



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 26, 2026 – 10:30 AM EDT

PDB ID : 7ZIM / pdb_00007zim
Title : JC Polyomavirus VP1 in complex with 3'-Sialyllactose glycomacromolecules
(aromatic linker)
Authors : Freytag, J.; Mueller, J.C.; Stehle, T.
Deposited on : 2022-04-08
Resolution : 1.55 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

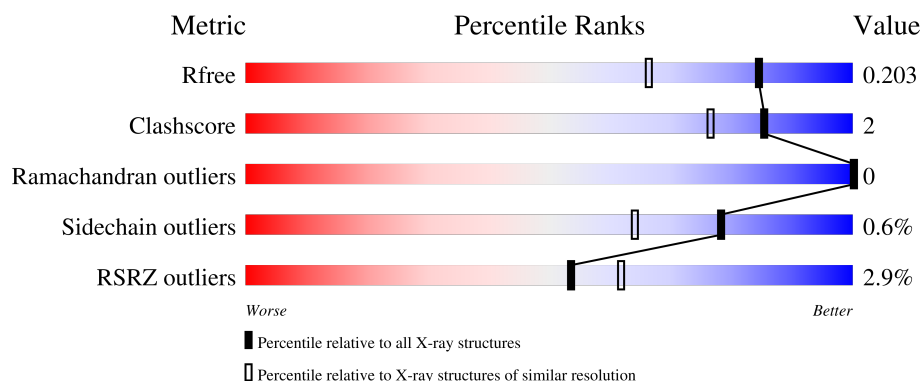
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.55 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.



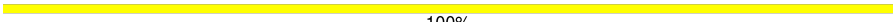
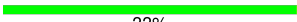
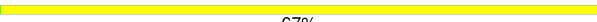
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2145 (1.56-1.56)
Clashscore	190562	2189 (1.56-1.56)
Ramachandran outliers	187476	2153 (1.56-1.56)
Sidechain outliers	187428	2150 (1.56-1.56)
RSRZ outliers	180081	2146 (1.56-1.56)

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	AAA	272	 3% 93% 5%
1	BBB	272	 3% 89% 5% 6%
1	CCC	272	 2% 92% 6%
1	DDD	272	 4% 91% 6%
1	EEE	272	 2% 91% 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	BaB	3	 100%
2	CaC	3	 33%  67%
3	A	2	 50%  50%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12254 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 Major capsid protein VP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	259	Total	C	N	O	S	0	7	0
			2040	1285	349	395	11			
1	BBB	256	Total	C	N	O	S	0	10	0
			2045	1286	352	396	11			
1	CCC	265	Total	C	N	O	S	0	16	0
			2169	1358	369	430	12			
1	DDD	265	Total	C	N	O	S	0	13	0
			2137	1340	368	417	12			
1	EEE	259	Total	C	N	O	S	0	5	0
			2050	1291	353	395	11			

There are 20 discrepancies between the modelled and reference sequences:

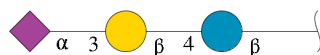
Chain	Residue	Modelled	Actual	Comment	Reference
AAA	18	GLY	-	expression tag	UNP P03089
AAA	19	SER	-	expression tag	UNP P03089
AAA	20	HIS	-	expression tag	UNP P03089
AAA	21	MET	-	expression tag	UNP P03089
BBB	18	GLY	-	expression tag	UNP P03089
BBB	19	SER	-	expression tag	UNP P03089
BBB	20	HIS	-	expression tag	UNP P03089
BBB	21	MET	-	expression tag	UNP P03089
CCC	18	GLY	-	expression tag	UNP P03089
CCC	19	SER	-	expression tag	UNP P03089
CCC	20	HIS	-	expression tag	UNP P03089
CCC	21	MET	-	expression tag	UNP P03089
DDD	18	GLY	-	expression tag	UNP P03089
DDD	19	SER	-	expression tag	UNP P03089
DDD	20	HIS	-	expression tag	UNP P03089
DDD	21	MET	-	expression tag	UNP P03089
EEE	18	GLY	-	expression tag	UNP P03089
EEE	19	SER	-	expression tag	UNP P03089
EEE	20	HIS	-	expression tag	UNP P03089

Continued on next page...

Continued from previous page...

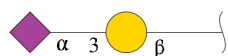
Chain	Residue	Modelled	Actual	Comment	Reference
EEE	21	MET	-	expression tag	UNP P03089

- Molecule 2 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose.



