



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 03:01 PM UTC

PDB ID : 1GQG / pdb_00001gqg
Title : Quercetin 2,3-dioxygenase in complex with the inhibitor diethyldithiocarbamate
Authors : Steiner, R.A.; Dijkstra, B.W.
Deposited on : 2001-11-23
Resolution : 1.70 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:

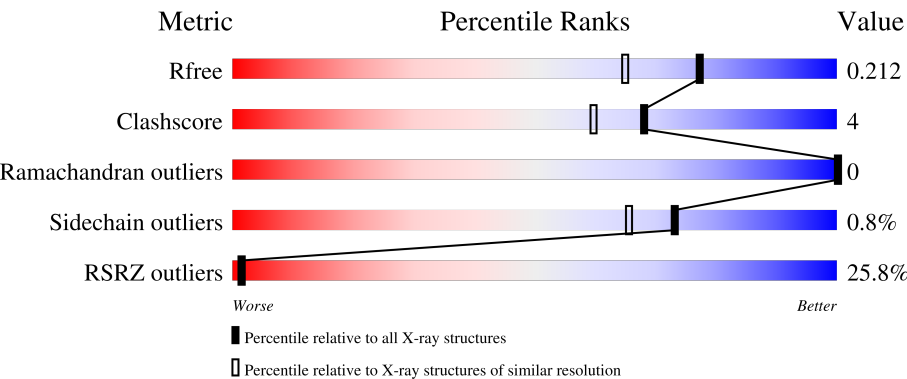
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	350	% 87%8%5%
1	B	350	% 91%. . 5%
1	C	350	3% 91%5% . .
1	D	350	94% 89%6% . 5%
2	E	3	33%33%33%

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Mol	Chain	Length	Quality of chain
2	F	3	
3	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
5	CU	D	1352	-	-	-	X

2 Entry composition [i](#)

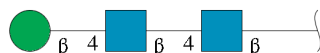
There are 7 unique types of molecules in this entry. The entry contains 12136 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 QUERCETIN 2,3-DIOXYGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	333	Total	C	N	O	S	0	8	0
			2595	1654	420	515	6			
1	B	334	Total	C	N	O	S	0	4	0
			2590	1648	421	516	5			
1	C	337	Total	C	N	O	S	0	3	0
			2605	1655	424	521	5			
1	D	333	Total	C	N	O	S	0	3	0
			2578	1642	419	512	5			

- Molecule 2 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



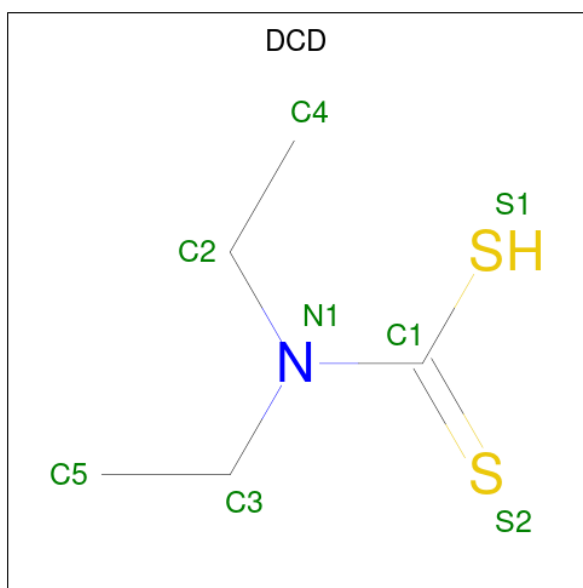
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	F	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 3 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
3	G	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is DIETHYLCARBAMODITHIOIC ACID (CCD ID: DCD) (formula: $C_5H_{11}NS_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	S	0	0
			8	5	1	2		
4	B	1	Total	C	N	S	0	0
			8	5	1	2		
4	C	1	Total	C	N	S	0	0
			8	5	1	2		
4	D	1	Total	C	N	S	0	0
			8	5	1	2		

- Molecule 5 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Cu	0	0
			1	1		
5	B	1	Total	Cu	0	0
			1	1		
5	C	1	Total	Cu	0	0
			1	1		
5	D	1	Total	Cu	0	0
			1	1		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	B	1	Total	C	N	O	0	0
			14	8	1	5		
6	B	1	Total	C	N	O	0	0
			14	8	1	5		
6	B	1	Total	C	N	O	0	0
			14	8	1	5		
6	C	1	Total	C	N	O	0	0
			14	8	1	5		
6	C	1	Total	C	N	O	0	0
			14	8	1	5		
6	C	1	Total	C	N	O	0	0
			14	8	1	5		
6	D	1	Total	C	N	O	0	0
			14	8	1	5		
6	D	1	Total	C	N	O	0	0
			14	8	1	5		
6	D	1	Total	C	N	O	0	0
			14	8	1	5		

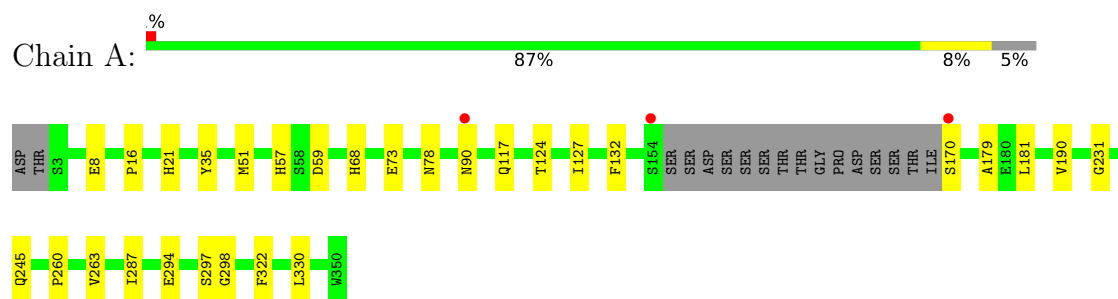
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	411	Total 411	O 411	0	0
7	B	346	Total 346	O 346	0	0
7	C	345	Total 345	O 345	0	0
7	D	342	Total 342	O 342	0	0

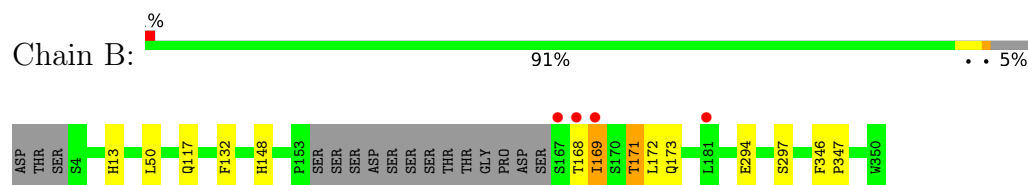
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

