Full wwPDB X-ray Structure Validation Report ⓘ

Sep 21, 2020 – 05:08 PM BST

PDB ID	:	4J3U
Title	:	Crystal structure of barley limit dextrinase in complex with maltosyl-S-betacyclodextrin
Authors	:	Sim, L.; Windahl, M.S.; Moeller, M.S.; Henriksen, A.
Deposited on	:	2013-02-06
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 following versions of software and data (see references ①) were used in the production of this report:

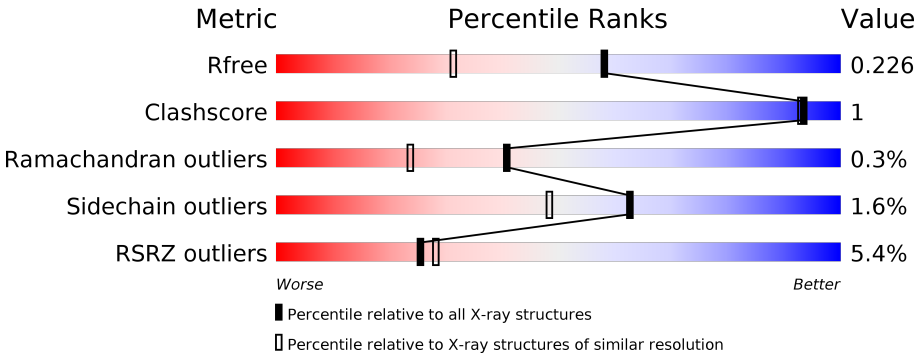
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.14.6
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.6

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (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 on 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 <=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	905	6% 92%
1	B	905	5% 92% 5%
2	C	9	33% 44% 22%
2	D	9	11% 89%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15402 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 Limit dextrinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	870	Total	C	N	O	S	0	9	0
			6799	4296	1163	1308	32			
1	B	864	Total	C	N	O	S	0	9	0
			6752	4274	1153	1293	32			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP Q9FYY0
A	-18	GLY	-	expression tag	UNP Q9FYY0
A	-17	SER	-	expression tag	UNP Q9FYY0
A	-16	SER	-	expression tag	UNP Q9FYY0
A	-15	HIS	-	expression tag	UNP Q9FYY0
A	-14	HIS	-	expression tag	UNP Q9FYY0
A	-13	HIS	-	expression tag	UNP Q9FYY0
A	-12	HIS	-	expression tag	UNP Q9FYY0
A	-11	HIS	-	expression tag	UNP Q9FYY0
A	-10	HIS	-	expression tag	UNP Q9FYY0
A	-9	SER	-	expression tag	UNP Q9FYY0
A	-8	SER	-	expression tag	UNP Q9FYY0
A	-7	GLY	-	expression tag	UNP Q9FYY0
A	-6	LEU	-	expression tag	UNP Q9FYY0
A	-5	VAL	-	expression tag	UNP Q9FYY0
A	-4	PRO	-	expression tag	UNP Q9FYY0
A	-3	ARG	-	expression tag	UNP Q9FYY0
A	-2	GLY	-	expression tag	UNP Q9FYY0
A	-1	SER	-	expression tag	UNP Q9FYY0
A	0	HIS	-	expression tag	UNP Q9FYY0
A	1	MET	-	expression tag	UNP Q9FYY0
A	82	ARG	LYS	SEE REMARK 999	UNP Q9FYY0
A	213	ALA	THR	SEE REMARK 999	UNP Q9FYY0
A	395	ARG	CYS	SEE REMARK 999	UNP Q9FYY0
B	-19	MET	-	expression tag	UNP Q9FYY0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	expression tag	UNP Q9FYY0
B	-17	SER	-	expression tag	UNP Q9FYY0
B	-16	SER	-	expression tag	UNP Q9FYY0
B	-15	HIS	-	expression tag	UNP Q9FYY0
B	-14	HIS	-	expression tag	UNP Q9FYY0
B	-13	HIS	-	expression tag	UNP Q9FYY0
B	-12	HIS	-	expression tag	UNP Q9FYY0
B	-11	HIS	-	expression tag	UNP Q9FYY0
B	-10	HIS	-	expression tag	UNP Q9FYY0
B	-9	SER	-	expression tag	UNP Q9FYY0
B	-8	SER	-	expression tag	UNP Q9FYY0
B	-7	GLY	-	expression tag	UNP Q9FYY0
B	-6	LEU	-	expression tag	UNP Q9FYY0
B	-5	VAL	-	expression tag	UNP Q9FYY0
B	-4	PRO	-	expression tag	UNP Q9FYY0
B	-3	ARG	-	expression tag	UNP Q9FYY0
B	-2	GLY	-	expression tag	UNP Q9FYY0
B	-1	SER	-	expression tag	UNP Q9FYY0
B	0	HIS	-	expression tag	UNP Q9FYY0
B	1	MET	-	expression tag	UNP Q9FYY0
B	82	ARG	LYS	SEE REMARK 999	UNP Q9FYY0
B	213	ALA	THR	SEE REMARK 999	UNP Q9FYY0
B	395	ARG	CYS	SEE REMARK 999	UNP Q9FYY0

- Molecule 2 is an oligosaccharide called Cyclic alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-[alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-1)]6-thio-alpha-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	9	Total	C	O	S	0	0	0
			99	54	44	1			
2	D	9	Total	C	O	S	0	0	0
			99	54	44	1			

- Molecule 3 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	12	Total	I	0	1
			13	13		
3	A	20	Total	I	0	2
			22	22		

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	2	Total Ca 2 2	0	0
4	A	2	Total Ca 2 2	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Cl 1 1	0	0
5	A	1	Total Cl 1 1	0	0

- Molecule 6 is water.