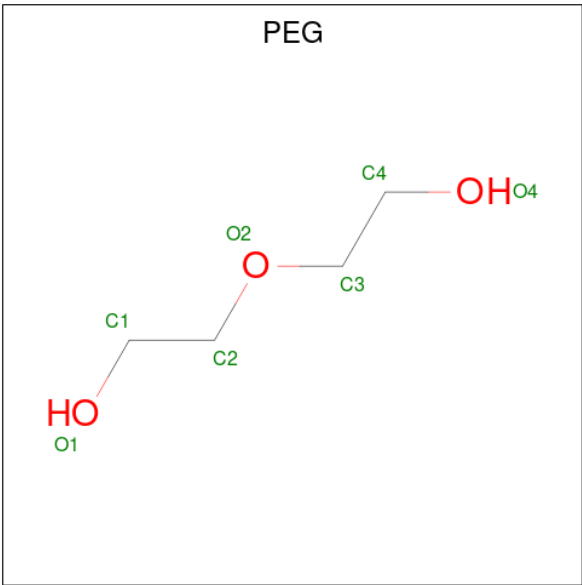
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	BaB	3	Total	C	N	O	0	0	0
			43	23	1	19			
2	CaC	3	Total	C	N	O	0	0	1
			32	17	1	14			

- Molecule 3 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	A	2	Total	C	N	O	0	0	1
			21	11	1	9			

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	AAA	1	Total	C	O	0	0
			7	4	3		
4	EEE	1	Total	C	O	0	0
			7	4	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	AAA	308	Total	O	0	0
			308	308		
5	BBB	320	Total	O	0	0
			320	320		
5	CCC	365	Total	O	0	0
			365	365		
5	DDD	383	Total	O	0	0
			383	383		
5	EEE	327	Total	O	0	0
			327	327		

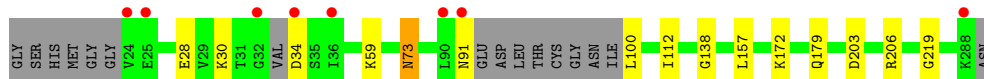
3 Residue-property plots [i](#)

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: Major capsid protein VP1



- Molecule 1: Major capsid protein VP1



- Molecule 1: Major capsid protein VP1



- Molecule 1: Major capsid protein VP1



- Molecule 1: Major capsid protein VP1



- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain BaB:  100%

BGC1
GAL2
SIA3

- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain CaC:  33%  67%

BGC1
GAL2
SIA3

- Molecule 3: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose

Chain A:  50%  50%

GAL1
SIA2

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	150.15Å 96.64Å 128.56Å 90.00° 110.49° 90.00°	Depositor
Resolution (Å)	44.80 – 1.55 44.80 – 1.55	Depositor EDS
% Data completeness (in resolution range)	99.8 (44.80-1.55) 99.9 (44.80-1.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.00 (at 1.55Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.167 , 0.191 0.180 , 0.203	Depositor DCC
R_{free} test set	4979 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å ²)	19.3	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 37.4	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	0.97	EDS
Total number of atoms	12254	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.68% 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: BGC, GAL, PEG, SIA

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	0.94	0/2096	1.04	0/2848
1	BBB	0.93	0/2101	1.02	0/2856
1	CCC	0.92	0/2232	1.02	0/3032
1	DDD	0.94	0/2194	1.05	0/2984
1	EEE	0.94	0/2101	1.04	0/2854
All	All	0.93	0/10724	1.03	0/14574

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 [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	2040	0	1970	6	0
1	BBB	2045	0	1973	11	0
1	CCC	2169	0	2088	14	0
1	DDD	2137	0	2058	12	0
1	EEE	2050	0	1981	9	0
2	BaB	43	0	37	0	0
2	CaC	32	0	26	0	0
3	A	21	0	17	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	AAA	7	0	10	0	0
4	EEE	7	0	10	0	0
5	AAA	308	0	0	1	0
5	BBB	320	0	0	3	0
5	CCC	365	0	0	5	0
5	DDD	383	0	0	1	0
5	EEE	327	0	0	1	0
All	All	12254	0	10170	45	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 2.

