



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:11 PM UTC

PDB ID : 3HT3 / pdb_00003ht3
Title : Crystal structure of fragment DNA polymerase I from *Bacillus stearothermophilus* V713P mutant bound to G:dCTP
Authors : Wu, E.Y.; Beese, L.S.
Deposited on : 2009-06-11
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

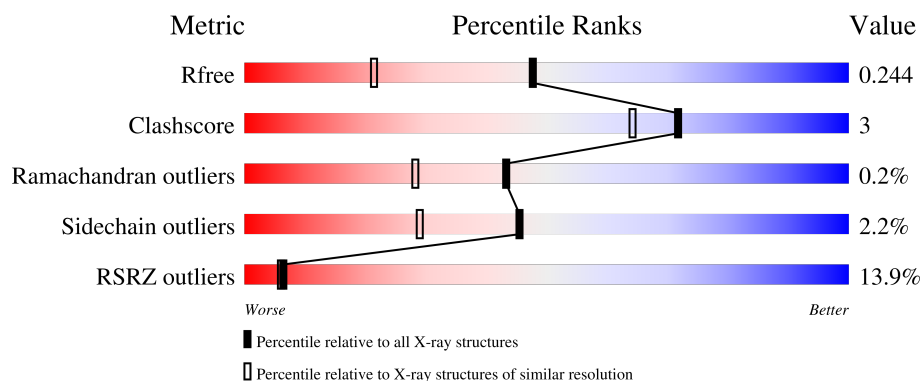
1 Overall quality at a glance

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	579	18% 92% 8%
1	D	579	9% 92% 7%
2	B	9	11% 78% 22%
2	E	9	22% 67% 33%
3	C	12	17% 92% 8%

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Mol	Chain	Length	Quality of chain
3	F	12	17% 100%
4	G	2	100%
4	H	2	100%
4	I	2	50% 50%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 11370 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 DNA polymerase I, large fragment.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	579	Total	C	N	O	S	0	5	0
			4678	2975	811	875	17			
1	D	579	Total	C	N	O	S	0	6	0
			4678	2978	810	872	18			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	598	ALA	ASP	engineered mutation	PDB 3HT3
A	713	PRO	VAL	engineered mutation	PDB 3HT3
D	598	ALA	ASP	engineered mutation	PDB 3HT3
D	713	PRO	VAL	engineered mutation	PDB 3HT3

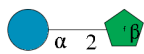
- Molecule 2 is a DNA chain called 5'-D(*CP*GP*AP*TP*CP*AP*CP*GP*(DOC))-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	9	Total	C	N	O	P	0	0	0
			178	86	34	50	8			
2	E	9	Total	C	N	O	P	0	0	0
			178	86	34	50	8			

- Molecule 3 is a DNA chain called 5'-D(*AP*CP*GP*GP*CP*GP*TP*GP*AP*TP*CP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	12	Total	C	N	O	P	0	0	0
			246	117	48	70	11			
3	F	12	Total	C	N	O	P	0	0	0
			246	117	48	70	11			

- Molecule 4 is an oligosaccharide called beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose.

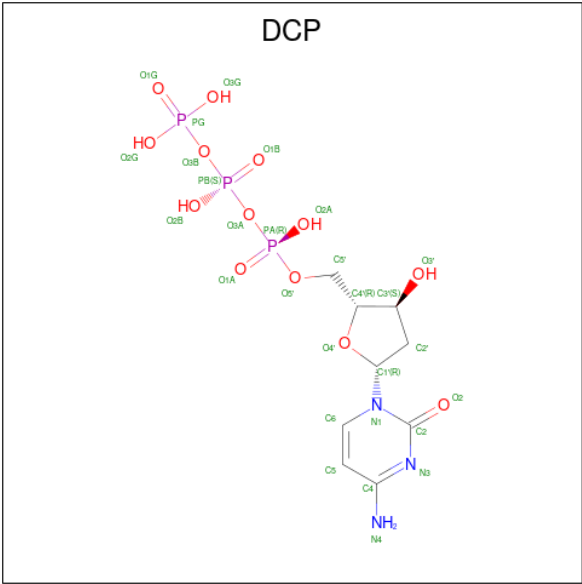


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
4	G	2	Total	C	O	0	0	0
			23	12	11			
4	H	2	Total	C	O	0	0	0
			23	12	11			
4	I	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		
5	D	1	Total	Mg	0	0
			1	1		

- Molecule 6 is 2'-DEOXYCYTIDINE-5'-TRIPHOSPHATE (CCD ID: DCP) (formula: C₉H₁₆N₃O₁₃P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			28	9	3	13	3		
6	A	1	Total	C	N	O	P	0	0
			28	9	3	13	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	D	1	Total	C	N	O	P	0	0
			28	9	3	13	3		

- Molecule 7 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	D	1	Total	O	S	0	0
			5	4	1		
7	D	1	Total	O	S	0	0
			5	4	1		
7	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	365	Total	O	0	0
			365	365		
8	D	521	Total	O	0	0
			521	521		
8	B	21	Total	O	0	0
			21	21		
8	C	32	Total	O	0	0
			32	32		
8	E	16	Total	O	0	0
			16	16		

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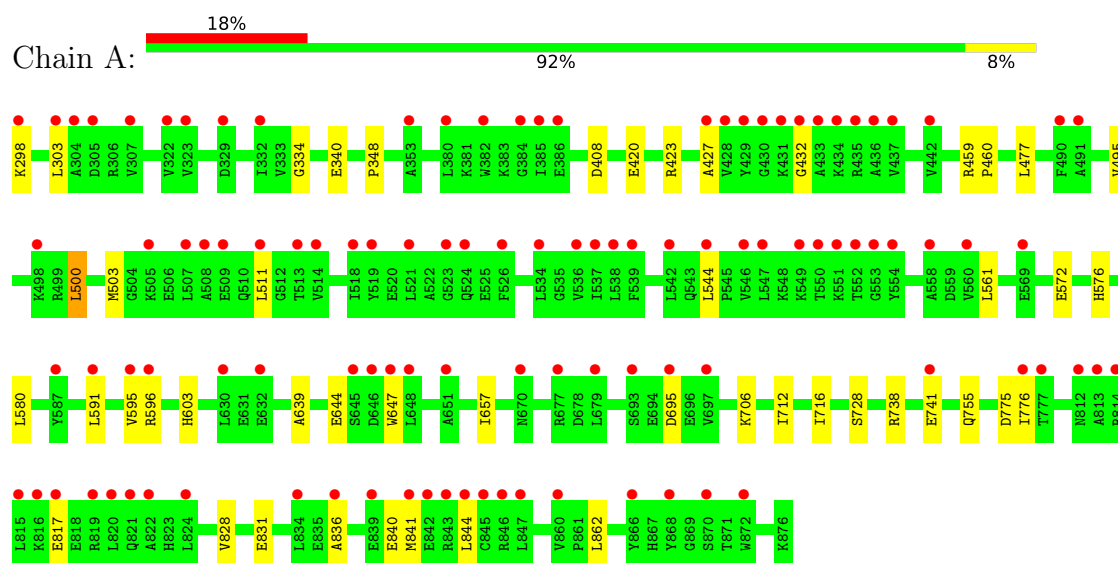
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	F	41	Total	O	0	0
			41	41		

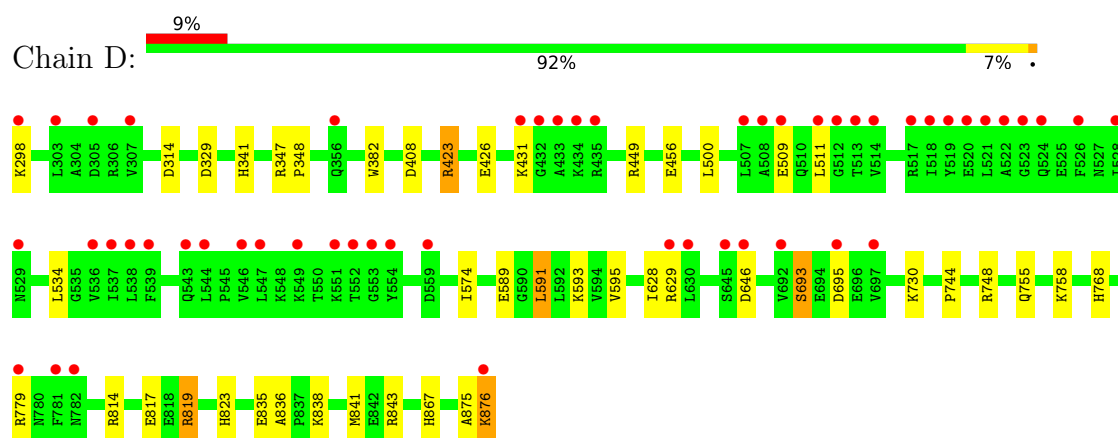
3 Residue-property plots [i](#)

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.