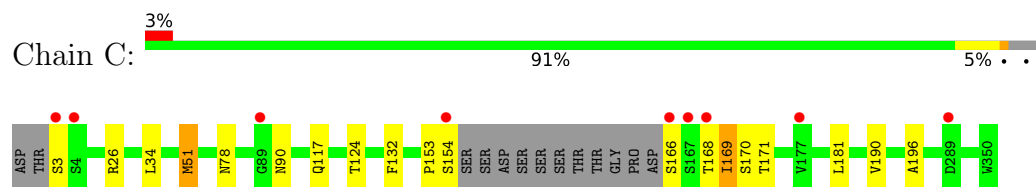
- Molecule 1: QUERCETIN 2,3-DIOXYGENASE



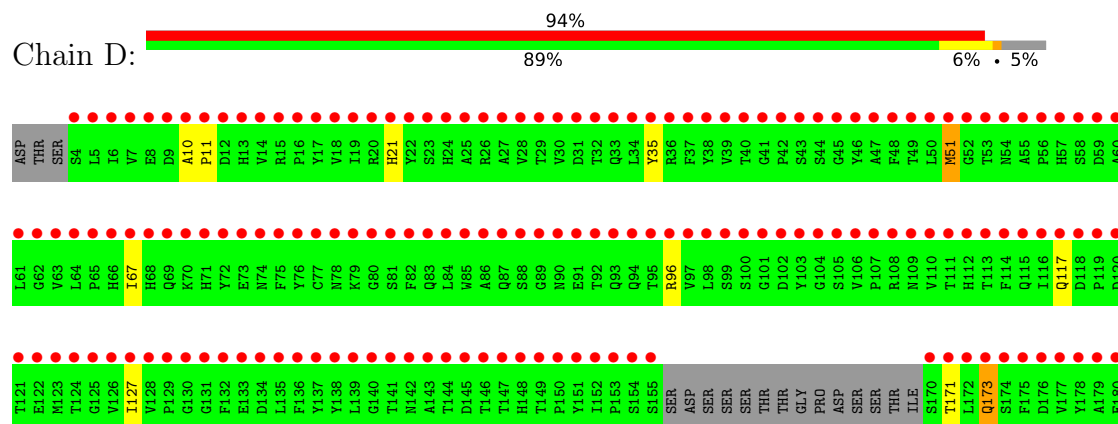
- Molecule 1: QUERCETIN 2,3-DIOXYGENASE

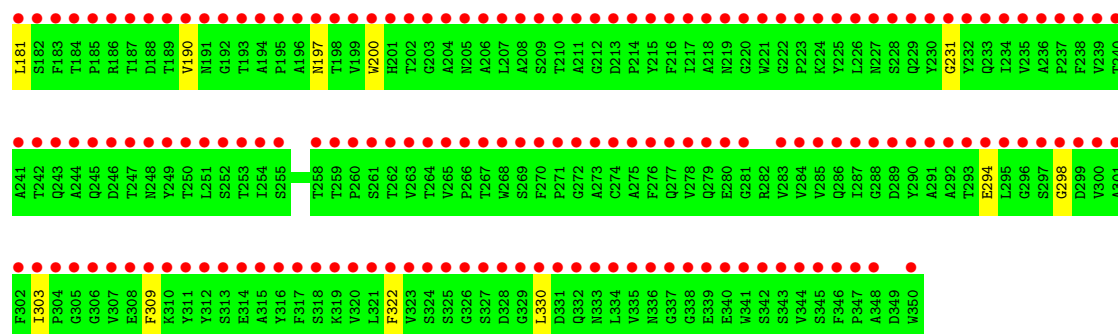


- Molecule 1: QUERCETIN 2,3-DIOXYGENASE



- Molecule 1: QUERCETIN 2,3-DIOXYGENASE





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



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



- Molecule 3: 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	108.94Å 55.65Å 123.86Å 90.00° 98.26° 90.00°	Depositor
Resolution (Å)	19.92 – 1.70 19.92 – 1.70	Depositor EDS
% Data completeness (in resolution range)	91.3 (19.92-1.70) 91.2 (19.92-1.70)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.64 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.161 , 0.183 0.198 , 0.212	Depositor DCC
R_{free} test set	7426 reflections (4.59%)	wwPDB-VP
Wilson B-factor (Å ²)	21.9	Xtriage
Anisotropy	0.617	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 42.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	12136	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.12% 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: DCD, CU, NAG, BMA

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	0.56	0/2710	0.88	1/3713 (0.0%)
1	B	0.50	0/2687	0.87	0/3684
1	C	0.49	1/2698 (0.0%)	0.85	1/3698 (0.0%)
1	D	0.51	1/2670 (0.0%)	0.87	1/3660 (0.0%)
All	All	0.52	2/10765 (0.0%)	0.86	3/14755 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	51	MET	SD-CE	-7.32	1.61	1.79
1	C	51	MET	SD-CE	-5.24	1.66	1.79

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	231	GLY	N-CA-C	-5.74	102.38	112.77
1	D	231	GLY	N-CA-C	-5.42	102.39	112.37
1	C	196	ALA	N-CA-C	5.17	116.92	111.28

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	8[A]	GLU	Sidechain
1	A	8[B]	GLU	Sidechain

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	2595	0	2405	26	0
1	B	2590	0	2399	14	0
1	C	2605	0	2411	20	0
1	D	2578	0	2385	16	0
2	E	39	0	34	1	0
2	F	39	0	34	1	0
3	G	28	0	25	1	0
4	A	8	0	10	1	0
4	B	8	0	11	0	0
4	C	8	0	10	2	0
4	D	8	0	11	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	42	0	39	0	0
6	B	56	0	52	0	0
6	C	42	0	39	0	0
6	D	42	0	39	0	0
7	A	411	0	0	6	0
7	B	346	0	0	4	0
7	C	345	0	0	4	0
7	D	342	0	0	4	0
All	All	12136	0	9904	75	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 4.

