



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 04:57 AM UTC

PDB ID : 9PI9 / pdb_00009pi9
Title : Sacituzumab Fab bound to Trop2 Dimer
Authors : Ferrao, R.; Lansdon, E.B.
Deposited on : 2025-07-10
Resolution : 1.56 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

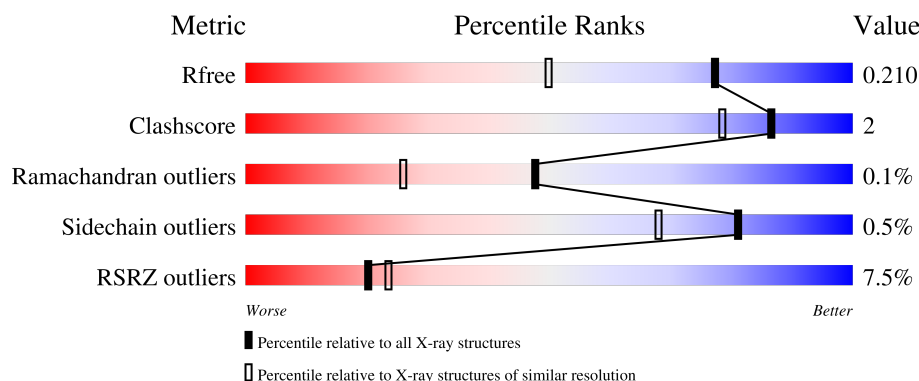
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.56 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.



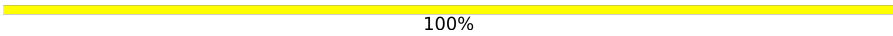
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2145 (1.56-1.56)
Clashscore	190562	2189 (1.56-1.56)
Ramachandran outliers	187476	2153 (1.56-1.56)
Sidechain outliers	187428	2150 (1.56-1.56)
RSRZ outliers	180081	2146 (1.56-1.56)

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	A	226	
1	C	226	
2	B	214	
2	D	214	
3	E	250	

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Mol	Chain	Length	Quality of chain
3	F	250	
4	G	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
8	CIT	E	303	-	-	X	-
8	CIT	F	301	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 11459 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 Sacituzumab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	218	Total	C	N	O	S	0	0	0
			1640	1047	267	320	6			
1	C	217	Total	C	N	O	S	0	1	0
			1638	1046	266	320	6			

- Molecule 2 is a protein called Sacituzumab Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	213	Total	C	N	O	S	0	3	0
			1642	1034	272	330	6			
2	D	213	Total	C	N	O	S	0	3	0
			1644	1035	271	332	6			

- Molecule 3 is a protein called Tumor-associated calcium signal transducer 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	231	Total	C	N	O	S	0	0	0
			1773	1098	327	333	15			
3	F	223	Total	C	N	O	S	0	1	0
			1742	1076	330	321	15			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	120	GLN	ASN	conflict	UNP P09758
E	208	GLN	ASN	conflict	UNP P09758
E	275	HIS	-	expression tag	UNP P09758
E	276	HIS	-	expression tag	UNP P09758
E	277	HIS	-	expression tag	UNP P09758
E	278	HIS	-	expression tag	UNP P09758
E	279	HIS	-	expression tag	UNP P09758
E	280	HIS	-	expression tag	UNP P09758

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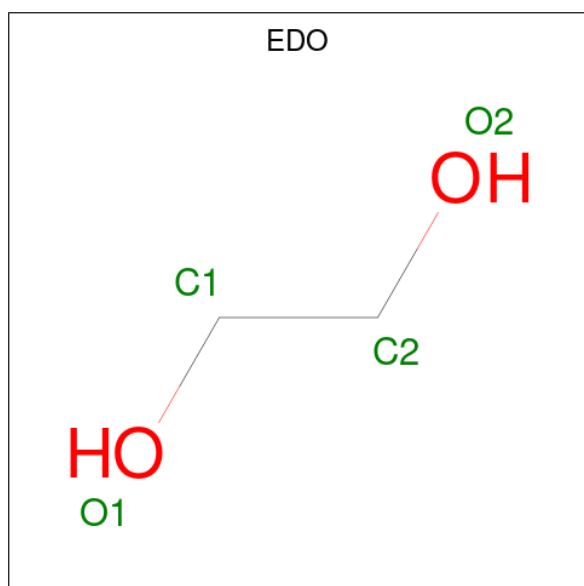
Chain	Residue	Modelled	Actual	Comment	Reference
F	120	GLN	ASN	conflict	UNP P09758
F	208	GLN	ASN	conflict	UNP P09758
F	275	HIS	-	expression tag	UNP P09758
F	276	HIS	-	expression tag	UNP P09758
F	277	HIS	-	expression tag	UNP P09758
F	278	HIS	-	expression tag	UNP P09758
F	279	HIS	-	expression tag	UNP P09758
F	280	HIS	-	expression tag	UNP P09758