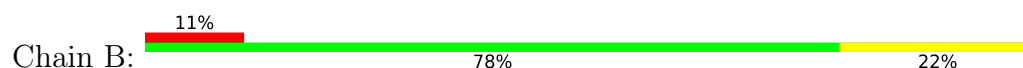
- Molecule 1: DNA polymerase I, large fragment



- Molecule 1: DNA polymerase I, large fragment



- Molecule 2: 5'-D(*CP*GP*AP*TP*CP*AP*CP*GP*(DOC))-3'

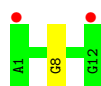




- Molecule 2: 5'-D(*CP*GP*AP*TP*CP*AP*CP*GP*(DOC))-3'



- Molecule 3: 5'-D(*AP*CP*GP*GP*CP*GP*TP*GP*AP*TP*CP*G)-3'



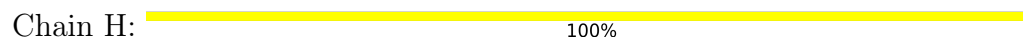
- Molecule 3: 5'-D(*AP*CP*GP*GP*CP*GP*TP*GP*AP*TP*CP*G)-3'



- Molecule 4: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose



- Molecule 4: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose



- Molecule 4: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	93.28Å 108.79Å 152.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.98 – 1.70 46.98 – 1.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.98-1.70) 99.8 (46.98-1.70)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.57 (at 1.70Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.210 , 0.247 0.208 , 0.244	Depositor DCC
R_{free} test set	7528 reflections (4.44%)	wwPDB-VP
Wilson B-factor (Å ²)	17.9	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 40.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11370	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% 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: DOC, GLC, MG, DCP, FRU, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.56	0/4775	0.79	0/6452
1	D	0.62	0/4781	0.80	0/6459
2	B	0.34	0/179	0.97	0/274
2	E	0.36	0/179	1.01	0/274
3	C	0.39	0/276	1.03	0/425
3	F	0.38	0/276	0.95	0/425
All	All	0.58	0/10466	0.82	0/14309

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4678	0	4736	28	0
1	D	4678	0	4751	37	0
2	B	178	0	102	1	0
2	E	178	0	102	2	0
3	C	246	0	136	1	0
3	F	246	0	136	0	0
4	G	23	0	21	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	23	0	21	2	0
4	I	23	0	21	0	0
5	A	1	0	0	0	0
5	D	1	0	0	0	0
6	A	56	0	24	1	0
6	D	28	0	12	0	0
7	D	15	0	0	0	0
8	A	365	0	0	8	0
8	B	21	0	0	0	0
8	C	32	0	0	1	0
8	D	521	0	0	9	0
8	E	16	0	0	0	0
8	F	41	0	0	0	0
All	All	11370	0	10062	67	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 3.

All (67) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:758:LYS:HE2	8:D:972:HOH:O	1.56	1.04
1:D:423:ARG:HG2	1:D:423:ARG:HH11	1.31	0.96
1:D:876:LYS:HE3	8:D:14:HOH:O	1.74	0.86
1:D:456:GLU:HG2	8:D:295:HOH:O	1.74	0.86
1:D:843:ARG:HD2	8:D:180:HOH:O	1.75	0.86
1:D:819:ARG:HH11	1:D:819:ARG:HG3	1.40	0.85
1:D:408:ASP:HB2	4:H:2:FRU:H11	1.65	0.78
1:D:693:SER:HB2	1:D:695:ASP:OD1	1.92	0.70
1:A:657:ILE:HD13	1:A:862:LEU:HD22	1.78	0.66
1:D:875:ALA:C	1:D:876:LYS:HG2	2.22	0.65
1:D:867:HIS:CG	1:D:876:LYS:HA	2.32	0.65
1:D:875:ALA:O	1:D:876:LYS:HG2	1.96	0.65
1:A:423:ARG:HH11	1:A:427:ALA:HB1	1.64	0.63
1:D:534:LEU:HD11	1:D:574:ILE:HD13	1.80	0.63
1:A:596:ARG:HD3	1:A:603:HIS:CD2	2.34	0.62
1:D:298:LYS:HB3	1:D:449:ARG:NH2	2.15	0.62
1:A:695:ASP:HB3	8:A:996:HOH:O	2.02	0.59
1:D:819:ARG:HG3	1:D:819:ARG:NH1	2.13	0.58
1:A:459:ARG:HG3	8:A:1107:HOH:O	2.04	0.57
1:A:596:ARG:HD3	1:A:603:HIS:HD2	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:840:GLU:HB3	8:A:1052:HOH:O	2.04	0.57
1:D:426:GLU:OE2	1:D:431:LYS:HD3	2.05	0.56
1:D:744:PRO:HB2	1:D:748[B]:ARG:HH12	1.73	0.54
1:D:629:ARG:HH22	2:E:29:DOC:H5	1.73	0.54
1:D:423:ARG:HG2	1:D:423:ARG:NH1	2.08	0.53
1:D:456:GLU:CG	8:D:295:HOH:O	2.44	0.53
1:A:591:LEU:O	1:A:595:VAL:HG23	2.10	0.52
1:D:836:ALA:HB3	1:D:841:MET:CE	2.40	0.52
1:D:591:LEU:O	1:D:595:VAL:HG23	2.11	0.51
1:A:408:ASP:HB2	4:G:2:FRU:H11	1.92	0.51
1:A:596:ARG:NH2	8:A:121:HOH:O	2.43	0.51
1:D:744:PRO:HB2	1:D:748[B]:ARG:NH1	2.26	0.50
1:D:408:ASP:HB2	4:H:2:FRU:C1	2.39	0.50
1:D:779:ARG:HD3	8:D:1115:HOH:O	2.12	0.48
1:A:706:LYS:HE3	6:A:201:DCP:O3B	2.14	0.48
1:D:646:ASP:HB3	1:D:838:LYS:HE3	1.96	0.48
1:A:738:ARG:HA	1:A:741:GLU:HG2	1.96	0.48
1:A:459:ARG:NH2	1:D:314:ASP:O	2.47	0.48
1:D:589:GLU:O	1:D:593:LYS:HG3	2.13	0.47
2:B:21:DC:H2''	2:B:22:DG:C8	2.49	0.47
2:E:21:DC:H2'	2:E:22:DG:C8	2.50	0.46
1:D:814:ARG:HA	1:D:817:GLU:HG2	1.98	0.46
1:A:459:ARG:HB3	1:A:460:PRO:HD3	1.98	0.45
1:A:500:LEU:HA	1:A:503:MET:HE3	1.99	0.45
1:A:334:GLY:HA2	1:A:348:PRO:HD3	2.00	0.44
1:A:828:VAL:HB	1:A:831:GLU:CG	2.48	0.44
1:D:341:HIS:HE1	8:D:930:HOH:O	1.99	0.44
1:D:768:HIS:HD2	8:D:1152:HOH:O	2.01	0.43
1:A:755[A]:GLN:HG2	8:A:1053:HOH:O	2.17	0.43
1:D:423:ARG:NH1	1:D:423:ARG:CG	2.79	0.43
1:D:823:HIS:HE1	1:D:835:GLU:OE2	2.02	0.43
1:D:867:HIS:CB	1:D:876:LYS:HA	2.48	0.43
1:D:755:GLN:HG2	8:D:126:HOH:O	2.19	0.42
1:A:738:ARG:HA	1:A:741:GLU:CG	2.50	0.42
1:A:500:LEU:HD13	1:A:639:ALA:CB	2.50	0.42
1:A:817:GLU:HG2	8:A:1143:HOH:O	2.19	0.42
1:A:576:HIS:CE1	1:A:580:LEU:HD11	2.55	0.42
1:A:775:ASP:HB2	8:A:67:HOH:O	2.20	0.41
1:A:712:ILE:HA	1:A:716:ILE:HG22	2.02	0.41
1:A:495:VAL:C	8:A:1025:HOH:O	2.64	0.41
1:D:329:ASP:H	1:D:382:TRP:CD1	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:836:ALA:HB3	1:A:841:MET:CE	2.50	0.40
1:D:534:LEU:HD11	1:D:574:ILE:CD1	2.50	0.40
1:A:644:GLU:HB2	1:A:647:TRP:CD1	2.57	0.40
1:D:347:ARG:HA	1:D:348:PRO:HD3	1.98	0.40
3:C:8:DG:H4'	8:C:587:HOH:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	582/579 (100%)	569 (98%)	12 (2%)	1 (0%)	43	28
1	D	583/579 (101%)	572 (98%)	10 (2%)	1 (0%)	43	28
All	All	1165/1158 (101%)	1141 (98%)	22 (2%)	2 (0%)	43	28

