



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 27, 2026 – 04:56 PM EDT

PDB ID : 1UZ8 / pdb_00001uz8
Title : anti-Lewis X Fab fragment in complex with Lewis X
Authors : Van Roon, A.M.M.; Pannu, N.S.; De Vrind, J.P.M.; Hokke, C.H.; Deelder, A.M.; Van Der marel, G.A.; Van Boom, J.H.; Abrahams, J.P.
Deposited on : 2004-03-05
Resolution : 1.80 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

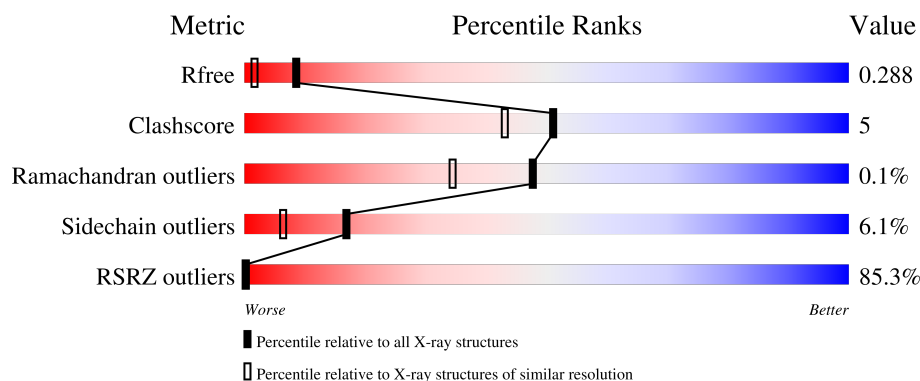
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	218	
1	L	218	
2	B	212	
2	H	212	
3	C	3	

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Mol	Chain	Length	Quality of chain
3	D	3	 67% 33%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7002 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.

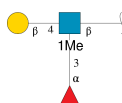
- Molecule 1 is a protein called IGG FAB (IGG3, KAPPA) LIGHT CHAIN 291-2G3-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	218	Total	C	N	O	S	0	3	0
			1704	1065	286	346	7			
1	L	218	Total	C	N	O	S	0	1	0
			1696	1061	282	346	7			

- Molecule 2 is a protein called IGG FAB (IGG3, KAPPA) HEAVY CHAIN 291-2G3-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	212	Total	C	N	O	S	0	2	0
			1619	1029	268	315	7			
2	H	212	Total	C	N	O	S	0	3	0
			1622	1031	268	316	7			

- Molecule 3 is an oligosaccharide called alpha-L-fucopyranose-(1-3)-[beta-D-galactopyranose-(1-4)]methyl 2-acetamido-2-deoxy-beta-D-glucopyranoside.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	3	Total	C	N	O	0	0	0
			37	21	1	15			
3	D	3	Total	C	N	O	0	0	0
			37	21	1	15			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	65	Total	O	0	0
			65	65		

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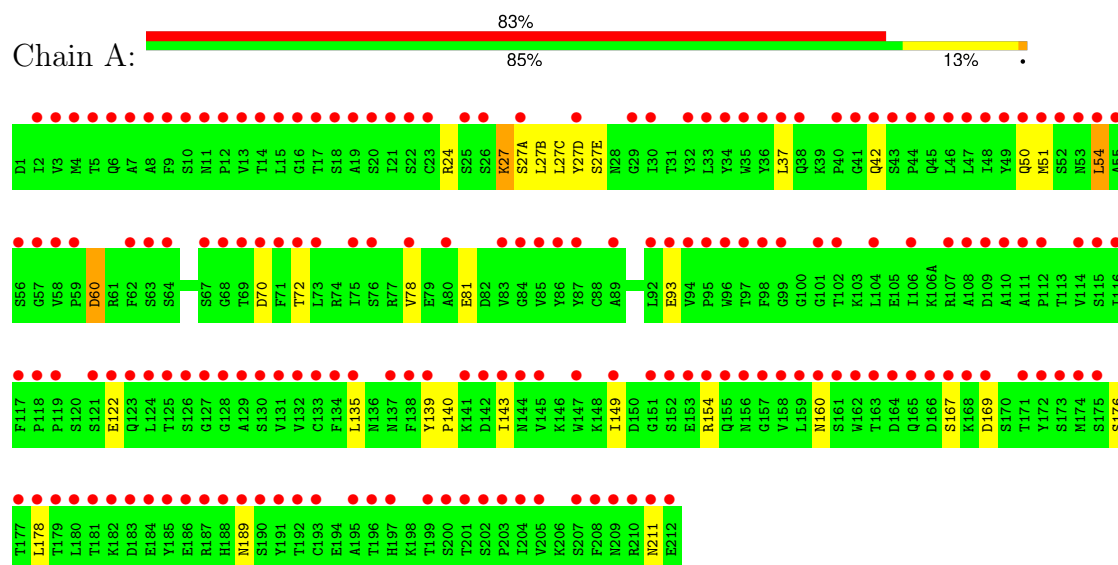
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	96	Total 96	O 96	0	0
4	H	92	Total 92	O 92	0	0
4	L	34	Total 34	O 34	0	0

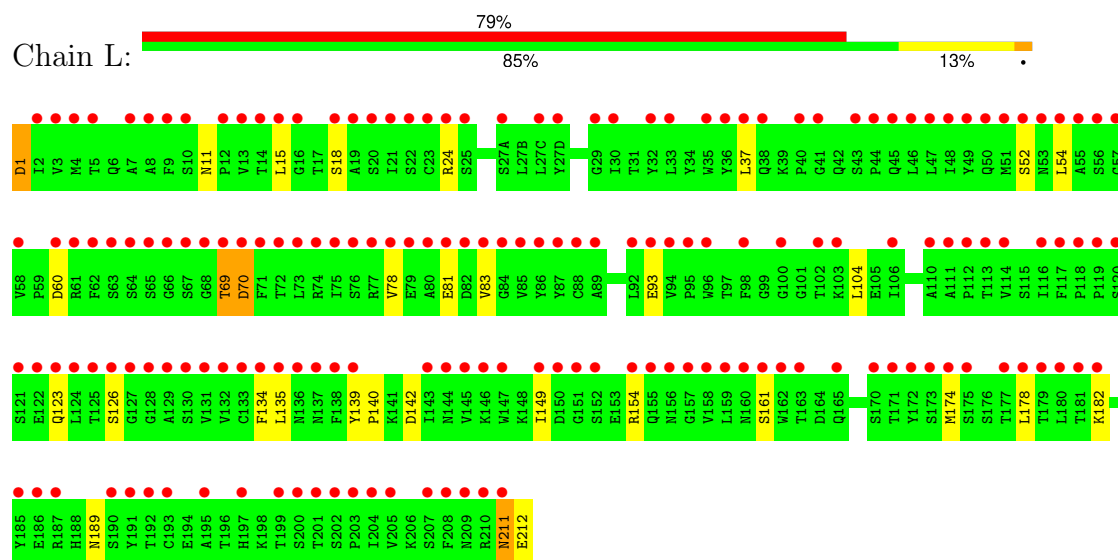
3 Residue-property plots

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.