All (45) 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:CCC:184[B]:GLU:HG2	5:CCC:585:HOH:O	1.82	0.78
1:AAA:218:GLY:O	1:EEE:223:PRO:CB	2.33	0.76
1:BBB:73:ASN:ND2	5:BBB:301:HOH:O	2.23	0.72
1:AAA:82:VAL:O	1:AAA:192[B]:ASN:ND2	2.23	0.70
1:EEE:203:ASP:OD2	1:EEE:206[B]:ARG:HD3	1.96	0.65
1:AAA:218:GLY:O	1:EEE:223:PRO:HB2	1.96	0.64
1:CCC:114:VAL:O	1:DDD:216[B]:LEU:HD13	1.98	0.64
1:CCC:206[B]:ARG:NH2	5:CCC:301:HOH:O	2.28	0.62
1:CCC:177[A]:GLN:HG2	5:CCC:561:HOH:O	2.02	0.60
1:BBB:203:ASP:OD2	1:BBB:206[B]:ARG:HD3	2.02	0.60
1:DDD:177[B]:GLN:HG2	5:DDD:657:HOH:O	2.02	0.59
1:BBB:59:LYS:HE3	5:BBB:318:HOH:O	2.03	0.57
1:AAA:138:GLY:HA2	1:AAA:219:GLY:O	2.07	0.54
1:CCC:203:ASP:OD2	1:CCC:206[B]:ARG:HD3	2.08	0.53
1:AAA:172:LYS:NZ	5:AAA:702:HOH:O	2.37	0.52
1:DDD:34:ASP:O	1:DDD:284:LYS:HE3	2.09	0.52
1:BBB:112[B]:ILE:HD11	1:CCC:204:PRO:HG3	1.92	0.51
1:BBB:28:GLU:OE2	1:BBB:30:LYS:NZ	2.41	0.51
1:DDD:118:MET:HE2	1:EEE:216:LEU:HD23	1.94	0.50
1:CCC:138:GLY:HA2	1:CCC:219:GLY:O	2.12	0.49
1:CCC:184[B]:GLU:HG3	5:CCC:444:HOH:O	2.14	0.48
1:DDD:68:GLU:H	1:DDD:68:GLU:CD	2.20	0.48
1:EEE:252[B]:TYR:HE2	5:EEE:615:HOH:O	1.98	0.47
1:BBB:172:LYS:NZ	5:BBB:304:HOH:O	2.45	0.47
1:CCC:203:ASP:OD2	1:CCC:206[B]:ARG:CD	2.63	0.46
1:CCC:137:GLN:HE21	1:CCC:221:ASN:HA	1.79	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EEE:218:GLY:O	1:EEE:222:VAL:HG11	2.16	0.45
1:AAA:218:GLY:O	1:EEE:223:PRO:HB3	2.15	0.45
1:BBB:157:LEU:O	1:BBB:179:GLN:HA	2.17	0.44
1:DDD:218:GLY:O	1:DDD:222:VAL:HG11	2.18	0.43
1:BBB:91:ASN:HD21	1:BBB:100:LEU:N	2.16	0.43
1:DDD:94[A]:LEU:HD23	1:DDD:94[A]:LEU:HA	1.77	0.43
1:BBB:112[B]:ILE:CD1	1:CCC:204:PRO:HG3	2.48	0.42
1:EEE:157:LEU:O	1:EEE:179:GLN:HA	2.19	0.42
1:DDD:152:GLU:HB3	1:DDD:206[B]:ARG:CZ	2.49	0.42
1:BBB:138:GLY:HA2	1:BBB:219:GLY:O	2.20	0.42
1:DDD:157:LEU:O	1:DDD:179:GLN:HA	2.20	0.41
1:CCC:157:LEU:O	1:CCC:179:GLN:HA	2.20	0.41
1:DDD:60[A]:SER:HB3	3:A:2:SIA:HO8	1.84	0.41
1:CCC:247:LYS:NZ	5:CCC:316:HOH:O	2.53	0.41
1:DDD:82:VAL:H	1:DDD:192[A]:ASN:HD21	1.68	0.41
1:BBB:34:ASP:N	1:BBB:34:ASP:OD1	2.53	0.41
1:EEE:264[B]:ASN:ND2	1:EEE:268:SER:OG	2.54	0.41
1:DDD:115:THR:HB	1:DDD:118:MET:HE3	2.03	0.40
1:CCC:119:ASN:C	1:CCC:119:ASN:OD1	2.64	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AAA	260/272 (96%)	253 (97%)	7 (3%)	0	100	100
1	BBB	260/272 (96%)	252 (97%)	8 (3%)	0	100	100
1	CCC	277/272 (102%)	266 (96%)	11 (4%)	0	100	100
1	DDD	274/272 (101%)	266 (97%)	8 (3%)	0	100	100
1	EEE	258/272 (95%)	250 (97%)	8 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1329/1360 (98%)	1287 (97%)	42 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	AAA	227/237 (96%)	226 (100%)	1 (0%)	84	73
1	BBB	229/237 (97%)	228 (100%)	1 (0%)	84	73
1	CCC	246/237 (104%)	244 (99%)	2 (1%)	73	56
1	DDD	240/237 (101%)	237 (99%)	3 (1%)	61	36
1	EEE	228/237 (96%)	227 (100%)	1 (0%)	84	73
All	All	1170/1185 (99%)	1162 (99%)	8 (1%)	78	59

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	67	PHE
1	BBB	73	ASN
1	CCC	30	LYS
1	CCC	94	LEU
1	DDD	94[A]	LEU
1	DDD	94[B]	LEU
1	DDD	123	ASN
1	EEE	220	GLU

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 ⓘ

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

5.5 Carbohydrates ⓘ

Of 8 monosaccharides modelled in this entry, 6 were used for Mogul analysis.

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	SIA	A	2	3	20,20,21	0.67	0	21,28,31	0.96	2 (9%)
2	BGC	BaB	1	2	12,12,12	0.87	1 (8%)	17,17,17	1.01	0
2	GAL	BaB	2	2	11,11,12	0.59	0	15,15,17	1.16	1 (6%)
2	SIA	BaB	3	2	20,20,21	0.89	1 (5%)	21,28,31	1.12	3 (14%)
2	GAL	CaC	2	2	11,11,12	0.70	0	15,15,17	2.26	4 (26%)
2	SIA	CaC	3	2	20,20,21	0.91	1 (5%)	21,28,31	1.31	3 (14%)

