



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:45 PM UTC

PDB ID : 2QPU / pdb_00002qpu
Title : Sugar tongs mutant S378P in complex with acarbose
Authors : Aghajari, N.; Jensen, M.H.; Tranier, S.; Haser, R.
Deposited on : 2007-07-25
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
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

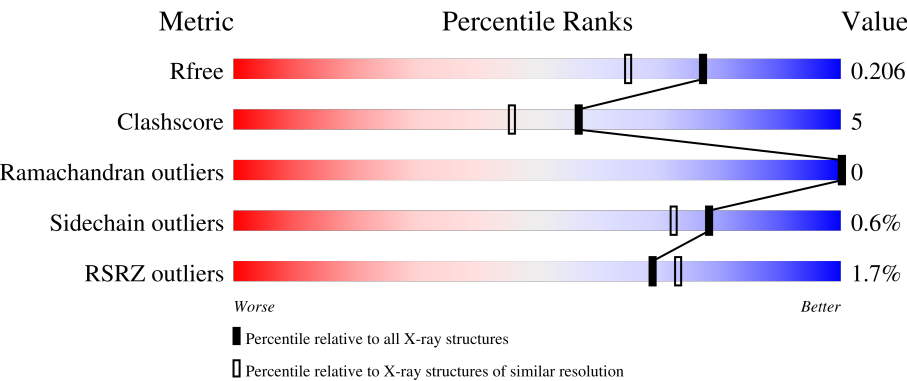
1 Overall quality at a glance i

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	405	% 86%13%
1	B	405	2% 85%15%
1	C	405	2% 87%13%
2	D	3	67%33%

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
4	EDO	A	2000	-	X	-	-
5	QPU	A	3000	X	-	-	-
5	QPU	A	4000	X	-	-	-
5	QPU	B	4000	X	-	-	-
5	QPU	C	3000	X	-	-	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 11424 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 Alpha-amylase type A isozyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	404	Total	C	N	O	S	0	1	0
			3148	2010	538	584	16			
1	B	404	Total	C	N	O	S	0	4	0
			3174	2028	543	586	17			
1	C	404	Total	C	N	O	S	0	4	0
			3172	2027	542	585	18			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	284	VAL	ALA	engineered mutation	UNP P00693
A	378	PRO	SER	engineered mutation	UNP P00693
B	284	VAL	ALA	engineered mutation	UNP P00693
B	378	PRO	SER	engineered mutation	UNP P00693
C	284	VAL	ALA	engineered mutation	UNP P00693
C	378	PRO	SER	engineered mutation	UNP P00693

- Molecule 2 is an oligosaccharide called 4,6-dideoxy-4-[[[(1S,4R,5S,6S)-4,5,6-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	3	Total	C	N	O	0	0	0
			44	25	1	18			

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	Ca	0	0
			4	4		
3	B	4	Total	Ca	0	0
			4	4		

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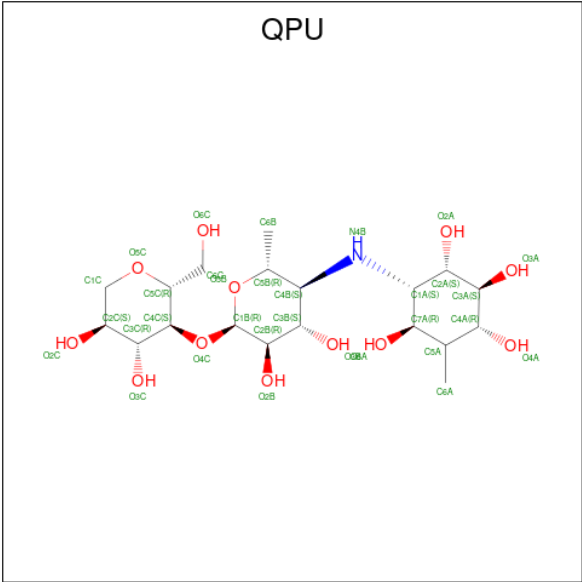
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	4	Total	Ca	0	0
			4	4		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



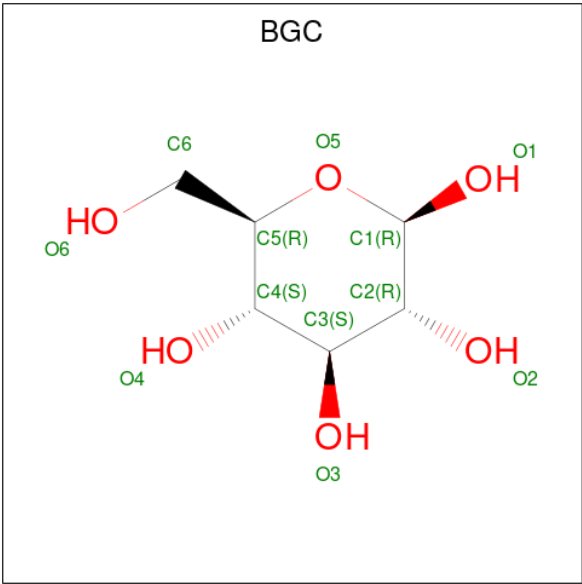
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is 1,5-anhydro-4-O-(4,6-dideoxy-4-[[[(1S,2S,3S,4R,5S,6R)-2,3,4,6-tetrahydroxy-5-methylcyclohexyl]amino}-alpha-D-glucopyranosyl)-D-glucitol (CCD ID: QPU) (formula: $C_{19}H_{35}NO_{12}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			32	19	1	12		
5	A	1	Total	C	N	O	0	0
			32	19	1	12		
5	B	1	Total	C	N	O	0	0
			32	19	1	12		
5	C	1	Total	C	N	O	0	0
			32	19	1	12		

- Molecule 6 is beta-D-glucopyranose (CCD ID: BGC) (formula: C₆H₁₂O₆).



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

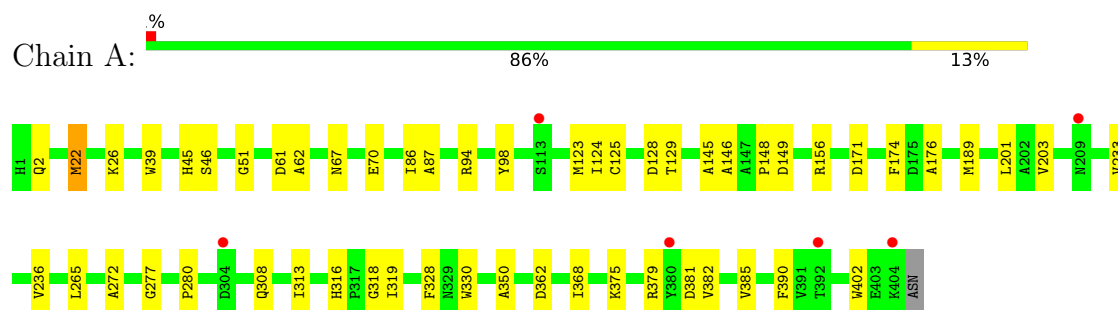
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	604	Total	O	0	0
			604	604		
7	B	526	Total	O	0	0
			526	526		
7	C	596	Total	O	0	0
			596	596		

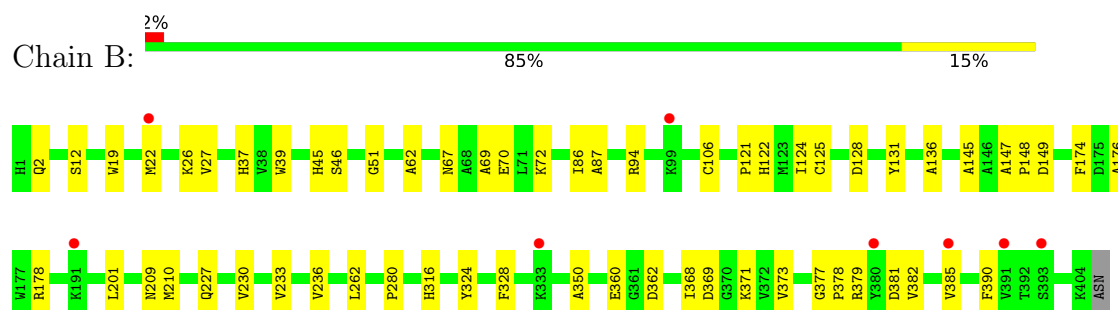
3 Residue-property plots

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.