- 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	G	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



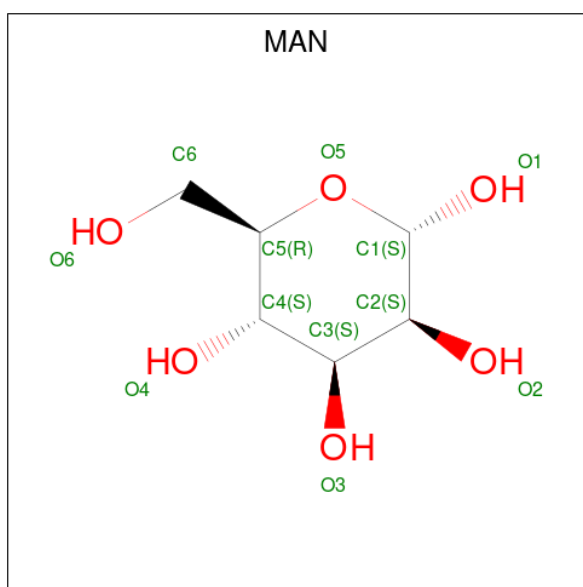
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		

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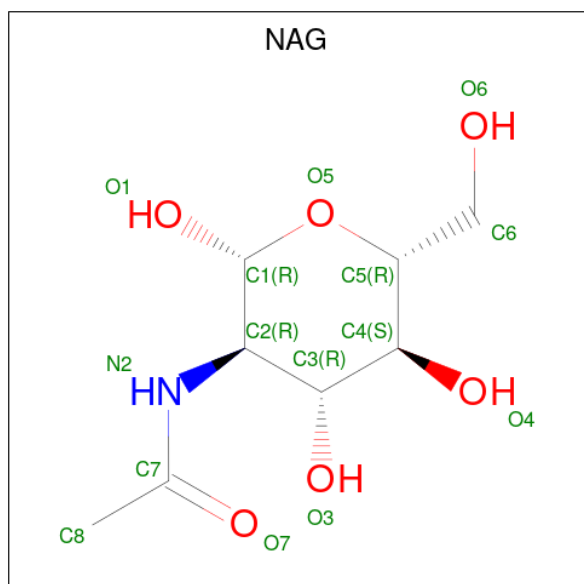
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	E	1	Total	C	O	0	0
			4	2	2		
5	E	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is alpha-D-mannopyranose (CCD ID: MAN) (formula: C₆H₁₂O₆).



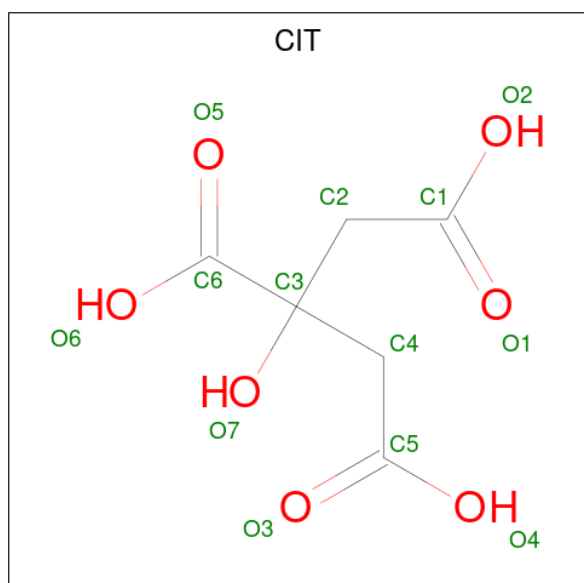
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	C	O	0	0
			12	6	6		

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	E	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 8 is CITRIC ACID (CCD ID: CIT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	E	1	Total	C	O	0	0
			13	6	7		
8	F	1	Total	C	O	0	0
			13	6	7		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	234	Total	O	0	0
			234	234		
9	B	265	Total	O	0	0
			265	265		
9	C	219	Total	O	0	0
			219	219		
9	D	273	Total	O	0	0
			273	273		
9	E	120	Total	O	0	0
			120	120		
9	F	141	Total	O	0	0
			141	141		

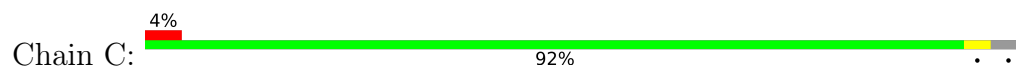
3 Residue-property plots [i](#)

