Full wwPDB X-ray Structure Validation Report ⓘ

Sep 27, 2023 – 12:09 AM EDT

PDB ID	:	6D1U
Title	:	Crystal structure of the human CLR:RAMP1 extracellular domain heterodimer in complex with adrenomedullin 2/intermedin
Authors	:	Pioszak, A.; Roehrkasse, A.
Deposited on	:	2018-04-12
Resolution	:	2.05 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:

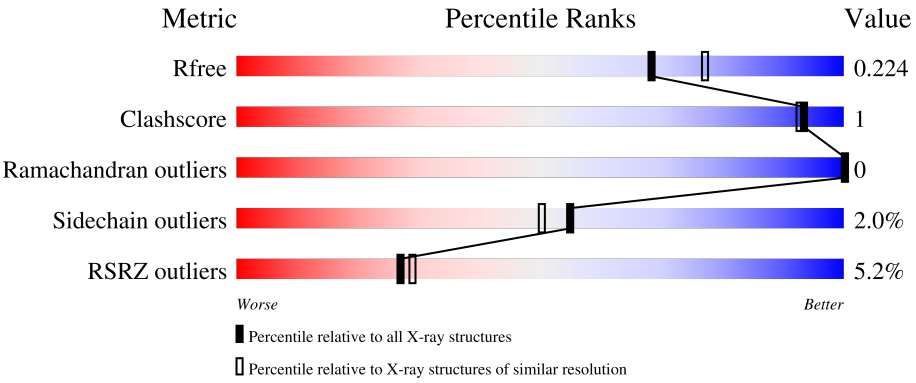
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 2.05 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	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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	89% · 7%
1	B	593	6% 89% · 7%
1	C	593	8% 90% 5% · ·
2	D	20	5% 60% 10% 30%
2	E	20	5% 85% 15%

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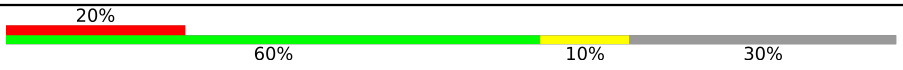
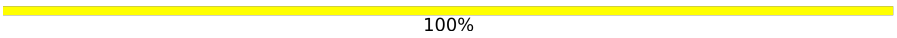
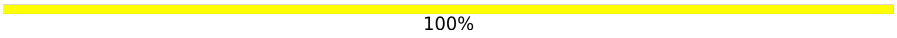
Mol	Chain	Length	Quality of chain
2	F	20	
3	G	2	
3	H	2	
3	I	2	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 14158 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	553	Total	C	N	O	S	0	3	0
			4388	2799	732	833	24			
1	B	553	Total	C	N	O	S	0	0	0
			4361	2784	725	829	23			
1	C	567	Total	C	N	O	S	0	0	0
			4494	2870	756	846	22			

There are 66 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
A	2149	HIS	-	expression tag	UNP Q16602
A	2150	HIS	-	expression tag	UNP Q16602

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Chain	Residue	Modelled	Actual	Comment	Reference
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	1023	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
C	2147	HIS	-	expression tag	UNP Q16602
C	2148	HIS	-	expression tag	UNP Q16602

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Chain	Residue	Modelled	Actual	Comment	Reference
C	2149	HIS	-	expression tag	UNP Q16602
C	2150	HIS	-	expression tag	UNP Q16602

- Molecule 2 is a protein called ADM2.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	D	14	Total C N O 96 58 16 22	0	0	1
2	E	17	Total C N O 120 71 23 26	0	0	1
2	F	14	Total C N O 96 58 16 22	0	0	1

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

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

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Na 1 1	0	0
4	C	3	Total Na 3 3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	293	Total O 293 293	0	0
5	B	104	Total O 104 104	0	0

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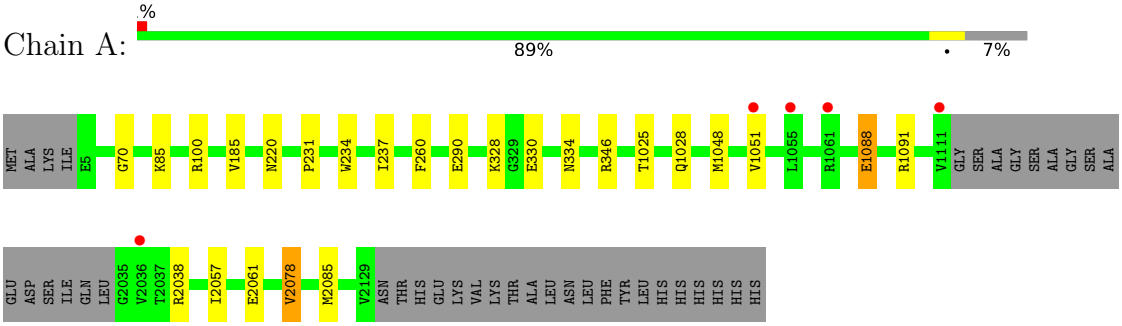
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	117	Total O 117 117	0	0
5	D	8	Total O 8 8	0	0
5	E	5	Total O 5 5	0	0
5	F	3	Total O 3 3	0	0

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.

