



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:58 PM UTC

PDB ID : 7BG0 / pdb_00007bg0
Title : Fusion of MBP and the backbone of the long-acting amylin analog AM833.
Authors : Johansson, E.
Deposited on : 2021-01-05
Resolution : 2.89 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

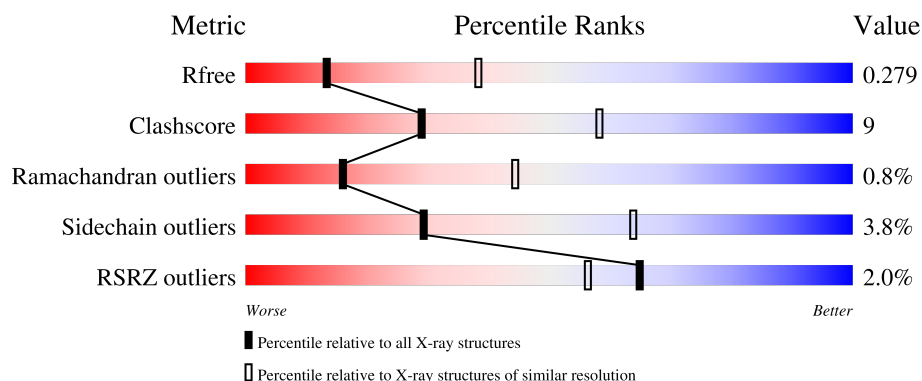
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.89 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	408	2% 79% 19% ..
1	B	408	75% 13% 9% .
1	D	408	3% 69% 19% 10% .
1	E	408	2% 77% 20% ..
2	C	2	50% 50%

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Mol	Chain	Length	Quality of chain
2	F	2	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11933 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/maltodextrin-binding periplasmic protein, Islet amyloid polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	403	Total	C	N	O	S	0	0	0
			3102	1991	512	591	8			
1	B	371	Total	C	N	O	S	0	0	0
			2863	1844	467	546	6			
1	D	366	Total	C	N	O	S	0	0	0
			2831	1825	460	540	6			
1	E	401	Total	C	N	O	S	0	0	0
			3091	1984	510	589	8			

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	26	MET	-	initiating methionine	UNP P0AEX9
A	385	ALA	GLU	engineered mutation	UNP P0AEX9
A	388	ALA	-	linker	UNP P0AEX9
A	389	ALA	-	linker	UNP P0AEX9
A	390	ALA	-	linker	UNP P0AEX9
A	391	GLN	-	linker	UNP P0AEX9
A	392	THR	-	linker	UNP P0AEX9
A	393	ASN	-	linker	UNP P0AEX9
A	394	ALA	-	linker	UNP P0AEX9
A	395	ALA	-	linker	UNP P0AEX9
A	396	ALA	-	linker	UNP P0AEX9
A	410	GLU	ASN	engineered mutation	UNP P10997
A	413	ARG	VAL	engineered mutation	UNP P10997
A	421	PRO	ALA	engineered mutation	UNP P10997
A	424	PRO	SER	engineered mutation	UNP P10997
A	425	PRO	SER	engineered mutation	UNP P10997
A	433	PRO	TYR	engineered mutation	UNP P10997
B	26	MET	-	initiating methionine	UNP P0AEX9
B	385	ALA	GLU	engineered mutation	UNP P0AEX9
B	388	ALA	-	linker	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	389	ALA	-	linker	UNP P0AEX9
B	390	ALA	-	linker	UNP P0AEX9
B	391	GLN	-	linker	UNP P0AEX9
B	392	THR	-	linker	UNP P0AEX9
B	393	ASN	-	linker	UNP P0AEX9
B	394	ALA	-	linker	UNP P0AEX9
B	395	ALA	-	linker	UNP P0AEX9
B	396	ALA	-	linker	UNP P0AEX9
B	410	GLU	ASN	engineered mutation	UNP P10997
B	413	ARG	VAL	engineered mutation	UNP P10997
B	421	PRO	ALA	engineered mutation	UNP P10997
B	424	PRO	SER	engineered mutation	UNP P10997
B	425	PRO	SER	engineered mutation	UNP P10997
B	433	PRO	TYR	engineered mutation	UNP P10997
D	26	MET	-	initiating methionine	UNP P0AEX9
D	385	ALA	GLU	engineered mutation	UNP P0AEX9
D	388	ALA	-	linker	UNP P0AEX9
D	389	ALA	-	linker	UNP P0AEX9
D	390	ALA	-	linker	UNP P0AEX9
D	391	GLN	-	linker	UNP P0AEX9
D	392	THR	-	linker	UNP P0AEX9
D	393	ASN	-	linker	UNP P0AEX9
D	394	ALA	-	linker	UNP P0AEX9
D	395	ALA	-	linker	UNP P0AEX9
D	396	ALA	-	linker	UNP P0AEX9
D	410	GLU	ASN	engineered mutation	UNP P10997
D	413	ARG	VAL	engineered mutation	UNP P10997
D	421	PRO	ALA	engineered mutation	UNP P10997
D	424	PRO	SER	engineered mutation	UNP P10997
D	425	PRO	SER	engineered mutation	UNP P10997
D	433	PRO	TYR	engineered mutation	UNP P10997
E	26	MET	-	initiating methionine	UNP P0AEX9
E	385	ALA	GLU	engineered mutation	UNP P0AEX9
E	388	ALA	-	linker	UNP P0AEX9
E	389	ALA	-	linker	UNP P0AEX9
E	390	ALA	-	linker	UNP P0AEX9
E	391	GLN	-	linker	UNP P0AEX9
E	392	THR	-	linker	UNP P0AEX9
E	393	ASN	-	linker	UNP P0AEX9
E	394	ALA	-	linker	UNP P0AEX9
E	395	ALA	-	linker	UNP P0AEX9
E	396	ALA	-	linker	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
E	410	GLU	ASN	engineered mutation	UNP P10997
E	413	ARG	VAL	engineered mutation	UNP P10997
E	421	PRO	ALA	engineered mutation	UNP P10997
E	424	PRO	SER	engineered mutation	UNP P10997
E	425	PRO	SER	engineered mutation	UNP P10997
E	433	PRO	TYR	engineered mutation	UNP P10997

- Molecule 2 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.