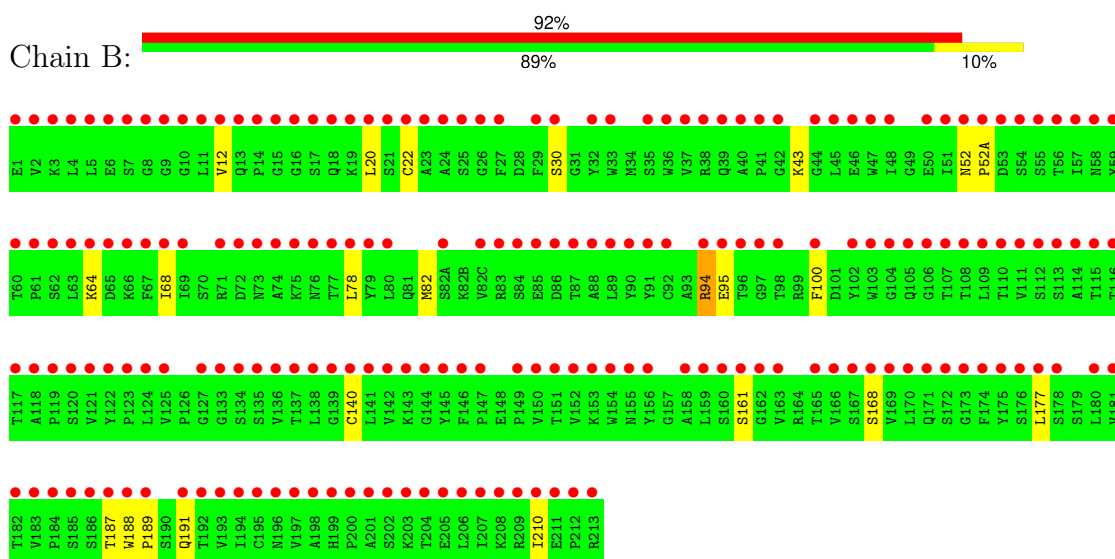
• Molecule 1: IGG FAB (IGG3, KAPPA) LIGHT CHAIN 291-2G3-A



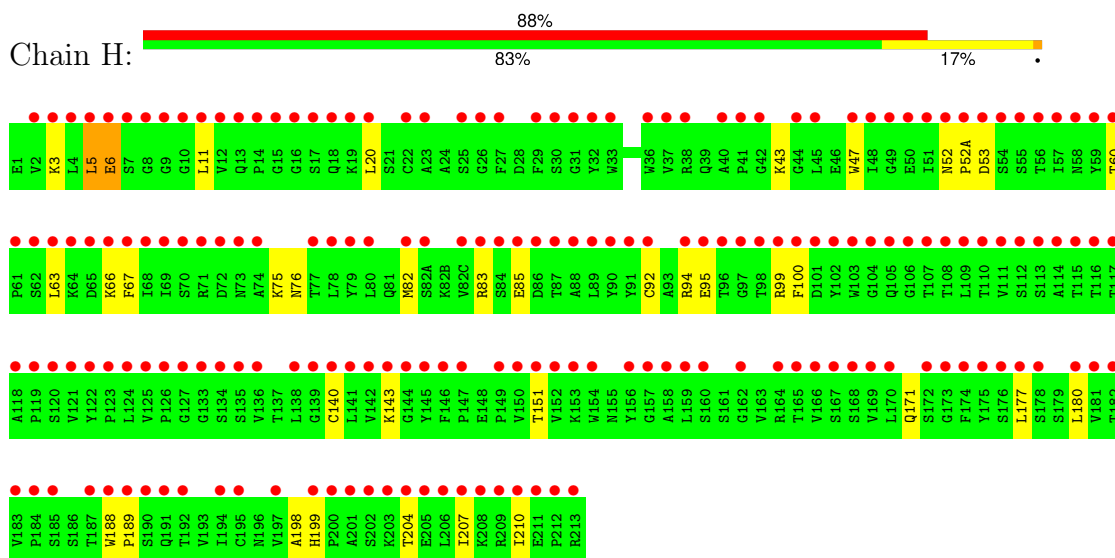
• Molecule 1: IGG FAB (IGG3, KAPPA) LIGHT CHAIN 291-2G3-A



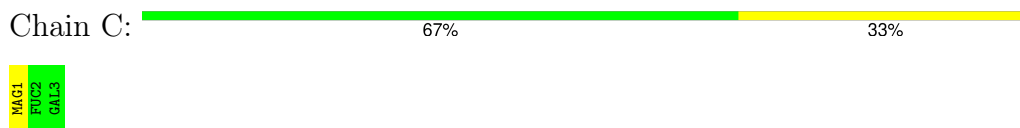
• Molecule 2: IGG FAB (IGG3, KAPPA) HEAVY CHAIN 291-2G3-A



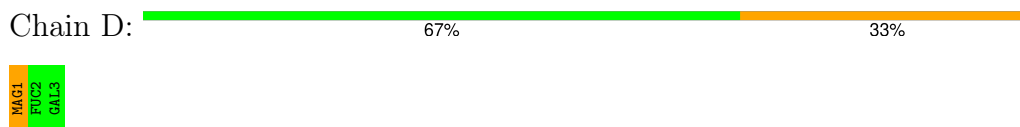
• Molecule 2: IGG FAB (IGG3, KAPPA) HEAVY CHAIN 291-2G3-A



• Molecule 3: alpha-L-fucopyranose-(1-3)-[beta-D-galactopyranose-(1-4)]methyl 2-acetamido-2-deoxy-beta-D-glucopyranoside



• Molecule 3: alpha-L-fucopyranose-(1-3)-[beta-D-galactopyranose-(1-4)]methyl 2-acetamido-2-deoxy-beta-D-glucopyranoside



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	45.10Å 60.78Å 91.56Å 95.98° 95.41° 101.71°	Depositor
Resolution (Å)	91.29 – 1.80 90.42 – 1.80	Depositor EDS
% Data completeness (in resolution range)	92.9 (91.29-1.80) 93.3 (90.42-1.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.85 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.2.0000	Depositor
R, R_{free}	0.210 , 0.247 0.264 , 0.288	Depositor DCC
R_{free} test set	4064 reflections (4.63%)	wwPDB-VP
Wilson B-factor (Å ²)	28.2	Xtriage
Anisotropy	0.273	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 133.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.67	EDS
Total number of atoms	7002	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 5.22% 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: GAL, MAG, FUC

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	0.35	0/1759	0.76	0/2387
1	L	0.34	0/1739	0.75	0/2362
2	B	0.44	0/1667	0.81	0/2269
2	H	0.42	0/1674	0.79	0/2279
All	All	0.39	0/6839	0.78	0/9297

