Full wwPDB X-ray Structure Validation Report ⓘ

Sep 24, 2023 – 05:32 PM EDT

PDB ID	:	5V6Y
Title	:	Crystal structure of the human CLR:RAMP1 extracellular domain heterodimer with bound high-affinity and altered selectivity adrenomedullin variant
Authors	:	Pioszak, A.; Booe, J.
Deposited on	:	2017-03-17
Resolution	:	2.80 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:

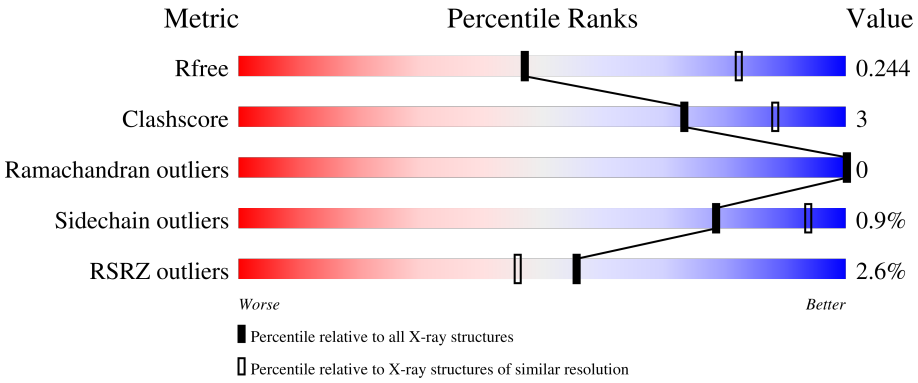
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	593	87% 6% 7%
1	B	593	2% 83% 9% 7%
1	C	593	2% 83% 9% 7%
1	D	593	5% 84% 9% 8%
2	E	17	76% 18% 6%

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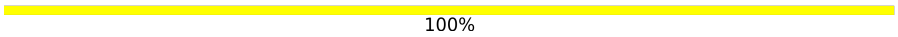
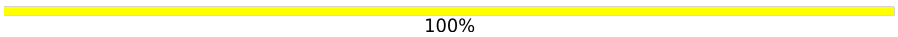
Mol	Chain	Length	Quality of chain
2	F	17	
2	G	17	
2	H	17	
3	I	2	
3	J	2	
3	K	2	
3	L	2	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 17855 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 Maltose-binding periplasmic protein,Receptor activity-modifying protein 1,Calcitonin gene-related peptide type 1 receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	550	Total	C	N	O	S	0	0	0
			4341	2773	720	825	23			
1	B	551	Total	C	N	O	S	0	0	0
			4349	2779	721	826	23			
1	C	549	Total	C	N	O	S	0	0	0
			4335	2770	718	824	23			
1	D	547	Total	C	N	O	S	0	0	0
			4278	2727	710	818	23			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP P0AEY0
A	369	ASN	-	linker	UNP P0AEY0
A	370	ALA	-	linker	UNP P0AEY0
A	371	ALA	-	linker	UNP P0AEY0
A	372	ALA	-	linker	UNP P0AEY0
A	373	GLU	-	linker	UNP P0AEY0
A	374	PHE	-	linker	UNP P0AEY0
A	2020	GLY	-	linker	UNP O60894
A	2021	SER	-	linker	UNP O60894
A	2022	ALA	-	linker	UNP O60894
A	2023	GLY	-	linker	UNP O60894
A	2024	SER	-	linker	UNP O60894
A	2025	ALA	-	linker	UNP O60894
A	2026	GLY	-	linker	UNP O60894
A	2027	SER	-	linker	UNP O60894
A	2028	ALA	-	linker	UNP O60894
A	2145	HIS	-	expression tag	UNP Q16602
A	2146	HIS	-	expression tag	UNP Q16602
A	2147	HIS	-	expression tag	UNP Q16602
A	2148	HIS	-	expression tag	UNP Q16602

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Chain	Residue	Modelled	Actual	Comment	Reference
A	2149	HIS	-	expression tag	UNP Q16602
A	2150	HIS	-	expression tag	UNP Q16602
B	1	MET	-	initiating methionine	UNP P0AEY0
B	369	ASN	-	linker	UNP P0AEY0
B	370	ALA	-	linker	UNP P0AEY0
B	371	ALA	-	linker	UNP P0AEY0
B	372	ALA	-	linker	UNP P0AEY0
B	373	GLU	-	linker	UNP P0AEY0
B	374	PHE	-	linker	UNP P0AEY0
B	2020	GLY	-	linker	UNP O60894
B	2021	SER	-	linker	UNP O60894
B	2022	ALA	-	linker	UNP O60894
B	2023	GLY	-	linker	UNP O60894
B	2024	SER	-	linker	UNP O60894
B	2025	ALA	-	linker	UNP O60894
B	2026	GLY	-	linker	UNP O60894
B	2027	SER	-	linker	UNP O60894
B	2028	ALA	-	linker	UNP O60894
B	2145	HIS	-	expression tag	UNP Q16602
B	2146	HIS	-	expression tag	UNP Q16602
B	2147	HIS	-	expression tag	UNP Q16602
B	2148	HIS	-	expression tag	UNP Q16602
B	2149	HIS	-	expression tag	UNP Q16602
B	2150	HIS	-	expression tag	UNP Q16602
C	1	MET	-	initiating methionine	UNP P0AEY0
C	369	ASN	-	linker	UNP P0AEY0
C	370	ALA	-	linker	UNP P0AEY0
C	371	ALA	-	linker	UNP P0AEY0
C	372	ALA	-	linker	UNP P0AEY0
C	373	GLU	-	linker	UNP P0AEY0
C	374	PHE	-	linker	UNP P0AEY0
C	2020	GLY	-	linker	UNP O60894
C	2021	SER	-	linker	UNP O60894
C	2022	ALA	-	linker	UNP O60894
C	2023	GLY	-	linker	UNP O60894
C	2024	SER	-	linker	UNP O60894
C	2025	ALA	-	linker	UNP O60894
C	2026	GLY	-	linker	UNP O60894
C	2027	SER	-	linker	UNP O60894
C	2028	ALA	-	linker	UNP O60894
C	2145	HIS	-	expression tag	UNP Q16602
C	2146	HIS	-	expression tag	UNP Q16602

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Chain	Residue	Modelled	Actual	Comment	Reference
C	2147	HIS	-	expression tag	UNP Q16602
C	2148	HIS	-	expression tag	UNP Q16602
C	2149	HIS	-	expression tag	UNP Q16602
C	2150	HIS	-	expression tag	UNP Q16602
D	1	MET	-	initiating methionine	UNP P0AEY0
D	369	ASN	-	linker	UNP P0AEY0
D	370	ALA	-	linker	UNP P0AEY0
D	371	ALA	-	linker	UNP P0AEY0
D	372	ALA	-	linker	UNP P0AEY0
D	373	GLU	-	linker	UNP P0AEY0
D	374	PHE	-	linker	UNP P0AEY0
D	2020	GLY	-	linker	UNP O60894
D	2021	SER	-	linker	UNP O60894
D	2022	ALA	-	linker	UNP O60894
D	2023	GLY	-	linker	UNP O60894
D	2024	SER	-	linker	UNP O60894
D	2025	ALA	-	linker	UNP O60894
D	2026	GLY	-	linker	UNP O60894
D	2027	SER	-	linker	UNP O60894
D	2028	ALA	-	linker	UNP O60894
D	2145	HIS	-	expression tag	UNP Q16602
D	2146	HIS	-	expression tag	UNP Q16602
D	2147	HIS	-	expression tag	UNP Q16602
D	2148	HIS	-	expression tag	UNP Q16602
D	2149	HIS	-	expression tag	UNP Q16602
D	2150	HIS	-	expression tag	UNP Q16602