All (75) 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:D:171:THR:HA	1:D:173:GLN:OE1	1.68	0.93
1:A:73:GLU:HG3	1:A:127[A]:ILE:HD12	1.55	0.86
1:A:181[B]:LEU:HD23	7:A:2103:HOH:O	1.79	0.82
1:A:78[B]:ASN:ND2	1:A:124:THR:OG1	2.12	0.82
1:B:297:SER:HB3	7:B:2270:HOH:O	1.86	0.76
1:A:260[B]:PRO:HG2	1:A:263:VAL:CG2	2.19	0.71
1:A:245:GLN:HG3	7:A:2285:HOH:O	1.91	0.71
1:A:57:HIS:HE1	1:A:59:ASP:OD1	1.75	0.68
1:D:173:GLN:H	1:D:173:GLN:CD	2.03	0.66
1:C:51:MET:HE2	4:C:1351:DCD:H3C2	1.77	0.66
1:C:190:VAL:HG11	2:F:1:NAG:H82	1.79	0.65
1:C:117:GLN:HB2	7:C:2155:HOH:O	1.97	0.65
1:A:170:SER:HB3	1:A:179:ALA:HB2	1.84	0.60
1:A:78[B]:ASN:HD21	1:A:124:THR:CB	2.15	0.60
1:C:169:ILE:CG2	1:C:170:SER:N	2.64	0.59
1:B:148:HIS:HE1	7:B:2004:HOH:O	1.86	0.59
1:C:181:LEU:HD12	1:C:181:LEU:H	1.69	0.58
1:B:169:ILE:O	1:B:173:GLN:HG3	2.04	0.57
1:B:117:GLN:HG3	7:D:2212:HOH:O	2.03	0.56
1:C:181:LEU:HD12	1:C:181:LEU:N	2.22	0.54
1:A:73:GLU:CG	1:A:127[A]:ILE:HD12	2.35	0.54
1:D:190:VAL:HG11	3:G:1:NAG:H82	1.89	0.54
1:A:179:ALA:HB1	1:A:181[A]:LEU:CD1	2.37	0.54
1:C:51:MET:CE	4:C:1351:DCD:H3C2	2.39	0.53
1:A:68:HIS:CE1	1:A:132:PHE:HZ	2.27	0.53
1:A:127[A]:ILE:HD11	4:A:1351:DCD:H5C1	1.92	0.52
1:A:190:VAL:HG11	2:E:1:NAG:H82	1.92	0.51
1:C:132:PHE:HB3	7:C:2081:HOH:O	2.10	0.51
1:A:35:TYR:HD2	1:A:51[B]:MET:CE	2.25	0.50
1:A:179:ALA:HB1	1:A:181[A]:LEU:HD12	1.94	0.50
1:A:260[B]:PRO:HG2	1:A:263:VAL:HG23	1.93	0.50
1:C:78[B]:ASN:ND2	1:C:124:THR:OG1	2.37	0.50
1:B:132:PHE:HB3	7:B:2066:HOH:O	2.11	0.49
1:B:168:THR:O	1:B:169:ILE:C	2.55	0.49
1:C:166:SER:O	1:C:169:ILE:HG22	2.13	0.49
1:A:16:PRO:HB3	1:A:287:ILE:HG21	1.96	0.48
1:C:132:PHE:CB	7:C:2081:HOH:O	2.62	0.47
1:A:294:GLU:HG2	7:A:2339:HOH:O	2.14	0.47
1:D:67:ILE:HD11	7:D:2145:HOH:O	2.14	0.46
1:B:13:HIS:HB2	1:C:171:THR:HG23	1.97	0.46
1:B:168:THR:O	1:B:171:THR:N	2.49	0.46
1:D:35:TYR:HD2	1:D:51:MET:HE3	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:34:LEU:C	1:C:34:LEU:HD23	2.40	0.46
1:B:294:GLU:HG2	7:B:2284:HOH:O	2.17	0.45
1:A:322:PHE:CZ	1:A:330:LEU:HB3	2.52	0.45
1:D:294:GLU:HG2	7:D:2288:HOH:O	2.17	0.45
1:C:169:ILE:HD12	1:C:169:ILE:HA	1.70	0.45
1:A:132:PHE:CB	7:A:2179:HOH:O	2.65	0.44
1:B:171:THR:HG22	7:C:2026:HOH:O	2.16	0.44
1:A:57:HIS:CE1	1:A:59:ASP:OD1	2.63	0.44
1:D:197:ASN:CG	1:D:197:ASN:O	2.59	0.44
1:D:171:THR:CA	1:D:173:GLN:OE1	2.54	0.43
1:C:90:ASN:OD1	1:C:90:ASN:C	2.62	0.43
1:C:169:ILE:HG22	1:C:170:SER:H	1.84	0.43
1:A:132:PHE:HB2	7:A:2179:HOH:O	2.18	0.43
1:A:170:SER:CB	1:A:179:ALA:HB2	2.49	0.42
1:D:21:HIS:CG	1:D:298:GLY:HA3	2.53	0.42
1:B:346:PHE:HB2	1:B:347:PRO:HD2	2.00	0.42
1:C:169:ILE:HG22	1:C:170:SER:N	2.33	0.42
1:C:153:PRO:O	1:C:154:SER:C	2.62	0.42
1:D:35:TYR:HD2	1:D:51:MET:CE	2.32	0.42
1:D:322:PHE:CZ	1:D:330:LEU:HB3	2.55	0.41
1:D:10:ALA:HA	1:D:11:PRO:HD3	1.90	0.41
1:C:169:ILE:HG23	1:C:170:SER:N	2.36	0.41
1:D:96:ARG:HD2	1:D:200:TRP:CD2	2.56	0.41
1:B:346:PHE:HB2	1:B:347:PRO:CD	2.50	0.41
1:A:57:HIS:HD2	1:A:117:GLN:O	2.02	0.41
1:A:21:HIS:CG	1:A:298:GLY:HA3	2.56	0.41
1:A:117:GLN:HB2	7:A:2166:HOH:O	2.20	0.41
1:B:172:LEU:HD23	1:B:172:LEU:HA	1.94	0.40
1:D:117:GLN:NE2	7:D:2149:HOH:O	2.54	0.40
1:C:26:ARG:HH11	1:C:26:ARG:HG2	1.86	0.40
1:D:303:ILE:HG21	1:D:309:PHE:CD1	2.56	0.40
1:B:50:LEU:C	1:B:50:LEU:HD23	2.46	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	337/350 (96%)	329 (98%)	8 (2%)	0	100	100
1	B	334/350 (95%)	325 (97%)	9 (3%)	0	100	100
1	C	336/350 (96%)	324 (96%)	12 (4%)	0	100	100
1	D	332/350 (95%)	323 (97%)	9 (3%)	0	100	100
All	All	1339/1400 (96%)	1301 (97%)	38 (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	A	284/294 (97%)	281 (99%)	3 (1%)	65	54
1	B	282/294 (96%)	280 (99%)	2 (1%)	76	69
1	C	284/294 (97%)	281 (99%)	3 (1%)	65	54
1	D	279/294 (95%)	277 (99%)	2 (1%)	76	69
All	All	1129/1176 (96%)	1119 (99%)	10 (1%)	73	62

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	ASN
1	A	297[A]	SER
1	A	297[B]	SER
1	B	169	ILE
1	B	171	THR
1	C	3	SER
1	C	168	THR
1	C	169	ILE

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Mol	Chain	Res	Type
1	D	173	GLN
1	D	181	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	HIS
1	A	332	GLN
1	A	336	ASN
1	B	74	ASN
1	B	83	GLN
1	B	148	HIS
1	B	173	GLN
1	B	332	GLN
1	B	336	ASN
1	C	74	ASN
1	C	83	GLN
1	C	332	GLN
1	C	336	ASN
1	D	74	ASN
1	D	332	GLN
1	D	336	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

8 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	$\# Z > 2$
2	NAG	E	1	1,2	14,14,15	0.45	0	17,19,21	1.16	2 (11%)
2	NAG	E	2	2	14,14,15	0.48	0	17,19,21	1.02	1 (5%)
2	BMA	E	3	2	11,11,12	0.59	0	15,15,17	0.53	0
2	NAG	F	1	1,2	14,14,15	0.50	0	17,19,21	0.99	0
2	NAG	F	2	2	14,14,15	0.50	0	17,19,21	1.07	0
2	BMA	F	3	2	11,11,12	0.63	0	15,15,17	0.52	0
3	NAG	G	1	3,1	14,14,15	0.54	0	17,19,21	1.37	2 (11%)
3	NAG	G	2	3	14,14,15	0.58	0	17,19,21	0.85	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
2	NAG	E	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	BMA	E	3	2	-	0/2/19/22	0/1/1/1
2	NAG	F	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	0/6/23/26	0/1/1/1
2	BMA	F	3	2	-	0/2/19/22	0/1/1/1
3	NAG	G	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	G	2	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	1	NAG	C2-N2-C7	-3.35	118.41	122.90
3	G	1	NAG	O5-C1-C2	-3.12	106.46	111.29
2	E	1	NAG	O5-C1-C2	-3.06	106.56	111.29
2	E	2	NAG	O4-C4-C3	-2.03	105.60	110.38
2	E	1	NAG	C2-N2-C7	-2.00	120.22	122.90

There are no chirality outliers.

All (4) torsion outliers are listed below:

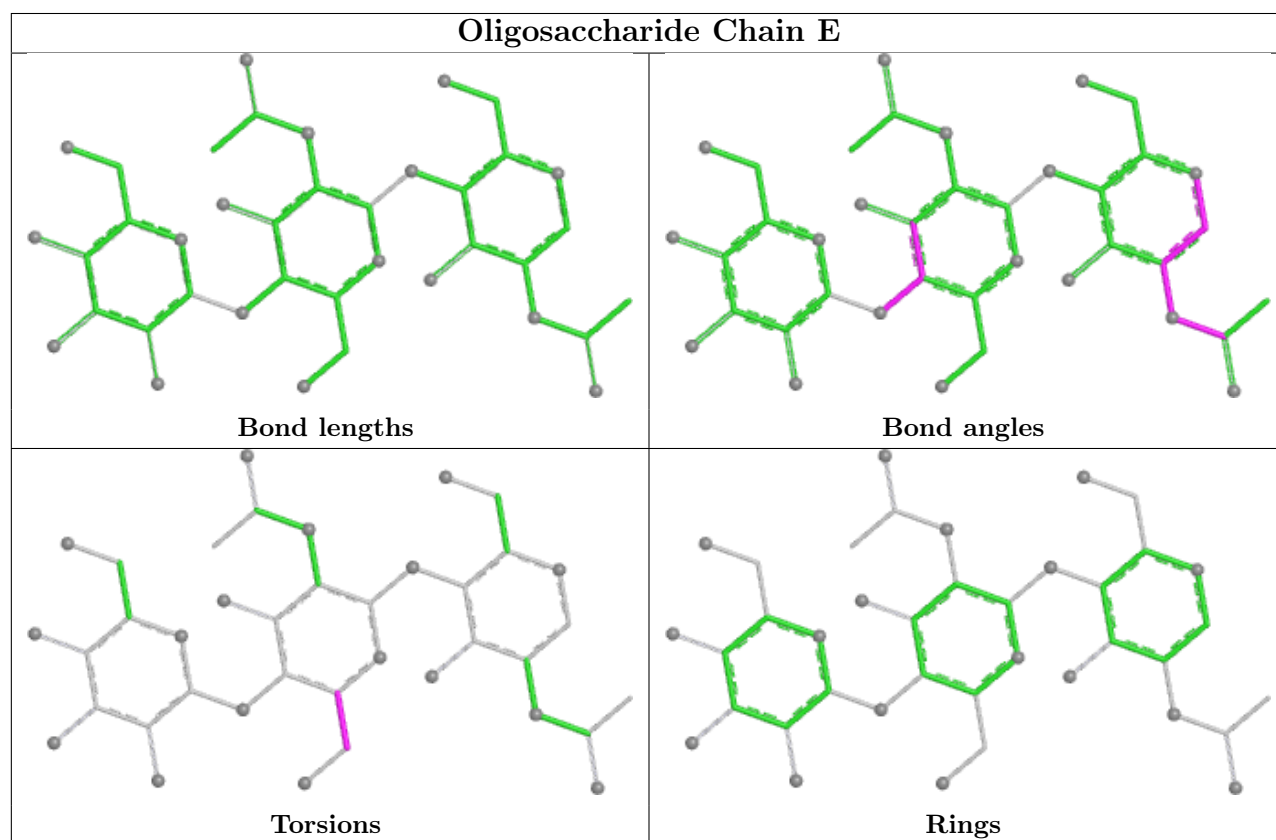
Mol	Chain	Res	Type	Atoms
2	E	2	NAG	C4-C5-C6-O6
3	G	1	NAG	C4-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
3	G	1	NAG	O5-C5-C6-O6

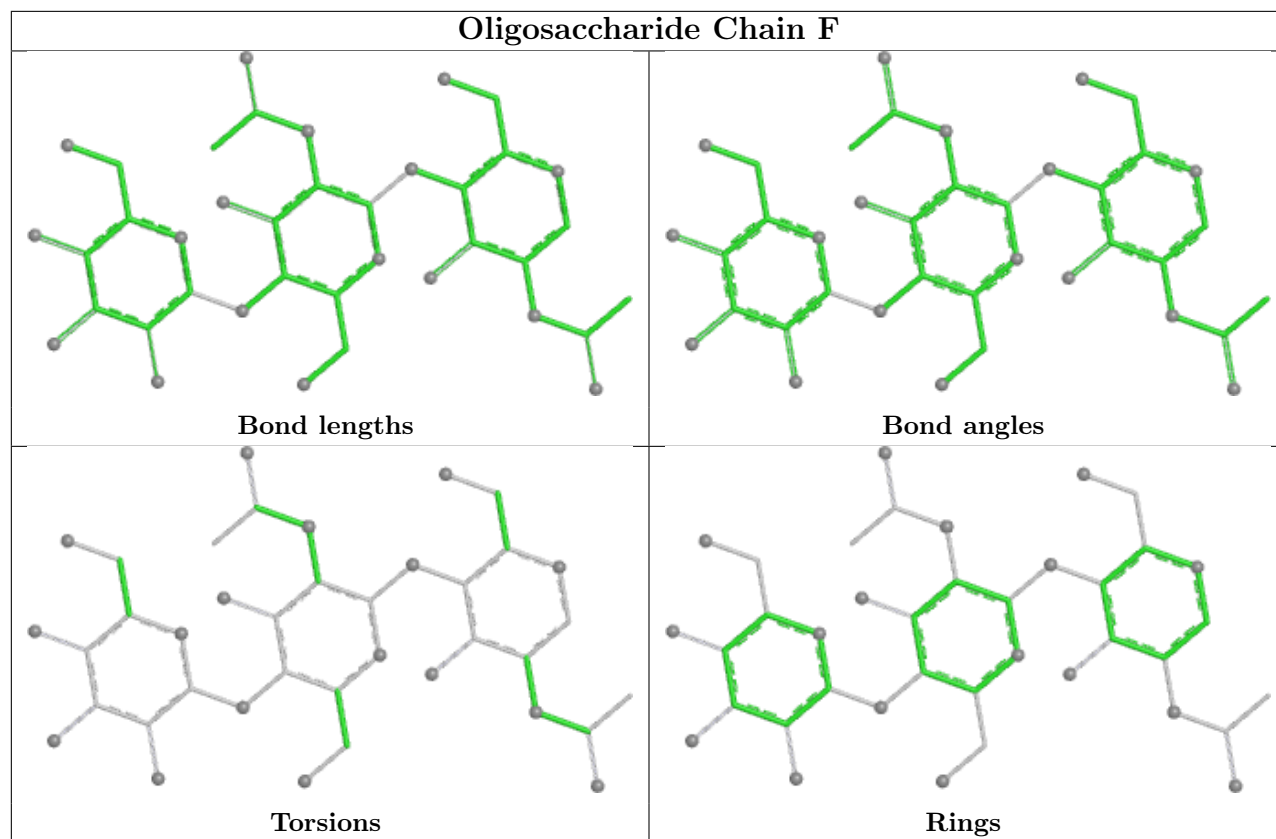
There are no ring outliers.