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	SIA	A	2	3	-	0/18/34/38	0/1/1/1
2	BGC	BaB	1	2	-	0/2/22/22	0/1/1/1
2	GAL	BaB	2	2	-	0/2/19/22	0/1/1/1
2	SIA	BaB	3	2	-	1/18/34/38	0/1/1/1
2	GAL	CaC	2	2	-	0/2/19/22	0/1/1/1
2	SIA	CaC	3	2	-	1/18/34/38	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	CaC	3	SIA	C3-C2	2.41	1.56	1.52
2	BaB	1	BGC	O1-C1	2.23	1.46	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	BaB	3	SIA	C3-C2	2.11	1.55	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	CaC	2	GAL	O3-C3-C2	5.48	121.25	110.05
2	CaC	2	GAL	C2-C3-C4	3.58	117.16	110.86
2	CaC	2	GAL	C3-C4-C5	3.53	116.64	110.23
2	CaC	3	SIA	O6-C2-C3	-3.43	105.95	110.56
2	CaC	3	SIA	O6-C2-C1	3.30	113.94	107.72
2	CaC	2	GAL	C1-O5-C5	3.27	116.56	112.19
2	BaB	2	GAL	O3-C3-C2	-2.85	104.23	110.05
2	BaB	3	SIA	O6-C2-C1	2.32	112.09	107.72
3	A	2	SIA	O1B-C1-C2	2.27	118.61	112.71
3	A	2	SIA	O6-C2-C3	-2.21	107.58	110.56
2	BaB	3	SIA	O1A-C1-C2	-2.17	118.16	122.85
2	CaC	3	SIA	O1A-C1-C2	-2.16	118.19	122.85
2	BaB	3	SIA	O1B-C1-C2	2.03	117.98	112.71

There are no chirality outliers.

All (2) torsion outliers are listed below:

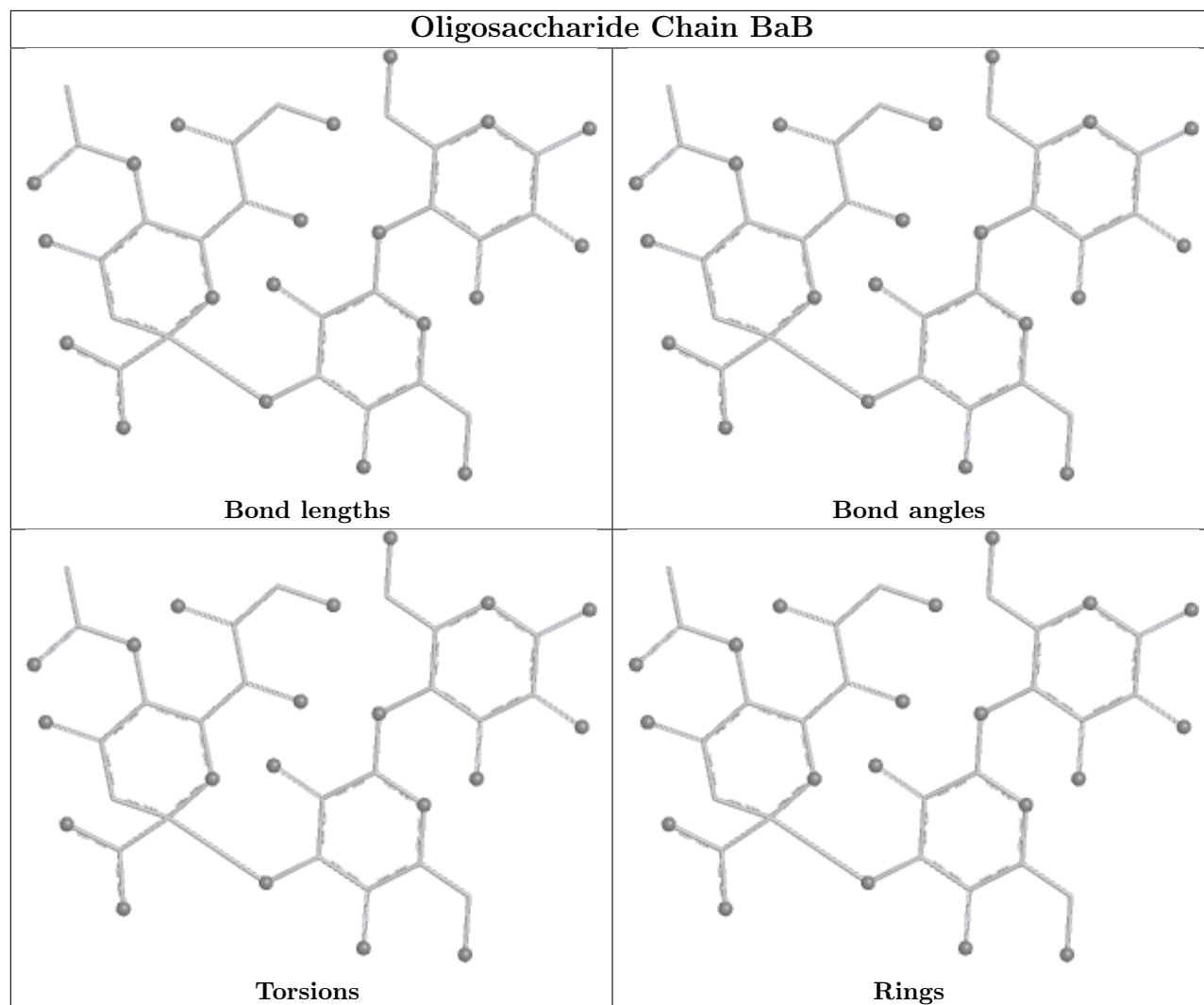
Mol	Chain	Res	Type	Atoms
2	CaC	3	SIA	C6-C7-C8-O8
2	BaB	3	SIA	C6-C7-C8-O8