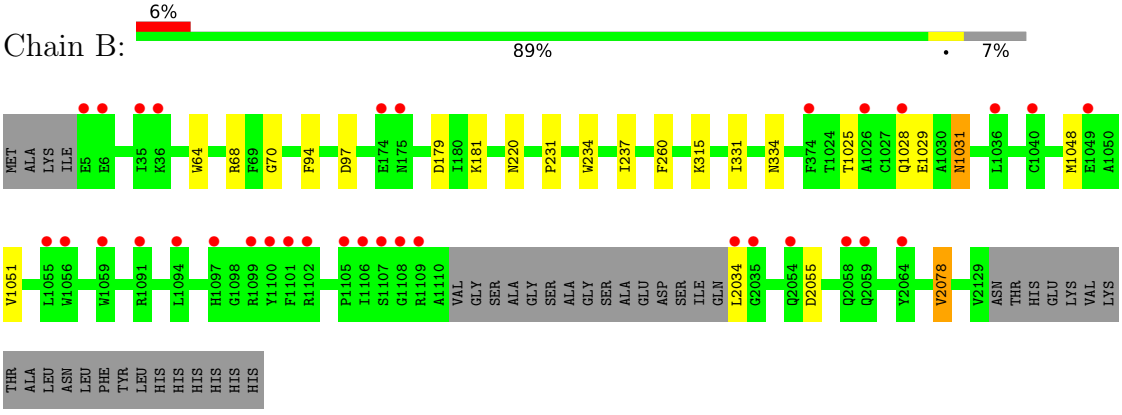
• Molecule 1: Maltose-binding periplasmic protein,Receptor activity-modifying protein 1,Calcitonin gene-related peptide type 1 receptor

Chain A:



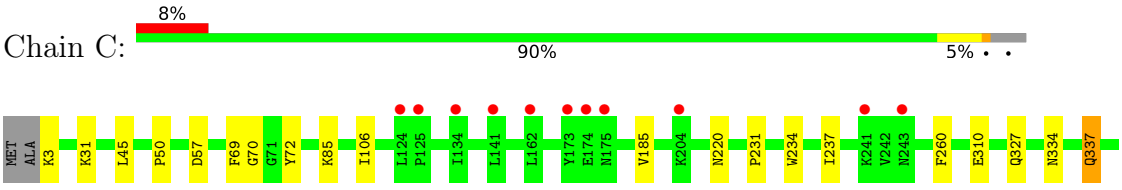
• Molecule 1: Maltose-binding periplasmic protein,Receptor activity-modifying protein 1,Calcitonin gene-related peptide type 1 receptor

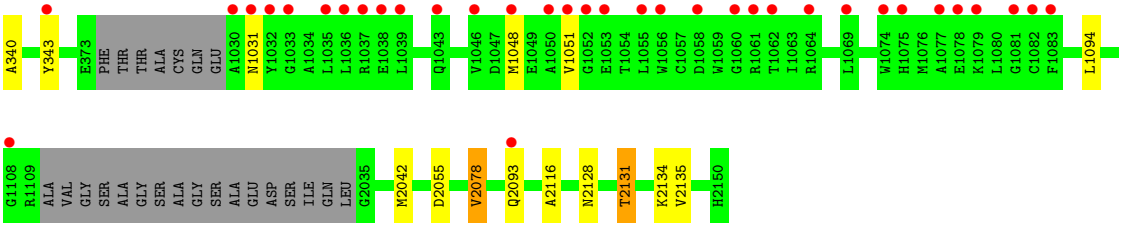
Chain B:



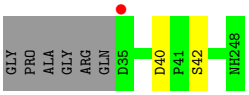
• Molecule 1: Maltose-binding periplasmic protein,Receptor activity-modifying protein 1,Calcitonin gene-related peptide type 1 receptor

Chain C:

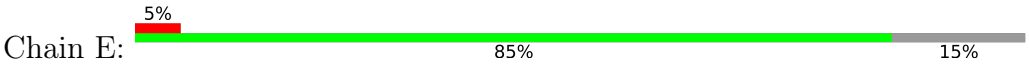


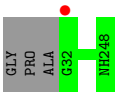


• Molecule 2: ADM2

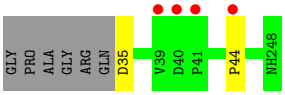


• Molecule 2: ADM2





• Molecule 2: ADM2



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

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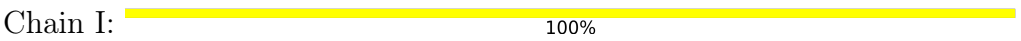

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	172.29Å 106.04Å 136.91Å 90.00° 122.53° 90.00°	Depositor
Resolution (Å)	45.64 – 2.05 45.63 – 2.04	Depositor EDS
% Data completeness (in resolution range)	98.6 (45.64-2.05) 97.7 (45.63-2.04)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.82 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.194 , 0.223 0.200 , 0.224	Depositor DCC
R_{free} test set	6618 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å^2)	46.3	Xtriage
Anisotropy	0.566	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 47.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	14158	wwPDB-VP
Average B, all atoms (Å^2)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.42% 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, NA, 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	0.70	1/4500 (0.0%)	0.77	4/6112 (0.1%)
1	B	0.62	0/4473	0.74	3/6077 (0.0%)
1	C	0.65	0/4613	0.76	2/6264 (0.0%)
2	D	0.72	0/99	0.65	0/137
2	E	0.80	0/123	0.87	0/168
2	F	0.56	0/99	0.67	0/137
All	All	0.66	1/13907 (0.0%)	0.76	9/18895 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1088	GLU	CD-OE1	-6.09	1.19	1.25