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: Sacituzumab Heavy Chain



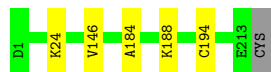
- Molecule 1: Sacituzumab Heavy Chain



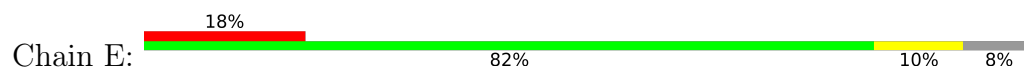
- Molecule 2: Sacituzumab Light Chain

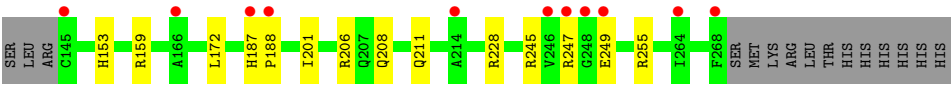


- Molecule 2: Sacituzumab Light Chain

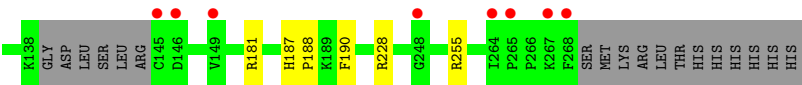
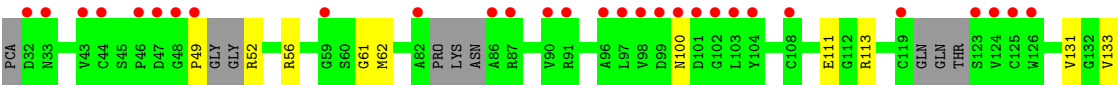
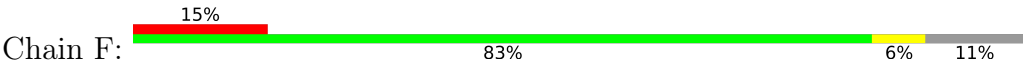


- Molecule 3: Tumor-associated calcium signal transducer 2

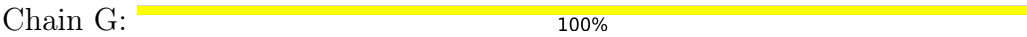




● Molecule 3: Tumor-associated calcium signal transducer 2



● 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	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	50.43Å 210.60Å 78.06Å 90.00° 105.56° 90.00°	Depositor
Resolution (Å)	47.34 – 1.56 47.34 – 1.56	Depositor EDS
% Data completeness (in resolution range)	99.6 (47.34-1.56) 91.7 (47.34-1.56)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.83 (at 1.56Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, R_{free}	0.181 , 0.211 0.180 , 0.210	Depositor DCC
R_{free} test set	2005 reflections (0.90%)	wwPDB-VP
Wilson B-factor (Å ²)	19.5	Xtriage
Anisotropy	0.350	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 38.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	11459	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.95% 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: EDO, MAN, CIT, NAG, PCA

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	A	0.54	0/1685	0.69	0/2297
1	C	0.51	0/1686	0.67	0/2298
2	B	0.57	0/1687	0.73	0/2294
2	D	0.55	0/1689	0.75	0/2297
3	E	0.41	0/1799	0.61	0/2434
3	F	0.44	0/1775	0.62	0/2396
All	All	0.51	0/10321	0.68	0/14016