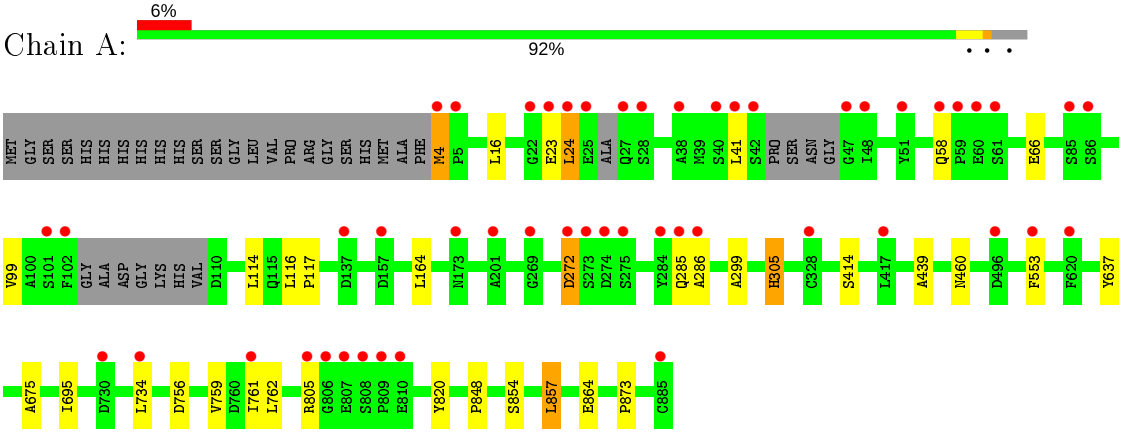
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	791	Total O 791 791	0	0
6	B	821	Total O 821 821	0	0

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.

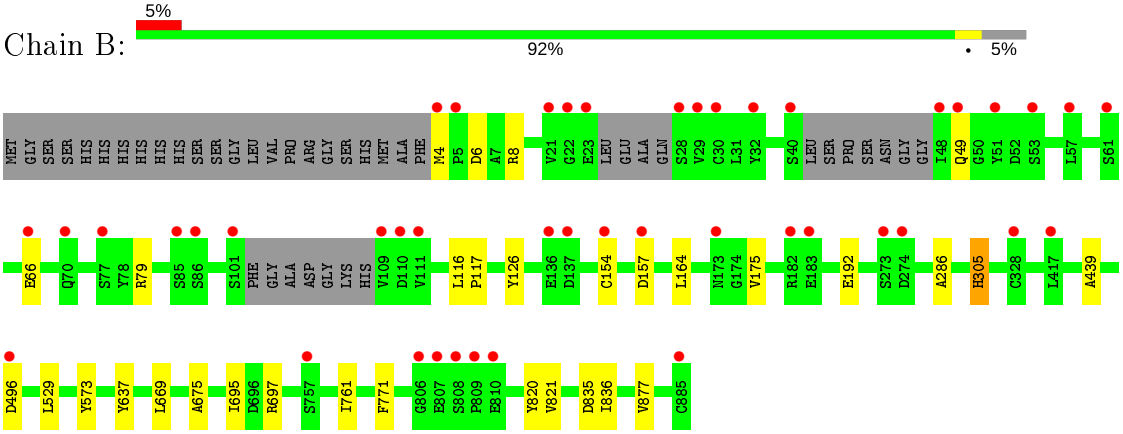
• Molecule 1: Limit dextrinase

Chain A:



• Molecule 1: Limit dextrinase

Chain B:



• Molecule 2: Cyclic alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-[alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-1)]6-thio-alpha-D-glucopyranose

Chain C:

• Molecule 2: Cyclic alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-[alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-1)]6-thio-alpha-D-glucopyranose

Chain D:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	195.43Å 84.61Å 121.79Å 90.00° 119.91° 90.00°	Depositor
Resolution (Å)	29.76 – 1.70 29.76 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.5 (29.76-1.70) 99.6 (29.76-1.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.19 (at 1.70Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.172 , 0.218 0.180 , 0.226	Depositor DCC
R_{free} test set	9417 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	15.2	Xtriage
Anisotropy	0.119	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 45.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	15402	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 36.88 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.6671e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: IOD, CA, GLC, SGD, CL

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	0.29	0/6982	0.54	1/9492 (0.0%)
1	B	0.29	0/6944	0.54	0/9441
All	All	0.29	0/13926	0.54	1/18933 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	734	LEU	CA-CB-CG	5.15	127.15	115.30

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	6799	0	6554	18	0
1	B	6752	0	6538	16	0
2	C	99	0	81	2	0
2	D	99	0	81	1	0
3	A	22	0	0	8	0
3	B	13	0	0	1	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	791	0	0	4	0
6	B	821	0	0	1	0
All	All	15402	0	13254	37	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 1.

