Full wwPDB X-ray Structure Validation Report (i)

Oct 7, 2023 – 03:37 PM EDT

PDB ID	:	6DKS
Title	:	Structure of the Rbpj-SHARP-DNA Repressor Complex
Authors	:	Kovall, R.A.; VanderWielen, B.D.; Yuan, Z.
Deposited on	:	2018-05-30
Resolution	:	2.78 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 (i) 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 (1)) were used in the production of this report:

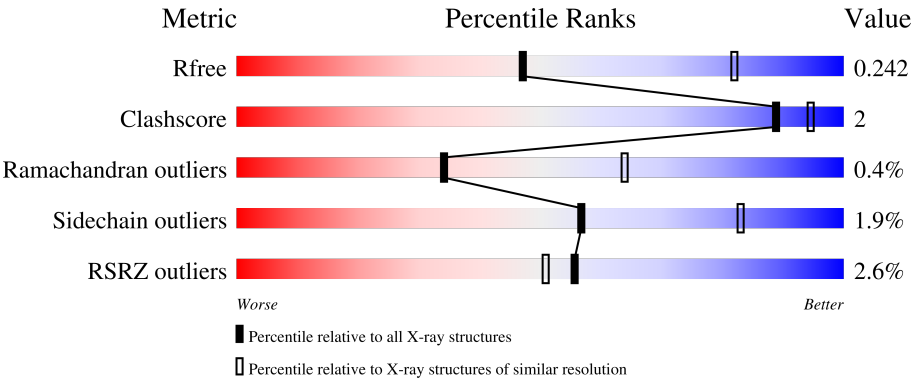
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.78 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	4107 (2.80-2.76)
Clashscore	141614	4575 (2.80-2.76)
Ramachandran outliers	138981	4487 (2.80-2.76)
Sidechain outliers	138945	4489 (2.80-2.76)
RSRZ outliers	127900	4027 (2.80-2.76)

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 <=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	15	13% 87% 13%
1	E	15	7% 100%
2	B	15	7% 87% 13%
2	F	15	87% 13%
3	C	422	3% 92% 6% ·

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Mol	Chain	Length	Quality of chain
3	G	422	3% 94% 6%
4	D	407	2% 93% 7%
4	H	407	% 94% 5%
5	I	2	50% 50%
5	J	2	50% 50%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 13438 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 DNA chain called DNA (5'-D(*AP*AP*TP*CP*TP*TP*TP*CP*CP*CP*AP*CP*AP*GP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	15	Total	C	N	O	P	0	0	0
			298	145	50	89	14			
1	E	15	Total	C	N	O	P	0	0	0
			298	145	50	89	14			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	15	Total	C	N	O	P	0	0	0
			311	149	61	87	14			
2	F	15	Total	C	N	O	P	0	0	0
			311	149	61	87	14			

- Molecule 3 is a protein called Recombining binding protein suppressor of hairless.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	417	Total	C	N	O	S	0	0	0
			3068	1954	529	561	24			
3	G	422	Total	C	N	O	S	0	1	0
			3137	1997	537	579	24			

- Molecule 4 is a protein called Maltose/maltodextrin-binding periplasmic protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	407	Total	C	N	O	S	0	0	0
			2997	1920	492	579	6			
4	H	405	Total	C	N	O	S	0	1	0
			2972	1908	483	575	6			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	367	ASN	-	expression tag	UNP P0AEY0
D	368	ALA	-	expression tag	UNP P0AEY0
D	369	ALA	-	expression tag	UNP P0AEY0
D	370	ALA	-	expression tag	UNP P0AEY0
D	2777	GLY	-	expression tag	UNP P0AEY0
D	2778	ALA	-	expression tag	UNP P0AEY0
D	2779	GLY	-	expression tag	UNP P0AEY0
D	2780	LEU	-	expression tag	UNP P0AEY0
D	2781	ARG	-	expression tag	UNP P0AEY0
D	2782	VAL	-	expression tag	UNP P0AEY0
D	2783	ASN	-	expression tag	UNP P0AEY0
D	2784	THR	-	expression tag	UNP P0AEY0
D	2785	SER	-	expression tag	UNP P0AEY0
D	2786	GLU	-	expression tag	UNP P0AEY0
D	2787	GLY	-	expression tag	UNP P0AEY0
D	2788	VAL	-	expression tag	UNP P0AEY0
D	2789	VAL	-	expression tag	UNP P0AEY0
D	2790	LEU	-	expression tag	UNP P0AEY0
D	2791	LEU	-	expression tag	UNP P0AEY0
D	2792	SER	-	expression tag	UNP P0AEY0
D	2793	TYR	-	expression tag	UNP P0AEY0
D	2794	SER	-	expression tag	UNP P0AEY0
D	2795	GLY	-	expression tag	UNP P0AEY0
D	2796	GLN	-	expression tag	UNP P0AEY0
D	2797	LYS	-	expression tag	UNP P0AEY0
D	2798	THR	-	expression tag	UNP P0AEY0
D	2799	GLU	-	expression tag	UNP P0AEY0
D	2800	GLY	-	expression tag	UNP P0AEY0
D	2801	PRO	-	expression tag	UNP P0AEY0
D	2802	GLN	-	expression tag	UNP P0AEY0
D	2803	ARG	-	expression tag	UNP P0AEY0
D	2804	ILE	-	expression tag	UNP P0AEY0
D	2805	SER	-	expression tag	UNP P0AEY0
D	2806	ALA	-	expression tag	UNP P0AEY0
D	2807	LYS	-	expression tag	UNP P0AEY0
D	2808	ILE	-	expression tag	UNP P0AEY0
D	2809	SER	-	expression tag	UNP P0AEY0
D	2810	GLN	-	expression tag	UNP P0AEY0
D	2811	ILE	-	expression tag	UNP P0AEY0
D	2812	PRO	-	expression tag	UNP P0AEY0
D	2813	PRO	-	expression tag	UNP P0AEY0
D	2814	ALA	-	expression tag	UNP P0AEY0
H	367	ASN	-	expression tag	UNP P0AEY0