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	2078	VAL	CB-CA-C	-7.78	96.62	111.40
1	A	2078	VAL	CB-CA-C	-7.37	97.40	111.40
1	A	346	ARG	NE-CZ-NH1	6.61	123.61	120.30
1	B	2055	ASP	CB-CG-OD1	6.27	123.94	118.30
1	A	2078	VAL	CG1-CB-CG2	6.12	120.70	110.90
1	A	100	ARG	NE-CZ-NH2	-5.71	117.44	120.30
1	C	2078	VAL	CG1-CB-CG2	5.42	119.57	110.90
1	B	2078	VAL	CB-CA-C	-5.33	101.27	111.40
1	B	97	ASP	CB-CG-OD2	-5.26	113.56	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	4388	0	4222	8	0
1	B	4361	0	4197	10	0
1	C	4494	0	4320	17	0
2	D	96	0	78	1	0
2	E	120	0	102	0	0
2	F	96	0	78	3	0
3	G	23	0	21	0	0
3	H	23	0	21	0	0
3	I	23	0	21	0	0
4	A	1	0	0	0	0
4	C	3	0	0	0	0
5	A	293	0	0	2	0
5	B	104	0	0	0	1
5	C	117	0	0	0	1
5	D	8	0	0	0	0
5	E	5	0	0	0	0
5	F	3	0	0	0	0
All	All	14158	0	13060	36	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (36) 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:337:GLN:NE2	1:C:337:GLN:H	1.87	0.73
1:C:337:GLN:H	1:C:337:GLN:HE21	1.48	0.59
1:C:2093:GLN:N	2:F:35:ASP:O	2.35	0.59
1:B:1029:GLU:HB3	1:B:1031:ASN:HD22	1.68	0.58
1:A:290:GLU:HG2	5:A:2552:HOH:O	2.04	0.57
1:C:340:ALA:HB2	1:C:2116:ALA:O	2.09	0.53
1:A:1088:GLU:OE1	1:A:1091[B]:ARG:NH1	2.43	0.51
1:A:328:LYS:NZ	5:A:2306:HOH:O	2.44	0.50
1:C:70:GLY:HA3	1:C:334:ASN:O	2.12	0.49
1:B:1048:MET:HA	1:B:1051:VAL:HG12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1029:GLU:CB	1:B:1031:ASN:HD22	2.25	0.49
1:C:1048:MET:HA	1:C:1051:VAL:HG12	1.94	0.49
1:C:2128:ASN:HB3	1:C:2131:THR:HG23	1.94	0.49
1:A:1048:MET:HA	1:A:1051:VAL:HG12	1.94	0.48
1:B:70:GLY:HA3	1:B:334:ASN:O	2.12	0.48
1:B:1025:THR:O	1:B:1028:GLN:HG2	2.13	0.48
1:C:343:TYR:CZ	2:F:44:PRO:HD2	2.49	0.48
1:A:1025:THR:O	1:A:1028:GLN:HG2	2.14	0.47
1:A:70:GLY:HA3	1:A:334:ASN:O	2.14	0.47
1:C:343:TYR:CE1	2:F:44:PRO:HD3	2.51	0.46
1:C:3:LYS:N	1:C:57:ASP:OD1	2.49	0.46
1:C:220:ASN:HD21	1:C:237:ILE:HG12	1.81	0.45
1:B:179:ASP:OD1	1:B:181:LYS:HG3	2.17	0.44
1:C:2135:VAL:O	1:C:2135:VAL:HG12	2.16	0.44
1:B:231:PRO:HA	1:B:234:TRP:CE2	2.53	0.44
1:C:231:PRO:HA	1:C:234:TRP:CE2	2.53	0.44
1:A:231:PRO:HA	1:A:234:TRP:CE2	2.53	0.43
1:C:50:PRO:HG3	1:C:72:TYR:CE1	2.54	0.43
1:C:69:PHE:HB3	1:C:106:ILE:HD12	2.00	0.43
1:C:337:GLN:NE2	1:C:337:GLN:N	2.64	0.43
2:D:40:ASP:OD2	2:D:42:SER:OG	2.29	0.43
1:A:220:ASN:HD21	1:A:237:ILE:HG12	1.83	0.42
1:B:64:TRP:CD1	1:B:68:ARG:HG3	2.54	0.42
1:B:94:PHE:CE1	1:B:331:ILE:HD12	2.55	0.41
1:C:1094:LEU:HD12	1:C:1094:LEU:HA	1.87	0.40
1:B:220:ASN:HD21	1:B:237:ILE:HG12	1.86	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:2330:HOH:O	5:C:2328:HOH:O[2_556]	2.11	0.09

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	552/593 (93%)	547 (99%)	5 (1%)	0	100	100
1	B	549/593 (93%)	545 (99%)	4 (1%)	0	100	100
1	C	561/593 (95%)	555 (99%)	6 (1%)	0	100	100
2	D	12/20 (60%)	12 (100%)	0	0	100	100
2	E	15/20 (75%)	15 (100%)	0	0	100	100
2	F	12/20 (60%)	12 (100%)	0	0	100	100
All	All	1701/1839 (92%)	1686 (99%)	15 (1%)	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	455/484 (94%)	445 (98%)	10 (2%)	52	46
1	B	452/484 (93%)	447 (99%)	5 (1%)	73	73
1	C	466/484 (96%)	452 (97%)	14 (3%)	41	34
2	D	12/15 (80%)	12 (100%)	0	100	100
2	E	14/15 (93%)	14 (100%)	0	100	100
2	F	12/15 (80%)	12 (100%)	0	100	100
All	All	1411/1497 (94%)	1382 (98%)	29 (2%)	55	48

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	85	LYS
1	A	185	VAL
1	A	260	PHE
1	A	330	GLU