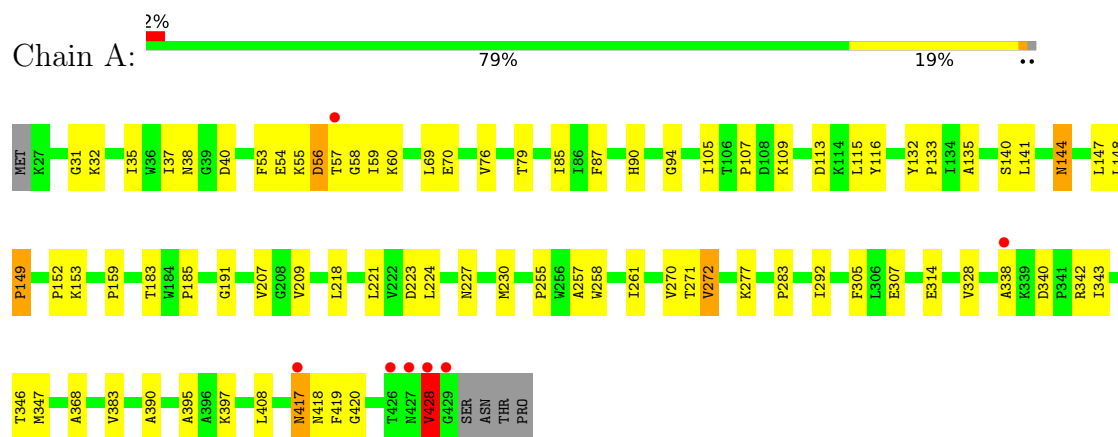


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	C	2	Total	C	O	0	0	0
			23	12	11			
2	F	2	Total	C	O	0	0	0
			23	12	11			

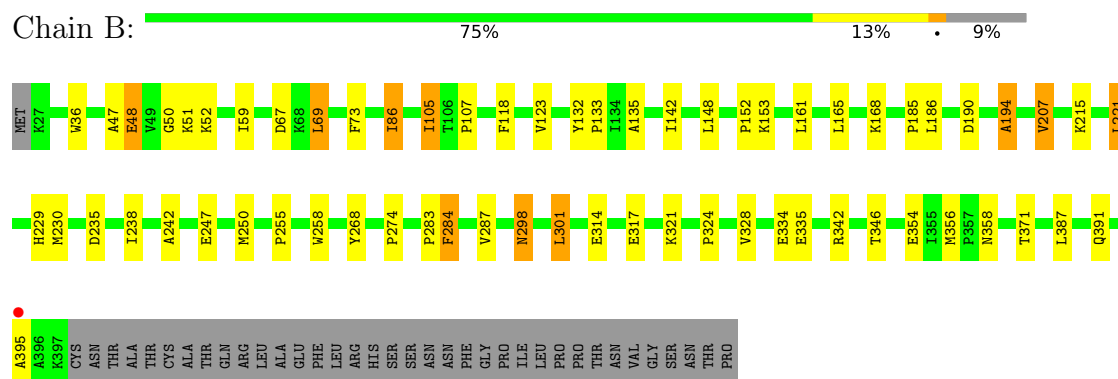
3 Residue-property plots

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.

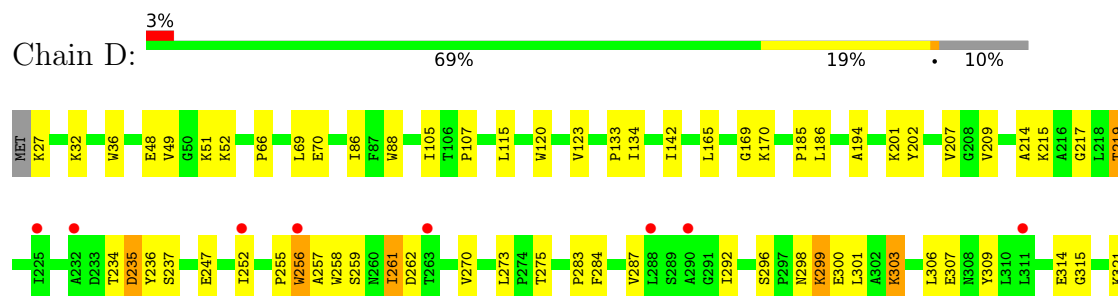
- Molecule 1: Maltose/maltodextrin-binding periplasmic protein, Islet amyloid polypeptide

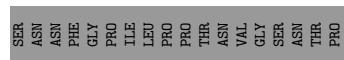


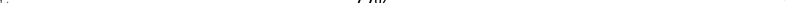
- Molecule 1: Maltose/maltodextrin-binding periplasmic protein, Islet amyloid polypeptide

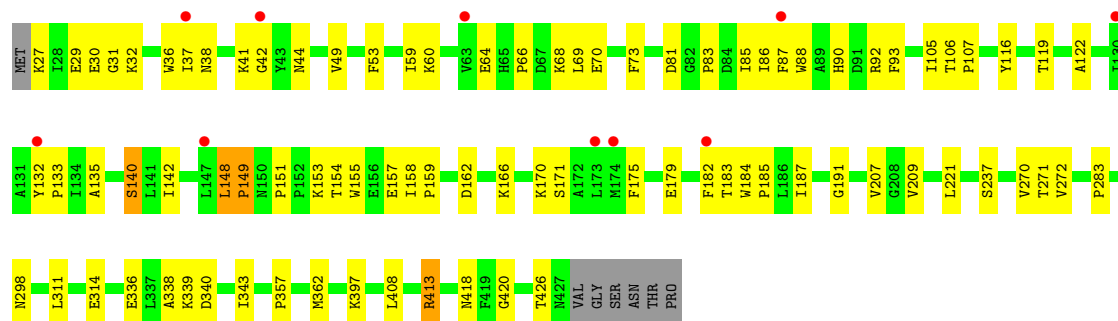


- Molecule 1: Maltose/maltodextrin-binding periplasmic protein, Islet amyloid polypeptide





- Chain E: 



- Chain C:  50% 50%



- Chain F: 50% 50%



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	179.13Å 179.13Å 150.21Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	37.55 – 2.89 37.55 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.4 (37.55-2.89) 87.3 (37.55-2.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 2.90Å)	Xtriage
Refinement program	PHENIX dev_3965	Depositor
R, R_{free}	0.220 , 0.279 0.220 , 0.279	Depositor DCC
R_{free} test set	1994 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	56.1	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 32.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.025 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	11933	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.82% 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: 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	0.17	0/3177	0.36	0/4318
1	B	0.15	0/2932	0.33	0/3982
1	D	0.16	0/2900	0.37	0/3939
1	E	0.15	0/3166	0.39	2/4303 (0.0%)
All	All	0.16	0/12175	0.36	2/16542 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	413	ARG	CB-CG-CD	-7.95	93.02	111.30
1	E	413	ARG	CG-CD-NE	5.67	124.48	112.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	413	ARG	Sidechain