All (37) 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)
3:A:914:IOD:I	6:A:1468:HOH:O	2.72	0.78
1:B:154[A]:CYS:SG	1:B:192:GLU:HG3	2.29	0.72
3:A:912:IOD:I	6:A:1606:HOH:O	2.80	0.69
1:A:675:ALA:CB	1:A:761[B]:ILE:HD13	2.31	0.60
1:A:23:GLU:O	1:A:24:LEU:CB	2.49	0.59
3:A:913:IOD:I	6:A:1509:HOH:O	2.87	0.58
1:B:675:ALA:HB3	1:B:761[B]:ILE:HD12	1.87	0.57
1:B:154[A]:CYS:SG	1:B:192:GLU:CG	2.92	0.56
1:B:675:ALA:CB	1:B:761[B]:ILE:HD12	2.37	0.55
1:B:836:ILE:HD12	1:B:836:ILE:N	2.22	0.55
1:B:6:ASP:OD2	1:B:8:ARG:NH1	2.41	0.53
1:A:553:PHE:HB3	2:C:5:GLC:H3	1.92	0.52
1:B:697[A]:ARG:NH2	6:B:1704:HOH:O	2.43	0.51
3:A:923:IOD:I	6:A:1573:HOH:O	2.89	0.51
1:A:286:ALA:HB3	3:A:925:IOD:I	2.82	0.50
1:A:756:ASP:OD2	1:A:854:SER:OG	2.25	0.50
1:A:848:PRO:HG2	3:A:924:IOD:I	2.82	0.49
1:A:414:SER:OG	3:A:922:IOD:I	2.92	0.48
1:A:4:MET:N	1:A:4:MET:SD	2.86	0.48
1:A:285:GLN:HG2	1:B:573:TYR:OH	2.13	0.48
1:B:126:TYR:CD1	1:B:175:VAL:HG21	2.49	0.47
1:B:116:LEU:N	1:B:117:PRO:CD	2.78	0.47
1:A:99:VAL:HG13	1:A:114:LEU:HD11	1.96	0.46
1:B:669:LEU:HD23	1:B:877:VAL:CG2	2.47	0.45
1:B:771:PHE:CZ	1:B:821:VAL:HG11	2.52	0.44
1:A:305:HIS:CD2	1:A:305:HIS:C	2.92	0.43
1:B:305:HIS:C	1:B:305:HIS:CD2	2.92	0.43
1:A:272[A]:ASP:OD1	1:A:272[A]:ASP:C	2.56	0.43
1:A:761[B]:ILE:HD12	1:A:762:LEU:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:553:PHE:HB2	2:C:6:GLC:H3	2.00	0.42
1:B:835:ASP:C	1:B:836:ILE:HD12	2.40	0.41
1:A:857:LEU:HD22	1:A:873:PRO:HB3	2.03	0.41
1:A:460:ASN:HA	3:A:929[A]:IOD:I	2.91	0.41
1:A:299:ALA:HB2	1:A:759:VAL:HG13	2.03	0.40
1:A:116:LEU:N	1:A:117:PRO:CD	2.84	0.40
1:B:286:ALA:HB3	3:B:917:IOD:I	2.92	0.40
1:B:697[A]:ARG:NH1	2:D:3:GLC:O3	2.55	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	871/905 (96%)	850 (98%)	18 (2%)	3 (0%)	41	24
1	B	865/905 (96%)	845 (98%)	18 (2%)	2 (0%)	47	30
All	All	1736/1810 (96%)	1695 (98%)	36 (2%)	5 (0%)	41	24

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	24	LEU
1	A	439	ALA
1	B	439	ALA
1	A	695	ILE
1	B	695	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	739/760 (97%)	725 (98%)	14 (2%)	57 41
1	B	736/760 (97%)	725 (98%)	11 (2%)	65 51
All	All	1475/1520 (97%)	1450 (98%)	25 (2%)	62 46

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	MET
1	A	16	LEU
1	A	41	LEU
1	A	58	GLN
1	A	66	GLU
1	A	164	LEU
1	A	272[A]	ASP
1	A	272[B]	ASP
1	A	305	HIS
1	A	637	TYR
1	A	805	ARG
1	A	820	TYR
1	A	857	LEU
1	A	864	GLU
1	B	4	MET
1	B	49	GLN
1	B	66	GLU
1	B	79	ARG
1	B	157	ASP
1	B	164	LEU
1	B	305	HIS
1	B	496	ASP
1	B	529	LEU
1	B	637	TYR
1	B	820	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	GLN
1	A	142	HIS
1	A	574	GLN
1	A	817	ASN
1	B	142	HIS
1	B	149	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