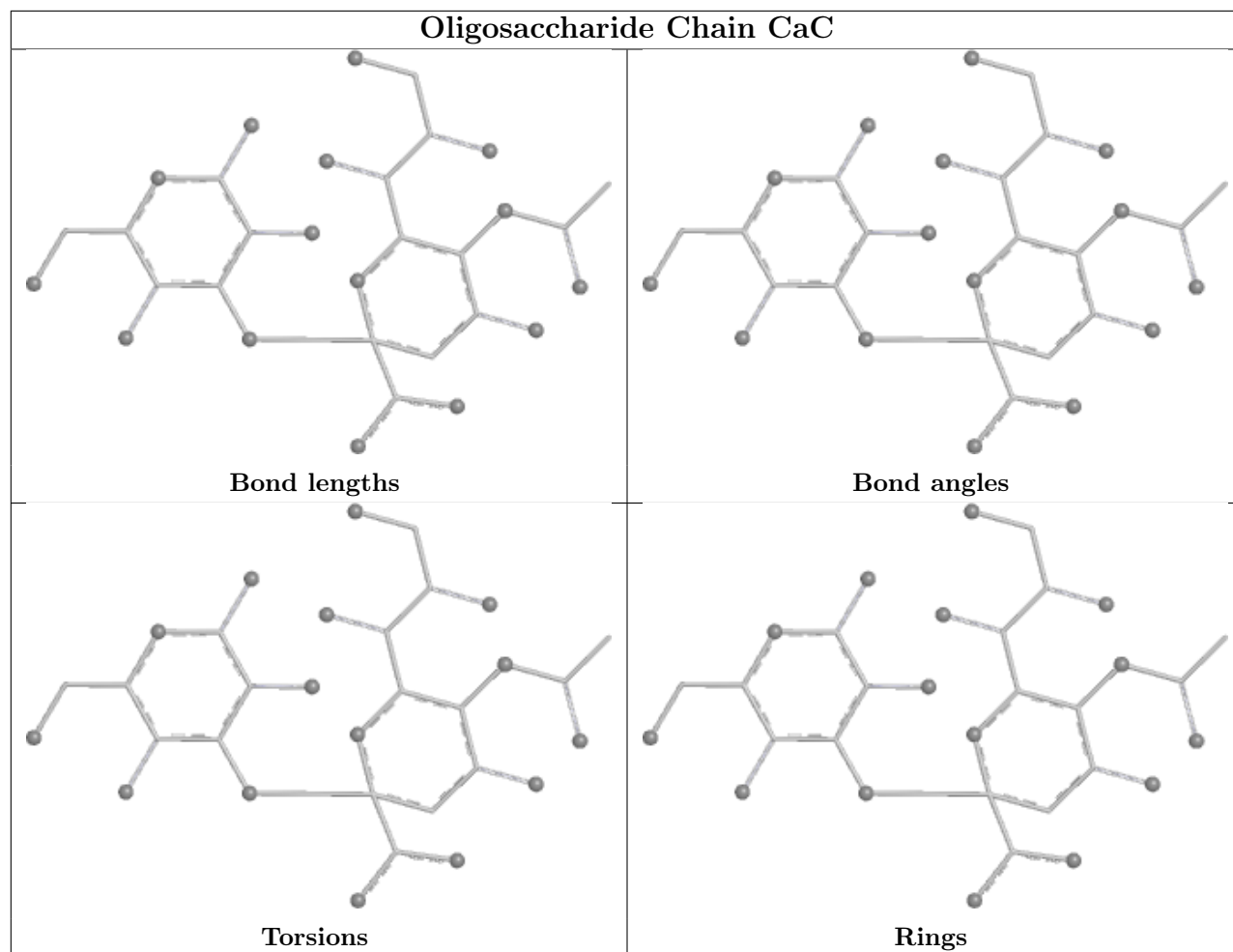
There are no ring outliers.