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	3102	0	3068	66	0
1	B	2863	0	2838	52	0
1	D	2831	0	2804	69	0
1	E	3091	0	3056	78	0
2	C	23	0	21	0	0
2	F	23	0	21	2	0
All	All	11933	0	11808	206	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (206) 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:A:105:ILE:HG22	1:A:107:PRO:HD3	1.56	0.87
1:E:183:THR:HG22	1:E:187:ILE:HD11	1.59	0.84
1:D:105:ILE:HG22	1:D:107:PRO:HD3	1.60	0.82
1:B:105:ILE:HG22	1:B:107:PRO:HD3	1.63	0.79
1:A:59:ILE:HG12	1:B:301:LEU:HD21	1.65	0.78
1:E:64:GLU:HG2	1:E:66:PRO:HD3	1.65	0.78
1:D:299:LYS:O	1:D:301:LEU:N	2.16	0.77
1:D:66:PRO:HD2	1:D:69:LEU:HD12	1.67	0.77
1:D:287:VAL:HB	1:E:90:HIS:HD2	1.50	0.75
1:D:36:TRP:HB3	1:D:69:LEU:HD11	1.70	0.72
1:D:356:MET:HB2	1:E:90:HIS:CE1	2.25	0.71
1:E:179:GLU:HB2	1:E:182:PHE:HE2	1.56	0.70
1:E:105:ILE:HG22	1:E:107:PRO:HD3	1.74	0.70
1:D:258:TRP:HB2	1:D:324:PRO:HG2	1.74	0.70
1:D:284:PHE:HD1	1:D:356:MET:HG2	1.56	0.69
1:A:417:ASN:N	1:A:417:ASN:OD1	2.25	0.68
1:E:179:GLU:HB2	1:E:182:PHE:CE2	2.28	0.67
1:E:357:PRO:HD2	1:E:362:MET:HE2	1.75	0.67
1:B:207:VAL:O	1:B:391:GLN:NE2	2.27	0.67
1:A:38:ASN:ND2	1:A:40:ASP:OD1	2.29	0.65
1:E:154:THR:OG1	1:E:157:GLU:HG2	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:298:ASN:N	1:B:298:ASN:OD1	2.29	0.65
1:E:66:PRO:HG2	1:E:69:LEU:HD13	1.80	0.64
1:E:338:ALA:HA	1:E:340:ASP:N	2.12	0.64
1:E:338:ALA:HB2	1:E:343:ILE:HB	1.80	0.64
1:A:338:ALA:HB2	1:A:343:ILE:HB	1.81	0.63
1:B:258:TRP:HB2	1:B:324:PRO:HG2	1.79	0.63
1:A:338:ALA:HA	1:A:340:ASP:N	2.14	0.62
1:A:32:LYS:O	1:B:298:ASN:ND2	2.22	0.61
1:A:90:HIS:HD2	1:B:287:VAL:HB	1.64	0.61
1:D:284:PHE:CD1	1:D:356:MET:HG2	2.35	0.60
1:E:153:LYS:N	1:E:157:GLU:OE2	2.29	0.60
1:D:298:ASN:ND2	1:E:29:GLU:O	2.35	0.59
1:A:59:ILE:HG12	1:B:301:LEU:CD2	2.32	0.59
1:D:306:LEU:HD21	1:E:85:ILE:HD13	1.86	0.58
1:B:268:TYR:OH	1:B:342:ARG:NH1	2.36	0.58
1:A:207:VAL:CG1	1:A:395:ALA:HB2	2.33	0.58
1:D:255:PRO:HB2	1:D:324:PRO:HB2	1.86	0.58
1:A:115:LEU:HD23	1:A:133:PRO:HG2	1.86	0.57
1:D:356:MET:HB2	1:E:90:HIS:HE1	1.69	0.57
1:E:36:TRP:CG	1:E:83:PRO:HG3	2.38	0.57
1:E:70:GLU:H	1:E:70:GLU:CD	2.12	0.57
1:D:298:ASN:OD1	1:E:31:GLY:N	2.38	0.57
1:E:88:TRP:HB3	1:E:93:PHE:HE1	1.69	0.56
1:D:270:VAL:HG22	1:E:142:ILE:HG22	1.86	0.56
1:E:32:LYS:HD3	1:E:60:LYS:HB3	1.88	0.56
1:B:235:ASP:OD2	1:B:238:ILE:HG12	2.06	0.55
1:A:90:HIS:CE1	1:B:356:MET:HB2	2.42	0.55
1:A:207:VAL:HG11	1:A:395:ALA:HB2	1.89	0.54
1:D:359:ILE:HD12	1:D:361:GLN:HB2	1.88	0.54
1:A:109:LYS:NZ	1:A:113:ASP:OD2	2.32	0.54
1:A:418:ASN:CG	1:A:419:PHE:H	2.16	0.54
1:D:49:VAL:HA	1:D:52:LYS:HE3	1.90	0.54
1:E:90:HIS:CD2	1:E:122:ALA:HB1	2.43	0.53
1:B:123:VAL:HG21	1:B:133:PRO:HD3	1.91	0.53
1:B:284:PHE:CD1	1:B:356:MET:HG2	2.43	0.53
1:A:54:GLU:O	1:A:58:GLY:HA2	2.09	0.53
1:D:275:THR:O	1:E:155:TRP:N	2.35	0.53
1:E:36:TRP:CD2	1:E:83:PRO:HG3	2.43	0.53
1:A:57:THR:O	1:A:59:ILE:HD12	2.08	0.53
1:E:105:ILE:HD12	1:E:132:TYR:CE1	2.43	0.53
1:D:323:LYS:HD3	1:E:42:GLY:HA2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:215:LYS:HD3	1:B:387:LEU:HD12	1.90	0.52