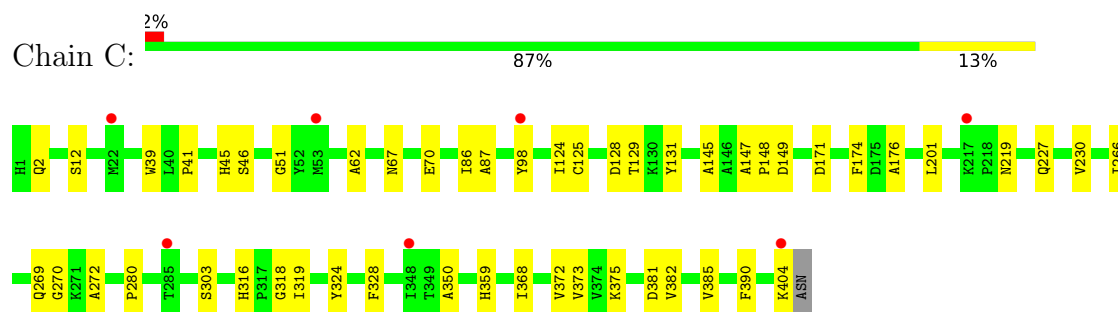
- Molecule 1: Alpha-amylase type A isozyme



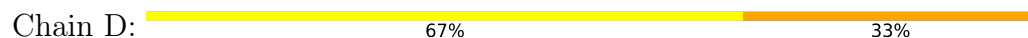
- Molecule 1: Alpha-amylase type A isozyme



- Molecule 1: Alpha-amylase type A isozyme



- Molecule 2: 4,6-dideoxy-4-[(1S,4R,5S,6S)-4,5,6-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-beta-D-glucopyranose





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	218.93Å 89.65Å 62.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.26 – 1.70 46.26 – 1.70	Depositor EDS
% Data completeness (in resolution range)	98.9 (46.26-1.70) 99.0 (46.26-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.15 (at 1.70Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.178 , 0.209 0.175 , 0.206	Depositor DCC
R_{free} test set	6781 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	11.7	Xtriage
Anisotropy	0.121	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 49.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11424	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.21% 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: QPU, GLC, CA, EDO, BGC, AC1

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	0.34	0/3241	0.90	12/4410 (0.3%)
1	B	0.34	0/3267	0.89	10/4442 (0.2%)
1	C	0.35	0/3267	0.90	13/4444 (0.3%)
All	All	0.34	0/9775	0.89	35/13296 (0.3%)

There are no bond length outliers.

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	128	ASP	N-CA-C	-7.62	98.97	109.71
1	A	316	HIS	N-CA-C	7.59	118.86	110.13
1	B	316	HIS	N-CA-C	7.49	118.74	110.13
1	C	316	HIS	N-CA-C	7.12	118.32	110.13
1	C	128	ASP	N-CA-C	-6.57	99.76	109.62
1	A	145	ALA	N-CA-C	6.54	119.24	111.33
1	B	128	ASP	N-CA-C	-6.40	100.02	109.62
1	C	145	ALA	N-CA-C	6.39	119.06	111.33
1	C	318	GLY	N-CA-C	-6.34	103.42	112.81
1	B	145	ALA	N-CA-C	6.24	118.88	111.71
1	C	381	ASP	N-CA-C	6.09	118.10	108.67
1	C	303	SER	N-CA-C	5.99	118.60	111.71
1	B	381	ASP	N-CA-C	5.94	118.41	108.73
1	A	98	TYR	N-CA-C	5.83	119.06	109.85
1	A	381	ASP	N-CA-C	5.83	118.22	108.96
1	B	147	ALA	N-CA-C	5.82	113.45	108.22
1	C	12	SER	N-CA-C	5.77	118.31	111.33
1	C	328	PHE	N-CA-C	5.72	120.39	113.41
1	A	129	THR	N-CA-C	5.71	119.76	112.34
1	C	41	PRO	N-CA-C	5.62	117.56	110.70
1	A	330	TRP	N-CA-C	-5.59	103.53	110.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	377	GLY	CA-C-N	5.58	125.11	119.19
1	B	377	GLY	C-N-CA	5.58	125.11	119.19
1	B	12	SER	N-CA-C	5.57	118.07	111.33
1	A	318	GLY	N-CA-C	-5.54	103.41	112.83
1	C	147	ALA	N-CA-C	5.37	113.05	108.22
1	C	129	THR	N-CA-C	5.34	118.90	112.38
1	B	27	VAL	N-CA-C	5.34	115.54	110.42
1	A	265	LEU	N-CA-C	5.26	119.26	113.21
1	C	98	TYR	N-CA-C	5.24	118.13	109.85
1	A	146	ALA	N-CA-C	5.13	119.16	113.01
1	A	313	ILE	N-CA-C	5.07	117.39	111.05
1	B	178	ARG	N-CA-C	-5.07	99.00	108.02
1	A	308	GLN	N-CA-C	-5.07	105.84	111.36
1	C	272	ALA	N-CA-C	-5.00	103.29	109.64

