



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:39 AM UTC

PDB ID : 6D1U / pdb_00006d1u
Title : Crystal structure of the human CLR:RAMP1 extracellular domain heterodimer in complex with adrenomedullin 2/intermedin
Authors : Pioszak, A.; Roehrkaske, 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

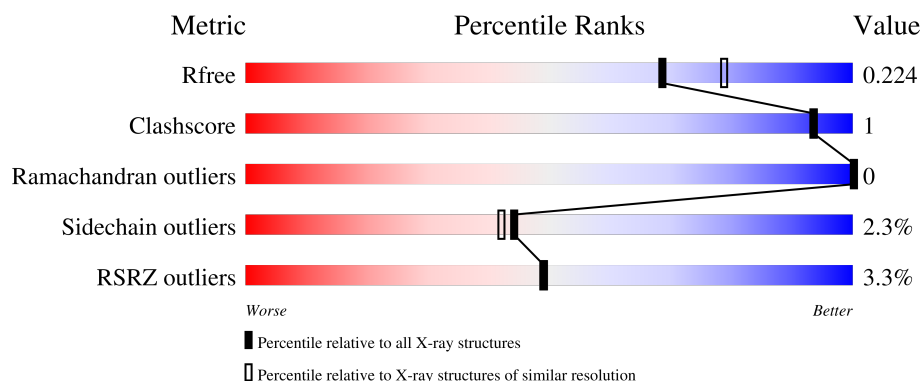
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

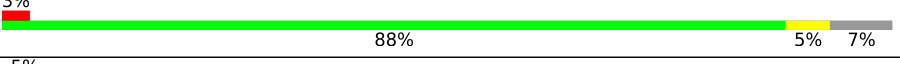
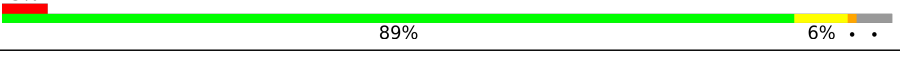
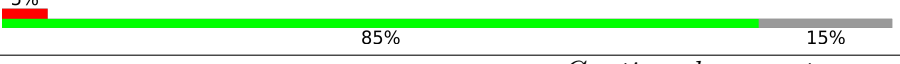
The reported resolution of this entry is 2.05 Å.

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.



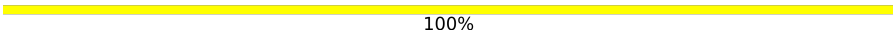
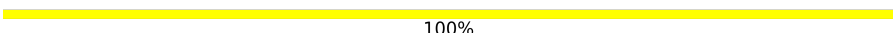
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	593	
1	B	593	
1	C	593	
2	D	20	
2	E	20	

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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

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	0	0	1
			96	58	16	22			
2	E	17	Total	C	N	O	0	0	1
			120	71	23	26			
2	F	14	Total	C	N	O	0	0	1
			96	58	16	22			

- 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	0	0	0
			23	12	11			
3	H	2	Total	C	O	0	0	0
			23	12	11			
3	I	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 5 is water.

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

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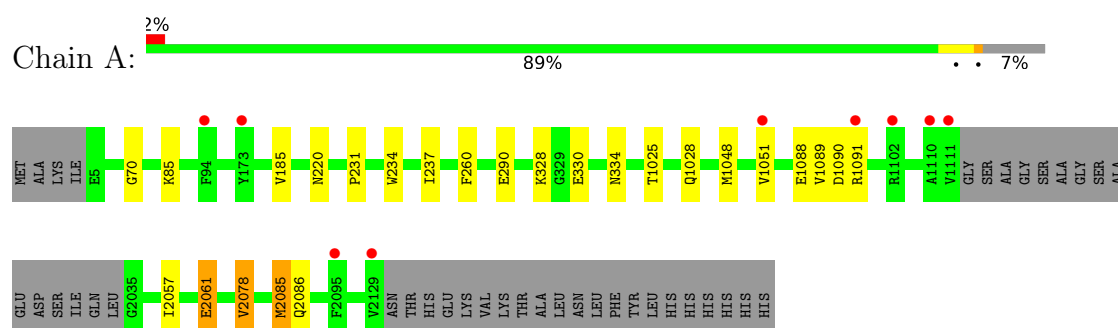
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	117	Total 117	O 117	0	0
5	D	8	Total 8	O 8	0	0
5	E	5	Total 5	O 5	0	0
5	F	3	Total 3	O 3	0	0