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Mol	Chain	Res	Type
1	A	2038	ARG
1	A	2057	ILE
1	A	2061	GLU
1	A	2078	VAL
1	A	2085[A]	MET
1	A	2085[B]	MET
1	B	260	PHE
1	B	315	LYS
1	B	1031	ASN
1	B	2034	LEU
1	B	2078	VAL
1	C	31	LYS
1	C	45	LEU
1	C	85	LYS
1	C	185	VAL
1	C	260	PHE
1	C	310	GLU
1	C	327	GLN
1	C	337	GLN
1	C	1031	ASN
1	C	2042	MET
1	C	2055	ASP
1	C	2078	VAL
1	C	2131	THR
1	C	2134	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	ASN
1	A	51	GLN
1	A	102	ASN
1	A	220	ASN
1	A	1045	GLN
1	B	51	GLN
1	B	102	ASN
1	B	220	ASN
1	B	1031	ASN
1	B	1045	GLN
1	B	2086	GLN
1	C	51	GLN
1	C	102	ASN

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Mol	Chain	Res	Type
1	C	220	ASN
1	C	327	GLN
1	C	337	GLN
1	C	1045	GLN
1	C	2045	GLN
1	C	2058	GLN
1	C	2086	GLN
2	D	45	HIS
2	E	34	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)

6 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	GLC	G	1	3	12,12,12	0.66	0	17,17,17	1.81	4 (23%)
3	GLC	G	2	3	11,11,12	0.99	0	15,15,17	1.22	2 (13%)
3	GLC	H	1	3	12,12,12	0.67	0	17,17,17	0.96	0
3	GLC	H	2	3	11,11,12	0.80	0	15,15,17	1.37	3 (20%)
3	GLC	I	1	3	12,12,12	0.67	0	17,17,17	1.56	2 (11%)
3	GLC	I	2	3	11,11,12	0.52	0	15,15,17	1.00	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	G	1	3	-	0/2/22/22	0/1/1/1
3	GLC	G	2	3	-	0/2/19/22	0/1/1/1
3	GLC	H	1	3	-	2/2/22/22	0/1/1/1
3	GLC	H	2	3	-	0/2/19/22	0/1/1/1
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

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	1	GLC	O5-C1-C2	4.60	118.49	110.28
3	I	1	GLC	O5-C1-C2	4.08	117.56	110.28
3	G	1	GLC	C1-O5-C5	3.13	119.57	113.66
3	H	2	GLC	C1-O5-C5	3.11	116.41	112.19
3	G	1	GLC	O3-C3-C2	-2.73	104.04	110.35
3	G	2	GLC	O2-C2-C3	2.70	115.55	110.14
3	G	2	GLC	C1-C2-C3	2.61	112.88	109.67
3	G	1	GLC	O1-C1-O5	-2.52	102.83	110.38
3	H	2	GLC	C2-C3-C4	-2.49	106.58	110.89
3	I	2	GLC	C1-O5-C5	2.38	115.42	112.19
3	I	1	GLC	O2-C2-C3	-2.08	105.53	110.35
3	H	2	GLC	O2-C2-C1	-2.08	104.91	109.15

There are no chirality outliers.

All (2) torsion outliers are listed below:

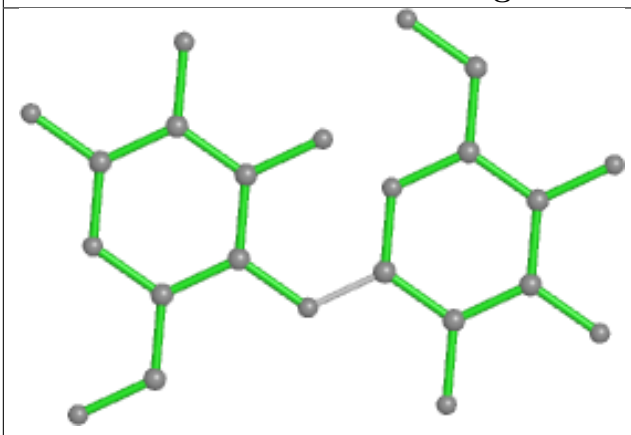
Mol	Chain	Res	Type	Atoms
3	H	1	GLC	C4-C5-C6-O6
3	H	1	GLC	O5-C5-C6-O6

There are no ring outliers.

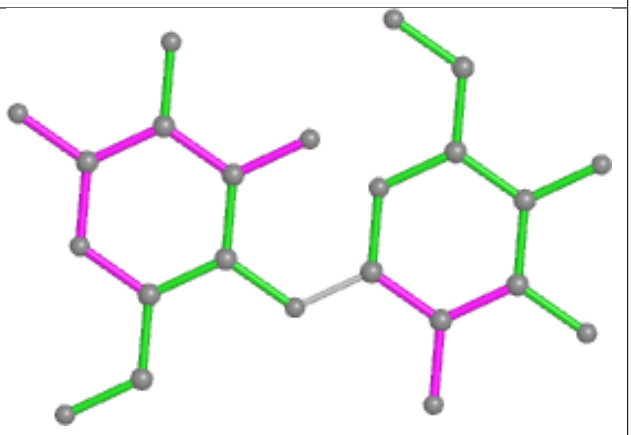
No monomer is involved in short contacts.

