



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 30, 2026 – 03:19 AM UTC

PDB ID : 2XQY / pdb_00002xqy
Title : CRYSTAL STRUCTURE OF PSEUDORABIES CORE FRAGMENT OF GLYCOPROTEIN H IN COMPLEX WITH FAB D6.3
Authors : Backovic, M.; Dubois, R.; Cockburn, J.; Sharff, A.; Vaney, M.; Granzow, H.; Klupp, B.; Bricogne, G.; Mettenleiter, T.; Rey, F.
Deposited on : 2010-09-08
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

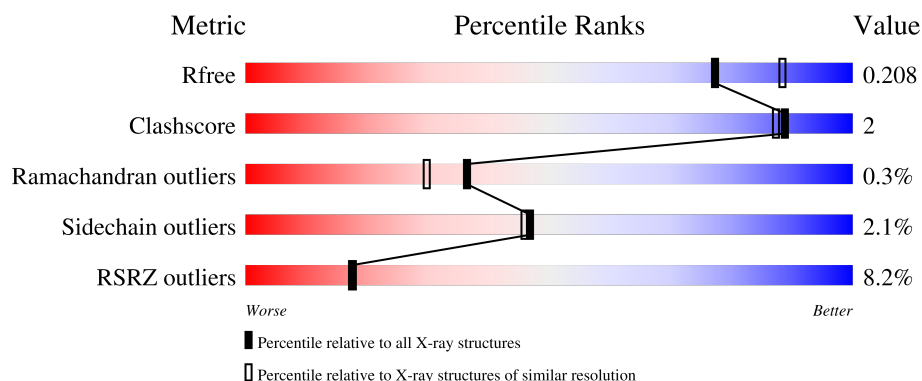
1 Overall quality at a glance

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.



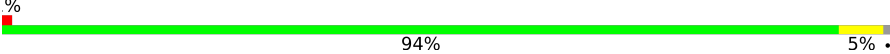
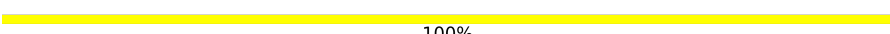
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

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	572	11% 74% 6% 19%
1	E	572	11% 74% 6% 19%
2	G	261	2% 81% 17%
2	J	261	3% 80% 17%
3	K	220	2% 95% 5%

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Mol	Chain	Length	Quality of chain
3	L	220	 % 94% 5% .
4	B	2	 100%
4	C	2	 100%
4	D	2	 100%
4	F	2	 100%
4	H	2	 100%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14739 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 ENVELOPE GLYCOPROTEIN H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	464	Total	C	N	O	S	0	0	0
			3475	2195	624	637	19			
1	E	464	Total	C	N	O	S	0	0	0
			3475	2195	624	637	19			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	105	ARG	-	expression tag	UNP P27416
A	106	SER	-	expression tag	UNP P27416
A	640	PHE	-	expression tag	UNP P27416
A	641	GLU	-	expression tag	UNP P27416
A	642	ASP	-	expression tag	UNP P27416
A	643	ASP	-	expression tag	UNP P27416
A	644	ASP	-	expression tag	UNP P27416
A	645	ASP	-	expression tag	UNP P27416
A	646	LYS	-	expression tag	UNP P27416
A	647	ALA	-	expression tag	UNP P27416
A	648	GLY	-	expression tag	UNP P27416
A	649	TRP	-	expression tag	UNP P27416
A	650	SER	-	expression tag	UNP P27416
A	651	HIS	-	expression tag	UNP P27416
A	652	PRO	-	expression tag	UNP P27416
A	653	GLN	-	expression tag	UNP P27416
A	654	PHE	-	expression tag	UNP P27416
A	655	GLU	-	expression tag	UNP P27416
A	656	LYS	-	expression tag	UNP P27416
A	657	GLY	-	expression tag	UNP P27416
A	658	GLY	-	expression tag	UNP P27416
A	659	GLY	-	expression tag	UNP P27416
A	660	SER	-	expression tag	UNP P27416
A	661	GLY	-	expression tag	UNP P27416
A	662	GLY	-	expression tag	UNP P27416

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Chain	Residue	Modelled	Actual	Comment	Reference
A	663	GLY	-	expression tag	UNP P27416
A	664	SER	-	expression tag	UNP P27416
A	665	GLY	-	expression tag	UNP P27416
A	666	GLY	-	expression tag	UNP P27416
A	667	GLY	-	expression tag	UNP P27416
A	668	SER	-	expression tag	UNP P27416
A	669	TRP	-	expression tag	UNP P27416
A	670	SER	-	expression tag	UNP P27416
A	671	HIS	-	expression tag	UNP P27416
A	672	PRO	-	expression tag	UNP P27416
A	673	GLN	-	expression tag	UNP P27416
A	674	PHE	-	expression tag	UNP P27416
A	675	GLU	-	expression tag	UNP P27416
A	676	LYS	-	expression tag	UNP P27416
E	105	ARG	-	expression tag	UNP P27416
E	106	SER	-	expression tag	UNP P27416
E	105	ARG	-	expression tag	UNP P27416
E	106	SER	-	expression tag	UNP P27416
E	640	PHE	-	expression tag	UNP P27416
E	641	GLU	-	expression tag	UNP P27416
E	642	ASP	-	expression tag	UNP P27416
E	643	ASP	-	expression tag	UNP P27416
E	644	ASP	-	expression tag	UNP P27416
E	645	ASP	-	expression tag	UNP P27416
E	646	LYS	-	expression tag	UNP P27416
E	647	ALA	-	expression tag	UNP P27416
E	648	GLY	-	expression tag	UNP P27416
E	649	TRP	-	expression tag	UNP P27416
E	650	SER	-	expression tag	UNP P27416
E	651	HIS	-	expression tag	UNP P27416
E	652	PRO	-	expression tag	UNP P27416
E	653	GLN	-	expression tag	UNP P27416
E	654	PHE	-	expression tag	UNP P27416
E	655	GLU	-	expression tag	UNP P27416
E	656	LYS	-	expression tag	UNP P27416
E	657	GLY	-	expression tag	UNP P27416
E	658	GLY	-	expression tag	UNP P27416
E	659	GLY	-	expression tag	UNP P27416
E	660	SER	-	expression tag	UNP P27416
E	661	GLY	-	expression tag	UNP P27416
E	662	GLY	-	expression tag	UNP P27416
E	663	GLY	-	expression tag	UNP P27416