1:A:347:MET:HE1	1:B:118:PHE:HZ	1.73	0.52
1:D:287:VAL:HB	1:E:90:HIS:CD2	2.40	0.52
1:E:116:TYR:O	1:E:119:THR:OG1	2.25	0.52
1:A:32:LYS:HA	1:A:59:ILE:CG2	2.39	0.52
1:B:36:TRP:HB3	1:B:69:LEU:HD13	1.92	0.51
1:E:37:ILE:HA	1:E:87:PHE:HB2	1.93	0.51
1:B:73:PHE:CG	1:B:86:ILE:HD12	2.45	0.51
1:D:255:PRO:O	1:D:258:TRP:N	2.35	0.51
1:A:347:MET:HE1	1:B:118:PHE:CZ	2.45	0.51
1:D:270:VAL:HG12	1:D:345:ALA:HB3	1.91	0.51
1:A:148:LEU:HD21	1:A:152:PRO:HD3	1.92	0.51
1:A:183:THR:HG23	1:B:221:LEU:HD13	1.91	0.51
1:D:258:TRP:CH2	1:D:342:ARG:HG3	2.46	0.51
1:A:328:VAL:HA	1:B:135:ALA:HA	1.93	0.51
1:D:298:ASN:HD21	1:E:30:GLU:HA	1.76	0.51
1:A:224:LEU:HD12	1:A:230:MET:HE2	1.93	0.50
1:D:283:PRO:HB3	1:E:185:PRO:HG3	1.92	0.50
1:A:31:GLY:O	1:A:59:ILE:HG23	2.11	0.50
1:B:317:GLU:HG2	1:B:321:LYS:HE2	1.93	0.50
1:E:418:ASN:C	1:E:420:GLY:H	2.19	0.50
1:B:317:GLU:O	1:B:321:LYS:HG3	2.11	0.50
1:E:148:LEU:HD11	1:E:151:PRO:HA	1.94	0.50
1:A:90:HIS:CD2	1:B:287:VAL:H	2.29	0.50
1:D:247:GLU:HA	1:E:170:LYS:HD2	1.94	0.50
1:D:284:PHE:HD2	1:E:184:TRP:CD1	2.30	0.50
1:D:287:VAL:H	1:E:90:HIS:CD2	2.30	0.50
1:A:305:PHE:HE1	1:B:50:GLY:HA2	1.77	0.49
1:D:185:PRO:HG3	1:E:283:PRO:HA	1.94	0.49
1:D:123:VAL:HG21	1:D:133:PRO:HD3	1.92	0.49
1:B:148:LEU:HD21	1:B:152:PRO:HD3	1.94	0.49
1:B:161:LEU:HG	1:B:165:LEU:HD12	1.95	0.49
1:A:223:ASP:O	1:A:227:ASN:ND2	2.46	0.49
1:D:303:LYS:HG3	1:D:307:GLU:OE1	2.13	0.49
1:A:144:ASN:HB3	1:A:147:LEU:HB2	1.93	0.48
1:D:256:TRP:HA	1:D:324:PRO:HD2	1.96	0.48
1:D:322:ASP:OD2	1:E:44:ASN:HB2	2.13	0.48
1:D:328:VAL:HA	1:E:135:ALA:HA	1.95	0.48
1:E:27:LYS:N	1:E:81:ASP:OD1	2.47	0.48
1:A:159:PRO:HA	1:B:229:HIS:CD2	2.49	0.48
1:E:106:THR:O	1:E:106:THR:OG1	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:349:ASN:ND2	1:E:140:SER:HA	2.29	0.48
1:A:305:PHE:CE1	1:B:50:GLY:HA2	2.49	0.47
1:D:142:ILE:HG12	1:E:270:VAL:HG22	1.95	0.47
1:A:418:ASN:C	1:A:420:GLY:H	2.23	0.47
1:D:247:GLU:O	1:E:170:LYS:HB3	2.14	0.47
1:E:36:TRP:HB3	1:E:69:LEU:HD11	1.96	0.46
1:E:187:ILE:HD12	1:E:187:ILE:H	1.80	0.46
1:D:215:LYS:O	1:D:219:THR:HB	2.15	0.46
1:A:270:VAL:HG22	1:B:142:ILE:HG12	1.98	0.46
1:A:283:PRO:HA	1:B:185:PRO:HG3	1.98	0.46
1:B:242:ALA:O	1:B:247:GLU:HB3	2.16	0.46
1:D:309:TYR:O	1:D:315:GLY:HA3	2.16	0.46
1:D:309:TYR:CE2	1:E:53:PHE:HD1	2.34	0.46
1:E:155:TRP:O	1:E:158:ILE:HD12	2.16	0.46
1:B:230:MET:HB3	1:B:230:MET:HE2	1.83	0.45
1:E:158:ILE:N	1:E:159:PRO:HD2	2.31	0.45
1:A:116:TYR:HE2	1:B:334:GLU:HG2	1.81	0.45
1:B:48:GLU:O	1:B:51:LYS:HB2	2.16	0.45
1:D:314:GLU:H	1:D:314:GLU:CD	2.24	0.45
1:A:70:GLU:OE1	1:A:70:GLU:N	2.36	0.45
1:A:135:ALA:HA	1:B:328:VAL:HA	1.99	0.45
1:E:73:PHE:CE1	1:E:86:ILE:HB	2.52	0.45
1:E:271:THR:OG1	1:E:272:VAL:N	2.50	0.45
1:A:76:VAL:O	1:A:79:THR:OG1	2.34	0.45
1:D:115:LEU:HB2	1:D:120:TRP:NE1	2.32	0.45
1:D:292:ILE:HG21	1:D:299:LYS:HE3	1.99	0.45
1:E:336:GLU:O	1:E:339:LYS:HG3	2.17	0.45
1:D:202:TYR:CZ	1:D:357:PRO:HG3	2.52	0.44
1:E:73:PHE:CD2	1:E:73:PHE:C	2.95	0.44
1:A:54:GLU:OE1	1:A:60:LYS:NZ	2.40	0.44
1:B:258:TRP:CH2	1:B:342:ARG:HG3	2.52	0.44
1:A:56:ASP:OD1	1:A:56:ASP:N	2.50	0.44