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	A	1640	0	1580	3	0
1	C	1638	0	1583	4	0
2	B	1642	0	1607	3	0
2	D	1644	0	1604	3	0
3	E	1773	0	1689	19	0
3	F	1742	0	1679	12	0
4	G	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	12	0	18	0	0
5	B	8	0	12	0	0
5	C	12	0	18	0	0
5	D	8	0	12	0	0
5	E	8	0	12	1	0
6	C	12	0	12	0	0
7	E	14	0	13	0	0
8	E	13	0	5	6	0
8	F	13	0	5	6	0
9	A	234	0	0	0	0
9	B	265	0	0	0	0
9	C	219	0	0	0	0
9	D	273	0	0	0	0
9	E	120	0	0	0	0
9	F	141	0	0	0	0
All	All	11459	0	9874	42	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 (42) 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:F:255:ARG:HE	8:F:301:CIT:H42	1.33	0.90
3:E:255:ARG:HE	8:E:303:CIT:H42	1.34	0.89
3:F:49:PRO:HD2	3:F:52:ARG:HD2	1.70	0.73
3:E:208:GLN:HB2	3:E:211:GLN:HG3	1.76	0.68
3:F:111:GLU:OE1	3:F:113:ARG:NH2	2.30	0.64
3:E:56:ARG:HH21	3:E:61:GLY:HA2	1.63	0.63
3:E:228:ARG:NH2	8:F:301:CIT:O7	2.33	0.61
3:E:228:ARG:HH22	8:F:301:CIT:H41	1.67	0.59
1:A:60:TYR:HB3	1:A:64:PHE:O	2.06	0.56
3:F:255:ARG:HE	8:F:301:CIT:C4	2.14	0.55
3:E:255:ARG:NE	8:E:303:CIT:H42	2.15	0.55
3:E:255:ARG:HE	8:E:303:CIT:C4	2.15	0.54
8:E:303:CIT:H41	3:F:228:ARG:HH22	1.73	0.54
3:F:56:ARG:HH21	3:F:61:GLY:HA3	1.72	0.54
3:E:153:HIS:HD2	3:E:206:ARG:HG2	1.74	0.52
3:E:45:SER:C	3:E:47:ASP:H	2.22	0.48
3:E:159:ARG:HH21	8:E:303:CIT:H41	1.79	0.46
3:E:42:THR:HG21	3:E:64:VAL:HG11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:ALA:HB1	1:A:108:PHE:HB3	1.97	0.45
3:E:100:ASN:HA	3:F:100:ASN:HA	1.99	0.45
3:F:131:VAL:HG23	3:F:133:VAL:HG23	1.97	0.45
2:B:37:GLN:HB2	2:B:47:LEU:HD11	2.00	0.44
1:C:61:THR:O	1:C:65:LYS:HG3	2.17	0.44
2:B:184:ALA:O	2:B:188:LYS:HG3	2.18	0.44
3:F:255:ARG:NE	8:F:301:CIT:H42	2.16	0.44
2:B:105:GLU:OE1	2:B:173:TYR:OH	2.27	0.44
1:A:105:TYR:CD1	3:E:245:ARG:HD2	2.53	0.44
3:E:255:ARG:HD2	3:E:255:ARG:C	2.43	0.43
3:E:172:LEU:HD21	3:E:201:ILE:HG23	1.99	0.43
2:D:184:ALA:O	2:D:188:LYS:HG3	2.19	0.43
1:C:203:ILE:HD13	1:C:218:ARG:HA	2.01	0.43
3:E:77:LYS:HG2	3:E:105:ASP:OD1	2.20	0.42
3:E:228:ARG:HH22	8:F:301:CIT:C4	2.32	0.42
1:C:31:ASN:OD1	5:E:301:EDO:H22	2.19	0.42
8:E:303:CIT:C4	3:F:228:ARG:HH22	2.32	0.42
2:D:24:LYS:HB2	2:D:24:LYS:HE2	1.84	0.41
3:F:187[B]:HIS:HB3	3:F:190:PHE:CD2	2.56	0.41
1:C:153:TYR:CE2	1:C:158:VAL:HG13	2.55	0.40
3:E:62:MET:HE3	3:E:62:MET:HB3	1.94	0.40
3:E:187:HIS:ND1	3:E:188:PRO:HD2	2.37	0.40
3:F:181:ARG:HD2	3:F:188:PRO:HG3	2.03	0.40
2:D:146:VAL:HG13	2:D:194[B]:CYS:SG	2.61	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	A	214/226 (95%)	209 (98%)	5 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	214/226 (95%)	211 (99%)	3 (1%)	0	100	100
2	B	214/214 (100%)	210 (98%)	4 (2%)	0	100	100
2	D	214/214 (100%)	210 (98%)	4 (2%)	0	100	100
3	E	225/250 (90%)	217 (96%)	7 (3%)	1 (0%)	30	13
3	F	214/250 (86%)	208 (97%)	6 (3%)	0	100	100
All	All	1295/1380 (94%)	1265 (98%)	29 (2%)	1 (0%)	48	26

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	247	ARG

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	A	181/190 (95%)	181 (100%)	0	100	100
1	C	182/190 (96%)	180 (99%)	2 (1%)	65	43
2	B	188/187 (100%)	188 (100%)	0	100	100
2	D	188/187 (100%)	188 (100%)	0	100	100
3	E	185/216 (86%)	182 (98%)	3 (2%)	55	28
3	F	185/216 (86%)	184 (100%)	1 (0%)	81	68
All	All	1109/1186 (94%)	1103 (100%)	6 (0%)	81	68

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	203	ILE
1	C	214	LYS
3	E	32	ASP
3	E	64	VAL
3	E	249	GLU

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Mol	Chain	Res	Type
3	F	62	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	160	GLN
1	C	39	GLN
2	D	27	GLN
2	D	38	GLN
2	D	189	HIS
3	E	54	GLN
3	E	152	HIS
3	E	198	GLN
3	E	208	GLN
3	E	252	GLN
3	F	198	GLN
3	F	208	GLN