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Chain	Residue	Modelled	Actual	Comment	Reference
E	664	SER	-	expression tag	UNP P27416
E	665	GLY	-	expression tag	UNP P27416
E	666	GLY	-	expression tag	UNP P27416
E	667	GLY	-	expression tag	UNP P27416
E	668	SER	-	expression tag	UNP P27416
E	669	TRP	-	expression tag	UNP P27416
E	670	SER	-	expression tag	UNP P27416
E	671	HIS	-	expression tag	UNP P27416
E	672	PRO	-	expression tag	UNP P27416
E	673	GLN	-	expression tag	UNP P27416
E	674	PHE	-	expression tag	UNP P27416
E	675	GLU	-	expression tag	UNP P27416
E	676	LYS	-	expression tag	UNP P27416

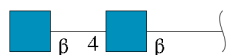
- Molecule 2 is a protein called A13-D6.3 MONOCLONAL ANTIBODY.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	216	Total	C	N	O	S	0	0	0
			1648	1044	270	327	7			
2	J	216	Total	C	N	O	S	0	0	0
			1648	1044	270	327	7			

- Molecule 3 is a protein called A13-D6.3 MONOCLONAL ANTIBODY.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	K	218	Total	C	N	O	S	0	1	0
			1698	1059	288	344	7			
3	L	218	Total	C	N	O	S	0	0	0
			1689	1054	285	343	7			

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	B	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	C	2	Total	C	N	O	0	0	0
			28	16	2	10			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	H	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	E	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	133	Total	O	0	0
			133	133		
6	E	160	Total	O	0	0
			160	160		
6	G	141	Total	O	0	0
			141	141		
6	J	180	Total	O	0	0
			180	180		
6	K	173	Total	O	0	0
			173	173		

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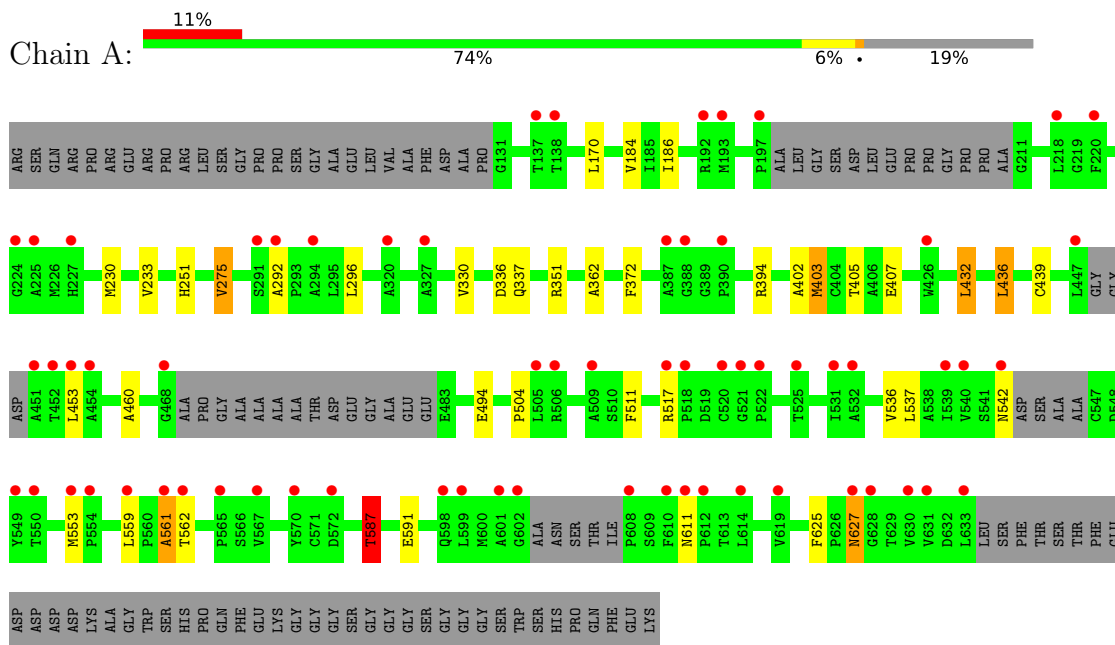
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	L	165	Total 165	O 165	0	0