1:A:148:LEU:HD12	1:A:149:PRO:HD2	1.99	0.44
1:D:273:LEU:HD22	1:D:349:ASN:ND2	2.32	0.44
1:D:207:VAL:O	1:D:391:GLN:NE2	2.51	0.44
1:D:214:ALA:HA	1:E:187:ILE:HG22	1.99	0.44
1:A:257:ALA:O	1:A:261:ILE:HG13	2.18	0.44
1:A:255:PRO:HA	1:A:258:TRP:CE2	2.52	0.44
1:D:270:VAL:HB	1:D:342:ARG:HB2	2.00	0.44
1:D:255:PRO:O	1:D:257:ALA:N	2.51	0.44
1:A:35:ILE:HG12	1:A:85:ILE:HB	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:70:GLU:HB3	1:D:88:TRP:CZ2	2.53	0.44
1:A:428:VAL:HG21	1:E:237:SER:HB3	1.99	0.43
1:A:53:PHE:O	1:A:57:THR:N	2.45	0.43
1:B:52:LYS:HE3	1:B:52:LYS:HB2	1.55	0.43
1:D:356:MET:HE3	1:D:366:TRP:HZ2	1.84	0.43
1:E:311:LEU:HD23	1:E:311:LEU:HA	1.89	0.43
1:E:338:ALA:HA	1:E:339:LYS:C	2.44	0.43
1:D:252:ILE:HD12	1:E:175:PHE:CD2	2.53	0.43
1:E:105:ILE:CG2	1:E:107:PRO:HD3	2.46	0.43
1:A:152:PRO:HD2	1:B:250:MET:HE1	2.00	0.43
1:E:92:ARG:NH1	2:F:2:GLC:O4	2.52	0.43
1:E:31:GLY:O	1:E:59:ILE:HG23	2.19	0.43
1:D:186:LEU:HD23	1:E:221:LEU:HB2	2.01	0.43
1:E:184:TRP:HA	1:E:187:ILE:CD1	2.49	0.43
1:D:261:ILE:H	1:D:261:ILE:HG13	1.71	0.42
1:E:162:ASP:O	1:E:166:LYS:HG3	2.19	0.42
1:A:368:ALA:HB1	1:A:390:ALA:HA	2.01	0.42
1:A:37:ILE:HA	1:A:87:PHE:HB2	2.01	0.42
1:D:217:GLY:HA3	1:E:187:ILE:HA	2.00	0.42
1:E:148:LEU:HD22	1:E:149:PRO:HD2	2.00	0.42
1:A:153:LYS:HA	1:A:153:LYS:HD2	1.78	0.42
1:A:292:ILE:HD12	1:B:105:ILE:HD11	2.02	0.42
1:B:67:ASP:OD1	1:E:237:SER:OG	2.30	0.42
1:B:255:PRO:HA	1:B:258:TRP:CD2	2.54	0.42
1:A:270:VAL:HB	1:A:342:ARG:HG2	2.02	0.42
1:A:94:GLY:HA3	1:B:358:ASN:O	2.20	0.42
1:A:314:GLU:H	1:A:314:GLU:CD	2.28	0.42
1:D:215:LYS:HD3	1:D:387:LEU:HD12	2.00	0.42
1:A:221:LEU:HB2	1:B:186:LEU:HD23	2.01	0.42
1:D:235:ASP:CG	1:D:236:TYR:N	2.78	0.42
1:A:218:LEU:HD23	1:A:383:VAL:HG13	2.02	0.41
1:B:47:ALA:O	1:B:51:LYS:HG3	2.20	0.41
1:A:141:LEU:HD22	1:B:274:PRO:HG3	2.02	0.41
1:E:41:LYS:HD3	1:E:41:LYS:HA	1.88	0.41
1:A:271:THR:OG1	1:A:272:VAL:N	2.53	0.41
1:D:27:LYS:HD2	1:D:27:LYS:HA	1.80	0.41
1:D:169:GLY:O	1:D:170:LYS:HD3	2.20	0.41
1:D:209:VAL:O	1:D:387:LEU:HD22	2.20	0.41
1:E:38:ASN:ND2	1:E:88:TRP:HZ3	2.18	0.41
1:E:68:LYS:HA	1:E:68:LYS:HD2	1.66	0.41
1:A:54:GLU:OE2	1:A:60:LYS:HD2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:GLU:OE1	1:B:132:TYR:OH	2.31	0.41
1:D:235:ASP:OD1	1:D:237:SER:N	2.53	0.41
1:D:298:ASN:ND2	1:E:30:GLU:HA	2.34	0.41
1:D:375:ASN:HB3	1:D:381:GLN:HB2	2.02	0.41
1:E:119:THR:HB	1:E:133:PRO:HB2	2.02	0.41
1:D:275:THR:OG1	1:E:154:THR:HG22	2.20	0.41
1:B:207:VAL:HG11	1:B:395:ALA:HB2	2.03	0.41
1:E:314:GLU:CD	1:E:314:GLU:H	2.29	0.41
1:D:48:GLU:OE1	1:D:51:LYS:HE3	2.21	0.41
1:D:366:TRP:CD1	2:F:2:GLC:H4	2.56	0.41
1:E:70:GLU:HB2	1:E:92:ARG:HD3	2.02	0.41
1:A:185:PRO:HG3	1:B:283:PRO:HA	2.03	0.41
1:A:277:LYS:HD3	1:B:190:ASP:CG	2.46	0.41
1:D:133:PRO:O	1:D:134:ILE:HD13	2.21	0.41
1:D:259:SER:HA	1:D:262:ASP:OD2	2.21	0.40
1:D:32:LYS:O	1:E:298:ASN:ND2	2.54	0.40
1:A:59:ILE:HG21	1:B:301:LEU:HD23	2.03	0.40
1:B:314:GLU:H	1:B:314:GLU:CD	2.30	0.40
1:A:105:ILE:HD12	1:A:132:TYR:CE1	2.56	0.40
1:A:207:VAL:HG23	1:B:194:ALA:O	2.21	0.40
1:A:428:VAL:HG11	1:E:237:SER:OG	2.21	0.40