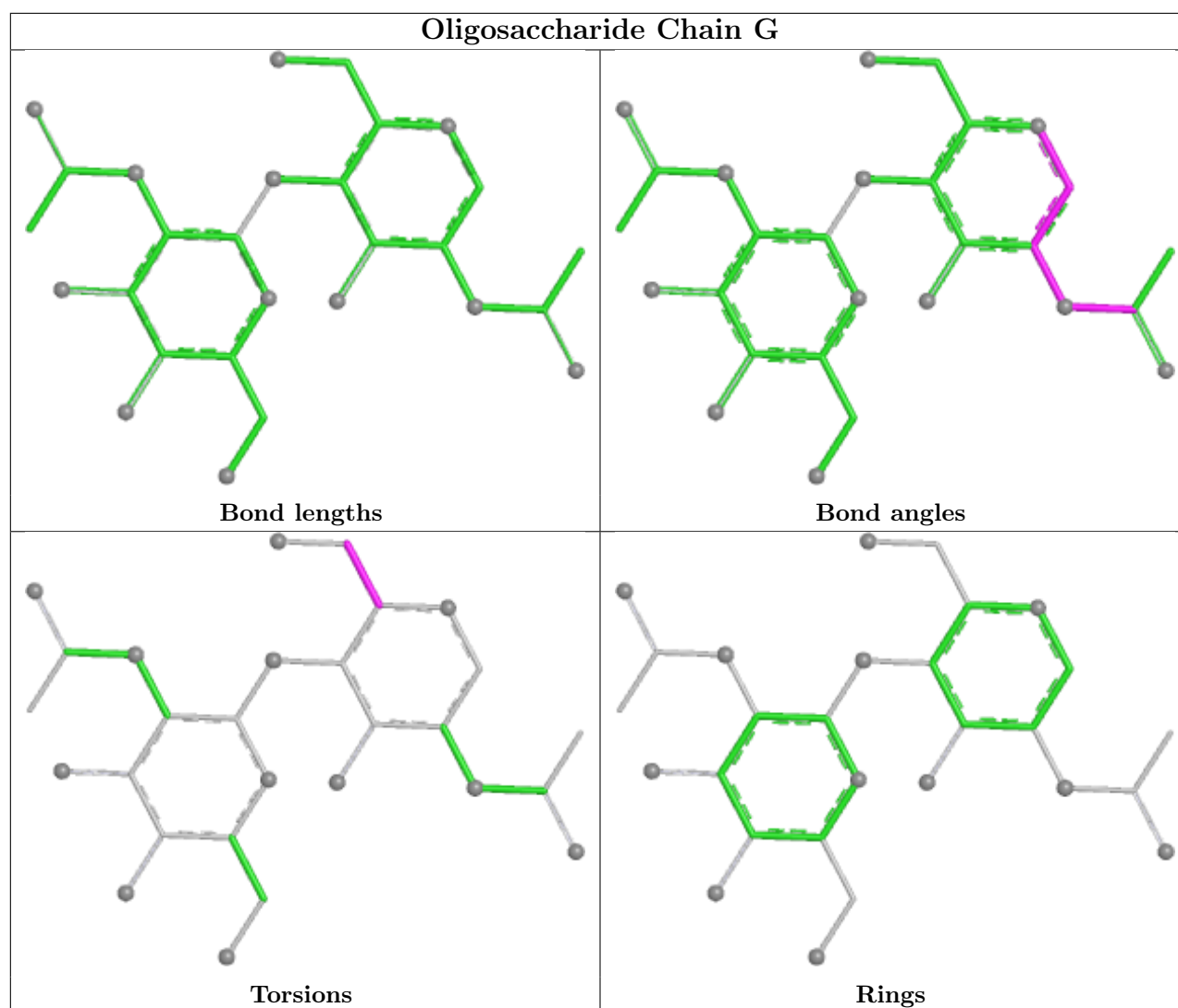
3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1	NAG	1	0
3	G	1	NAG	1	0
2	F	1	NAG	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](#)

Of 21 ligands modelled in this entry, 4 are monoatomic - leaving 17 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	$\# Z > 2$
6	NAG	D	1357	1	14,14,15	0.64	0	17,19,21	1.11	1 (5%)
6	NAG	A	1356	1	14,14,15	0.60	0	17,19,21	0.91	1 (5%)
6	NAG	A	1353	1	14,14,15	0.46	0	17,19,21	0.85	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	B	1355	1	14,14,15	0.66	0	17,19,21	1.49	2 (11%)
4	DCD	A	1351	5	6,7,7	0.97	0	6,8,8	0.93	0
4	DCD	C	1351	5	6,7,7	1.09	1 (16%)	6,8,8	0.58	0
6	NAG	A	1357	1	14,14,15	0.63	0	17,19,21	0.85	0
6	NAG	C	1353	1	14,14,15	0.48	0	17,19,21	0.60	0
4	DCD	D	1351	5	6,7,7	1.61	1 (16%)	6,8,8	1.46	1 (16%)
4	DCD	B	1351	5	6,7,7	1.33	1 (16%)	6,8,8	0.91	0
6	NAG	C	1356	1	14,14,15	0.60	0	17,19,21	1.03	1 (5%)
6	NAG	D	1353	1	14,14,15	0.51	0	17,19,21	1.24	2 (11%)
6	NAG	B	1356	1	14,14,15	0.59	0	17,19,21	0.77	0
6	NAG	D	1356	1	14,14,15	0.51	0	17,19,21	0.91	0
6	NAG	B	1353	1	14,14,15	0.60	0	17,19,21	0.89	1 (5%)
6	NAG	C	1357	1	14,14,15	0.64	0	17,19,21	1.26	2 (11%)
6	NAG	B	1354	1	14,14,15	0.55	0	17,19,21	1.26	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
6	NAG	D	1357	1	-	0/6/23/26	0/1/1/1
6	NAG	A	1356	1	-	0/6/23/26	0/1/1/1
6	NAG	A	1353	1	-	0/6/23/26	0/1/1/1
6	NAG	B	1355	1	-	0/6/23/26	0/1/1/1
4	DCD	A	1351	5	-	0/8/8/8	-
4	DCD	C	1351	5	-	0/8/8/8	-
6	NAG	A	1357	1	-	0/6/23/26	0/1/1/1
6	NAG	C	1353	1	-	0/6/23/26	0/1/1/1
4	DCD	D	1351	5	-	0/8/8/8	-
4	DCD	B	1351	5	-	0/8/8/8	-
6	NAG	C	1356	1	-	0/6/23/26	0/1/1/1
6	NAG	D	1353	1	-	0/6/23/26	0/1/1/1
6	NAG	B	1356	1	-	0/6/23/26	0/1/1/1
6	NAG	D	1356	1	-	0/6/23/26	0/1/1/1
6	NAG	B	1353	1	-	0/6/23/26	0/1/1/1
6	NAG	C	1357	1	-	0/6/23/26	0/1/1/1
6	NAG	B	1354	1	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1351	DCD	C1-S2	-3.54	1.59	1.66
4	B	1351	DCD	C1-S2	-3.05	1.60	1.66
4	C	1351	DCD	C1-S2	-2.35	1.61	1.66

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1355	NAG	O5-C1-C2	-4.42	104.46	111.29
6	B	1354	NAG	C2-N2-C7	-4.10	117.40	122.90
6	C	1357	NAG	O5-C1-C2	-3.33	106.14	111.29
4	D	1351	DCD	S2-C1-N1	-3.14	117.98	123.70
6	B	1355	NAG	C2-N2-C7	-2.93	118.97	122.90
6	D	1353	NAG	C6-C5-C4	-2.87	105.98	113.02
6	D	1357	NAG	O5-C1-C2	-2.56	107.33	111.29
6	C	1356	NAG	O5-C1-C2	-2.50	107.42	111.29
6	B	1353	NAG	C2-N2-C7	-2.13	120.05	122.90
6	C	1357	NAG	C2-N2-C7	-2.12	120.05	122.90
6	D	1353	NAG	C4-C3-C2	-2.07	107.99	111.02
6	A	1356	NAG	C2-N2-C7	-2.04	120.17	122.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1351	DCD	1	0
4	C	1351	DCD	2	0

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	A	333/350 (95%)	-0.04	3 (0%) 81 83	10, 15, 20, 27	8 (2%)
1	B	334/350 (95%)	0.04	4 (1%) 76 80	11, 15, 19, 28	4 (1%)
1	C	337/350 (96%)	0.29	9 (2%) 56 60	10, 15, 20, 34	3 (0%)
1	D	333/350 (95%)	5.01	329 (98%) 0 0	9, 15, 20, 34	3 (0%)
All	All	1337/1400 (95%)	1.32	345 (25%) 1 1	9, 15, 20, 34	18 (1%)

All (345) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	155	SER	12.7
1	D	154	SER	12.1
1	D	138	TYR	11.4
1	D	170	SER	10.4
1	D	262	THR	10.3
1	D	181	LEU	9.7
1	D	137	TYR	9.6
1	D	263	VAL	9.5
1	D	171	THR	9.4
1	D	117	GLN	9.3
1	D	190	VAL	9.3
1	D	289	ASP	9.3
1	D	342	SER	9.2
1	D	183	PHE	9.0
1	D	132	PHE	8.8
1	D	27	ALA	8.7
1	D	261	SER	8.6
1	D	116	ILE	8.5
1	D	80	GLY	8.5
1	D	63	VAL	8.3
1	D	28	VAL	8.2