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	A	1704	0	1636	10	0
1	L	1696	0	1630	18	0
2	B	1619	0	1596	17	0
2	H	1622	0	1599	26	0
3	C	37	0	35	0	0
3	D	37	0	35	1	0
4	A	65	0	0	0	0
4	B	96	0	0	1	0
4	H	92	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	L	34	0	0	1	0
All	All	7002	0	6531	69	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 (69) 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:L:189:ASN:HD21	1:L:211:ASN:HB3	1.48	0.78
2:H:94:ARG:HD2	2:H:100:PHE:O	1.83	0.78
2:H:20:LEU:HG	2:H:82:MET:CE	2.13	0.77
2:H:20:LEU:HG	2:H:82:MET:HE2	1.70	0.72
2:B:20:LEU:HD11	2:B:82:MET:CE	2.21	0.71
2:H:151[B]:THR:HG22	4:H:2065:HOH:O	1.98	0.63
1:A:60:ASP:N	1:A:60:ASP:OD1	2.30	0.61
2:B:20:LEU:HG	2:B:82:MET:HE3	1.83	0.60
2:H:180:LEU:HD13	1:L:134:PHE:CD1	2.37	0.59
2:B:20:LEU:HD11	2:B:82:MET:HE1	1.85	0.57
2:H:66:LYS:HE2	2:H:67:PHE:HE1	1.70	0.57
1:A:149:ILE:HD11	1:A:178:LEU:HD21	1.87	0.55
2:B:20:LEU:CD1	2:B:82:MET:CE	2.85	0.55
2:B:177:LEU:C	2:B:177:LEU:HD12	2.33	0.54
1:L:69:THR:HG22	1:L:70:ASP:OD1	2.07	0.54
1:L:123:GLN:O	1:L:126:SER:OG	2.25	0.53
1:L:211:ASN:ND2	1:L:212:GLU:HG3	2.24	0.53
2:H:66:LYS:HE2	2:H:67:PHE:CE1	2.44	0.51
2:B:22:CYS:HB3	2:B:78:LEU:HB3	1.92	0.51
2:H:20:LEU:CG	2:H:82:MET:CE	2.86	0.50
2:H:52:ASN:HB2	2:H:52(A):PRO:HD2	1.93	0.50
2:H:20:LEU:HD11	2:H:82:MET:HE1	1.94	0.48
1:L:15:LEU:HA	1:L:78:VAL:HG23	1.95	0.48
2:B:140[B]:CYS:SG	2:B:210:ILE:HD11	2.54	0.48
2:H:180:LEU:HD13	1:L:134:PHE:CE1	2.49	0.48
2:B:20:LEU:CG	2:B:82:MET:HE3	2.42	0.47
1:L:149:ILE:HD11	1:L:178:LEU:HD21	1.97	0.47
2:B:52:ASN:HB2	2:B:52(A):PRO:HD2	1.97	0.47
1:A:160:ASN:HD22	1:A:176:SER:HA	1.80	0.47
1:L:60:ASP:OD1	1:L:60:ASP:N	2.44	0.46
2:H:52:ASN:HB2	2:H:52(A):PRO:CD	2.46	0.46
2:H:53:ASP:C	2:H:53:ASP:OD1	2.58	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:6:GLU:OE1	2:H:6:GLU:N	2.45	0.46
2:B:187:THR:O	2:B:191:GLN:HB2	2.16	0.45
2:B:52:ASN:HB2	2:B:52(A):PRO:CD	2.46	0.45
1:A:169:ASP:OD1	1:A:169:ASP:C	2.59	0.45
2:H:94:ARG:HD3	2:H:100:PHE:HB3	1.97	0.44
2:B:30:SER:O	2:B:52(A):PRO:HB3	2.17	0.44
2:H:11:LEU:HD23	2:H:11:LEU:C	2.42	0.44
2:B:94:ARG:HD2	2:B:100:PHE:O	2.17	0.44
1:L:83:VAL:HG23	1:L:104:LEU:O	2.18	0.44
2:H:199:HIS:HB3	2:H:204:THR:HB	2.01	0.43
1:A:135:LEU:HD23	1:A:143:ILE:HD13	2.00	0.43
2:H:3:LYS:HD3	2:H:5:LEU:HD23	2.01	0.43
1:L:139:TYR:CG	1:L:140:PRO:HA	2.54	0.43
1:L:93:GLU:HA	3:D:1:MAG:HM3	2.01	0.43
2:B:12:VAL:HG23	4:B:2003:HOH:O	2.18	0.42
2:H:177:LEU:C	2:H:177:LEU:HD12	2.45	0.42
2:H:140[B]:CYS:SG	2:H:210:ILE:HD11	2.59	0.42
1:L:182:LYS:HE3	4:L:2030:HOH:O	2.19	0.42
1:A:139:TYR:CG	1:A:140:PRO:HA	2.55	0.42
1:L:135:LEU:HB2	1:L:174:MET:HG3	2.02	0.42
1:L:149:ILE:HD12	1:L:154:ARG:HD3	2.01	0.41
2:H:47:TRP:O	2:H:60:THR:OG1	2.32	0.41
1:A:27:LYS:HE2	1:A:93:GLU:OE2	2.20	0.41
2:B:168:SER:HA	2:B:177:LEU:HB3	2.03	0.41
2:H:20:LEU:CD1	2:H:82:MET:CE	2.99	0.41
1:L:211:ASN:HD21	1:L:212:GLU:HG3	1.86	0.41
2:H:151[A]:THR:OG1	2:H:198:ALA:HB3	2.21	0.41
1:L:54:LEU:HD11	1:L:60:ASP:HA	2.03	0.41
1:A:189:ASN:HD21	1:A:211:ASN:H	1.69	0.41
2:B:94:ARG:O	2:B:95:GLU:C	2.64	0.41
1:A:50:GLN:O	1:A:51:MET:HB3	2.21	0.40
2:B:188:TRP:CG	2:B:189:PRO:HA	2.56	0.40
2:H:188:TRP:CG	2:H:189:PRO:HA	2.55	0.40
1:A:54:LEU:HD12	1:A:54:LEU:HA	1.88	0.40
2:H:75:LYS:O	2:H:76:ASN:HB2	2.22	0.40
1:L:1:ASP:OD1	1:L:1:ASP:N	2.49	0.40
2:H:67:PHE:N	2:H:67:PHE:CD1	2.89	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	A	219/218 (100%)	213 (97%)	6 (3%)	0	100	100
1	L	217/218 (100%)	212 (98%)	5 (2%)	0	100	100
2	B	210/212 (99%)	207 (99%)	3 (1%)	0	100	100
2	H	211/212 (100%)	207 (98%)	3 (1%)	1 (0%)	24	14
All	All	857/860 (100%)	839 (98%)	17 (2%)	1 (0%)	48	34

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	95	GLU

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	196/193 (102%)	177 (90%)	19 (10%)	8	2
1	L	194/193 (100%)	182 (94%)	12 (6%)	16	6
2	B	183/181 (101%)	178 (97%)	5 (3%)	39	27
2	H	184/181 (102%)	173 (94%)	11 (6%)	17	7
All	All	757/748 (101%)	710 (94%)	47 (6%)	17	6

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	ARG
1	A	27	LYS
1	A	27(A)	SER
1	A	27(B)	LEU
1	A	27(C)	LEU
1	A	27(D)	TYR
1	A	27(E)	SER
1	A	37	LEU
1	A	42	GLN
1	A	54	LEU
1	A	60	ASP
1	A	70	ASP
1	A	72	THR
1	A	78	VAL
1	A	81	GLU
1	A	122[A]	GLU
1	A	122[B]	GLU
1	A	154	ARG
1	A	167	SER
2	B	43	LYS
2	B	64	LYS
2	B	68	ILE
2	B	94	ARG
2	B	161	SER
2	H	5	LEU
2	H	6	GLU
2	H	43	LYS
2	H	63	LEU
2	H	83	ARG
2	H	85	GLU
2	H	92	CYS
2	H	99	ARG
2	H	143	LYS
2	H	171	GLN
2	H	207	ILE
1	L	1	ASP
1	L	11	ASN
1	L	18	SER
1	L	24	ARG
1	L	37	LEU
1	L	52	SER
1	L	69	THR
1	L	70	ASP

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Mol	Chain	Res	Type
1	L	81	GLU
1	L	142	ASP
1	L	161	SER
1	L	211	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	136	ASN
1	A	156	ASN
1	A	160	ASN
1	A	189	ASN
1	L	50	GLN
1	L	136	ASN
1	L	189	ASN
1	L	211	ASN

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 ⓘ

6 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	MAG	C	1	3	16,16,16	0.47	0	22,22,22	1.19	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	FUC	C	2	3	10,10,11	0.63	0	14,14,16	0.88	0
3	GAL	C	3	3	11,11,12	0.72	0	15,15,17	0.82	0
3	MAG	D	1	3	16,16,16	0.48	0	22,22,22	1.44	2 (9%)
3	FUC	D	2	3	10,10,11	0.63	0	14,14,16	0.69	0
3	GAL	D	3	3	11,11,12	0.74	0	15,15,17	0.79	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
3	MAG	C	1	3	-	0/8/28/28	0/1/1/1
3	FUC	C	2	3	-	-	0/1/1/1
3	GAL	C	3	3	-	0/2/19/22	0/1/1/1
3	MAG	D	1	3	-	2/8/28/28	0/1/1/1
3	FUC	D	2	3	-	-	0/1/1/1
3	GAL	D	3	3	-	0/2/19/22	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(°)
3	D	1	MAG	CM-O1-C1	4.54	120.16	113.26
3	C	1	MAG	CM-O1-C1	3.81	119.05	113.26
3	D	1	MAG	O5-C5-C4	-2.42	105.34	109.70

There are no chirality outliers.