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	3148	0	2999	27	0
1	B	3174	0	3033	33	0
1	C	3172	0	3033	26	0
2	D	44	0	30	1	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0
3	C	4	0	0	0	0
4	A	4	0	6	0	0
4	B	4	0	4	0	0
5	A	64	0	68	0	0
5	B	32	0	34	2	0
5	C	32	0	34	1	0
6	C	12	0	12	0	0
7	A	604	0	0	0	0
7	B	526	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	C	596	0	0	3	0
All	All	11424	0	9253	88	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 (88) 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:B:106:CYS:SG	1:B:121:PRO:HG3	2.15	0.86
1:C:382:VAL:O	1:C:385:VAL:HG12	1.84	0.78
1:A:2:GLN:NE2	1:A:319:ILE:HD13	1.98	0.77
1:C:2:GLN:NE2	1:C:319:ILE:HD13	2.09	0.68
1:C:368:ILE:HB	1:C:372:VAL:CG1	2.30	0.62
1:A:382:VAL:O	1:A:385:VAL:HG12	2.00	0.61
1:C:269:GLN:HG3	7:C:4640:HOH:O	1.99	0.61
5:C:3000:QPU:H7A	5:C:3000:QPU:H6BB	1.84	0.60
1:C:45:HIS:HB2	1:C:62:ALA:HB3	1.84	0.59
1:B:209:ASN:HD22	1:B:210:MET:H	1.48	0.59
1:A:368:ILE:HD12	1:A:368:ILE:N	2.18	0.58
1:A:233:VAL:O	1:A:236:VAL:HG12	2.04	0.58
1:C:368:ILE:HB	1:C:372:VAL:HG13	1.85	0.58
1:B:209:ASN:HD22	1:B:210:MET:N	2.02	0.58
1:B:2:GLN:HE21	1:B:37:HIS:CE1	2.22	0.57
1:B:67:ASN:OD1	1:B:70:GLU:HG3	2.05	0.56
1:B:362:ASP:OD2	1:B:379:ARG:HB2	2.04	0.56
1:B:368:ILE:HD12	1:B:368:ILE:N	2.24	0.53
1:C:87:ALA:HB2	1:C:174:PHE:CD1	2.44	0.52
1:B:201:LEU:C	1:B:201:LEU:HD12	2.35	0.52
1:A:46:SER:CB	1:A:51:GLY:HA2	2.39	0.52
1:B:382:VAL:O	1:B:385:VAL:HG12	2.10	0.51
1:A:45:HIS:HB2	1:A:62:ALA:HB3	1.91	0.51
1:B:45:HIS:HB2	1:B:62:ALA:HB3	1.93	0.51
1:B:233:VAL:O	1:B:236:VAL:HG12	2.11	0.50
1:B:362:ASP:HB2	1:B:378:PRO:HG2	1.93	0.50
1:C:219:ASN:HB3	7:C:4241:HOH:O	2.12	0.50
1:B:369:ASP:O	1:B:371:LYS:HG3	2.12	0.49
1:A:201:LEU:HD12	1:A:201:LEU:C	2.37	0.49
1:A:67:ASN:OD1	1:A:70:GLU:HG3	2.12	0.49
1:B:94:ARG:O	1:B:148:PRO:HD2	2.13	0.48
1:B:230:VAL:HG11	5:B:4000:QPU:H1B	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:280:PRO:HB2	1:C:350:ALA:O	2.12	0.48
1:A:189:MET:HA	1:A:189:MET:HE2	1.96	0.48
1:A:2:GLN:HE21	1:A:319:ILE:HD13	1.75	0.48
1:B:87:ALA:HB2	1:B:174:PHE:CD1	2.49	0.48
1:A:123:MET:CE	1:A:156:ARG:HD3	2.43	0.48
1:A:176:ALA:HB1	1:A:201:LEU:O	2.14	0.48
1:B:373:VAL:HG23	1:B:390:PHE:CE2	2.49	0.48
1:C:67:ASN:OD1	1:C:70:GLU:HG3	2.15	0.47
1:A:61:ASP:OD1	1:A:67:ASN:HB2	2.15	0.47
1:C:266:ILE:HD11	1:C:270:GLY:HA2	1.97	0.47
1:A:362:ASP:OD2	1:A:379:ARG:HB2	2.15	0.46
1:C:39:TRP:HA	1:C:86:ILE:HB	1.97	0.46
1:A:375:LYS:HD3	1:A:375:LYS:C	2.41	0.46
1:C:131:TYR:CG	1:C:148:PRO:HG3	2.51	0.46
1:B:280:PRO:HB2	1:B:350:ALA:O	2.16	0.46
1:B:19:TRP:CH2	1:B:22[B]:MET:HE1	2.51	0.45
1:B:86:ILE:HG12	1:B:176:ALA:HB3	1.98	0.45
1:C:368:ILE:N	1:C:368:ILE:HD12	2.31	0.45
1:C:46:SER:CB	1:C:51:GLY:HA2	2.46	0.45
1:C:176:ALA:HB1	1:C:201:LEU:O	2.17	0.45
1:A:87:ALA:HB2	1:A:174:PHE:CD1	2.52	0.44
1:A:22:MET:HE2	1:A:22:MET:C	2.42	0.44
1:A:280:PRO:HB2	1:A:350:ALA:O	2.17	0.44
1:A:375:LYS:HG3	1:A:382:VAL:HG21	1.98	0.44
1:B:209:ASN:ND2	1:B:210:MET:N	2.64	0.44
1:C:201:LEU:C	1:C:201:LEU:HD12	2.42	0.44
1:C:227:GLN:HA	1:C:230:VAL:HG22	2.00	0.43
1:A:86:ILE:HG12	1:A:176:ALA:HB3	2.00	0.43
1:B:26:LYS:HD2	1:B:328:PHE:CE1	2.54	0.43
1:C:359:HIS:HE1	7:C:4583:HOH:O	2.01	0.43
1:C:375:LYS:HG3	1:C:382:VAL:HG21	2.00	0.43
1:A:26:LYS:HD2	1:A:328:PHE:CE1	2.54	0.43
1:B:26:LYS:HD2	1:B:328:PHE:CZ	2.53	0.43
1:B:124:ILE:O	1:B:125:CYS:C	2.61	0.43
1:C:124:ILE:O	1:C:125:CYS:C	2.62	0.43
1:A:390:PHE:HB3	1:A:402:TRP:HB3	2.00	0.43
1:C:373:VAL:HG23	1:C:390:PHE:CE2	2.54	0.42
1:B:227:GLN:HE22	5:B:4000:QPU:C2C	2.33	0.42
1:B:324:TYR:CD1	1:B:324:TYR:C	2.97	0.42
1:B:69:ALA:HA	1:B:72:LYS:NZ	2.34	0.42
2:D:1:BGC:H6C2	2:D:2:GLC:H5	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:375:LYS:C	1:C:375:LYS:HD3	2.45	0.42
1:A:203:VAL:HG13	1:A:203:VAL:O	2.20	0.42
1:B:131:TYR:CG	1:B:148:PRO:HG3	2.54	0.42
1:B:122:HIS:O	1:B:136:ALA:HB2	2.20	0.41
1:C:390:PHE:CE2	1:C:404:LYS:HB2	2.55	0.41
1:A:94:ARG:O	1:A:148:PRO:HD2	2.21	0.41
1:A:272:ALA:O	1:A:277:GLY:HA3	2.20	0.41
1:B:39:TRP:HA	1:B:86:ILE:HB	2.02	0.41
1:A:39:TRP:HA	1:A:86:ILE:HB	2.03	0.41
1:B:176:ALA:HB1	1:B:201:LEU:O	2.21	0.41
1:B:46:SER:CB	1:B:51:GLY:HA2	2.51	0.41
1:B:262:LEU:HB2	1:B:360:GLU:O	2.21	0.41
1:C:324:TYR:CD1	1:C:324:TYR:C	2.99	0.40
1:A:124:ILE:O	1:A:125:CYS:C	2.64	0.40
1:C:87:ALA:HB2	1:C:174:PHE:CG	2.57	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	403/405 (100%)	390 (97%)	13 (3%)	0	100	100
1	B	406/405 (100%)	391 (96%)	15 (4%)	0	100	100
1	C	406/405 (100%)	394 (97%)	12 (3%)	0	100	100
All	All	1215/1215 (100%)	1175 (97%)	40 (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	319/319 (100%)	316 (99%)	3 (1%)	70	62
1	B	322/319 (101%)	321 (100%)	1 (0%)	86	83
1	C	322/319 (101%)	320 (99%)	2 (1%)	78	72
All	All	963/957 (101%)	957 (99%)	6 (1%)	78	72

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

Mol	Chain	Res	Type
1	A	22	MET
1	A	149	ASP
1	A	171	ASP
1	B	149	ASP
1	C	149	ASP
1	C	171	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	15	GLN
1	A	21	ASN
1	A	84	GLN
1	A	228	ASN
1	A	329	ASN
1	A	397	ASN
1	B	2	GLN
1	B	6	GLN
1	B	15	GLN
1	B	209	ASN
1	B	227	GLN
1	B	228	ASN
1	B	231	ASN
1	B	329	ASN

