



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 30, 2022 – 12:29 am GMT

PDB ID : 6ZJG
Title : Crystal structure of ACPA E4 in complex with CII-C-48-CIT
Authors : Ge, C.; Holmdahl, R.
Deposited on : 2020-06-29
Resolution : 2.45 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 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

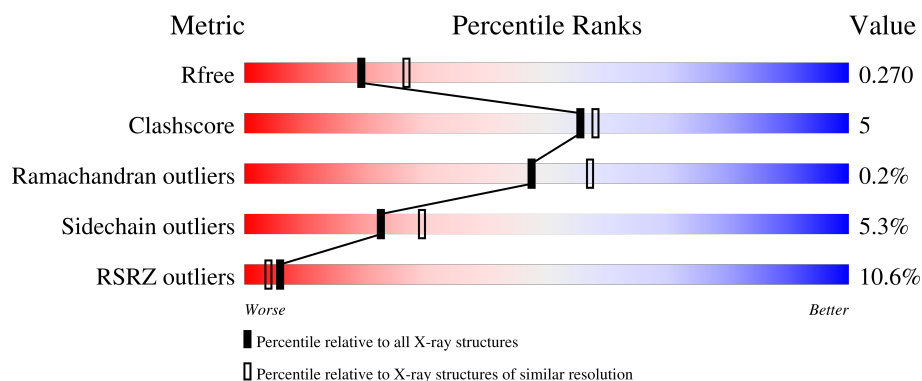
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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	B	18	
2	HHH	221	
3	LLL	216	
4	A	2	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6585 atoms, of which 3224 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-48-CIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	9	Total	C	H	N	O	0	0	0
			129	39	64	12	14			

- Molecule 2 is a protein called ACPA E4 Fab fragment - heavy chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	HHH	216	Total	C	H	N	O	S	92	0	0
			3193	1021	1580	265	318	9			

- Molecule 3 is a protein called ACPA E4 Fab fragment - light chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	LLL	212	Total	C	H	N	O	S	98	0	0
			3163	1005	1553	276	323	6			

- 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	A	2	Total	C	H	N	O	5	0	0
			55	16	27	2	10			

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	HHH	21	Total	O	0	0
			21	21		

Continued on next page...

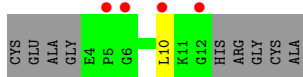
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	LLL	24	Total	O	0	0
			24	24		

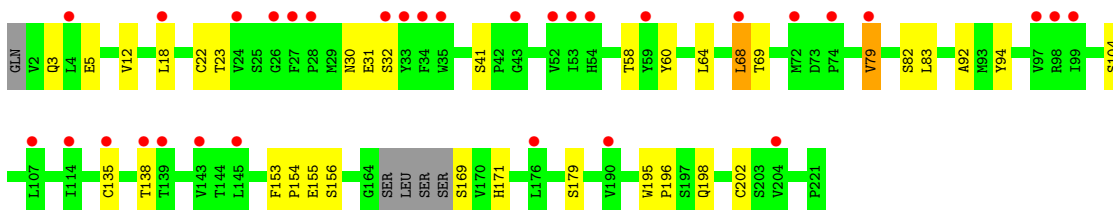
3 Residue-property plots [i](#)

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.

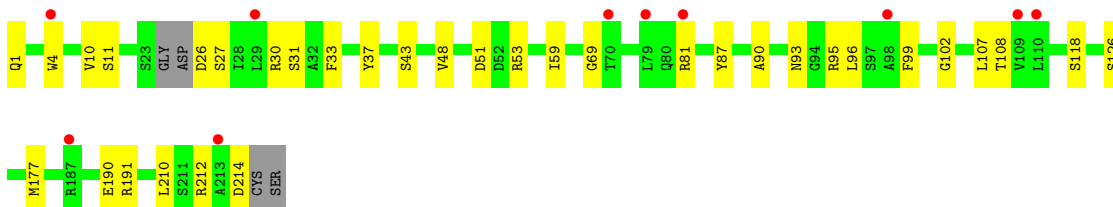
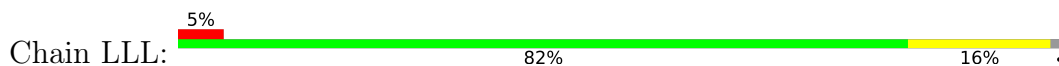
- Molecule 1: CII-C-48-CIT