- Molecule 2 is a protein called ADM.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	16	Total	C	N	O	0	0	1
			118	80	19	19			
2	F	16	Total	C	N	O	0	1	1
			138	94	24	20			
2	G	14	Total	C	N	O	0	0	1
			111	76	20	15			
2	H	14	Total	C	N	O	0	0	1
			90	61	15	14			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	45	TRP	SER	engineered mutation	UNP P35318
E	46	LEU	LYS	engineered mutation	UNP P35318
E	50	TRP	GLN	engineered mutation	UNP P35318
E	52	PHE	TYR	engineered mutation	UNP P35318
E	53	NH2	-	amidation	UNP P35318
F	45	TRP	SER	engineered mutation	UNP P35318
F	46	LEU	LYS	engineered mutation	UNP P35318
F	50	TRP	GLN	engineered mutation	UNP P35318
F	52	PHE	TYR	engineered mutation	UNP P35318
F	53	NH2	-	amidation	UNP P35318
G	45	TRP	SER	engineered mutation	UNP P35318
G	46	LEU	LYS	engineered mutation	UNP P35318
G	50	TRP	GLN	engineered mutation	UNP P35318
G	52	PHE	TYR	engineered mutation	UNP P35318
G	53	NH2	-	amidation	UNP P35318
H	45	TRP	SER	engineered mutation	UNP P35318
H	46	LEU	LYS	engineered mutation	UNP P35318
H	50	TRP	GLN	engineered mutation	UNP P35318
H	52	PHE	TYR	engineered mutation	UNP P35318
H	53	NH2	-	amidation	UNP P35318

- Molecule 3 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.

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

- Molecule 4 is water.

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

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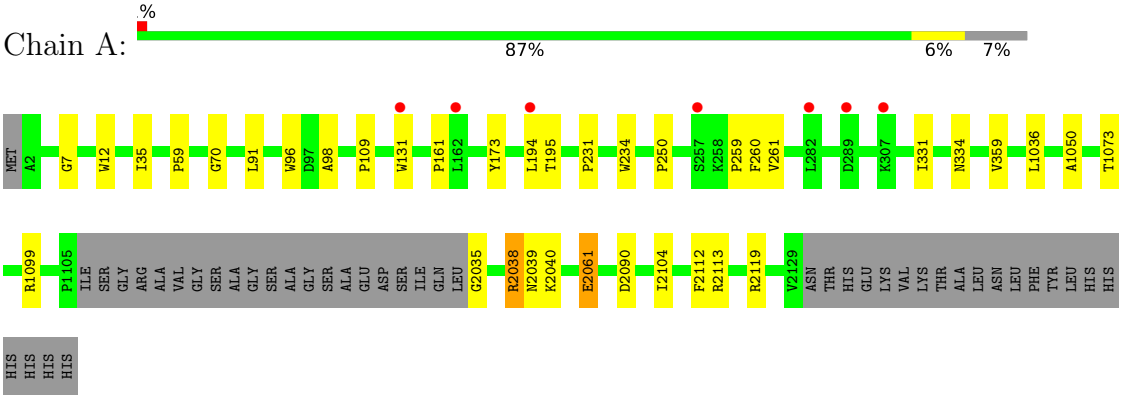
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total O 1 1	0	0

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.

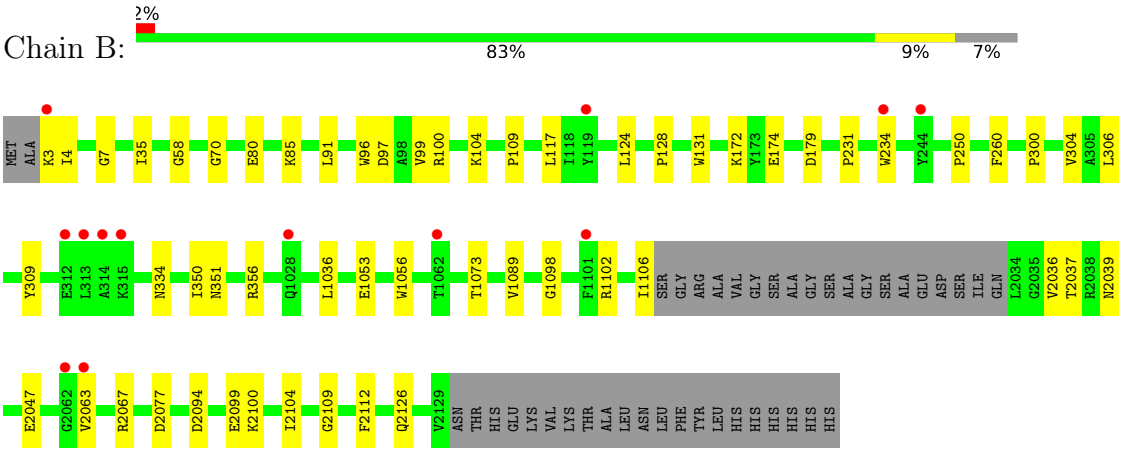
• Molecule 1: Maltose-binding periplasmic protein,Receptor activity-modifying protein 1,Calcitonin gene-related peptide type 1 receptor

Chain A:



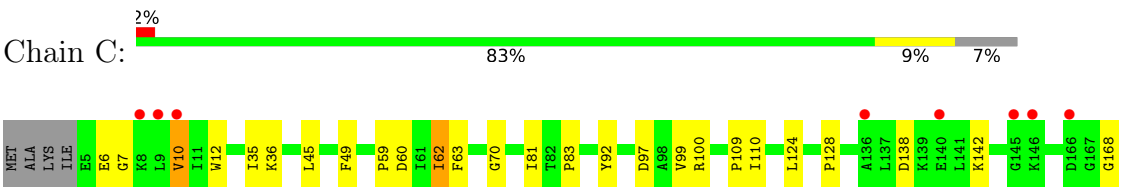
• Molecule 1: Maltose-binding periplasmic protein,Receptor activity-modifying protein 1,Calcitonin gene-related peptide type 1 receptor

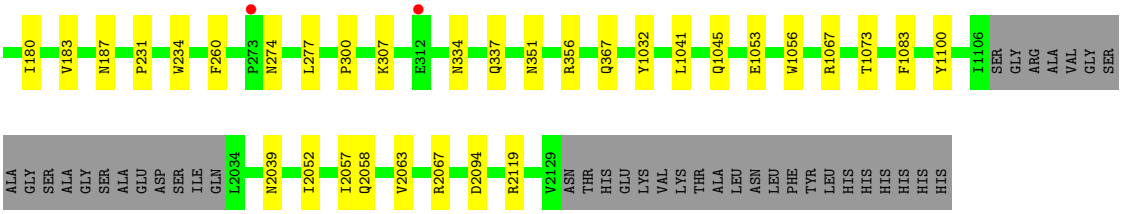
Chain B:



• Molecule 1: Maltose-binding periplasmic protein,Receptor activity-modifying protein 1,Calcitonin gene-related peptide type 1 receptor

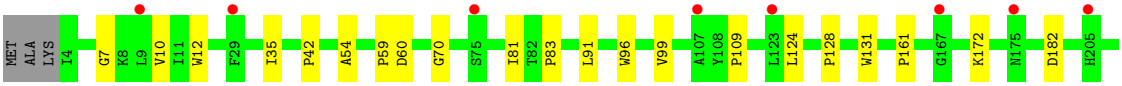
Chain C:

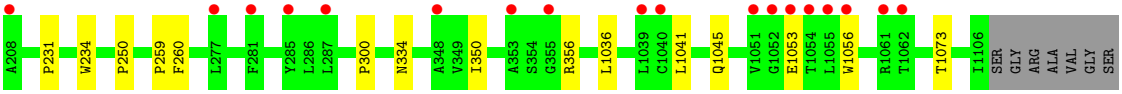


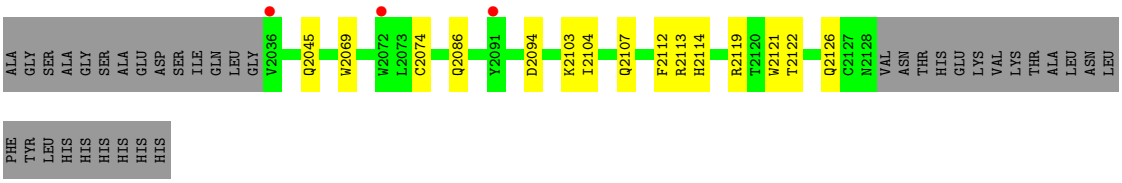


• Molecule 1: Maltose-binding periplasmic protein,Receptor activity-modifying protein 1,Calcitonin gene-related peptide type 1 receptor

Chain D:

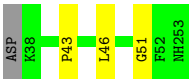






• Molecule 2: ADM

Chain E:

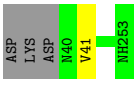


• Molecule 2: ADM

Chain F:

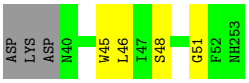
• Molecule 2: ADM

Chain G:



• Molecule 2: ADM

Chain H:

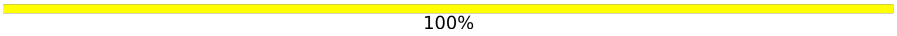


• Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain I:

• Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain J:

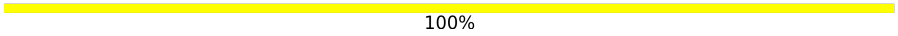


• Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain K:

• Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	195.50Å 69.44Å 200.00Å 90.00° 99.43° 90.00°	Depositor
Resolution (Å)	45.11 – 2.80 45.11 – 2.80	Depositor EDS
% Data completeness (in resolution range)	94.1 (45.11-2.80) 87.7 (45.11-2.80)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.15 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.212 , 0.244 0.212 , 0.244	Depositor DCC
R_{free} test set	2000 reflections (3.23%)	wwPDB-VP
Wilson B-factor (Å^2)	80.0	Xtriage
Anisotropy	0.475	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 55.6	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	0.94	EDS
Total number of atoms	17855	wwPDB-VP
Average B, all atoms (Å^2)	118.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.86% 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: NH2, 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	0.24	0/4453	0.39	0/6050
1	B	0.24	0/4461	0.39	0/6061
1	C	0.24	0/4447	0.39	0/6043
1	D	0.24	0/4385	0.40	0/5961
2	E	0.22	0/123	0.32	0/171
2	F	0.21	0/145	0.31	0/201
2	G	0.25	0/116	0.36	0/160
2	H	0.26	0/93	0.36	0/129
All	All	0.24	0/18223	0.39	0/24776

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	4341	0	4178	21	1
1	B	4349	0	4186	31	1
1	C	4335	0	4171	31	1
1	D	4278	0	4095	29	0
2	E	118	0	100	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	138	0	120	1	0
2	G	111	0	105	1	0
2	H	90	0	73	2	0
3	I	23	0	21	0	0
3	J	23	0	21	0	0
3	K	23	0	21	0	0
3	L	23	0	21	0	0
4	A	2	0	0	0	0
4	B	1	0	0	0	0
All	All	17855	0	17112	116	2