18 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	SGD	C	1	2	11,11,12	0.70	1 (9%)	15,15,17	0.88	0
2	GLC	C	2	2	11,11,12	0.25	0	15,15,17	0.72	0
2	GLC	C	3	2	11,11,12	0.21	0	15,15,17	0.57	0
2	GLC	C	4	2	11,11,12	0.28	0	15,15,17	1.02	1 (6%)
2	GLC	C	5	2	11,11,12	0.40	0	15,15,17	0.97	1 (6%)
2	GLC	C	6	2	11,11,12	0.30	0	15,15,17	1.36	2 (13%)
2	GLC	C	7	2	11,11,12	0.30	0	15,15,17	0.90	0
2	GLC	C	8	2	11,11,12	0.27	0	15,15,17	0.84	2 (13%)
2	GLC	C	9	2	11,11,12	0.21	0	15,15,17	0.76	1 (6%)
2	SGD	D	1	2	11,11,12	0.69	1 (9%)	15,15,17	0.83	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	GLC	D	2	2	11,11,12	0.27	0	15,15,17	0.68	0
2	GLC	D	3	2	11,11,12	0.31	0	15,15,17	0.61	0
2	GLC	D	4	2	11,11,12	0.25	0	15,15,17	1.45	1 (6%)
2	GLC	D	5	2	11,11,12	0.27	0	15,15,17	0.88	1 (6%)
2	GLC	D	6	2	11,11,12	0.27	0	15,15,17	1.10	1 (6%)
2	GLC	D	7	2	11,11,12	0.23	0	15,15,17	0.91	1 (6%)
2	GLC	D	8	2	11,11,12	0.28	0	15,15,17	0.74	1 (6%)
2	GLC	D	9	2	11,11,12	0.26	0	15,15,17	0.79	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	SGD	C	1	2	-	0/2/19/22	0/1/1/1
2	GLC	C	2	2	-	0/2/19/22	0/1/1/1
2	GLC	C	3	2	-	0/2/19/22	0/1/1/1
2	GLC	C	4	2	-	2/2/19/22	0/1/1/1
2	GLC	C	5	2	-	0/2/19/22	0/1/1/1
2	GLC	C	6	2	-	0/2/19/22	0/1/1/1
2	GLC	C	7	2	-	0/2/19/22	0/1/1/1
2	GLC	C	8	2	-	0/2/19/22	0/1/1/1
2	GLC	C	9	2	-	0/2/19/22	0/1/1/1
2	SGD	D	1	2	-	0/2/19/22	0/1/1/1
2	GLC	D	2	2	-	0/2/19/22	0/1/1/1
2	GLC	D	3	2	-	0/2/19/22	0/1/1/1
2	GLC	D	4	2	-	1/2/19/22	0/1/1/1
2	GLC	D	5	2	-	0/2/19/22	0/1/1/1
2	GLC	D	6	2	-	0/2/19/22	0/1/1/1
2	GLC	D	7	2	-	0/2/19/22	0/1/1/1
2	GLC	D	8	2	-	0/2/19/22	0/1/1/1
2	GLC	D	9	2	-	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	SGD	C6-S1	-2.09	1.77	1.81
2	D	1	SGD	C6-S1	-2.02	1.77	1.81

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	4	GLC	C1-O5-C5	4.72	118.58	112.19
2	C	6	GLC	C1-O5-C5	4.10	117.75	112.19
2	D	6	GLC	C1-O5-C5	3.23	116.56	112.19
2	C	4	GLC	C1-O5-C5	2.87	116.08	112.19
2	D	5	GLC	C1-O5-C5	2.84	116.05	112.19
2	C	5	GLC	C1-O5-C5	2.69	115.84	112.19
2	C	6	GLC	O5-C1-C2	-2.29	107.24	110.77
2	D	9	GLC	C1-O5-C5	2.21	115.18	112.19
2	D	8	GLC	C1-O5-C5	2.10	115.04	112.19
2	C	8	GLC	C1-O5-C5	2.09	115.02	112.19
2	C	9	GLC	C1-O5-C5	2.01	114.91	112.19
2	D	7	GLC	C1-O5-C5	2.01	114.91	112.19
2	C	8	GLC	C1-C2-C3	2.01	112.14	109.67

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	4	GLC	O5-C5-C6-O6
2	C	4	GLC	C4-C5-C6-O6
2	D	4	GLC	C4-C5-C6-O6

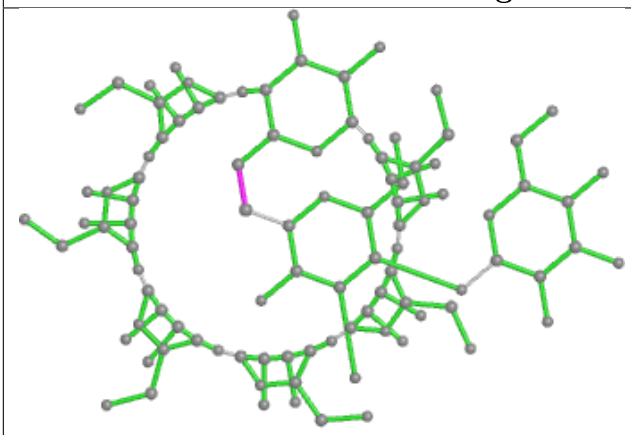
There are no ring outliers.

3 monomers are involved in 3 short contacts:

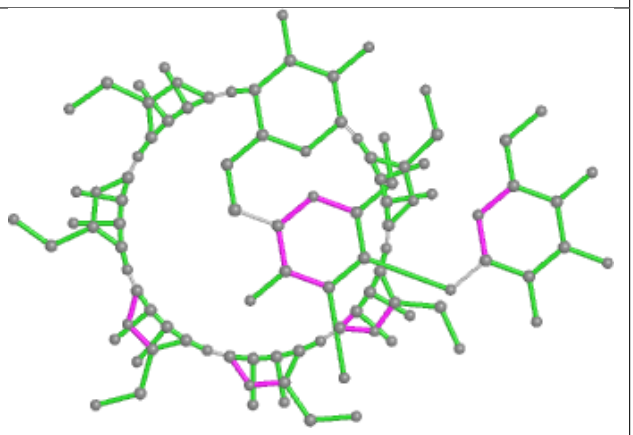
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	5	GLC	1	0
2	D	3	GLC	1	0
2	C	6	GLC	1	0