- Molecule 2: ACPA E4 Fab fragment - heavy chain



- Molecule 3: ACPA E4 Fab fragment - light chain



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



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	77.18Å 151.77Å 97.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	75.89 – 2.45 75.89 – 2.45	Depositor EDS
% Data completeness (in resolution range)	100.0 (75.89-2.45) 100.0 (75.89-2.45)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.48 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.8.0258, REFMAC 5.8.0258	Depositor
R, R_{free}	0.223 , 0.265 0.226 , 0.270	Depositor DCC
R_{free} test set	1129 reflections (5.29%)	wwPDB-VP
Wilson B-factor (Å ²)	57.6	Xtriage
Anisotropy	0.156	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6585	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.55% 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: CIR, 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	B	0.78	0/53	0.78	0/67
2	HHH	0.70	0/1659	0.85	0/2276
3	LLL	0.69	0/1649	0.89	1/2250 (0.0%)
All	All	0.70	0/3361	0.87	1/4593 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	LLL	53	ARG	CB-CA-C	-5.15	100.09	110.40

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	B	65	64	60	0	0
2	HHH	1613	1580	1575	19	0
3	LLL	1610	1553	1549	20	0
4	A	28	27	25	0	0
5	HHH	21	0	0	1	0
5	LLL	24	0	0	1	0
All	All	3361	3224	3209	33	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 5.

All (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)
3:LLL:81:ARG:NH2	5:LLL:401:HOH:O	2.04	0.83
2:HHH:171:HIS:HB3	3:LLL:177:MET:CE	2.27	0.64
3:LLL:1:GLN:CD	3:LLL:1:GLN:H1	1.99	0.64
3:LLL:93:ASN:OD1	3:LLL:95:ARG:HB3	2.00	0.61
3:LLL:210:LEU:O	3:LLL:210:LEU:HD12	2.01	0.60
2:HHH:68:LEU:HD13	2:HHH:83:LEU:HD13	1.88	0.55
2:HHH:5:GLU:O	2:HHH:22:CYS:HA	2.07	0.54
3:LLL:190:GLU:O	3:LLL:212:ARG:NH2	2.41	0.54
3:LLL:30:ARG:HB2	3:LLL:69:GLY:HA2	1.92	0.52
2:HHH:58:THR:HG21	2:HHH:60:TYR:OH	2.10	0.51
3:LLL:210:LEU:HD12	3:LLL:210:LEU:C	2.32	0.50
2:HHH:22:CYS:HB3	2:HHH:79:VAL:HG13	1.93	0.49
3:LLL:90:ALA:HB1	3:LLL:99:PHE:CZ	2.48	0.49
3:LLL:10:VAL:O	3:LLL:107:LEU:HA	2.15	0.46
2:HHH:135:CYS:SG	3:LLL:214:ASP:OD2	2.75	0.45
2:HHH:64:LEU:HB3	2:HHH:68:LEU:HD22	1.98	0.45
2:HHH:30:ASN:ND2	5:HHH:302:HOH:O	2.50	0.44
3:LLL:11:SER:HA	3:LLL:108:THR:O	2.17	0.44
2:HHH:92:ALA:HB3	2:HHH:94:TYR:CE1	2.52	0.44
2:HHH:171:HIS:HB3	3:LLL:177:MET:HE2	1.97	0.44
2:HHH:195:TRP:CG	2:HHH:196:PRO:HA	2.53	0.44
2:HHH:171:HIS:CB	3:LLL:177:MET:HE1	2.48	0.43
2:HHH:171:HIS:CB	3:LLL:177:MET:CE	2.96	0.43
2:HHH:171:HIS:HA	3:LLL:177:MET:HE1	2.00	0.43
2:HHH:155:GLU:HA	2:HHH:156:SER:HA	1.82	0.43
2:HHH:153:PHE:HA	2:HHH:154:PRO:HA	1.87	0.42
2:HHH:202:CYS:O	2:HHH:202:CYS:SG	2.77	0.42
3:LLL:33:PHE:HB3	3:LLL:51:ASP:HA	2.01	0.42
2:HHH:12:VAL:HG21	2:HHH:18:LEU:HD13	2.01	0.41
3:LLL:37:TYR:O	3:LLL:87:TYR:HA	2.21	0.41
3:LLL:4:TRP:HB2	3:LLL:102:GLY:HA2	2.03	0.40
2:HHH:69:THR:HB	2:HHH:82:SER:HB3	2.03	0.40
3:LLL:48:VAL:HG22	3:LLL:59:ILE:HD12	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	4/18 (22%)	2 (50%)	2 (50%)	0	100	100
2	HHH	212/221 (96%)	198 (93%)	13 (6%)	1 (0%)	29	34
3	LLL	208/216 (96%)	197 (95%)	11 (5%)	0	100	100
All	All	424/455 (93%)	397 (94%)	26 (6%)	1 (0%)	47	57

