



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:49 AM UTC

PDB ID : 9FYZ / pdb_00009fyz
Title : Crystal structure of SusA amylase from Bacteroides thetaiotaomicron covalently bound to alpha-1,6 branched pseudo-trisaccharide activity-based probe
Authors : Pickles, I.B.; Moroz, O.; Davies, G.
Deposited on : 2024-07-04
Resolution : 2.43 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

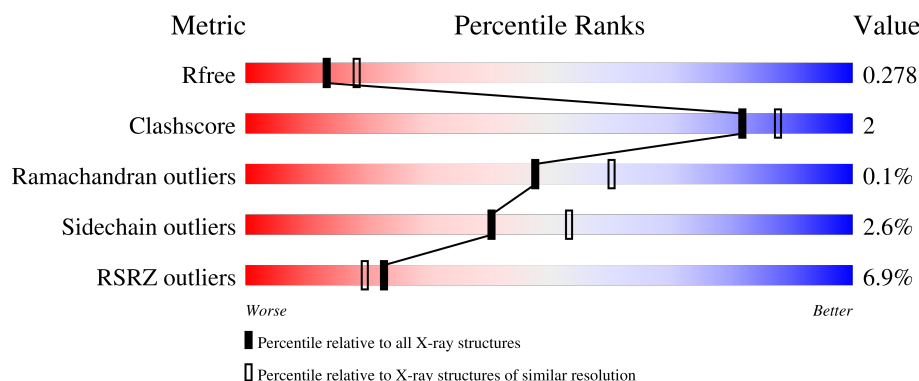
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.43 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	2340 (2.46-2.42)
Clashscore	190562	2400 (2.46-2.42)
Ramachandran outliers	187476	2379 (2.46-2.42)
Sidechain outliers	187428	2379 (2.46-2.42)
RSRZ outliers	180081	2340 (2.46-2.42)

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	610	88% 9% .
1	B	610	4% 87% 9% ..
1	C	610	7% 88% 8% ..
1	D	610	8% 90% 7% ..
1	E	610	7% 89% 7% ..

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Mol	Chain	Length	Quality of chain
1	F	610	15% 87% 9%
2	G	2	100%
2	H	2	100%
2	I	2	100%
2	J	2	100%
2	K	2	100%
2	L	2	50% 50%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 28807 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 Neopullulanase SusA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	594	Total	C	N	O	S	0	0	0
			4797	3060	799	917	21			
1	B	591	Total	C	N	O	S	0	0	0
			4753	3033	793	906	21			
1	C	590	Total	C	N	O	S	0	0	0
			4621	2936	771	893	21			
1	D	594	Total	C	N	O	S	0	0	0
			4624	2942	778	883	21			
1	E	593	Total	C	N	O	S	0	0	0
			4512	2857	767	867	21			
1	F	589	Total	C	N	O	S	0	0	0
			4495	2837	763	874	21			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	8	MET	-	initiating methionine	UNP Q8A1G0
A	9	HIS	-	expression tag	UNP Q8A1G0
A	10	HIS	-	expression tag	UNP Q8A1G0
A	11	HIS	-	expression tag	UNP Q8A1G0
A	12	HIS	-	expression tag	UNP Q8A1G0
A	13	HIS	-	expression tag	UNP Q8A1G0
A	14	HIS	-	expression tag	UNP Q8A1G0
A	15	GLU	-	expression tag	UNP Q8A1G0
A	16	ASN	-	expression tag	UNP Q8A1G0
A	17	LEU	-	expression tag	UNP Q8A1G0
A	18	TYR	-	expression tag	UNP Q8A1G0
A	19	PHE	-	expression tag	UNP Q8A1G0
A	20	GLN	-	expression tag	UNP Q8A1G0
A	21	GLY	-	expression tag	UNP Q8A1G0
B	8	MET	-	initiating methionine	UNP Q8A1G0
B	9	HIS	-	expression tag	UNP Q8A1G0
B	10	HIS	-	expression tag	UNP Q8A1G0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	11	HIS	-	expression tag	UNP Q8A1G0
B	12	HIS	-	expression tag	UNP Q8A1G0
B	13	HIS	-	expression tag	UNP Q8A1G0
B	14	HIS	-	expression tag	UNP Q8A1G0
B	15	GLU	-	expression tag	UNP Q8A1G0
B	16	ASN	-	expression tag	UNP Q8A1G0
B	17	LEU	-	expression tag	UNP Q8A1G0
B	18	TYR	-	expression tag	UNP Q8A1G0
B	19	PHE	-	expression tag	UNP Q8A1G0
B	20	GLN	-	expression tag	UNP Q8A1G0
B	21	GLY	-	expression tag	UNP Q8A1G0
C	8	MET	-	initiating methionine	UNP Q8A1G0
C	9	HIS	-	expression tag	UNP Q8A1G0
C	10	HIS	-	expression tag	UNP Q8A1G0
C	11	HIS	-	expression tag	UNP Q8A1G0
C	12	HIS	-	expression tag	UNP Q8A1G0
C	13	HIS	-	expression tag	UNP Q8A1G0
C	14	HIS	-	expression tag	UNP Q8A1G0
C	15	GLU	-	expression tag	UNP Q8A1G0
C	16	ASN	-	expression tag	UNP Q8A1G0
C	17	LEU	-	expression tag	UNP Q8A1G0
C	18	TYR	-	expression tag	UNP Q8A1G0
C	19	PHE	-	expression tag	UNP Q8A1G0
C	20	GLN	-	expression tag	UNP Q8A1G0
C	21	GLY	-	expression tag	UNP Q8A1G0
D	8	MET	-	initiating methionine	UNP Q8A1G0
D	9	HIS	-	expression tag	UNP Q8A1G0
D	10	HIS	-	expression tag	UNP Q8A1G0
D	11	HIS	-	expression tag	UNP Q8A1G0
D	12	HIS	-	expression tag	UNP Q8A1G0
D	13	HIS	-	expression tag	UNP Q8A1G0
D	14	HIS	-	expression tag	UNP Q8A1G0
D	15	GLU	-	expression tag	UNP Q8A1G0
D	16	ASN	-	expression tag	UNP Q8A1G0
D	17	LEU	-	expression tag	UNP Q8A1G0
D	18	TYR	-	expression tag	UNP Q8A1G0
D	19	PHE	-	expression tag	UNP Q8A1G0
D	20	GLN	-	expression tag	UNP Q8A1G0
D	21	GLY	-	expression tag	UNP Q8A1G0
E	8	MET	-	initiating methionine	UNP Q8A1G0
E	9	HIS	-	expression tag	UNP Q8A1G0
E	10	HIS	-	expression tag	UNP Q8A1G0

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Chain	Residue	Modelled	Actual	Comment	Reference
E	11	HIS	-	expression tag	UNP Q8A1G0
E	12	HIS	-	expression tag	UNP Q8A1G0
E	13	HIS	-	expression tag	UNP Q8A1G0
E	14	HIS	-	expression tag	UNP Q8A1G0
E	15	GLU	-	expression tag	UNP Q8A1G0
E	16	ASN	-	expression tag	UNP Q8A1G0
E	17	LEU	-	expression tag	UNP Q8A1G0
E	18	TYR	-	expression tag	UNP Q8A1G0
E	19	PHE	-	expression tag	UNP Q8A1G0
E	20	GLN	-	expression tag	UNP Q8A1G0
E	21	GLY	-	expression tag	UNP Q8A1G0
F	8	MET	-	initiating methionine	UNP Q8A1G0
F	9	HIS	-	expression tag	UNP Q8A1G0
F	10	HIS	-	expression tag	UNP Q8A1G0
F	11	HIS	-	expression tag	UNP Q8A1G0
F	12	HIS	-	expression tag	UNP Q8A1G0
F	13	HIS	-	expression tag	UNP Q8A1G0
F	14	HIS	-	expression tag	UNP Q8A1G0
F	15	GLU	-	expression tag	UNP Q8A1G0
F	16	ASN	-	expression tag	UNP Q8A1G0
F	17	LEU	-	expression tag	UNP Q8A1G0
F	18	TYR	-	expression tag	UNP Q8A1G0
F	19	PHE	-	expression tag	UNP Q8A1G0
F	20	GLN	-	expression tag	UNP Q8A1G0
F	21	GLY	-	expression tag	UNP Q8A1G0

- Molecule 2 is an oligosaccharide called alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose.



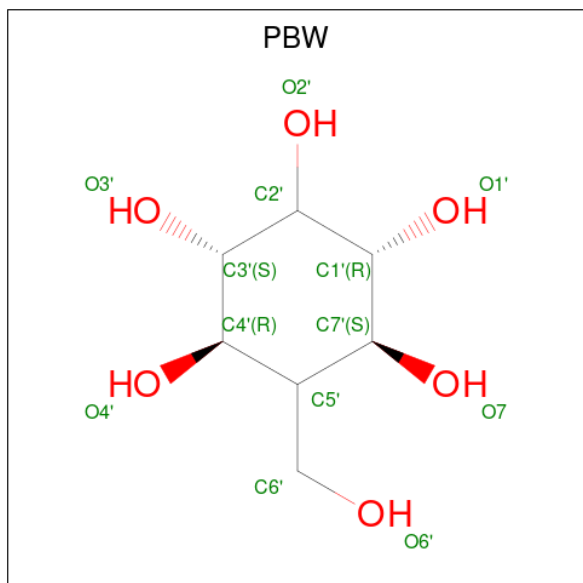
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	G	2	Total	C	O	0	0	0
			22	12	10			
2	H	2	Total	C	O	0	0	0
			22	12	10			
2	I	2	Total	C	O	0	0	0
			22	12	10			
2	J	2	Total	C	O	0	0	0
			22	12	10			

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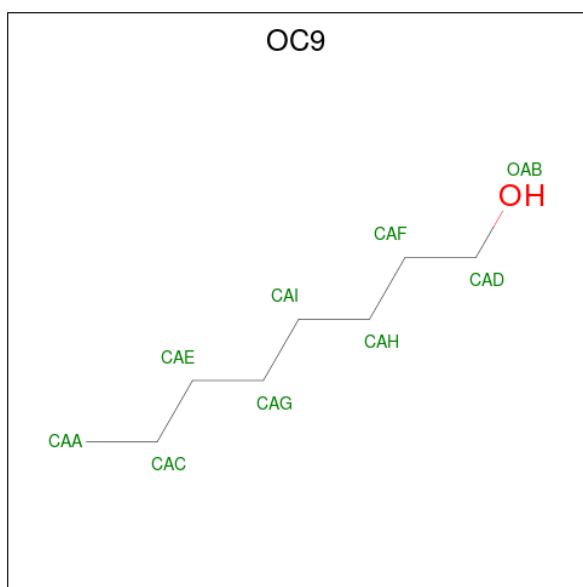
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	K	2	Total	C	O	0	0	0
			22	12	10			
2	L	2	Total	C	O	0	0	0
			22	12	10			

- Molecule 3 is (1 {S},4 {S},5 {R})-6-(hydroxymethyl)cyclohexane-1,2,3,4,5-pentol (CCD ID: PBW) (formula: C₇H₁₄O₆) (labeled as "Ligand of Interest" by depositor).



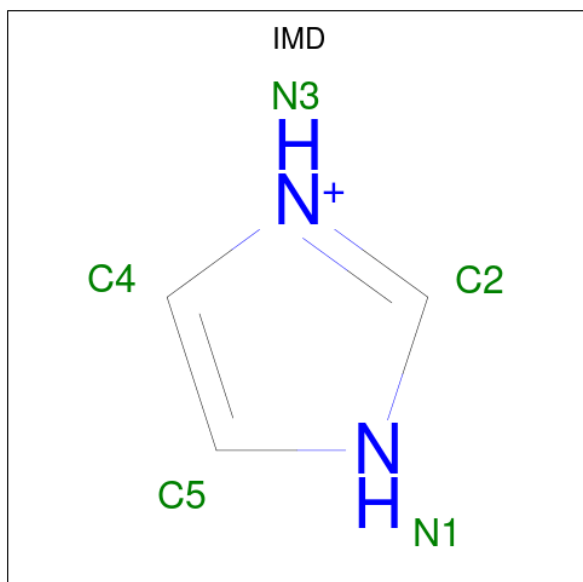
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			12	7	5		
3	B	1	Total	C	O	0	0
			12	7	5		
3	C	1	Total	C	O	0	0
			12	7	5		
3	D	1	Total	C	O	0	0
			12	7	5		
3	E	1	Total	C	O	0	0
			12	7	5		
3	F	1	Total	C	O	0	0
			12	7	5		

- Molecule 4 is OCTAN-1-OL (CCD ID: OC9) (formula: C₈H₁₈O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C 4 4	0	0
4	B	1	Total C 4 4	0	0
4	C	1	Total C 2 2	0	0
4	D	1	Total C 3 3	0	0
4	E	1	Total C 2 2	0	0

- Molecule 5 is IMIDAZOLE (CCD ID: IMD) (formula: $C_3H_5N_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N 5 3 2	0	0
5	A	1	Total C N 5 3 2	0	0
5	A	1	Total C N 5 3 2	0	0
5	B	1	Total C N 5 3 2	0	0
5	C	1	Total C N 5 3 2	0	0
5	C	1	Total C N 5 3 2	0	0
5	C	1	Total C N 5 3 2	0	0
5	D	1	Total C N 5 3 2	0	0
5	D	1	Total C N 5 3 2	0	0
5	D	1	Total C N 5 3 2	0	0
5	E	1	Total C N 5 3 2	0	0
5	F	1	Total C N 5 3 2	0	0

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	2	Total Ca 2 2	0	0
6	B	2	Total Ca 2 2	0	0
6	C	2	Total Ca 2 2	0	0
6	D	2	Total Ca 2 2	0	0
6	E	2	Total Ca 2 2	0	0
6	F	2	Total Ca 2 2	0	0

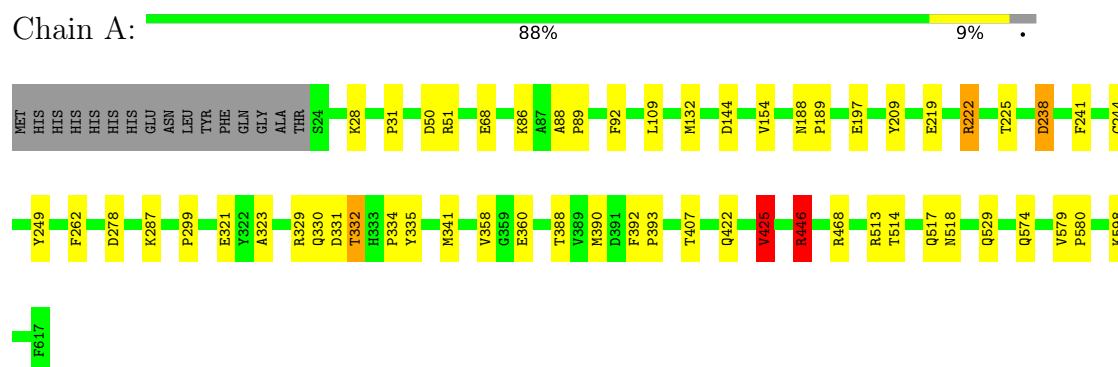
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	295	Total 295	O 295	0	0
7	B	180	Total 180	O 180	0	0
7	C	84	Total 84	O 84	0	0
7	D	68	Total 68	O 68	0	0
7	E	42	Total 42	O 42	0	0
7	F	45	Total 45	O 45	0	0

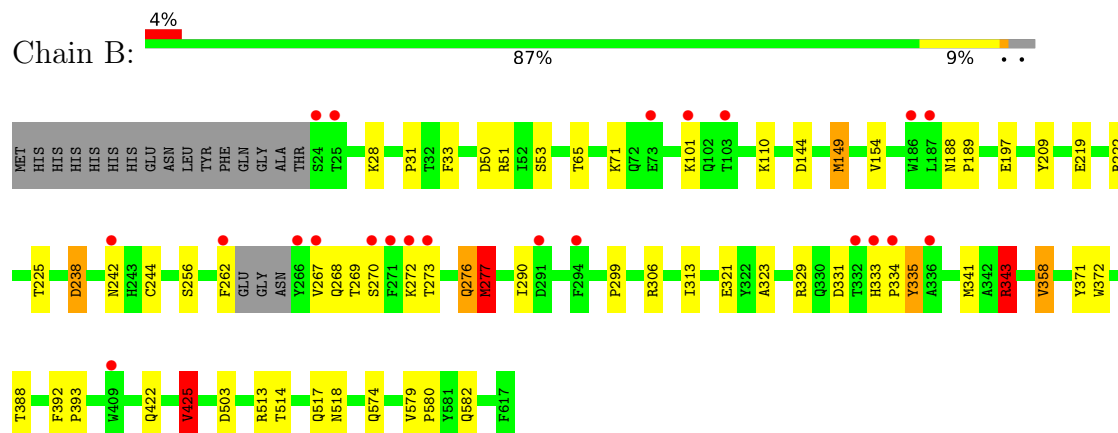
3 Residue-property plots [i](#)

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.