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Mol	Chain	Res	Type
1	C	2	GLN
1	C	6	GLN
1	C	15	GLN
1	C	219	ASN
1	C	227	GLN
1	C	228	ASN
1	C	269	GLN
1	C	308	GLN
1	C	329	ASN
1	C	359	HIS
1	C	397	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 ⓘ

3 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	BGC	D	1	2	12,12,12	0.93	0	17,17,17	0.49	0
2	GLC	D	2	2	11,11,12	1.25	2 (18%)	15,15,17	0.63	0
2	AC1	D	3	2	21,22,23	3.72	3 (14%)	22,32,34	0.83	1 (4%)

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	BGC	D	1	2	-	0/2/22/22	0/1/1/1
2	GLC	D	2	2	-	0/2/19/22	0/1/1/1
2	AC1	D	3	2	-	3/6/43/46	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	3	AC1	C7B-C5B	15.64	1.54	1.32
2	D	3	AC1	C4A-C5B	4.43	1.55	1.51
2	D	3	AC1	C1B-C7B	3.66	1.55	1.50
2	D	2	GLC	C4-C5	2.22	1.57	1.53
2	D	2	GLC	O5-C5	2.09	1.47	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	3	AC1	C3B-C4A-C5B	-2.09	108.38	111.67

There are no chirality outliers.

All (3) torsion outliers are listed below:

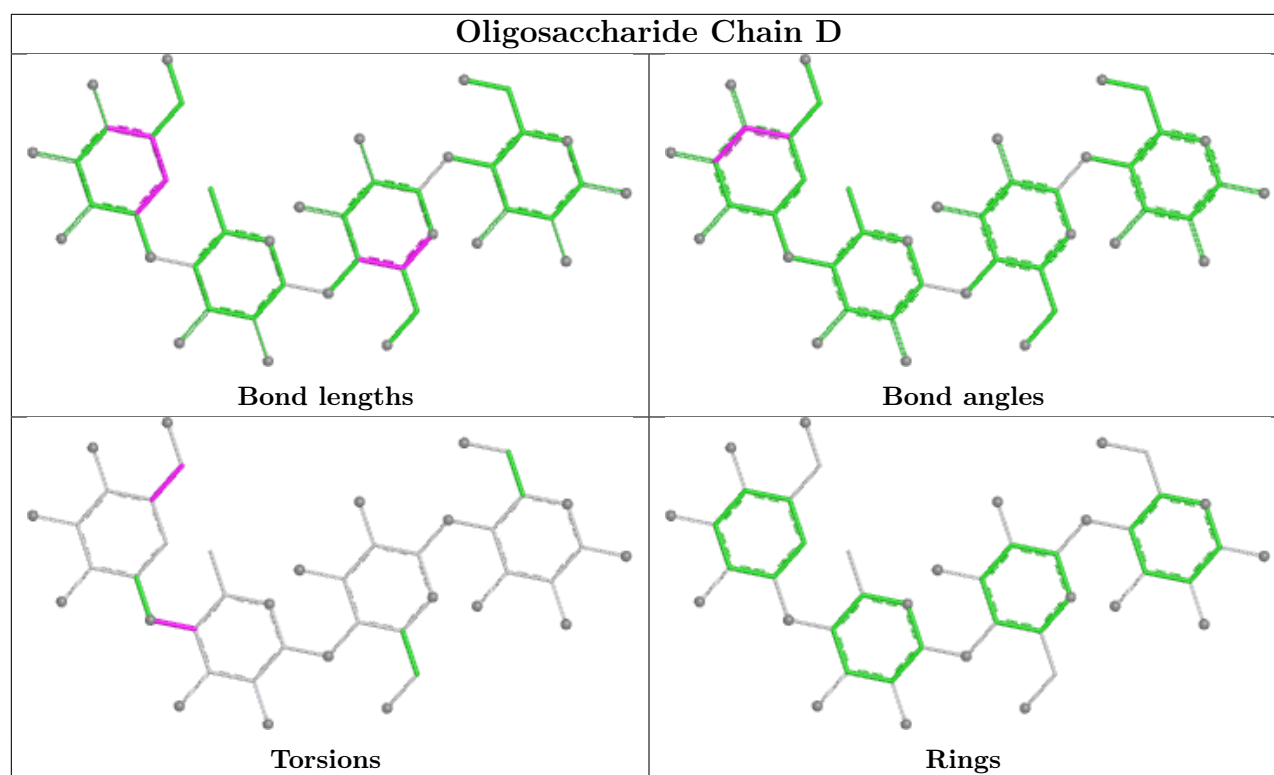
Mol	Chain	Res	Type	Atoms
2	D	3	AC1	C3-C4-N4A-C1B
2	D	3	AC1	C4A-C5B-C6B-O6B
2	D	3	AC1	C7B-C5B-C6B-O6B

There are no ring outliers.

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1	BGC	1	0
2	D	2	GLC	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 19 ligands modelled in this entry, 12 are monoatomic - leaving 7 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$
4	EDO	B	2001	3	3,3,3	2.24	2 (66%)	2,2,2	0.43	0
5	QPU	A	4000	-	32,34,34	0.85	1 (3%)	48,51,51	1.73	4 (8%)
5	QPU	C	3000	-	32,34,34	0.86	1 (3%)	48,51,51	1.68	4 (8%)
6	BGC	C	4000	-	12,12,12	0.34	0	17,17,17	0.40	0
5	QPU	A	3000	-	32,34,34	0.86	1 (3%)	48,51,51	1.71	5 (10%)
4	EDO	A	2000	-	3,3,3	2.22	2 (66%)	2,2,2	0.46	0
5	QPU	B	4000	-	32,34,34	0.96	1 (3%)	48,51,51	1.69	4 (8%)

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	QPU	C	3000	-	1/1/15/16	3/10/71/71	0/3/3/3
5	QPU	A	4000	-	1/1/15/16	4/10/71/71	0/3/3/3
4	EDO	B	2001	3	-	0/1/1/1	-
6	BGC	C	4000	-	-	0/2/22/22	0/1/1/1
5	QPU	A	3000	-	1/1/15/16	6/10/71/71	0/3/3/3
4	EDO	A	2000	-	-	1/1/1/1	-
5	QPU	B	4000	-	1/1/15/16	4/10/71/71	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	2001	EDO	O2-C2	2.99	1.57	1.42
4	A	2000	EDO	O2-C2	2.96	1.57	1.42
5	B	4000	QPU	O5C-C5C	2.37	1.48	1.43
4	A	2000	EDO	O1-C1	2.35	1.54	1.42
4	B	2001	EDO	O1-C1	2.35	1.54	1.42
5	A	4000	QPU	O5C-C5C	2.20	1.47	1.43
5	A	3000	QPU	O5C-C5C	2.06	1.47	1.43
5	C	3000	QPU	O5C-C5C	2.05	1.47	1.43