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 (116) 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:C:97:ASP:OD1	1:C:100:ARG:NH1	2.00	0.95
1:B:80:GLU:OE2	1:B:104:LYS:NZ	2.09	0.85
1:C:1067:ARG:NH1	1:C:2039:ASN:OD1	2.09	0.85
1:B:97:ASP:OD1	1:B:100:ARG:NH1	2.24	0.69
1:C:274:ASN:HB3	1:C:277:LEU:HB2	1.78	0.64
1:B:351:ASN:OD1	1:B:356:ARG:NH2	2.24	0.64
1:C:6:GLU:O	1:C:274:ASN:ND2	2.31	0.63
1:B:350:ILE:HG22	1:B:356:ARG:HH22	1.65	0.61
1:D:234:TRP:HB2	1:D:300:PRO:HG2	1.85	0.59
1:C:234:TRP:HB2	1:C:300:PRO:HG2	1.84	0.59
1:D:12:TRP:CD2	1:D:59:PRO:HG3	2.37	0.59
1:C:124:LEU:HD21	1:C:128:PRO:HD3	1.85	0.58
1:A:2035:GLY:O	1:A:2039:ASN:N	2.34	0.58
1:C:10:VAL:HG23	1:C:60:ASP:H	1.67	0.58
1:D:124:LEU:HD21	1:D:128:PRO:HD3	1.85	0.58
1:D:172:LYS:HD2	1:D:182:ASP:OD2	2.04	0.57
1:B:124:LEU:HD21	1:B:128:PRO:HD3	1.86	0.57
1:C:356:ARG:HB3	2:G:41:VAL:HG11	1.87	0.57
1:D:1036:LEU:HD22	1:D:1073:THR:HG22	1.85	0.56
1:B:117:LEU:HD22	1:B:250:PRO:HD3	1.89	0.54
1:D:2074:CYS:O	1:D:2086:GLN:NE2	2.36	0.54
1:C:49:PHE:CG	1:C:62:ILE:HD12	2.43	0.53
1:B:4:ILE:HD11	1:B:58:GLY:O	2.08	0.53
1:B:2099:GLU:HG2	1:B:2126:GLN:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:LEU:HD13	1:A:109:PRO:HG2	1.91	0.52
1:A:2040:LYS:NZ	1:A:2090:ASP:OD1	2.42	0.52
1:D:2104:ILE:HB	1:D:2112:PHE:HB2	1.92	0.52
1:B:91:LEU:HD12	1:B:96:TRP:CZ2	2.44	0.52
1:D:91:LEU:HD12	1:D:96:TRP:CZ2	2.45	0.52
1:D:54:ALA:O	1:D:2107:GLN:HG3	2.09	0.51
1:B:1036:LEU:HD22	1:B:1073:THR:HG22	1.93	0.51
1:A:1036:LEU:HD22	1:A:1073:THR:HG22	1.92	0.51
1:B:70:GLY:HA3	1:B:334:ASN:O	2.11	0.51
1:D:91:LEU:HD13	1:D:109:PRO:HG2	1.93	0.50
1:C:12:TRP:CD2	1:C:59:PRO:HG3	2.46	0.50
1:C:351:ASN:HA	1:C:356:ARG:HD2	1.93	0.50
1:B:91:LEU:HD13	1:B:109:PRO:HG2	1.93	0.50
1:D:2114:HIS:HD2	1:D:2121:TRP:CE2	2.31	0.49
1:A:161:PRO:HG3	1:A:259:PRO:HA	1.95	0.49
1:A:70:GLY:HA3	1:A:334:ASN:O	2.13	0.48
1:A:91:LEU:HD12	1:A:96:TRP:CZ2	2.48	0.48
1:A:2104:ILE:HB	1:A:2112:PHE:HB2	1.95	0.48
1:C:231:PRO:HA	1:C:234:TRP:CE2	2.49	0.48
1:D:70:GLY:HA3	1:D:334:ASN:O	2.13	0.48
1:D:99:VAL:HG21	1:D:109:PRO:HD3	1.96	0.48
1:B:231:PRO:HA	1:B:234:TRP:CE2	2.49	0.48
2:H:46:LEU:HA	2:H:51:GLY:HA3	1.96	0.47
1:A:7:GLY:O	1:A:35:ILE:HG23	2.14	0.47
1:D:131:TRP:CD1	1:D:250:PRO:HB2	2.49	0.47
1:A:12:TRP:CD2	1:A:59:PRO:HG3	2.50	0.47
1:A:231:PRO:HA	1:A:234:TRP:CE2	2.50	0.47
1:C:1041:LEU:O	1:C:1045:GLN:HG3	2.14	0.47
1:B:7:GLY:O	1:B:35:ILE:HG23	2.14	0.47
1:B:2104:ILE:HB	1:B:2112:PHE:HB2	1.97	0.47
1:D:12:TRP:CE2	1:D:42:PRO:HG2	2.50	0.47
1:A:194:LEU:HD23	1:A:359:VAL:HG13	1.97	0.46
1:B:99:VAL:HG21	1:B:109:PRO:HD3	1.97	0.46
1:A:2061:GLU:H	1:A:2061:GLU:HG2	1.49	0.46
1:B:1098:GLY:CA	1:B:1102:ARG:HH11	2.29	0.46
1:C:180:ILE:HD13	1:C:337:GLN:HG3	1.98	0.46
1:D:2113:ARG:HA	1:D:2119:ARG:O	2.16	0.46
1:A:2038:ARG:HD2	1:A:2038:ARG:HA	1.69	0.45
1:B:234:TRP:HB2	1:B:300:PRO:HG2	1.97	0.45
1:C:63:PHE:HE2	1:C:110:ILE:HG13	1.81	0.45
1:D:231:PRO:HA	1:D:234:TRP:CE2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:TRP:CD1	1:A:250:PRO:HB2	2.51	0.45
1:B:2099:GLU:HG3	1:B:2100:LYS:H	1.81	0.45
1:D:1053:GLU:HG2	1:D:1056:TRP:CZ2	2.52	0.45
1:C:2094:ASP:OD1	1:C:2094:ASP:N	2.37	0.45
1:C:2052:ILE:HG23	1:C:2067:ARG:HD2	1.99	0.44
1:B:131:TRP:NE1	1:B:250:PRO:HG2	2.32	0.44
1:D:2045:GLN:HB2	1:D:2069:TRP:CZ2	2.53	0.44
2:E:43:PRO:HG2	2:E:46:LEU:HD12	1.99	0.44
1:B:2094:ASP:OD1	1:B:2094:ASP:N	2.51	0.44
1:A:195:THR:HA	1:A:359:VAL:HG21	2.00	0.44
1:C:70:GLY:HA3	1:C:334:ASN:O	2.18	0.44
1:B:304:VAL:HG21	1:B:309:TYR:HD2	1.83	0.43
1:C:12:TRP:CE2	1:C:59:PRO:HG3	2.53	0.43
1:C:1045:GLN:HG2	1:C:1100:TYR:OH	2.17	0.43
1:D:2094:ASP:OD1	1:D:2094:ASP:N	2.49	0.43
1:B:1053:GLU:HG2	1:B:1056:TRP:CH2	2.54	0.43
1:B:91:LEU:HD23	1:B:306:LEU:HA	2.01	0.43
1:C:1032:TYR:OH	1:C:1073:THR:O	2.34	0.43
1:C:1053:GLU:HG2	1:C:1056:TRP:CZ2	2.54	0.43
1:D:2103:LYS:HB2	1:D:2122:THR:HG23	2.00	0.43
1:B:1098:GLY:O	1:B:1102:ARG:NH1	2.52	0.43
1:C:1083:PHE:HB2	1:C:2119:ARG:CZ	2.49	0.42
2:H:45:TRP:O	2:H:48:SER:OG	2.25	0.42
1:A:261:VAL:HB	1:A:331:ILE:HA	2.01	0.42
1:A:2113:ARG:HA	1:A:2119:ARG:O	2.19	0.42
1:D:12:TRP:CG	1:D:59:PRO:HG3	2.55	0.42
1:D:2114:HIS:HD2	1:D:2121:TRP:CD2	2.38	0.42
1:B:1106:ILE:HG22	1:B:2047:GLU:HG2	2.01	0.42
1:B:2037:THR:OG1	2:F:39:ASP:HB2	2.20	0.42
1:C:183:VAL:HB	1:C:367:GLN:OE1	2.20	0.42
1:A:98:ALA:HB2	1:A:331:ILE:HD11	2.01	0.42
1:C:168:GLY:HA2	1:C:187:ASN:HD21	1.85	0.42
1:C:2057:ILE:HD12	1:C:2057:ILE:HA	1.97	0.42
1:B:2063:VAL:HG12	1:B:2109:GLY:HA3	2.02	0.42
1:C:92:TYR:CD2	1:C:307:LYS:HG2	2.54	0.42
1:D:1041:LEU:O	1:D:1045:GLN:HG3	2.19	0.42
1:D:161:PRO:HG3	1:D:259:PRO:HA	2.02	0.41
1:D:10:VAL:N	1:D:60:ASP:OD1	2.34	0.41
1:D:7:GLY:O	1:D:35:ILE:HG23	2.20	0.41
1:A:12:TRP:CG	1:A:59:PRO:HG3	2.56	0.41
1:B:172:LYS:HG3	1:B:174:GLU:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:99:VAL:HG21	1:C:109:PRO:HD3	2.03	0.41
1:D:350:ILE:HG22	1:D:356:ARG:HH22	1.86	0.41
1:B:2036:VAL:HG23	1:B:2039:ASN:H	1.86	0.41
1:C:81:ILE:HG13	1:C:83:PRO:HD3	2.03	0.41
1:C:138:ASP:O	1:C:142:LYS:N	2.54	0.41
2:E:46:LEU:HA	2:E:51:GLY:HA3	2.03	0.40
1:A:2040:LYS:NZ	1:A:2090:ASP:CG	2.75	0.40
1:C:7:GLY:O	1:C:35:ILE:HG23	2.22	0.40
1:D:81:ILE:HG13	1:D:83:PRO:HD3	2.03	0.40
1:B:2067:ARG:NE	1:B:2077:ASP:OD2	2.50	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:85:LYS:NZ	1:B:179:ASP:OD2[4_655]	1.80	0.40
1:A:1050:ALA:O	1:C:36:LYS:NZ[3_545]	1.97	0.23

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	546/593 (92%)	535 (98%)	11 (2%)	0	100	100
1	B	547/593 (92%)	534 (98%)	13 (2%)	0	100	100
1	C	545/593 (92%)	532 (98%)	13 (2%)	0	100	100
1	D	543/593 (92%)	529 (97%)	14 (3%)	0	100	100
2	E	14/17 (82%)	14 (100%)	0	0	100	100
2	F	15/17 (88%)	14 (93%)	1 (7%)	0	100	100
2	G	12/17 (71%)	12 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	12/17 (71%)	12 (100%)	0	0	100	100
All	All	2234/2440 (92%)	2182 (98%)	52 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	450/484 (93%)	445 (99%)	5 (1%)	73	92
1	B	451/484 (93%)	448 (99%)	3 (1%)	84	95
1	C	450/484 (93%)	444 (99%)	6 (1%)	69	91
1	D	440/484 (91%)	438 (100%)	2 (0%)	88	96
2	E	11/14 (79%)	11 (100%)	0	100	100
2	F	13/14 (93%)	12 (92%)	1 (8%)	13	35
2	G	11/14 (79%)	11 (100%)	0	100	100
2	H	7/14 (50%)	7 (100%)	0	100	100
All	All	1833/1992 (92%)	1816 (99%)	17 (1%)	78	94

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	173	TYR
1	A	260	PHE
1	A	1099	ARG
1	A	2038	ARG
1	A	2061	GLU
1	B	3	LYS
1	B	260	PHE
1	B	1089	VAL
1	C	10	VAL
1	C	45	LEU

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Mol	Chain	Res	Type
1	C	62	ILE
1	C	260	PHE
1	C	2058	GLN
1	C	2063	VAL
1	D	260	PHE
1	D	2126	GLN
2	F	39	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1028	GLN
1	D	2045	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)