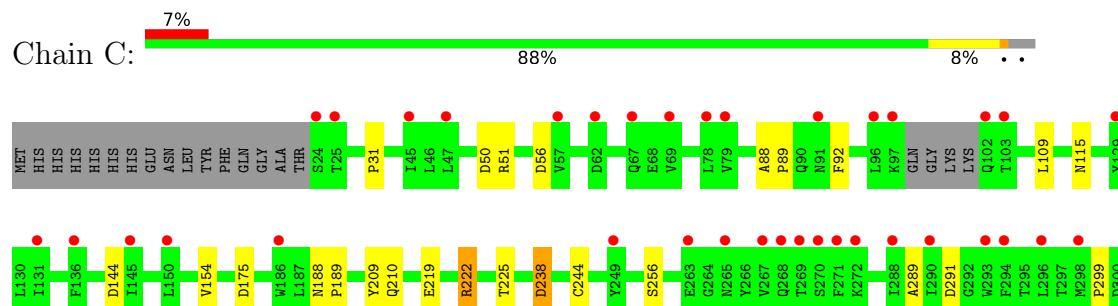
• Molecule 1: Neopullulanase SusA

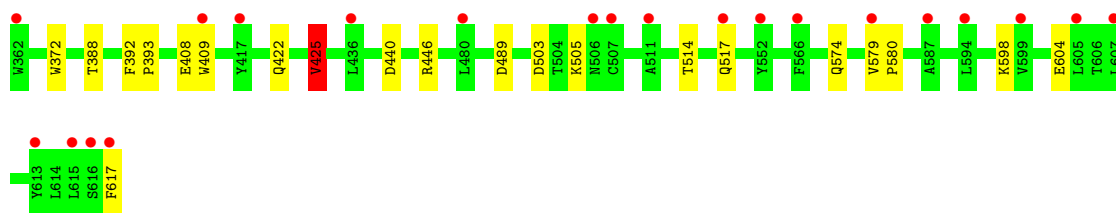


• Molecule 1: Neopullulanase SusA

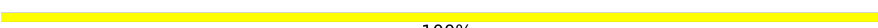


• Molecule 1: Neopullulanase SusA



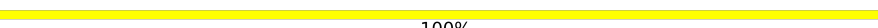


- Molecule 2: alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose

Chain G:  100%

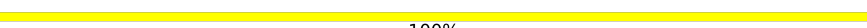
GLC1
GLC2

- Molecule 2: alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose

Chain H:  100%

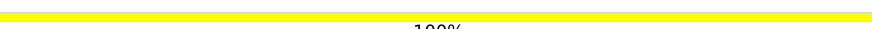
GLC1
GLC2

- Molecule 2: alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose

Chain I:  100%

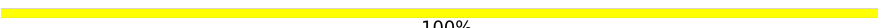
GLC1
GLC2

- Molecule 2: alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose

Chain J:  100%

GLC1
GLC2

- Molecule 2: alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose

Chain K:  100%

GLC1
GLC2

- Molecule 2: alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose

Chain L:  50% 50%

GLC1
GLC2

4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	105.98Å 105.98Å 753.69Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	58.25 – 2.43 58.25 – 2.43	Depositor EDS
% Data completeness (in resolution range)	100.0 (58.25-2.43) 100.0 (58.25-2.43)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 2.42Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.230 , 0.281 0.230 , 0.278	Depositor DCC
R_{free} test set	9306 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	58.0	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 57.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.017 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	28807	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.87% 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: IMD, CA, GLC, OC9, PBW

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	0.69	1/4921 (0.0%)	1.02	7/6683 (0.1%)
1	B	0.63	1/4874 (0.0%)	1.03	10/6619 (0.2%)
1	C	0.56	1/4743 (0.0%)	0.95	6/6464 (0.1%)
1	D	0.54	1/4745 (0.0%)	0.95	6/6469 (0.1%)
1	E	0.53	1/4633 (0.0%)	0.97	8/6330 (0.1%)
1	F	0.54	1/4613 (0.0%)	0.95	10/6297 (0.2%)
All	All	0.59	6/28529 (0.0%)	0.98	47/38862 (0.1%)

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	3
1	B	0	2
1	C	0	4
1	D	0	4
1	E	0	4
1	F	0	2
All	All	0	19

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	331	ASP	CG-OD2	5.75	1.36	1.25
1	A	331	ASP	CG-OD2	5.61	1.36	1.25
1	F	331	ASP	CG-OD2	5.50	1.35	1.25
1	D	331	ASP	CG-OD2	5.43	1.35	1.25
1	E	331	ASP	CG-OD2	5.36	1.35	1.25
1	B	331	ASP	CG-OD2	5.24	1.35	1.25

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	531	ARG	NE-CZ-NH1	-16.74	104.76	121.50
1	B	149	MET	CG-SD-CE	-11.12	76.44	100.90
1	F	68	GLU	N-CA-CB	-7.32	98.03	110.99
1	A	321	GLU	CB-CA-C	-7.13	99.69	110.88
1	C	321	GLU	CB-CA-C	-6.65	100.44	110.88
1	A	68	GLU	N-CA-CB	-6.64	99.24	110.99
1	D	321	GLU	CB-CA-C	-6.61	100.50	110.88
1	E	321	GLU	CB-CA-C	-6.49	100.69	110.88
1	B	321	GLU	CB-CA-C	-6.45	100.76	110.88
1	F	321	GLU	CB-CA-C	-6.45	100.76	110.88
1	E	300	ASP	CA-CB-CG	6.34	118.94	112.60
1	A	278	ASP	CA-CB-CG	6.20	118.80	112.60
1	B	65	THR	CA-CB-OG1	-6.14	100.39	109.60
1	B	321	GLU	N-CA-CB	6.01	118.72	110.01
1	E	531	ARG	NE-CZ-NH2	5.97	124.57	119.20
1	C	321	GLU	N-CA-CB	5.92	118.59	110.01
1	E	278	ASP	CA-CB-CG	5.89	118.49	112.60
1	A	425	VAL	CB-CA-C	-5.87	103.06	112.16
1	B	331	ASP	CB-CG-OD2	-5.85	104.94	118.40
1	D	278	ASP	CA-CB-CG	5.84	118.44	112.60
1	F	425	VAL	CB-CA-C	-5.83	102.82	112.26
1	D	321	GLU	N-CA-CB	5.82	118.45	110.01
1	B	425	VAL	CB-CA-C	-5.76	102.93	112.26
1	A	425	VAL	N-CA-CB	5.75	120.49	110.65
1	F	321	GLU	N-CA-CB	5.64	118.19	110.01
1	E	425	VAL	CB-CA-C	-5.63	103.14	112.26
1	B	503	ASP	CA-CB-CG	5.61	118.21	112.60
1	F	446	ARG	NE-CZ-NH1	-5.57	115.93	121.50
1	C	425	VAL	CB-CA-C	-5.55	103.26	112.26
1	E	321	GLU	N-CA-CB	5.54	118.04	110.01
1	C	577	ASP	CA-CB-CG	5.52	118.12	112.60
1	B	262	PHE	CA-C-O	-5.50	111.45	120.80
1	D	425	VAL	CB-CA-C	-5.47	103.39	112.26
1	A	321	GLU	N-CA-CB	5.47	117.95	110.01
1	F	62	ASP	CA-CB-CG	5.47	118.07	112.60
1	B	277	MET	CG-SD-CE	5.43	112.85	100.90
1	C	503	ASP	CA-CB-CG	5.42	118.02	112.60
1	C	425	VAL	N-CA-CB	5.42	120.57	110.77
1	D	339	ASP	CA-CB-CG	5.41	118.01	112.60
1	B	425	VAL	N-CA-CB	5.39	120.52	110.77
1	F	278	ASP	CA-CB-CG	5.28	117.88	112.60
1	F	503	ASP	CA-CB-CG	5.22	117.82	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	68	GLU	CB-CA-C	5.20	119.22	109.86
1	E	503	ASP	CA-CB-CG	5.17	117.78	112.60
1	D	425	VAL	N-CA-CB	5.10	120.00	110.77
1	F	617	PHE	CA-CB-CG	5.06	118.86	113.80
1	A	241	PHE	CA-CB-CG	5.04	118.84	113.80

There are no chirality outliers.

All (19) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	222	ARG	Sidechain
1	A	446	ARG	Sidechain
1	A	468	ARG	Sidechain
1	B	306	ARG	Sidechain
1	B	343	ARG	Sidechain
1	C	222	ARG	Sidechain
1	C	304	ARG	Sidechain
1	C	329	ARG	Sidechain
1	C	446	ARG	Sidechain
1	D	113	ARG	Sidechain
1	D	222	ARG	Sidechain
1	D	304	ARG	Sidechain
1	D	446	ARG	Sidechain
1	E	222	ARG	Sidechain
1	E	446	ARG	Sidechain
1	E	51	ARG	Sidechain
1	E	531	ARG	Sidechain
1	F	112	ARG	Sidechain
1	F	113	ARG	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	4797	0	4568	25	0
1	B	4753	0	4523	26	0
1	C	4621	0	4192	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	4624	0	4209	19	0
1	E	4512	0	3964	19	0
1	F	4495	0	3917	22	0
2	G	22	0	18	0	0
2	H	22	0	18	0	0
2	I	22	0	18	0	0
2	J	22	0	18	0	0
2	K	22	0	18	0	0
2	L	22	0	19	2	0
3	A	12	0	0	0	0
3	B	12	0	0	0	0
3	C	12	0	0	0	0
3	D	12	0	0	1	0
3	E	12	0	0	0	0
3	F	12	0	0	1	0
4	A	4	0	4	0	0
4	B	4	0	4	0	0
4	C	2	0	0	0	0
4	D	3	0	2	0	0
4	E	2	0	0	0	0
5	A	15	0	15	0	0
5	B	5	0	5	0	0
5	C	15	0	15	3	0
5	D	15	0	15	1	0
5	E	5	0	5	0	0
5	F	5	0	5	0	0
6	A	2	0	0	0	0
6	B	2	0	0	0	0
6	C	2	0	0	0	0
6	D	2	0	0	0	0
6	E	2	0	0	0	0
6	F	2	0	0	0	0
7	A	295	0	0	3	1
7	B	180	0	0	0	0
7	C	84	0	0	1	1
7	D	68	0	0	0	0
7	E	42	0	0	0	0
7	F	45	0	0	2	0
All	All	28807	0	25552	134	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (134) 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:290:ILE:HG12	1:B:335:TYR:CZ	2.38	0.58
1:B:269:THR:HG21	1:B:334:PRO:HB3	1.86	0.57
1:B:276:GLN:HB3	1:B:277:MET:HE3	1.91	0.52
1:C:289:ALA:O	1:C:291:ASP:N	2.34	0.51
1:B:277:MET:HE2	1:B:371:TYR:CD1	2.47	0.50
1:D:440:ASP:OD1	3:D:701:PBW:O3'	2.30	0.49
1:E:509:ASP:O	1:E:511:ALA:O	2.31	0.49
1:E:51:ARG:NH1	1:E:51:ARG:HG3	2.27	0.49
1:C:332:THR:HG22	1:C:335:TYR:CD1	2.48	0.48
1:C:115:ASN:HA	5:C:703:IMD:H5	1.95	0.48
1:A:446:ARG:HG3	7:A:1077:HOH:O	2.14	0.48
1:A:514:THR:OG1	1:A:517:GLN:HG3	2.14	0.48
1:B:313:ILE:HD11	1:B:343:ARG:HD3	1.96	0.48
1:F:332:THR:HG22	1:F:335:TYR:CD1	2.50	0.47
1:A:219:GLU:OE2	1:A:222:ARG:NH1	2.48	0.47
1:F:408:GLU:HG3	1:F:409:TRP:CD1	2.49	0.47
1:A:88:ALA:HB1	1:A:89:PRO:HD2	1.96	0.47
1:C:422:GLN:O	1:C:425:VAL:HG22	2.15	0.47
1:A:332:THR:HG22	1:A:335:TYR:CD1	2.50	0.46
1:B:276:GLN:CB	1:B:277:MET:HE3	2.46	0.46
1:F:149:MET:N	7:F:805:HOH:O	2.48	0.46
1:E:422:GLN:O	1:E:425:VAL:HG22	2.15	0.46
1:B:270:SER:HB2	1:B:272:LYS:HE2	1.97	0.46
1:F:422:GLN:O	1:F:425:VAL:HG22	2.15	0.46
1:A:334:PRO:HD3	1:A:360:GLU:O	2.16	0.46
1:B:225:THR:HG21	1:B:323:ALA:O	2.16	0.46
1:C:334:PRO:HD3	1:C:360:GLU:O	2.15	0.46
1:D:244:CYS:O	1:D:299:PRO:HD2	2.16	0.46
1:D:334:PRO:HD3	1:D:360:GLU:O	2.17	0.45
1:A:244:CYS:O	1:A:299:PRO:HD2	2.16	0.45
1:B:422:GLN:O	1:B:425:VAL:HG22	2.17	0.45
1:F:514:THR:OG1	1:F:517:GLN:HG3	2.16	0.45
1:C:611:GLU:OE2	7:C:801:HOH:O	2.21	0.45
1:B:392:PHE:N	1:B:393:PRO:CD	2.80	0.45
1:B:514:THR:OG1	1:B:517:GLN:HG3	2.16	0.45
1:C:526:LYS:NZ	5:C:705:IMD:C2	2.80	0.45
1:D:332:THR:HG22	1:D:335:TYR:CD1	2.52	0.45
1:C:244:CYS:O	1:C:299:PRO:HD2	2.16	0.44
1:D:422:GLN:O	1:D:425:VAL:HG22	2.17	0.44
1:E:334:PRO:HD3	1:E:360:GLU:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:244:CYS:O	1:F:299:PRO:HD2	2.17	0.44
1:C:330:GLN:HG2	1:C:341:MET:CE	2.47	0.44
1:E:332:THR:HG22	1:E:335:TYR:CD1	2.52	0.44
1:E:514:THR:OG1	1:E:517:GLN:HG3	2.17	0.44
1:D:225:THR:HG21	1:D:323:ALA:O	2.17	0.44
1:F:334:PRO:HD3	1:F:360:GLU:O	2.17	0.44
1:A:249:TYR:N	7:A:812:HOH:O	2.40	0.44
1:D:514:THR:OG1	1:D:517:GLN:HG3	2.17	0.44
1:D:188:ASN:HB3	1:D:189:PRO:CD	2.47	0.44
1:A:392:PHE:N	1:A:393:PRO:CD	2.81	0.44
1:E:244:CYS:O	1:E:299:PRO:HD2	2.18	0.44
1:F:188:ASN:HB3	1:F:189:PRO:CD	2.47	0.44
1:A:579:VAL:N	1:A:580:PRO:CD	2.81	0.44
1:A:330:GLN:HG2	1:A:341:MET:CE	2.48	0.43
1:C:219:GLU:OE2	1:C:222:ARG:NH1	2.51	0.43
1:F:489:ASP:OD2	2:L:1:GLC:O3	2.29	0.43
1:C:514:THR:OG1	1:C:517:GLN:HG3	2.19	0.43
1:C:92:PHE:HE2	1:C:109:LEU:HD13	1.83	0.43
1:F:358:VAL:HA	1:F:388:THR:O	2.18	0.43
1:B:358:VAL:HA	1:B:388:THR:O	2.18	0.43
1:E:358:VAL:HA	1:E:388:THR:O	2.18	0.43
1:F:440:ASP:OD1	3:F:701:PBW:O3'	2.37	0.43
1:C:458:LYS:HD2	5:C:704:IMD:H5	2.00	0.43
1:D:31:PRO:HB3	1:D:209:TYR:CE1	2.53	0.43
1:B:219:GLU:OE2	1:B:222:ARG:NH1	2.51	0.43
1:D:358:VAL:HA	1:D:388:THR:O	2.19	0.43
1:E:31:PRO:HB3	1:E:209:TYR:CE1	2.54	0.43
1:A:50:ASP:O	1:A:51:ARG:C	2.62	0.43
1:B:238:ASP:OD1	1:B:329:ARG:HD2	2.19	0.43
1:D:50:ASP:O	1:D:51:ARG:C	2.62	0.43
1:B:333:HIS:N	1:B:334:PRO:HD2	2.34	0.42
1:F:31:PRO:HB3	1:F:209:TYR:CE1	2.53	0.42
1:B:244:CYS:O	1:B:299:PRO:HD2	2.19	0.42
1:E:188:ASN:HB3	1:E:189:PRO:CD	2.48	0.42
1:F:88:ALA:HB1	1:F:89:PRO:HD2	2.01	0.42
1:A:188:ASN:HB3	1:A:189:PRO:CD	2.49	0.42
1:C:225:THR:HG21	1:C:323:ALA:O	2.19	0.42
1:D:238:ASP:OD1	1:D:329:ARG:HD2	2.19	0.42
1:A:358:VAL:HA	1:A:388:THR:O	2.19	0.42
1:F:330:GLN:HG2	1:F:341:MET:CE	2.50	0.42
1:B:188:ASN:HB3	1:B:189:PRO:CD	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:238:ASP:OD1	1:C:329:ARG:HD2	2.20	0.42
1:C:358:VAL:HA	1:C:388:THR:O	2.18	0.42
1:D:392:PHE:N	1:D:393:PRO:CD	2.82	0.42
1:A:144:ASP:HB3	1:A:154:VAL:HG11	2.00	0.42
1:A:238:ASP:OD1	1:A:329:ARG:HD2	2.20	0.42
1:A:360:GLU:HA	1:A:390:MET:SD	2.60	0.42
1:B:31:PRO:HB3	1:B:209:TYR:CE1	2.55	0.42
1:B:144:ASP:HB3	1:B:154:VAL:HG11	2.01	0.42
1:C:50:ASP:O	1:C:51:ARG:C	2.62	0.42
1:D:579:VAL:N	1:D:580:PRO:CD	2.83	0.42
1:E:144:ASP:HB3	1:E:154:VAL:HG11	2.01	0.42
1:E:579:VAL:N	1:E:580:PRO:CD	2.82	0.42
1:C:144:ASP:HB3	1:C:154:VAL:HG11	2.01	0.42
1:C:392:PHE:N	1:C:393:PRO:CD	2.82	0.42
1:D:88:ALA:HB1	1:D:89:PRO:HD2	2.01	0.42
1:E:50:ASP:O	1:E:51:ARG:C	2.62	0.42
1:A:407:THR:HB	7:A:985:HOH:O	2.19	0.42
1:A:31:PRO:HB3	1:A:209:TYR:CE1	2.55	0.41
1:A:92:PHE:HE2	1:A:109:LEU:HD13	1.85	0.41
1:F:144:ASP:HB3	1:F:154:VAL:HG11	2.01	0.41
1:F:392:PHE:N	1:F:393:PRO:CD	2.83	0.41
1:B:50:ASP:O	1:B:51:ARG:C	2.63	0.41
1:B:513:ARG:HD2	1:B:518:ASN:OD1	2.20	0.41
1:E:392:PHE:N	1:E:393:PRO:CD	2.83	0.41
1:A:225:THR:HG21	1:A:323:ALA:O	2.20	0.41
1:A:513:ARG:HD2	1:A:518:ASN:OD1	2.20	0.41
1:D:144:ASP:HB3	1:D:154:VAL:HG11	2.01	0.41
1:E:330:GLN:HG2	1:E:341:MET:CE	2.50	0.41
1:F:50:ASP:O	1:F:51:ARG:C	2.63	0.41
1:F:238:ASP:OD1	1:F:329:ARG:HD2	2.21	0.41
1:C:31:PRO:HB3	1:C:209:TYR:CE1	2.55	0.41
1:B:579:VAL:N	1:B:580:PRO:CD	2.83	0.41
1:F:254:MET:HB2	7:F:804:HOH:O	2.20	0.41
1:A:262:PHE:CE1	1:A:287:LYS:HE2	2.55	0.41
1:B:53:SER:O	1:B:71:LYS:HD2	2.20	0.41
1:E:238:ASP:OD1	1:E:329:ARG:HD2	2.20	0.41
1:D:33:PHE:CE1	1:D:110:LYS:HE2	2.56	0.41
1:A:422:GLN:O	1:A:425:VAL:HG22	2.21	0.40
1:A:579:VAL:N	1:A:580:PRO:HD2	2.35	0.40
1:C:88:ALA:HB1	1:C:89:PRO:HD2	2.03	0.40
1:C:513:ARG:HD2	1:C:518:ASN:OD1	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:88:ALA:HB1	1:E:89:PRO:HD2	2.02	0.40
1:E:225:THR:HG21	1:E:323:ALA:O	2.20	0.40
1:E:513:ARG:HD2	1:E:518:ASN:OD1	2.20	0.40
1:F:201:HIS:CD2	2:L:1:GLC:H2	2.56	0.40
1:B:313:ILE:CD1	1:B:343:ARG:HD3	2.51	0.40
1:C:188:ASN:HB3	1:C:189:PRO:CD	2.51	0.40
1:D:330:GLN:HG2	1:D:341:MET:CE	2.51	0.40
1:F:579:VAL:N	1:F:580:PRO:CD	2.84	0.40
1:B:33:PHE:CE1	1:B:110:LYS:HE2	2.56	0.40
1:B:277:MET:HE1	1:B:372:TRP:HE1	1.85	0.40
1:D:610:ARG:O	5:D:704:IMD:C2	2.70	0.40
1:F:277:MET:HE1	1:F:372:TRP:HE1	1.86	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1057:HOH:O	7:C:849:HOH:O[4_665]	2.06	0.14