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	$\# Z > 2$
3	PCA	E	31	3	7,8,9	0.73	0	9,10,12	1.28	2 (22%)

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	PCA	E	31	3	-	0/0/11/13	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	31	PCA	CB-CA-N	2.28	109.51	103.24
3	E	31	PCA	CB-CG-CD	2.08	107.63	104.41

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 [i](#)

2 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	G	1	4,3	14,14,15	0.79	0	17,19,21	1.21	1 (5%)
4	NAG	G	2	4	14,14,15	0.66	0	17,19,21	1.23	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	G	1	4,3	-	0/6/23/26	0/1/1/1
4	NAG	G	2	4	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
4	G	2	NAG	C1-O5-C5	3.47	116.84	112.19
4	G	1	NAG	C1-C2-N2	2.19	113.89	110.43

There are no chirality outliers.

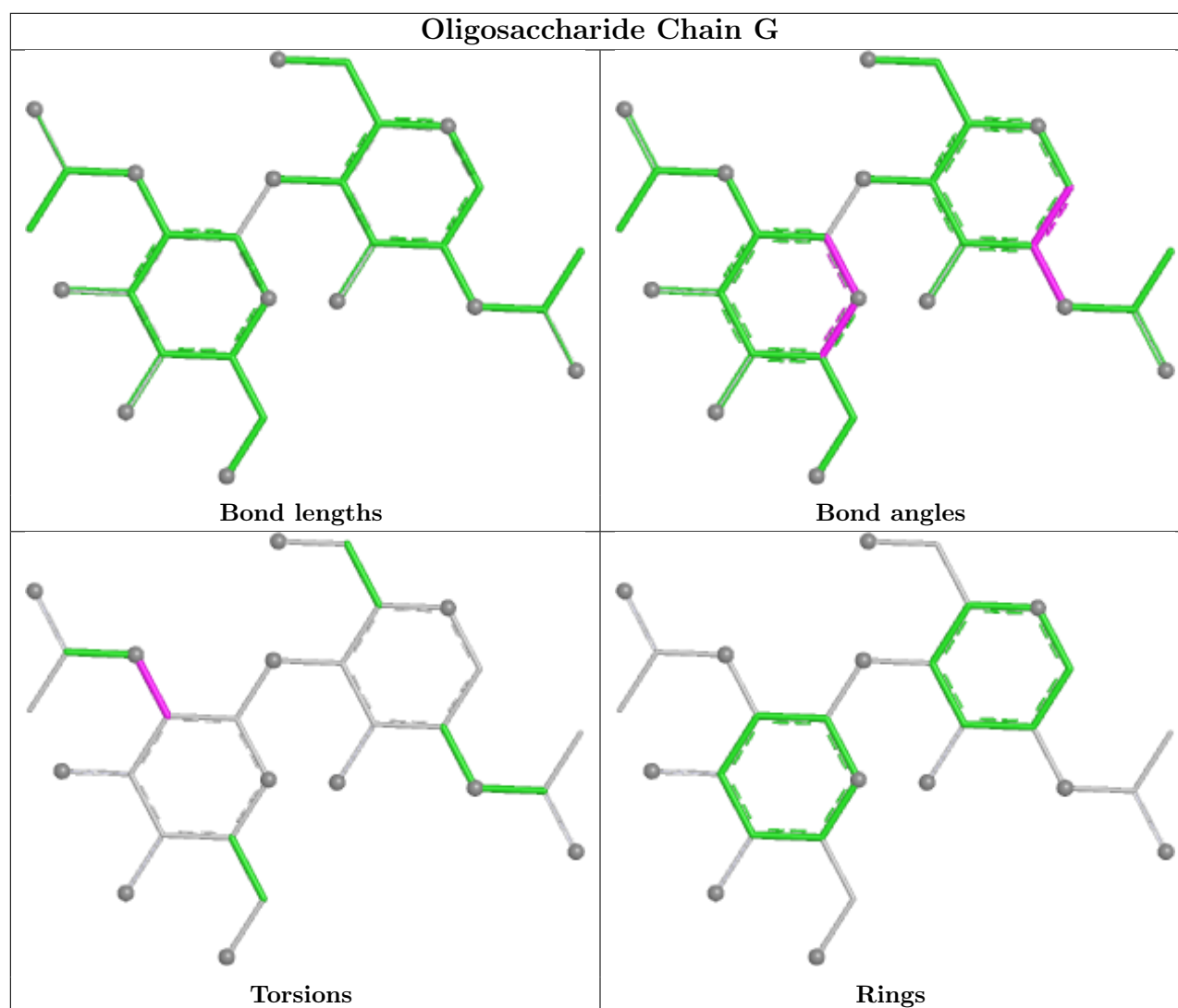
All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	2	NAG	C1-C2-N2-C7