8 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	$\#\|Z\|>2$
3	GLC	I	1	3	12,12,12	0.79	0	17,17,17	0.84	1 (5%)
3	GLC	I	2	3	11,11,12	0.97	0	15,15,17	0.83	0
3	GLC	J	1	3	12,12,12	0.79	0	17,17,17	0.85	1 (5%)
3	GLC	J	2	3	11,11,12	0.94	0	15,15,17	0.79	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	GLC	K	1	3	12,12,12	0.79	0	17,17,17	0.86	1 (5%)
3	GLC	K	2	3	11,11,12	0.94	0	15,15,17	0.88	0
3	GLC	L	1	3	12,12,12	0.79	0	17,17,17	0.84	1 (5%)
3	GLC	L	2	3	11,11,12	1.00	0	15,15,17	0.87	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
3	GLC	I	1	3	-	0/2/22/22	0/1/1/1
3	GLC	I	2	3	-	0/2/19/22	0/1/1/1
3	GLC	J	1	3	-	0/2/22/22	0/1/1/1
3	GLC	J	2	3	-	0/2/19/22	0/1/1/1
3	GLC	K	1	3	-	0/2/22/22	0/1/1/1
3	GLC	K	2	3	-	0/2/19/22	0/1/1/1
3	GLC	L	1	3	-	0/2/22/22	0/1/1/1
3	GLC	L	2	3	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	L	1	GLC	C1-O5-C5	-2.61	108.74	113.66
3	I	1	GLC	C1-O5-C5	-2.59	108.77	113.66
3	J	1	GLC	C1-O5-C5	-2.57	108.81	113.66
3	K	1	GLC	C1-O5-C5	-2.56	108.83	113.66
3	J	2	GLC	C6-C5-C4	-2.11	108.05	113.00
3	L	2	GLC	C1-O5-C5	-2.07	109.39	112.19

There are no chirality outliers.

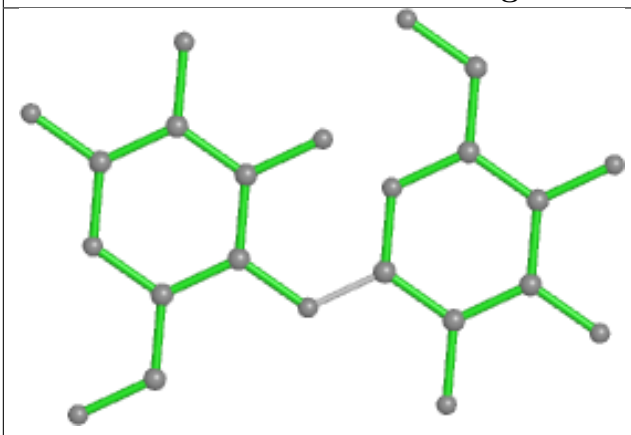
There are no torsion outliers.

There are no ring outliers.

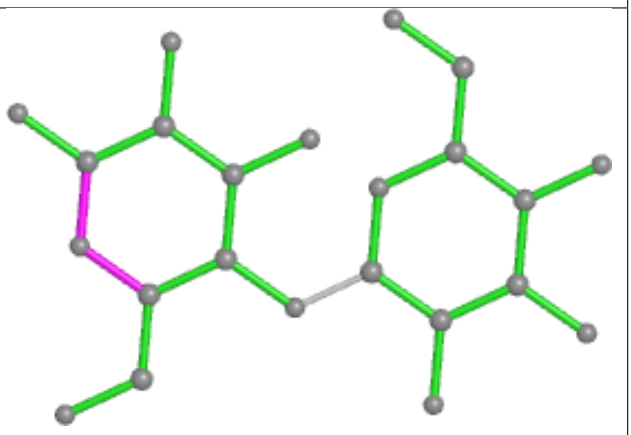
No monomer is involved in short contacts.