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	4000	QPU	C7A-C5A-C4A	6.89	120.99	109.23
5	A	3000	QPU	C7A-C5A-C4A	6.82	120.87	109.23
5	A	4000	QPU	C7A-C5A-C4A	6.80	120.84	109.23
5	C	3000	QPU	C7A-C5A-C4A	6.63	120.56	109.23
5	C	3000	QPU	C6A-C5A-C4A	5.64	119.93	112.13
5	A	4000	QPU	C6A-C5A-C4A	5.62	119.90	112.13
5	A	3000	QPU	C6A-C5A-C4A	5.53	119.78	112.13
5	B	4000	QPU	C6A-C5A-C4A	5.43	119.63	112.13
5	C	3000	QPU	C6A-C5A-C7A	5.34	119.51	112.13
5	B	4000	QPU	C6A-C5A-C7A	5.25	119.38	112.13
5	A	3000	QPU	C6A-C5A-C7A	5.22	119.35	112.13
5	A	4000	QPU	C6A-C5A-C7A	5.16	119.25	112.13
5	A	4000	QPU	C1A-N4B-C4B	-3.94	109.44	116.38
5	A	3000	QPU	C1A-N4B-C4B	-3.70	109.86	116.38
5	C	3000	QPU	C1A-N4B-C4B	-2.78	111.48	116.38
5	B	4000	QPU	C1A-N4B-C4B	-2.75	111.53	116.38
5	A	3000	QPU	C4A-C3A-C2A	-2.02	107.29	110.83

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	3000	QPU	C5A
5	A	4000	QPU	C5A
5	B	4000	QPU	C5A
5	C	3000	QPU	C5A

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	3000	QPU	C3B-C4B-N4B-C1A
5	C	3000	QPU	C5B-C4B-N4B-C1A
5	A	3000	QPU	C4C-C5C-C6C-O6C
5	A	3000	QPU	O5C-C5C-C6C-O6C
5	A	4000	QPU	O5C-C5C-C6C-O6C
5	A	4000	QPU	C4C-C5C-C6C-O6C
5	B	4000	QPU	C4C-C5C-C6C-O6C
5	A	3000	QPU	C2A-C1A-N4B-C4B
5	A	3000	QPU	C5B-C4B-N4B-C1A
5	A	4000	QPU	C3B-C4B-N4B-C1A
5	B	4000	QPU	C3B-C4B-N4B-C1A
5	A	3000	QPU	O5B-C1B-O4C-C4C
5	A	3000	QPU	C2B-C1B-O4C-C4C
5	C	3000	QPU	C4C-C5C-C6C-O6C
5	B	4000	QPU	O5C-C5C-C6C-O6C
4	A	2000	EDO	O1-C1-C2-O2
5	A	4000	QPU	C7A-C1A-N4B-C4B
5	B	4000	QPU	C7A-C1A-N4B-C4B

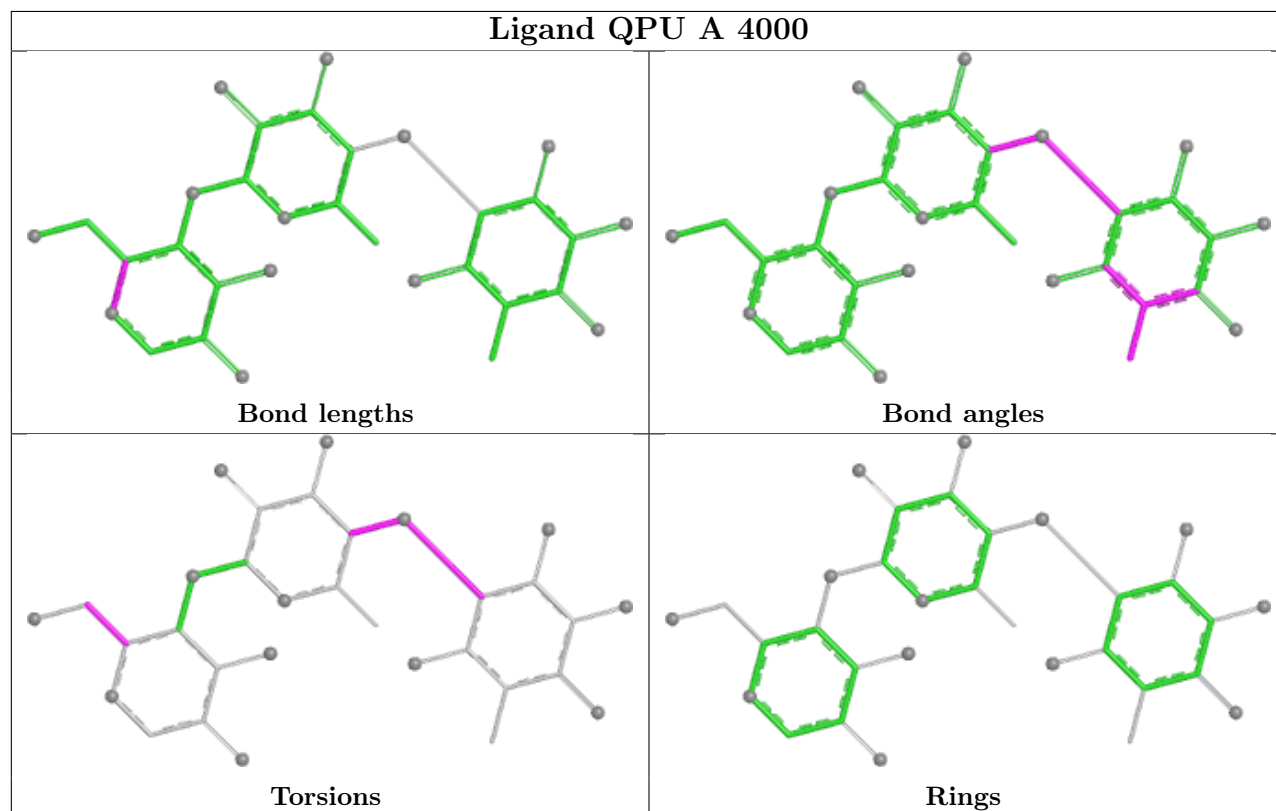
There are no ring outliers.