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Chain	Residue	Modelled	Actual	Comment	Reference
H	368	ALA	-	expression tag	UNP P0AEY0
H	369	ALA	-	expression tag	UNP P0AEY0
H	370	ALA	-	expression tag	UNP P0AEY0
H	2777	GLY	-	expression tag	UNP P0AEY0
H	2778	ALA	-	expression tag	UNP P0AEY0
H	2779	GLY	-	expression tag	UNP P0AEY0
H	2780	LEU	-	expression tag	UNP P0AEY0
H	2781	ARG	-	expression tag	UNP P0AEY0
H	2782	VAL	-	expression tag	UNP P0AEY0
H	2783	ASN	-	expression tag	UNP P0AEY0
H	2784	THR	-	expression tag	UNP P0AEY0
H	2785	SER	-	expression tag	UNP P0AEY0
H	2786	GLU	-	expression tag	UNP P0AEY0
H	2787	GLY	-	expression tag	UNP P0AEY0
H	2788	VAL	-	expression tag	UNP P0AEY0
H	2789	VAL	-	expression tag	UNP P0AEY0
H	2790	LEU	-	expression tag	UNP P0AEY0
H	2791	LEU	-	expression tag	UNP P0AEY0
H	2792	SER	-	expression tag	UNP P0AEY0
H	2793	TYR	-	expression tag	UNP P0AEY0
H	2794	SER	-	expression tag	UNP P0AEY0
H	2795	GLY	-	expression tag	UNP P0AEY0
H	2796	GLN	-	expression tag	UNP P0AEY0
H	2797	LYS	-	expression tag	UNP P0AEY0
H	2798	THR	-	expression tag	UNP P0AEY0
H	2799	GLU	-	expression tag	UNP P0AEY0
H	2800	GLY	-	expression tag	UNP P0AEY0
H	2801	PRO	-	expression tag	UNP P0AEY0
H	2802	GLN	-	expression tag	UNP P0AEY0
H	2803	ARG	-	expression tag	UNP P0AEY0
H	2804	ILE	-	expression tag	UNP P0AEY0
H	2805	SER	-	expression tag	UNP P0AEY0
H	2806	ALA	-	expression tag	UNP P0AEY0
H	2807	LYS	-	expression tag	UNP P0AEY0
H	2808	ILE	-	expression tag	UNP P0AEY0
H	2809	SER	-	expression tag	UNP P0AEY0
H	2810	GLN	-	expression tag	UNP P0AEY0
H	2811	ILE	-	expression tag	UNP P0AEY0
H	2812	PRO	-	expression tag	UNP P0AEY0
H	2813	PRO	-	expression tag	UNP P0AEY0
H	2814	ALA	-	expression tag	UNP P0AEY0

- Molecule 5 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.

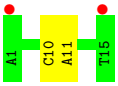
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	I	2	Total C O 23 12 11	0	0	0
5	J	2	Total C O 23 12 11	0	0	0

3 Residue-property plots

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

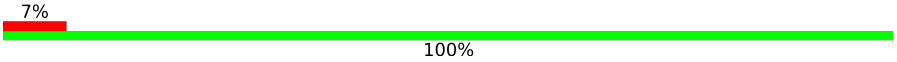
• Molecule 1: DNA (5'-D(*AP*AP*TP*CP*TP*TP*TP*CP*CP*CP*AP*CP*AP*GP*T)-3')

Chain A:



• Molecule 1: DNA (5'-D(*AP*AP*TP*CP*TP*TP*TP*CP*CP*CP*AP*CP*AP*GP*T)-3')

Chain E:



• Molecule 2: DNA (5'-D(*TP*TP*AP*CP*TP*GP*TP*GP*GP*GP*AP*AP*AP*GP*A)-3')