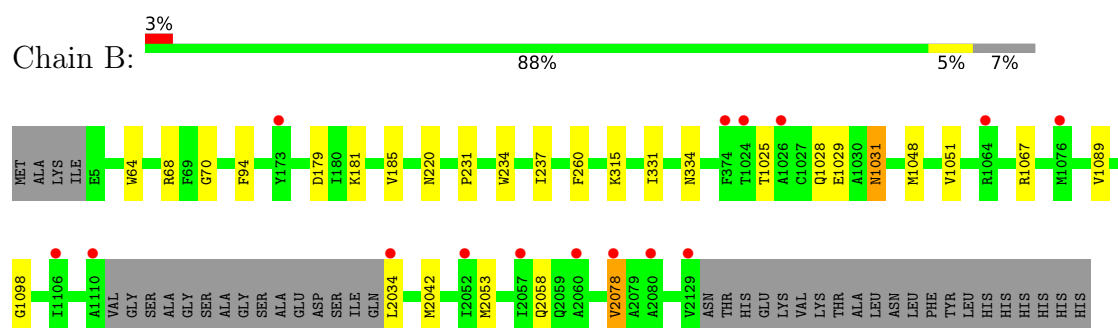
3 Residue-property plots [i](#)

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.

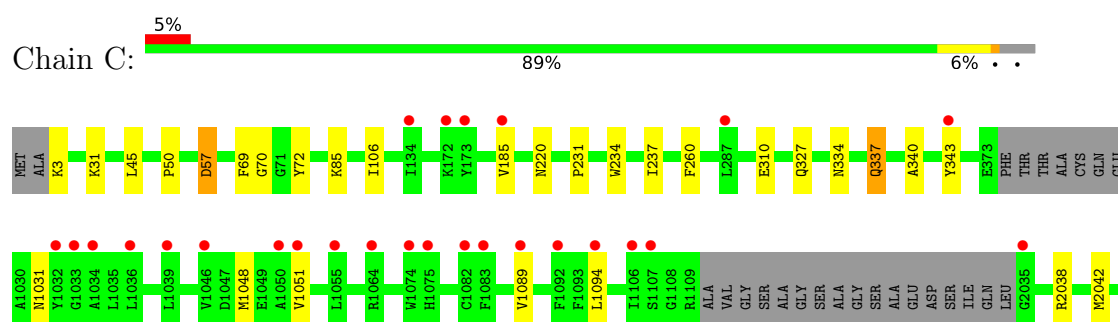
- Molecule 1: Maltose-binding periplasmic protein, Receptor activity-modifying protein 1, Calcinon gene-related peptide type 1 receptor

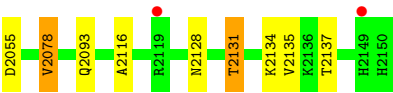


- Molecule 1: Maltose-binding periplasmic protein, Receptor activity-modifying protein 1, Calcinon gene-related peptide type 1 receptor

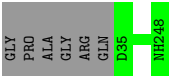


- Molecule 1: Maltose-binding periplasmic protein, Receptor activity-modifying protein 1, Calcinon gene-related peptide type 1 receptor

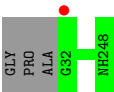
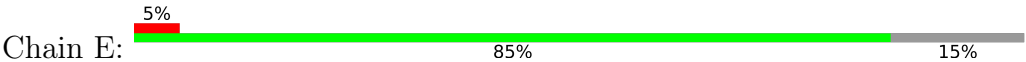




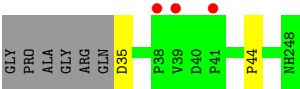
● Molecule 2: ADM2



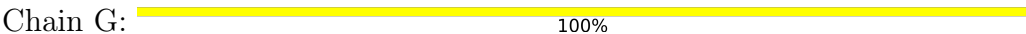
● Molecule 2: ADM2



● Molecule 2: ADM2



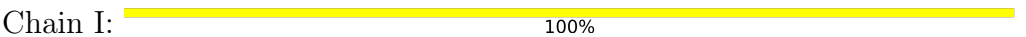
● Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose



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



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



4 Data and refinement statistics

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 45.64 – 2.05	Depositor EDS
% Data completeness (in resolution range)	98.6 (45.64-2.05) 98.6 (45.64-2.05)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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 (5.02%)	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)	0.31 , 39.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, GLC, NH2

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	0.88	1/4500 (0.0%)	0.91	2/6112 (0.0%)
1	B	0.81	0/4473	0.89	2/6077 (0.0%)
1	C	0.85	0/4613	0.92	3/6264 (0.0%)
2	D	0.87	0/99	0.76	0/137
2	E	1.04	0/123	0.99	0/168
2	F	0.79	0/99	0.79	0/137
All	All	0.85	1/13907 (0.0%)	0.91	7/18895 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1090	ASP	CA-C	5.04	1.59	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	2078	VAL	CB-CA-C	-8.09	96.62	111.18
1	A	2078	VAL	CB-CA-C	-7.65	97.40	111.18
1	A	2061	GLU	N-CA-C	6.15	120.62	113.18
1	C	57	ASP	CA-C-N	-6.00	112.45	121.87
1	C	57	ASP	C-N-CA	-6.00	112.45	121.87
1	B	2058	GLN	N-CA-C	5.34	118.22	110.42
1	B	2078	VAL	CB-CA-C	-5.27	101.27	110.71

