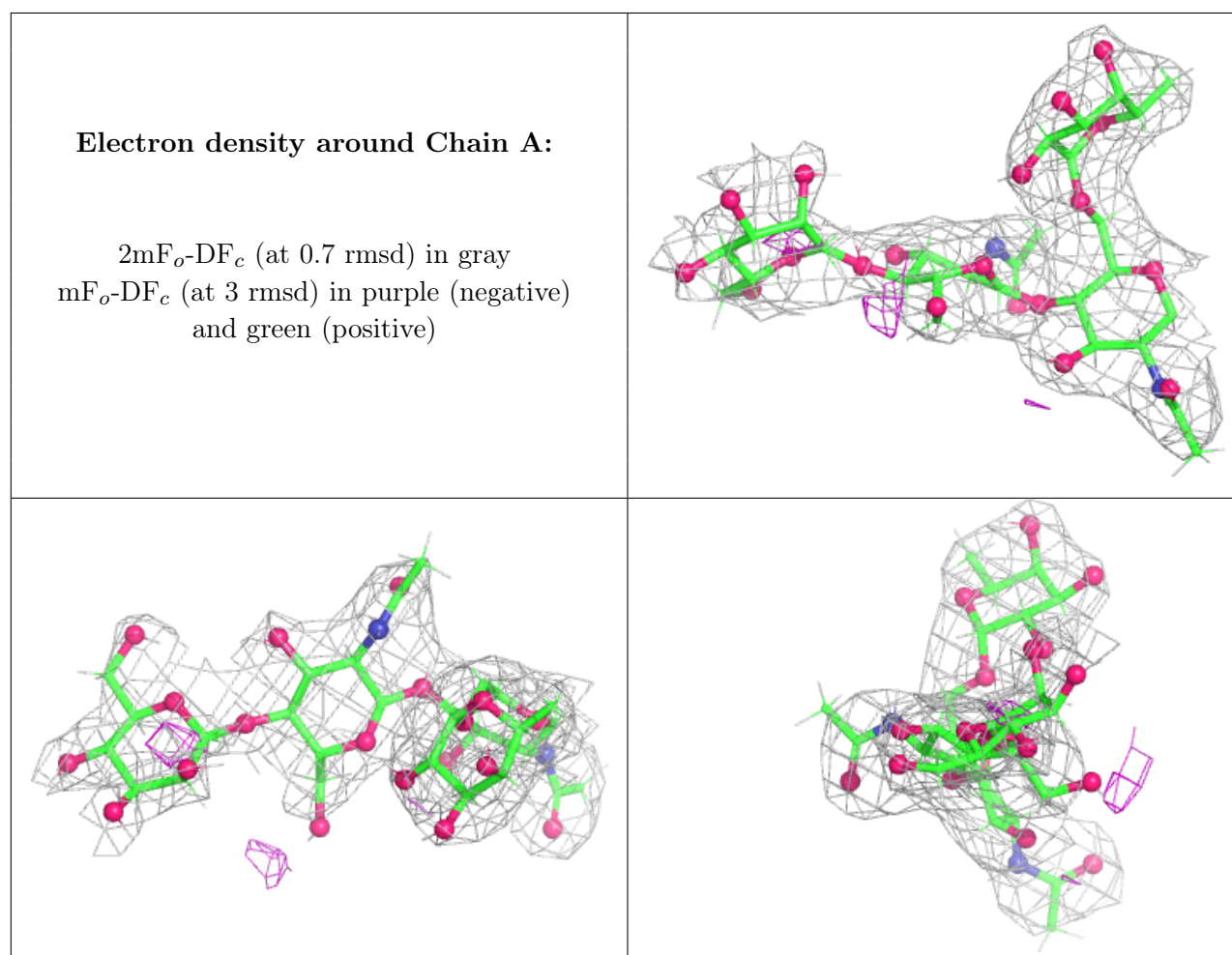
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	CIR	BBB	601	11/12	0.95	0.20	35,37,39,39	0

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, 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	BMA	A	3	11/12	0.65	0.43	30,80,82,83	4
4	NAG	A	2	14/15	0.90	0.28	30,64,68,72	2
4	NAG	A	1	14/15	0.95	0.16	30,51,53,54	1
4	FUC	A	4	10/11	0.95	0.25	30,47,48,48	3

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 ⓘ

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
5	ZN	HHH	302	1/1	0.98	0.08	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	ZN	BBB	701	1/1	0.99	0.13	30,30,30,30	0
5	ZN	HHH	303	1/1	0.99	0.16	49,49,49,49	0
5	ZN	HHH	301	1/1	1.00	0.12	39,39,39,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.