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

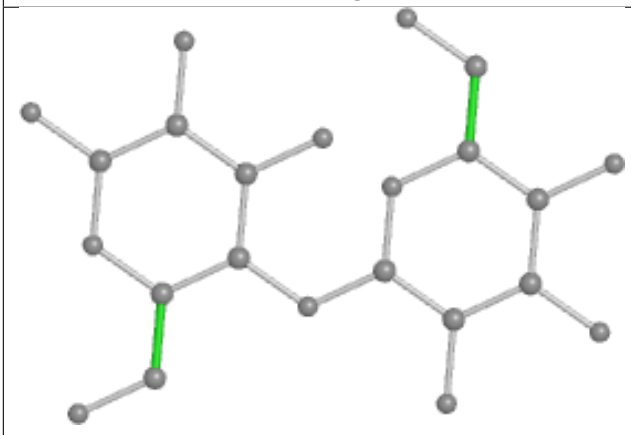
Oligosaccharide Chain I



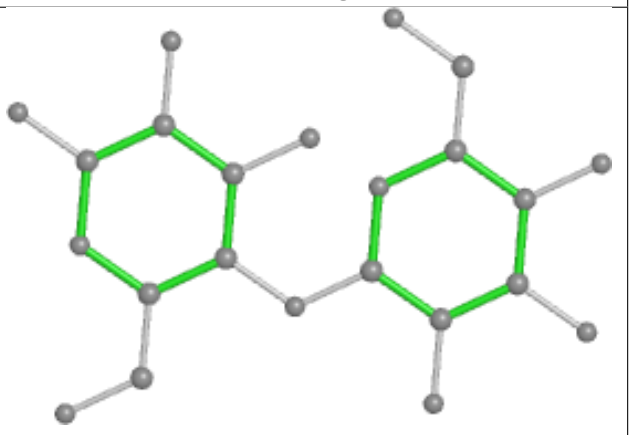
Bond lengths



Bond angles

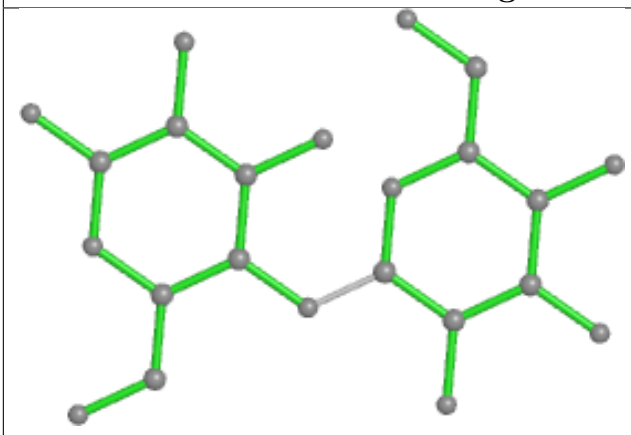


Torsions

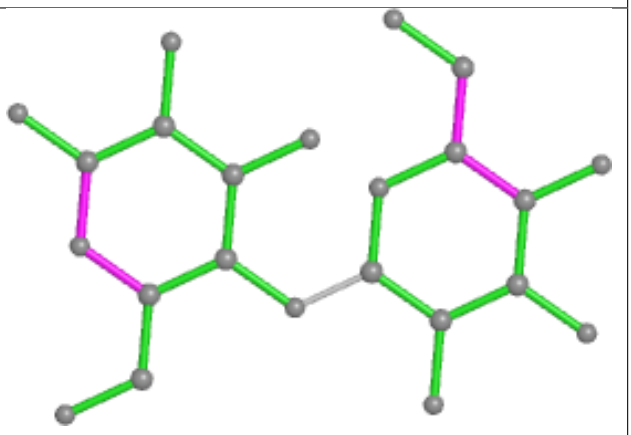


Rings

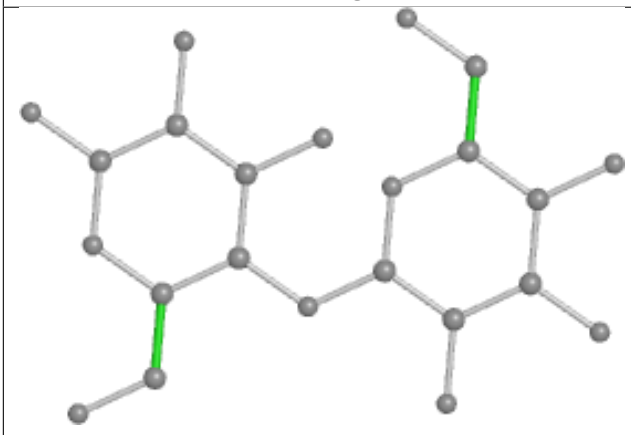
Oligosaccharide Chain J



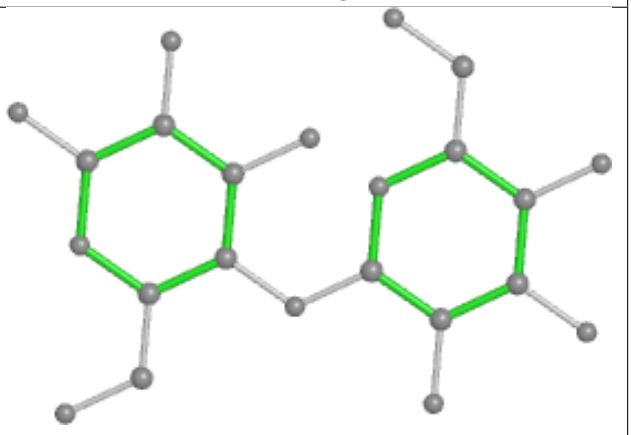
Bond lengths



Bond angles

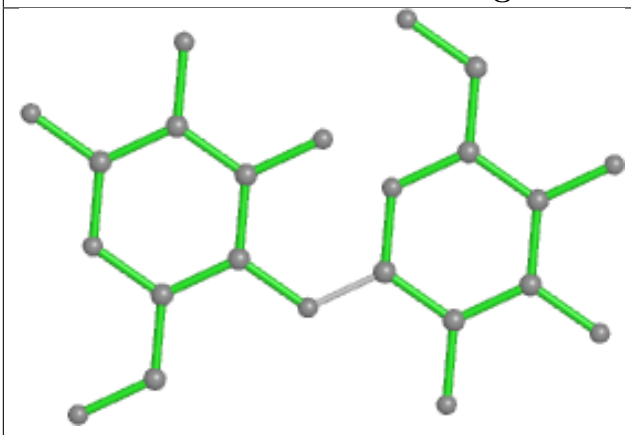


Torsions

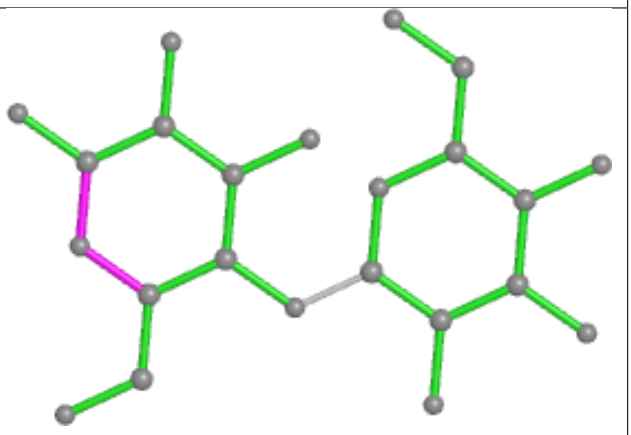


Rings

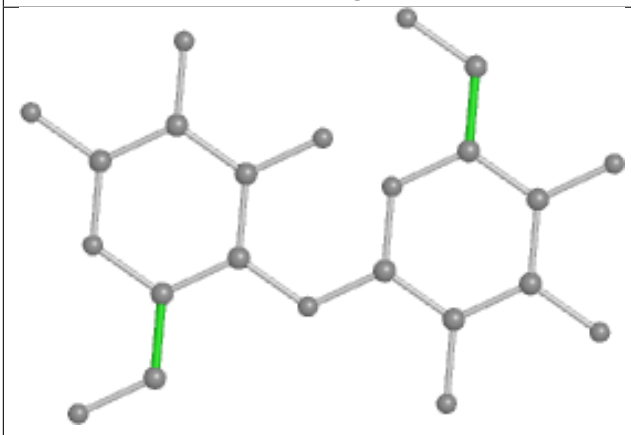
Oligosaccharide Chain K



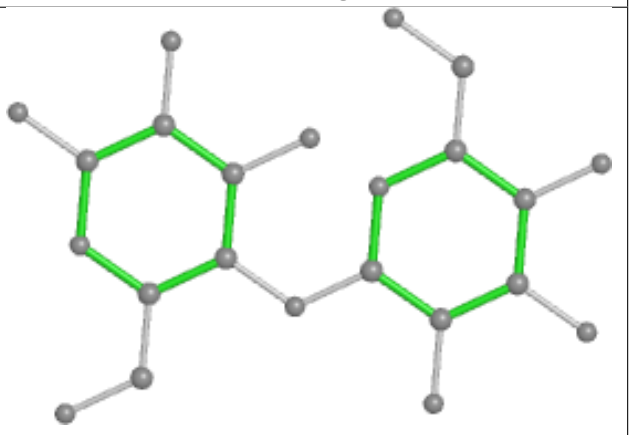
Bond lengths



Bond angles

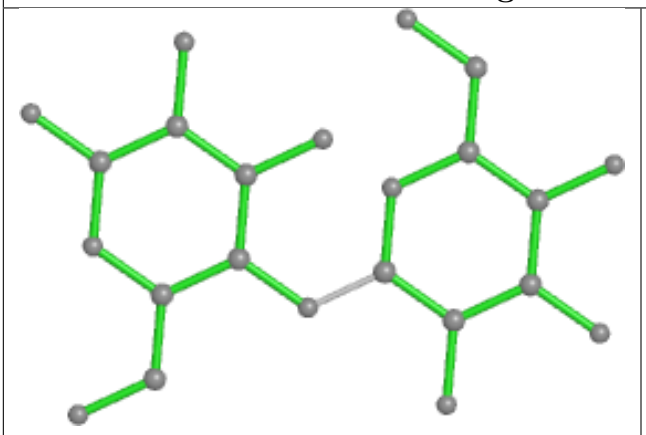


Torsions

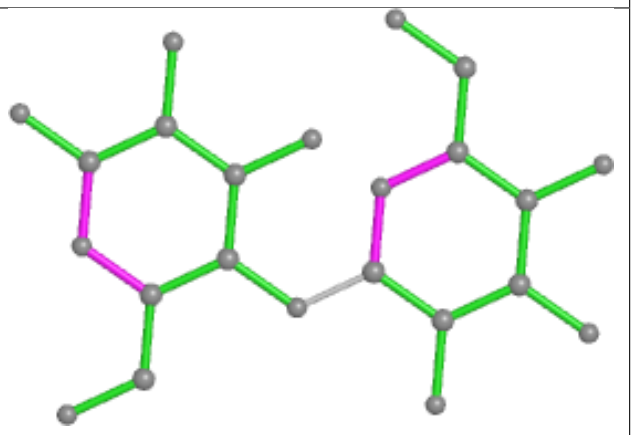


Rings

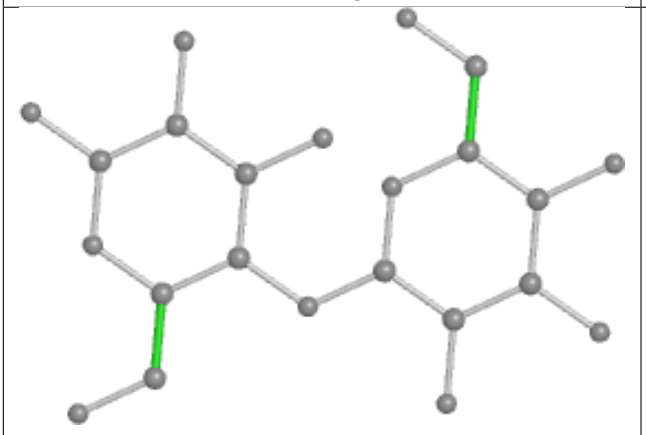
Oligosaccharide Chain L



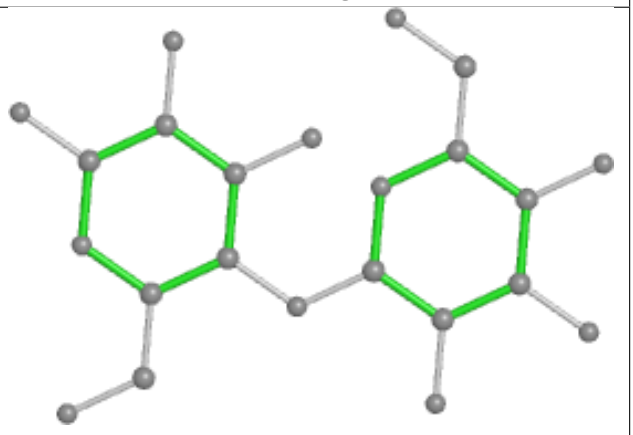
Bond lengths



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	550/593 (92%)	-0.16	7 (1%) 77 72	71, 108, 156, 199	0
1	B	551/593 (92%)	-0.05	13 (2%) 59 49	58, 111, 180, 214	0
1	C	549/593 (92%)	-0.08	10 (1%) 68 61	58, 103, 161, 211	0
1	D	547/593 (92%)	0.20	29 (5%) 26 17	82, 138, 186, 246	0
2	E	15/17 (88%)	-0.15	0 100 100	97, 113, 175, 192	0
2	F	15/17 (88%)	-0.28	0 100 100	64, 81, 144, 148	0
2	G	13/17 (76%)	0.16	0 100 100	55, 67, 128, 148	0
2	H	13/17 (76%)	0.09	0 100 100	145, 177, 218, 254	0
All	All	2253/2440 (92%)	-0.02	59 (2%) 56 46	55, 115, 175, 254	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	119	TYR	5.5
1	D	175	ASN	5.1
1	B	1101	PHE	4.7
1	D	1040	CYS	4.5
1	C	9	LEU	4.2
1	D	1055	LEU	4.2