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	592/610 (97%)	575 (97%)	17 (3%)	0	100	100
1	B	587/610 (96%)	564 (96%)	21 (4%)	2 (0%)	36	44
1	C	586/610 (96%)	567 (97%)	19 (3%)	0	100	100
1	D	592/610 (97%)	573 (97%)	19 (3%)	0	100	100
1	E	591/610 (97%)	571 (97%)	20 (3%)	0	100	100
1	F	583/610 (96%)	565 (97%)	18 (3%)	0	100	100
All	All	3531/3660 (96%)	3415 (97%)	114 (3%)	2 (0%)	48	60

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	335	TYR
1	B	268	GLN

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	513/537 (96%)	502 (98%)	11 (2%)	47	60
1	B	506/537 (94%)	489 (97%)	17 (3%)	32	45
1	C	467/537 (87%)	457 (98%)	10 (2%)	47	60
1	D	462/537 (86%)	453 (98%)	9 (2%)	50	63
1	E	432/537 (80%)	418 (97%)	14 (3%)	34	46
1	F	430/537 (80%)	418 (97%)	12 (3%)	38	51
All	All	2810/3222 (87%)	2737 (97%)	73 (3%)	40	53

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	LYS
1	A	86	LYS
1	A	132	MET
1	A	197	GLU
1	A	238	ASP
1	A	332	THR
1	A	425	VAL
1	A	446	ARG
1	A	529	GLN
1	A	574	GLN
1	A	598	LYS
1	B	28	LYS
1	B	101	LYS
1	B	149	MET
1	B	197	GLU

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Mol	Chain	Res	Type
1	B	238	ASP
1	B	242	ASN
1	B	256	SER
1	B	267	VAL
1	B	273	THR
1	B	276	GLN
1	B	277	MET
1	B	341	MET
1	B	343	ARG
1	B	358	VAL
1	B	425	VAL
1	B	574	GLN
1	B	582	GLN
1	C	56	ASP
1	C	175	ASP
1	C	210	GLN
1	C	238	ASP
1	C	256	SER
1	C	332	THR
1	C	358	VAL
1	C	425	VAL
1	C	446	ARG
1	C	574	GLN
1	D	102	GLN
1	D	238	ASP
1	D	256	SER
1	D	332	THR
1	D	358	VAL
1	D	425	VAL
1	D	446	ARG
1	D	574	GLN
1	D	602	ARG
1	E	51	ARG
1	E	102	GLN
1	E	153	ASN
1	E	175	ASP
1	E	197	GLU
1	E	238	ASP
1	E	256	SER
1	E	332	THR
1	E	358	VAL
1	E	407	THR

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Mol	Chain	Res	Type
1	E	425	VAL
1	E	446	ARG
1	E	531	ARG
1	E	574	GLN
1	F	32	THR
1	F	102	GLN
1	F	175	ASP
1	F	238	ASP
1	F	332	THR
1	F	349	ASN
1	F	358	VAL
1	F	425	VAL
1	F	505	LYS
1	F	574	GLN
1	F	598	LYS
1	F	604	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	276	GLN
1	B	44	GLN
1	B	399	ASN
1	B	603	ASN
1	E	102	GLN
1	F	349	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 ⓘ

12 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	GLC	G	1	3,4,2	11,11,12	1.39	2 (18%)	15,15,17	1.52	3 (20%)
2	GLC	G	2	2	11,11,12	0.73	0	15,15,17	1.33	2 (13%)
2	GLC	H	1	3,4,2	11,11,12	1.53	2 (18%)	15,15,17	1.03	1 (6%)
2	GLC	H	2	2	11,11,12	0.89	1 (9%)	15,15,17	1.16	1 (6%)
2	GLC	I	1	3,4,2	11,11,12	1.14	0	15,15,17	1.27	3 (20%)
2	GLC	I	2	2	11,11,12	0.59	0	15,15,17	0.83	1 (6%)
2	GLC	J	1	3,4,2	11,11,12	0.91	0	15,15,17	1.26	1 (6%)
2	GLC	J	2	2	11,11,12	0.50	0	15,15,17	1.21	2 (13%)
2	GLC	K	1	3,4,2	11,11,12	1.20	1 (9%)	15,15,17	1.17	1 (6%)
2	GLC	K	2	2	11,11,12	0.63	0	15,15,17	1.35	2 (13%)
2	GLC	L	1	3,2	11,11,12	1.09	1 (9%)	15,15,17	1.49	2 (13%)
2	GLC	L	2	2	11,11,12	0.74	1 (9%)	15,15,17	1.18	1 (6%)

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	GLC	G	1	3,4,2	-	0/2/19/22	0/1/1/1
2	GLC	G	2	2	-	2/2/19/22	0/1/1/1
2	GLC	H	1	3,4,2	-	0/2/19/22	0/1/1/1
2	GLC	H	2	2	-	0/2/19/22	0/1/1/1
2	GLC	I	1	3,4,2	-	0/2/19/22	0/1/1/1
2	GLC	I	2	2	-	2/2/19/22	0/1/1/1
2	GLC	J	1	3,4,2	-	0/2/19/22	0/1/1/1
2	GLC	J	2	2	-	2/2/19/22	0/1/1/1
2	GLC	K	1	3,4,2	-	0/2/19/22	0/1/1/1
2	GLC	K	2	2	-	2/2/19/22	0/1/1/1
2	GLC	L	1	3,2	-	0/2/19/22	0/1/1/1
2	GLC	L	2	2	-	0/2/19/22	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1	GLC	O5-C5	3.27	1.49	1.43
2	G	1	GLC	C1-C2	-2.81	1.45	1.52
2	H	2	GLC	O5-C5	2.76	1.48	1.43
2	K	1	GLC	O5-C1	-2.51	1.39	1.43
2	H	1	GLC	C2-C3	-2.45	1.48	1.52
2	L	1	GLC	O5-C5	2.29	1.47	1.43
2	L	2	GLC	C2-C3	2.17	1.55	1.52
2	G	1	GLC	O5-C1	-2.12	1.40	1.43

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	1	GLC	C1-C2-C3	-4.35	103.31	109.64
2	J	1	GLC	C1-C2-C3	-3.63	104.35	109.64
2	K	2	GLC	C3-C4-C5	3.41	116.41	110.23
2	H	2	GLC	C1-O5-C5	3.31	116.62	112.19
2	K	1	GLC	C1-C2-C3	-3.21	104.97	109.64
2	G	1	GLC	C1-C2-C3	-2.93	105.37	109.64
2	J	2	GLC	C3-C4-C5	2.89	115.48	110.23
2	G	2	GLC	C1-O5-C5	2.70	115.80	112.19
2	L	2	GLC	C1-C2-C3	2.52	113.32	109.64
2	I	1	GLC	C1-O5-C5	2.47	115.50	112.19
2	K	2	GLC	C2-C3-C4	2.45	115.17	110.86
2	I	1	GLC	C1-C2-C3	-2.42	106.12	109.64
2	L	1	GLC	O2-C2-C1	2.40	114.72	109.22
2	G	1	GLC	O4-C4-C5	-2.31	103.63	109.32
2	G	2	GLC	O4-C4-C3	-2.27	105.04	110.38
2	J	2	GLC	C2-C3-C4	2.13	114.61	110.86
2	I	2	GLC	C1-C2-C3	2.10	112.71	109.64
2	I	1	GLC	O2-C2-C1	2.08	113.99	109.22
2	G	1	GLC	O3-C3-C2	-2.08	105.82	110.05
2	H	1	GLC	O3-C3-C2	-2.01	105.95	110.05

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	K	2	GLC	O5-C5-C6-O6
2	I	2	GLC	O5-C5-C6-O6
2	J	2	GLC	O5-C5-C6-O6
2	J	2	GLC	C4-C5-C6-O6

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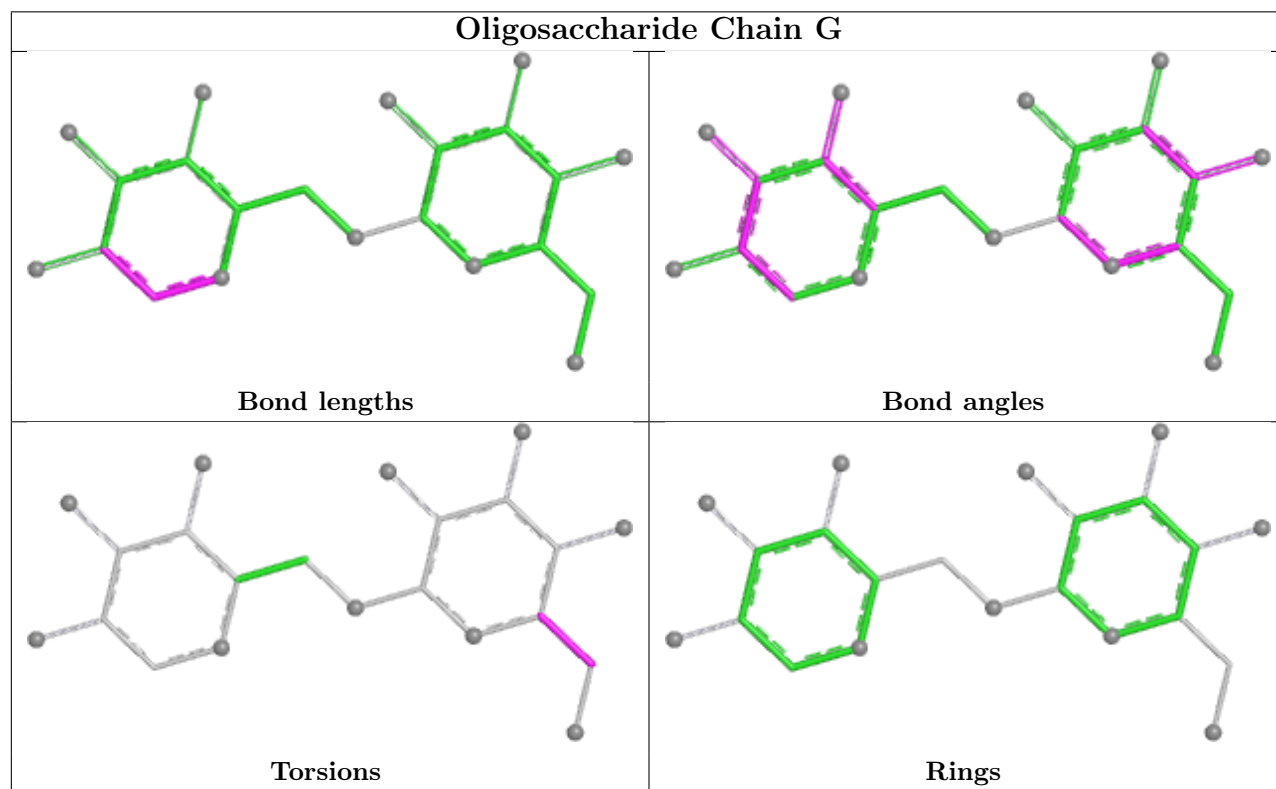
Mol	Chain	Res	Type	Atoms
2	I	2	GLC	C4-C5-C6-O6
2	K	2	GLC	C4-C5-C6-O6
2	G	2	GLC	C4-C5-C6-O6
2	G	2	GLC	O5-C5-C6-O6

There are no ring outliers.

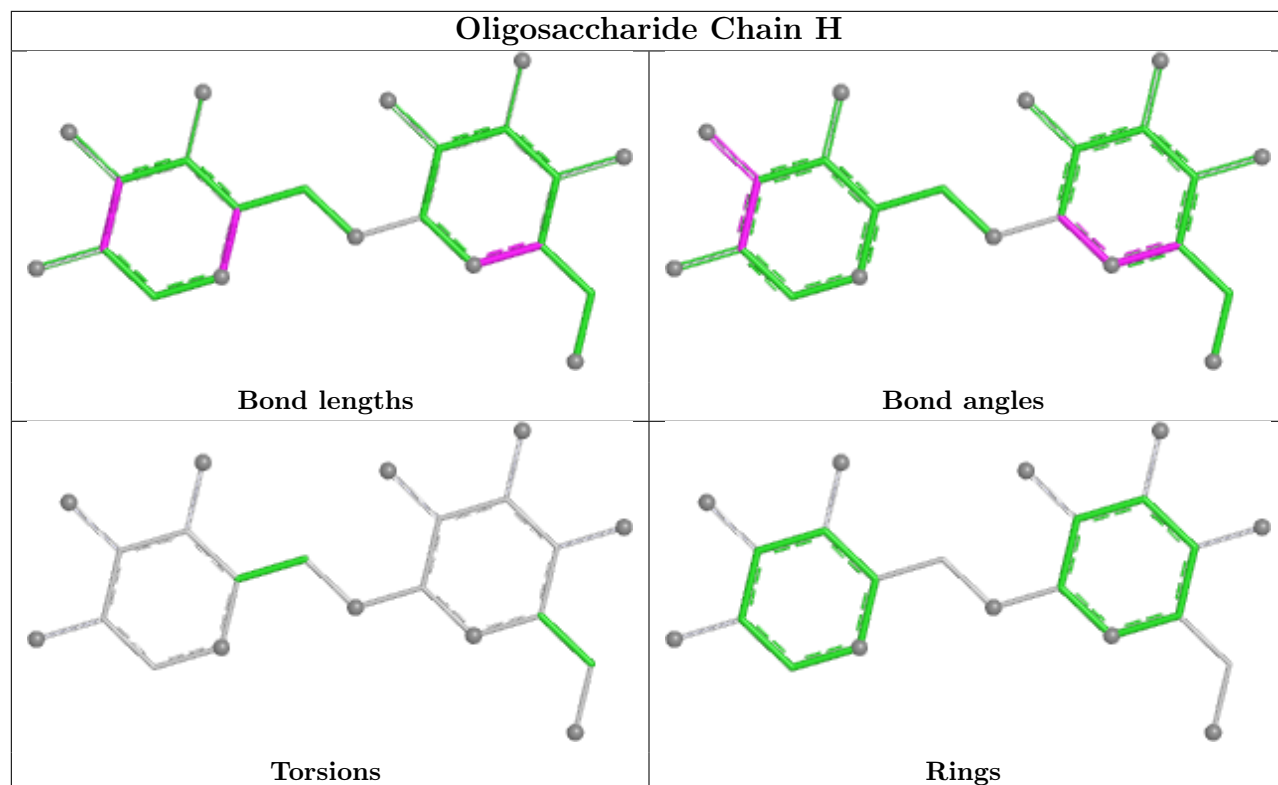
1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L	1	GLC	2	0

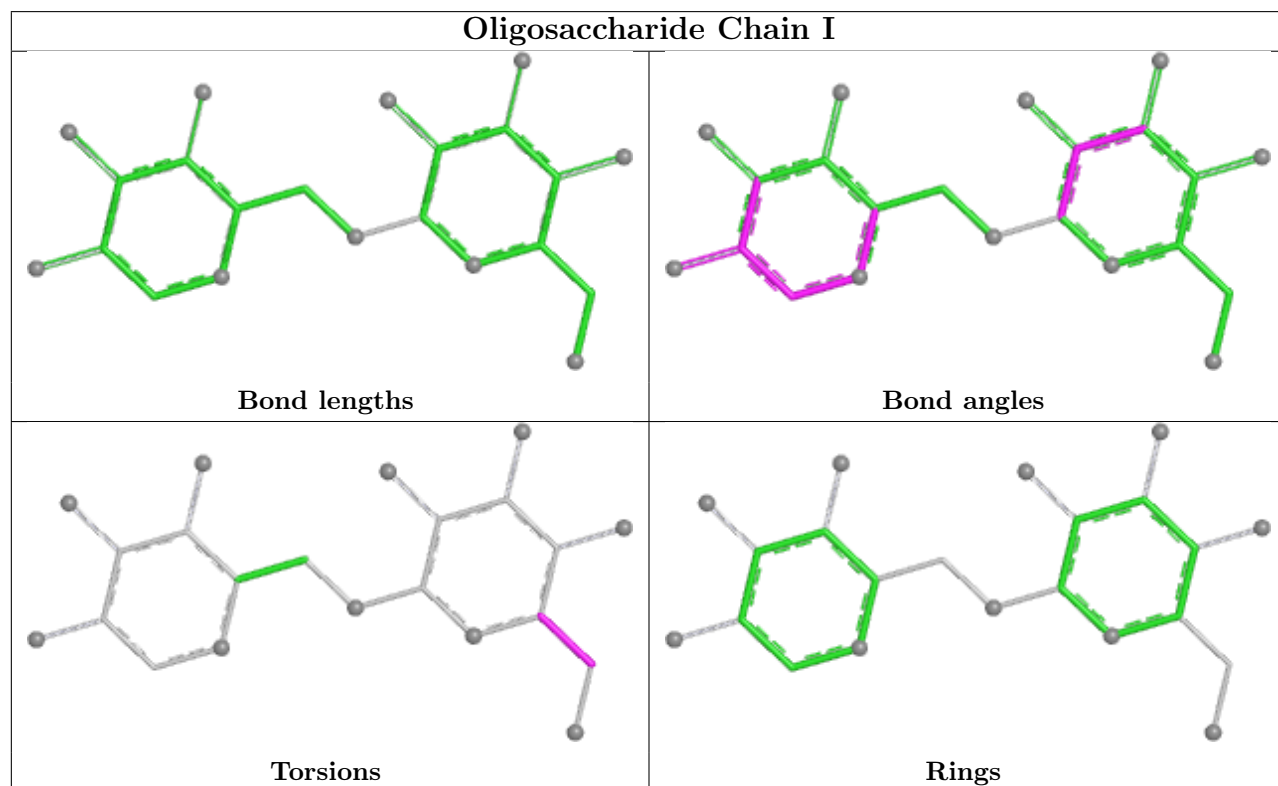
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