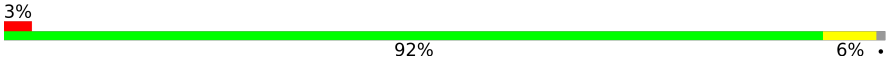
Chain B:

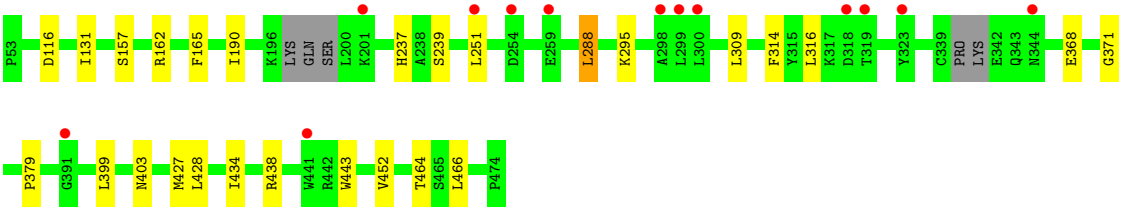
• Molecule 2: DNA (5'-D(*TP*TP*AP*CP*TP*GP*TP*GP*GP*GP*AP*AP*AP*GP*A)-3')

Chain F:

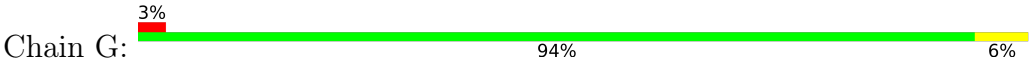
• Molecule 3: Recombining binding protein suppressor of hairless

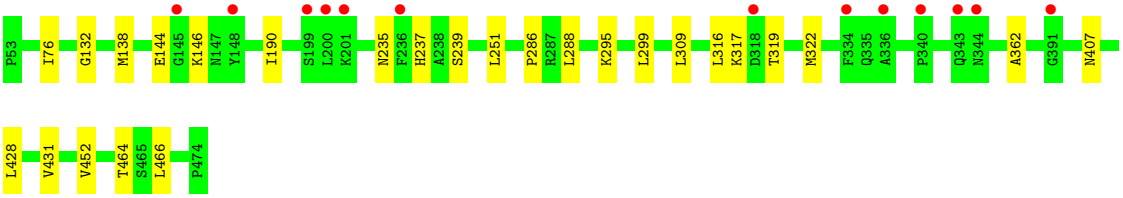
Chain C:



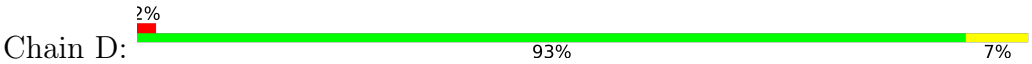


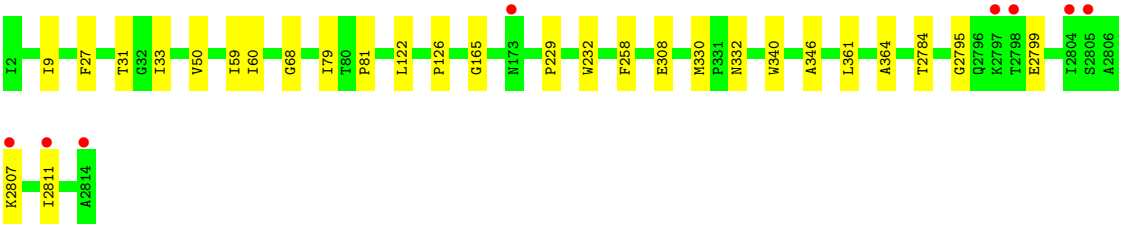
• Molecule 3: Recombining binding protein suppressor of hairless



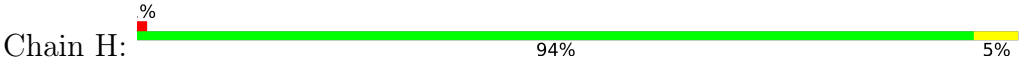


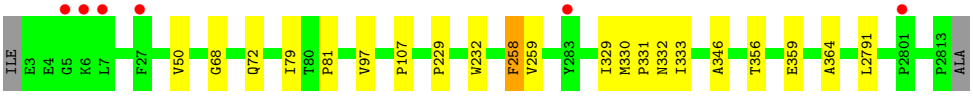
• Molecule 4: Maltose/maltodextrin-binding periplasmic protein





• Molecule 4: Maltose/maltodextrin-binding periplasmic protein





• Molecule 5: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

• Molecule 5: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	54.45Å 231.57Å 90.26Å 90.00° 99.88° 90.00°	Depositor
Resolution (Å)	38.53 – 2.78 38.53 – 2.78	Depositor EDS
% Data completeness (in resolution range)	98.8 (38.53-2.78) 99.2 (38.53-2.78)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.80 (at 2.77Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.195 , 0.228 0.206 , 0.242	Depositor DCC
R_{free} test set	2756 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	59.7	Xtriage
Anisotropy	0.558	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 43.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	13438	wwPDB-VP
Average B, all atoms (Å^2)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.64% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: GLC