There are no symmetry-related clashes.

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	401/408 (98%)	380 (95%)	17 (4%)	4 (1%)	12	39
1	B	369/408 (90%)	350 (95%)	18 (5%)	1 (0%)	36	65
1	D	364/408 (89%)	345 (95%)	14 (4%)	5 (1%)	9	30
1	E	399/408 (98%)	380 (95%)	16 (4%)	3 (1%)	16	44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1533/1632 (94%)	1455 (95%)	65 (4%)	13 (1%)	16	44

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	428	VAL
1	D	256	TRP
1	D	300	GLU
1	E	149	PRO
1	D	234	THR
1	A	149	PRO
1	B	194	ALA
1	D	194	ALA
1	E	191	GLY
1	E	397	LYS
1	A	397	LYS
1	D	299	LYS
1	A	191	GLY

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	319/324 (98%)	308 (97%)	11 (3%)	32	66
1	B	292/324 (90%)	276 (94%)	16 (6%)	19	50
1	D	290/324 (90%)	279 (96%)	11 (4%)	29	64
1	E	318/324 (98%)	310 (98%)	8 (2%)	42	74
All	All	1219/1296 (94%)	1173 (96%)	46 (4%)	29	64

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	LYS
1	A	56	ASP

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Mol	Chain	Res	Type
1	A	69	LEU
1	A	140	SER
1	A	144	ASN
1	A	209	VAL
1	A	272	VAL
1	A	346	THR
1	A	408	LEU
1	A	417	ASN
1	A	428	VAL
1	B	48	GLU
1	B	59	ILE
1	B	69	LEU
1	B	86	ILE
1	B	105	ILE
1	B	153	LYS
1	B	168	LYS
1	B	207	VAL
1	B	221	LEU
1	B	284	PHE
1	B	298	ASN
1	B	301	LEU
1	B	335	GLU
1	B	346	THR
1	B	354	GLU
1	B	371	THR
1	D	86	ILE
1	D	165	LEU
1	D	201	LYS
1	D	219	THR
1	D	235	ASP
1	D	261	ILE
1	D	296	SER
1	D	303	LYS
1	D	321	LYS
1	D	371	THR
1	D	382	THR
1	E	49	VAL
1	E	140	SER
1	E	148	LEU
1	E	171	SER
1	E	207	VAL
1	E	209	VAL

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Mol	Chain	Res	Type
1	E	408	LEU
1	E	426	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	90	HIS
1	A	98	GLN
1	A	227	ASN
1	A	375	ASN
1	A	381	GLN
1	B	227	ASN
1	B	231	ASN
1	B	267	ASN
1	B	381	GLN
1	D	227	ASN
1	E	90	HIS
1	E	227	ASN
1	E	375	ASN
1	E	381	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

4 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GLC	C	1	2	12,12,12	0.52	0	17,17,17	0.56	0
2	GLC	C	2	2	11,11,12	0.56	0	15,15,17	0.83	1 (6%)
2	GLC	F	1	2	12,12,12	0.55	0	17,17,17	0.97	0
2	GLC	F	2	2	11,11,12	0.53	0	15,15,17	0.95	1 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	C	1	2	-	2/2/22/22	0/1/1/1
2	GLC	C	2	2	-	0/2/19/22	0/1/1/1
2	GLC	F	1	2	-	2/2/22/22	0/1/1/1
2	GLC	F	2	2	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	2	GLC	C1-O5-C5	2.80	115.93	112.19
2	C	2	GLC	C1-O5-C5	2.24	115.19	112.19

There are no chirality outliers.

All (4) torsion outliers are listed below:

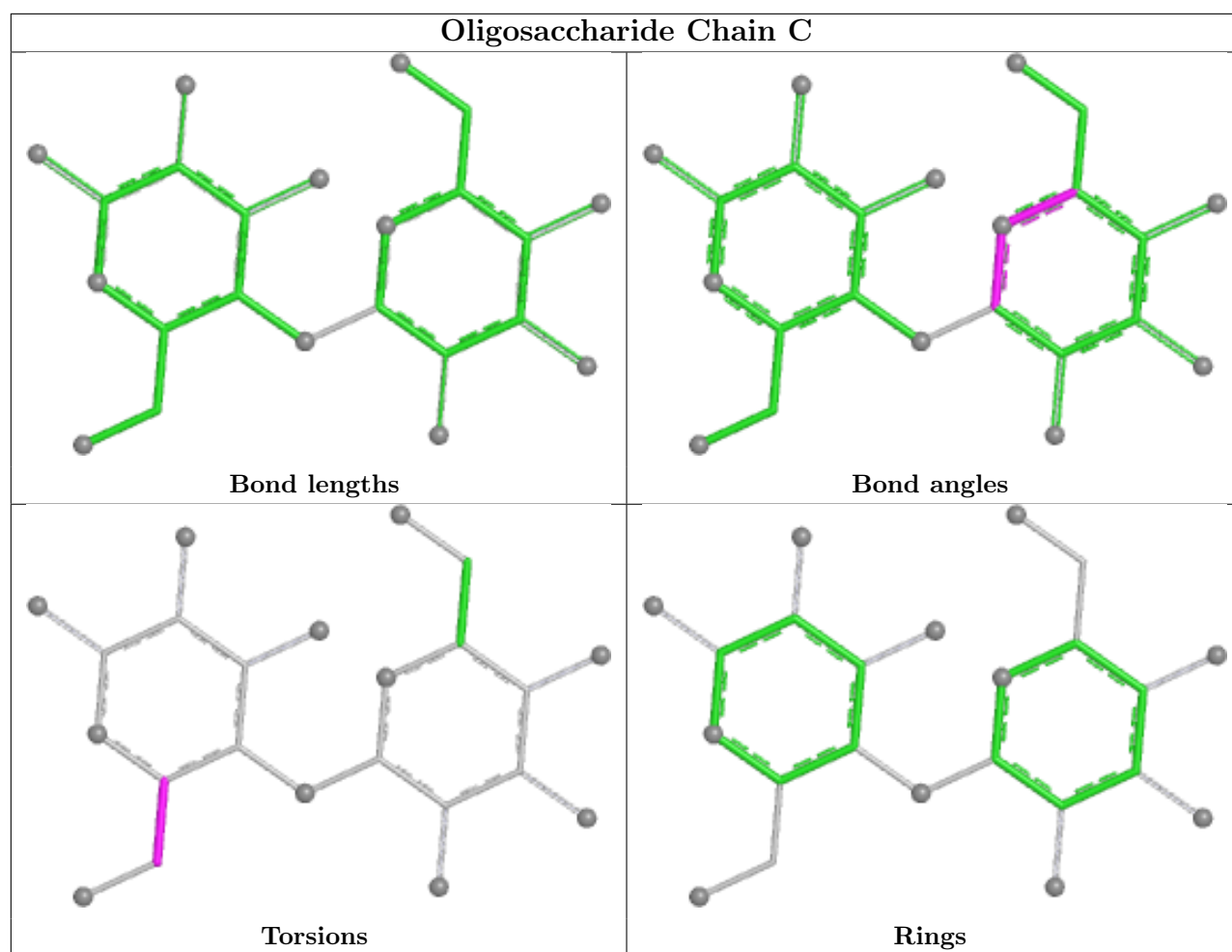
Mol	Chain	Res	Type	Atoms
2	F	1	GLC	C4-C5-C6-O6
2	F	1	GLC	O5-C5-C6-O6
2	C	1	GLC	C4-C5-C6-O6
2	C	1	GLC	O5-C5-C6-O6