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	432	GLY
1	D	628	ILE

5.3.2 Protein sidechains [i](#)

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	500/495 (101%)	486 (97%)	14 (3%)	38	21
1	D	501/495 (101%)	492 (98%)	9 (2%)	51	36
All	All	1001/990 (101%)	978 (98%)	23 (2%)	45	27

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	298	LYS
1	A	303	LEU
1	A	340	GLU
1	A	420[A]	GLU
1	A	420[B]	GLU
1	A	477	LEU
1	A	500	LEU
1	A	511	LEU
1	A	544	LEU
1	A	561	LEU
1	A	572	GLU
1	A	728	SER
1	A	776	ILE
1	A	844	LEU
1	D	423	ARG
1	D	500	LEU
1	D	509	GLU
1	D	511	LEU
1	D	591	LEU
1	D	693	SER
1	D	730	LYS
1	D	819	ARG
1	D	876	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	356	GLN
1	A	468	ASN
1	A	470	GLN
1	A	579	GLN
1	A	704	GLN
1	A	782	ASN
1	A	821	GLN

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Mol	Chain	Res	Type
1	A	867	HIS
1	D	341	HIS
1	D	418	GLN
1	D	468	ASN
1	D	470	GLN
1	D	524	GLN
1	D	723	GLN
1	D	755	GLN
1	D	768	HIS
1	D	823	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	DOC	B	29	3,2	16,19,20	0.85	0	20,26,29	1.02	0
2	DOC	E	29	3,2	16,19,20	0.86	0	20,26,29	0.99	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DOC	B	29	3,2	-	0/7/18/19	0/2/2/2
2	DOC	E	29	3,2	-	0/7/18/19	0/2/2/2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	29	DOC	1	0

5.5 Carbohydrates

6 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	GLC	G	1	4	11,11,12	0.57	0	15,15,17	1.21	1 (6%)
4	FRU	G	2	4	11,12,12	0.57	0	10,18,18	0.79	0
4	GLC	H	1	4	11,11,12	0.45	0	15,15,17	0.96	1 (6%)
4	FRU	H	2	4	11,12,12	0.58	0	10,18,18	0.71	0
4	GLC	I	1	4	11,11,12	0.52	0	15,15,17	0.86	1 (6%)
4	FRU	I	2	4	11,12,12	0.55	0	10,18,18	0.80	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
4	GLC	G	1	4	-	0/2/19/22	0/1/1/1
4	FRU	G	2	4	-	0/5/24/24	0/1/1/1
4	GLC	H	1	4	-	0/2/19/22	0/1/1/1
4	FRU	H	2	4	-	0/5/24/24	0/1/1/1
4	GLC	I	1	4	-	0/2/19/22	0/1/1/1
4	FRU	I	2	4	-	0/5/24/24	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	1	GLC	C1-O5-C5	4.36	118.03	112.19
4	H	1	GLC	C1-O5-C5	3.02	116.23	112.19
4	I	1	GLC	C1-O5-C5	2.45	115.47	112.19

There are no chirality outliers.

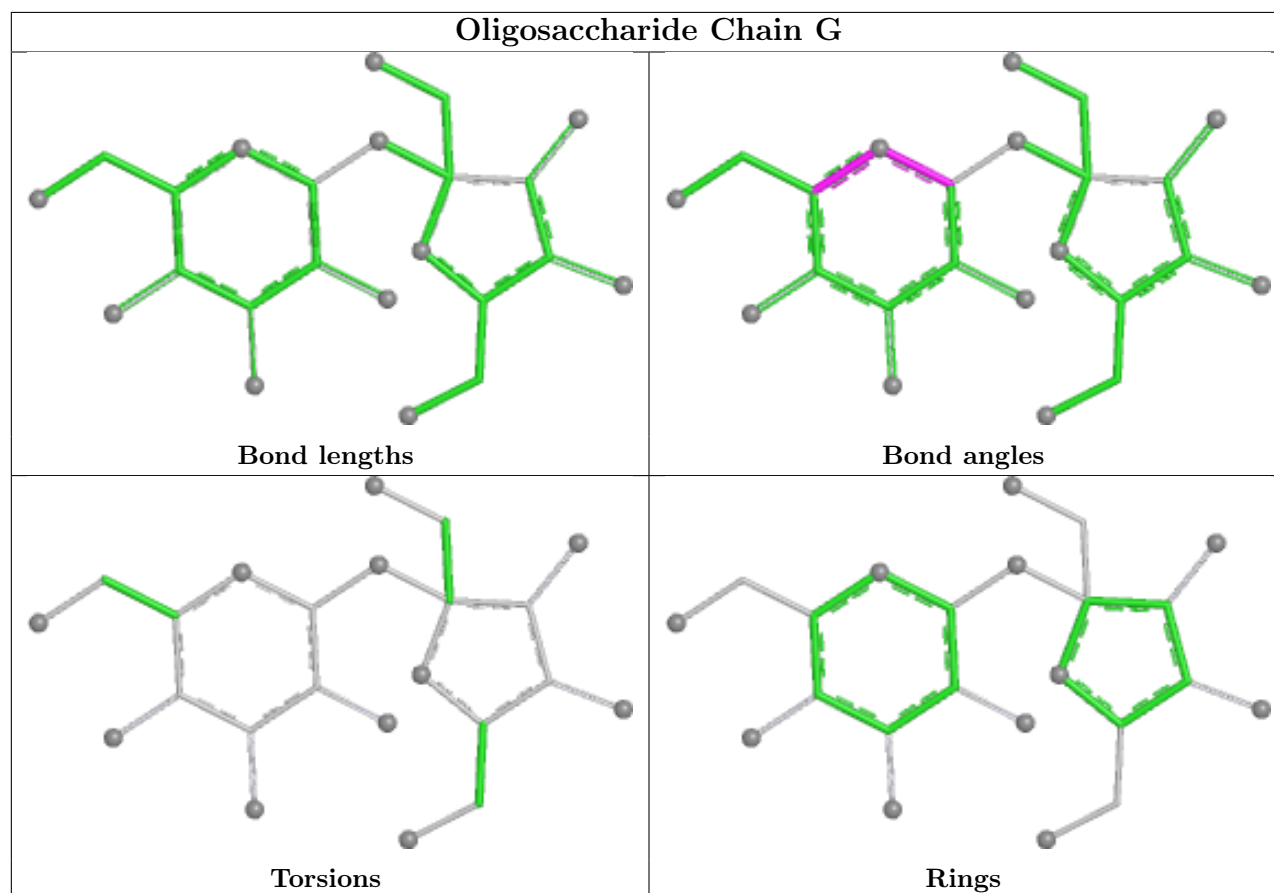
There are no torsion outliers.

There are no ring outliers.