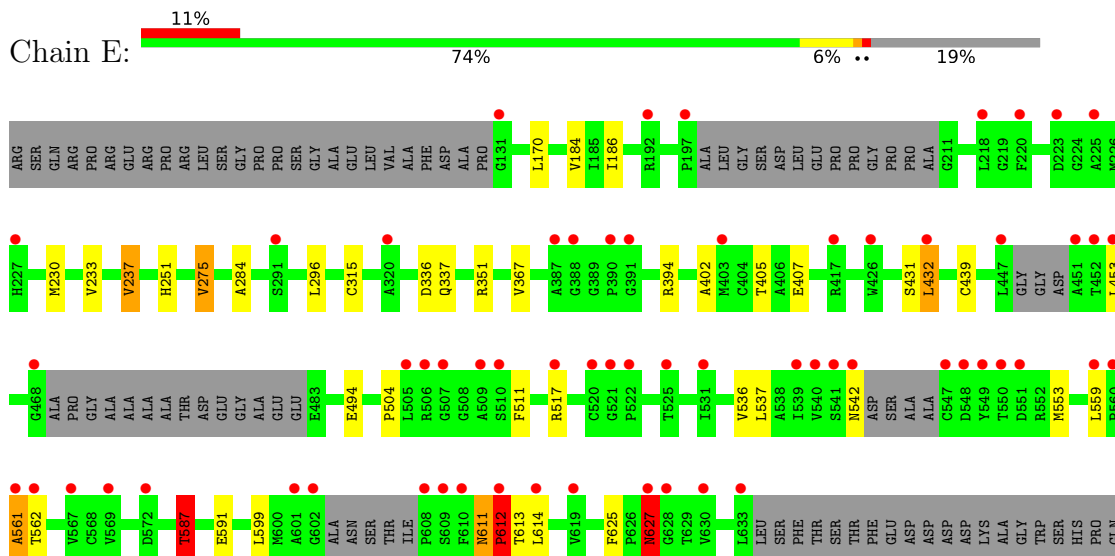
3 Residue-property plots

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: ENVELOPE GLYCOPROTEIN H



- Molecule 1: ENVELOPE GLYCOPROTEIN H



PHE GLU LYS GLY GLY GLY SER GLY GLY GLY SER GLY GLY GLY SER TRP SER HIS PRO GLN PHE GLU LYS

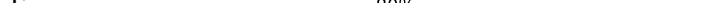
● Molecule 2: A13-D6.3 MONOCLONAL ANTIBODY

Chain G: 2% 81% 17%

ARG	SER	LVS	LEU	LEU	ASP	Q1	K38	P41	G42	R43	I48	K115	C128	G129	ASP	THR	T132	S156	N196	R213	ALA	SER	ASP	ASP	ASP	ASP	ASP	LVS	ALA	GLY	TRP	SER	SER	THR	PRO	GLN	PHE	GLU	LVS	GLY	GLY	GLY	GLY	SER	GLY	GLY	GLY	SER	TRP	SER
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HIS
PRO
GLN
PHE
GLU
LYS

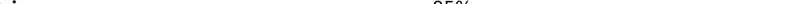
• Molecule 2: A13-D6.3 MONOCLONAL ANTIBODY

Chain J: 

ARG	SER	LYS	LEU	LEU	ASP	Q1	K38	P41	R42	R43	I48	V127	G128	G129	ASP	THR	T132	I138	E148	S156	I159	D173	N196	R213	ALA	SER	ASP	ASP	ASP	ASP	LYS	ALA	GLY	TRP	SER	HIS	PRO	GLN	PHE	GLU	LYS	GLY	GLY	SER	GLY	GLY	GLY
-----	-----	-----	-----	-----	-----	----	-----	-----	-----	-----	-----	------	------	------	-----	-----	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

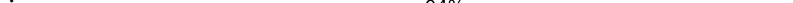
SER
GLY
GLY
GLY
SER
TRP
SER
HIS
PRO
GLN
PHE
GLU
LYS

● Molecule 3: A13-D6.3 MONOCLONAL ANTIBODY

Chain K: 

Category	Count
ARG	1
SER	1
D1	1
Y30	1
Y36	1
S56	1
Q89	1
P113	1
I144	1
I150	1
Q156	1
L179	1
C194	1
H198	1
K199	1
T200	1
S201	1
T202	1
C214	1

• Molecule 3: A13-D6.3 MONOCLONAL ANTIBODY

Chain L:  94% 5% 1%

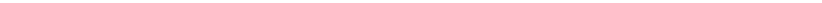
Amino Acid Category	Number of Residues (approx.)
ARG	10
SER	10
D1	10
Y30	10
P40	10
S56	10
I106	10
T126	10
P141	10
I150	10
D165	10
L179	10
T197	10
H198	10
K199	10
T200	10
S201	10
T202	10
C214	10

- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B: 100%

NAG1
NAG2

- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:  100%

MAG1
MAG2

- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:  100%MAG1
MAG2

- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  100%MAG1
MAG2

- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  100%MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	82.31Å 100.63Å 161.83Å 90.00° 94.02° 90.00°	Depositor
Resolution (Å)	58.12 – 2.05 58.12 – 2.05	Depositor EDS
% Data completeness (in resolution range)	91.8 (58.12-2.05) 92.1 (58.12-2.05)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.09 (at 2.05Å)	Xtrriage
Refinement program	BUSTER 2.11.0	Depositor
R, R_{free}	0.188 , 0.205 0.190 , 0.208	Depositor DCC
R_{free} test set	7603 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	49.7	Xtrriage
Anisotropy	0.308	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 58.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	14739	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 29.05 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.6582e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG

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	0.86	1/3544 (0.0%)	1.24	7/4826 (0.1%)
1	E	0.84	0/3544	1.26	14/4826 (0.3%)
2	G	0.80	0/1691	0.96	0/2309
2	J	0.86	0/1691	0.97	0/2309
3	K	0.83	0/1742	1.02	0/2367
3	L	0.87	0/1730	1.03	2/2353 (0.1%)
All	All	0.84	1/13942 (0.0%)	1.13	23/18990 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	403	MET	SD-CE	-14.03	1.44	1.79