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	0.99	0/332	0.93	0/509
1	E	1.00	0/332	0.92	0/509
2	B	0.93	0/350	0.88	0/540
2	F	0.97	0/350	0.92	0/540
3	C	0.38	0/3137	0.59	0/4270
3	G	0.38	0/3211	0.59	0/4378
4	D	0.40	0/3070	0.59	0/4197
4	H	0.41	0/3045	0.60	0/4171
All	All	0.48	0/13827	0.64	0/19114

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	298	0	172	1	0
1	E	298	0	172	0	0
2	B	311	0	171	1	0
2	F	311	0	171	1	0
3	C	3068	0	2836	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	3137	0	2889	10	0
4	D	2997	0	2815	13	0
4	H	2972	0	2772	10	0
5	I	23	0	21	0	0
5	J	23	0	21	0	0
All	All	13438	0	12040	48	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 2.

All (48) 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:G:464:THR:HG22	3:G:466:LEU:H	1.53	0.74
3:C:464:THR:HG22	3:C:466:LEU:H	1.53	0.73
4:H:68:GLY:HA3	4:H:332:ASN:O	1.99	0.63
4:D:68:GLY:HA3	4:D:332:ASN:O	2.01	0.60
4:D:79:ILE:HG22	4:D:81:PRO:HD3	1.83	0.59
3:C:131:ILE:CG2	3:C:162:ARG:HH22	2.15	0.59
3:G:452:VAL:O	3:G:464:THR:HB	2.03	0.58
3:C:131:ILE:HG22	3:C:162:ARG:HH22	1.68	0.58
3:C:452:VAL:O	3:C:464:THR:HB	2.04	0.57
4:D:27:PHE:O	4:D:31:THR:HG22	2.05	0.57
3:G:316:LEU:O	3:G:319:THR:HG22	2.06	0.55
3:G:190:ILE:HD11	3:G:309:LEU:HD12	1.91	0.53
3:C:190:ILE:HD11	3:C:309:LEU:HD12	1.91	0.53
3:C:379:PRO:HB2	3:C:403:ASN:HB3	1.90	0.53
3:C:288:LEU:HD13	3:C:314:PHE:HD2	1.74	0.52
3:C:131:ILE:HG23	3:C:165:PHE:CD2	2.46	0.51
3:G:319:THR:HG21	3:G:322:MET:HB2	1.96	0.47
3:C:466:LEU:HD23	4:D:2795:GLY:HA2	1.98	0.46
4:D:9:ILE:HG12	4:D:59:ILE:HB	1.96	0.46
3:G:319:THR:HG23	3:G:322:MET:H	1.81	0.45
3:G:286:PRO:O	3:G:288:LEU:HG	2.15	0.45
4:H:97:VAL:HG21	4:H:107:PRO:HD3	1.99	0.45
2:B:2:DT:H2"	2:B:3:DA:C8	2.51	0.45
3:C:316:LEU:HD21	4:D:2811:ILE:HD12	1.99	0.45
4:D:31:THR:HG23	4:D:33:ILE:H	1.82	0.45
4:H:259:VAL:HB	4:H:329:ILE:HA	1.99	0.45
4:H:79:ILE:HD12	4:H:81:PRO:HD3	1.98	0.44
4:D:122:LEU:HD21	4:D:126:PRO:HD3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:399:LEU:HB2	3:C:427:MET:HB3	1.99	0.44
4:D:330:MET:CE	4:D:340:TRP:HZ2	2.31	0.43
3:C:368:GLU:HB3	3:C:371:GLY:O	2.19	0.43
3:G:431:VAL:HG11	4:H:2791:LEU:HD13	2.02	0.42
4:H:346:ALA:HB2	4:H:364:ALA:HB2	2.01	0.42
3:G:76:ILE:HB	3:G:362:ALA:HB3	2.01	0.42
4:H:356:THR:HG23	4:H:359:GLU:H	1.84	0.42
3:C:237:HIS:CE1	3:C:239:SER:HB2	2.55	0.42
2:F:2:DT:H2"	2:F:3:DA:C8	2.55	0.41
3:C:288:LEU:HD13	3:C:314:PHE:CD2	2.55	0.41
3:G:237:HIS:CE1	3:G:239:SER:HB2	2.56	0.41
3:C:434:ILE:HG22	4:D:2784:THR:HG21	2.02	0.41
3:C:466:LEU:CD2	4:D:2795:GLY:HA2	2.50	0.41
4:H:258:PHE:CD1	4:H:330:MET:HG2	2.56	0.41
4:D:229:PRO:HA	4:D:232:TRP:CE2	2.55	0.41
3:C:438:ARG:HB3	3:C:443:TRP:HA	2.02	0.41
4:H:229:PRO:HA	4:H:232:TRP:CE2	2.56	0.40
4:D:346:ALA:HB2	4:D:364:ALA:HB2	2.03	0.40
4:H:331:PRO:HB2	4:H:333:ILE:HG12	2.03	0.40
1:A:10:DC:H2"	1:A:11:DA:C8	2.56	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
3	C	411/422 (97%)	394 (96%)	16 (4%)	1 (0%)	47 76
3	G	421/422 (100%)	405 (96%)	13 (3%)	3 (1%)	22 50
4	D	405/407 (100%)	392 (97%)	11 (3%)	2 (0%)	29 58
4	H	404/407 (99%)	390 (96%)	14 (4%)	0	100 100
All	All	1641/1658 (99%)	1581 (96%)	54 (3%)	6 (0%)	34 64