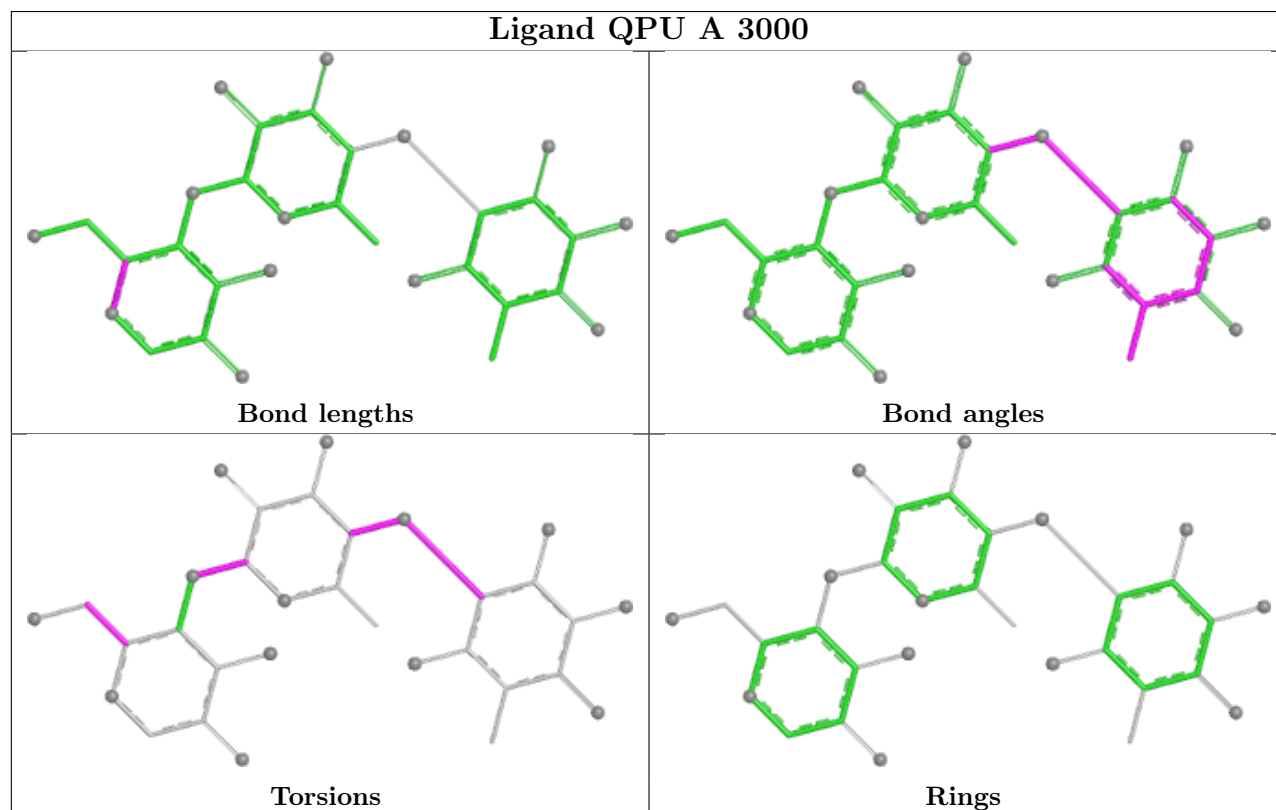
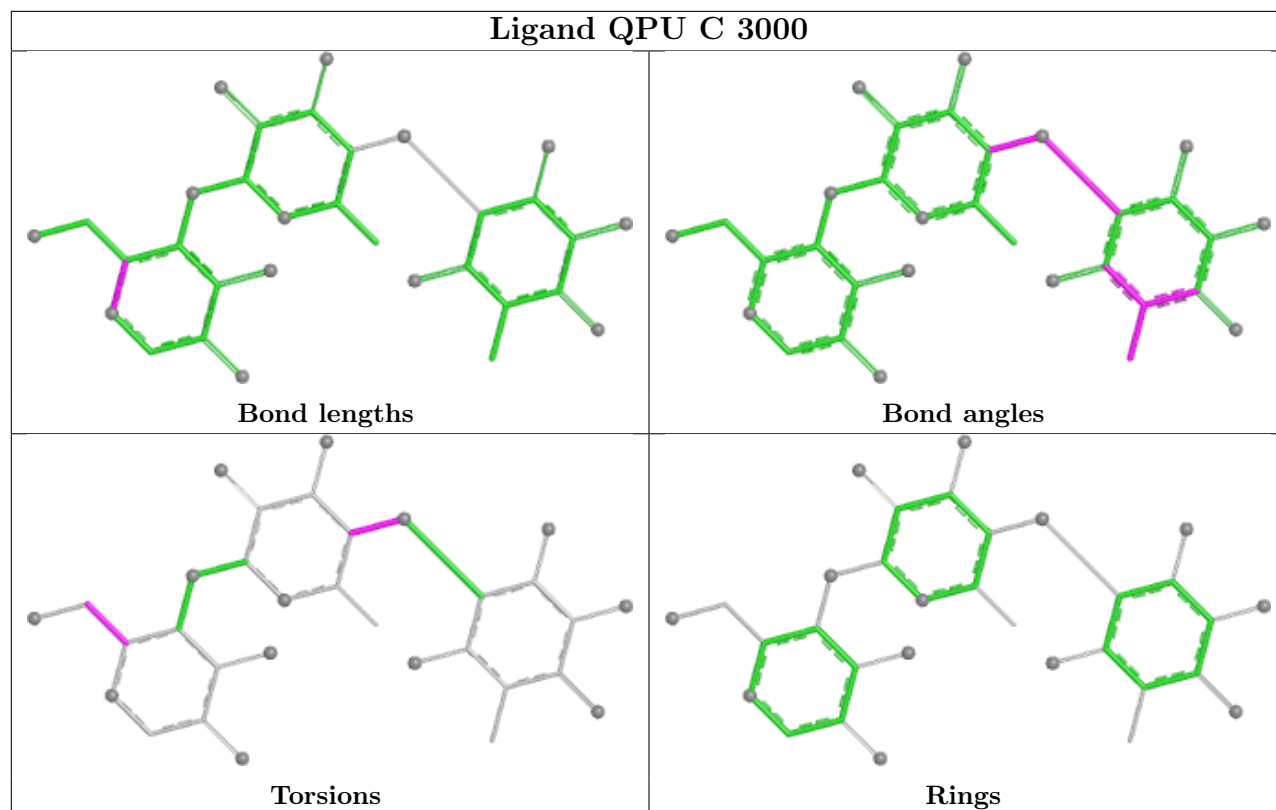
2 monomers are involved in 3 short contacts:

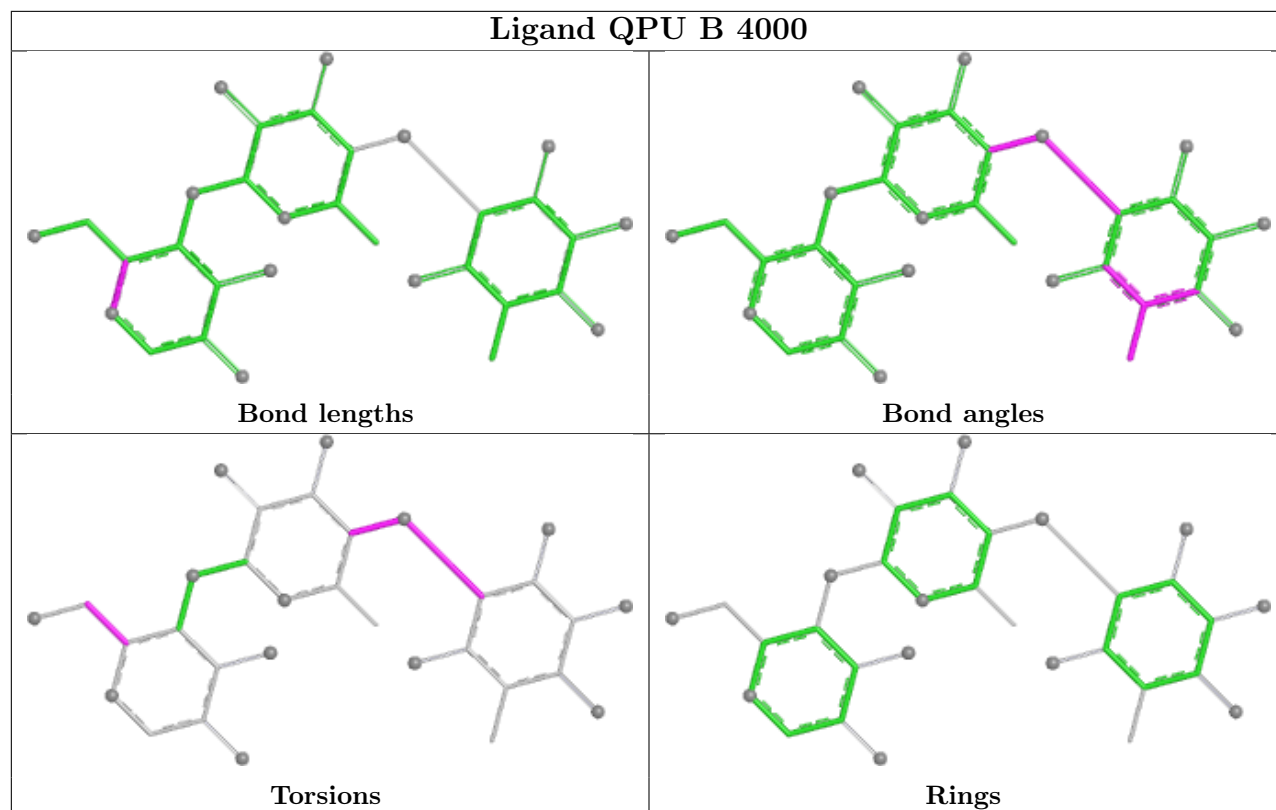
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	3000	QPU	1	0
5	B	4000	QPU	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