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	HHH	179	SER

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	5/10 (50%)	4 (80%)	1 (20%)	1	0
2	HHH	188/193 (97%)	177 (94%)	11 (6%)	19	25
3	LLL	181/184 (98%)	173 (96%)	8 (4%)	28	37
All	All	374/387 (97%)	354 (95%)	20 (5%)	22	29

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	10	LEU
2	HHH	3	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	HHH	23	THR
2	HHH	31	GLU
2	HHH	32	SER
2	HHH	41	SER
2	HHH	68	LEU
2	HHH	79	VAL
2	HHH	104	SER
2	HHH	138	THR
2	HHH	169	SER
2	HHH	198	GLN
3	LLL	26	ASP
3	LLL	27	SER
3	LLL	31	SER
3	LLL	43	SER
3	LLL	96	LEU
3	LLL	118	SER
3	LLL	126	SER
3	LLL	191	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	B	8	1	9,10,11	0.97	0	6,11,13	1.10	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
1	CIR	B	8	1	-	0/8/9/11	-

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.

5.5 Carbohydrates

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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	A	1	3,4	14,14,15	0.50	0	17,19,21	1.31	2 (11%)
4	NAG	A	2	4	14,14,15	0.91	1 (7%)	17,19,21	1.66	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
4	NAG	A	1	3,4	-	2/6/23/26	0/1/1/1
4	NAG	A	2	4	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2	NAG	C1-C2	2.48	1.56	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2	NAG	C1-O5-C5	4.47	118.25	112.19
4	A	1	NAG	O5-C1-C2	-2.73	106.98	111.29
4	A	1	NAG	C1-O5-C5	2.40	115.44	112.19
4	A	2	NAG	O7-C7-C8	-2.33	117.73	122.06
4	A	2	NAG	C2-N2-C7	2.16	125.97	122.90

There are no chirality outliers.