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	2799	GLU
3	C	295	LYS
3	G	144	GLU
3	G	295	LYS
4	D	165	GLY
3	G	132	GLY

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	
3	C	297/372 (80%)	292 (98%)	5 (2%)	60	85
3	G	306/372 (82%)	298 (97%)	8 (3%)	46	76
4	D	286/323 (88%)	280 (98%)	6 (2%)	53	81
4	H	282/323 (87%)	279 (99%)	3 (1%)	73	90
All	All	1171/1390 (84%)	1149 (98%)	22 (2%)	57	83

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	116	ASP
3	C	157	SER
3	C	251	LEU
3	C	288	LEU
3	C	428	LEU
4	D	50	VAL
4	D	60	ILE
4	D	258	PHE
4	D	308	GLU
4	D	361	LEU
4	D	2807	LYS
3	G	138	MET
3	G	146	LYS
3	G	235	ASN

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Mol	Chain	Res	Type
3	G	251	LEU
3	G	299	LEU
3	G	317	LYS
3	G	407	ASN
3	G	428	LEU
4	H	50	VAL
4	H	72	GLN
4	H	258	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	457	ASN
3	G	164	HIS
3	G	407	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

4 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	$\#\|Z\| > 2$
5	GLC	I	1	5	12,12,12	0.30	0	17,17,17	0.45	0
5	GLC	I	2	5	11,11,12	0.33	0	15,15,17	0.88	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	GLC	J	1	5	12,12,12	0.33	0	17,17,17	0.66	0
5	GLC	J	2	5	11,11,12	0.34	0	15,15,17	0.58	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
5	GLC	I	1	5	-	0/2/22/22	0/1/1/1
5	GLC	I	2	5	-	0/2/19/22	0/1/1/1
5	GLC	J	1	5	-	0/2/22/22	0/1/1/1
5	GLC	J	2	5	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	I	2	GLC	C1-O5-C5	3.19	116.51	112.19
5	J	2	GLC	C1-O5-C5	2.02	114.93	112.19

There are no chirality outliers.

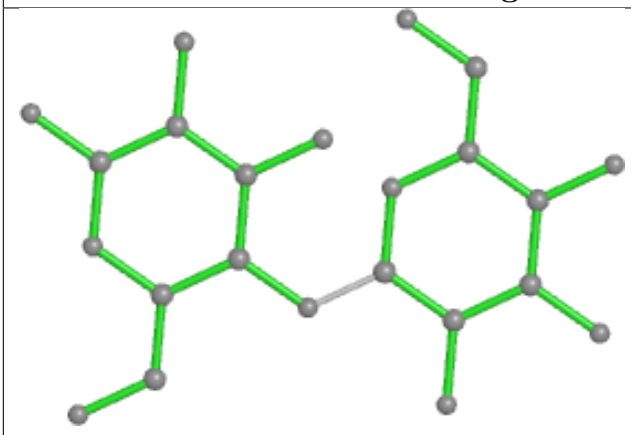
There are no torsion outliers.

There are no ring outliers.

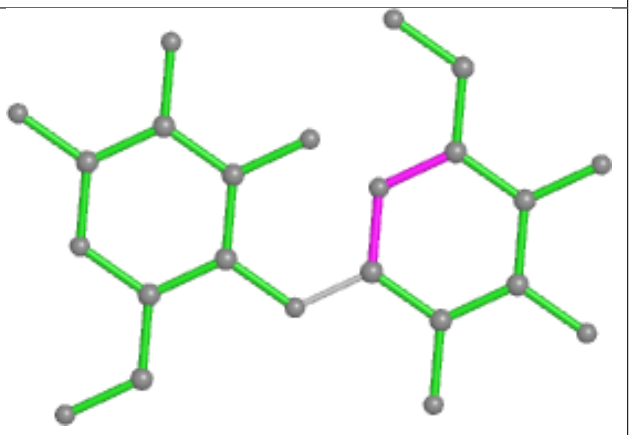
No monomer is involved in short contacts.