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

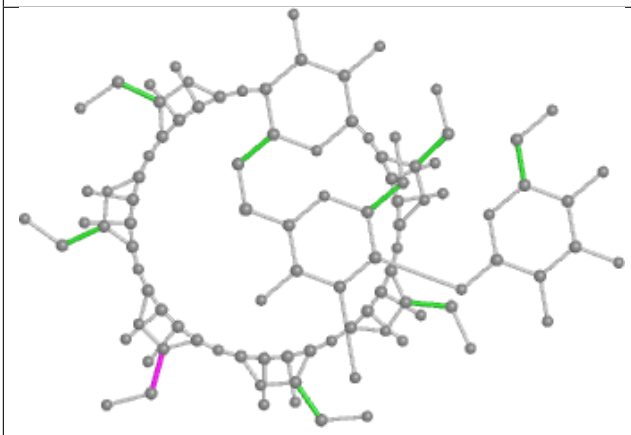
Oligosaccharide Chain C



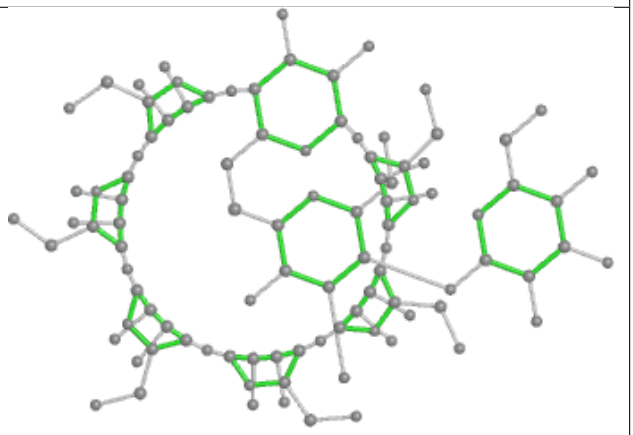
Bond lengths



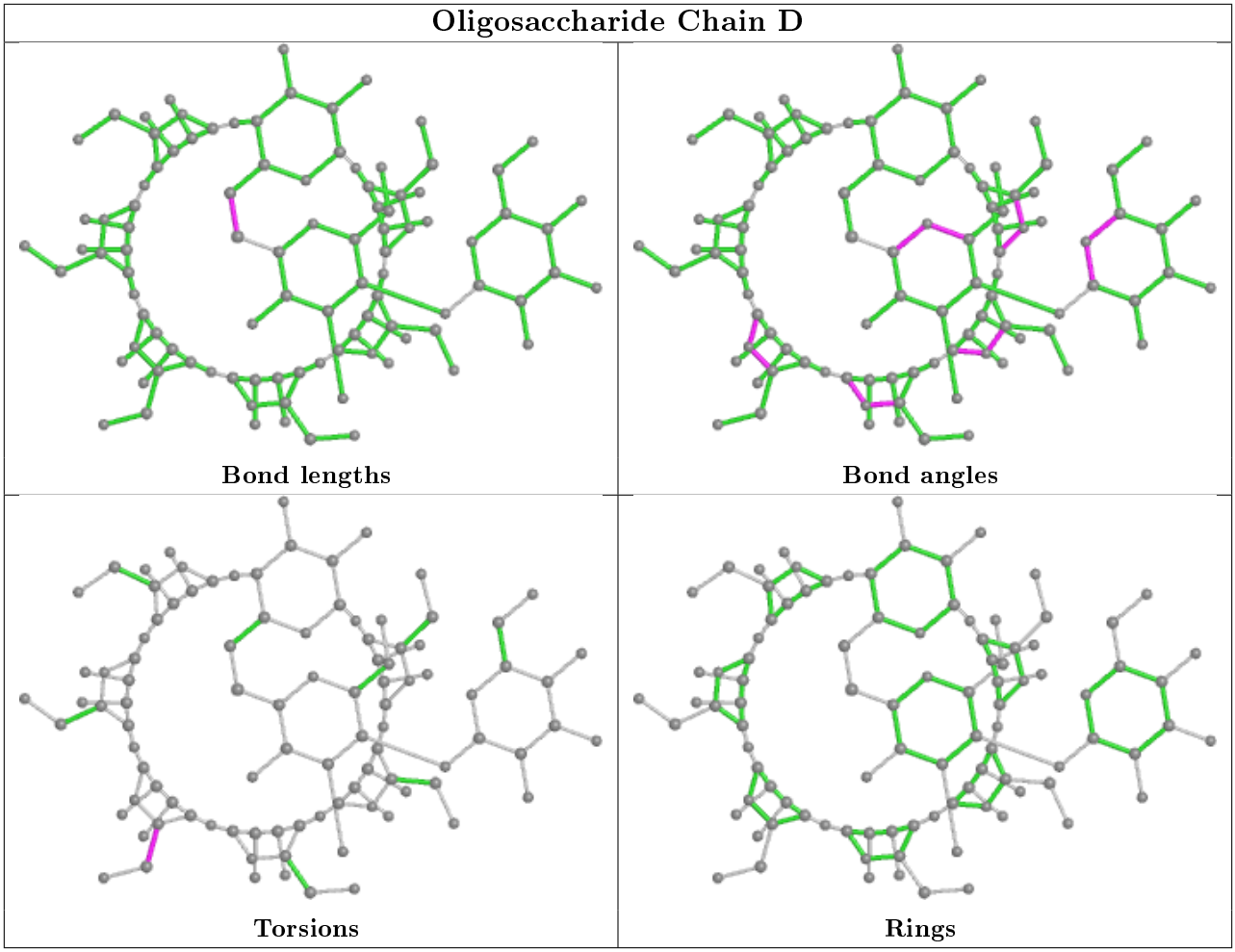
Bond angles



Torsions



Rings



5.6 Ligand geometry

Of 41 ligands modelled in this entry, 41 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