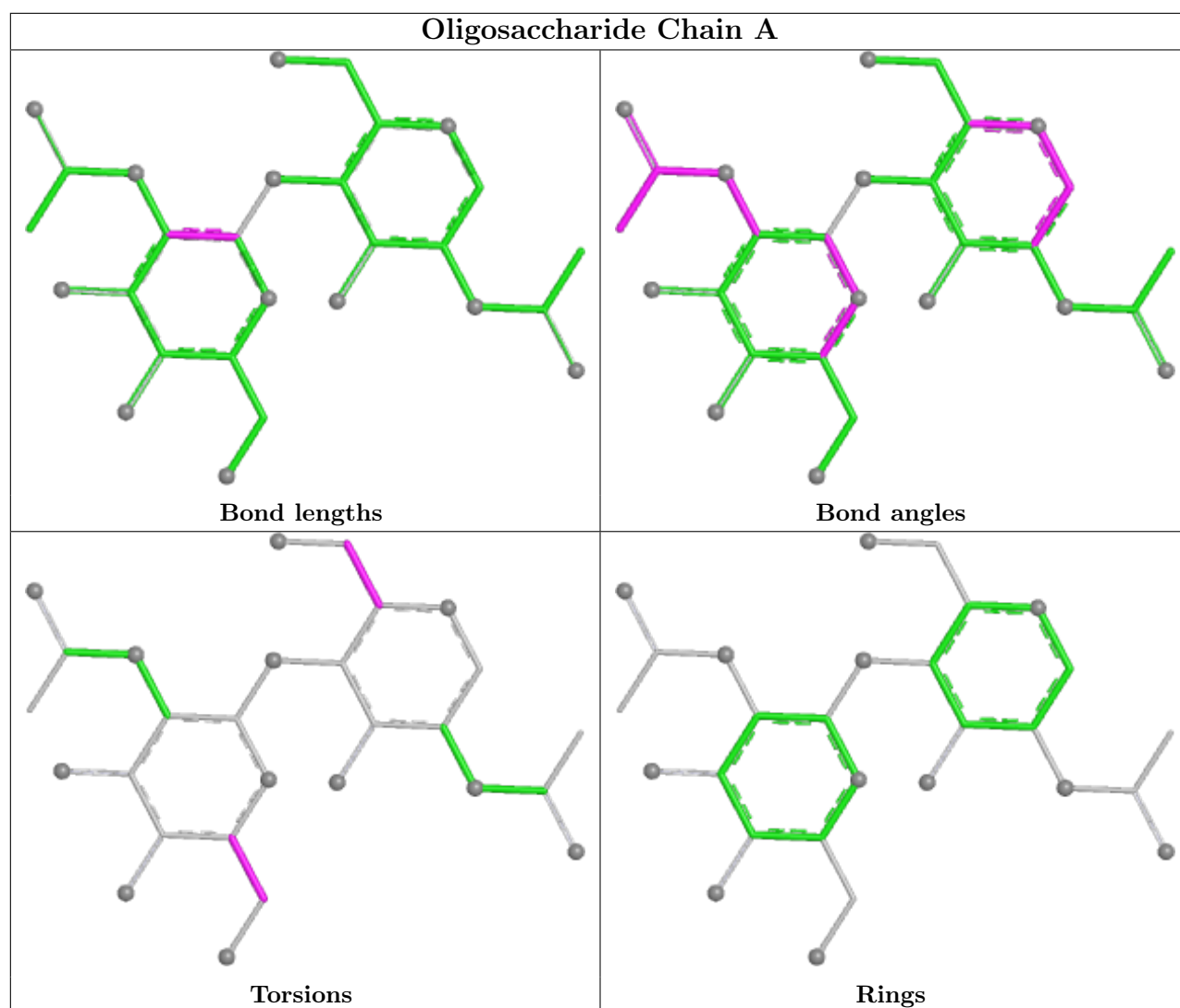
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	2	NAG	O5-C5-C6-O6
4	A	1	NAG	O5-C5-C6-O6
4	A	1	NAG	C4-C5-C6-O6
4	A	2	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.



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

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	B	8/18 (44%)	2.56	4 (50%) 0 0	83, 96, 126, 127	0
2	HHH	216/221 (97%)	1.06	32 (14%) 2 1	39, 66, 107, 127	0
3	LLL	212/216 (98%)	0.78	10 (4%) 31 29	40, 58, 90, 114	0
All	All	436/455 (95%)	0.95	46 (10%) 6 4	39, 61, 104, 127	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	HHH	138	THR	8.5
1	B	5	PRO	5.4
2	HHH	33	TYR	4.5
2	HHH	35	TRP	4.1
1	B	6	GLY	4.0
2	HHH	139	THR	4.0
3	LLL	29	LEU	3.6
2	HHH	28	PRO	3.5
2	HHH	24	VAL	3.4
2	HHH	54	HIS	3.4
2	HHH	27	PHE	3.3
2	HHH	135	CYS	3.3
1	B	12	GLY	3.3
2	HHH	53	ILE	3.2
3	LLL	213	ALA	3.2
2	HHH	34	PHE	3.1
2	HHH	143	VAL	2.9
2	HHH	32	SER	2.8
2	HHH	176	LEU	2.8
2	HHH	52	VAL	2.8
3	LLL	98	ALA	2.7
2	HHH	99	ILE	2.7
1	B	10	LEU	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	LLL	4	TRP	2.6
2	HHH	59	TYR	2.6
2	HHH	204	VAL	2.5
2	HHH	72	MET	2.5
2	HHH	190	VAL	2.4
2	HHH	74	PRO	2.4
3	LLL	70	THR	2.4
2	HHH	107	LEU	2.4
2	HHH	26	GLY	2.4
3	LLL	81	ARG	2.4
2	HHH	79	VAL	2.3
2	HHH	98	ARG	2.3
2	HHH	4	LEU	2.3
2	HHH	68	LEU	2.2
3	LLL	187	ARG	2.2
2	HHH	43	GLY	2.2
2	HHH	97	VAL	2.2
2	HHH	145	LEU	2.1
3	LLL	109	VAL	2.1
2	HHH	114	ILE	2.1
2	HHH	18	LEU	2.1
3	LLL	79	LEU	2.0
3	LLL	110	LEU	2.0

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.