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	612	PRO	CA-C-N	7.79	135.72	121.70
1	E	612	PRO	C-N-CA	7.79	135.72	121.70
1	A	627	ASN	CA-CB-CG	7.26	119.86	112.60
1	E	627	ASN	CA-CB-CG	7.22	119.82	112.60
1	E	439	CYS	N-CA-C	6.95	118.93	111.36
1	E	587	THR	CB-CA-C	6.71	120.49	111.70
1	A	439	CYS	N-CA-C	6.61	118.56	111.36
1	A	587	THR	CB-CA-C	6.54	120.27	111.70
1	A	275	VAL	N-CA-CB	6.24	119.94	110.58
1	E	275	VAL	N-CA-CB	6.18	119.85	110.58
1	E	611	ASN	CA-CB-CG	6.06	118.66	112.60
1	A	561	ALA	CA-C-N	5.70	131.96	121.70
1	A	561	ALA	C-N-CA	5.70	131.96	121.70
1	E	561	ALA	CA-C-N	5.62	131.82	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	561	ALA	C-N-CA	5.62	131.82	121.70
3	L	106	ILE	CB-CA-C	5.35	118.12	110.84
1	E	284	ALA	CA-C-N	5.13	127.40	120.38
1	E	284	ALA	C-N-CA	5.13	127.40	120.38
1	E	431	SER	CA-C-N	5.12	127.40	120.38
1	E	431	SER	C-N-CA	5.12	127.40	120.38
3	L	197	THR	CB-CA-C	5.09	118.53	110.19
1	A	611	ASN	CA-CB-CG	5.08	117.68	112.60
1	E	237	VAL	N-CA-CB	5.00	117.34	110.54

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	3475	0	3463	18	0
1	E	3475	0	3463	18	0
2	G	1648	0	1601	3	0
2	J	1648	0	1601	4	0
3	K	1698	0	1624	6	0
3	L	1689	0	1611	6	0
4	B	28	0	25	0	0
4	C	28	0	25	0	0
4	D	28	0	25	0	0
4	F	28	0	25	0	0
4	H	28	0	25	0	0
5	E	14	0	13	1	0
6	A	133	0	0	0	0
6	E	160	0	0	1	0
6	G	141	0	0	0	0
6	J	180	0	0	1	0
6	K	173	0	0	1	0
6	L	165	0	0	0	0
All	All	14739	0	13501	51	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (51) 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:E:612:PRO:HB2	1:E:613:THR:HB	1.45	0.95
2:G:156:SER:H	2:G:196:ASN:HD21	1.30	0.77
1:A:337:GLN:HG2	3:L:56:SER:HB2	1.74	0.70
2:J:156:SER:H	2:J:196:ASN:HD21	1.40	0.69
3:L:150:ILE:HD11	3:L:179:LEU:HD21	1.81	0.61
1:A:362:ALA:HB1	1:A:403:MET:HE1	1.85	0.57
1:A:251:HIS:CD2	1:A:432:LEU:H	2.22	0.57
1:E:296:LEU:HD23	1:E:336:ASP:HB3	1.86	0.56
1:A:296:LEU:HD23	1:A:336:ASP:HB3	1.86	0.56
1:E:612:PRO:HB2	1:E:613:THR:CB	2.29	0.56
1:E:394:ARG:HG3	1:E:504:PRO:HB2	1.88	0.56
1:E:337:GLN:HG2	3:K:56:SER:HB2	1.86	0.55
1:A:337:GLN:CG	3:L:56:SER:HB2	2.37	0.55
1:A:394:ARG:HG3	1:A:504:PRO:HB2	1.89	0.55
2:J:148:GLU:OE2	6:J:1201:HOH:O	2.18	0.55
3:K:150:ILE:HD11	3:K:179:LEU:HD21	1.90	0.54
1:A:184:VAL:HG11	1:A:233:VAL:HG11	1.89	0.54
1:A:436:LEU:HG	1:A:460:ALA:HB2	1.89	0.54
1:E:251:HIS:CD2	1:E:432:LEU:H	2.25	0.53
1:A:517:ARG:HA	1:A:536:VAL:HG11	1.92	0.52
1:E:517:ARG:HA	1:E:536:VAL:HG11	1.92	0.52
1:A:625:PHE:C	1:A:627:ASN:H	2.18	0.51
1:E:170:LEU:HD23	1:E:186:ILE:HD12	1.95	0.49
1:E:511:PHE:CD1	1:E:537:LEU:HD21	2.47	0.49
1:A:511:PHE:CD1	1:A:537:LEU:HD21	2.47	0.48
1:A:405:THR:HG22	1:A:407:GLU:H	1.77	0.48
1:E:402:ALA:HA	1:E:587:THR:HG22	1.96	0.48
1:E:405:THR:HG22	1:E:407:GLU:H	1.78	0.47
3:L:141:PRO:O	3:L:198:HIS:HE1	1.98	0.47
3:K:113:PRO:HG3	3:K:144:ILE:HD11	1.95	0.47
2:J:156:SER:H	2:J:196:ASN:ND2	2.09	0.47
1:A:170:LEU:HD23	1:A:186:ILE:HD12	1.97	0.46
1:A:402:ALA:HA	1:A:587:THR:HG22	1.98	0.46
3:L:40:PRO:HG2	3:L:165:ASP:CG	2.40	0.46
1:E:625:PHE:C	1:E:627:ASN:H	2.24	0.46
2:J:38:LYS:HB2	2:J:48:ILE:HD11	1.98	0.46
1:E:184:VAL:HG11	1:E:233:VAL:HG11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:315:CYS:HB3	6:E:1272:HOH:O	2.17	0.44
2:G:38:LYS:HB2	2:G:48:ILE:HD11	1.99	0.44
1:A:372:PHE:CZ	1:A:403:MET:HE2	2.53	0.44
3:L:198:HIS:HD2	3:L:200:THR:OG1	2.00	0.44
3:K:198:HIS:HD2	3:K:200:THR:OG1	2.01	0.43
1:A:494:GLU:HB3	1:A:542:ASN:HD21	1.84	0.42
1:E:337:GLN:CG	3:K:56:SER:HB2	2.49	0.42
2:G:115:LYS:HE2	6:K:318:HOH:O	2.18	0.42
1:A:292:ALA:O	1:A:330:VAL:HG11	2.19	0.42
1:E:494:GLU:HB3	1:E:542:ASN:HD21	1.85	0.42
3:K:36:TYR:HE2	3:K:89:GLN:HE21	1.68	0.42
1:E:599:LEU:HD12	1:E:611:ASN:HB2	2.02	0.41
1:E:625:PHE:CD1	5:E:1103:NAG:H61	2.56	0.40
1:A:511:PHE:HD1	1:A:537:LEU:HD21	1.87	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	452/572 (79%)	434 (96%)	17 (4%)	1 (0%)	43	37
1	E	452/572 (79%)	433 (96%)	15 (3%)	4 (1%)	14	7
2	G	212/261 (81%)	206 (97%)	6 (3%)	0	100	100
2	J	212/261 (81%)	207 (98%)	5 (2%)	0	100	100
3	K	217/220 (99%)	213 (98%)	4 (2%)	0	100	100
3	L	216/220 (98%)	209 (97%)	7 (3%)	0	100	100
All	All	1761/2106 (84%)	1702 (97%)	54 (3%)	5 (0%)	36	30