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	4388	0	4222	9	0
1	B	4361	0	4197	12	0
1	C	4494	0	4320	17	0
2	D	96	0	78	0	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	38	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 (38) 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:A:2085[B]:MET:HE3	1:A:2086:GLN:HA	1.84	0.58
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1048:MET:HA	1:B:1051:VAL:HG12	1.94	0.49
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:B:1098:GLY:CA	1:B:2053:MET:HE1	2.47	0.45
1:B:1067:ARG:HG3	1:B:2042:MET:HE3	1.98	0.45
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
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

5.3.1 Protein backbone

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

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%)	45	44
1	B	452/484 (93%)	445 (98%)	7 (2%)	57	58
1	C	466/484 (96%)	449 (96%)	17 (4%)	31	26
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%)	1377 (98%)	34 (2%)	44	40

All (34) 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
1	A	1089	VAL
1	A	2057	ILE
1	A	2061	GLU
1	A	2078	VAL
1	A	2085[A]	MET
1	A	2085[B]	MET
1	B	185	VAL
1	B	260	PHE
1	B	315	LYS
1	B	1031	ASN
1	B	1089	VAL
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	1089	VAL
1	C	2038	ARG
1	C	2042	MET
1	C	2055	ASP
1	C	2078	VAL
1	C	2131	THR
1	C	2134	LYS
1	C	2137	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	ASN
1	A	51	GLN
1	A	102	ASN

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Mol	Chain	Res	Type
1	A	203	ASN
1	A	220	ASN
1	A	2045	GLN
1	B	20	ASN
1	B	51	GLN
1	B	102	ASN
1	B	203	ASN
1	B	220	ASN
1	B	1031	ASN
1	B	2045	GLN
1	B	2086	GLN
1	C	20	ASN
1	C	51	GLN
1	C	102	ASN
1	C	203	ASN
1	C	220	ASN
1	C	327	GLN
1	C	337	GLN
1	C	2039	ASN
1	C	2045	GLN
1	C	2058	GLN
1	C	2086	GLN
1	C	2148	HIS
1	C	2150	HIS
2	D	45	HIS

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	1.15	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	0.79	0	15,15,17	1.33	2 (13%)
3	GLC	I	1	3	12,12,12	0.67	0	17,17,17	1.55	2 (11%)
3	GLC	I	2	3	11,11,12	0.51	0	15,15,17	0.97	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 (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	1	GLC	O5-C1-C2	4.66	118.49	110.30
3	I	1	GLC	O5-C1-C2	4.13	117.56	110.30
3	H	2	GLC	C1-O5-C5	3.15	116.41	112.19
3	G	1	GLC	C1-O5-C5	3.06	119.57	113.65
3	G	1	GLC	O3-C3-C2	-2.69	104.04	110.38
3	G	2	GLC	O2-C2-C3	2.61	115.55	110.15
3	G	1	GLC	O1-C1-O5	-2.55	102.83	110.41
3	H	2	GLC	C2-C3-C4	-2.43	106.58	110.86
3	I	2	GLC	C1-O5-C5	2.41	115.42	112.19
3	G	2	GLC	C1-C2-C3	2.22	112.88	109.64
3	I	1	GLC	O2-C2-C3	-2.06	105.53	110.38

There are no chirality outliers.