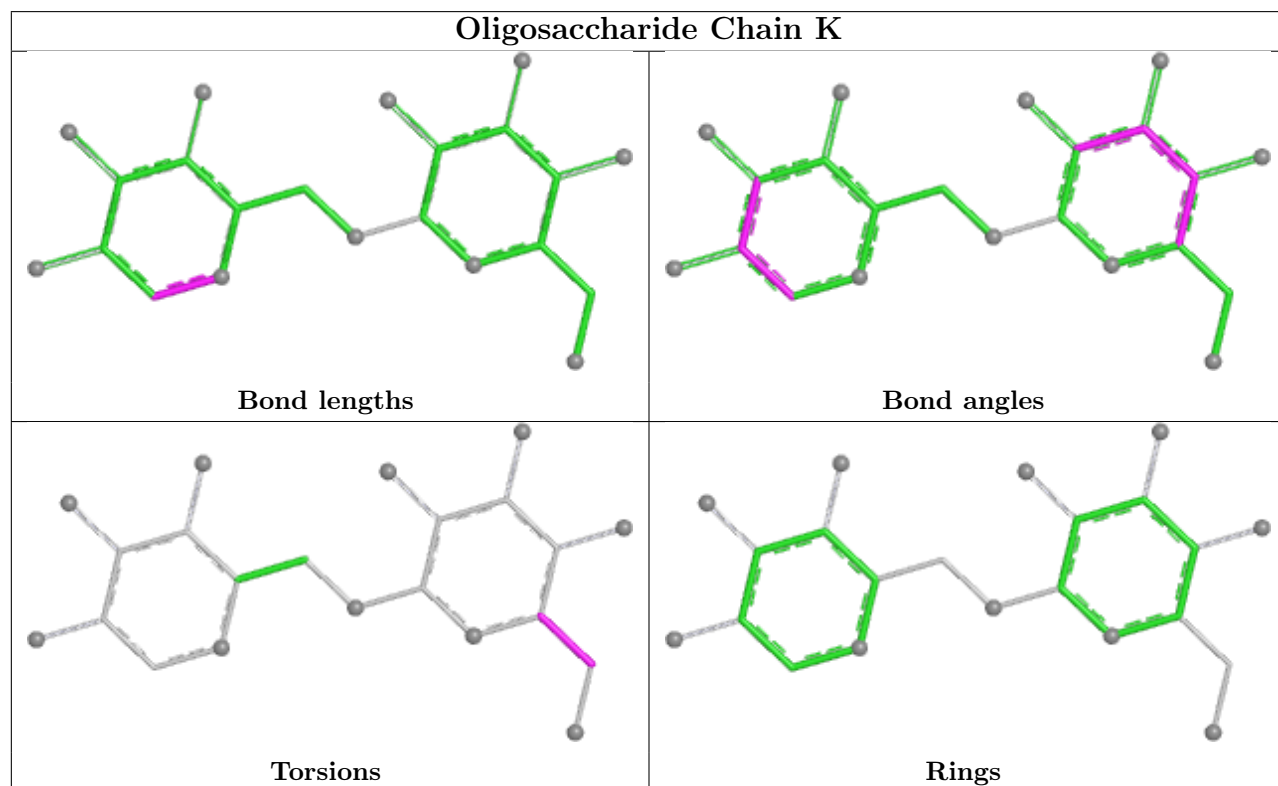
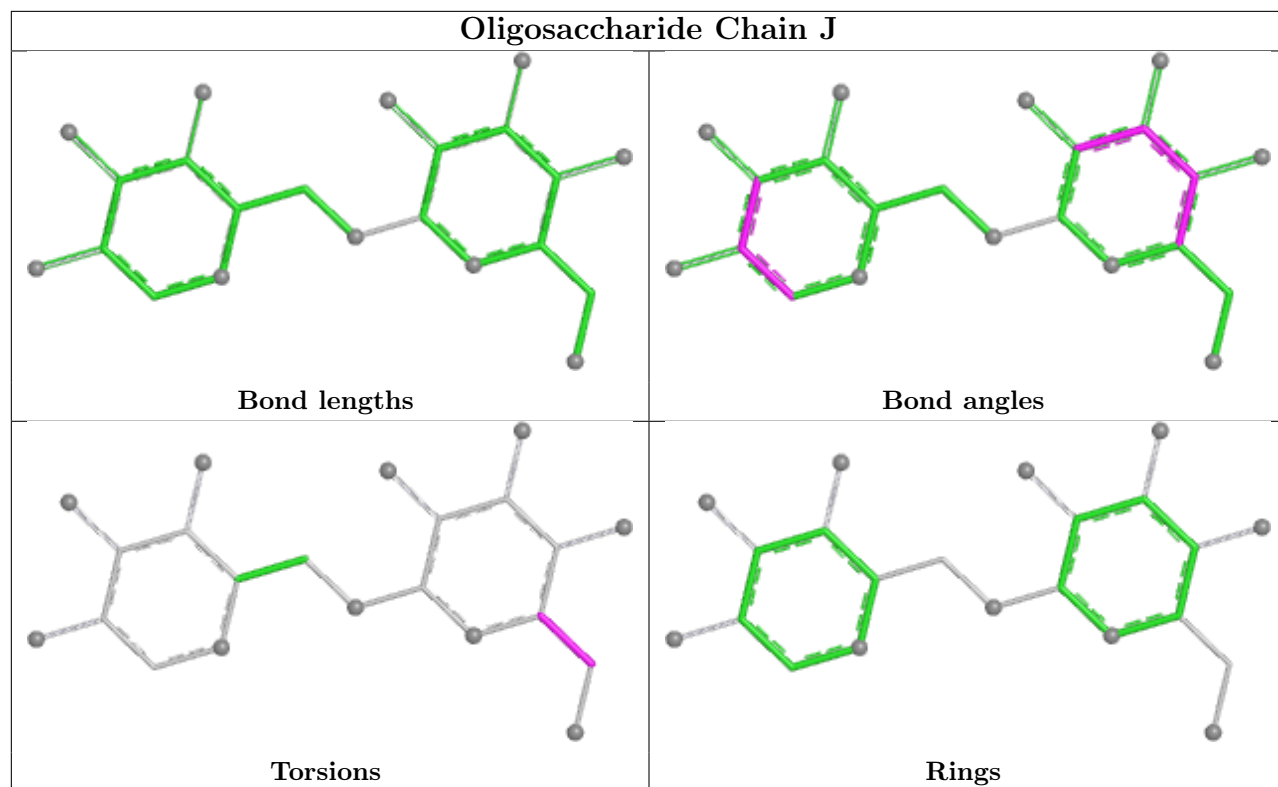


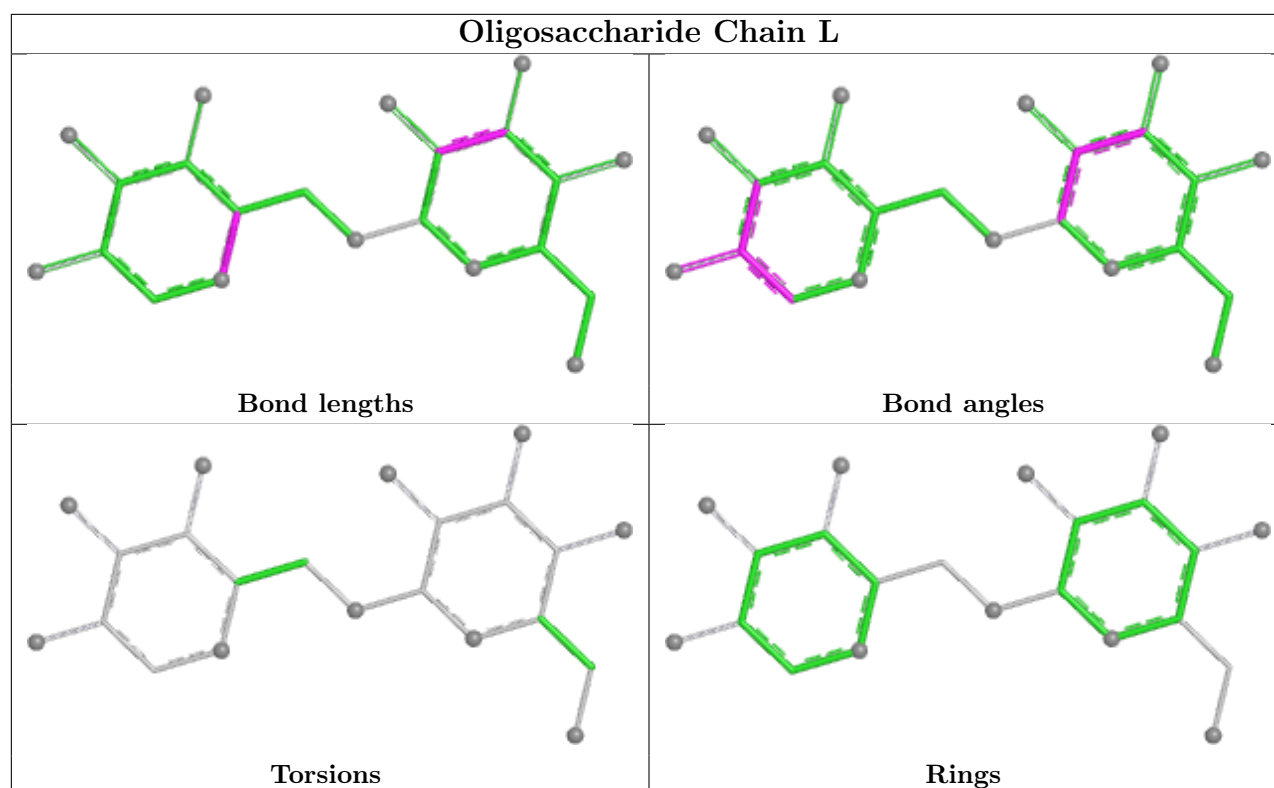
Oligosaccharide Chain H



Oligosaccharide Chain I







5.6 Ligand geometry [i](#)

Of 35 ligands modelled in this entry, 12 are monoatomic - leaving 23 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	$\# Z > 2$
5	IMD	A	704	-	5,5,5	0.25	0	5,5,5	0.67	0
5	IMD	B	703	-	5,5,5	0.26	0	5,5,5	0.56	0
4	OC9	C	702	2	1,1,8	0.49	0	-		
5	IMD	C	705	-	5,5,5	0.39	0	5,5,5	0.62	0
3	PBW	A	701	2,1	12,12,13	1.79	2 (16%)	14,17,19	2.10	1 (7%)
5	IMD	D	705	-	5,5,5	0.37	0	5,5,5	0.54	0
3	PBW	C	701	2,1	12,12,13	0.45	0	14,17,19	3.02	2 (14%)
3	PBW	D	701	2,1	12,12,13	0.62	0	14,17,19	2.64	1 (7%)
4	OC9	A	702	2	3,3,8	0.47	0	2,2,7	0.23	0
5	IMD	F	702	-	5,5,5	0.59	0	5,5,5	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	OC9	B	702	2	3,3,8	0.58	0	2,2,7	0.17	0
5	IMD	A	703	-	5,5,5	0.50	0	5,5,5	0.68	0
5	IMD	C	704	-	5,5,5	0.38	0	5,5,5	0.57	0
5	IMD	D	704	-	5,5,5	0.38	0	5,5,5	0.41	0
5	IMD	C	703	-	5,5,5	0.38	0	5,5,5	0.50	0
3	PBW	E	701	2,1	12,12,13	0.54	0	14,17,19	2.43	1 (7%)
4	OC9	E	702	2	1,1,8	0.44	0	-		
3	PBW	F	701	2,1	12,12,13	0.73	0	14,17,19	3.07	2 (14%)
5	IMD	E	703	-	5,5,5	0.30	0	5,5,5	0.60	0
3	PBW	B	701	2,1	12,12,13	0.54	0	14,17,19	2.98	1 (7%)
5	IMD	D	703	-	5,5,5	0.46	0	5,5,5	0.55	0
5	IMD	A	705	-	5,5,5	0.36	0	5,5,5	0.38	0
4	OC9	D	702	2	2,2,8	0.46	0	1,1,7	0.51	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	IMD	A	704	-	-	-	0/1/1/1
5	IMD	B	703	-	-	-	0/1/1/1
5	IMD	C	705	-	-	-	0/1/1/1
3	PBW	A	701	2,1	-	0/2/22/26	0/1/1/1
5	IMD	D	705	-	-	-	0/1/1/1
3	PBW	C	701	2,1	-	0/2/22/26	0/1/1/1
3	PBW	D	701	2,1	-	2/2/22/26	0/1/1/1
4	OC9	A	702	2	-	0/1/1/6	-
5	IMD	F	702	-	-	-	0/1/1/1
4	OC9	B	702	2	-	0/1/1/6	-
5	IMD	A	703	-	-	-	0/1/1/1
5	IMD	C	704	-	-	-	0/1/1/1
5	IMD	D	704	-	-	-	0/1/1/1
5	IMD	C	703	-	-	-	0/1/1/1
3	PBW	E	701	2,1	-	0/2/22/26	0/1/1/1
3	PBW	F	701	2,1	-	0/2/22/26	0/1/1/1
5	IMD	E	703	-	-	-	0/1/1/1
3	PBW	B	701	2,1	-	0/2/22/26	0/1/1/1
5	IMD	D	703	-	-	-	0/1/1/1
5	IMD	A	705	-	-	-	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	701	PBW	C2'-C3'	-4.38	1.45	1.52
3	A	701	PBW	C5'-C4'	-3.60	1.49	1.53

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	701	PBW	C7'-C1'-C2'	10.96	124.23	111.50
3	B	701	PBW	C7'-C1'-C2'	10.84	124.09	111.50
3	F	701	PBW	C7'-C1'-C2'	10.81	124.06	111.50
3	D	701	PBW	C7'-C1'-C2'	9.50	122.53	111.50
3	E	701	PBW	C7'-C1'-C2'	8.52	121.40	111.50
3	A	701	PBW	C7'-C1'-C2'	7.06	119.70	111.50
3	F	701	PBW	C2'-C3'-C4'	-2.64	106.22	110.86
3	C	701	PBW	C1'-C2'-C3'	2.10	113.69	110.67

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	701	PBW	C4'-C5'-C6'-O6'
3	D	701	PBW	C7'-C5'-C6'-O6'

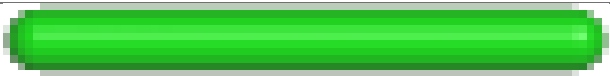
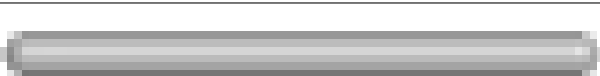
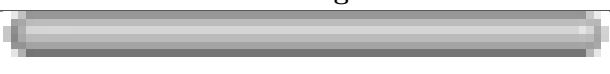
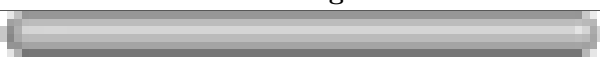
There are no ring outliers.