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

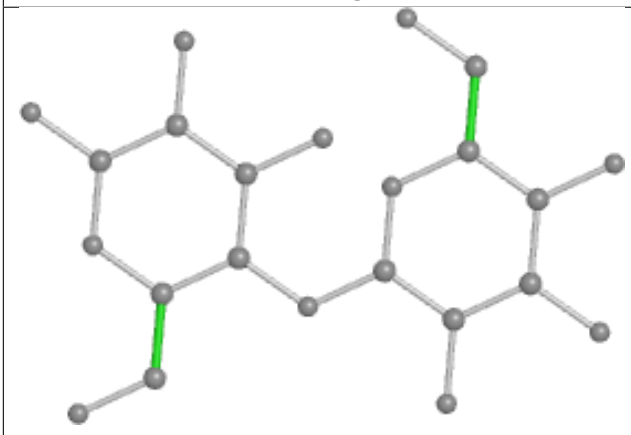
Oligosaccharide Chain G



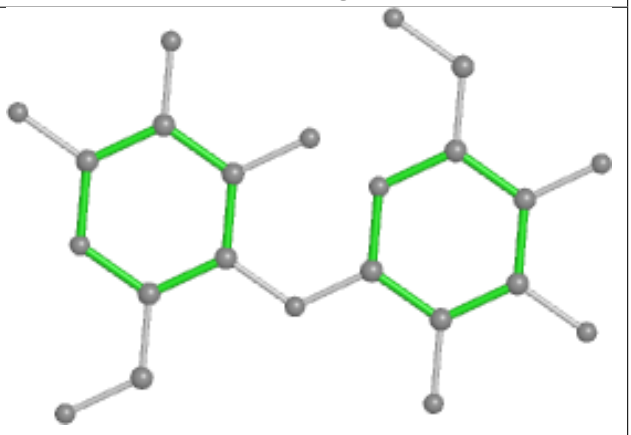
Bond lengths



Bond angles

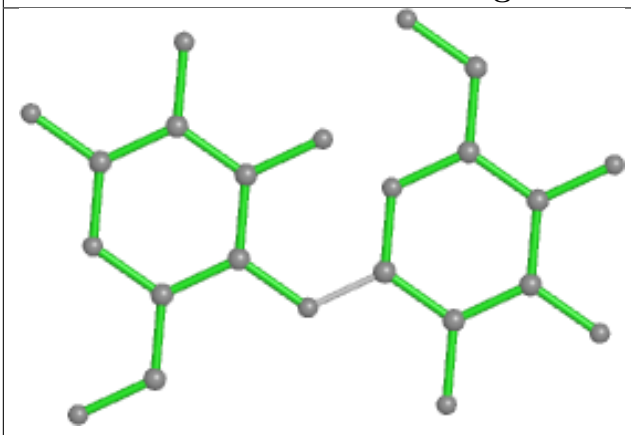


Torsions

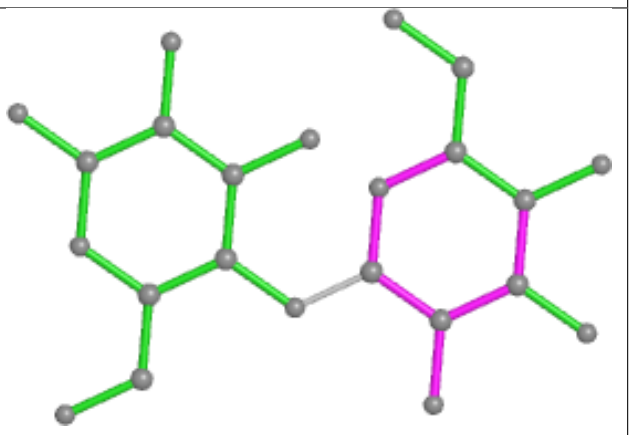


Rings

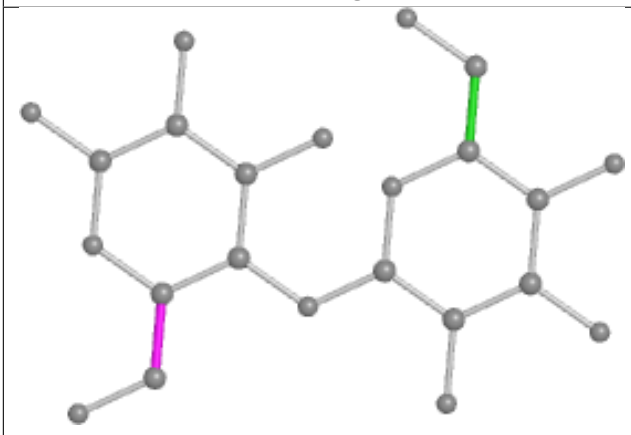
Oligosaccharide Chain H



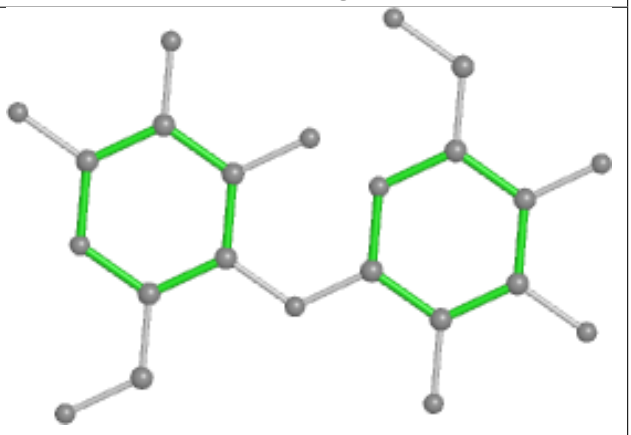
Bond lengths



Bond angles

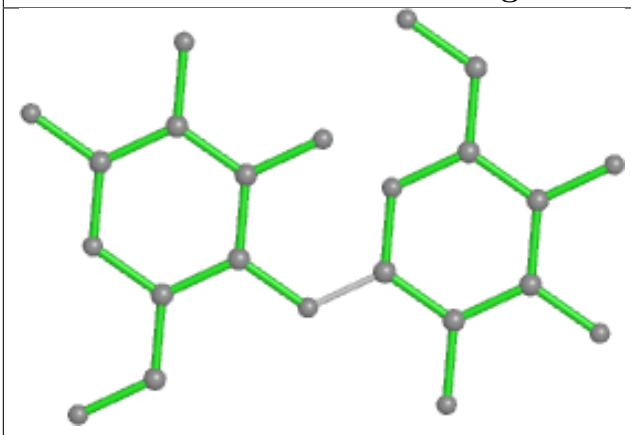


Torsions

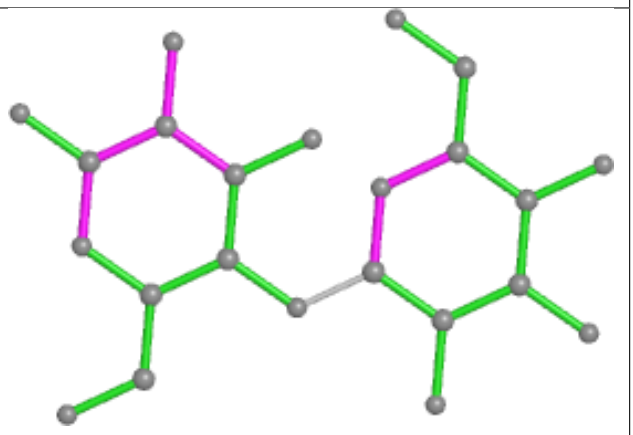


Rings

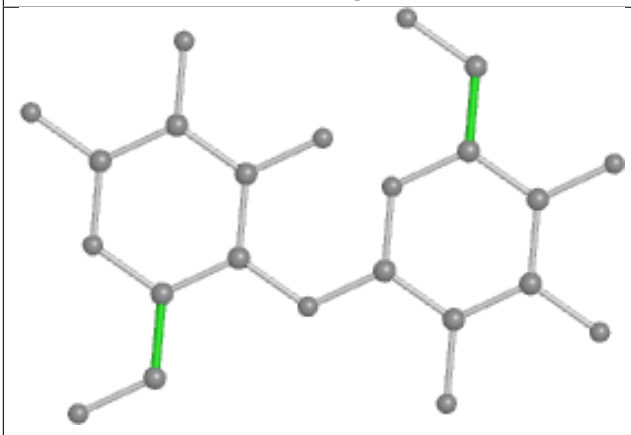
Oligosaccharide Chain I



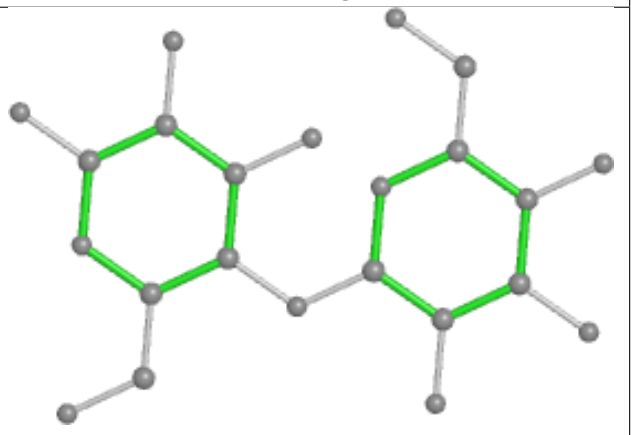
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 4 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 (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	553/593 (93%)	-0.10	5 (0%) 84 86	34, 53, 84, 104	0