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](#)

16 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	$\# Z > 2$
5	EDO	B	302	-	3,3,3	0.21	0	2,2,2	0.48	0
5	EDO	B	301	-	3,3,3	0.22	0	2,2,2	0.59	0
5	EDO	D	301	-	3,3,3	0.16	0	2,2,2	0.66	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	EDO	E	304	-	3,3,3	0.33	0	2,2,2	0.38	0
6	MAN	C	304	-	12,12,12	0.51	0	17,17,17	0.86	0
5	EDO	A	302	-	3,3,3	0.42	0	2,2,2	0.26	0
5	EDO	C	302	-	3,3,3	0.43	0	2,2,2	0.52	0
5	EDO	E	301	-	3,3,3	0.35	0	2,2,2	0.69	0
8	CIT	F	301	-	12,12,12	1.42	1 (8%)	17,17,17	1.48	5 (29%)
5	EDO	A	303	-	3,3,3	0.43	0	2,2,2	0.31	0
5	EDO	D	302	-	3,3,3	0.30	0	2,2,2	0.61	0
5	EDO	C	301	-	3,3,3	0.29	0	2,2,2	0.17	0
8	CIT	E	303	-	12,12,12	1.70	1 (8%)	17,17,17	1.82	5 (29%)
5	EDO	C	303	-	3,3,3	0.27	0	2,2,2	0.55	0
7	NAG	E	302	3	14,14,15	0.71	0	17,19,21	1.29	1 (5%)
5	EDO	A	301	-	3,3,3	0.36	0	2,2,2	0.72	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
5	EDO	B	302	-	-	0/1/1/1	-
5	EDO	B	301	-	-	0/1/1/1	-
5	EDO	D	301	-	-	0/1/1/1	-
5	EDO	E	304	-	-	0/1/1/1	-
6	MAN	C	304	-	-	0/2/22/22	0/1/1/1
5	EDO	A	302	-	-	0/1/1/1	-
5	EDO	C	302	-	-	0/1/1/1	-
5	EDO	E	301	-	-	0/1/1/1	-
8	CIT	F	301	-	-	1/16/16/16	-
5	EDO	A	303	-	-	0/1/1/1	-
5	EDO	D	302	-	-	1/1/1/1	-
5	EDO	C	301	-	-	0/1/1/1	-
8	CIT	E	303	-	-	9/16/16/16	-
5	EDO	C	303	-	-	0/1/1/1	-
7	NAG	E	302	3	-	0/6/23/26	0/1/1/1
5	EDO	A	301	-	-	0/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	E	303	CIT	C3-C6	3.97	1.57	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	F	301	CIT	C3-C6	2.92	1.56	1.53

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	E	303	CIT	O5-C6-C3	-3.86	114.61	122.09
8	E	303	CIT	O6-C6-C3	3.57	119.98	113.14
8	E	303	CIT	C3-C4-C5	3.07	122.32	113.92
8	F	301	CIT	O5-C6-C3	-2.97	116.34	122.09
8	F	301	CIT	C3-C4-C5	2.84	121.68	113.92
7	E	302	NAG	C1-C2-N2	2.75	114.77	110.43
8	E	303	CIT	C4-C3-C2	2.44	115.56	109.31
8	F	301	CIT	O6-C6-C3	2.32	117.60	113.14
8	E	303	CIT	C2-C3-C6	-2.26	105.03	110.03
8	F	301	CIT	C4-C3-C2	2.11	114.72	109.31
8	F	301	CIT	O1-C1-C2	-2.08	117.05	122.95

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	E	303	CIT	C2-C3-C4-C5
8	E	303	CIT	C6-C3-C4-C5
8	E	303	CIT	O7-C3-C6-O5
8	E	303	CIT	O7-C3-C6-O6
8	E	303	CIT	C4-C3-C6-O5
8	E	303	CIT	C4-C3-C6-O6
8	E	303	CIT	O7-C3-C4-C5
8	E	303	CIT	C1-C2-C3-O7
5	D	302	EDO	O1-C1-C2-O2
8	F	301	CIT	C1-C2-C3-O7
8	E	303	CIT	C1-C2-C3-C4

There are no ring outliers.