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

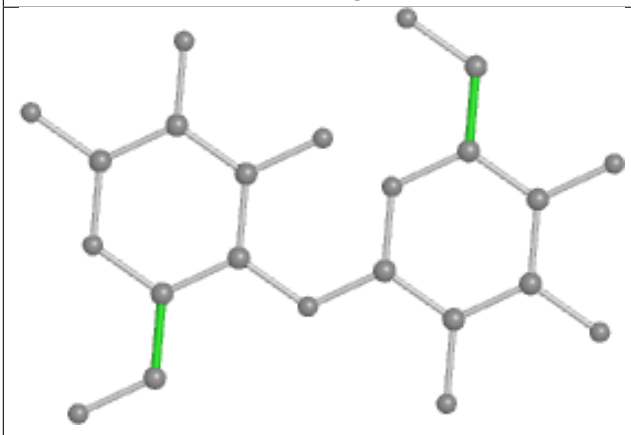
Oligosaccharide Chain I



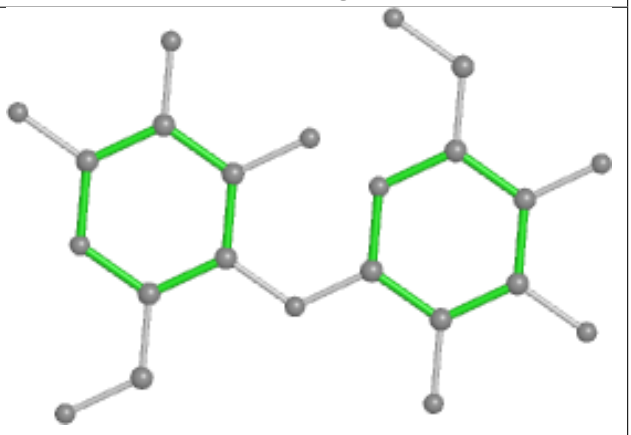
Bond lengths



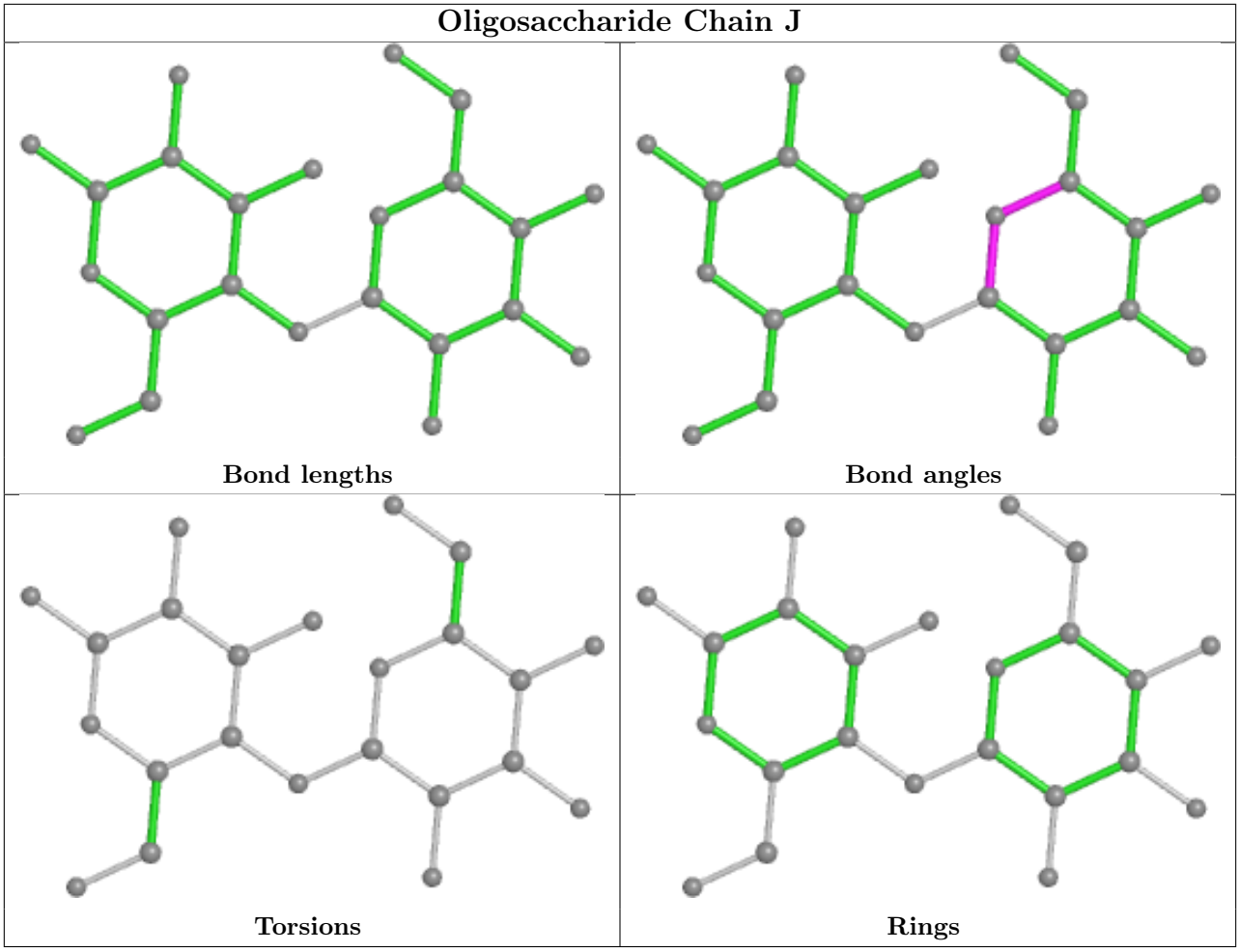
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

There are no ligands in this entry.