1	C	166	ASP	4.2
1	D	1051	VAL	4.1
1	B	1062	THR	4.0
1	D	167	GLY	3.7
1	A	289	ASP	3.6
1	D	1061	ARG	3.6
1	D	1062	THR	3.5
1	D	281	PHE	3.5
1	B	313	LEU	3.4
1	D	1039	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	29	PHE	3.4
1	D	348	ALA	3.4
1	B	2062	GLY	3.1
1	C	8	LYS	3.1
1	D	353	ALA	3.0
1	D	205	HIS	3.0
1	D	107	ALA	2.9
1	B	244	TYR	2.9
1	D	1053	GLU	2.9
1	D	9	LEU	2.9
1	D	277	LEU	2.9
1	A	162	LEU	2.9
1	D	1052	GLY	2.8
1	A	131	TRP	2.8
1	B	234	TRP	2.7
1	B	1028	GLN	2.7
1	C	312	GLU	2.6
1	A	282	LEU	2.6
1	C	145	GLY	2.5
1	D	208	ALA	2.5
1	A	307	LYS	2.5
1	D	287	LEU	2.5
1	C	10	VAL	2.4
1	B	312	GLU	2.4
1	D	355	GLY	2.4
1	A	257	SER	2.4
1	C	273	PRO	2.4
1	D	2091	TYR	2.4
1	C	136	ALA	2.4
1	D	123	LEU	2.3
1	D	1054	THR	2.3
1	A	194	LEU	2.3
1	D	2072	TRP	2.3
1	D	285	TYR	2.2
1	C	146	LYS	2.2
1	C	140	GLU	2.1
1	D	1056	TRP	2.1
1	B	2063	VAL	2.1
1	D	75	SER	2.1
1	B	314	ALA	2.0
1	D	2036	VAL	2.0
1	B	315	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	3	LYS	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)

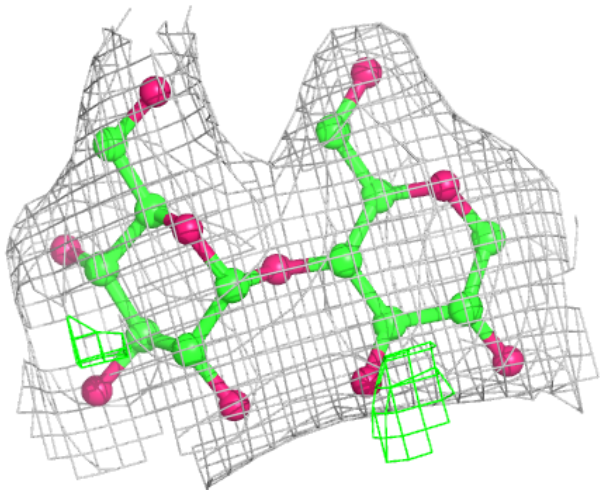
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

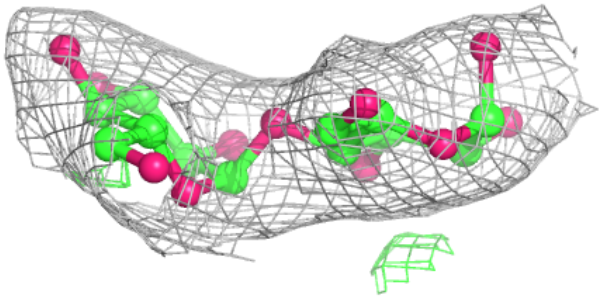
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GLC	J	1	12/12	0.97	0.20	67,79,86,92	0
3	GLC	K	1	12/12	0.97	0.22	72,78,86,89	0
3	GLC	L	1	12/12	0.97	0.19	95,102,110,113	0
3	GLC	I	2	11/12	0.98	0.18	70,73,78,81	0
3	GLC	K	2	11/12	0.98	0.23	61,65,69,70	0
3	GLC	I	1	12/12	0.98	0.18	72,76,85,86	0
3	GLC	L	2	11/12	0.98	0.14	90,93,103,105	0
3	GLC	J	2	11/12	0.99	0.17	60,63,67,73	0

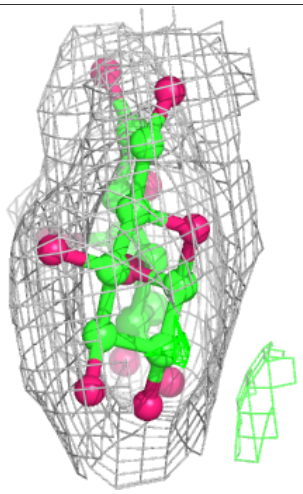
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