3 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	301	EDO	1	0
8	F	301	CIT	6	0
8	E	303	CIT	6	0

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	A	218/226 (96%)	0.15	6 (2%)	55	63	15, 25, 50, 64	0
1	C	217/226 (96%)	0.16	8 (3%)	45	53	15, 26, 53, 65	1 (0%)
2	B	213/214 (99%)	-0.13	1 (0%)	87	90	14, 23, 43, 58	3 (1%)
2	D	213/214 (99%)	-0.11	0	100	100	14, 24, 44, 57	3 (1%)
3	E	230/250 (92%)	1.00	46 (20%)	3	3	19, 40, 72, 83	0
3	F	223/250 (89%)	0.85	37 (16%)	4	5	17, 35, 73, 93	1 (0%)
All	All	1314/1380 (95%)	0.33	98 (7%)	20	23	14, 28, 63, 93	8 (0%)

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	103	LEU	6.4
3	E	123	SER	5.9
3	F	268	PHE	5.6
3	E	140	ASP	5.5
3	F	98	VAL	5.1
3	E	124	VAL	4.7
3	F	123	SER	4.5
1	C	195	SER	4.3
3	E	57	ALA	4.1
3	E	63	ALA	4.1
3	F	82	ALA	4.0
3	E	214	ALA	3.9
3	F	119	CYS	3.9
3	F	32	ASP	3.8
3	E	60	SER	3.7
3	F	97	LEU	3.7
3	F	145	CYS	3.7
3	E	119	CYS	3.6
3	E	83	PRO	3.5

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Mol	Chain	Res	Type	RSRZ
3	F	86	ALA	3.5
3	E	58	LEU	3.5
3	F	49	PRO	3.4
3	E	103	LEU	3.4
3	F	124	VAL	3.3
3	E	100	ASN	3.2
1	A	198	GLY	3.2
1	A	1	GLN	3.1
3	E	59	GLY	3.1
3	F	48	GLY	3.1
3	F	104	TYR	3.0
3	F	126	TRP	3.0
1	C	222	LYS	3.0
3	E	84	LYS	3.0
3	E	47	ASP	3.0
3	E	43	VAL	3.0
3	E	264	ILE	2.9
3	F	91	ARG	2.9
1	A	66	GLY	2.9
1	C	221	PRO	2.8
1	C	65	LYS	2.8
3	E	33	ASN	2.8
3	F	102	GLY	2.8
1	A	142	GLY	2.7
3	E	187	HIS	2.7
3	E	49	PRO	2.7
3	F	149	VAL	2.7
3	E	62	MET	2.6
3	F	265	PRO	2.6
1	C	66	GLY	2.6
3	E	248	GLY	2.6
3	E	86	ALA	2.6
3	F	96	ALA	2.6
3	F	125	CYS	2.5
3	F	248	GLY	2.5
1	A	137	LYS	2.5
3	E	52	ARG	2.5
3	F	101	ASP	2.5
3	F	264	ILE	2.5
3	E	85	ASN	2.5
3	F	90	VAL	2.5
3	E	46	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
3	F	146	ASP	2.4
3	E	268	PHE	2.4
3	E	82	ALA	2.4
3	F	46	PRO	2.4
3	F	108	CYS	2.3
3	E	98	VAL	2.3
3	E	247	ARG	2.3
1	A	222	LYS	2.3
3	E	166	ALA	2.3
3	F	100	ASN	2.2
3	E	110	PRO	2.2
3	F	47	ASP	2.2
3	E	246	VAL	2.2
3	E	145	CYS	2.2
3	E	139	GLY	2.2
1	C	194	SER	2.2
3	F	99	ASP	2.2
3	E	51	GLY	2.2
3	E	249	GLU	2.2
3	F	267	LYS	2.2
3	E	188	PRO	2.1
3	E	97	LEU	2.1
1	C	203	ILE	2.1
3	E	101	ASP	2.1
3	E	61	GLY	2.1
3	F	43	VAL	2.1
3	E	44	CYS	2.1
3	F	87	ARG	2.1
3	E	94	GLU	2.1
3	E	32	ASP	2.1
3	F	33	ASN	2.1
3	E	54	GLN	2.0
3	F	44	CYS	2.0
1	C	198	GLY	2.0
3	F	59	GLY	2.0
2	B	213	GLU	2.0
3	E	104	TYR	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.