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Mol	Chain	Res	Type	RSRZ
1	D	143	ALA	8.2
1	D	58	SER	8.1
1	D	328	ASP	8.0
1	D	34	LEU	8.0
1	D	146	THR	8.0
1	D	153	PRO	7.9
1	D	55	ALA	7.7
1	D	189	THR	7.6
1	D	37	PHE	7.6
1	D	75	PHE	7.5
1	D	177	VAL	7.5
1	D	152	ILE	7.4
1	D	89	GLY	7.4
1	D	82	PHE	7.4
1	D	175	PHE	7.3
1	D	67	ILE	7.2
1	D	29	THR	7.2
1	D	173	GLN	7.2
1	D	150	PRO	7.2
1	D	139	LEU	7.1
1	D	182	SER	7.1
1	D	350	TRP	7.0
1	D	98	LEU	7.0
1	D	151	TYR	7.0
1	D	14	VAL	7.0
1	D	97	VAL	7.0
1	D	178	TYR	7.0
1	D	216	PHE	7.0
1	D	225	TYR	7.0
1	D	115	GLN	6.9
1	D	110	VAL	6.9
1	D	77	CYS	6.8
1	D	90	ASN	6.8
1	D	172	LEU	6.8
1	D	22	TYR	6.7
1	D	54	ASN	6.7
1	D	290	TYR	6.7
1	D	57	HIS	6.7
1	D	120	ASP	6.7
1	D	6	ILE	6.6
1	D	35	TYR	6.6
1	D	214	PRO	6.5

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Mol	Chain	Res	Type	RSRZ
1	D	341	TRP	6.5
1	D	81	SER	6.5
1	D	144	THR	6.5
1	D	78	ASN	6.5
1	D	61	LEU	6.5
1	D	127[A]	ILE	6.5
1	D	149	THR	6.4
1	D	141	THR	6.4
1	D	84	LEU	6.3
1	D	46	TYR	6.3
1	D	228[A]	SER	6.3
1	D	106	VAL	6.3
1	D	230	TYR	6.2
1	D	30	VAL	6.2
1	D	135	LEU	6.2
1	D	207	LEU	6.2
1	D	85	TRP	6.2
1	D	121	THR	6.1
1	D	226	LEU	6.1
1	D	51	MET	6.1
1	D	229	GLN	6.1
1	D	327	SER	6.1
1	D	208	ALA	6.0
1	D	107	PRO	5.9
1	D	136	PHE	5.9
1	D	4	SER	5.9
1	D	211	ALA	5.9
1	D	217	ILE	5.9
1	D	31	ASP	5.9
1	D	111	THR	5.8
1	D	303	ILE	5.8
1	D	99	SER	5.8
1	D	64	LEU	5.8
1	D	5	LEU	5.8
1	D	72	TYR	5.7
1	D	259	THR	5.7
1	D	7	VAL	5.7
1	D	101	GLY	5.6
1	D	60	ALA	5.6
1	D	335	VAL	5.6
1	D	340	GLU	5.5
1	D	238	PHE	5.5

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Mol	Chain	Res	Type	RSRZ
1	D	113	THR	5.5
1	D	147	THR	5.5
1	D	184	THR	5.5
1	D	23	SER	5.5
1	D	131	GLY	5.5
1	D	19	ILE	5.5
1	D	56	PRO	5.5
1	D	200	TRP	5.5
1	D	32	THR	5.5
1	D	193	THR	5.5
1	D	128	VAL	5.5
1	D	33	GLN	5.4
1	D	69	GLN	5.4
1	D	24	HIS	5.4
1	D	123	MET	5.4
1	D	215	TYR	5.4
1	D	50	LEU	5.4
1	D	100[A]	SER	5.3
1	D	48	PHE	5.3
1	D	264	THR	5.3
1	D	47	ALA	5.3
1	D	76	TYR	5.2
1	D	52	GLY	5.2
1	D	59	ASP	5.2
1	D	71	HIS	5.2
1	D	92	THR	5.2
1	D	17	TYR	5.2
1	D	260	PRO	5.2
1	D	249	TYR	5.1
1	D	191	ASN	5.1
1	D	134	ASP	5.1
1	D	114	PHE	5.1
1	D	247	THR	5.1
1	D	38	TYR	5.0
1	D	10	ALA	5.0
1	D	86	ALA	5.0
1	D	298	GLY	5.0
1	D	142	ASN	5.0
1	D	62	GLY	4.9
1	D	70	LYS	4.9
1	D	39	VAL	4.9
1	D	293	THR	4.8

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Mol	Chain	Res	Type	RSRZ
1	D	66	HIS	4.8
1	D	9	ASP	4.8
1	D	130	GLY	4.8
1	C	167	SER	4.8
1	D	213	ASP	4.8
1	D	306	GLY	4.8
1	D	187	THR	4.8
1	D	42	PRO	4.8
1	D	221	TRP	4.8
1	D	180	GLU	4.8
1	D	336	ASN	4.7
1	D	8	GLU	4.7
1	D	129	PRO	4.7
1	D	252	SER	4.7
1	D	297	SER	4.7
1	D	79	LYS	4.7
1	D	104	GLY	4.7
1	D	192	GLY	4.7
1	D	53	THR	4.6
1	D	145	ASP	4.6
1	D	103	TYR	4.6
1	D	235	VAL	4.6
1	D	194	ALA	4.6
1	D	309	PHE	4.6
1	D	312	TYR	4.6
1	D	308	GLU	4.6
1	D	202	THR	4.5
1	D	18	VAL	4.5
1	D	251	LEU	4.5
1	D	339	GLU	4.5
1	D	271	PRO	4.5
1	D	73	GLU	4.5
1	D	188	ASP	4.5
1	D	246	ASP	4.5
1	D	11	PRO	4.5
1	D	108	ARG	4.5
1	D	21	HIS	4.5
1	D	242	THR	4.5
1	D	13	HIS	4.4
1	D	65	PRO	4.4
1	D	124	THR	4.4
1	D	87	GLN	4.4