All (2) torsion outliers are listed below:

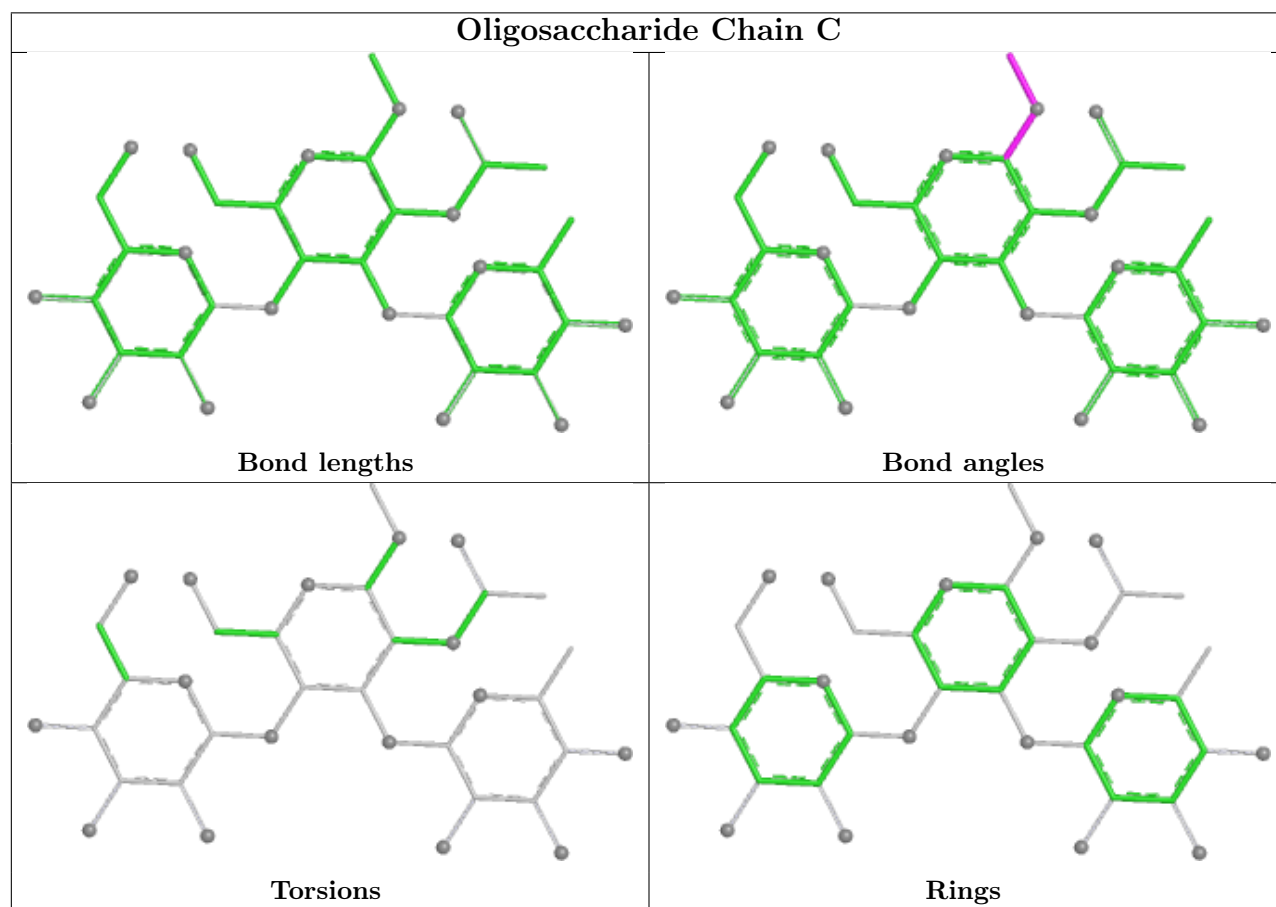
Mol	Chain	Res	Type	Atoms
3	D	1	MAG	O5-C5-C6-O6
3	D	1	MAG	C4-C5-C6-O6

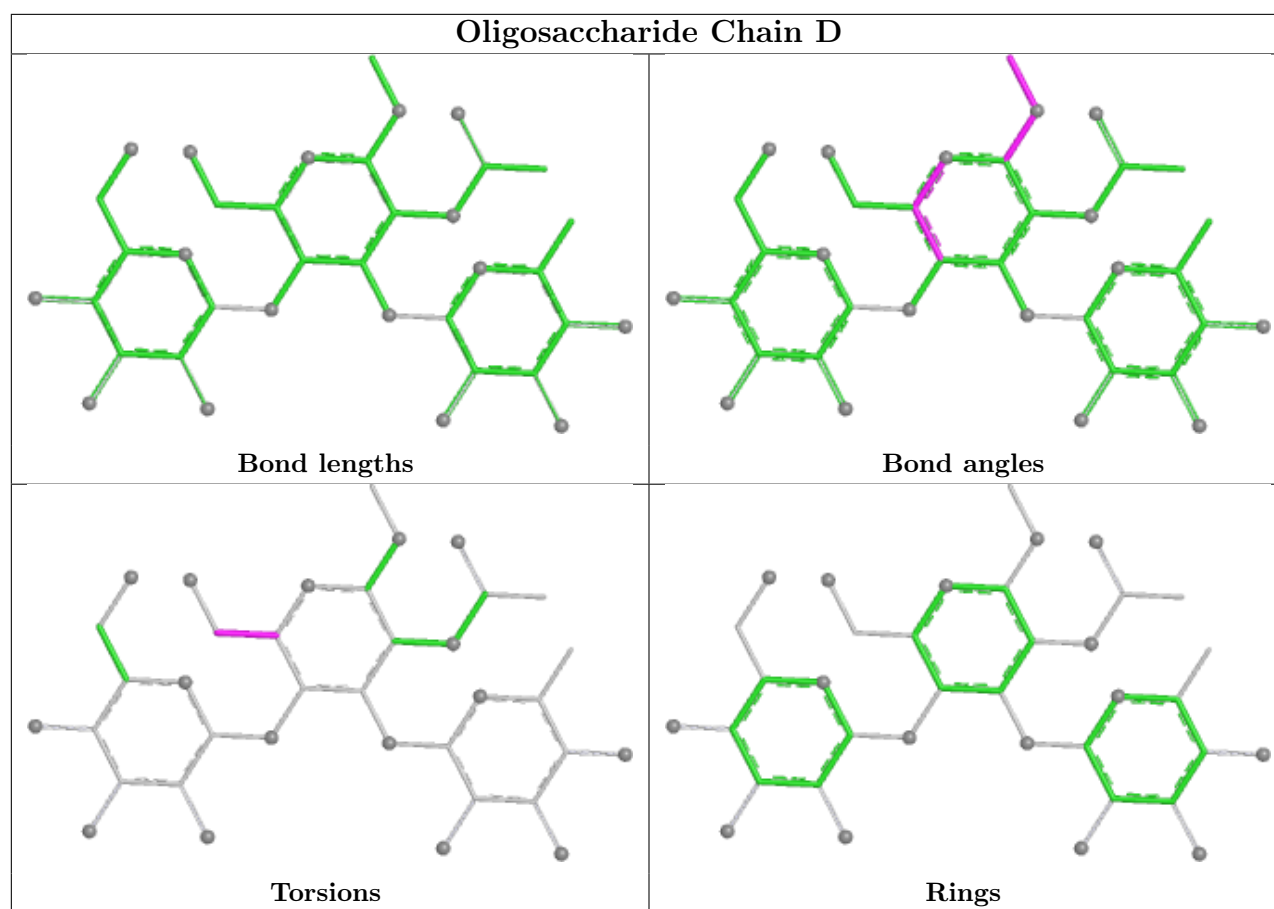
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1	MAG	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](#)

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	1
2	H	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	127:GLY	C	133:GLY	N	12.07
1	H	127:GLY	C	133:GLY	N	10.79

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	218/218 (100%)	2.99	181 (83%) 0 0	22, 42, 56, 63	3 (1%)
1	L	218/218 (100%)	2.85	172 (78%) 0 0	29, 46, 61, 69	1 (0%)
2	B	212/212 (100%)	3.26	194 (91%) 0 0	22, 42, 56, 64	2 (0%)
2	H	212/212 (100%)	3.30	187 (88%) 0 0	23, 39, 49, 57	3 (1%)
All	All	860/860 (100%)	3.10	734 (85%) 0 0	22, 42, 58, 69	9 (1%)