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	627	ASN
1	A	561	ALA
1	E	561	ALA
1	E	614	LEU
1	E	612	PRO

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	347/423 (82%)	336 (97%)	11 (3%)	34	29
1	E	347/423 (82%)	335 (96%)	12 (4%)	32	27
2	G	189/222 (85%)	188 (100%)	1 (0%)	81	85
2	J	189/222 (85%)	186 (98%)	3 (2%)	55	56
3	K	192/193 (100%)	191 (100%)	1 (0%)	81	85
3	L	191/193 (99%)	188 (98%)	3 (2%)	55	56
All	All	1455/1676 (87%)	1424 (98%)	31 (2%)	47	46

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	230	MET
1	A	275	VAL
1	A	351	ARG
1	A	432	LEU
1	A	436	LEU
1	A	453	LEU
1	A	553	MET
1	A	559	LEU
1	A	562	THR
1	A	587	THR
1	A	591	GLU
1	E	230	MET
1	E	237	VAL
1	E	275	VAL

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Mol	Chain	Res	Type
1	E	351	ARG
1	E	367	VAL
1	E	432	LEU
1	E	453	LEU
1	E	553	MET
1	E	559	LEU
1	E	562	THR
1	E	587	THR
1	E	591	GLU
2	G	196	ASN
2	J	43	ARG
2	J	173	ASP
2	J	196	ASN
3	K	202	THR
3	L	106	ILE
3	L	202	THR
3	L	214	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	246	GLN
1	A	251	HIS
1	A	260	GLN
1	A	542	ASN
1	A	557	GLN
1	A	615	HIS
1	E	246	GLN
1	E	251	HIS
1	E	260	GLN
1	E	337	GLN
1	E	542	ASN
1	E	557	GLN
1	E	611	ASN
2	G	39	GLN
2	G	105	GLN
2	G	196	ASN
2	J	196	ASN
3	K	89	GLN
3	K	190	ASN
3	K	198	HIS
3	K	210	ASN

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Mol	Chain	Res	Type
3	K	212	ASN
3	L	38	GLN
3	L	89	GLN
3	L	190	ASN
3	L	198	HIS
3	L	212	ASN

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 ⓘ

10 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
4	NAG	B	1	1,4	14,14,15	1.41	2 (14%)	17,19,21	1.61	3 (17%)
4	NAG	B	2	4	14,14,15	1.44	2 (14%)	17,19,21	1.23	2 (11%)
4	NAG	C	1	1,4	14,14,15	1.59	1 (7%)	17,19,21	1.72	4 (23%)
4	NAG	C	2	4	14,14,15	1.54	2 (14%)	17,19,21	1.46	2 (11%)
4	NAG	D	1	1,4	14,14,15	1.34	3 (21%)	17,19,21	1.57	3 (17%)
4	NAG	D	2	4	14,14,15	1.45	2 (14%)	17,19,21	1.11	2 (11%)
4	NAG	F	1	2,4	14,14,15	2.01	3 (21%)	17,19,21	2.35	6 (35%)
4	NAG	F	2	4	14,14,15	2.08	2 (14%)	17,19,21	2.16	4 (23%)
4	NAG	H	1	2,4	14,14,15	1.99	5 (35%)	17,19,21	2.41	6 (35%)
4	NAG	H	2	4	14,14,15	2.14	4 (28%)	17,19,21	2.01	4 (23%)

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
4	NAG	B	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	2	4	-	1/6/23/26	0/1/1/1
4	NAG	C	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	C	2	4	-	1/6/23/26	0/1/1/1
4	NAG	D	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	1/6/23/26	0/1/1/1
4	NAG	F	1	2,4	-	2/6/23/26	0/1/1/1
4	NAG	F	2	4	-	2/6/23/26	0/1/1/1
4	NAG	H	1	2,4	-	2/6/23/26	0/1/1/1
4	NAG	H	2	4	-	2/6/23/26	0/1/1/1