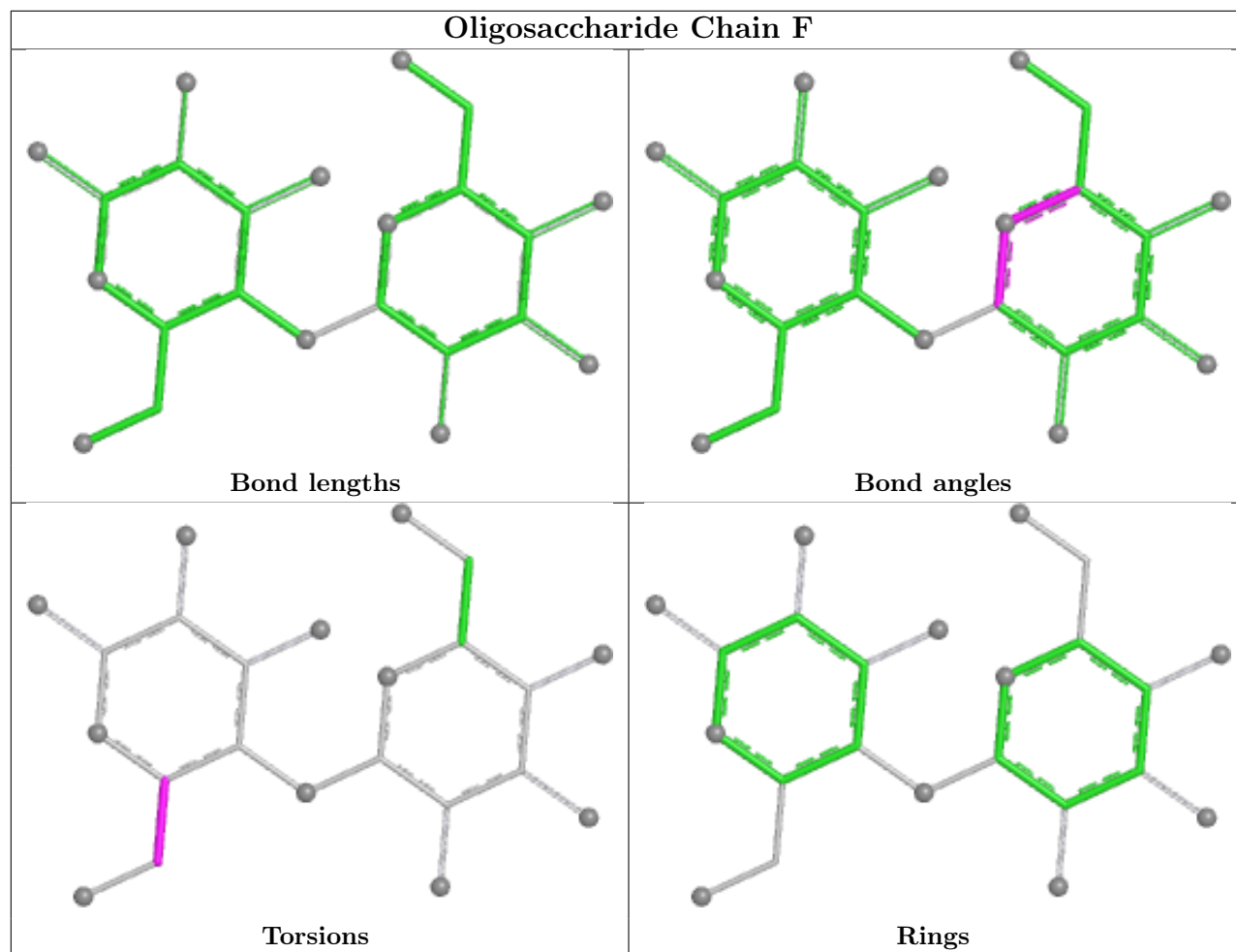
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	2	GLC	2	0

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





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, 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	403/408 (98%)	-0.14	7 (1%) 69 61	32, 53, 92, 114	0
1	B	371/408 (90%)	-0.13	1 (0%) 90 87	35, 57, 83, 98	0
1	D	366/408 (89%)	0.38	13 (3%) 46 38	35, 82, 119, 128	0
1	E	401/408 (98%)	0.24	10 (2%) 58 48	34, 66, 122, 134	0
All	All	1541/1632 (94%)	0.08	31 (2%) 65 56	32, 60, 117, 134	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	173	LEU	3.8
1	A	57	THR	3.4
1	D	325	LEU	3.2
1	A	428	VAL	3.1
1	E	87	PHE	2.7
1	D	326	GLY	2.7
1	D	311	LEU	2.6
1	D	290	ALA	2.5
1	B	395	ALA	2.5
1	A	427	ASN	2.5
1	E	130	ILE	2.4
1	D	369	VAL	2.4
1	A	426	THR	2.4
1	D	390	ALA	2.4
1	A	429	GLY	2.3
1	D	232	ALA	2.3
1	E	37	ILE	2.3
1	E	147	LEU	2.3
1	D	256	TRP	2.3
1	D	225	ILE	2.2
1	D	252	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	327	ALA	2.2
1	D	288	LEU	2.2
1	E	182	PHE	2.2
1	A	338	ALA	2.2
1	E	174	MET	2.1
1	E	42	GLY	2.1
1	A	417	ASN	2.1
1	D	263	THR	2.1
1	E	132	TYR	2.1
1	E	63	VAL	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](#)