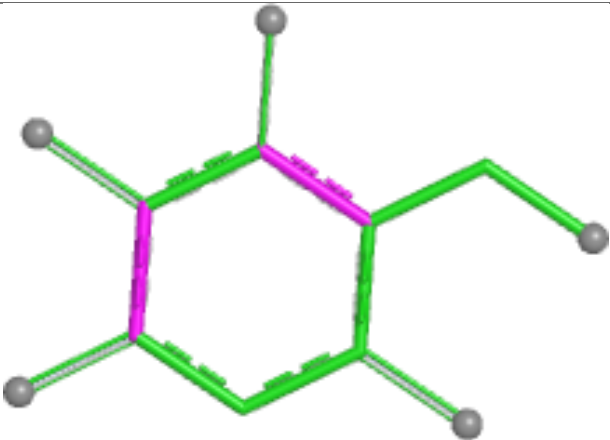
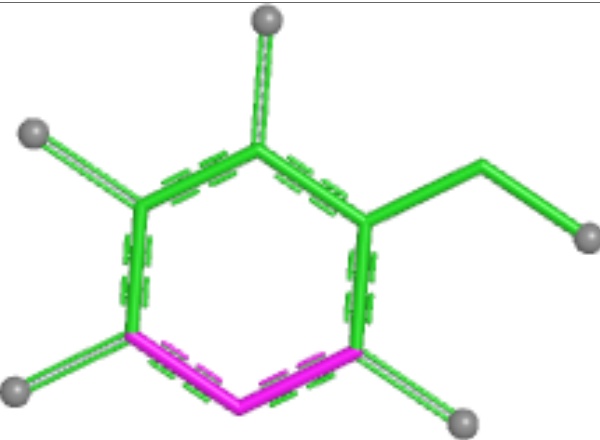
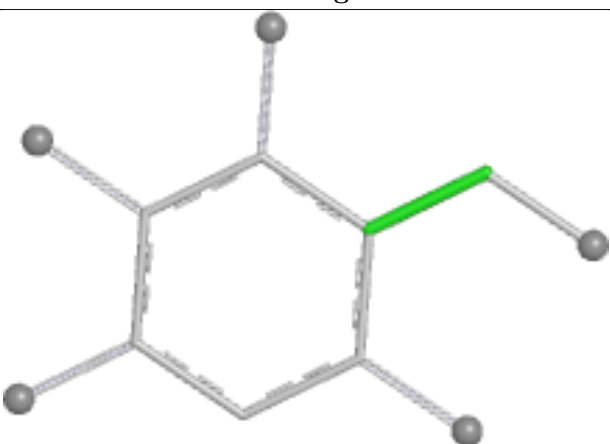
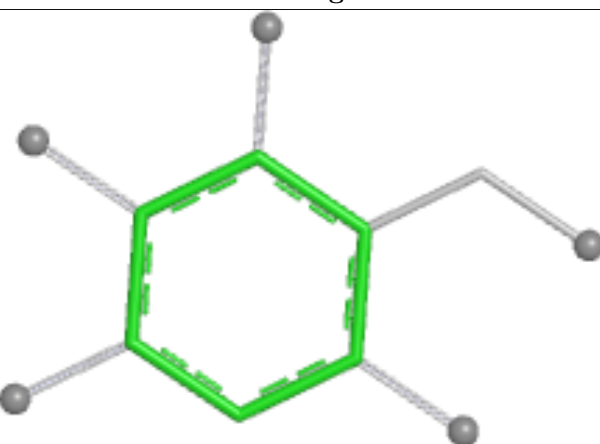
6 monomers are involved in 6 short contacts:

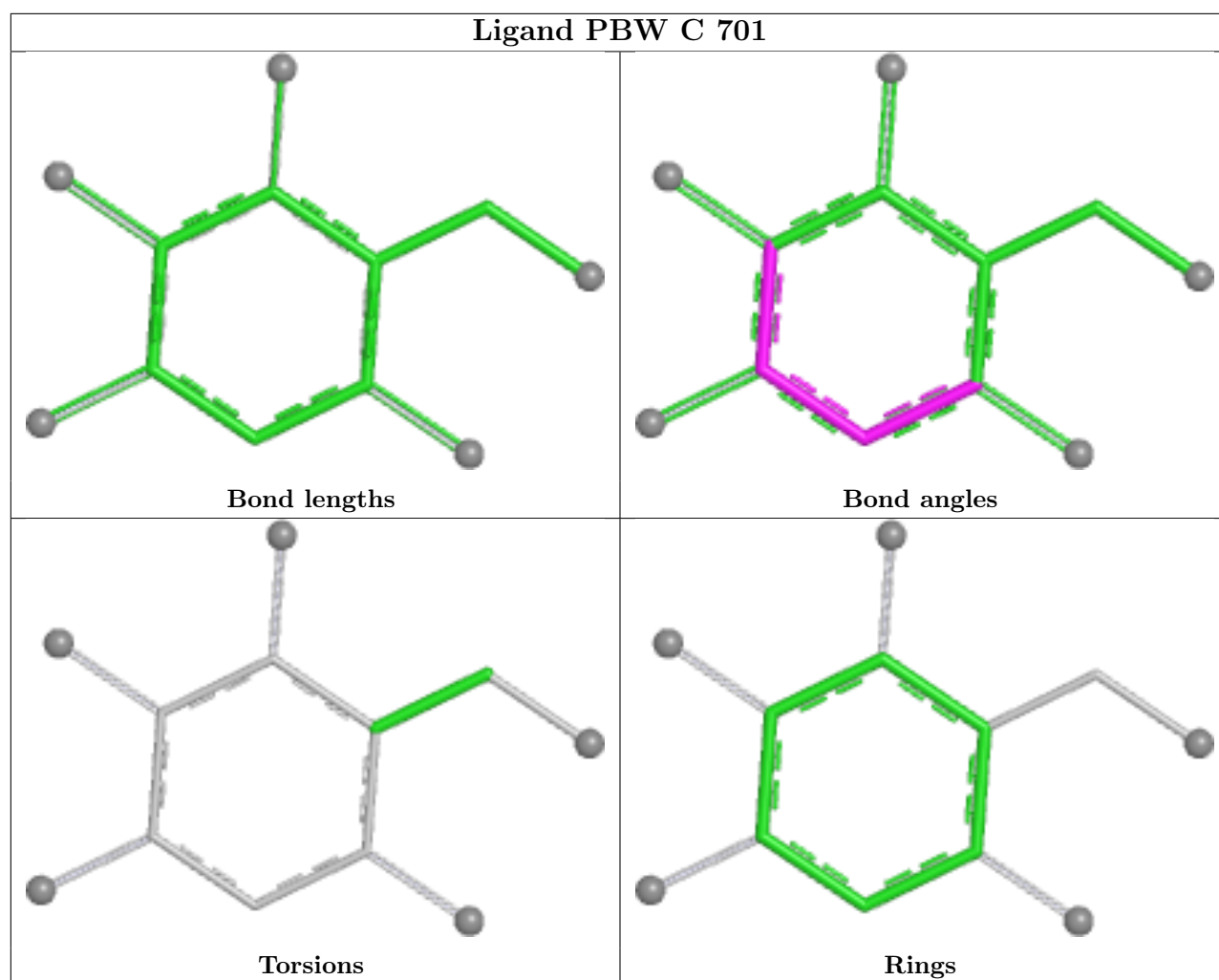
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	705	IMD	1	0
3	D	701	PBW	1	0
5	C	704	IMD	1	0
5	D	704	IMD	1	0
5	C	703	IMD	1	0
3	F	701	PBW	1	0

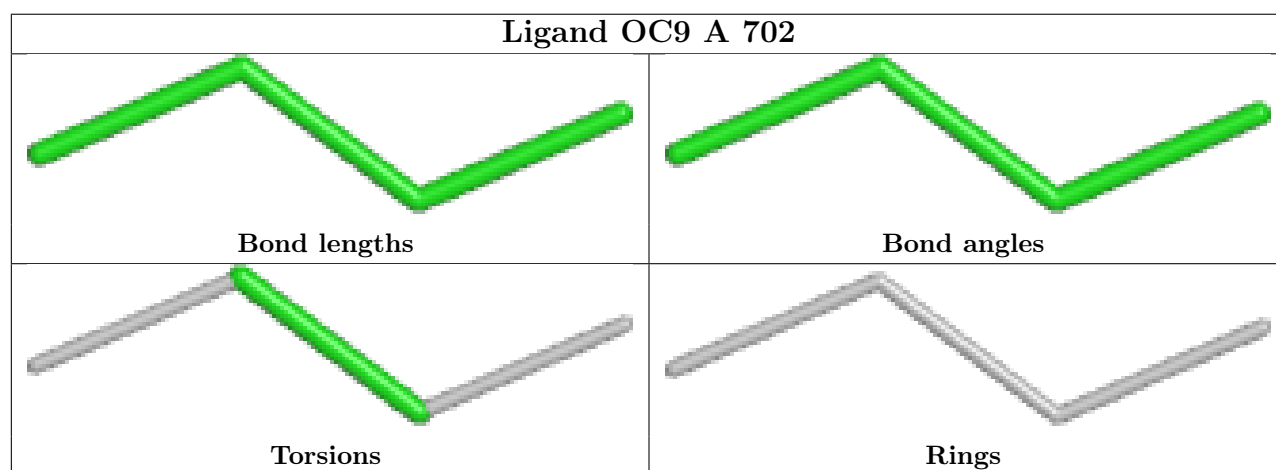
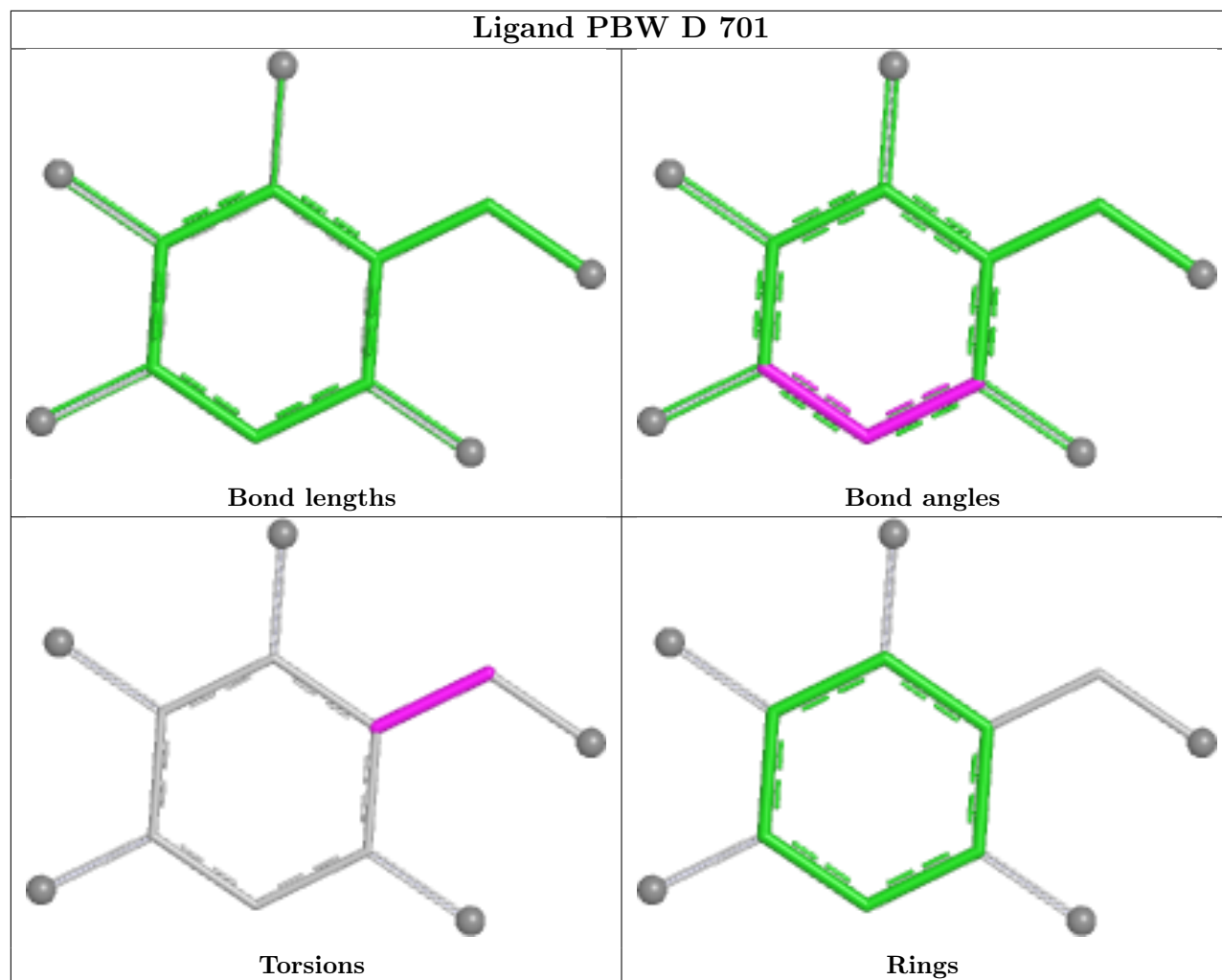
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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

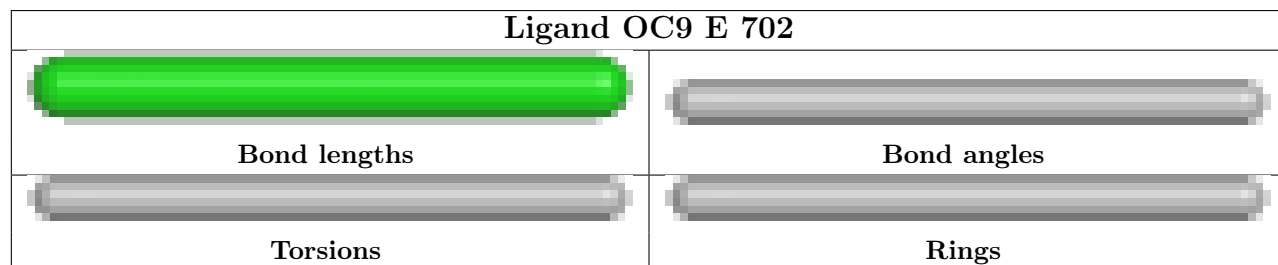
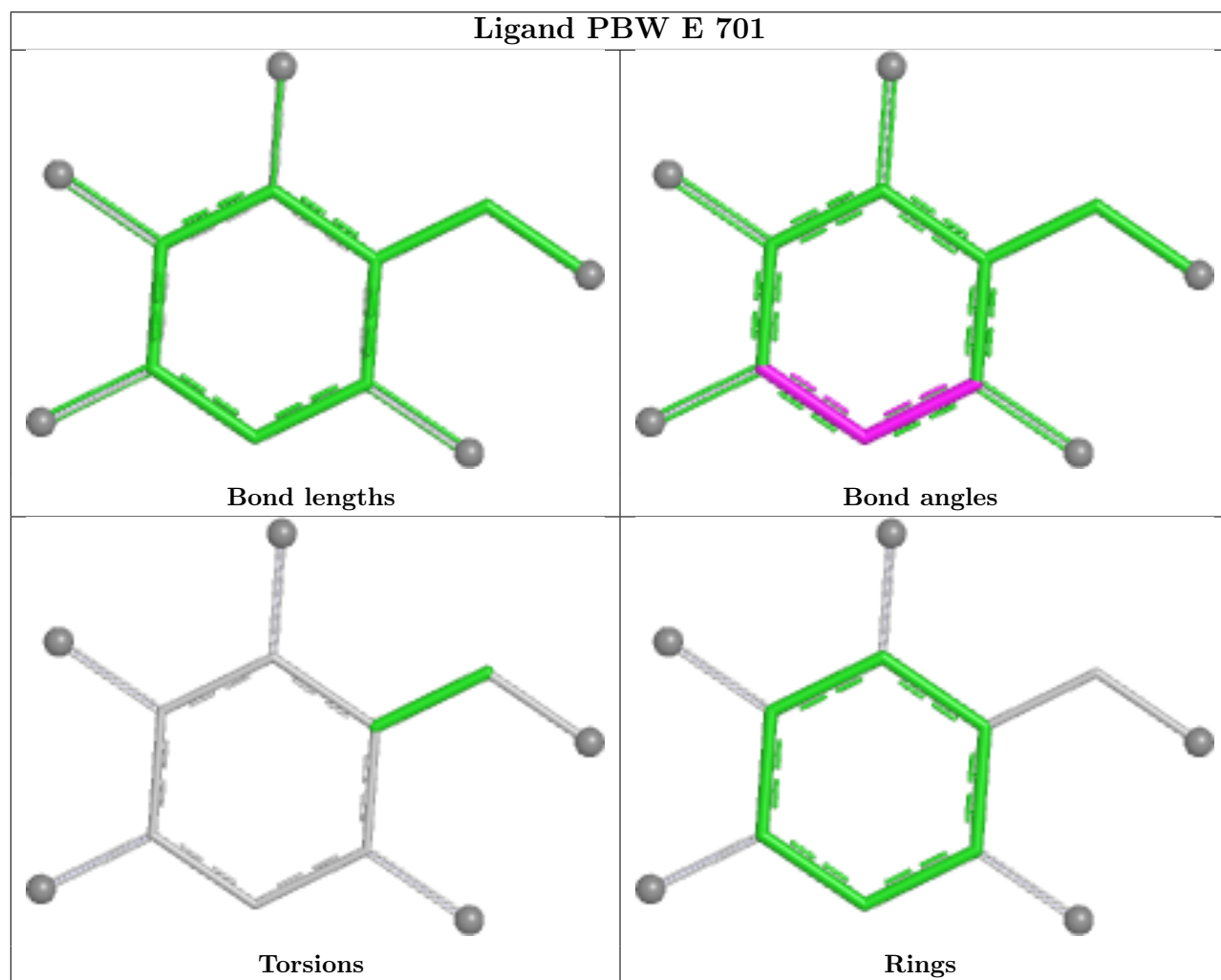
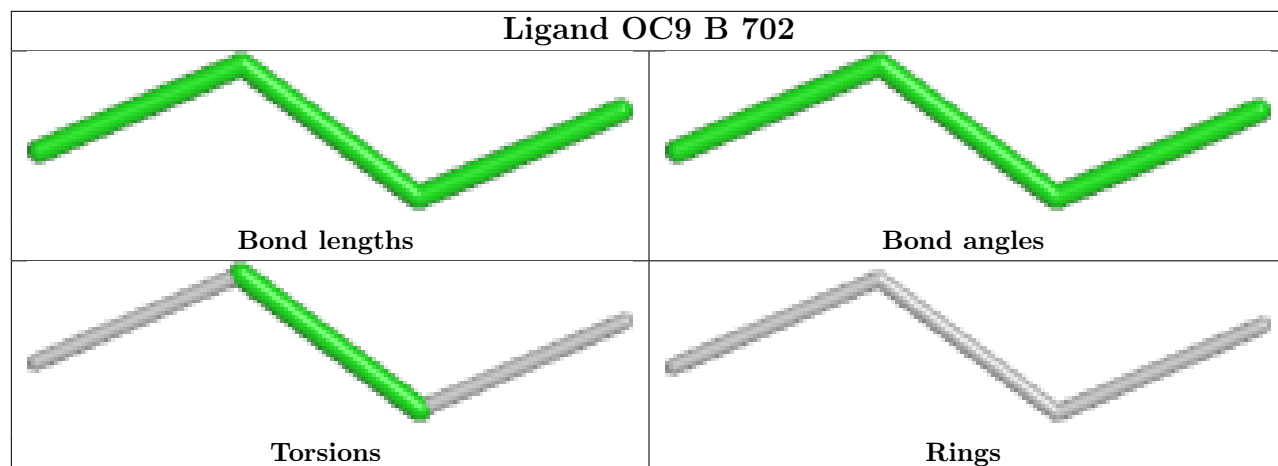
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