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	2	NAG	C1-C2	5.86	1.60	1.52
4	H	2	NAG	C1-C2	5.82	1.60	1.52
4	F	1	NAG	C1-C2	4.81	1.58	1.52
4	H	1	NAG	C1-C2	4.45	1.58	1.52
4	C	2	NAG	C1-C2	4.15	1.58	1.52
4	C	1	NAG	C1-C2	4.08	1.57	1.52
4	D	2	NAG	C1-C2	3.40	1.57	1.52
4	B	2	NAG	C1-C2	3.13	1.56	1.52
4	F	1	NAG	C4-C5	2.96	1.59	1.53
4	H	2	NAG	C2-N2	2.81	1.50	1.46
4	H	1	NAG	C4-C5	2.78	1.58	1.53
4	B	1	NAG	C1-C2	2.72	1.56	1.52
4	H	2	NAG	C3-C2	2.55	1.57	1.52
4	F	2	NAG	C3-C2	2.53	1.57	1.52
4	B	1	NAG	C3-C2	2.45	1.57	1.52
4	D	2	NAG	C3-C2	2.40	1.57	1.52
4	D	1	NAG	C1-C2	2.29	1.55	1.52
4	D	1	NAG	C3-C2	2.24	1.57	1.52
4	B	2	NAG	C3-C2	2.21	1.57	1.52
4	D	1	NAG	O5-C1	2.21	1.47	1.43
4	H	1	NAG	O5-C5	2.15	1.47	1.43
4	H	1	NAG	C2-N2	2.08	1.49	1.46
4	C	2	NAG	C3-C2	2.08	1.56	1.52
4	F	1	NAG	O5-C5	2.07	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	1	NAG	O4-C4	2.06	1.48	1.43
4	H	2	NAG	C4-C3	2.00	1.57	1.52

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	2	NAG	C1-C2-N2	5.51	119.12	110.43
4	F	2	NAG	C4-C3-C2	5.35	118.86	111.02
4	H	2	NAG	C4-C3-C2	5.14	118.55	111.02
4	H	2	NAG	C1-C2-N2	4.68	117.81	110.43
4	H	1	NAG	C1-O5-C5	4.60	118.35	112.19
4	H	1	NAG	C2-N2-C7	4.38	128.77	122.90
4	H	1	NAG	O4-C4-C3	-4.37	100.07	110.38
4	C	2	NAG	C1-C2-N2	4.36	117.31	110.43
4	F	1	NAG	O4-C4-C3	-4.35	100.13	110.38
4	F	1	NAG	C1-O5-C5	4.29	117.94	112.19
4	B	1	NAG	C1-O5-C5	4.12	117.71	112.19
4	C	1	NAG	C1-O5-C5	4.12	117.70	112.19
4	D	1	NAG	C1-O5-C5	3.95	117.47	112.19
4	F	1	NAG	C4-C3-C2	3.71	116.46	111.02
4	F	1	NAG	C2-N2-C7	3.50	127.59	122.90
4	H	1	NAG	C4-C3-C2	3.22	115.73	111.02
4	F	1	NAG	C1-C2-N2	2.98	115.13	110.43
4	B	1	NAG	C1-C2-N2	2.96	115.10	110.43
4	D	1	NAG	C1-C2-N2	2.94	115.07	110.43
4	F	1	NAG	O4-C4-C5	2.89	116.44	109.32
4	H	1	NAG	C1-C2-N2	2.83	114.89	110.43
4	C	2	NAG	C1-O5-C5	2.73	115.85	112.19
4	C	1	NAG	O4-C4-C3	2.52	116.31	110.38
4	H	2	NAG	C2-N2-C7	2.50	126.25	122.90
4	F	2	NAG	C2-N2-C7	2.47	126.21	122.90
4	B	2	NAG	O4-C4-C5	2.37	115.17	109.32
4	H	2	NAG	O5-C1-C2	2.28	114.83	111.29
4	C	1	NAG	O5-C1-C2	2.26	114.78	111.29
4	H	1	NAG	O4-C4-C5	2.23	114.82	109.32
4	B	1	NAG	C8-C7-N2	-2.12	112.61	116.12
4	D	2	NAG	C6-C5-C4	2.12	118.21	113.02
4	C	1	NAG	C2-N2-C7	2.11	125.72	122.90
4	D	1	NAG	C8-C7-N2	-2.06	112.69	116.12
4	B	2	NAG	C6-C5-C4	2.04	118.03	113.02
4	D	2	NAG	O4-C4-C5	2.03	114.33	109.32
4	F	2	NAG	O5-C1-C2	2.02	114.42	111.29

There are no chirality outliers.