All (734) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	10	GLY	7.1
2	H	52(A)	PRO	6.9
2	H	10	GLY	6.7
2	B	4	LEU	6.2
2	B	52(A)	PRO	6.2
2	H	7	SER	6.2
2	B	16	GLY	6.2
2	B	136	VAL	6.0
2	H	97	GLY	6.0
2	B	116	THR	5.7
2	B	172	SER	5.7
1	L	41	GLY	5.7
2	B	59	TYR	5.7
1	L	47	LEU	5.7
2	H	8	GLY	5.6
2	B	54	SER	5.6
1	A	209	ASN	5.5
1	A	128	GLY	5.5
2	H	22	CYS	5.4
2	H	162	GLY	5.4
1	L	46	LEU	5.4

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Mol	Chain	Res	Type	RSRZ
1	A	124	LEU	5.3
1	L	49	TYR	5.3
2	H	115	THR	5.3
2	B	175	TYR	5.2
2	H	12	VAL	5.2
1	A	118	PRO	5.2
2	H	110	THR	5.1
1	A	117	PHE	5.1
2	H	147	PRO	5.1
2	B	7	SER	5.1
2	H	188	TRP	5.1
1	A	14	THR	5.1
2	B	97	GLY	5.1
2	B	163	VAL	5.1
2	H	169	VAL	5.0
1	L	57	GLY	5.0
1	L	118	PRO	5.0
2	B	61	PRO	5.0
1	L	208	PHE	5.0
2	B	142	VAL	5.0
2	H	16	GLY	5.0
1	A	129	ALA	4.9
2	B	207	ILE	4.9
1	A	111	ALA	4.9
2	B	22	CYS	4.9
1	A	19	ALA	4.8
2	H	154	TRP	4.8
2	B	174	PHE	4.8
1	L	162	TRP	4.8
2	H	11	LEU	4.8
1	A	9	PHE	4.7
2	H	166	VAL	4.7
2	H	52	ASN	4.7
2	H	212	PRO	4.7
2	B	36	TRP	4.7
1	A	23	CYS	4.7
1	L	171	THR	4.7
2	H	141	LEU	4.7
2	B	146	PHE	4.6
1	L	86	TYR	4.6
2	H	9	GLY	4.6
1	L	179	THR	4.6

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Mol	Chain	Res	Type	RSRZ
2	B	12	VAL	4.6
1	L	37	LEU	4.6
1	L	8	ALA	4.6
2	H	125	VAL	4.6
2	H	183	VAL	4.6
2	H	4	LEU	4.6
1	L	163	THR	4.5
2	H	87	THR	4.5
2	H	117	THR	4.5
1	A	205	VAL	4.5
1	L	144	ASN	4.5
2	H	140[A]	CYS	4.5
2	B	42	GLY	4.5
1	A	59	PRO	4.5
2	B	119	PRO	4.5
1	A	108	ALA	4.5
2	H	201	ALA	4.5
1	L	134	PHE	4.4
1	A	13	VAL	4.4
2	H	160	SER	4.4
1	A	145	VAL	4.4
2	B	154	TRP	4.4
2	B	156	TYR	4.4
2	B	169	VAL	4.4
1	A	40	PRO	4.4
2	H	56	THR	4.4
2	H	96	THR	4.4
2	B	198	ALA	4.4
2	B	138	LEU	4.4
2	H	170	LEU	4.4
2	H	206	LEU	4.4
2	H	91	TYR	4.4
1	A	116	ILE	4.4
2	H	57	ILE	4.4
2	H	176	SER	4.3
2	B	206	LEU	4.3
1	A	48	ILE	4.3
1	A	95	PRO	4.3
2	H	174	PHE	4.3
2	H	89	LEU	4.3
2	H	122	TYR	4.3
2	H	36	TRP	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	8	ALA	4.3
1	L	145	VAL	4.3
2	B	18	GLN	4.3
1	A	125	THR	4.2
1	L	124	LEU	4.2
2	B	11	LEU	4.2
2	B	204	THR	4.2
2	H	116	THR	4.2
2	H	177	LEU	4.2
2	H	150	VAL	4.2
1	L	75	ILE	4.2
1	A	161	SER	4.2
2	B	88	ALA	4.2
2	H	42	GLY	4.2
2	H	103	TRP	4.2
1	L	192	THR	4.2
2	B	111	VAL	4.2
2	B	51	ILE	4.2
2	H	69	ILE	4.2
2	B	151	THR	4.2
2	B	159	LEU	4.2
1	A	200	SER	4.2
1	L	68	GLY	4.2
1	A	49	TYR	4.2
1	A	162	TRP	4.2
2	H	33	TRP	4.2
1	L	48	ILE	4.1
2	B	125	VAL	4.1
2	H	213	ARG	4.1
2	B	145	TYR	4.1
2	B	29	PHE	4.1
1	A	75	ILE	4.1
1	A	132	VAL	4.1
1	A	149	ILE	4.1
2	B	25	SER	4.1
1	L	178	LEU	4.1
2	B	20	LEU	4.1
2	B	63	LEU	4.1
2	H	159	LEU	4.1
2	H	50	GLU	4.1
1	A	139	TYR	4.1
1	A	164	ASP	4.1

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Mol	Chain	Res	Type	RSRZ
1	L	10	SER	4.1
1	A	127	GLY	4.1
2	H	44	GLY	4.1
1	A	208	PHE	4.0
2	B	57	ILE	4.0
1	A	35	TRP	4.0
2	B	47	TRP	4.0
1	L	40	PRO	4.0
2	B	60	THR	4.0
2	B	177	LEU	4.0
1	L	158	VAL	4.0
2	H	197	VAL	4.0
2	H	108	THR	4.0
2	H	145	TYR	4.0
2	H	175	TYR	4.0
2	B	104	GLY	4.0
1	A	187[A]	ARG	4.0
1	L	159	LEU	4.0
1	L	195	ALA	4.0
1	A	190	SER	4.0
2	H	113	SER	4.0
1	A	15	LEU	4.0
2	H	88	ALA	4.0
1	A	152	SER	4.0
1	A	138	PHE	4.0
1	L	69	THR	3.9
1	A	147	TRP	3.9
2	B	201	ALA	3.9
1	L	143	ILE	3.9
2	B	115	THR	3.9
2	H	51	ILE	3.9
1	L	185	TYR	3.9
1	A	16	GLY	3.9
1	A	157	GLY	3.9
1	L	205	VAL	3.9
1	L	117	PHE	3.9
2	B	185	SER	3.9
1	A	180	LEU	3.9
2	H	6	GLU	3.9
2	B	8	GLY	3.9
1	L	82	ASP	3.9
1	L	149	ILE	3.9

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Mol	Chain	Res	Type	RSRZ
2	H	121	VAL	3.9
2	B	21	SER	3.8
2	H	32	TYR	3.8
1	A	195	ALA	3.8
2	B	9	GLY	3.8
2	H	173	GLY	3.8
1	L	193	CYS	3.8
2	B	48	ILE	3.8
1	A	134	PHE	3.8
1	L	136	ASN	3.8
2	H	61	PRO	3.8
1	A	181	THR	3.8
2	H	47	TRP	3.8
1	L	62	PHE	3.8
1	L	63	SER	3.8
1	L	121	SER	3.8
1	A	36	TYR	3.8
1	L	36	TYR	3.8
2	B	200	PRO	3.8
1	A	179	THR	3.8
1	L	199	THR	3.8
1	A	211	ASN	3.8
2	B	210	ILE	3.8
1	L	126	SER	3.8
2	H	37	VAL	3.8
2	H	152	VAL	3.8
2	H	53	ASP	3.7
1	L	127	GLY	3.7
2	H	31	GLY	3.7
2	H	184	PRO	3.7
2	B	78	LEU	3.7
2	B	102	TYR	3.7
2	H	85	GLU	3.7
2	H	74	ALA	3.7
1	A	182[A]	LYS	3.7
1	L	85	VAL	3.7
1	L	35	TRP	3.7
1	A	174	MET	3.7
1	A	41	GLY	3.7
1	A	137	ASN	3.7
2	B	41	PRO	3.7
1	L	201	THR	3.7