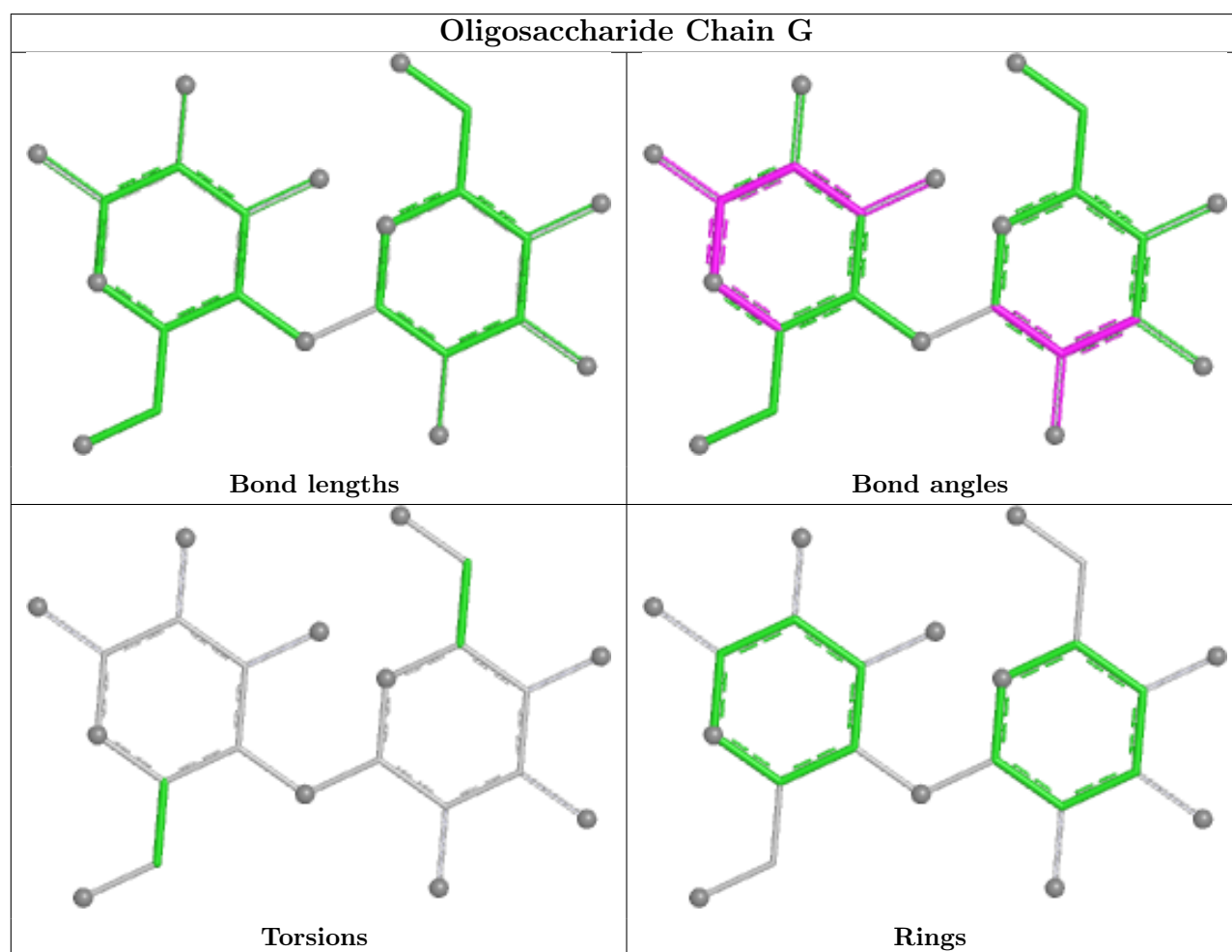
All (2) torsion outliers are listed below:

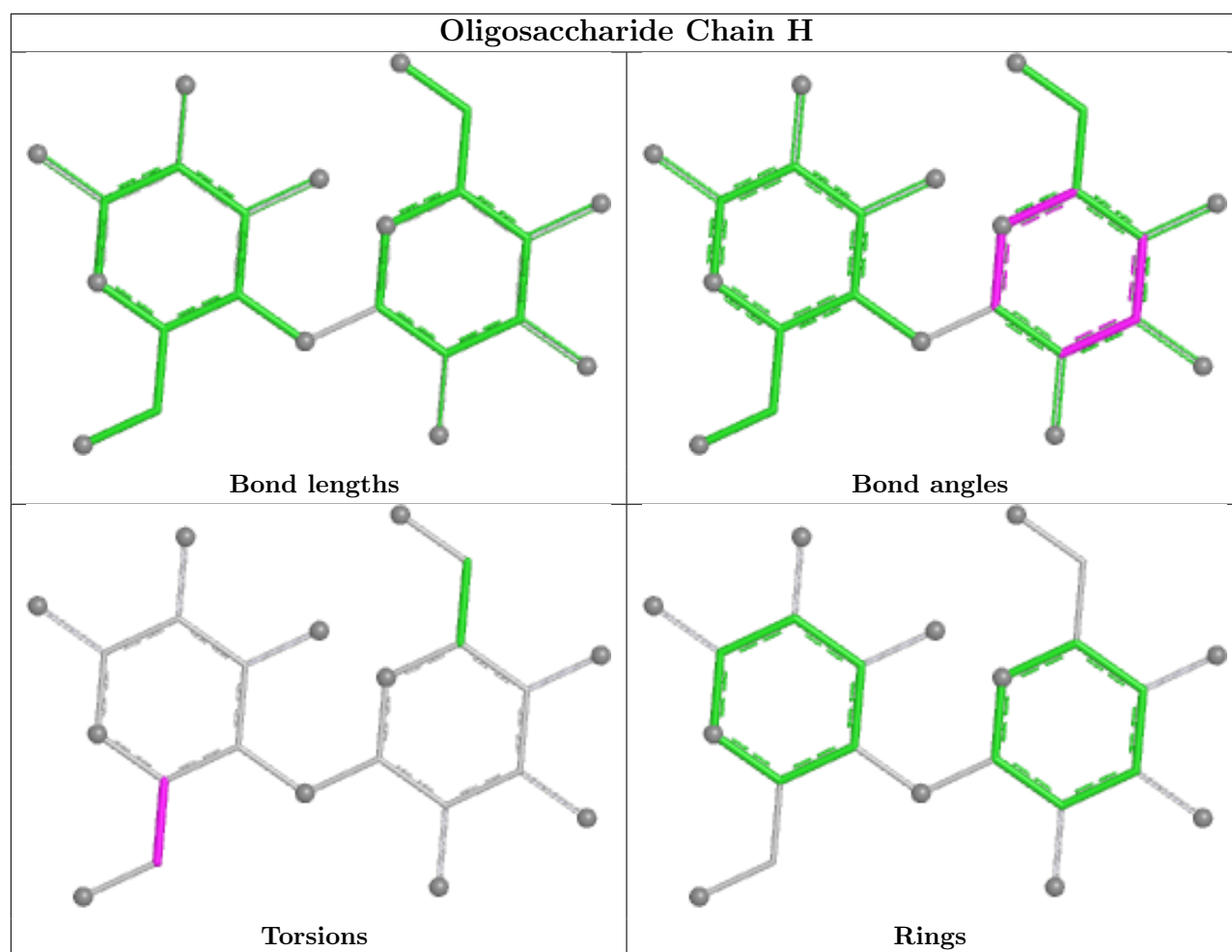
Mol	Chain	Res	Type	Atoms
3	H	1	GLC	C4-C5-C6-O6
3	H	1	GLC	O5-C5-C6-O6