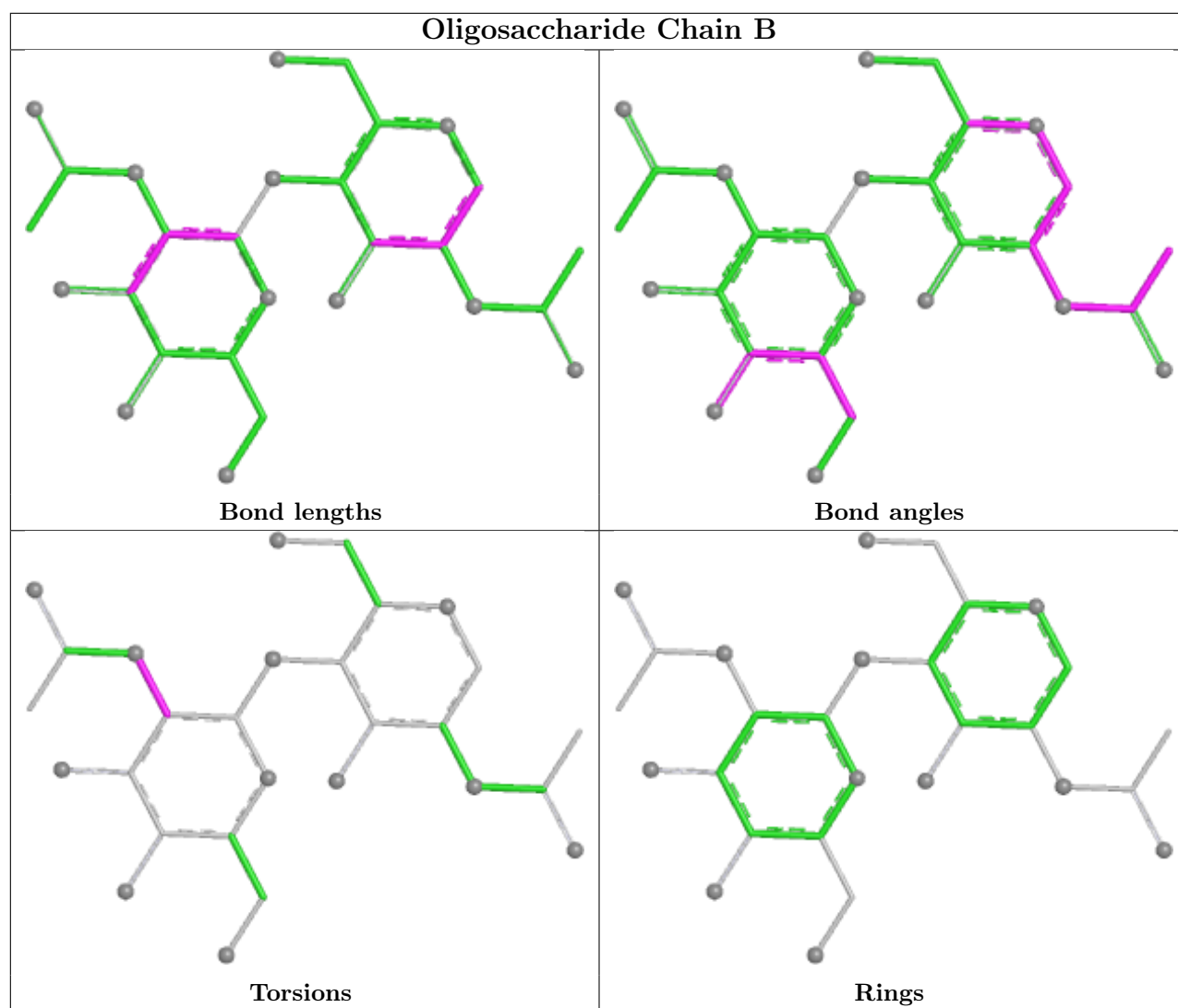
All (12) torsion outliers are listed below:

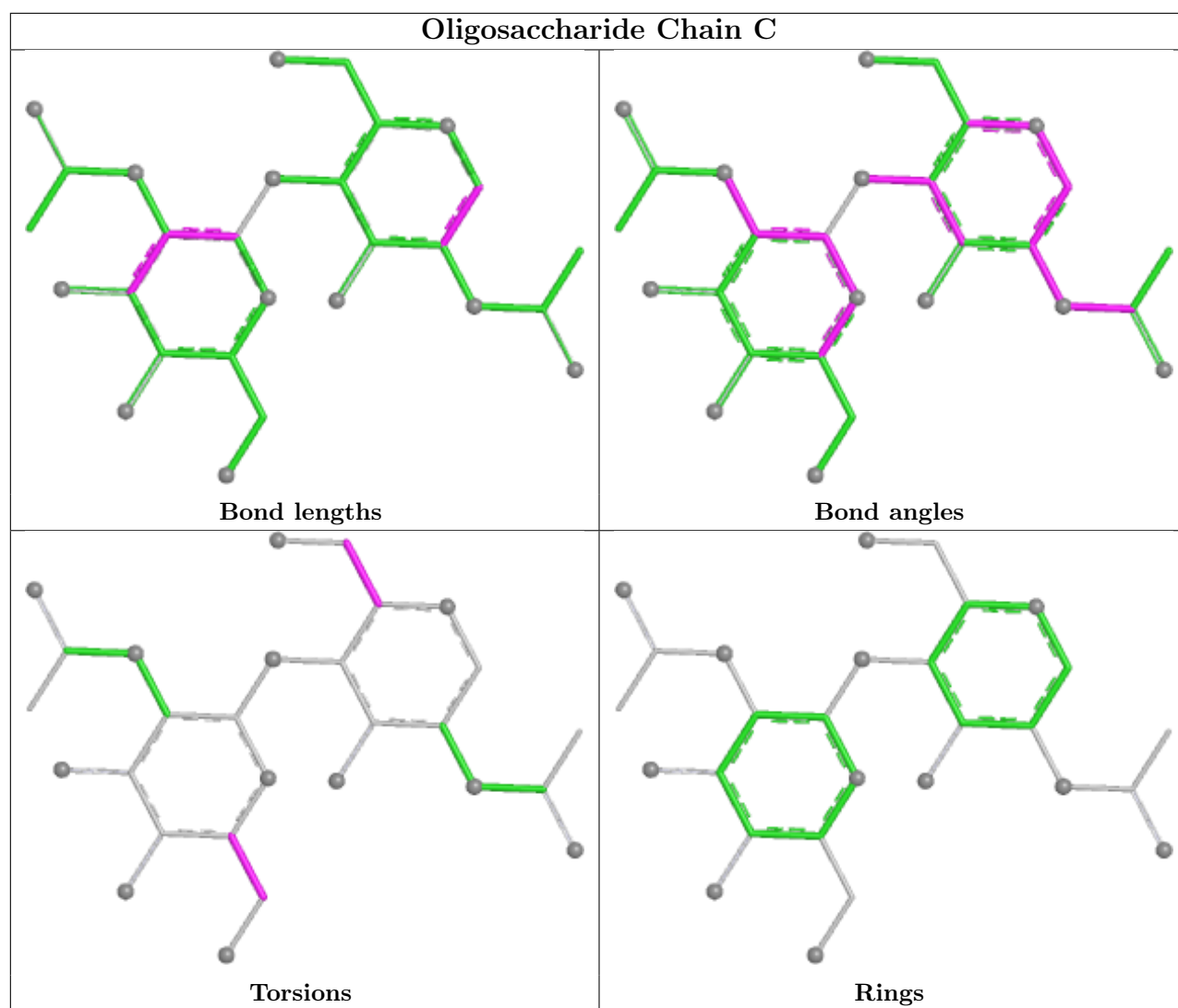
Mol	Chain	Res	Type	Atoms
4	F	2	NAG	O5-C5-C6-O6
4	H	2	NAG	O5-C5-C6-O6
4	F	2	NAG	C4-C5-C6-O6
4	H	2	NAG	C4-C5-C6-O6
4	H	1	NAG	C4-C5-C6-O6
4	F	1	NAG	C4-C5-C6-O6
4	H	1	NAG	O5-C5-C6-O6
4	F	1	NAG	O5-C5-C6-O6
4	C	1	NAG	O5-C5-C6-O6
4	C	2	NAG	O5-C5-C6-O6
4	B	2	NAG	C1-C2-N2-C7
4	D	2	NAG	C1-C2-N2-C7