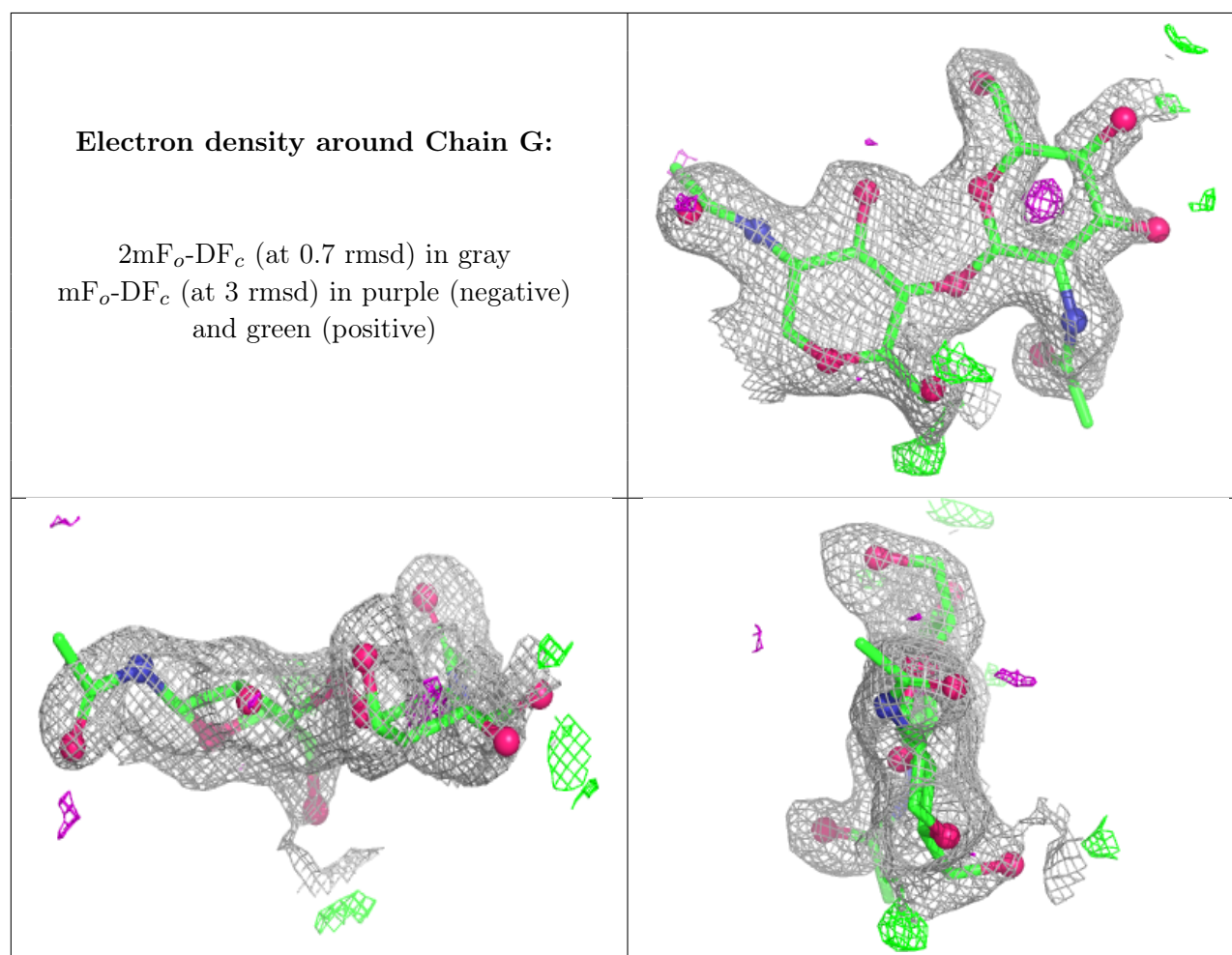
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	PCA	E	31	8/9	0.91	0.15	29,48,54,55	0

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(Å ²)	Q<0.9
4	NAG	G	2	14/15	0.64	0.17	65,81,90,91	0
4	NAG	G	1	14/15	0.83	0.12	40,48,65,67	0

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



6.4 Ligands

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
8	CIT	E	303	13/13	0.62	0.17	44,65,76,83	0
8	CIT	F	301	13/13	0.64	0.16	34,61,69,71	0
5	EDO	E	304	4/4	0.71	0.20	39,41,42,46	0
6	MAN	C	304	12/12	0.80	0.13	36,41,48,55	0
5	EDO	E	301	4/4	0.81	0.16	35,37,37,42	0
5	EDO	B	301	4/4	0.85	0.12	31,32,40,42	0
7	NAG	E	302	14/15	0.85	0.12	44,60,66,69	0
5	EDO	B	302	4/4	0.90	0.10	31,32,33,34	0
5	EDO	D	302	4/4	0.90	0.11	30,33,38,53	0
5	EDO	D	301	4/4	0.91	0.10	30,31,33,33	0
5	EDO	A	301	4/4	0.92	0.11	22,26,32,33	0
5	EDO	C	302	4/4	0.94	0.10	21,25,33,33	0
5	EDO	A	302	4/4	0.95	0.09	22,30,31,33	0
5	EDO	C	303	4/4	0.95	0.10	23,29,37,38	0
5	EDO	A	303	4/4	0.96	0.13	21,23,36,41	0
5	EDO	C	301	4/4	0.96	0.08	22,27,35,37	0

6.5 Other polymers

There are no such residues in this entry.