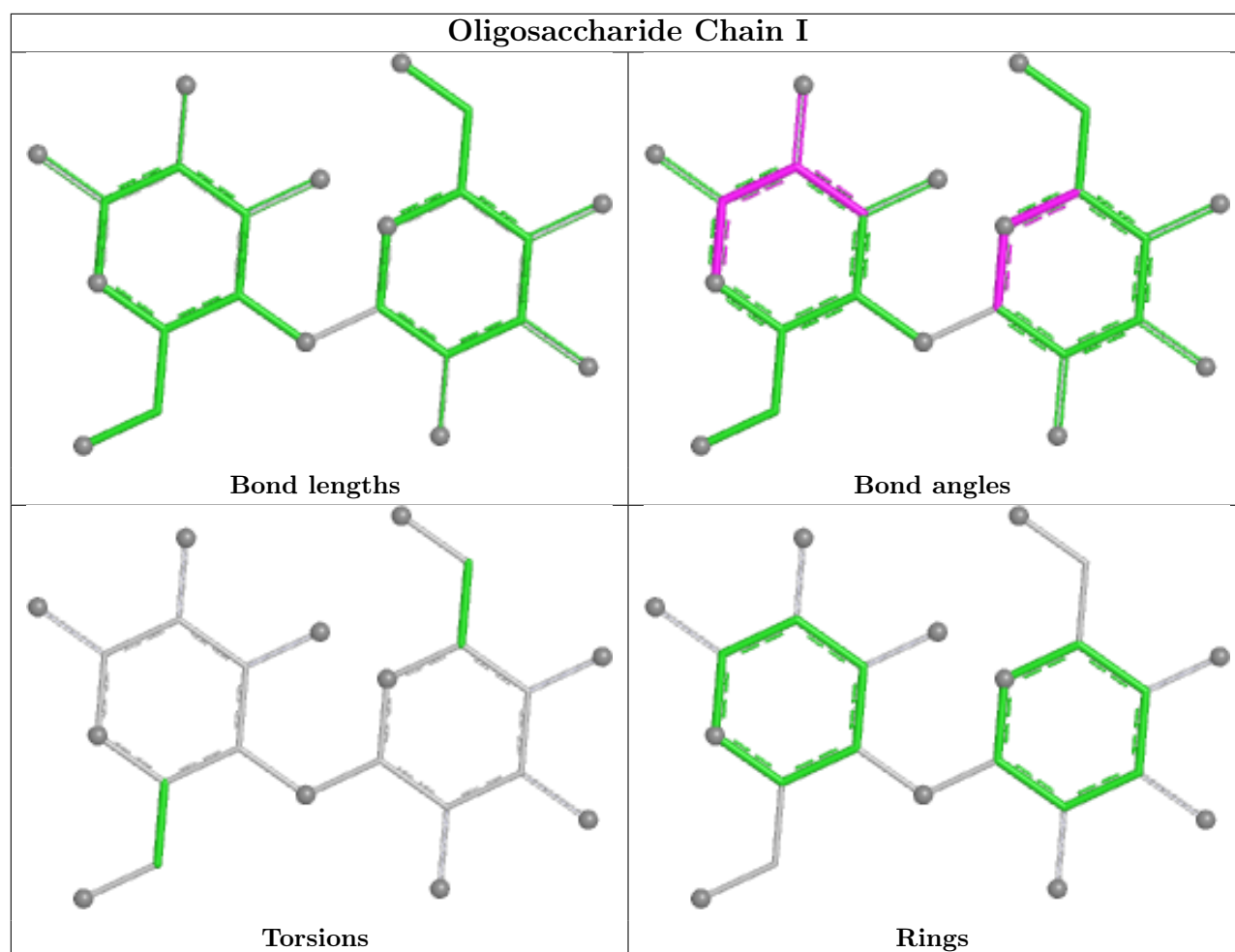
There are no ring outliers.