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Mol	Chain	Res	Type	RSRZ
2	B	77	THR	3.7
2	H	118	ALA	3.7
1	A	20	SER	3.7
2	B	17	SER	3.7
2	B	92	CYS	3.7
1	A	123	GLN	3.7
2	B	183	VAL	3.7
2	H	139	GLY	3.7
1	L	209	ASN	3.7
2	H	149	PRO	3.7
2	H	109	LEU	3.7
1	A	185	TYR	3.7
1	L	172	TYR	3.7
2	H	90	TYR	3.7
2	H	102	TYR	3.7
2	H	55	SER	3.7
2	H	211	GLU	3.7
2	H	15	GLY	3.7
2	B	66	LYS	3.7
2	B	203	LYS	3.7
1	A	130	SER	3.6
1	L	129	ALA	3.6
1	L	191	TYR	3.6
2	B	52	ASN	3.6
2	H	194	ILE	3.6
1	A	98	PHE	3.6
1	L	72	THR	3.6
2	B	87	THR	3.6
2	B	212	PRO	3.6
2	H	107	THR	3.6
2	B	160	SER	3.6
1	A	68	GLY	3.6
1	A	192	THR	3.6
1	L	14	THR	3.6
2	B	56	THR	3.6
1	A	167	SER	3.6
2	B	176	SER	3.6
1	A	178	LEU	3.6
2	H	124	LEU	3.6
1	L	7	ALA	3.6
2	B	24	ALA	3.6
2	B	13	GLN	3.6

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Mol	Chain	Res	Type	RSRZ
2	H	68	ILE	3.6
2	H	77	THR	3.6
2	H	189	PRO	3.6
1	L	64	SER	3.6
1	L	15	LEU	3.6
2	B	23	ALA	3.5
1	L	147	TRP	3.5
1	L	128	GLY	3.5
2	B	173	GLY	3.5
2	B	121	VAL	3.5
2	B	40	ALA	3.5
1	A	29	GLY	3.5
2	H	79	TYR	3.5
2	H	156	TYR	3.5
2	B	103	TRP	3.5
2	H	195	CYS	3.5
1	A	17	THR	3.5
1	A	177	THR	3.5
1	L	12	PRO	3.5
1	L	181	THR	3.5
2	H	204	THR	3.5
1	A	58	VAL	3.5
1	A	85	VAL	3.5
1	L	132	VAL	3.5
1	A	159	LEU	3.5
2	B	109	LEU	3.5
2	H	20	LEU	3.5
2	H	23	ALA	3.5
1	A	25	SER	3.5
2	B	90	TYR	3.5
2	B	122	TYR	3.5
2	B	140[A]	CYS	3.5
2	B	117	THR	3.5
2	B	149	PRO	3.5
2	H	13	GLN	3.5
1	A	3	VAL	3.5
1	L	114	VAL	3.5
1	A	4	MET	3.5
1	A	110	ALA	3.5
2	B	170	LEU	3.5
2	H	158	ALA	3.5
2	H	112	SER	3.4

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Mol	Chain	Res	Type	RSRZ
2	B	50	GLU	3.4
1	A	196	THR	3.4
1	A	21	ILE	3.4
1	L	2	ILE	3.4
2	H	210	ILE	3.4
2	B	141	LEU	3.4
2	H	63	LEU	3.4
1	L	211	ASN	3.4
1	L	174	MET	3.4
1	L	96	TRP	3.4
2	B	39	GLN	3.4
2	H	114	ALA	3.4
2	H	178	SER	3.4
1	L	156	ASN	3.4
2	B	184	PRO	3.4
1	L	87	TYR	3.4
1	L	157	GLY	3.4
1	A	53	ASN	3.4
1	L	9	PHE	3.4
1	A	112	PRO	3.4
2	H	66	LYS	3.3
1	A	186	GLU	3.3
1	L	18	SER	3.3
1	L	13	VAL	3.3
1	A	54	LEU	3.3
1	A	92	LEU	3.3
1	L	182	LYS	3.3
2	B	110	THR	3.3
2	H	14	PRO	3.3
2	B	26	GLY	3.3
1	A	175	SER	3.3
2	B	62	SER	3.3
2	B	178	SER	3.3
2	H	172	SER	3.3
2	H	202	SER	3.3
1	L	80	ALA	3.3
1	L	33	LEU	3.3
2	B	5	LEU	3.3
1	L	125	THR	3.3
2	B	96	THR	3.3
1	A	12	PRO	3.3
2	H	41	PRO	3.3