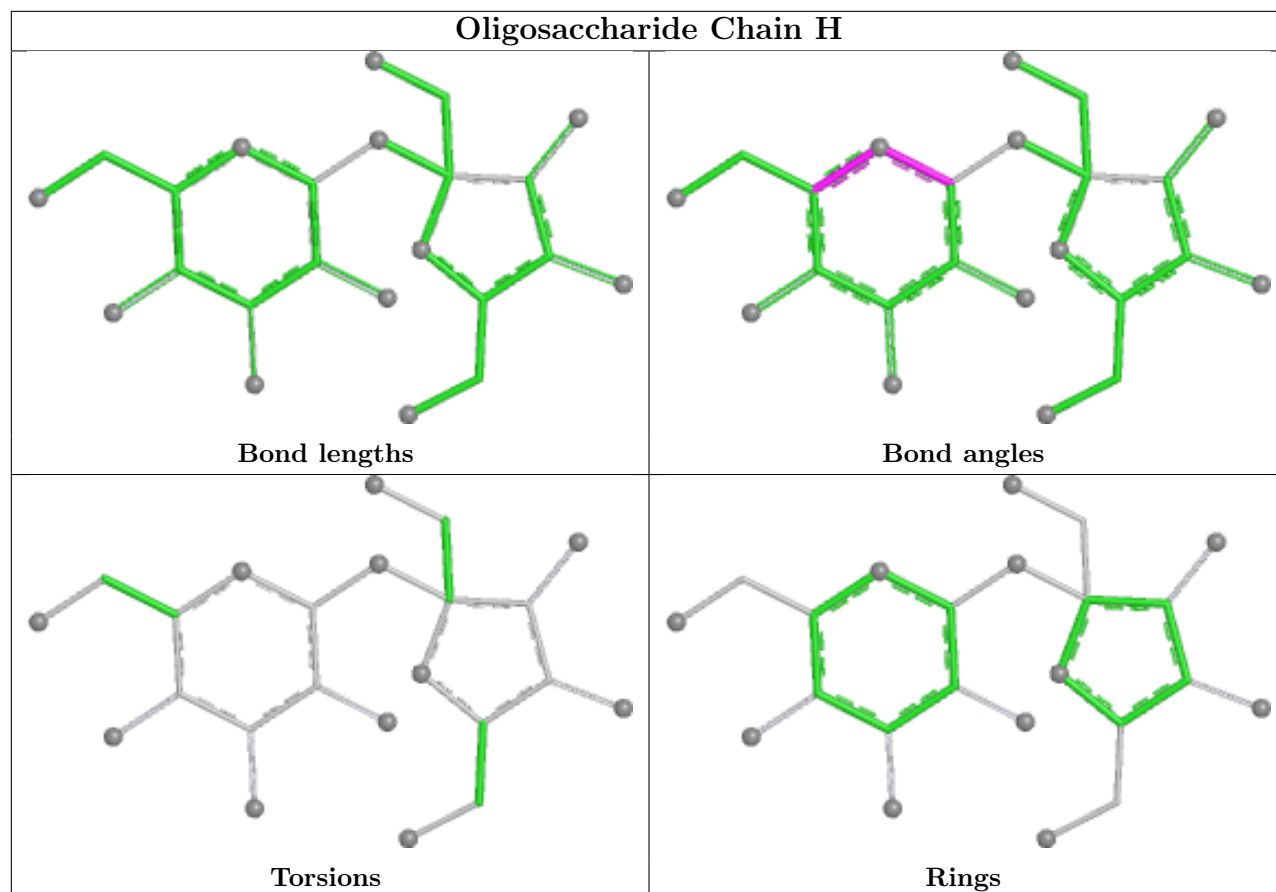
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	2	FRU	1	0
4	H	2	FRU	2	0

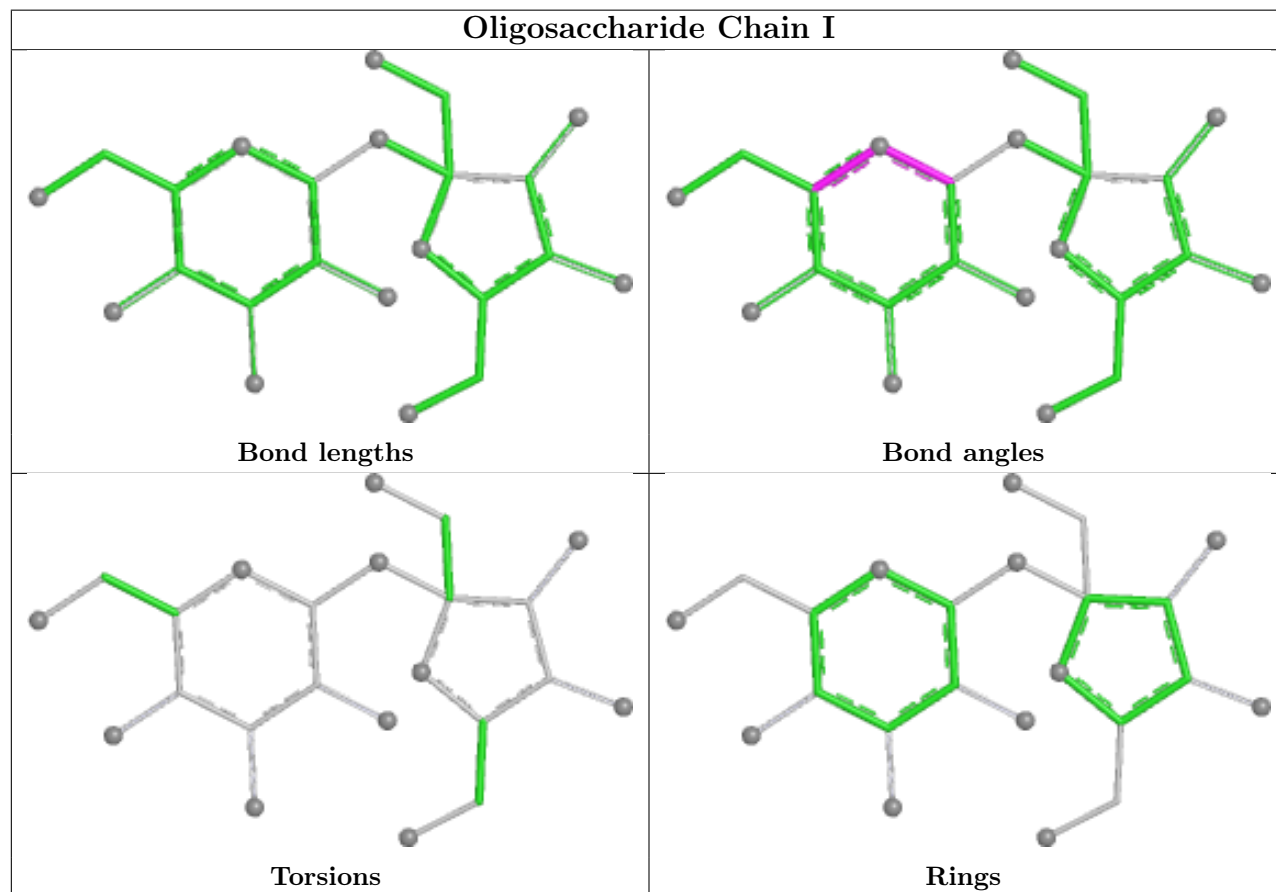
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



Oligosaccharide Chain H



Oligosaccharide Chain I



5.6 Ligand geometry

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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$
7	SO4	D	2	-	4,4,4	0.24	0	6,6,6	0.09	0
7	SO4	D	1	-	4,4,4	0.26	0	6,6,6	0.35	0
6	DCP	D	202	5	28,29,29	1.24	3 (10%)	41,45,45	1.22	5 (12%)
6	DCP	A	201	5	28,29,29	1.14	3 (10%)	41,45,45	1.06	0
6	DCP	A	203	-	28,29,29	1.09	3 (10%)	41,45,45	0.96	0
7	SO4	D	3	-	4,4,4	0.27	0	6,6,6	0.10	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
6	DCP	A	201	5	-	2/22/34/34	0/2/2/2
6	DCP	A	203	-	-	9/22/34/34	0/2/2/2
6	DCP	D	202	5	-	4/22/34/34	0/2/2/2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	202	DCP	PB-O3A	3.57	1.63	1.59
6	D	202	DCP	PA-O3A	3.00	1.62	1.59
6	A	203	DCP	PA-O3A	2.98	1.62	1.59
6	A	201	DCP	PB-O3A	2.83	1.62	1.59
6	A	201	DCP	PA-O3A	2.69	1.62	1.59
6	D	202	DCP	PB-O3B	2.67	1.62	1.59
6	A	203	DCP	PB-O3A	2.41	1.62	1.59
6	A	201	DCP	PB-O3B	2.13	1.61	1.59
6	A	203	DCP	C6-C5	2.03	1.39	1.35

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	202	DCP	C2'-C1'-N1	-3.17	105.89	113.81
6	D	202	DCP	O2A-PA-O1A	2.27	123.00	112.44
6	D	202	DCP	O3B-PB-O1B	-2.22	104.01	110.70
6	D	202	DCP	O3A-PB-O1B	-2.16	104.20	110.70
6	D	202	DCP	O3G-PG-O2G	2.12	115.75	107.80