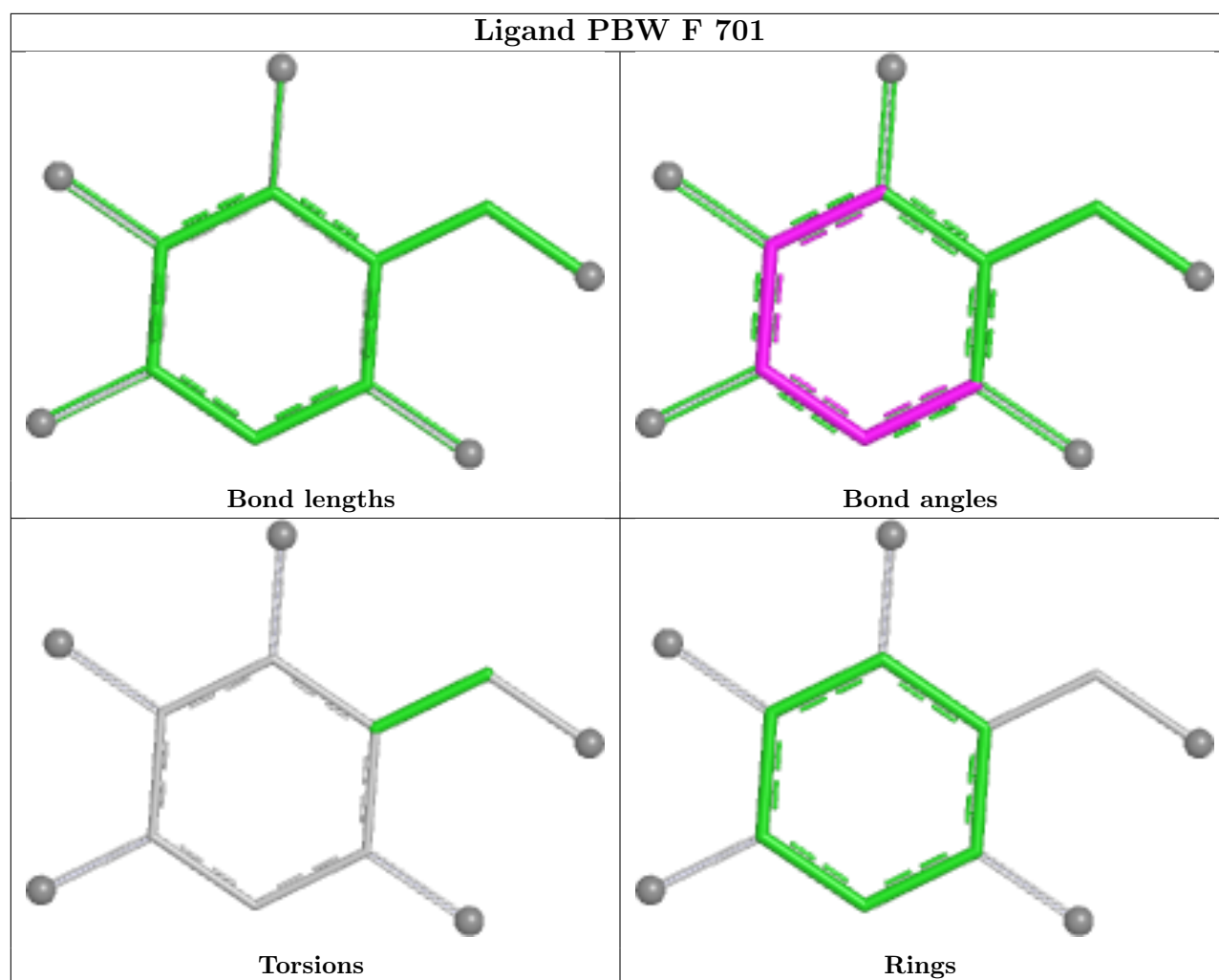
Ligand OC9 C 702	
	
Bond lengths	Bond angles
	
Torsions	Rings

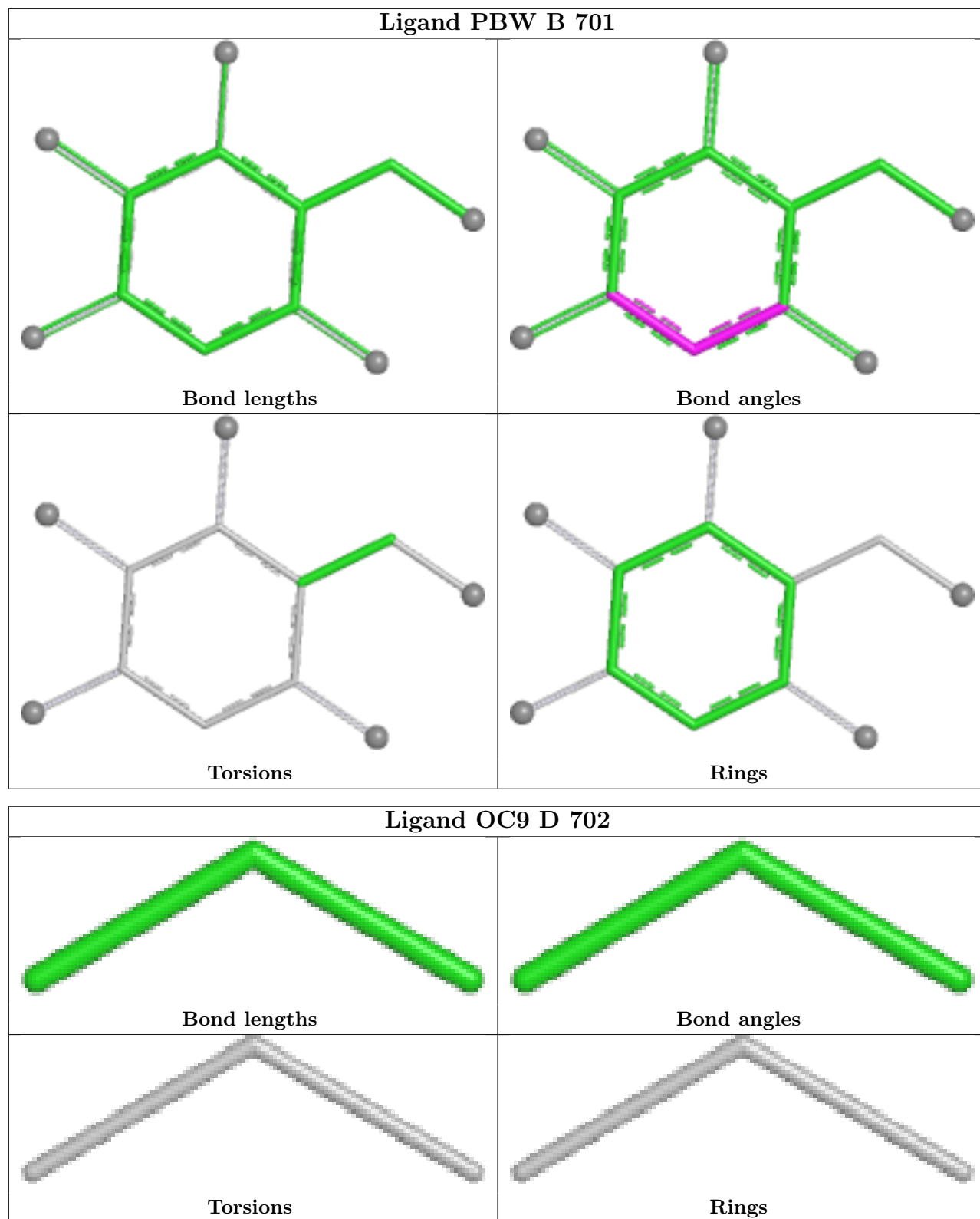
Ligand PBW A 701	
	
Bond lengths	Bond angles
	
Torsions	Rings











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	594/610 (97%)	-0.23	0	100	100	26, 43, 69, 98	0
1	B	591/610 (96%)	0.23	22 (3%)	45	43	34, 56, 89, 168	0
1	C	590/610 (96%)	0.63	41 (6%)	23	19	48, 74, 112, 161	0
1	D	594/610 (97%)	0.85	46 (7%)	19	16	50, 83, 120, 151	0
1	E	593/610 (97%)	0.86	45 (7%)	20	17	48, 90, 126, 159	0
1	F	589/610 (96%)	1.15	90 (15%)	5	3	51, 92, 119, 144	0
All	All	3551/3660 (97%)	0.58	244 (6%)	23	19	26, 74, 116, 168	0

All (244) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	333	HIS	5.7
1	C	24	SER	5.4
1	F	93	ASP	5.1
1	C	333	HIS	5.1
1	B	267	VAL	5.1
1	D	129	TYR	5.0
1	B	271	PHE	4.9
1	B	273	THR	4.6
1	B	266	TYR	4.4
1	D	475	TYR	4.4
1	B	270	SER	4.3
1	B	291	ASP	4.2
1	E	537	ILE	4.1
1	F	132	MET	4.0
1	B	25	THR	4.0
1	B	101	LYS	4.0
1	B	334	PRO	3.9
1	F	506	ASN	3.8
1	D	24	SER	3.8

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Mol	Chain	Res	Type	RSRZ
1	F	60	SER	3.8
1	E	190	ILE	3.7
1	F	25	THR	3.7
1	F	92	PHE	3.6
1	C	290	ILE	3.6
1	E	25	THR	3.5
1	E	603	ASN	3.5
1	F	26	ILE	3.5
1	C	79	VAL	3.4
1	D	182	VAL	3.4
1	B	272	LYS	3.4
1	F	97	LYS	3.4
1	C	67	GLN	3.3
1	B	409	TRP	3.3
1	E	319	TRP	3.3
1	C	296	LEU	3.3
1	E	613	TYR	3.3
1	C	270	SER	3.3
1	C	145	ILE	3.3
1	F	145	ILE	3.3
1	F	613	TYR	3.3
1	C	25	THR	3.3
1	E	221	PHE	3.2
1	C	62	ASP	3.2
1	E	523	PHE	3.2
1	B	262	PHE	3.2
1	F	150	LEU	3.2
1	D	476	GLY	3.2
1	D	512	ASN	3.1
1	B	103	THR	3.1
1	C	294	PHE	3.1
1	D	128	LEU	3.1
1	F	190	ILE	3.1
1	F	78	LEU	3.0
1	F	47	LEU	3.0
1	C	269	THR	3.0
1	C	129	TYR	3.0
1	D	176	TYR	3.0
1	D	507	CYS	3.0
1	B	24	SER	3.0
1	C	97	LYS	3.0
1	F	172	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	409	TRP	3.0
1	E	600	GLU	3.0
1	D	599	VAL	2.9
1	D	504	THR	2.9
1	D	587	ALA	2.9
1	E	45	ILE	2.9
1	F	579	VAL	2.9
1	F	33	PHE	2.9
1	F	67	GLN	2.9
1	F	197	GLU	2.9
1	F	186	TRP	2.9
1	F	617	PHE	2.9
1	C	263	GLU	2.9
1	B	242	ASN	2.8
1	F	319	TRP	2.8
1	F	188	ASN	2.8
1	F	79	VAL	2.8
1	E	33	PHE	2.8
1	F	24	SER	2.8
1	C	45	ILE	2.7
1	B	186	TRP	2.7
1	C	293	TRP	2.7
1	C	136	PHE	2.7
1	E	139	GLY	2.7
1	D	185	ILE	2.7
1	E	188	ASN	2.7
1	F	210	GLN	2.7
1	D	474	TYR	2.7
1	E	259	TRP	2.7
1	D	506	ASN	2.7
1	F	176	TYR	2.6
1	C	272	LYS	2.6
1	F	106	PRO	2.6
1	C	78	LEU	2.6
1	F	54	SER	2.6
1	E	129	TYR	2.6
1	C	617	PHE	2.6
1	F	34	TRP	2.6
1	F	52	ILE	2.6
1	F	130	LEU	2.6
1	D	175	ASP	2.5
1	F	164	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	480	LEU	2.5
1	F	607	LEU	2.5
1	E	26	ILE	2.5
1	C	102	GLN	2.5
1	E	599	VAL	2.5
1	D	161	ALA	2.5
1	B	332	THR	2.5
1	F	181	GLY	2.5
1	F	107	TYR	2.5
1	E	136	PHE	2.5
1	F	566	PHE	2.5
1	F	189	PRO	2.4
1	D	509	ASP	2.4
1	E	457	TYR	2.4
1	B	187	LEU	2.4
1	C	91	ASN	2.4
1	E	349	ASN	2.4
1	E	147	PRO	2.4
1	F	159	PRO	2.4
1	F	45	ILE	2.4
1	E	98	GLN	2.4
1	E	527	LEU	2.4
1	F	605	LEU	2.4
1	F	162	ARG	2.4
1	E	176	TYR	2.4
1	F	200	TYR	2.4
1	F	322	TYR	2.4
1	C	57	VAL	2.4
1	D	153	ASN	2.4
1	F	167	LEU	2.4
1	F	333	HIS	2.4
1	F	311	TYR	2.4
1	F	599	VAL	2.4
1	F	228	ALA	2.4
1	F	336	ALA	2.4
1	E	189	PRO	2.3
1	C	96	LEU	2.3
1	F	240	ILE	2.3
1	F	312	LEU	2.3
1	F	517	GLN	2.3
1	D	160	PHE	2.3
1	D	552	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	553	VAL	2.3
1	B	336	ALA	2.3
1	E	605	LEU	2.3
1	F	146	ILE	2.3
1	D	521	PHE	2.3
1	F	129	TYR	2.3
1	F	133	PRO	2.3
1	F	511	ALA	2.3
1	F	32	THR	2.3
1	D	162	ARG	2.3
1	F	409	TRP	2.3
1	D	130	LEU	2.3
1	F	241	PHE	2.3
1	F	294	PHE	2.3
1	D	208	TYR	2.3
1	D	613	TYR	2.3
1	D	133	PRO	2.3
1	D	159	PRO	2.3
1	C	268	GLN	2.3
1	F	344	TRP	2.3
1	F	362	TRP	2.3
1	E	104	LYS	2.3
1	F	235	VAL	2.3
1	E	589	SER	2.2
1	F	258	ASP	2.2
1	E	69	VAL	2.2
1	C	265	ASN	2.2
1	F	208	TYR	2.2
1	E	481	MET	2.2
1	F	95	ILE	2.2
1	F	616	SER	2.2
1	C	301	PHE	2.2
1	C	249	TYR	2.2
1	F	209	TYR	2.2
1	C	298	MET	2.2
1	F	224	LEU	2.2
1	C	288	ILE	2.2
1	F	315	SER	2.2
1	F	207	ASP	2.2
1	B	294	PHE	2.2
1	C	271	PHE	2.2
1	F	160	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	587	ALA	2.2
1	E	409	TRP	2.2
1	D	523	PHE	2.2
1	C	69	VAL	2.1
1	D	472	GLN	2.1
1	F	594	LEU	2.1
1	F	270	SER	2.1
1	E	501	PRO	2.1
1	C	341	MET	2.1
1	F	341	MET	2.1
1	D	157	ASN	2.1
1	D	152	GLY	2.1
1	F	103	THR	2.1
1	F	180	LEU	2.1
1	C	131	ILE	2.1
1	D	200	TYR	2.1
1	E	219	GLU	2.1
1	D	155	ASP	2.1
1	D	199	SER	2.1
1	F	272	LYS	2.1
1	D	136	PHE	2.1
1	E	496	PHE	2.1
1	C	267	VAL	2.1
1	E	235	VAL	2.1
1	C	186	TRP	2.1
1	C	362	TRP	2.1
1	E	587	ALA	2.1
1	C	150	LEU	2.1
1	D	167	LEU	2.1
1	F	507	CYS	2.1
1	F	61	ALA	2.1
1	C	47	LEU	2.1
1	F	292	GLY	2.1
1	D	479	ILE	2.1
1	F	226	GLN	2.0
1	D	69	VAL	2.0
1	E	154	VAL	2.0
1	E	591	PHE	2.0
1	E	567	LEU	2.0
1	F	615	LEU	2.0
1	C	103	THR	2.0
1	D	424	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	473	ILE	2.0
1	F	417	TYR	2.0
1	F	552	TYR	2.0
1	D	398	MET	2.0
1	D	163	HIS	2.0
1	E	402	PHE	2.0
1	B	73	GLU	2.0
1	E	180	LEU	2.0
1	E	224	LEU	2.0
1	E	394	LEU	2.0
1	F	436	LEU	2.0
1	E	99	GLY	2.0
1	F	139	GLY	2.0
1	D	32	THR	2.0
1	E	114	PRO	2.0

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

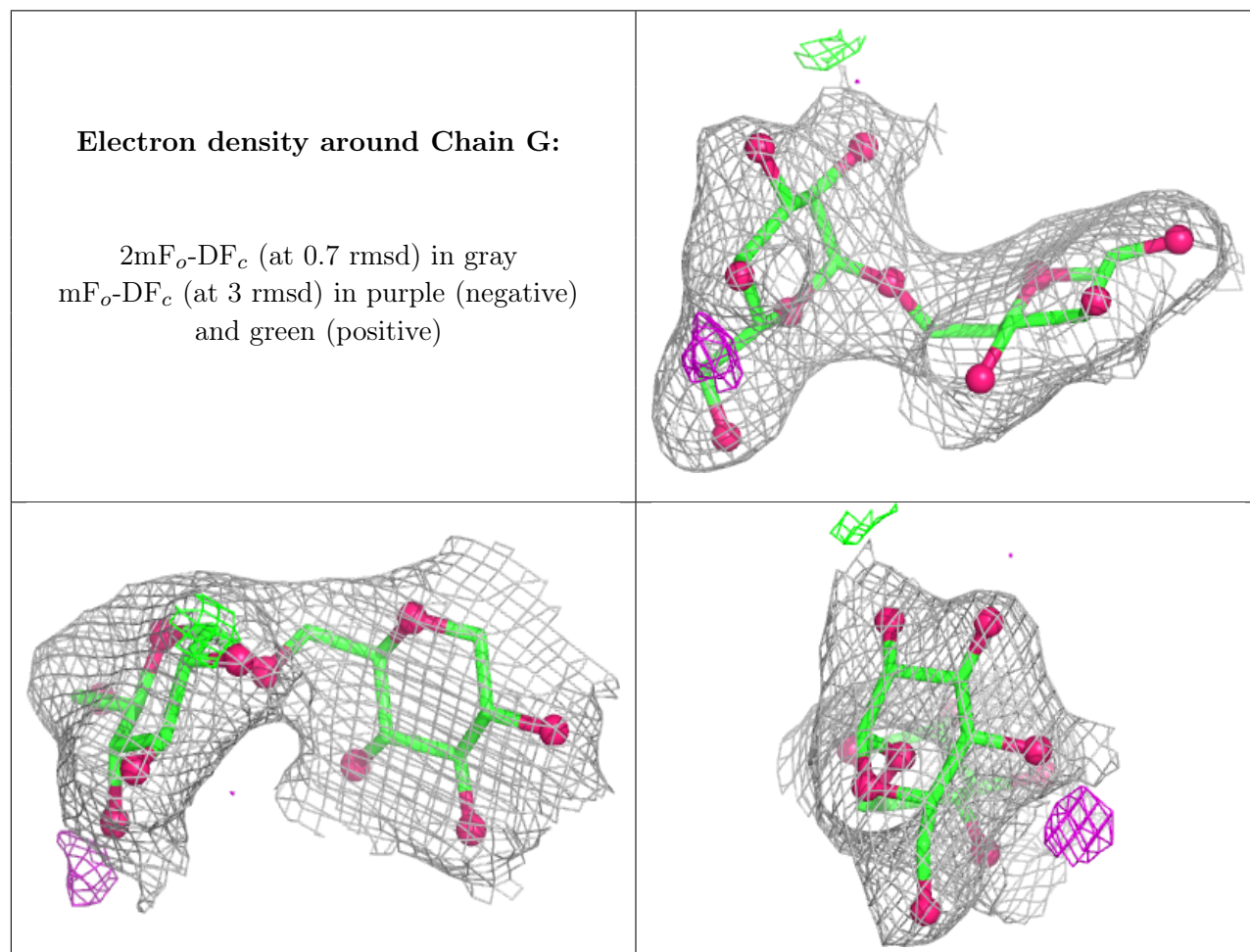
There are no non-standard protein/DNA/RNA residues in this entry.