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Mol	Chain	Res	Type	RSRZ
2	H	127	GLY	3.3
1	A	10	SER	3.3
1	A	131	VAL	3.3
1	L	131	VAL	3.3
1	A	135	LEU	3.3
2	B	192	THR	3.3
2	B	72	ASP	3.3
2	B	67	PHE	3.3
2	B	15	GLY	3.3
1	A	115	SER	3.3
2	B	202	SER	3.3
1	A	133	CYS	3.3
1	A	184	GLU	3.2
2	B	37	VAL	3.2
1	L	98	PHE	3.2
2	B	27	PHE	3.2
1	A	126	SER	3.2
2	B	144	GLY	3.2
1	A	2	ILE	3.2
1	A	86	TYR	3.2
1	A	191	TYR	3.2
1	A	114	VAL	3.2
2	H	187	THR	3.2
1	L	135	LEU	3.2
1	A	84	GLY	3.2
1	L	207	SER	3.2
1	L	197	HIS	3.2
2	H	209	ARG	3.2
1	A	203	PRO	3.2
1	L	83	VAL	3.2
2	B	73	ASN	3.2
1	A	37	LEU	3.2
2	B	124	LEU	3.2
2	B	153	LYS	3.2
1	A	50	GLN	3.2
1	A	207	SER	3.2
1	L	29	GLY	3.2
2	B	30	SER	3.2
2	B	134	SER	3.2
2	H	54	SER	3.2
2	B	188	TRP	3.1
1	A	11	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	106	ILE	3.1
1	A	87	TYR	3.1
1	A	172	TYR	3.1
2	H	200	PRO	3.1
1	A	46	LEU	3.1
1	L	54	LEU	3.1
1	L	152	SER	3.1
2	B	150	VAL	3.1
2	H	190	SER	3.1
2	B	65	ASP	3.1
2	H	191	GLN	3.1
1	L	113	THR	3.1
2	H	98	THR	3.1
2	B	189	PRO	3.1
1	L	27(A)	SER	3.1
2	B	33	TRP	3.1
2	B	120	SER	3.1
2	H	48	ILE	3.1
2	H	185	SER	3.1
2	B	80	LEU	3.1
2	B	82(C)	VAL	3.1
2	H	2	VAL	3.1
1	L	123	GLN	3.1
1	A	160	ASN	3.1
1	A	55	ALA	3.1
1	A	67	SER	3.1
2	B	118	ALA	3.1
2	H	17	SER	3.1
2	H	70	SER	3.1
1	L	30	ILE	3.1
1	A	93	GLU	3.1
1	L	92	LEU	3.1
2	B	45	LEU	3.1
2	B	79	TYR	3.1
2	H	59	TYR	3.1
2	H	72	ASP	3.1
1	A	156	ASN	3.1
2	H	146	PHE	3.1
1	L	133	CYS	3.1
1	A	43	SER	3.1
2	H	120	SER	3.1
1	L	55	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
2	H	26	GLY	3.1
2	H	207	ILE	3.0
1	A	34	TYR	3.0
1	L	139	TYR	3.0
1	A	76	SER	3.0
2	B	35	SER	3.0
1	L	88	CYS	3.0
1	L	16	GLY	3.0
1	L	112	PRO	3.0
1	A	30	ILE	3.0
1	A	154	ARG	3.0
1	A	189	ASN	3.0
1	L	160	ASN	3.0
2	H	73	ASN	3.0
2	B	193	VAL	3.0
2	H	111	VAL	3.0
2	H	119	PRO	3.0
2	H	144	GLY	3.0
1	A	6	GLN	3.0
1	L	19	ALA	3.0
1	A	210	ARG	3.0
1	A	78	VAL	3.0
1	A	158	VAL	3.0
2	B	32	TYR	3.0
2	H	82(C)	VAL	3.0
1	L	65	SER	3.0
1	L	161	SER	3.0
2	H	30	SER	3.0
1	A	38	GLN	3.0
1	L	150	ASP	3.0
1	A	101	GLY	3.0
1	L	84	GLY	3.0
1	L	61	ARG	3.0
1	L	3	VAL	2.9
1	L	58	VAL	2.9
1	L	78	VAL	2.9
2	H	84	SER	2.9
1	A	201	THR	2.9
2	B	133	GLY	2.9
1	A	47	LEU	2.9
1	L	20	SER	2.9
2	B	64	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
2	H	168	SER	2.9
1	A	199	THR	2.9
1	L	122[A]	GLU	2.9
2	B	100	PHE	2.9
1	L	23	CYS	2.9
2	H	18	GLN	2.9
1	A	168	LYS	2.9
1	A	56	SER	2.9
2	B	161	SER	2.9
2	H	135	SER	2.9
2	B	107	THR	2.9
1	L	119	PRO	2.9
1	A	188	HIS	2.9
2	H	67	PHE	2.9
1	L	67	SER	2.9
1	L	200	SER	2.9
1	L	73	LEU	2.9
2	H	49	GLY	2.9
2	H	133	GLY	2.9
2	H	136	VAL	2.8
1	L	77	ARG	2.8
2	B	85	GLU	2.8
1	L	120	SER	2.8
2	B	55	SER	2.8
2	H	80	LEU	2.8
2	H	151[A]	THR	2.8
1	L	44	PRO	2.8
2	B	6	GLU	2.8
2	B	74	ALA	2.8
2	H	100	PHE	2.8
1	A	193	CYS	2.8
2	H	104	GLY	2.8
1	A	204	ILE	2.8
2	B	71	ARG	2.8
1	A	171	THR	2.8
2	H	199	HIS	2.8
1	A	22	SER	2.8
2	B	155	ASN	2.8
1	L	27(C)	LEU	2.8
2	B	182	THR	2.8
1	A	51	MET	2.8
1	L	4	MET	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	181	VAL	2.8
2	B	196	ASN	2.7
2	H	29	PHE	2.7
2	H	167[A]	SER	2.7
1	A	155	GLN	2.7
2	B	197	VAL	2.7
1	L	53	ASN	2.7
1	L	79	GLU	2.7
2	B	19	LYS	2.7
2	B	98	THR	2.7
1	L	202	SER	2.7
2	B	213	ARG	2.7
2	B	58	ASN	2.7
1	L	110	ALA	2.7
1	L	71	PHE	2.7
1	L	138	PHE	2.7
1	A	18	SER	2.7
2	B	95	GLU	2.7
2	B	205	GLU	2.7
2	H	142	VAL	2.7
1	L	111	ALA	2.6
2	B	127	GLY	2.6
1	L	190	SER	2.6
2	B	186	SER	2.6
1	L	180	LEU	2.6
2	B	194	ILE	2.6
2	B	2	VAL	2.6
2	B	166	VAL	2.6
1	A	142	ASP	2.6
2	B	46	GLU	2.6
1	L	146	LYS	2.6
1	L	177	THR	2.6
2	B	165	THR	2.6
2	H	3	LYS	2.6
2	H	153	LYS	2.6
2	B	84	SER	2.6
2	B	147	PRO	2.6
2	H	126	PRO	2.6
1	A	107	ARG	2.6
1	L	70	ASP	2.6
1	L	100	GLY	2.6
1	A	7	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	80	ALA	2.6
1	A	27(A)	SER	2.6
2	B	168	SER	2.6
2	H	182	THR	2.6
1	A	44	PRO	2.6
2	B	209	ARG	2.6
1	A	70	ASP	2.6
1	A	99	GLY	2.6
2	B	3	LYS	2.6
2	B	75	LYS	2.6
1	A	94	VAL	2.6
1	A	52	SER	2.6
1	A	64	SER	2.6
1	A	202	SER	2.6
2	B	113	SER	2.6
1	L	210	ARG	2.5
2	B	94	ARG	2.5
2	H	78	LEU	2.5
2	H	138	LEU	2.5
1	L	21	ILE	2.5
2	H	40	ALA	2.5
1	L	76	SER	2.5
2	H	60	THR	2.5
1	A	122[A]	GLU	2.5
1	L	32	TYR	2.5
1	A	33	LEU	2.5
1	L	116	ILE	2.5
1	L	25	SER	2.5
1	A	89	ALA	2.5
2	B	137	THR	2.5
2	B	187	THR	2.5
2	H	205	GLU	2.5
2	H	92	CYS	2.5
2	B	91	TYR	2.5
1	A	71	PHE	2.5
2	B	89	LEU	2.5
1	A	26	SER	2.5
1	L	106	ILE	2.5
2	B	69	ILE	2.5
1	L	50	GLN	2.5
2	B	114	ALA	2.5
1	A	69	THR	2.5

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Mol	Chain	Res	Type	RSRZ
2	H	86	ASP	2.5
2	H	123	PRO	2.5
2	H	83	ARG	2.4
2	H	5	LEU	2.4
2	H	180	LEU	2.4
2	H	165	THR	2.4
1	L	94	VAL	2.4
1	A	57	GLY	2.4
2	B	44	GLY	2.4
1	A	45	GLN	2.4
2	B	105	GLN	2.4
2	B	195	CYS	2.4
1	A	121	SER	2.4
1	L	51	MET	2.4
1	A	143	ILE	2.4
2	B	53	ASP	2.4
2	B	68	ILE	2.4
2	H	101	ASP	2.4
1	A	5	THR	2.4
1	A	119	PRO	2.4
2	B	211	GLU	2.4
1	L	66	GLY	2.4
2	H	157	GLY	2.4
2	H	82	MET	2.4
1	L	170	SER	2.4
2	H	25	SER	2.4
2	H	203	LYS	2.4
2	H	27	PHE	2.4
1	A	97	THR	2.4
1	L	102	THR	2.4
1	A	42	GLN	2.4
1	L	38	GLN	2.4
1	L	203	PRO	2.4
2	B	123	PRO	2.4
1	A	144	ASN	2.4
2	B	76	ASN	2.4
2	B	106	GLY	2.4
2	H	181	VAL	2.4
1	A	173	SER	2.4
1	L	43	SER	2.4
2	H	64	LYS	2.4
2	B	86	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
2	H	105	GLN	2.3
1	L	204	ILE	2.3
2	H	58	ASN	2.3
2	B	139	GLY	2.3
1	A	83	VAL	2.3
1	L	130	SER	2.3
2	H	45	LEU	2.3
1	A	72	THR	2.3
2	H	208	LYS	2.3
1	L	56	SER	2.3
2	B	112	SER	2.3
2	H	99	ARG	2.3
1	A	166	ASP	2.3
2	B	180	LEU	2.3
1	A	163	THR	2.3
1	L	89	ALA	2.3
2	B	158	ALA	2.3
2	B	135	SER	2.3
2	H	192	THR	2.3
1	A	32	TYR	2.2
2	B	82(A)	SER	2.2
1	L	103	LYS	2.2
2	B	108	THR	2.2
1	A	212	GLU	2.2
1	A	109	ASP	2.2
2	H	62	SER	2.2
2	H	65	ASP	2.2
1	A	27(D)	TYR	2.2
1	A	197	HIS	2.2
1	A	141	LYS	2.2
1	L	81	GLU	2.2
1	L	5	THR	2.2
1	A	165	GLN	2.2
1	L	155	GLN	2.2
1	A	151	GLY	2.2
1	L	173	SER	2.2
1	A	96	TRP	2.2
2	B	38	ARG	2.2
2	H	71	ARG	2.2
2	B	1	GLU	2.2
2	B	152	VAL	2.2
2	B	171	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	L	60	ASP	2.2
1	L	151	GLY	2.2
2	H	38	ARG	2.2
2	H	164	ARG	2.2
1	A	153	GLU	2.1
1	L	165	GLN	2.1
1	A	102	THR	2.1
1	A	169	ASP	2.1
1	A	63	SER	2.1
1	L	175	SER	2.1
2	H	82(A)	SER	2.1
1	L	95	PRO	2.1
1	L	154	ARG	2.1
2	B	143	LYS	2.1
2	H	143	LYS	2.1
1	L	186	GLU	2.1
1	L	22	SER	2.1
1	L	24	ARG	2.1
1	L	187	ARG	2.1
2	H	95	GLU	2.1
1	A	104	LEU	2.1
1	L	137	ASN	2.1
1	A	62	PHE	2.1
1	L	74	ARG	2.1
2	B	83	ARG	2.1
2	B	167[A]	SER	2.1
2	H	94	ARG	2.1
2	H	19	LYS	2.1
2	H	106	GLY	2.1
1	A	183	ASP	2.1
2	B	208	LYS	2.0
1	L	27(D)	TYR	2.0
1	L	45	GLN	2.0
2	B	14	PRO	2.0
1	A	73	LEU	2.0
1	L	93	GLU	2.0
1	L	52	SER	2.0
2	H	134	SER	2.0
2	B	191	GLN	2.0
2	B	199	HIS	2.0
2	B	162	GLY	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](#)