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	203	DCP	O4'-C4'-C5'-O5'
6	A	203	DCP	PB-O3B-PG-O2G
6	A	203	DCP	PB-O3B-PG-O3G
6	A	203	DCP	C3'-C4'-C5'-O5'
6	A	203	DCP	PG-O3B-PB-O2B
6	D	202	DCP	PB-O3A-PA-O2A
6	A	203	DCP	C5'-O5'-PA-O3A
6	D	202	DCP	PB-O3B-PG-O1G
6	A	203	DCP	PA-O3A-PB-O2B
6	A	201	DCP	PB-O3A-PA-O1A
6	A	201	DCP	PG-O3B-PB-O1B
6	A	203	DCP	PA-O3A-PB-O1B
6	A	203	DCP	PG-O3B-PB-O1B
6	D	202	DCP	PB-O3A-PA-O1A
6	D	202	DCP	PA-O3A-PB-O2B

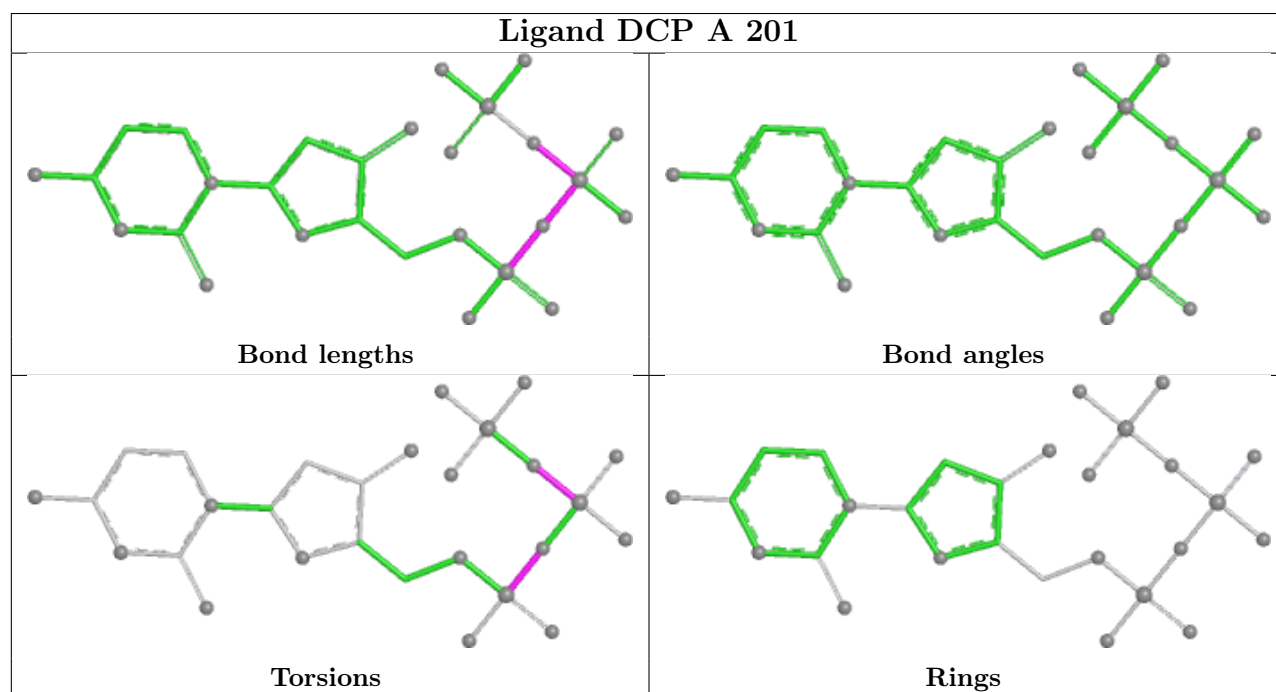
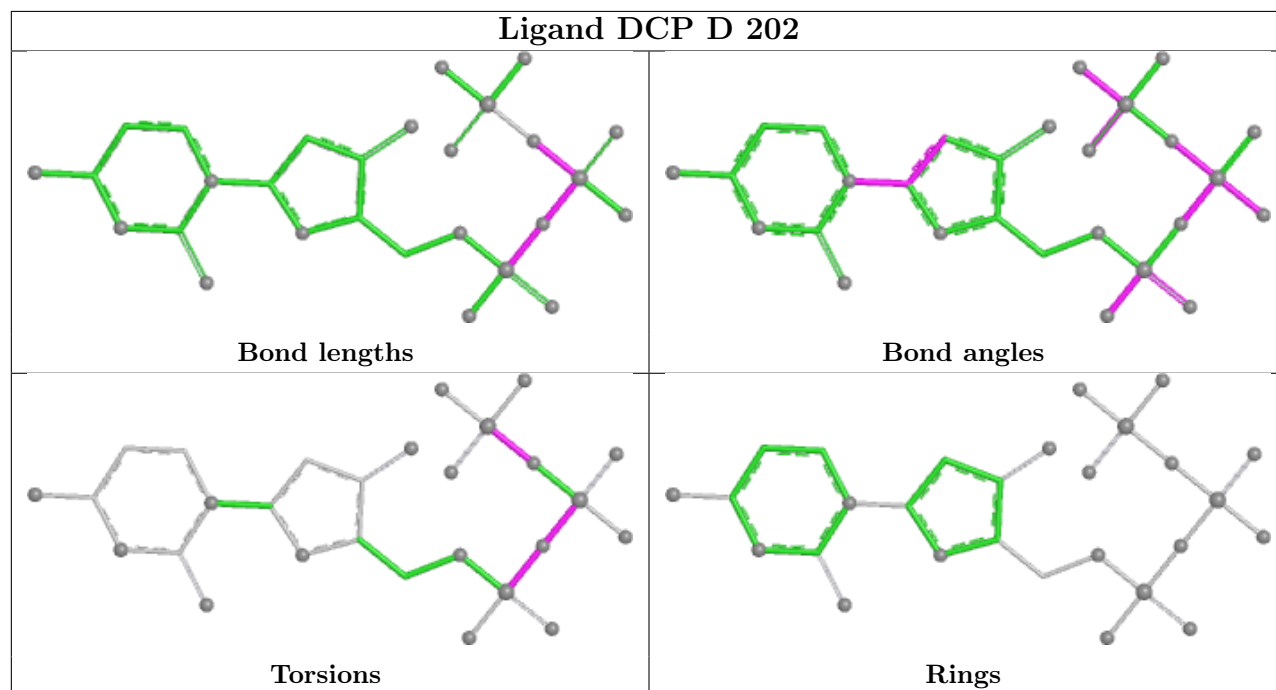
There are no ring outliers.

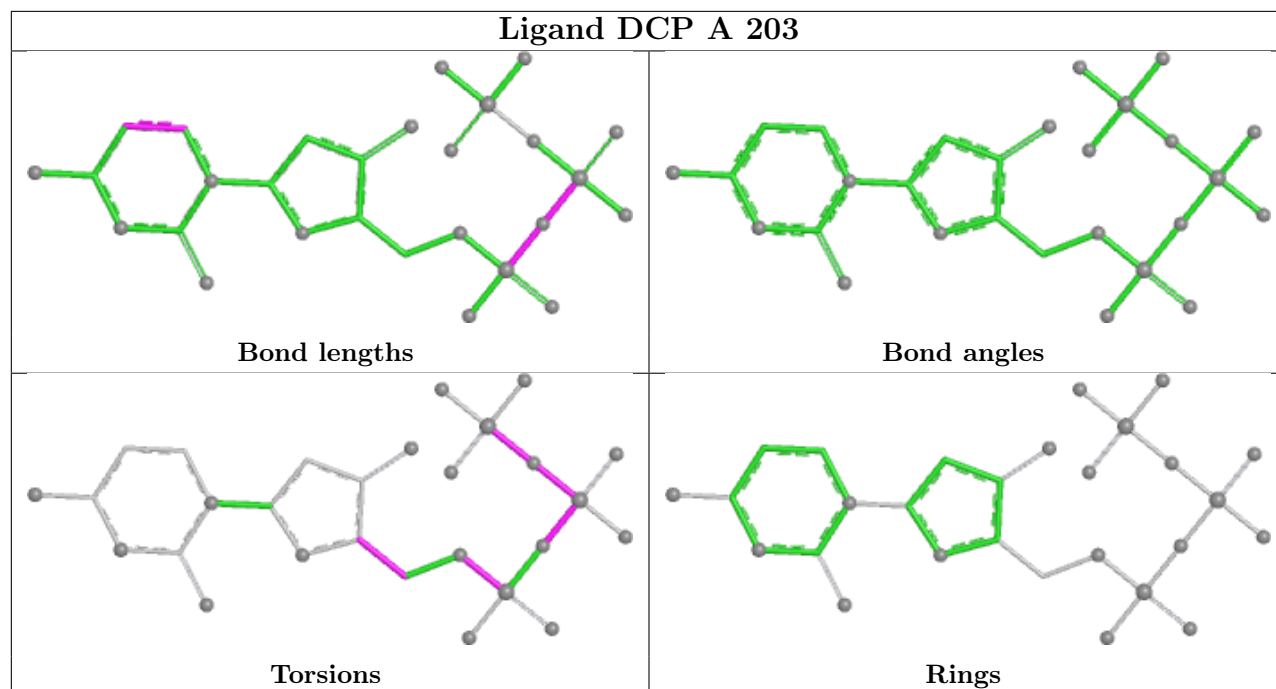
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	201	DCP	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.