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, 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	15/15 (100%)	0.28	2 (13%) 3 2	104, 115, 151, 156	0
1	E	15/15 (100%)	0.11	1 (6%) 17 13	82, 111, 144, 147	0
2	B	15/15 (100%)	0.36	1 (6%) 17 13	84, 131, 147, 154	0
2	F	15/15 (100%)	0.11	0 100 100	81, 112, 152, 156	0
3	C	417/422 (98%)	-0.01	13 (3%) 49 44	33, 69, 134, 165	0
3	G	422/422 (100%)	-0.04	13 (3%) 49 44	33, 67, 123, 164	0
4	D	407/407 (100%)	-0.02	8 (1%) 65 61	51, 74, 109, 154	0
4	H	405/407 (99%)	-0.12	6 (1%) 73 71	43, 70, 110, 138	0
All	All	1711/1718 (99%)	-0.04	44 (2%) 56 51	33, 72, 128, 165	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	H	5	GLY	3.6
3	G	340	PRO	3.6
3	C	441	TRP	3.3
3	G	334	PHE	3.2
3	G	391	GLY	3.1
1	A	15	DT	3.0
3	G	200	LEU	3.0
4	H	27	PHE	2.9
3	C	318	ASP	2.8
4	H	2801	PRO	2.8
3	G	336	ALA	2.7
3	C	391	GLY	2.7
3	C	300	LEU	2.6
3	C	319	THR	2.6
1	A	1	DA	2.5
4	H	7	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
3	C	344	ASN	2.5
2	B	1	DT	2.5
4	D	2797	LYS	2.4
3	C	254	ASP	2.4
3	C	201	LYS	2.4
3	G	201	LYS	2.4
3	C	251	LEU	2.4
4	D	2804	ILE	2.4
3	C	298	ALA	2.4
4	D	2798	THR	2.4
3	G	145	GLY	2.4
3	G	148	TYR	2.3
4	D	2811	ILE	2.3
1	E	3	DT	2.3
4	H	6	LYS	2.3
3	G	318	ASP	2.2
3	C	323	TYR	2.2
4	D	173	ASN	2.2
3	G	343	GLN	2.2
4	D	2814	ALA	2.1
4	D	2807	LYS	2.1
3	G	199	SER	2.1
3	G	236	PHE	2.1
4	H	283	TYR	2.0
3	C	259	GLU	2.0
3	C	299	LEU	2.0
4	D	2805	SER	2.0
3	G	344	ASN	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)

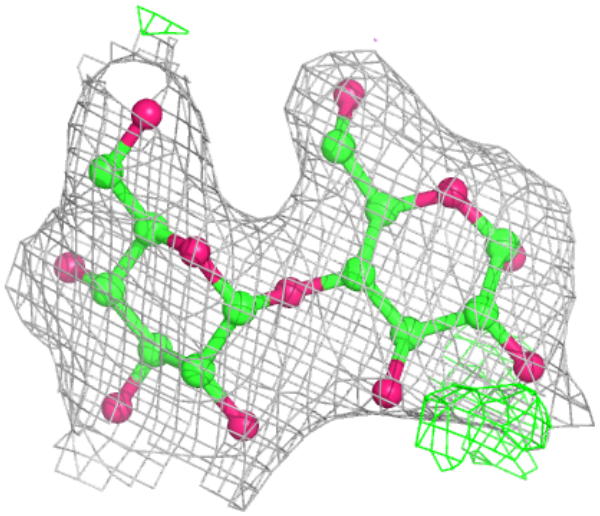
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

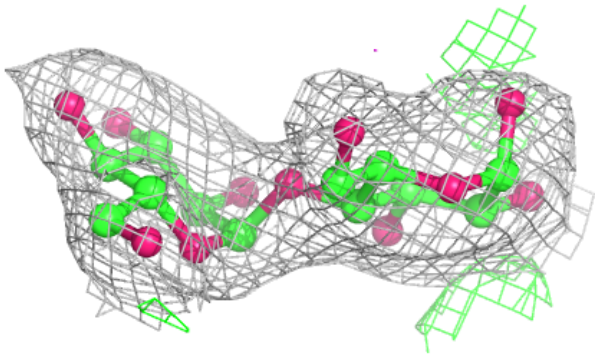
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	GLC	I	1	12/12	0.97	0.23	53,60,63,66	0
5	GLC	J	1	12/12	0.97	0.19	58,60,62,63	0
5	GLC	I	2	11/12	0.98	0.18	49,50,51,51	0
5	GLC	J	2	11/12	0.98	0.17	51,55,56,57	0