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.

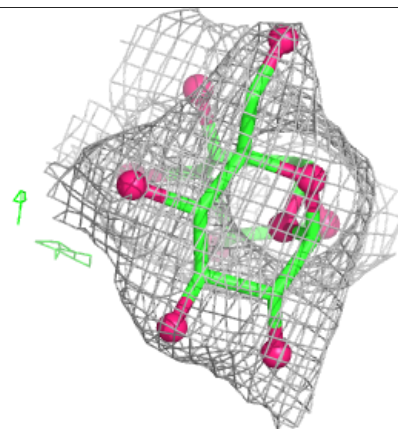
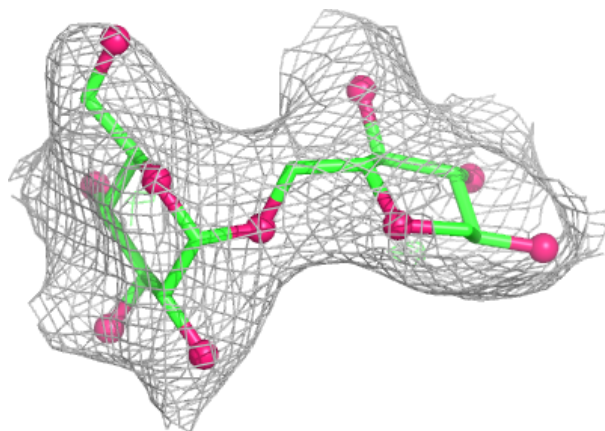
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GLC	J	2	11/12	0.84	0.13	89,94,103,104	0
2	GLC	L	2	11/12	0.85	0.10	84,96,106,110	0
2	GLC	I	2	11/12	0.86	0.11	64,79,99,99	0
2	GLC	K	2	11/12	0.88	0.10	77,89,95,95	0
2	GLC	I	1	11/12	0.91	0.09	69,77,82,84	0
2	GLC	J	1	11/12	0.92	0.10	65,80,85,111	0
2	GLC	G	2	11/12	0.93	0.07	39,45,50,59	0
2	GLC	L	1	11/12	0.94	0.07	73,79,87,92	0
2	GLC	H	1	11/12	0.94	0.07	47,59,72,73	0
2	GLC	K	1	11/12	0.95	0.07	69,81,88,93	0
2	GLC	H	2	11/12	0.95	0.07	62,69,77,93	0
2	GLC	G	1	11/12	0.98	0.05	30,32,37,42	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.



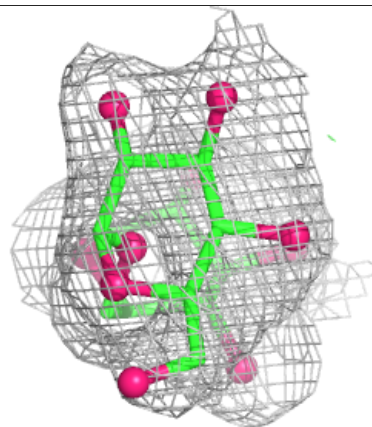
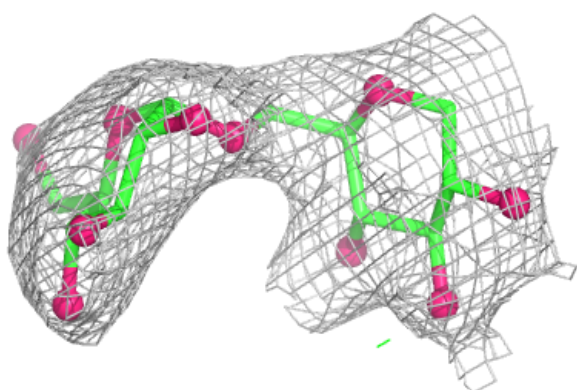
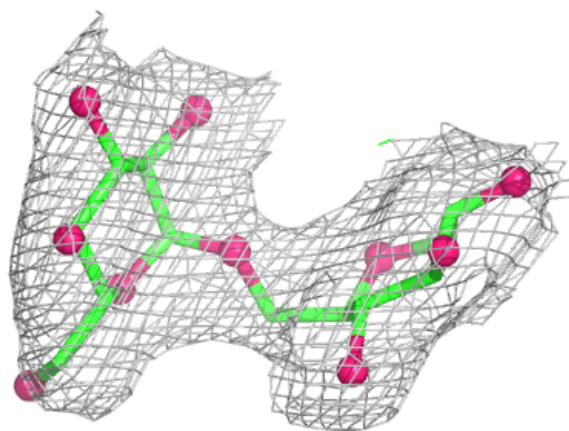
Electron density around Chain H:

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

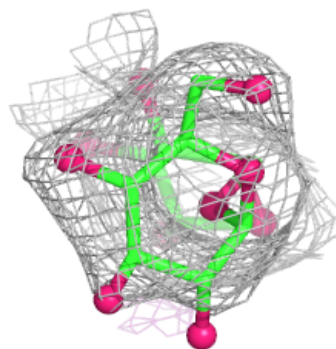
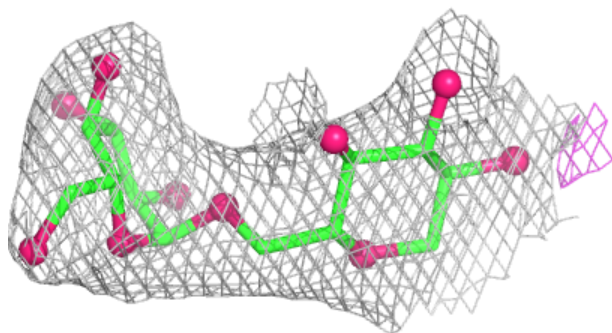
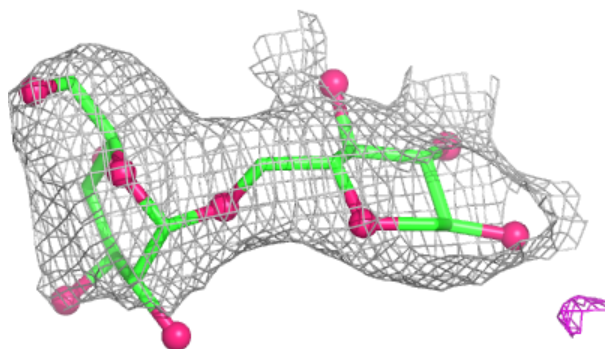


Electron density around Chain I:

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

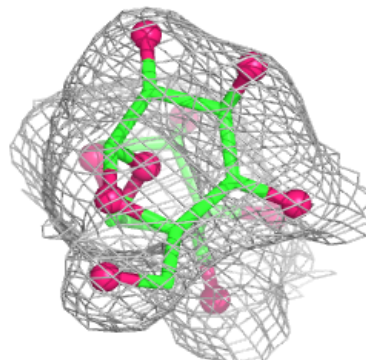
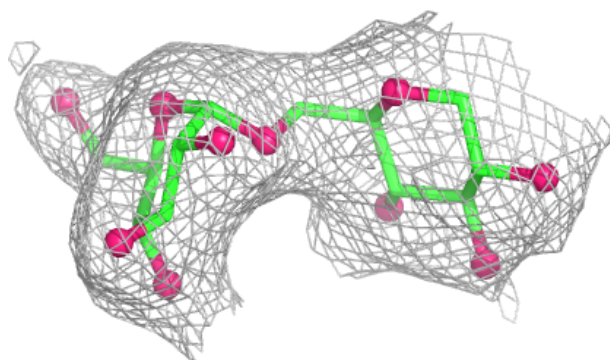
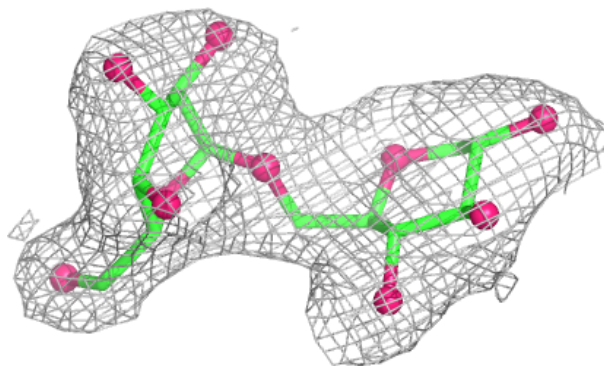
**Electron density around Chain J:**

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

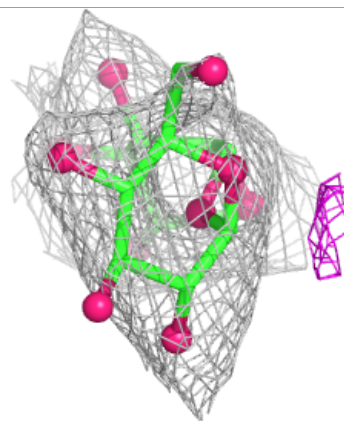
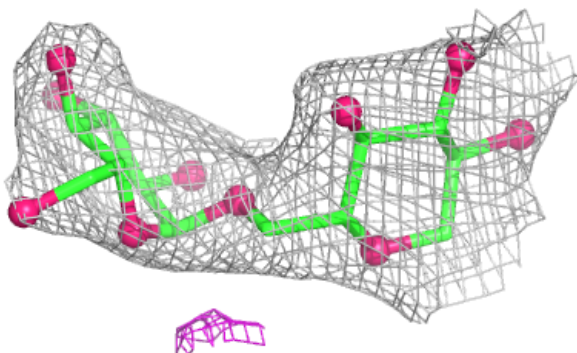
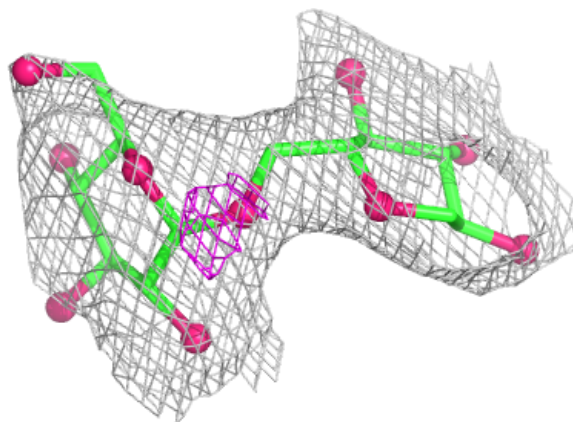


Electron density around Chain K:

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

**Electron density around Chain L:**

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



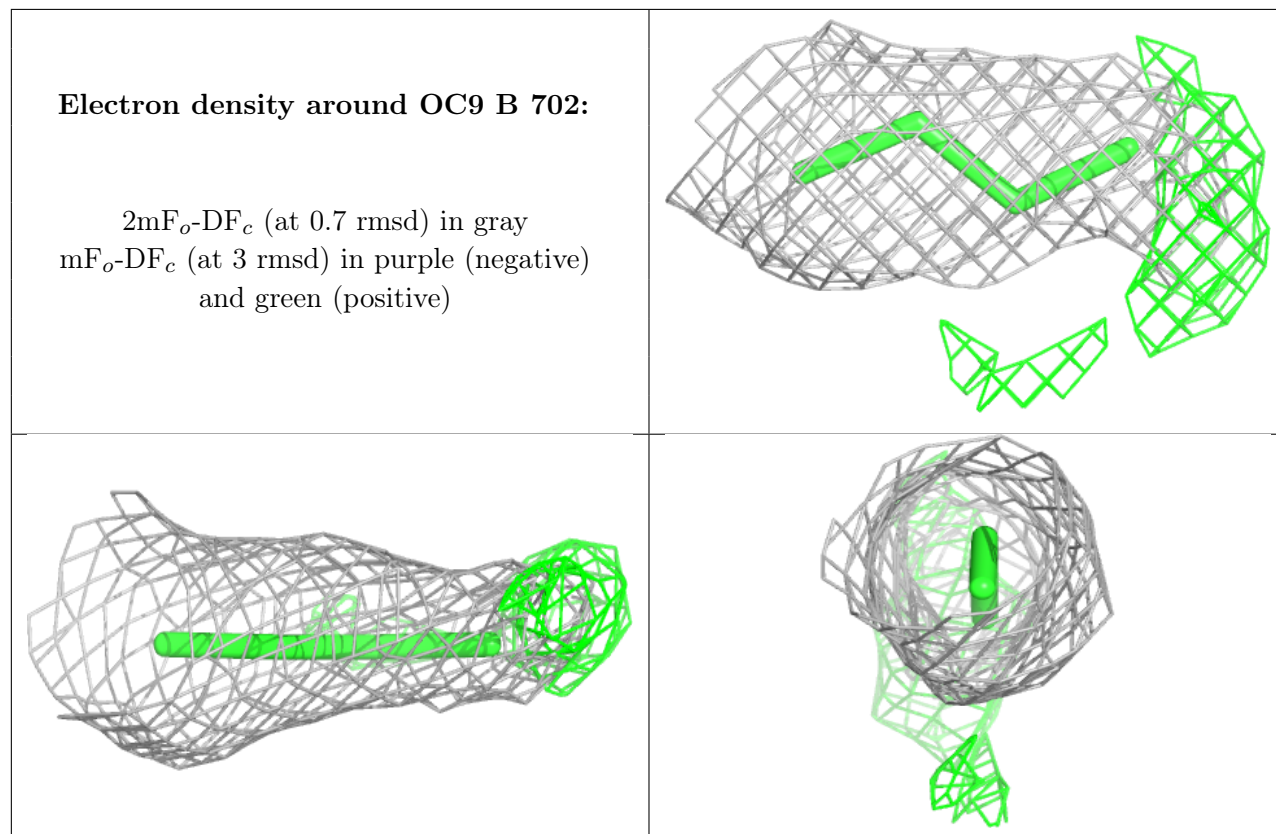
6.4 Ligands ⓘ

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(Å ²)	Q<0.9
4	OC9	B	702	4/9	0.63	0.36	74,75,83,88	0
5	IMD	E	703	5/5	0.72	0.20	88,96,102,103	0
4	OC9	C	702	2/9	0.74	0.36	84,84,84,88	0
5	IMD	C	704	5/5	0.78	0.20	75,84,91,95	0
5	IMD	D	703	5/5	0.79	0.23	83,93,96,99	0
4	OC9	D	702	3/9	0.80	0.23	78,78,86,99	0
4	OC9	E	702	2/9	0.80	0.38	96,96,96,105	0
5	IMD	C	703	5/5	0.80	0.14	96,96,97,100	0
6	CA	C	707	1/1	0.80	0.12	135,135,135,135	0
5	IMD	A	704	5/5	0.85	0.17	57,67,76,79	0
5	IMD	D	705	5/5	0.85	0.13	65,68,71,71	0
6	CA	B	705	1/1	0.89	0.10	93,93,93,93	0
5	IMD	C	705	5/5	0.89	0.13	56,62,72,74	0
5	IMD	D	704	5/5	0.90	0.13	88,92,92,93	0
5	IMD	F	702	5/5	0.90	0.12	78,80,82,85	0
3	PBW	C	701	12/13	0.91	0.09	68,79,89,90	0
5	IMD	B	703	5/5	0.91	0.15	58,58,67,75	0
3	PBW	F	701	12/13	0.91	0.08	77,90,97,98	0
6	CA	F	704	1/1	0.92	0.08	128,128,128,128	0
4	OC9	A	702	4/9	0.93	0.12	42,45,51,57	0
3	PBW	E	701	12/13	0.93	0.08	64,74,84,85	0
5	IMD	A	705	5/5	0.93	0.15	58,62,65,73	0
3	PBW	B	701	12/13	0.94	0.07	51,61,72,84	0
5	IMD	A	703	5/5	0.94	0.10	35,43,44,49	0
3	PBW	D	701	12/13	0.95	0.08	63,68,72,74	0
6	CA	E	704	1/1	0.95	0.05	77,77,77,77	0
6	CA	C	706	1/1	0.95	0.06	102,102,102,102	0
6	CA	F	703	1/1	0.96	0.06	99,99,99,99	0
3	PBW	A	701	12/13	0.97	0.06	29,33,48,48	0
6	CA	E	705	1/1	0.97	0.06	131,131,131,131	0
6	CA	D	706	1/1	0.98	0.07	105,105,105,105	0
6	CA	A	707	1/1	0.99	0.04	43,43,43,43	0
6	CA	B	704	1/1	0.99	0.10	73,73,73,73	0
6	CA	A	706	1/1	0.99	0.10	58,58,58,58	0
6	CA	D	707	1/1	0.99	0.03	75,75,75,75	0

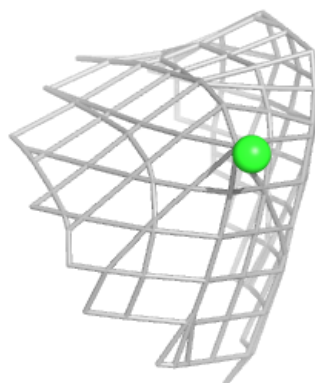
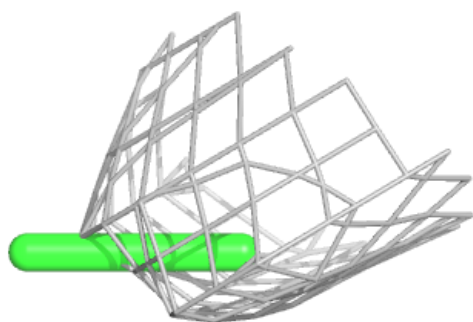
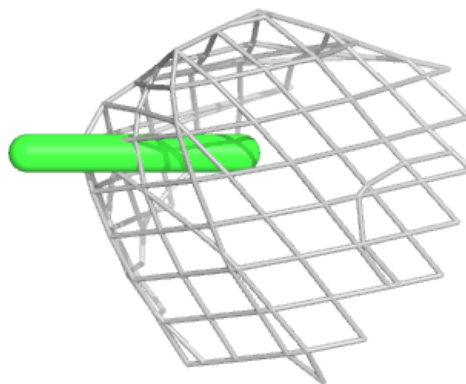
The following is a graphical depiction of the model fit to experimental electron density of all

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.