1	B	553/593 (93%)	0.14	33 (5%) 21 23	45, 70, 107, 138	0
1	C	567/593 (95%)	0.45	46 (8%) 12 12	37, 71, 114, 149	0
2	D	13/20 (65%)	0.53	1 (7%) 13 14	51, 68, 103, 119	0
2	E	16/20 (80%)	-0.17	1 (6%) 20 21	54, 61, 78, 78	0
2	F	13/20 (65%)	1.57	4 (30%) 0 0	73, 99, 108, 108	0
All	All	1715/1839 (93%)	0.17	90 (5%) 27 29	34, 65, 106, 149	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1082	CYS	8.1
1	C	1083	PHE	6.6
1	C	1039	LEU	6.6
1	C	1051	VAL	6.5
1	C	1038	GLU	5.7
1	C	1030	ALA	5.6
1	C	1033	GLY	5.4
1	C	1075	HIS	5.3
1	C	1074	TRP	5.3
1	C	1052	GLY	4.9
1	C	1055	LEU	4.8
1	C	1108	GLY	4.8
1	C	1081	GLY	4.8
1	B	1108	GLY	4.6
1	B	1100	TYR	4.4
1	C	1078	GLU	4.3
1	C	125	PRO	4.3
1	A	2036	VAL	4.1
1	C	174	GLU	4.0