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	579/579 (100%)	1.06	107 (18%) 3 3	10, 26, 42, 50	5 (0%)
1	D	579/579 (100%)	0.19	53 (9%) 14 15	6, 15, 38, 45	6 (1%)
2	B	8/9 (88%)	0.50	1 (12%) 8 8	14, 25, 45, 49	0
2	E	8/9 (88%)	0.62	2 (25%) 2 1	11, 28, 50, 57	0
3	C	12/12 (100%)	0.57	2 (16%) 4 4	11, 26, 43, 61	0
3	F	12/12 (100%)	0.51	2 (16%) 4 4	8, 20, 47, 67	0
All	All	1198/1200 (99%)	0.62	167 (13%) 6 6	6, 21, 41, 67	11 (0%)

All (167) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	820	LEU	5.9
1	A	844	LEU	5.1
1	D	433	ALA	4.8
1	A	523	GLY	4.8
1	A	647	TRP	4.4
1	A	437	VAL	3.9
1	A	815	LEU	3.7
1	D	518	ILE	3.7
1	A	819	ARG	3.6
1	A	550	THR	3.6
1	A	847	LEU	3.6
1	A	518	ILE	3.6
1	D	305	ASP	3.6
1	D	554	TYR	3.6
1	A	332	ILE	3.5
1	A	741	GLU	3.5
1	A	679	LEU	3.5
1	D	514	VAL	3.4
3	F	1	DA	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	429	TYR	3.4
1	D	645	SER	3.4
1	A	822	ALA	3.3
1	D	508	ALA	3.3
1	A	490	PHE	3.3
1	A	554	TYR	3.3
1	D	432	GLY	3.3
1	D	551	LYS	3.2
1	A	382	TRP	3.2
1	A	648	LEU	3.2
1	D	553	GLY	3.2
1	D	519	TYR	3.1
1	A	845	CYS	3.1
1	A	427	ALA	3.1
1	D	522	ALA	3.1
1	D	523	GLY	3.1
1	D	876	LYS	3.1
3	C	1	DA	3.1
1	D	521	LEU	3.1
1	D	559	ASP	3.1
1	A	521	LEU	3.0
1	D	511	LEU	3.0
1	A	507	LEU	3.0
1	A	813	ALA	3.0
2	E	21	DC	3.0
1	A	514	VAL	3.0
1	A	816	LYS	3.0
1	A	519	TYR	2.9
1	A	551	LYS	2.9
1	A	491	ALA	2.9
1	A	511	LEU	2.9
1	A	630	LEU	2.9
1	A	430	GLY	2.9
1	A	329	ASP	2.9
1	A	432	GLY	2.8
1	A	534	LEU	2.8
1	A	821	GLN	2.8
1	D	513	THR	2.8
1	A	595	VAL	2.8
1	A	547	LEU	2.8
1	D	782	ASN	2.8
1	A	646	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	526	PHE	2.8
1	A	846	ARG	2.8
1	A	645	SER	2.8
1	A	428	VAL	2.7
1	A	542	LEU	2.7
1	A	670	ASN	2.6
1	D	434	LYS	2.6
1	D	552	THR	2.6
1	A	384	GLY	2.6
1	A	544	LEU	2.6
1	D	781	PHE	2.6
1	D	298	LYS	2.6
1	A	843	ARG	2.6
1	D	509	GLU	2.6
1	D	646	ASP	2.6
1	D	695	ASP	2.6
1	D	356	GLN	2.6
1	A	591	LEU	2.6
1	A	842	GLU	2.6
1	A	298	LYS	2.5
1	A	814	ARG	2.5
1	D	536	VAL	2.5
1	D	539	PHE	2.5
1	A	323	VAL	2.5
1	A	695	ASP	2.5
1	A	651	ALA	2.5
1	A	553	GLY	2.5
1	A	552	THR	2.5
1	A	385	ILE	2.5
1	A	839	GLU	2.5
1	D	529	ASN	2.4
1	A	841	MET	2.4
1	A	558	ALA	2.4
1	A	307	VAL	2.4
1	A	776	ILE	2.4
1	A	870	SER	2.4
1	D	528	ILE	2.4
2	E	22	DG	2.4
1	A	498	LYS	2.4
1	D	544	LEU	2.4
1	D	526	PHE	2.4
1	D	517	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	512	GLY	2.4
1	D	303	LEU	2.4
1	A	435	ARG	2.4
1	D	692	VAL	2.4
1	A	569	GLU	2.3
1	D	538	LEU	2.3
1	D	547	LEU	2.3
1	D	779	ARG	2.3
1	A	587	TYR	2.3
1	A	536	VAL	2.3
1	D	307	VAL	2.3
1	D	524	GLN	2.3
2	B	21	DC	2.3
1	A	386	GLU	2.3
1	A	431	LYS	2.3
1	A	549	LYS	2.3
1	A	513	THR	2.3
1	A	836	ALA	2.3
1	A	539	PHE	2.3
3	F	2	DC	2.3
1	A	537	ILE	2.3
1	A	322	VAL	2.3
1	A	442	VAL	2.3
1	A	697	VAL	2.3
1	A	433	ALA	2.3
1	D	431	LYS	2.3
1	A	596	ARG	2.2
1	D	507	LEU	2.2
1	A	305	ASP	2.2
1	A	866	TYR	2.2
1	A	304	ALA	2.2
1	A	353	ALA	2.2
1	A	508	ALA	2.2
1	A	434	LYS	2.2
1	A	538	LEU	2.2
1	A	824	LEU	2.2
1	A	509	GLU	2.2
1	A	868	TYR	2.2
1	D	629	ARG	2.2
1	A	560	VAL	2.1
1	D	697	VAL	2.1
1	D	435	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	380	LEU	2.1
1	A	524	GLN	2.1
1	D	549	LYS	2.1
1	A	303	LEU	2.1
1	A	834	LEU	2.1
1	D	630	LEU	2.1
1	A	817	GLU	2.1
1	D	520	GLU	2.1
1	D	543	GLN	2.1
1	A	677	ARG	2.1
1	D	537	ILE	2.1
1	A	505	LYS	2.1
1	A	860	VAL	2.1
1	D	546	VAL	2.1
1	A	632	GLU	2.1
1	A	693	SER	2.1
1	A	872	TRP	2.1
3	C	12	DG	2.1
1	A	436	ALA	2.0
1	A	777	THR	2.0
1	A	812	ASN	2.0
1	A	546	VAL	2.0