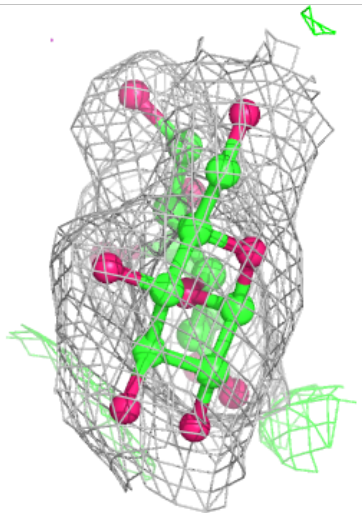
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain I:

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

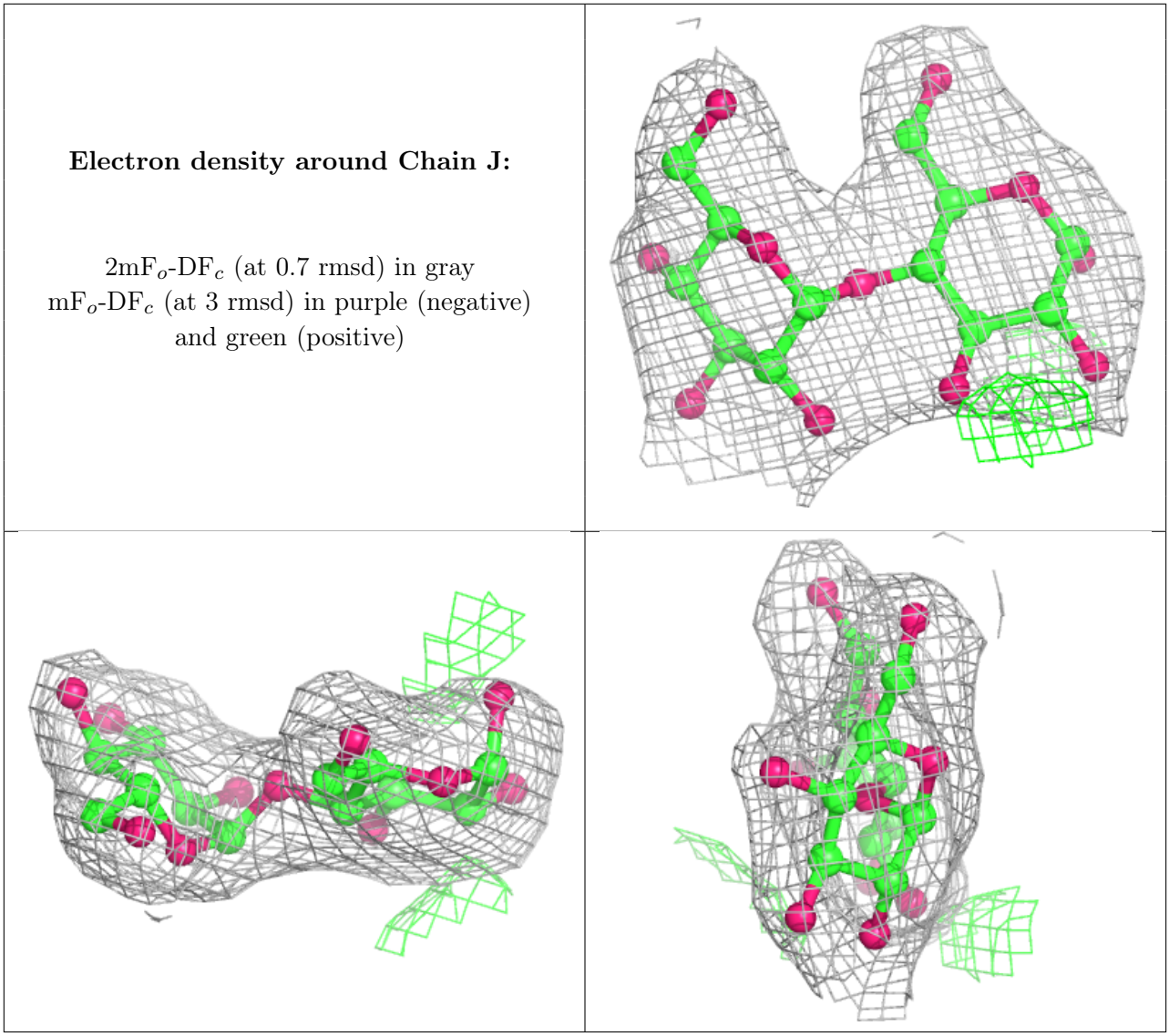






Electron density around Chain J:

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



6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.