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Mol	Chain	Res	Type	RSRZ
1	D	43	SER	4.4
1	D	174	SER	4.4
1	D	337	GLY	4.4
1	D	333	ASN	4.3
1	D	40	THR	4.3
1	D	49	THR	4.3
1	D	218	ALA	4.3
1	D	273	ALA	4.3
1	D	140	GLY	4.3
1	D	185	PRO	4.3
1	D	95	THR	4.3
1	D	323	VAL	4.3
1	D	288	GLY	4.3
1	D	199	VAL	4.3
1	D	239	VAL	4.3
1	D	278	VAL	4.3
1	D	223	PRO	4.3
1	D	326	GLY	4.2
1	D	205	ASN	4.2
1	D	300	VAL	4.2
1	D	206	ALA	4.2
1	D	270	PHE	4.2
1	D	302	PHE	4.2
1	D	198	THR	4.2
1	D	236	ALA	4.1
1	D	244	ALA	4.1
1	D	275	ALA	4.1
1	D	102	ASP	4.1
1	D	119	PRO	4.1
1	D	176	ASP	4.1
1	D	91	GLU	4.1
1	D	179	ALA	4.1
1	D	201	HIS	4.1
1	D	126	VAL	4.1
1	D	310	LYS	4.1
1	D	83	GLN	4.1
1	D	276	PHE	4.0
1	D	25	ALA	4.0
1	D	274	CYS	4.0
1	D	315	ALA	4.0
1	D	269	SER	3.9
1	D	272	GLY	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	250	THR	3.9
1	D	292	ALA	3.9
1	D	266	PRO	3.9
1	C	168	THR	3.8
1	D	209	SER	3.8
1	D	291	ALA	3.8
1	D	118	ASP	3.8
1	D	44	SER	3.8
1	D	321	LEU	3.8
1	D	212	GLY	3.8
1	D	268	TRP	3.8
1	D	232	TYR	3.8
1	D	301	ALA	3.7
1	D	26	ARG	3.7
1	D	122	GLU	3.7
1	D	237	PRO	3.7
1	D	41	GLY	3.7
1	D	304	PRO	3.6
1	D	204	ALA	3.6
1	D	133	GLU	3.6
1	D	68	HIS	3.6
1	D	241	ALA	3.6
1	D	344	VAL	3.6
1	C	4	SER	3.6
1	D	325	SER	3.6
1	D	286	GLN	3.6
1	D	195	PRO	3.6
1	D	234	ILE	3.6
1	D	258	THR	3.6
1	D	96	ARG	3.6
1	D	317	PHE	3.6
1	D	219	ASN	3.6
1	D	320	VAL	3.6
1	D	36	ARG	3.5
1	D	296	GLY	3.5
1	D	319	LYS	3.5
1	D	93	GLN	3.5
1	D	88	SER	3.5
1	D	330	LEU	3.5
1	D	196	ALA	3.4
1	D	243	GLN	3.4
1	D	203	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	338	GLY	3.4
1	C	166	SER	3.4
1	D	287	ILE	3.3
1	D	283	VAL	3.3
1	D	94	GLN	3.3
1	D	316	TYR	3.3
1	D	267	THR	3.3
1	D	245	GLN	3.3
1	D	231	GLY	3.2
1	D	329	GLY	3.2
1	D	332	GLN	3.2
1	D	285	VAL	3.2
1	D	125	GLY	3.2
1	D	210	THR	3.2
1	D	322	PHE	3.2
1	D	224	LYS	3.2
1	D	284	VAL	3.2
1	D	307	VAL	3.2
1	D	12	ASP	3.1
1	D	74	ASN	3.1
1	D	109	ASN	3.1
1	D	248	ASN	3.1
1	D	331	ASP	3.1
1	D	305	GLY	3.1
1	D	254	ILE	3.1
1	D	299	ASP	3.1
1	B	169	ILE	3.0
1	D	240	THR	3.0
1	D	294	GLU	3.0
1	D	45	GLY	3.0
1	D	220	GLY	3.0
1	D	334	LEU	3.0
1	D	105	SER	3.0
1	D	265	VAL	3.0
1	B	167	SER	3.0
1	D	15	ARG	2.9
1	D	112	HIS	2.9
1	D	253	THR	2.9
1	D	197	ASN	2.9
1	D	16	PRO	2.9
1	D	148	HIS	2.9
1	D	314	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	295	LEU	2.8
1	D	324	SER	2.8
1	C	89	GLY	2.8
1	D	222	GLY	2.8
1	D	279	GLN	2.8
1	B	168	THR	2.8
1	D	255	SER	2.8
1	D	345	SER	2.8
1	B	181	LEU	2.7
1	A	90	ASN	2.7
1	A	154	SER	2.7
1	D	281	GLY	2.6
1	D	280	GLU	2.6
1	D	20	ARG	2.6
1	D	311	TYR	2.6
1	C	3	SER	2.6
1	D	347	PRO	2.6
1	D	318	SER	2.5
1	D	186	ARG	2.5
1	C	154	SER	2.5
1	D	346	PHE	2.4
1	D	277	GLN	2.4
1	D	343	SER	2.4
1	D	227	ASN	2.3
1	D	348	ALA	2.2
1	C	177	VAL	2.2
1	D	313	SER	2.2
1	A	170	SER	2.2
1	D	233	GLN	2.1
1	C	289	ASP	2.1

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

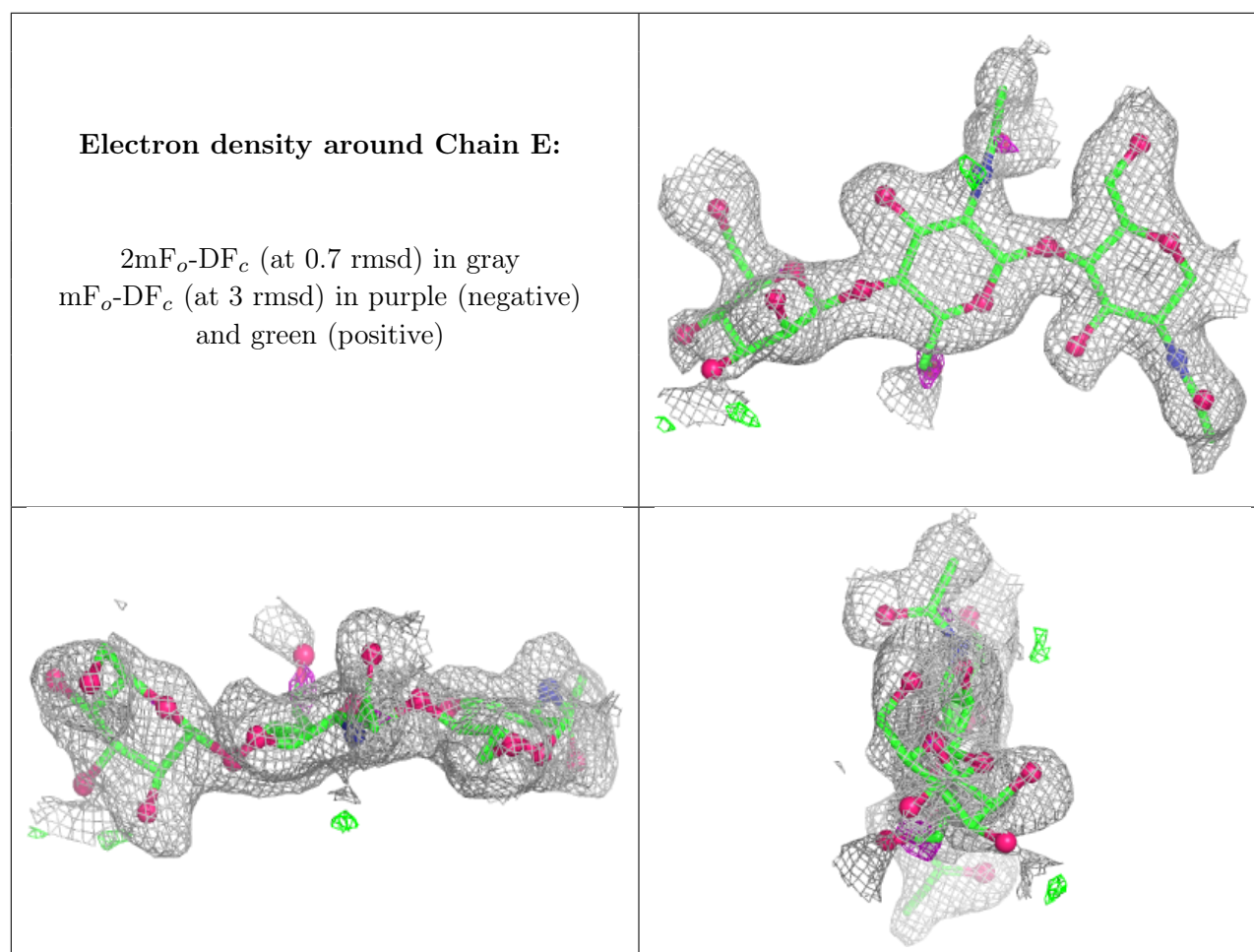
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

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.