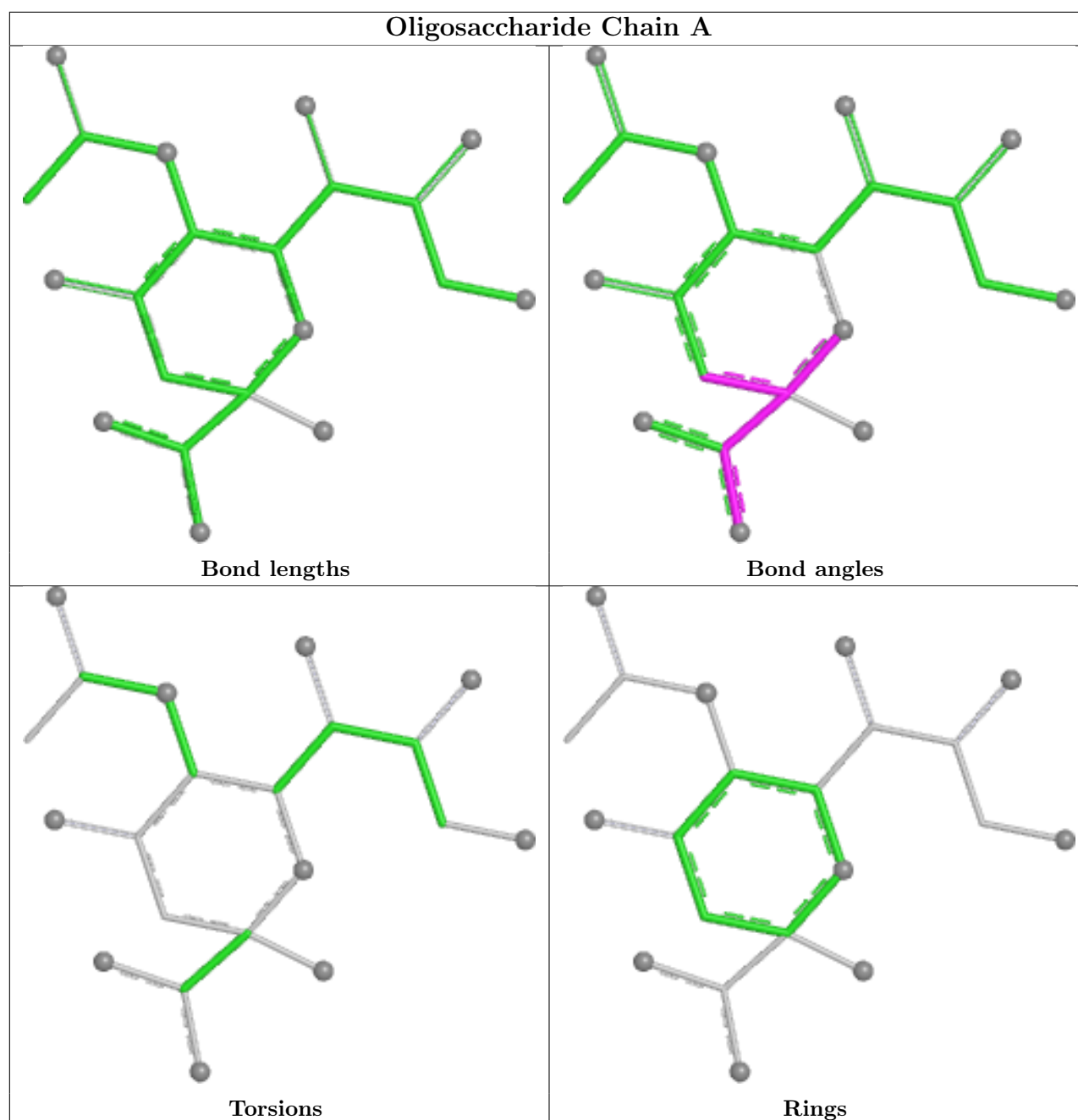
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2	SIA	1	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](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PEG	EEE	501	-	6,6,6	0.23	0	5,5,5	0.13	0
4	PEG	AAA	601	-	6,6,6	0.20	0	5,5,5	0.14	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	PEG	EEE	501	-	-	2/4/4/4	-
4	PEG	AAA	601	-	-	3/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	AAA	601	PEG	O1-C1-C2-O2
4	EEE	501	PEG	O2-C3-C4-O4
4	EEE	501	PEG	O1-C1-C2-O2
4	AAA	601	PEG	O2-C3-C4-O4
4	AAA	601	PEG	C1-C2-O2-C3

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

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	AAA	259/272 (95%)	-0.10	9 (3%)	47	55	8, 17, 32, 61	7 (2%)
1	BBB	256/272 (94%)	-0.08	8 (3%)	51	60	8, 17, 34, 57	10 (3%)
1	CCC	265/272 (97%)	-0.16	6 (2%)	61	69	7, 17, 31, 58	16 (6%)
1	DDD	265/272 (97%)	-0.13	10 (3%)	44	52	8, 16, 32, 58	13 (4%)
1	EEE	259/272 (95%)	-0.11	5 (1%)	66	75	8, 17, 33, 55	5 (1%)
All	All	1304/1360 (95%)	-0.12	38 (2%)	53	62	7, 17, 33, 61	51 (3%)