5.7 Other polymers

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, 95^{th} 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	870/905 (96%)	0.19	50 (5%)	23	26	8, 16, 38, 56	1 (0%)
1	B	864/905 (95%)	0.18	44 (5%)	28	31	7, 16, 40, 61	2 (0%)
All	All	1734/1810 (95%)	0.19	94 (5%)	25	28	7, 16, 39, 61	3 (0%)

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	885	CYS	12.2
1	B	5	PRO	9.2
1	A	885	CYS	9.0
1	B	4	MET	8.8
1	A	5	PRO	8.3
1	A	24	LEU	8.0
1	A	806	GLY	6.8
1	A	4	MET	6.5
1	A	808	SER	6.5
1	A	102	PHE	6.4
1	B	808	SER	6.3
1	B	806	GLY	5.3
1	B	109	VAL	5.2
1	A	810	GLU	5.0
1	B	23	GLU	4.6
1	A	807	GLU	4.6
1	A	47	GLY	4.5
1	B	28	SER	4.5
1	A	27	GLN	4.5
1	B	48	ILE	4.5
1	A	284	TYR	4.4
1	B	807	GLU	4.4
1	A	201	ALA	4.1
1	A	274	ASP	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	85	SER	3.8
1	A	41	LEU	3.7
1	B	101	SER	3.6
1	B	328	CYS	3.6
1	A	61	SER	3.6
1	A	51	TYR	3.6
1	A	58	GLN	3.6
1	A	42	SER	3.6
1	A	157	ASP	3.5
1	A	809	PRO	3.5
1	B	173	ASN	3.5
1	B	154[A]	CYS	3.5
1	A	86	SER	3.4
1	B	137	ASP	3.3
1	B	810	GLU	3.3
1	B	111	VAL	3.3
1	B	32	TYR	3.2
1	A	85	SER	3.2
1	A	273	SER	3.2
1	B	86	SER	3.1
1	A	620	PHE	3.1
1	B	496	ASP	3.0
1	B	30	CYS	3.0
1	A	805	ARG	2.9
1	B	40	SER	2.9
1	B	66	GLU	2.8
1	B	49	GLN	2.8
1	A	25	GLU	2.8
1	B	29	VAL	2.8
1	A	285	GLN	2.8
1	A	496	ASP	2.8
1	A	137	ASP	2.7
1	A	40[A]	SER	2.7
1	B	809	PRO	2.6
1	A	417	LEU	2.6
1	B	22	GLY	2.5
1	A	59	PRO	2.5
1	A	23	GLU	2.5
1	A	60	GLU	2.5
1	A	730	ASP	2.5
1	B	51	TYR	2.5
1	B	757	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	136	GLU	2.4
1	B	273	SER	2.4
1	B	70	GLN	2.4
1	A	328	CYS	2.4
1	B	417	LEU	2.4
1	A	173	ASN	2.4
1	B	274	ASP	2.3
1	A	286	ALA	2.3
1	B	53	SER	2.3
1	A	275	SER	2.2
1	A	38	ALA	2.2
1	A	48	ILE	2.2
1	A	101	SER	2.2
1	B	110	ASP	2.2
1	A	272[A]	ASP	2.2
1	A	553	PHE	2.2
1	B	77	SER	2.2
1	A	761[A]	ILE	2.2
1	A	22	GLY	2.1
1	A	28	SER	2.1
1	B	21	VAL	2.1
1	B	182	ARG	2.1
1	A	734	LEU	2.1
1	B	61	SER	2.1
1	B	57	LEU	2.0
1	A	269	GLY	2.0
1	B	183	GLU	2.0
1	B	157	ASP	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)

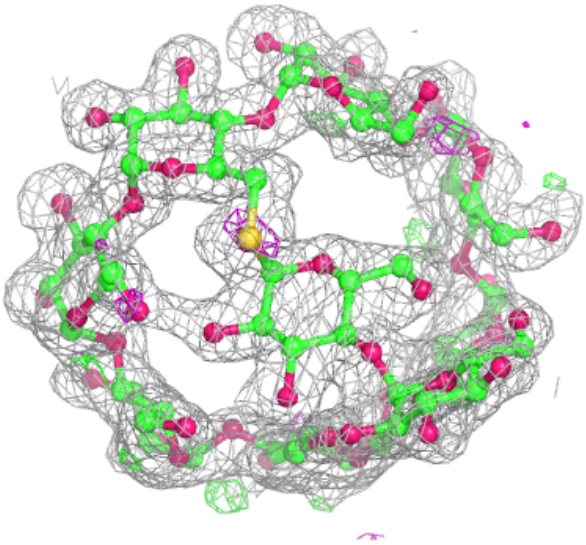
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