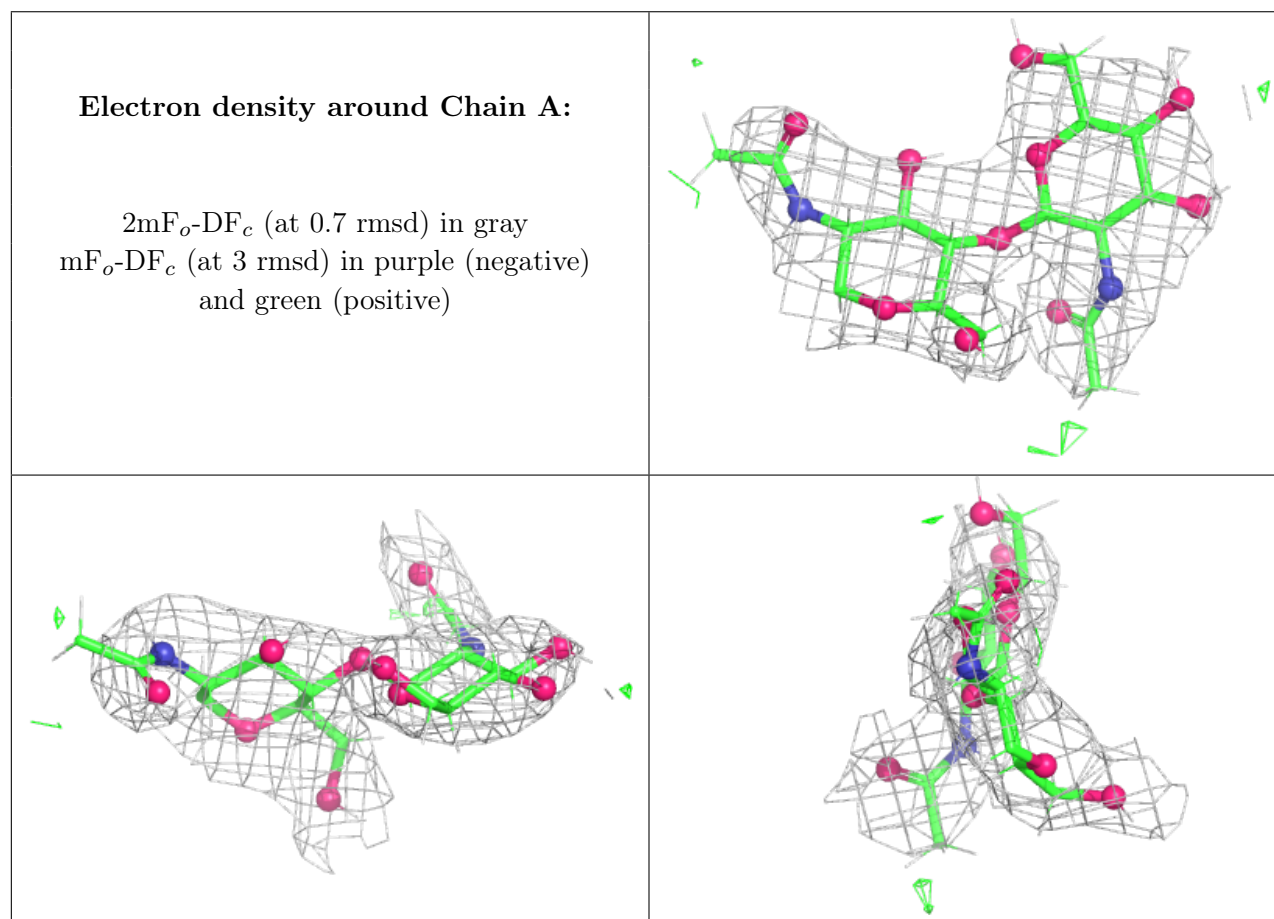
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	CIR	B	8	11/12	0.92	0.26	70,75,80,81	0

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	NAG	A	2	14/15	0.85	0.21	30,91,99,101	3
4	NAG	A	1	14/15	0.89	0.20	30,83,88,90	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.



6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.