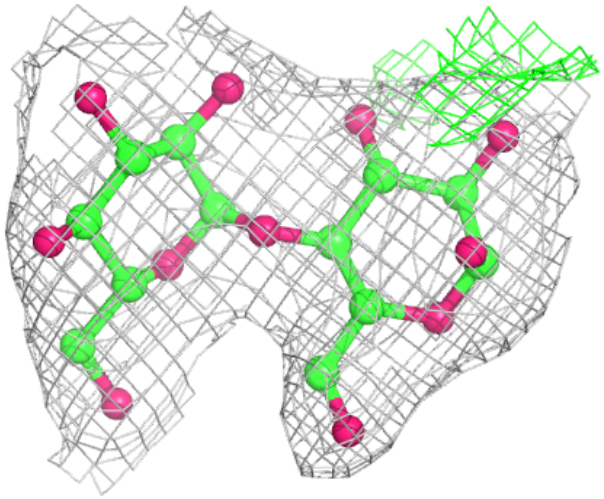


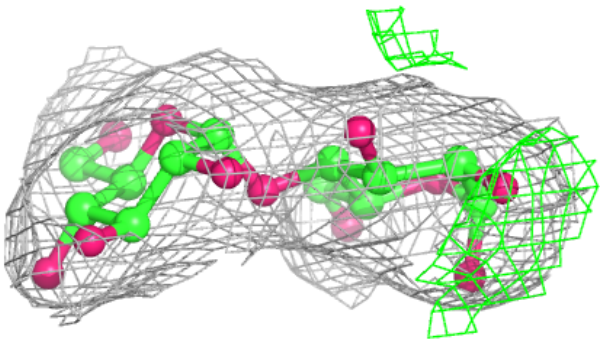


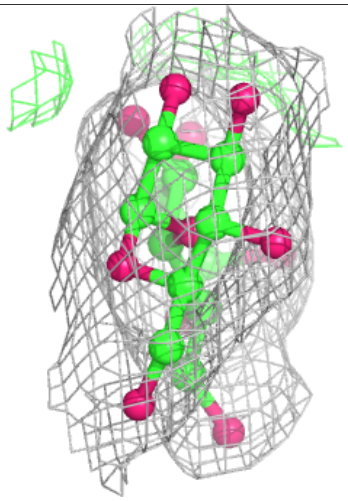


Electron density around Chain J:

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

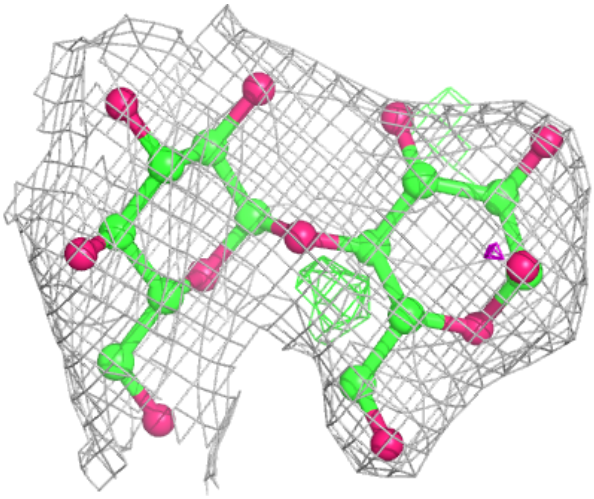


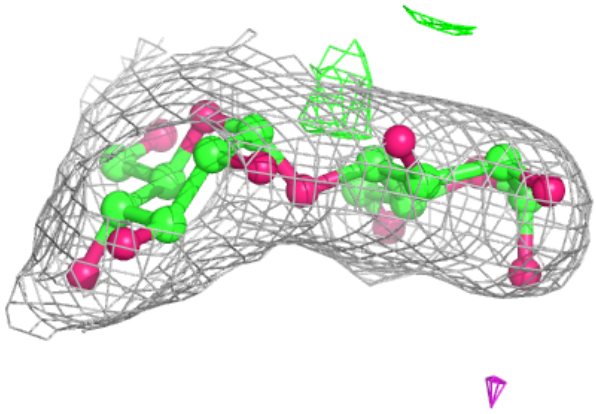


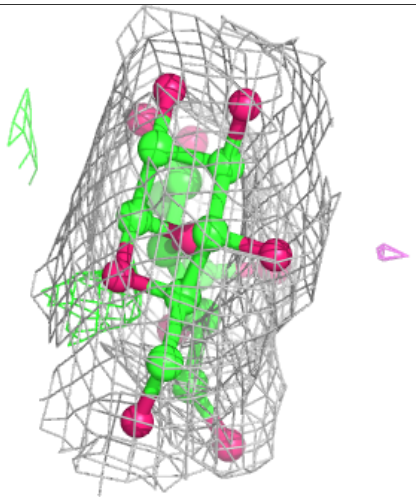


Electron density around Chain K:

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

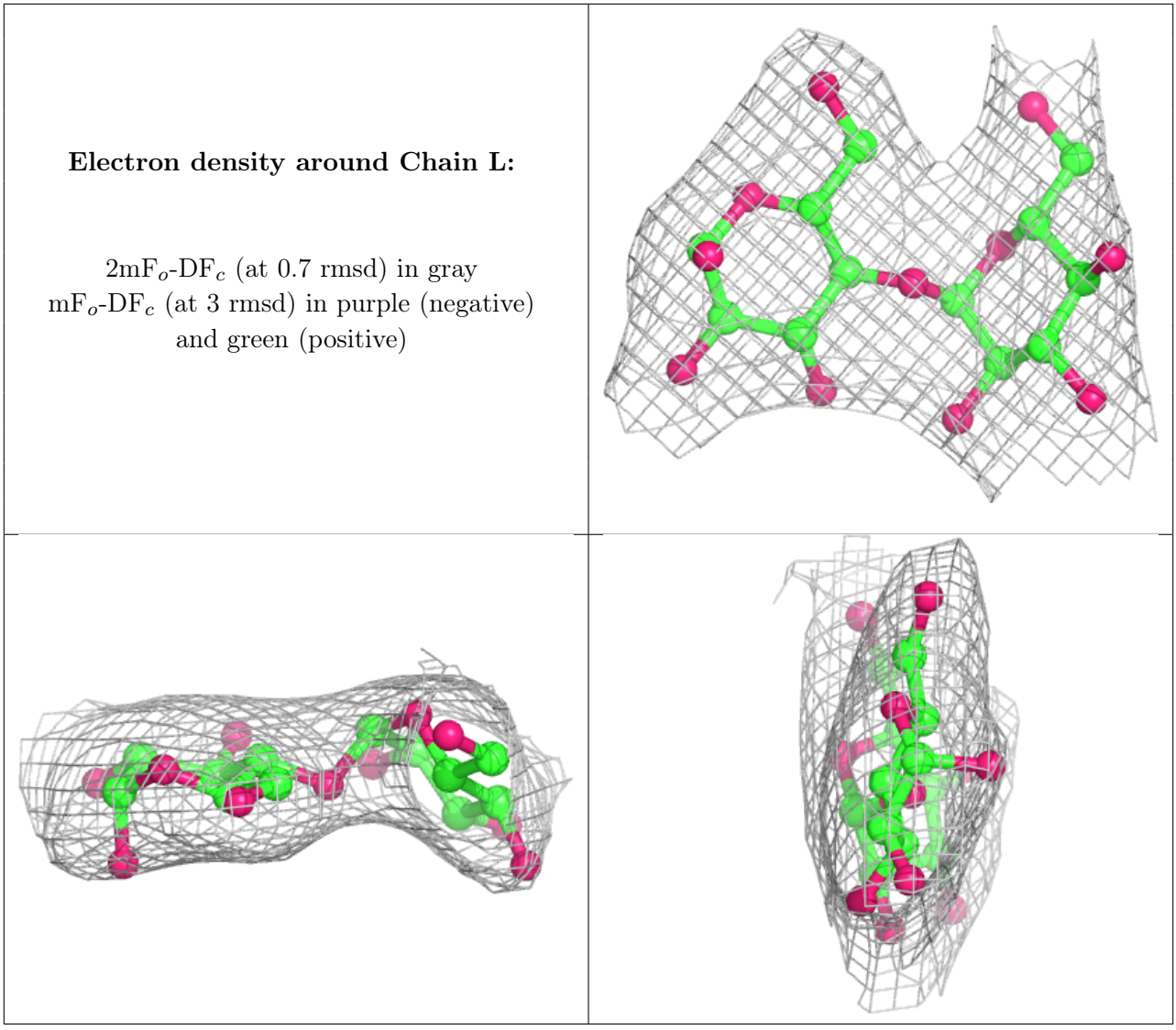






Electron density around Chain L:

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



6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.