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Mol	Chain	Res	Type	RSRZ
1	C	343	TYR	4.0
1	C	1046	VAL	3.9
2	F	39	VAL	3.9
1	B	1055	LEU	3.8
1	B	1028	GLN	3.8
1	B	5	GLU	3.7
2	D	35	ASP	3.7
1	C	1050	ALA	3.6
1	B	1106	ILE	3.6
1	C	134	ILE	3.5
1	B	1107	SER	3.5
1	C	1064	ARG	3.4
1	B	1036	LEU	3.4
1	C	1079	LYS	3.4
1	C	1032	TYR	3.4
1	B	6	GLU	3.3
1	B	1094	LEU	3.2
1	B	1101	PHE	3.1
1	C	1035	LEU	3.1
1	B	2035	GLY	3.1
1	B	2054	GLN	3.1
2	E	32	GLY	3.0
1	B	2058	GLN	3.0
1	B	1102	ARG	3.0
1	B	174	GLU	3.0
1	C	124	LEU	3.0
1	B	1026	ALA	2.9
1	C	1036	LEU	2.9
1	B	1056	TRP	2.9
1	C	1053	GLU	2.9
1	C	1056	TRP	2.9
1	B	175	ASN	2.9
1	C	1061	ARG	2.8
1	B	1105	PRO	2.7
1	B	1099	ARG	2.7
2	F	41	PRO	2.6
1	C	1062	THR	2.6
2	F	40	ASP	2.6
1	C	1048	MET	2.6
1	B	1059	TRP	2.6
1	C	1060	GLY	2.6
1	B	1109	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	35	ILE	2.5
1	C	141	LEU	2.5
1	C	2093	GLN	2.5
1	B	2034	LEU	2.4
1	C	173	TYR	2.4
1	B	374	PHE	2.4
1	C	1077	ALA	2.4
1	B	2059	GLN	2.3
1	C	1031	ASN	2.3
1	B	1049	GLU	2.3
1	C	175	ASN	2.3
1	A	1111	VAL	2.3
1	C	1037	ARG	2.2
1	C	162	LEU	2.2
1	C	243	ASN	2.2
1	B	36	LYS	2.1
1	C	241	LYS	2.1
1	B	1040	CYS	2.1
1	A	1055	LEU	2.1
1	B	2064	TYR	2.1
1	C	1043	GLN	2.1
1	A	1051	VAL	2.1
1	B	1091	ARG	2.1
1	C	1058	ASP	2.0
1	C	1069	LEU	2.0
1	B	1097	HIS	2.0
1	A	1061	ARG	2.0
1	C	204	LYS	2.0
2	F	44	PRO	2.0

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

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

6.3 Carbohydrates (i)

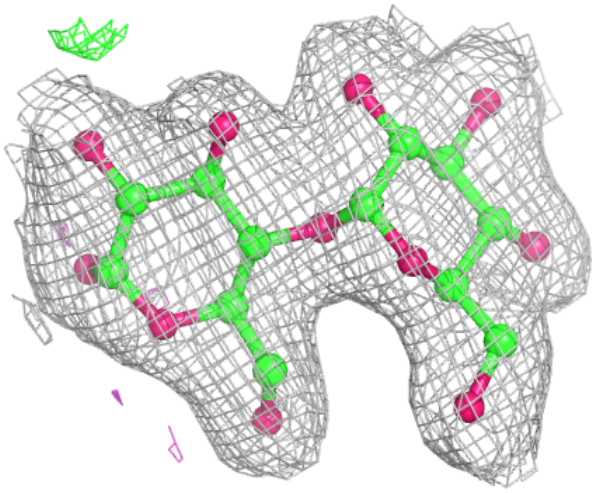
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

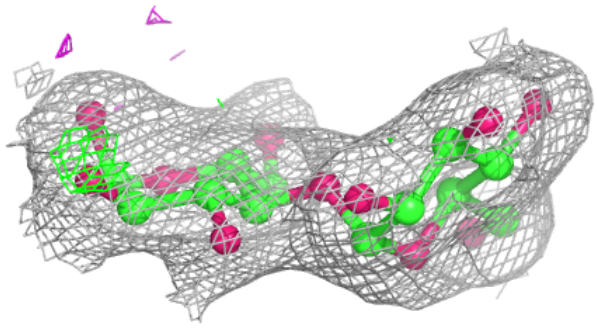
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GLC	H	1	12/12	0.97	0.10	49,53,55,55	0
3	GLC	I	2	11/12	0.97	0.13	50,53,54,55	0
3	GLC	H	2	11/12	0.98	0.11	44,47,49,49	0
3	GLC	I	1	12/12	0.98	0.13	52,54,57,59	0
3	GLC	G	1	12/12	0.98	0.11	40,45,51,52	0
3	GLC	G	2	11/12	0.99	0.14	36,38,40,41	0

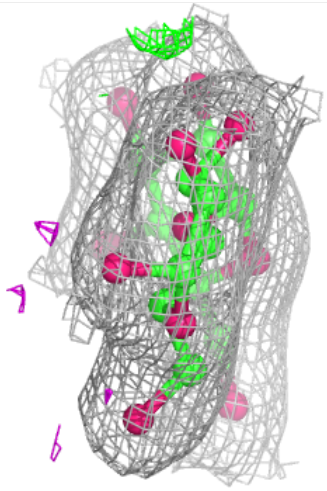
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain G:

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

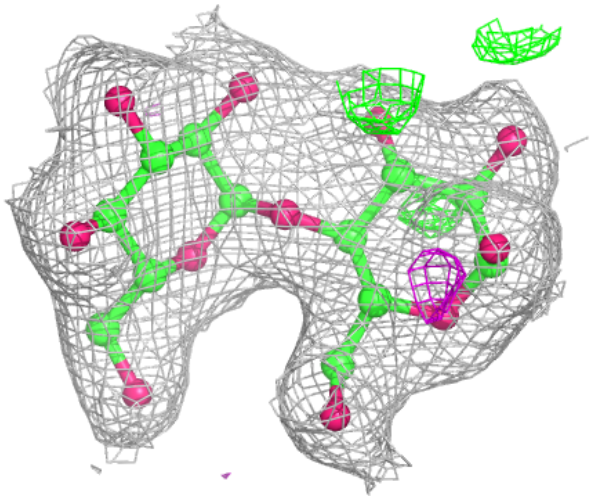


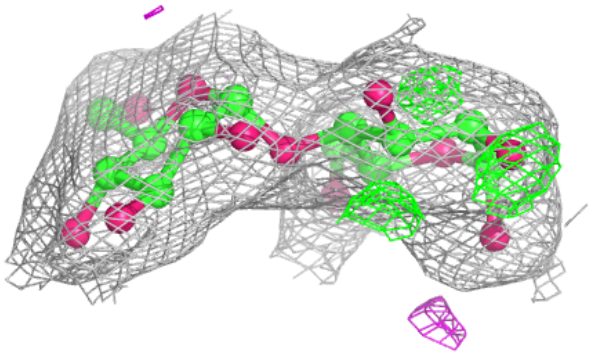


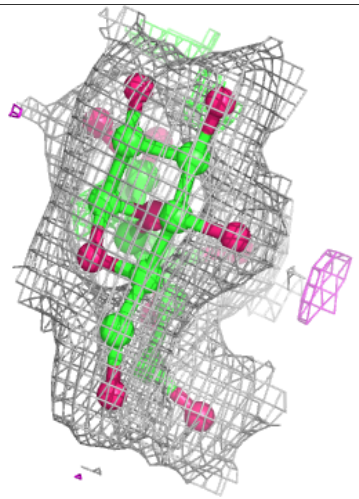


Electron density around Chain H:

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

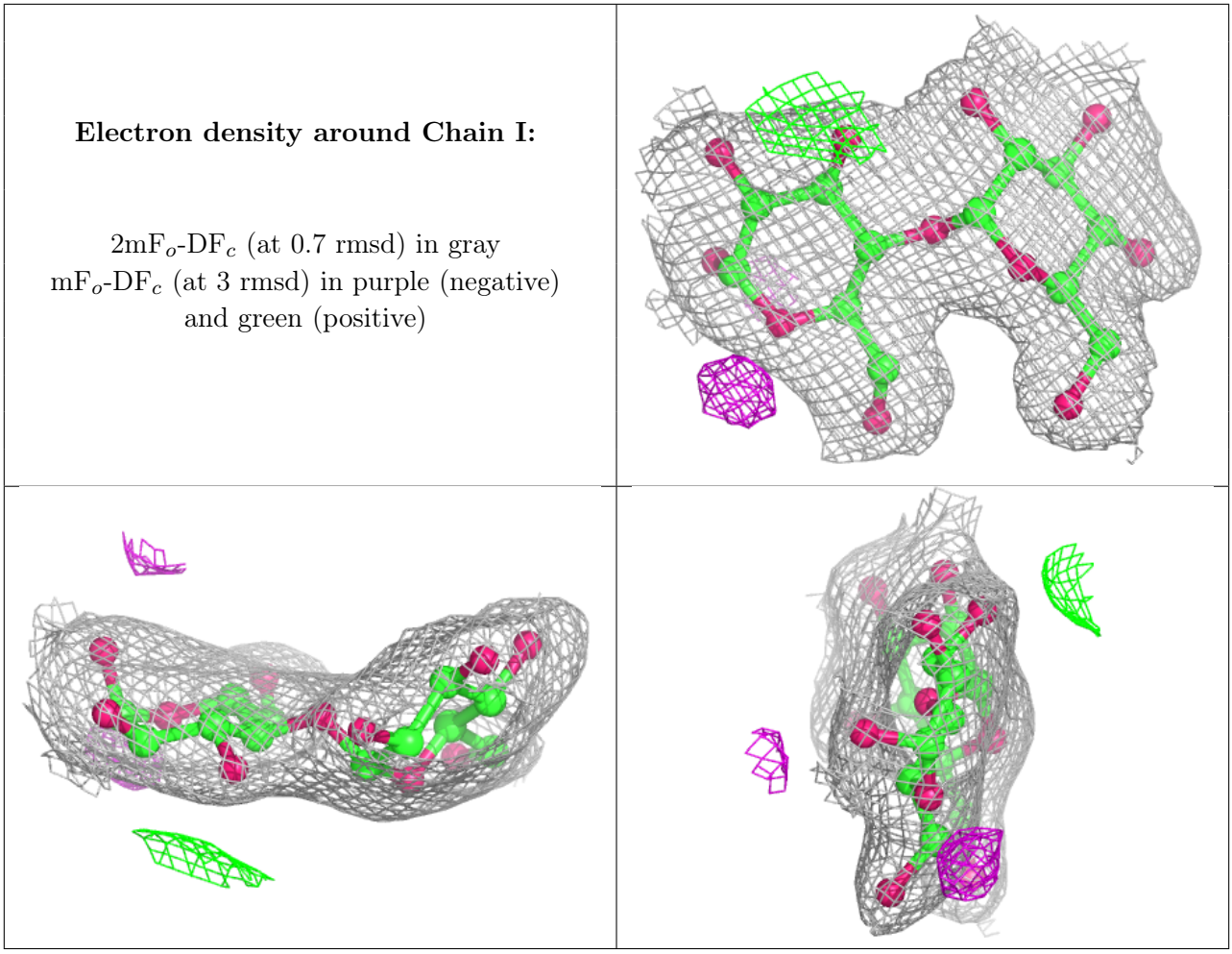






Electron density around Chain I:

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



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
4	NA	A	2202	1/1	0.88	0.19	61,61,61,61	0
4	NA	C	2203	1/1	0.91	0.07	52,52,52,52	0
4	NA	C	2204	1/1	0.92	0.08	60,60,60,60	0
4	NA	C	2202	1/1	0.99	0.10	42,42,42,42	0

6.5 Other polymers

There are no such residues in this entry.