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	404/405 (99%)	-0.12	6 (1%) 72 76	7, 12, 21, 30	1 (0%)
1	B	404/405 (99%)	-0.18	8 (1%) 65 69	4, 11, 21, 31	5 (1%)
1	C	404/405 (99%)	-0.21	7 (1%) 69 73	1, 10, 18, 30	5 (1%)
All	All	1212/1215 (99%)	-0.17	21 (1%) 69 73	1, 11, 20, 31	11 (0%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	22[A]	MET	6.5
1	C	53[A]	MET	6.4
1	C	348[A]	ILE	5.8
1	C	285	THR	4.8
1	C	217[A]	LYS	4.1
1	B	191	LYS	4.1
1	B	333[A]	LYS	3.7
1	C	98	TYR	3.4
1	B	22[A]	MET	3.4
1	B	380	TYR	3.3
1	A	392[A]	THR	2.9
1	B	391[A]	VAL	2.7
1	B	385	VAL	2.5
1	C	404	LYS	2.3
1	A	380	TYR	2.3
1	A	113	SER	2.3
1	B	99[A]	LYS	2.2
1	A	209	ASN	2.2
1	A	404	LYS	2.1
1	A	304	ASP	2.1
1	B	393	SER	2.0

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

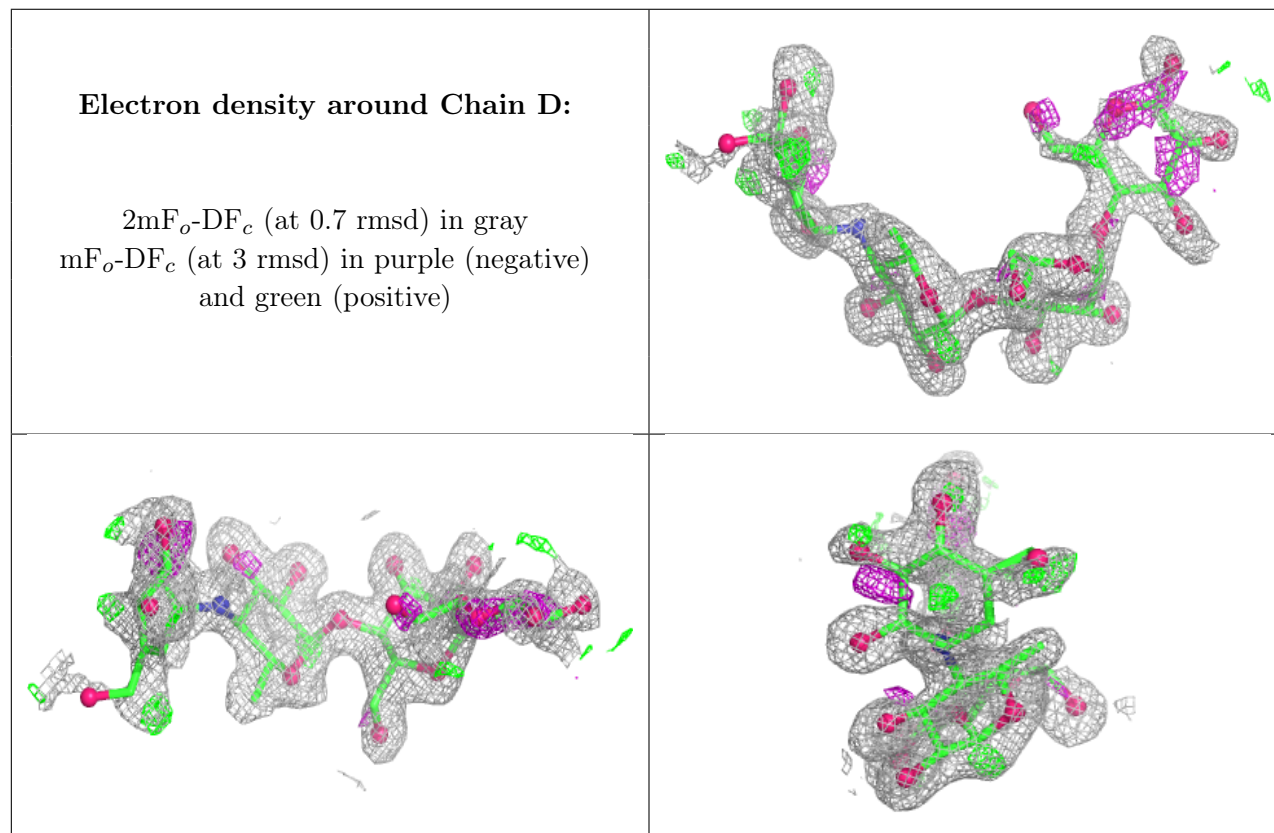
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	BGC	D	1	12/12	0.69	0.16	29,32,34,34	0
2	AC1	D	3	21/22	0.77	0.16	22,31,41,45	0
2	GLC	D	2	11/12	0.84	0.11	23,25,27,27	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