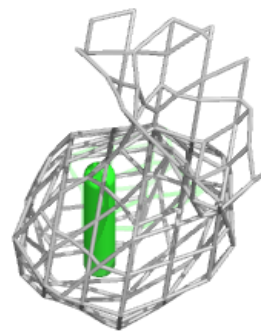
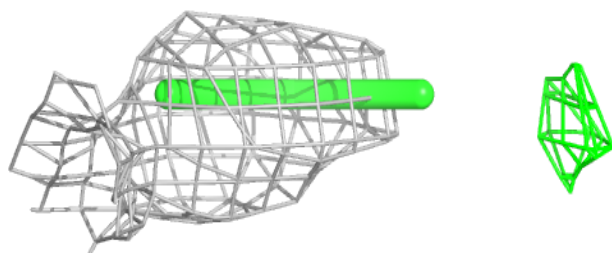
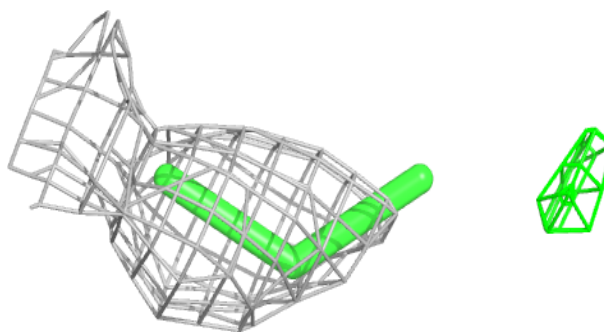


Electron density around OC9 C 702:

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

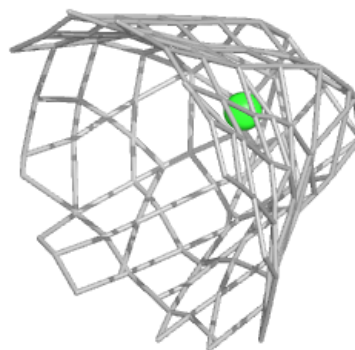
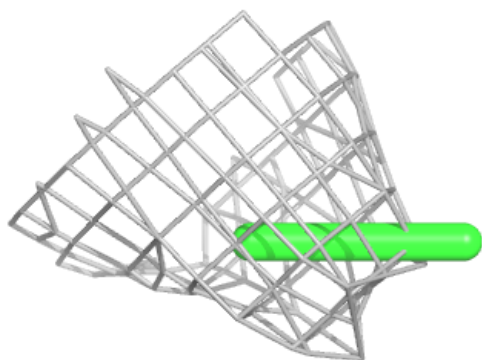
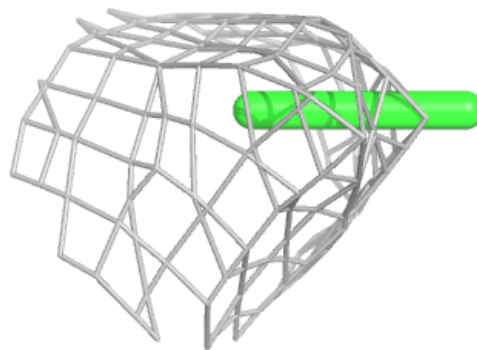
**Electron density around OC9 D 702:**

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



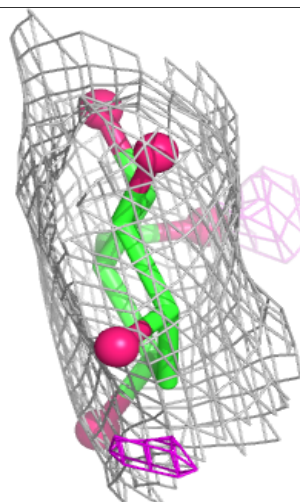
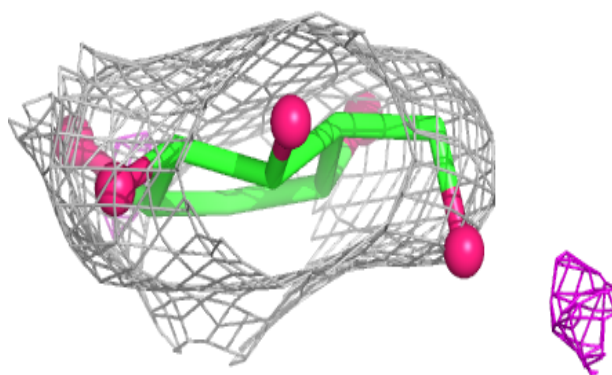
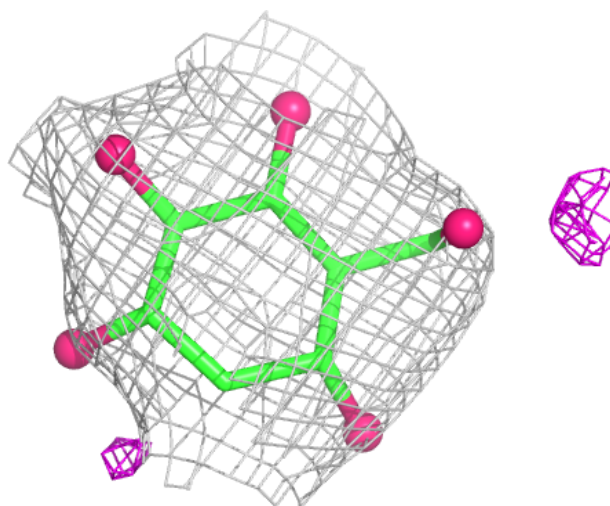
Electron density around OC9 E 702:

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



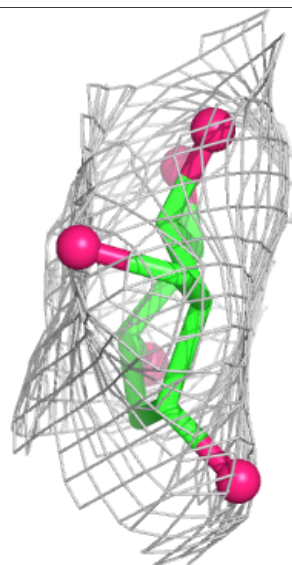
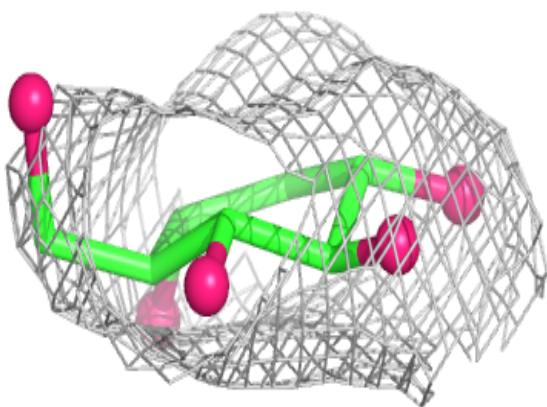
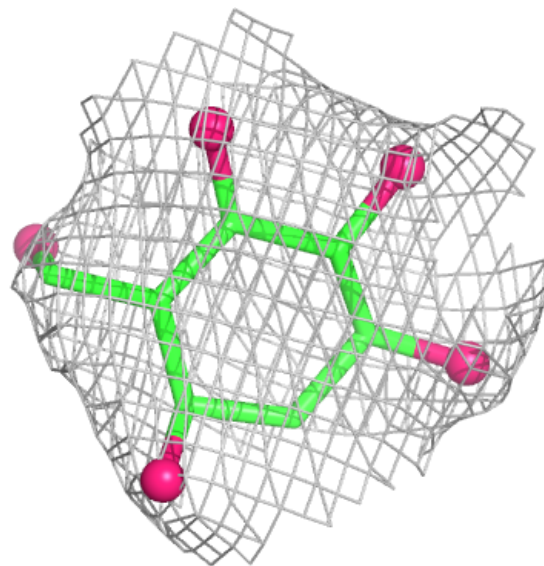
Electron density around PBW C 701:

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



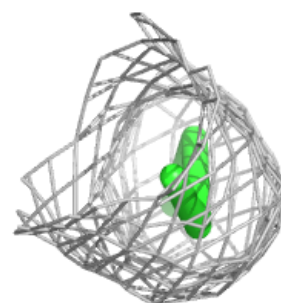
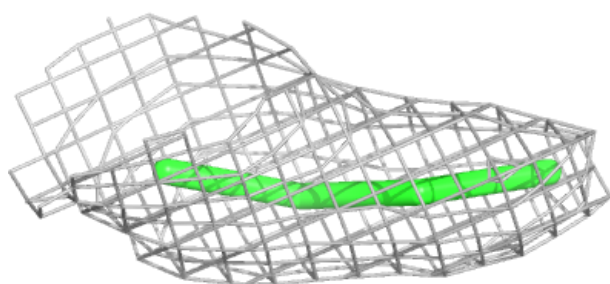
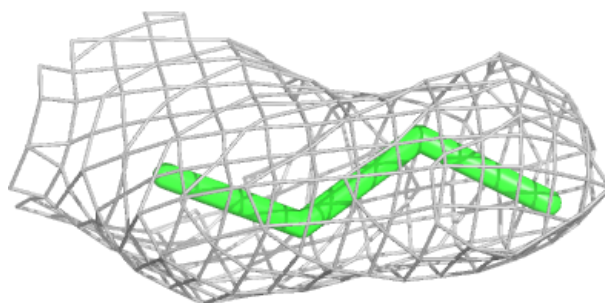
Electron density around PBW F 701:

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



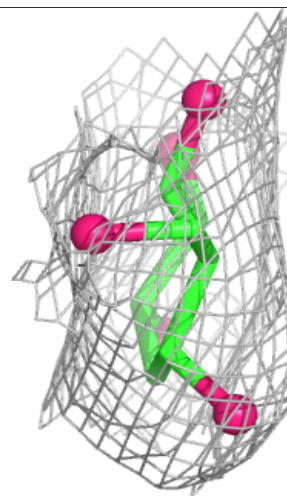
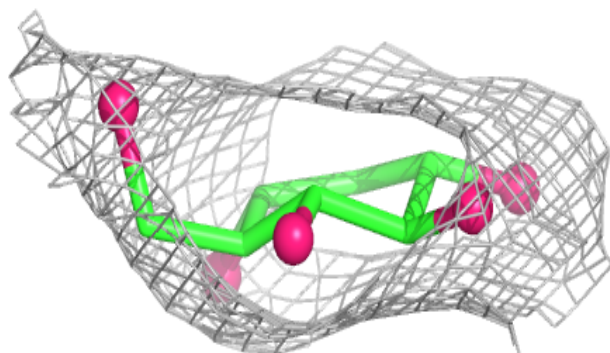
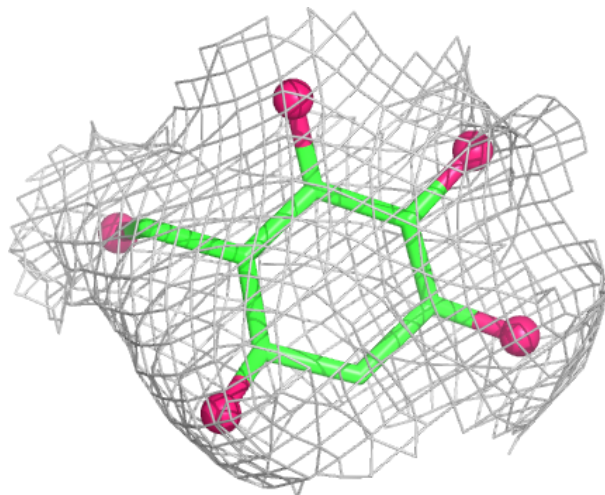
Electron density around OC9 A 702:

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



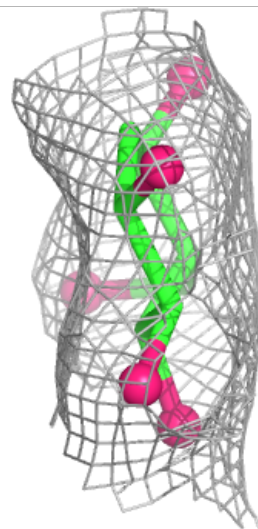
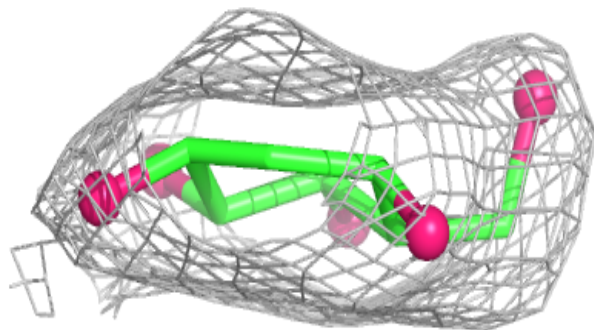
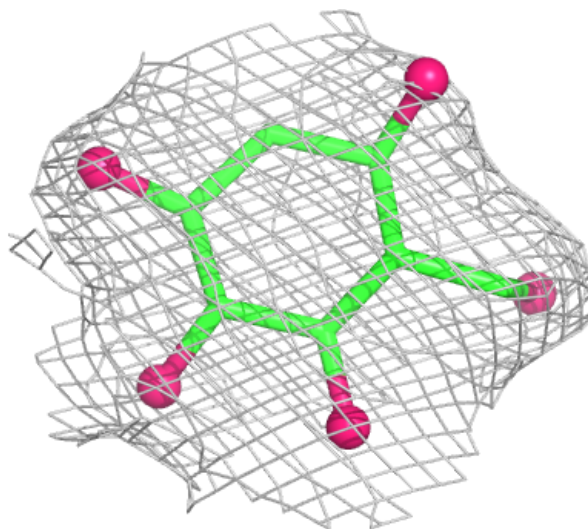
Electron density around PBW E 701:

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



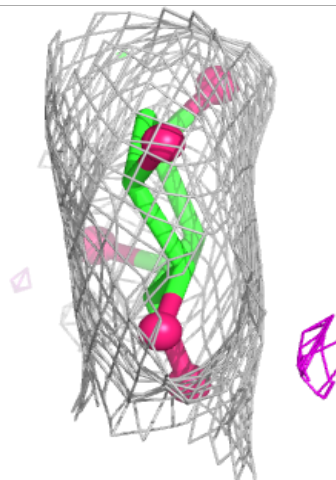
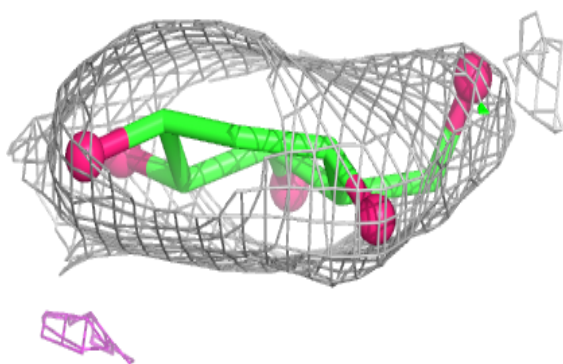
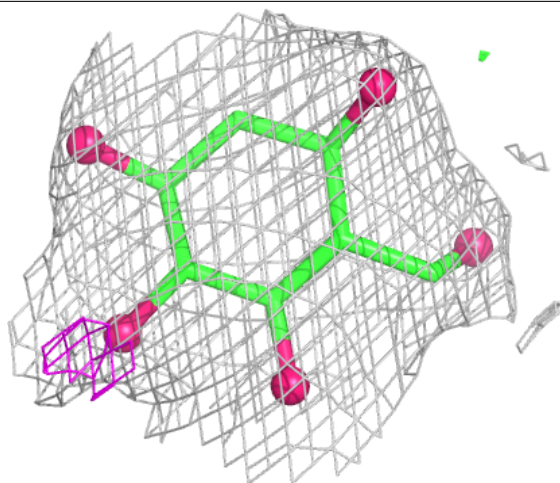
Electron density around PBW B 701:

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



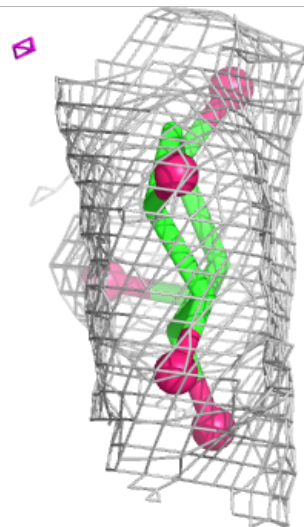
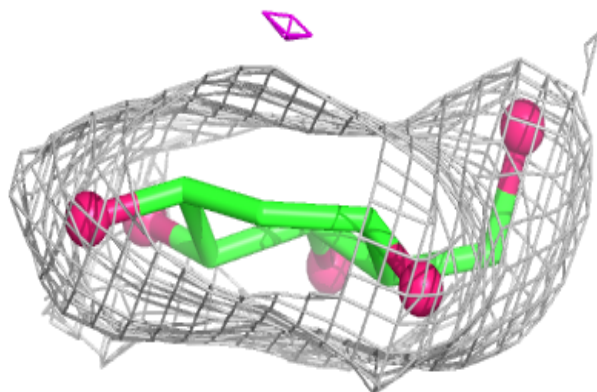
Electron density around PBW D 701:

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



Electron density around PBW A 701:

$2mF_o-DF_c$ (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.