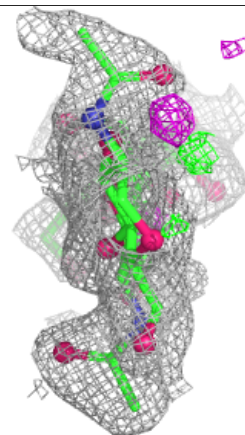
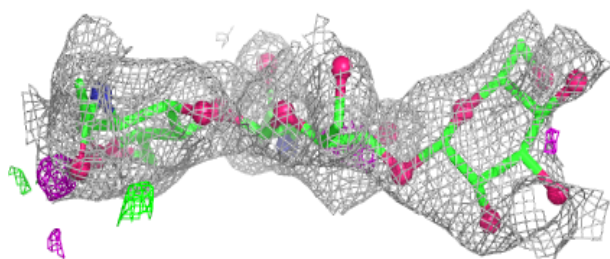
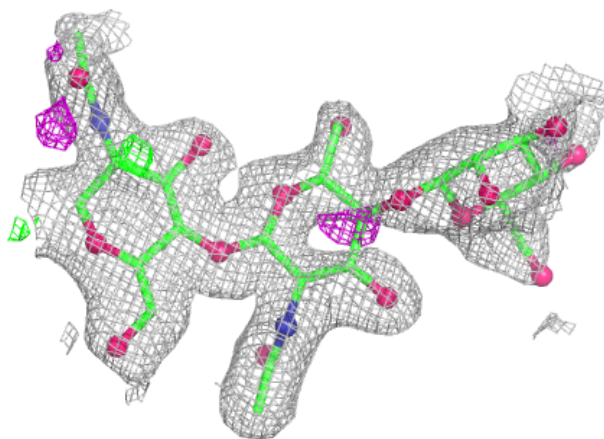
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	BMA	E	3	11/12	0.67	0.13	48,49,50,50	0
2	BMA	F	3	11/12	0.68	0.11	52,55,56,56	0
3	NAG	G	1	14/15	0.74	0.13	31,36,39,40	0
2	NAG	E	2	14/15	0.75	0.12	36,41,44,46	0
2	NAG	F	1	14/15	0.76	0.12	31,36,42,45	0
2	NAG	F	2	14/15	0.78	0.12	35,40,43,48	0
2	NAG	E	1	14/15	0.82	0.10	31,36,39,40	0
3	NAG	G	2	14/15	0.82	0.10	36,39,43,45	0

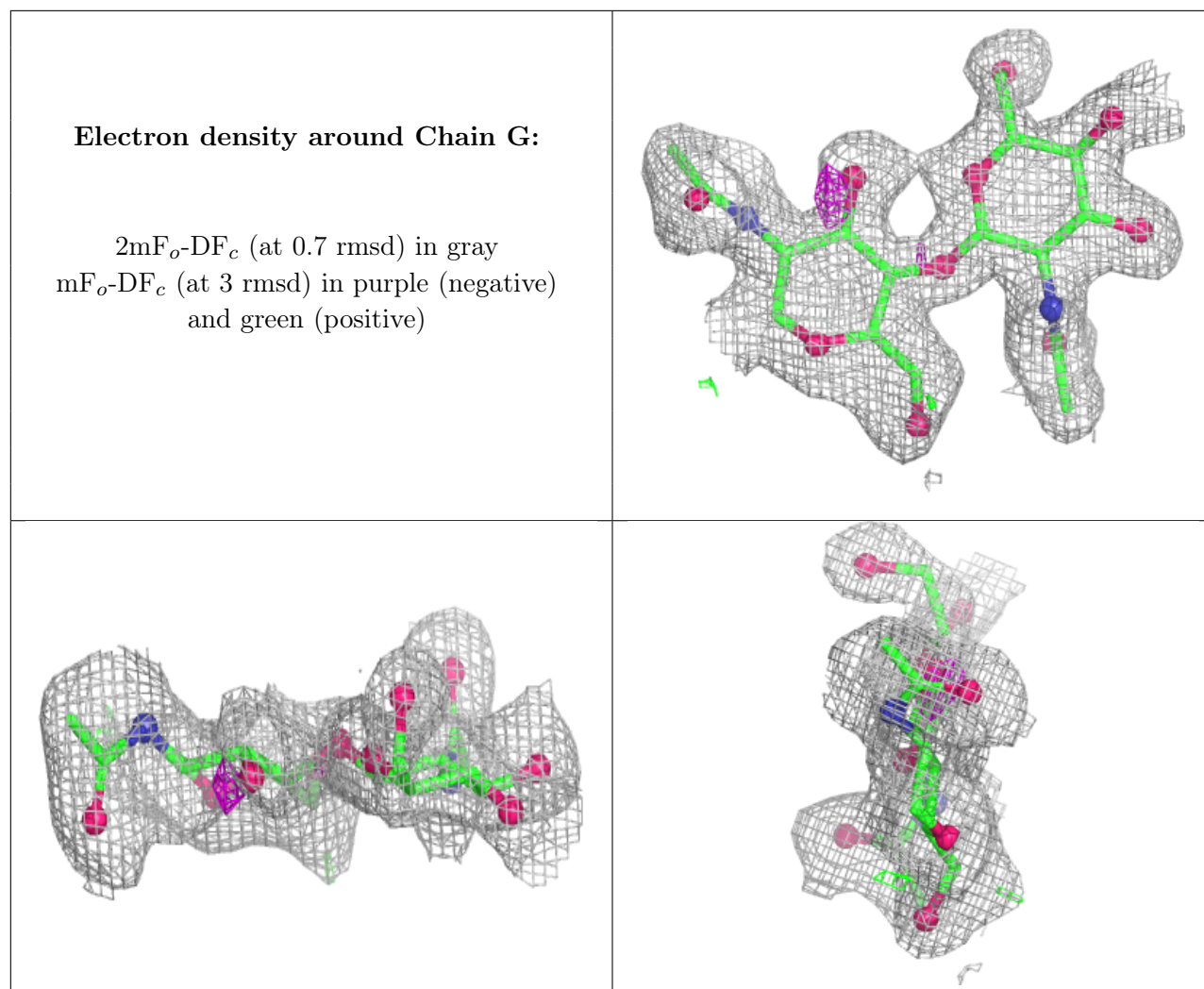
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



Electron density around Chain F:

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





6.4 Ligands ⓘ

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
5	CU	D	1352	1/1	0.43	0.48	17,17,17,17	0
6	NAG	A	1357	14/15	0.68	0.13	32,36,42,44	0
6	NAG	D	1356	14/15	0.72	0.12	29,33,37,38	0
6	NAG	B	1354	14/15	0.74	0.12	40,45,47,48	0
6	NAG	D	1353	14/15	0.76	0.12	33,39,42,43	0
6	NAG	B	1355	14/15	0.78	0.11	28,34,45,46	0
6	NAG	C	1353	14/15	0.78	0.12	34,39,44,46	0
6	NAG	B	1356	14/15	0.80	0.11	35,42,45,45	0
6	NAG	D	1357	14/15	0.81	0.11	32,38,44,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	DCD	D	1351	8/8	0.82	0.34	19,20,23,23	0
6	NAG	C	1357	14/15	0.83	0.11	32,39,42,43	0
6	NAG	C	1356	14/15	0.84	0.10	34,39,46,46	0
6	NAG	A	1356	14/15	0.86	0.10	27,32,41,43	0
6	NAG	B	1353	14/15	0.89	0.07	29,34,38,38	0
6	NAG	A	1353	14/15	0.89	0.08	26,32,35,36	0
4	DCD	C	1351	8/8	0.91	0.11	20,21,22,23	0
4	DCD	B	1351	8/8	0.96	0.09	22,23,24,24	0
4	DCD	A	1351	8/8	0.97	0.07	17,18,20,20	0
5	CU	B	1352	1/1	0.98	0.03	17,17,17,17	0
5	CU	C	1352	1/1	0.98	0.04	17,17,17,17	0
5	CU	A	1352	1/1	0.99	0.03	17,17,17,17	0

6.5 Other polymers [i](#)

There are no such residues in this entry.