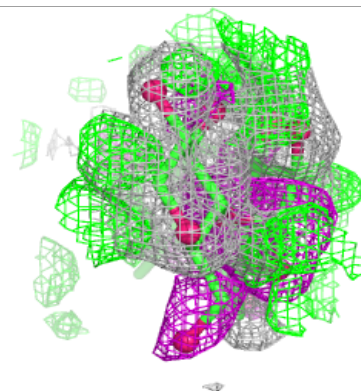
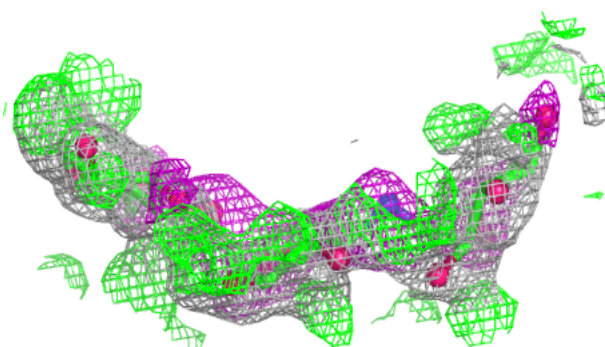
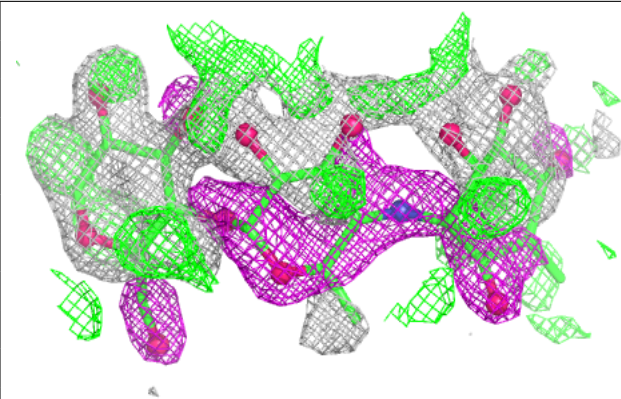
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	QPU	A	3000	32/32	0.41	0.23	26,29,32,33	0
5	QPU	B	4000	32/32	0.62	0.17	24,29,38,39	0
6	BGC	C	4000	12/12	0.74	0.14	26,28,30,31	0
5	QPU	A	4000	32/32	0.79	0.17	18,25,39,43	0
4	EDO	A	2000	4/4	0.82	0.14	28,29,30,34	0
5	QPU	C	3000	32/32	0.84	0.18	20,28,37,38	0
4	EDO	B	2001	4/4	0.86	0.16	24,26,27,27	0
3	CA	A	501	1/1	0.97	0.03	18,18,18,18	0
3	CA	A	500	1/1	0.99	0.02	10,10,10,10	0
3	CA	A	502	1/1	0.99	0.02	12,12,12,12	0
3	CA	A	503	1/1	0.99	0.15	29,29,29,29	0
3	CA	B	501	1/1	0.99	0.05	16,16,16,16	0
3	CA	B	503	1/1	0.99	0.08	19,19,19,19	0
3	CA	C	501	1/1	0.99	0.04	15,15,15,15	0
3	CA	C	503	1/1	0.99	0.10	23,23,23,23	0
3	CA	B	500	1/1	1.00	0.01	9,9,9,9	0
3	CA	C	500	1/1	1.00	0.01	7,7,7,7	0
3	CA	B	502	1/1	1.00	0.06	13,13,13,13	0
3	CA	C	502	1/1	1.00	0.01	11,11,11,11	0

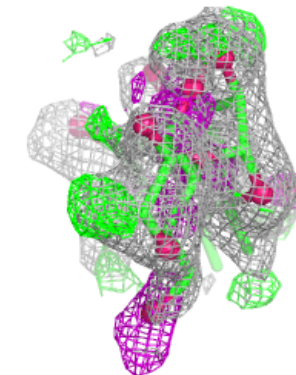
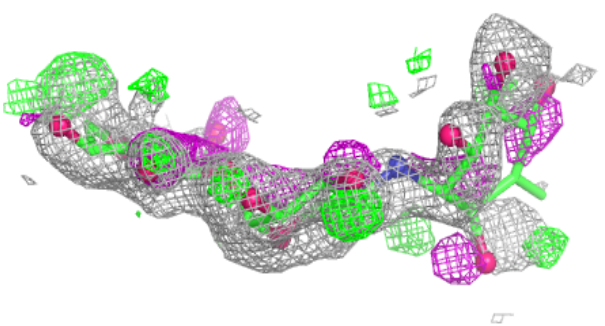
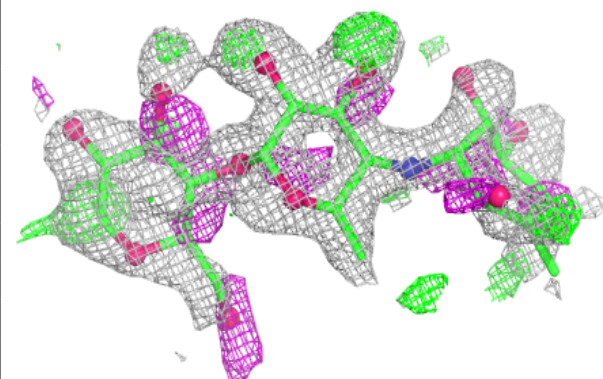
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around QPU A 3000:

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

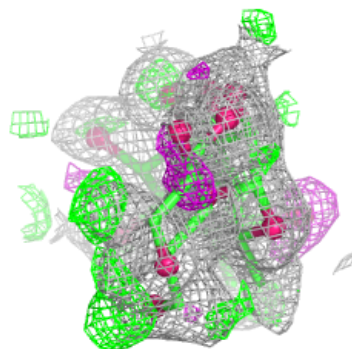
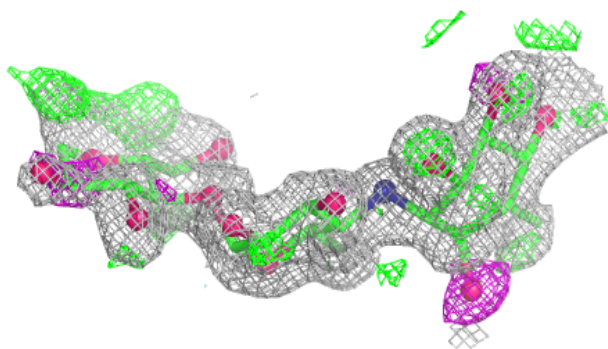
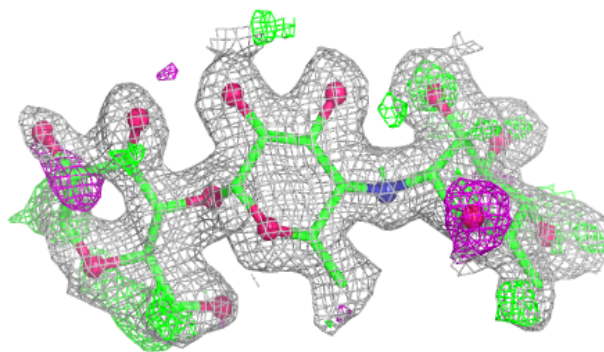
**Electron density around QPU B 4000:**

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

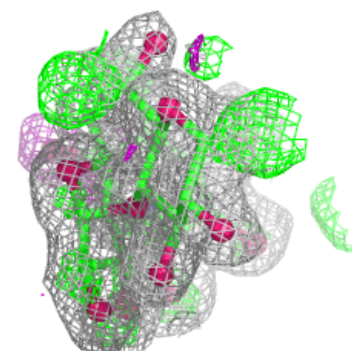
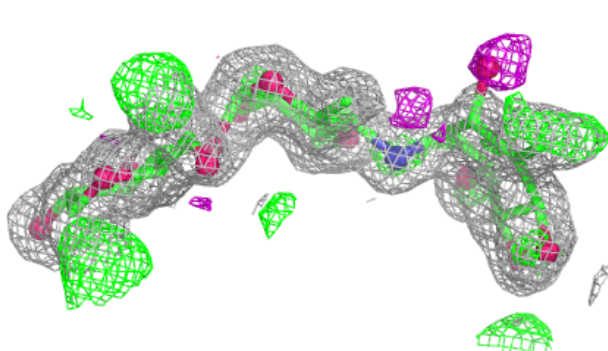
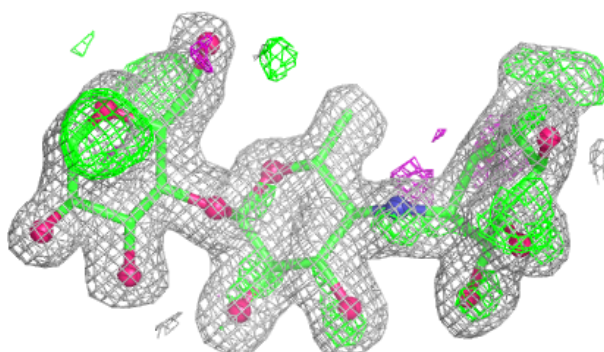


Electron density around QPU A 4000:

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

**Electron density around QPU C 3000:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.