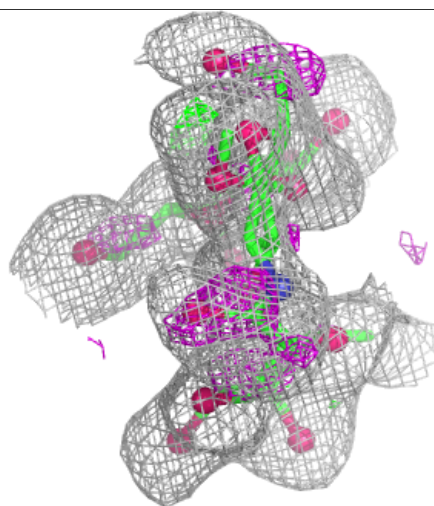
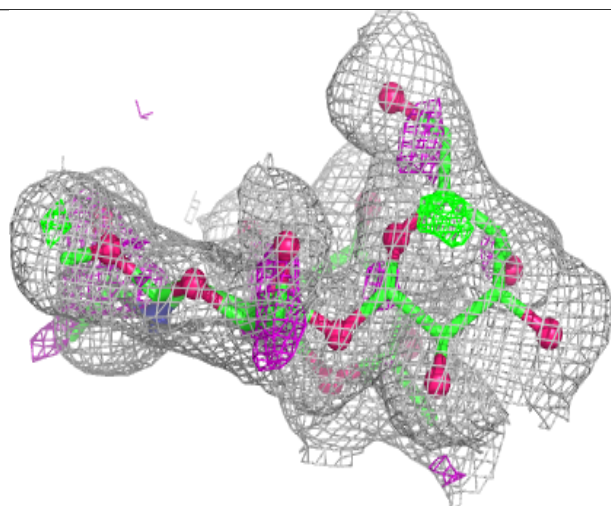
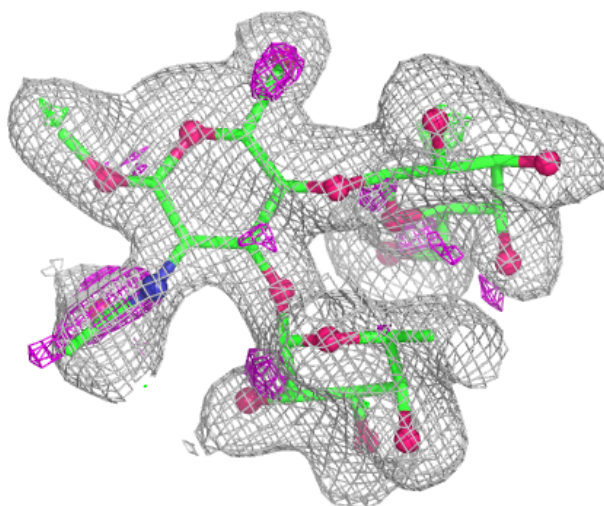
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

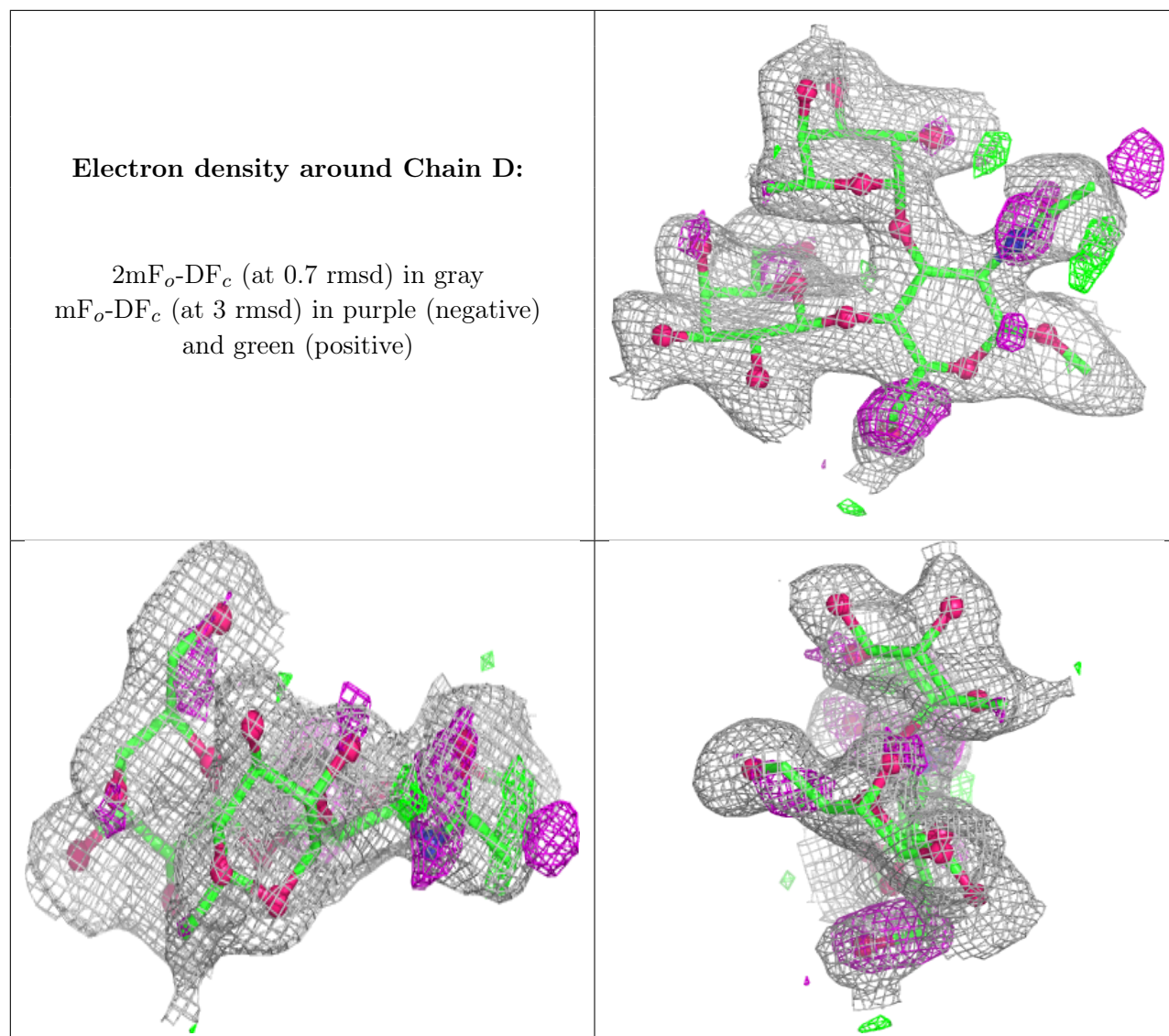
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MAG	C	1	16/16	-	-	39,41,44,45	0
3	FUC	C	2	10/11	-	-	43,44,46,46	0
3	GAL	C	3	11/12	-	-	39,41,43,43	0
3	MAG	D	1	16/16	-	-	34,37,39,40	0
3	FUC	D	2	10/11	-	-	36,38,40,40	0
3	GAL	D	3	11/12	-	-	33,36,38,38	0

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.

Electron density around Chain C:

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





6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.