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

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

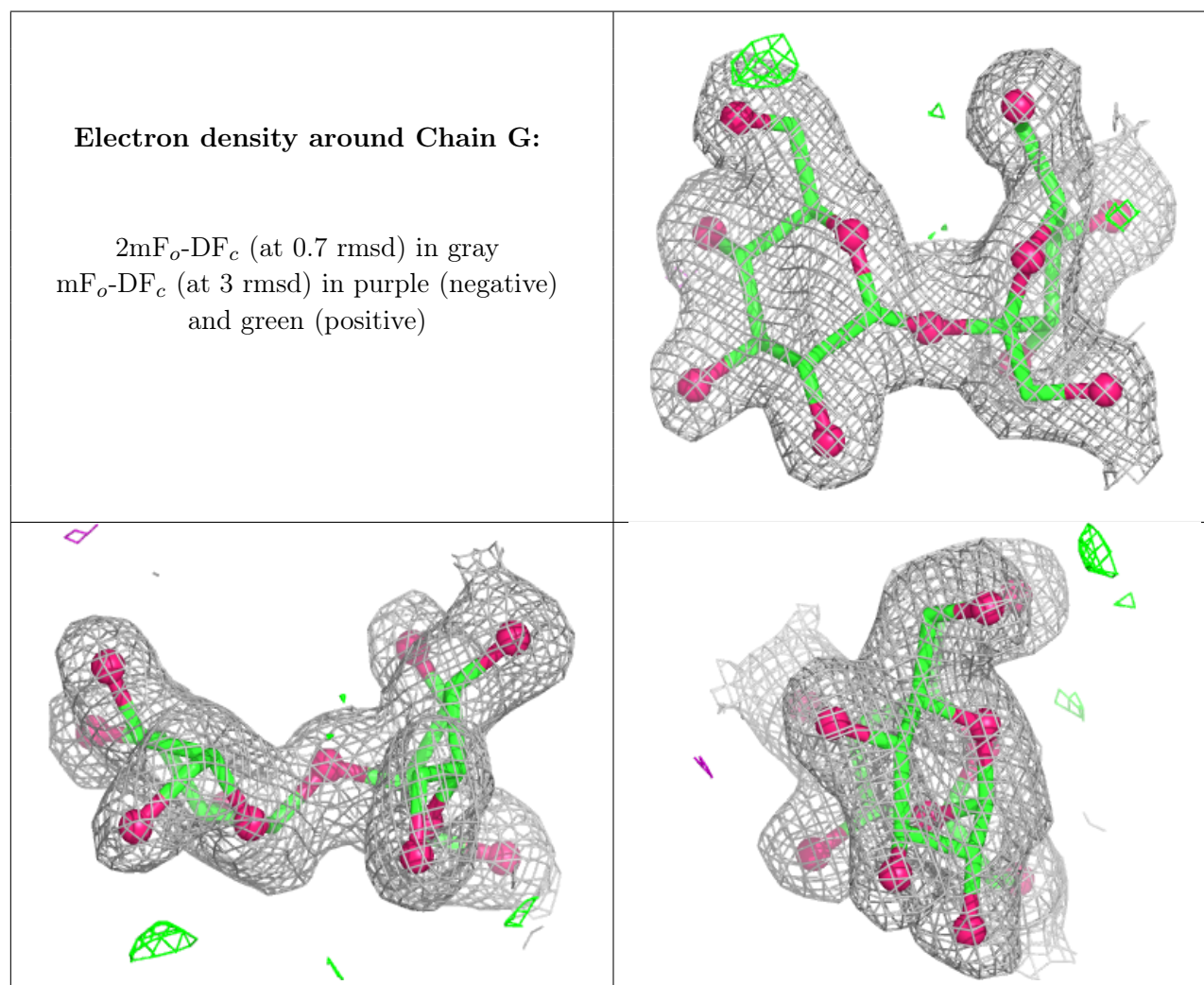
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	DOC	B	29	18/19	0.97	0.05	13,14,18,20	0
2	DOC	E	29	18/19	0.98	0.04	8,10,16,18	0

6.3 Carbohydrates [i](#)

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

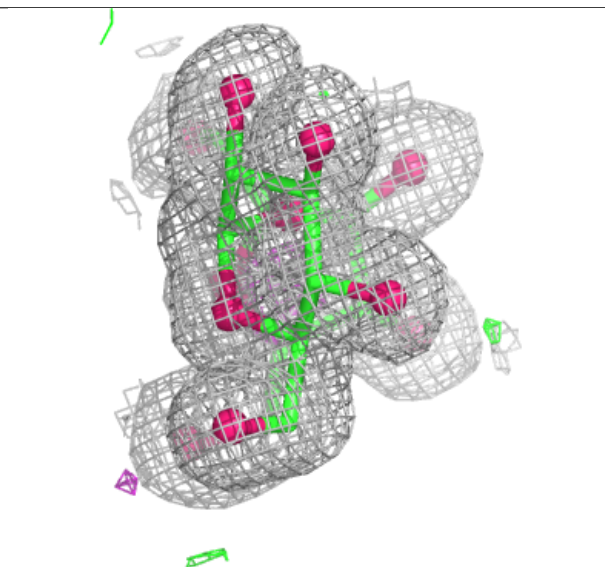
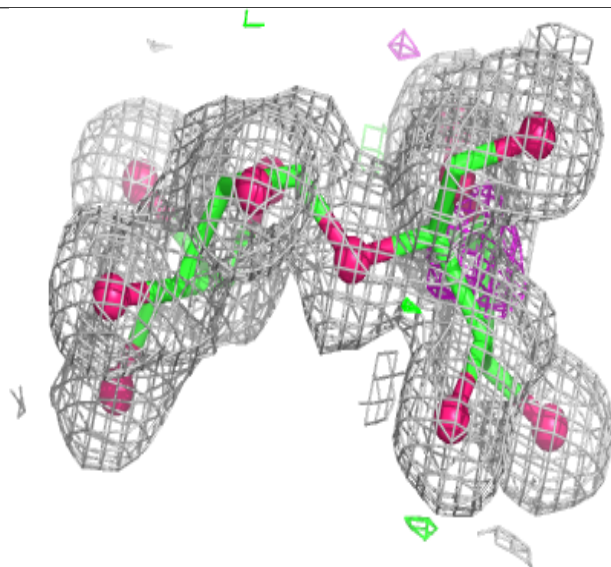
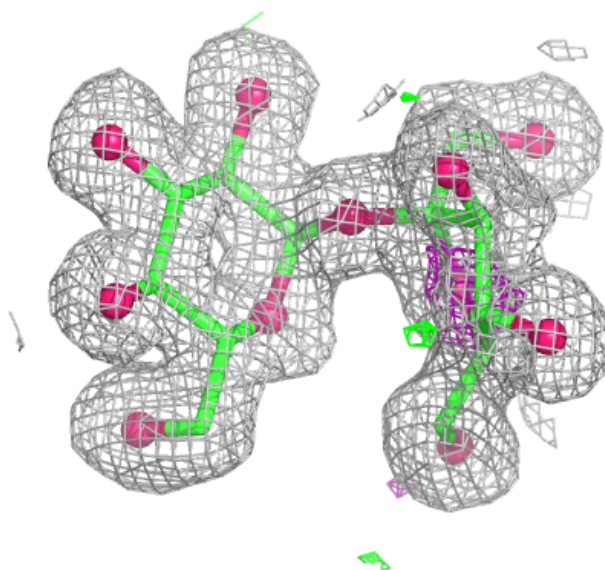
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	FRU	G	2	12/12	0.86	0.11	23,29,30,31	0
4	GLC	G	1	11/12	0.90	0.09	28,30,32,32	0
4	FRU	H	2	12/12	0.94	0.07	11,14,15,15	0
4	GLC	H	1	11/12	0.95	0.07	15,16,19,20	0
4	GLC	I	1	11/12	0.95	0.07	15,16,17,18	0
4	FRU	I	2	12/12	0.96	0.06	15,17,19,20	0