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.







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 ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	553/593 (93%)	-0.02	9 (1%) 70 72	22, 53, 84, 104	3 (0%)
1	B	553/593 (93%)	0.37	15 (2%) 56 58	45, 70, 107, 138	0
1	C	567/593 (95%)	0.47	28 (4%) 35 35	37, 71, 114, 149	0
2	D	13/20 (65%)	0.66	0 100 100	51, 68, 103, 119	0
2	E	16/20 (80%)	0.14	1 (6%) 26 26	54, 61, 78, 78	0
2	F	13/20 (65%)	1.66	3 (23%) 2 1	73, 99, 108, 108	0
All	All	1715/1839 (93%)	0.29	56 (3%) 49 49	22, 65, 106, 149	3 (0%)

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	32	GLY	4.3
1	C	1083	PHE	4.3
2	F	39	VAL	4.2
1	B	2057	ILE	4.0
1	C	1046	VAL	3.9
1	A	2129	VAL	3.7
1	B	1110	ALA	3.5
1	C	343	TYR	3.4
1	C	1033	GLY	3.3
1	B	2060	ALA	3.3
2	F	41	PRO	3.2
1	B	1106	ILE	3.1
1	C	1106	ILE	3.0
1	C	1032	TYR	2.9
1	C	1107	SER	2.9
1	C	1082	CYS	2.9
1	C	172	LYS	2.9
1	C	1039	LEU	2.8
1	B	2052	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	374	PHE	2.7
1	B	2034	LEU	2.7
1	A	1091[A]	ARG	2.7
1	C	1075	HIS	2.6
1	C	1055	LEU	2.6
1	A	1111	VAL	2.6
1	C	1051	VAL	2.6
1	A	1051	VAL	2.5
1	C	185	VAL	2.4
1	A	1110	ALA	2.4
1	C	1034	ALA	2.4
1	B	1076	MET	2.4
1	C	1092	PHE	2.4
1	B	2129	VAL	2.4
1	B	1024	THR	2.3
1	C	2119	ARG	2.2
1	B	2080	ALA	2.2
1	A	94	PHE	2.2
1	C	2035	GLY	2.2
1	C	1050	ALA	2.2
1	C	1036	LEU	2.2
1	C	287	LEU	2.1
1	B	173	TYR	2.1
1	C	173	TYR	2.1
2	F	38	PRO	2.1
1	C	2149	HIS	2.1
1	A	1102	ARG	2.1
1	C	1064	ARG	2.1
1	B	2078	VAL	2.1
1	C	1089	VAL	2.1
1	A	173	TYR	2.1
1	A	2095	PHE	2.1
1	C	1074	TRP	2.1
1	B	1026	ALA	2.1
1	C	1094	LEU	2.0
1	C	134	ILE	2.0
1	B	1064	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