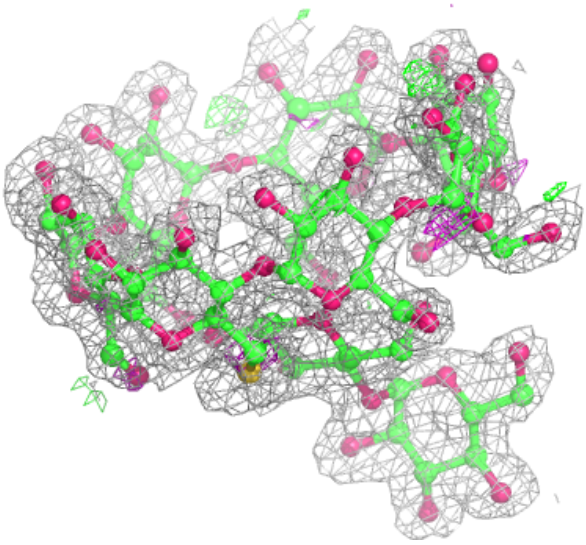
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GLC	C	3	11/12	0.75	0.24	30,34,39,39	0
2	GLC	C	5	11/12	0.77	0.25	37,42,44,45	0
2	GLC	D	5	11/12	0.85	0.16	27,34,37,38	0
2	GLC	C	8	11/12	0.87	0.12	28,30,35,36	0
2	GLC	C	4	11/12	0.87	0.23	38,41,45,46	0
2	GLC	D	3	11/12	0.89	0.14	22,24,27,28	0
2	GLC	D	4	11/12	0.90	0.16	29,30,34,38	0
2	GLC	C	6	11/12	0.91	0.10	25,30,33,34	0
2	GLC	D	8	11/12	0.91	0.14	22,24,27,28	0
2	GLC	C	2	11/12	0.92	0.14	21,23,26,27	0
2	GLC	C	7	11/12	0.92	0.10	17,19,25,32	0
2	GLC	D	9	11/12	0.93	0.13	28,30,33,34	0
2	GLC	C	9	11/12	0.93	0.13	26,27,30,31	0
2	GLC	D	6	11/12	0.93	0.10	17,21,27,29	0
2	SGD	C	1	11/12	0.94	0.08	15,17,22,27	0
2	GLC	D	7	11/12	0.95	0.07	15,16,22,26	0
2	GLC	D	2	11/12	0.96	0.08	16,18,20,22	0
2	SGD	D	1	11/12	0.97	0.07	13,15,17,21	0

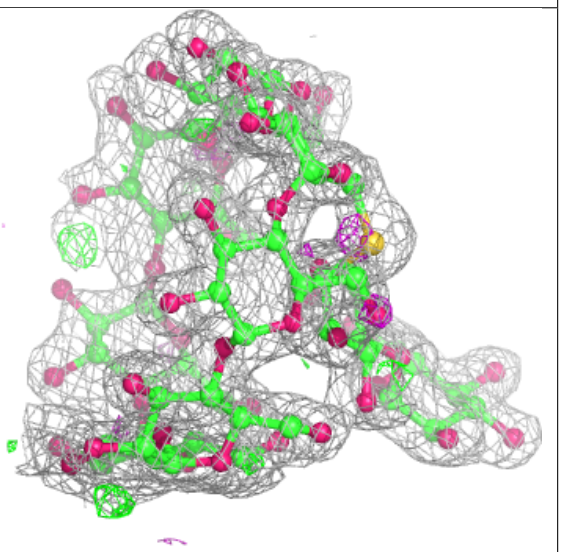
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain C:

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

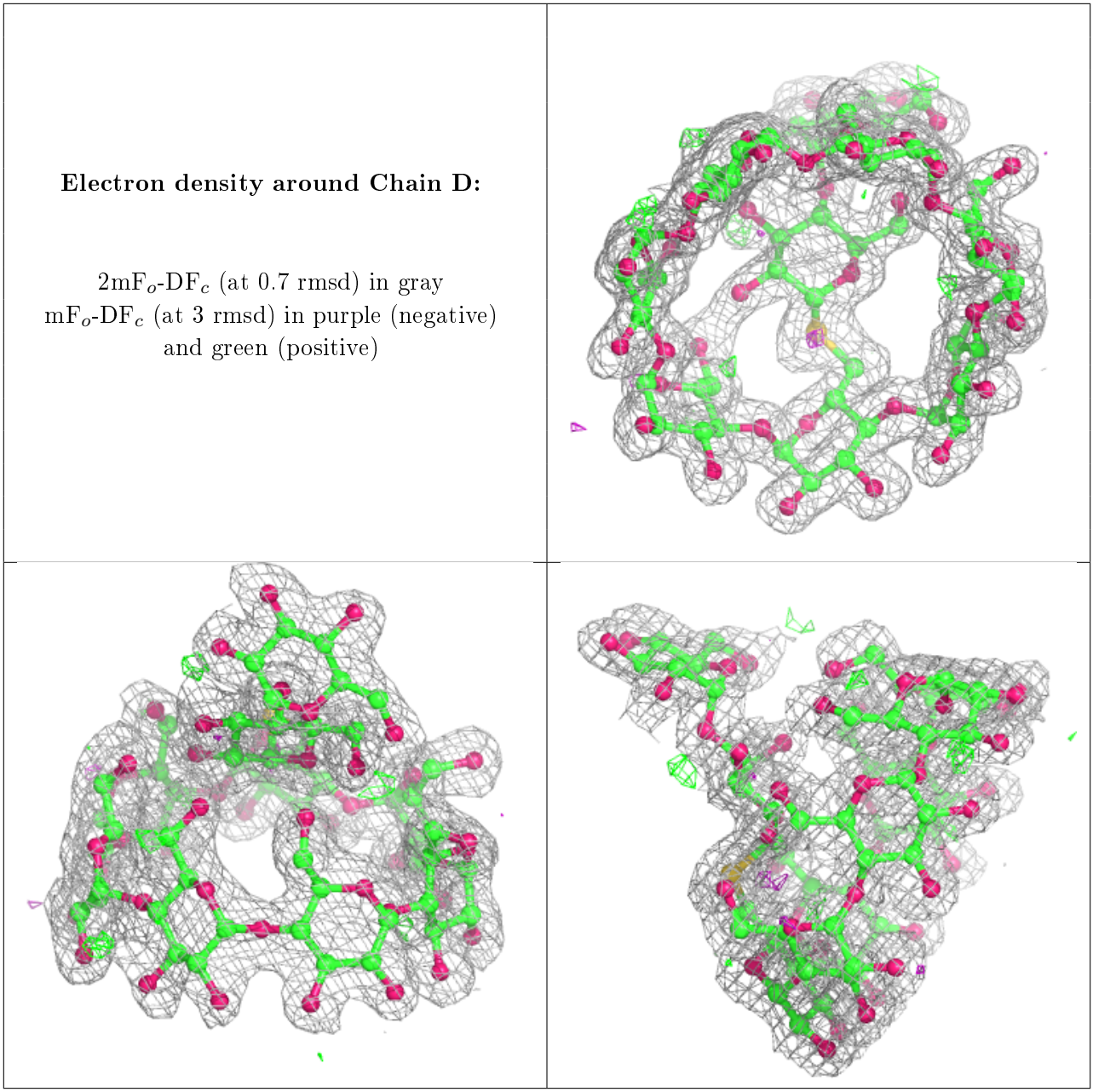






Electron density around Chain D:

$2mF_o$-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, 95^{th} 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
3	IOD	A	929[B]	1/1	0.94	0.16	62,62,62,62	1
3	IOD	A	929[A]	1/1	0.94	0.16	57,57,57,57	1
3	IOD	B	911	1/1	0.95	0.12	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	IOD	B	912	1/1	0.96	0.24	53,53,53,53	1
3	IOD	A	927	1/1	0.97	0.06	63,63,63,63	1
3	IOD	A	924	1/1	0.97	0.09	42,42,42,42	1
3	IOD	A	925	1/1	0.98	0.13	44,44,44,44	1
3	IOD	B	918	1/1	0.98	0.13	61,61,61,61	1
3	IOD	A	915	1/1	0.98	0.20	66,66,66,66	1
3	IOD	A	912	1/1	0.99	0.11	42,42,42,42	1
3	IOD	A	916	1/1	0.99	0.08	63,63,63,63	1
3	IOD	A	911	1/1	0.99	0.20	44,44,44,44	1
3	IOD	A	923	1/1	0.99	0.10	49,49,49,49	1
3	IOD	A	926	1/1	0.99	0.11	47,47,47,47	1
3	IOD	A	928[B]	1/1	0.99	0.06	38,38,38,38	1
5	CL	A	932	1/1	0.99	0.02	28,28,28,28	0
3	IOD	A	928[A]	1/1	0.99	0.06	31,31,31,31	1
3	IOD	B	913	1/1	0.99	0.02	32,32,32,32	1
3	IOD	A	921	1/1	0.99	0.07	55,55,55,55	1
3	IOD	B	921[B]	1/1	0.99	0.07	38,38,38,38	1
3	IOD	B	921[A]	1/1	0.99	0.07	35,35,35,35	1
3	IOD	A	919	1/1	0.99	0.05	41,41,41,41	1
3	IOD	B	920	1/1	0.99	0.14	49,49,49,49	0
3	IOD	A	913	1/1	1.00	0.10	35,35,35,35	1
3	IOD	A	922	1/1	1.00	0.04	30,30,30,30	1
4	CA	A	931	1/1	1.00	0.04	12,12,12,12	0
3	IOD	A	914	1/1	1.00	0.06	35,35,35,35	1
3	IOD	A	910	1/1	1.00	0.03	26,26,26,26	1
3	IOD	B	919	1/1	1.00	0.14	49,49,49,49	0
3	IOD	A	918	1/1	1.00	0.02	27,27,27,27	1
3	IOD	B	916	1/1	1.00	0.07	43,43,43,43	1
4	CA	B	923	1/1	1.00	0.03	10,10,10,10	0
3	IOD	B	917	1/1	1.00	0.05	31,31,31,31	1
3	IOD	A	917	1/1	1.00	0.08	16,16,16,16	1
3	IOD	B	914	1/1	1.00	0.05	19,19,19,19	1
4	CA	A	930	1/1	1.00	0.02	11,11,11,11	0
5	CL	B	924	1/1	1.00	0.04	16,16,16,16	0
3	IOD	A	920	1/1	1.00	0.03	29,29,29,29	1
3	IOD	B	915	1/1	1.00	0.02	27,27,27,27	1
4	CA	B	922	1/1	1.00	0.02	12,12,12,12	0
3	IOD	B	910	1/1	1.00	0.02	34,34,34,34	0

6.5 Other polymers (i)

There are no such residues in this entry.