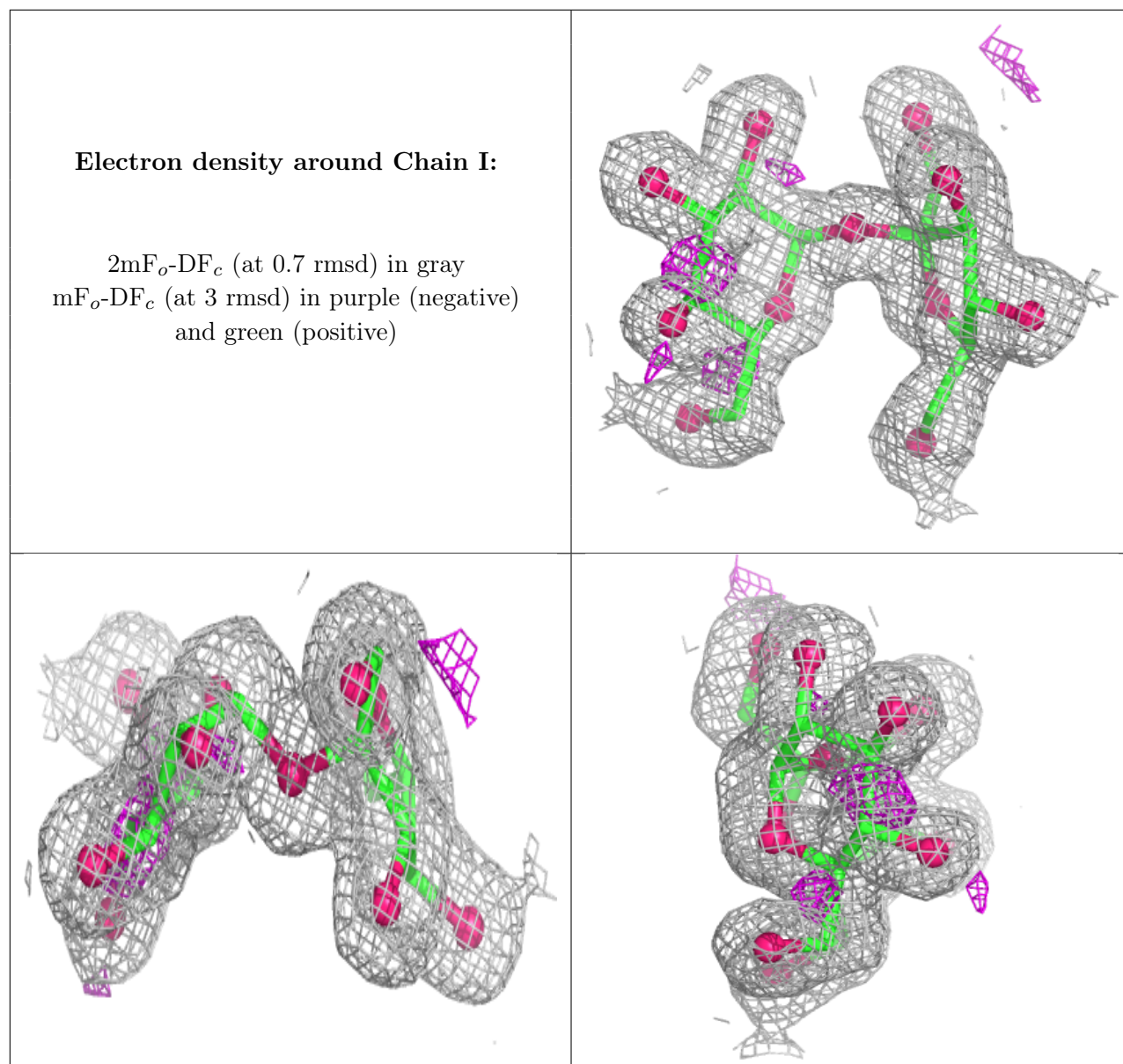
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



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)





6.4 Ligands [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
6	DCP	A	203	28/28	0.70	0.32	23,38,51,51	8
7	SO4	D	3	5/5	0.80	0.14	38,39,40,40	0
7	SO4	D	2	5/5	0.85	0.11	64,64,64,64	0
5	MG	A	200	1/1	0.86	0.19	39,39,39,39	0
6	DCP	A	201	28/28	0.92	0.09	25,28,38,39	0

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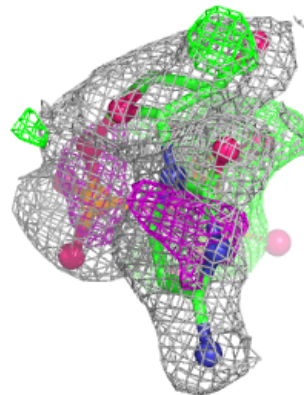
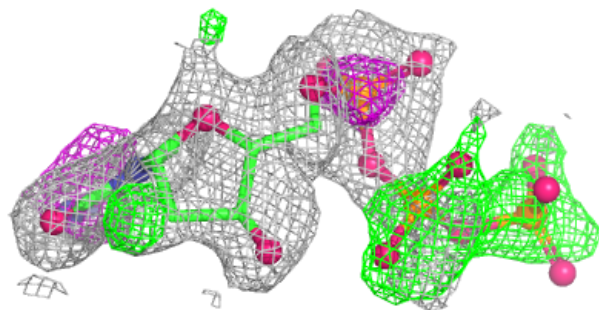
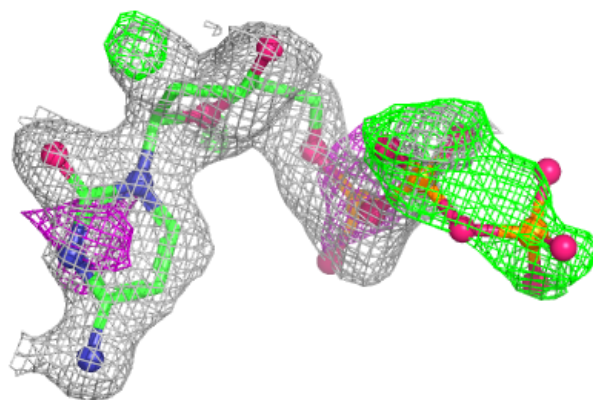
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	SO4	D	1	5/5	0.94	0.12	26,28,31,32	0
5	MG	D	200	1/1	0.96	0.09	17,17,17,17	0
6	DCP	D	202	28/28	0.97	0.07	16,18,21,24	0

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.

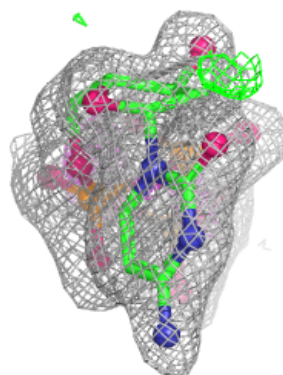
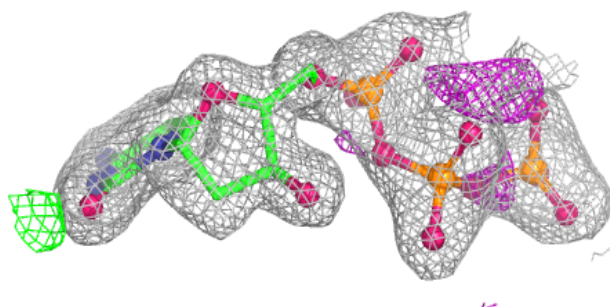
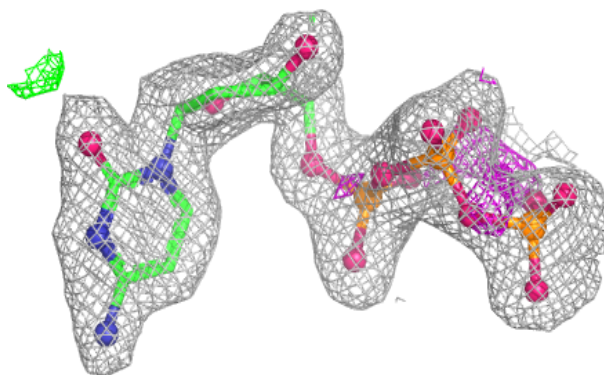
Electron density around DCP A 203:

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

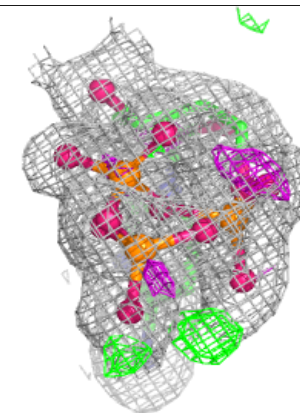
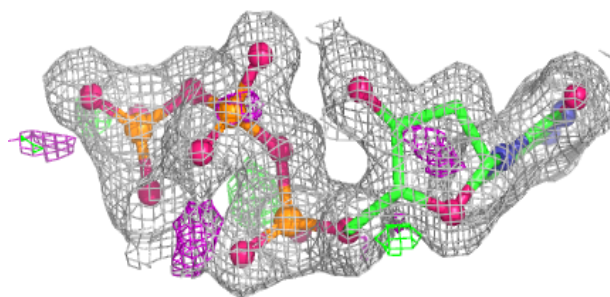
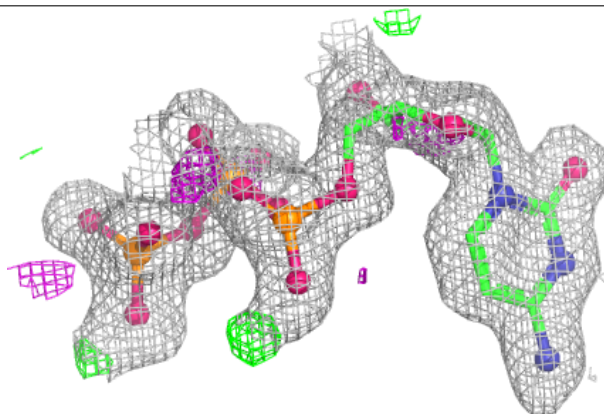


Electron density around DCP A 201:

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

**Electron density around DCP D 202:**

$2mF_o-DF_c$ (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.