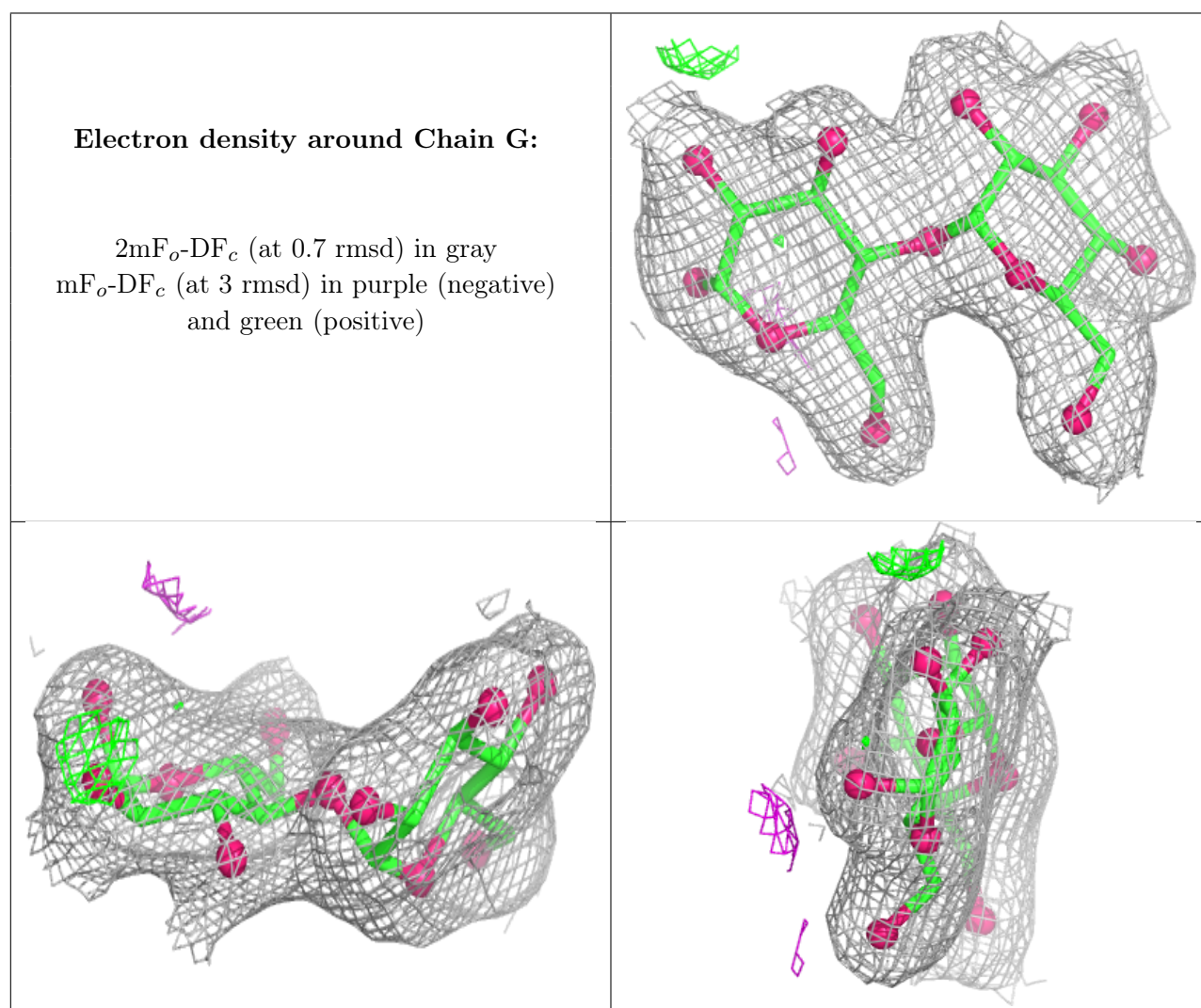
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

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

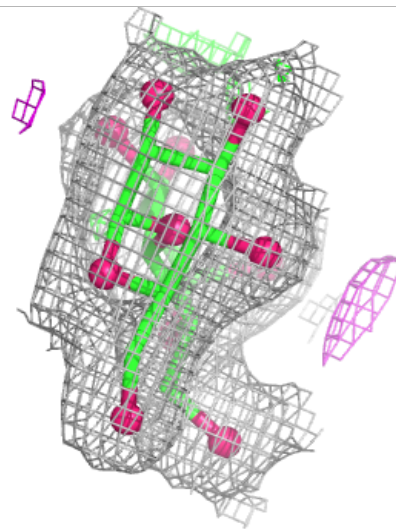
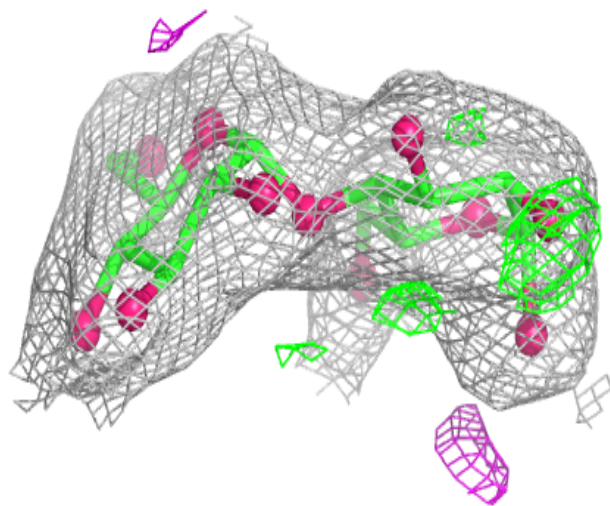
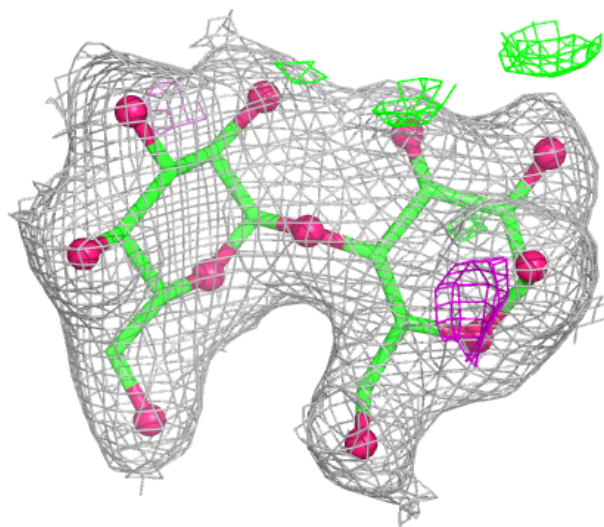
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	GLC	G	1	12/12	0.96	0.06	40,45,51,52	0
3	GLC	H	1	12/12	0.96	0.07	49,53,55,55	0
3	GLC	I	2	11/12	0.96	0.07	50,53,54,55	0
3	GLC	I	1	12/12	0.97	0.06	52,54,57,59	0
3	GLC	H	2	11/12	0.97	0.06	44,47,49,49	0
3	GLC	G	2	11/12	0.98	0.05	36,38,40,41	0