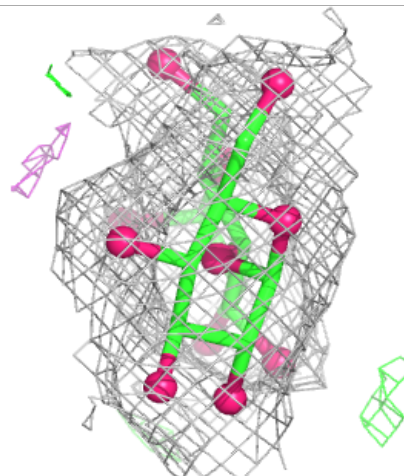
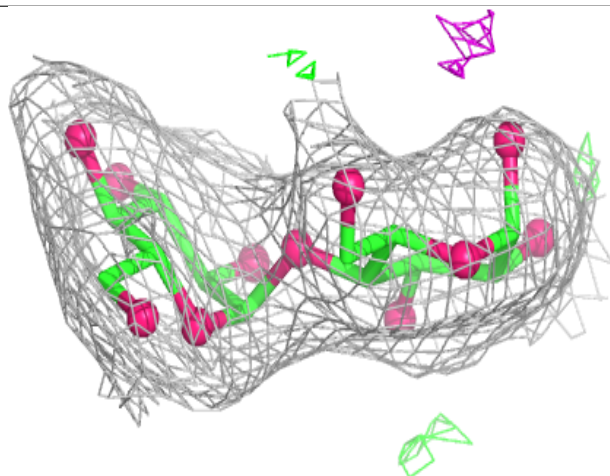
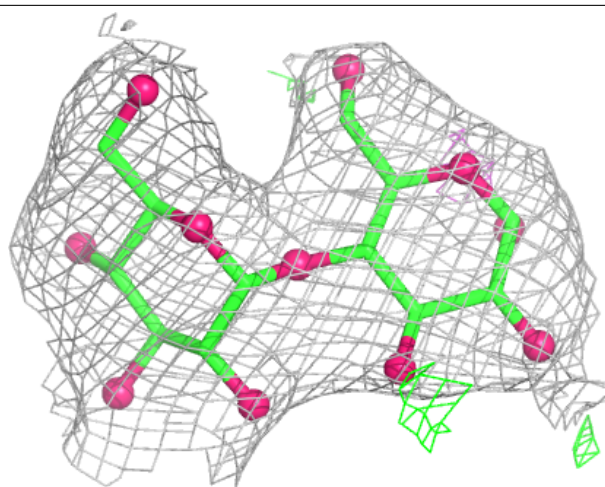
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

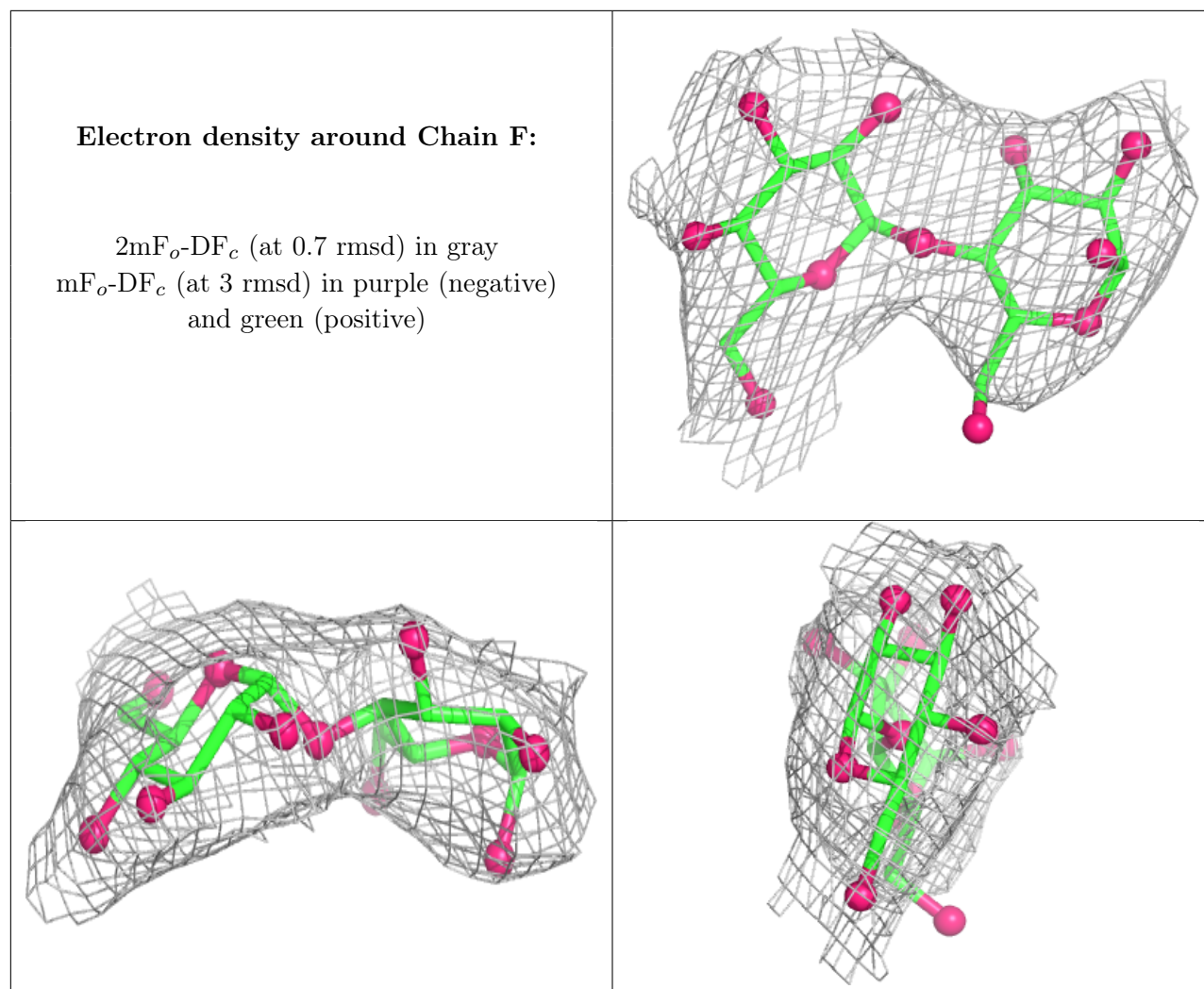
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GLC	C	1	12/12	-	-	42,51,56,57	0
2	GLC	C	2	11/12	-	-	41,43,48,49	0
2	GLC	F	1	12/12	0.89	0.09	91,96,101,101	0
2	GLC	F	2	11/12	0.92	0.07	79,83,87,89	0

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

Electron density around Chain C:

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





6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.