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	24	VAL	5.2
1	CCC	24	VAL	5.0
1	AAA	24	VAL	4.8
1	DDD	24	VAL	4.8
1	BBB	32	GLY	4.7
1	EEE	24	VAL	4.6
1	AAA	67	PHE	4.1
1	DDD	34	ASP	4.1
1	AAA	98	ASN	4.0
1	DDD	32	GLY	3.9
1	EEE	289	ASN	3.9
1	EEE	34	ASP	3.5
1	CCC	32	GLY	3.3
1	EEE	32	GLY	3.2
1	AAA	289	ASN	3.2
1	DDD	289	ASN	3.2
1	DDD	95	THR	3.2
1	DDD	96	CYS	3.2
1	AAA	34	ASP	3.0
1	CCC	34	ASP	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	CCC	95	THR	3.0
1	EEE	98	ASN	2.9
1	BBB	34	ASP	2.8
1	CCC	289	ASN	2.7
1	AAA	222	VAL	2.7
1	BBB	288	LYS	2.5
1	BBB	91	ASN	2.4
1	AAA	193	LYS	2.4
1	AAA	65	ASP	2.3
1	CCC	96	CYS	2.3
1	DDD	222	VAL	2.2
1	BBB	90	LEU	2.2
1	AAA	218	GLY	2.1
1	DDD	94[A]	LEU	2.1
1	BBB	36	ILE	2.1
1	BBB	25	GLU	2.1
1	DDD	25	GLU	2.1
1	DDD	68	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

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

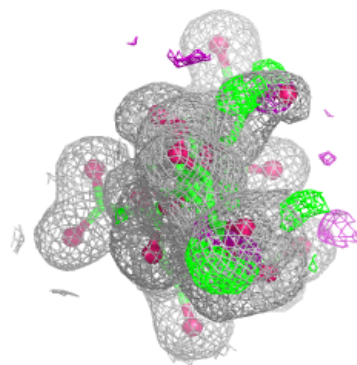
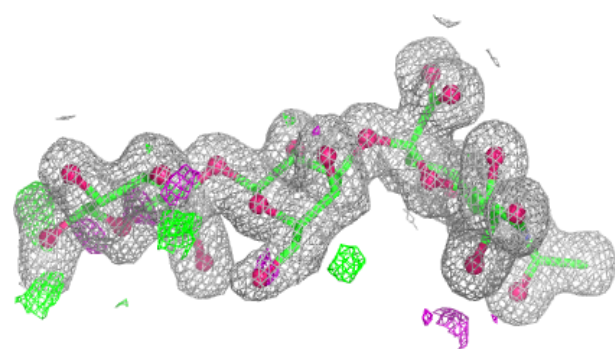
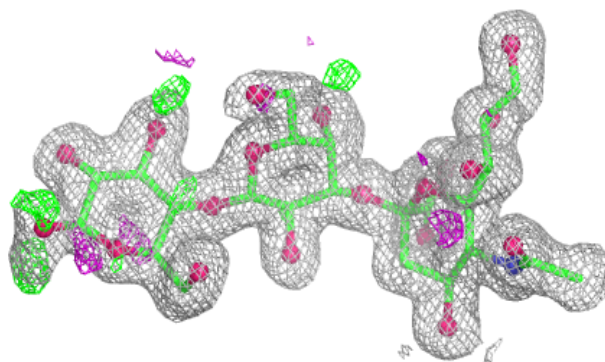
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	BGC	BaB	1	12/12	-	-	22,31,35,36	0
2	GAL	BaB	2	11/12	-	-	16,20,27,34	0
2	SIA	BaB	3	20/21	-	-	15,16,18,18	0
2	BGC	CaC	1	1/12	-	-	52,52,52,52	0
2	GAL	CaC	2	11/12	-	-	27,47,54,60	0
2	SIA	CaC	3	20/21	-	-	15,17,20,20	0
3	GAL	A	1	1/12	-	-	20,20,20,20	0
3	SIA	A	2	20/21	-	-	17,18,21,23	0

The following is a graphical depiction of the model fit to experimental electron density for oligosac-

charide. Each fit is shown from different orientation to approximate a three-dimensional view.

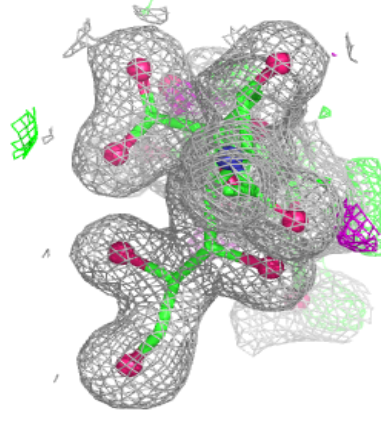
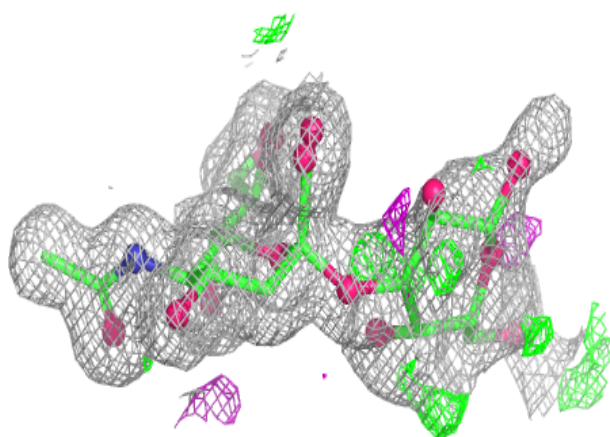
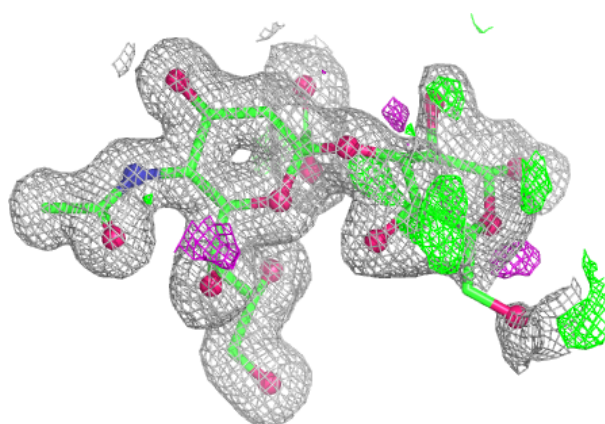
Electron density around Chain BaB:

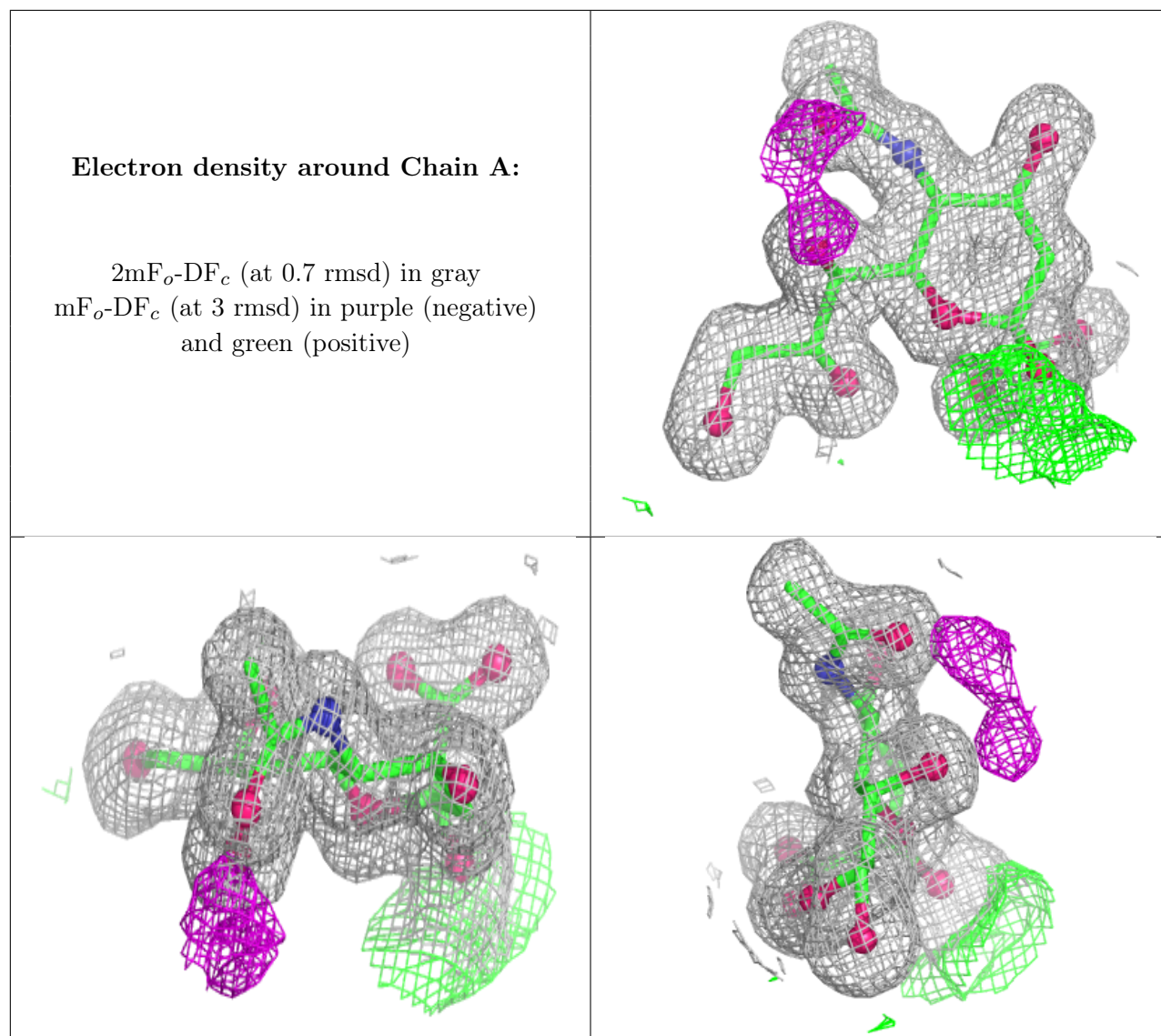
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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 [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
4	PEG	AAA	601	7/7	0.73	0.20	51,54,64,65	0
4	PEG	EEE	501	7/7	0.82	0.19	45,52,54,56	0

6.5 Other polymers [i](#)

There are no such residues in this entry.