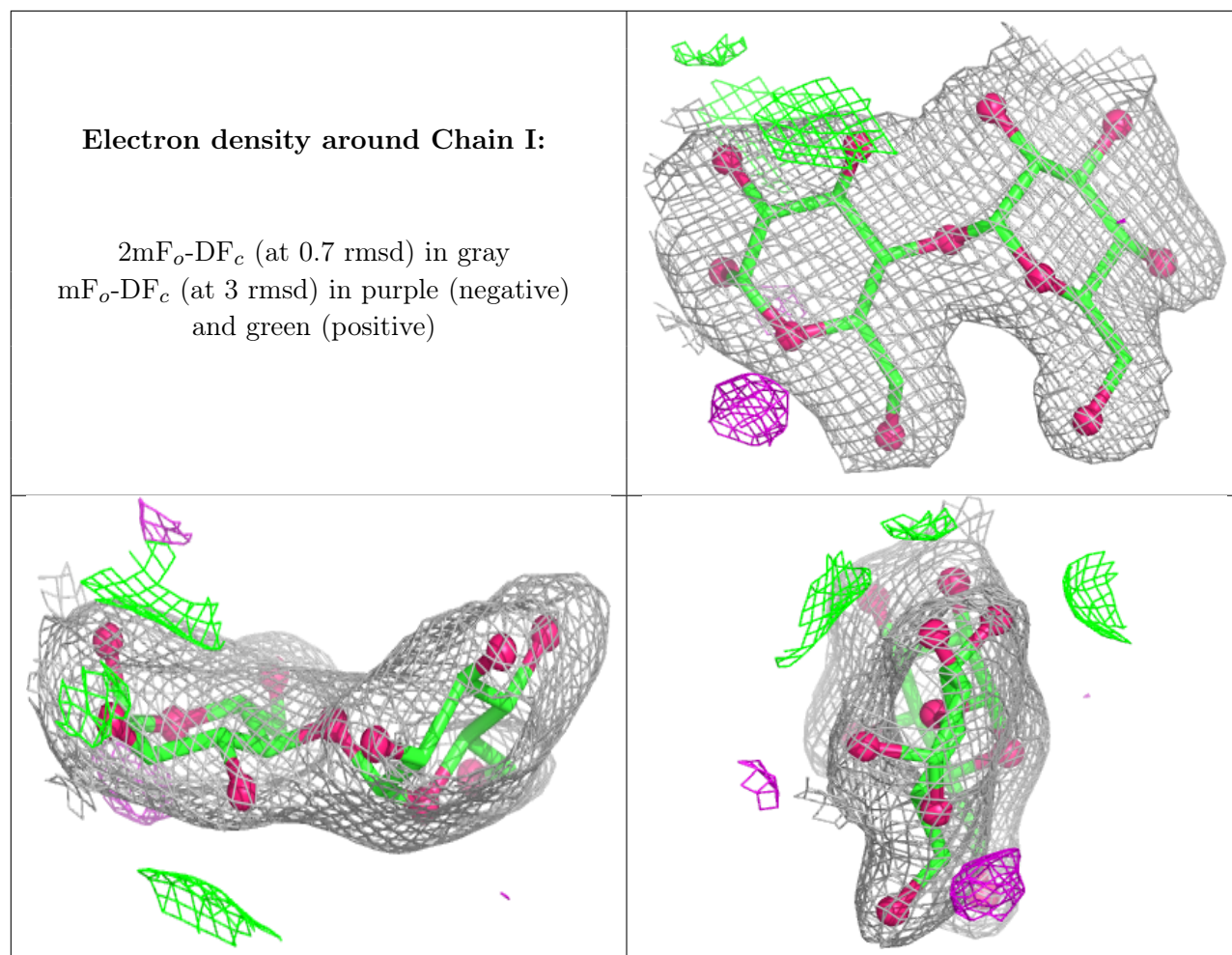
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



Electron density around Chain H:

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





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NA	A	2202	1/1	0.92	0.17	61,61,61,61	0
4	NA	C	2204	1/1	0.93	0.06	60,60,60,60	0
4	NA	C	2203	1/1	0.96	0.07	52,52,52,52	0
4	NA	C	2202	1/1	0.98	0.03	42,42,42,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.