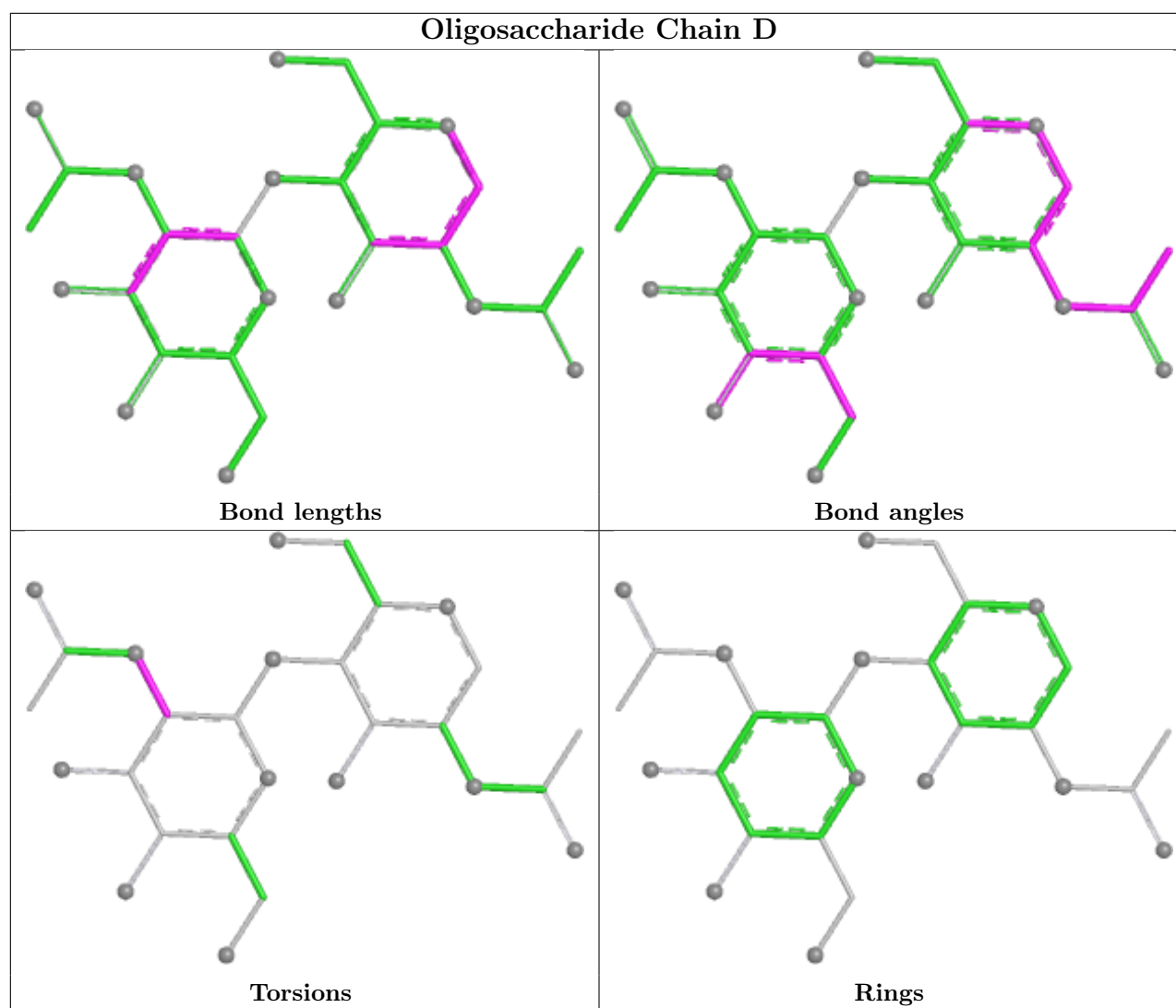
There are no ring outliers.

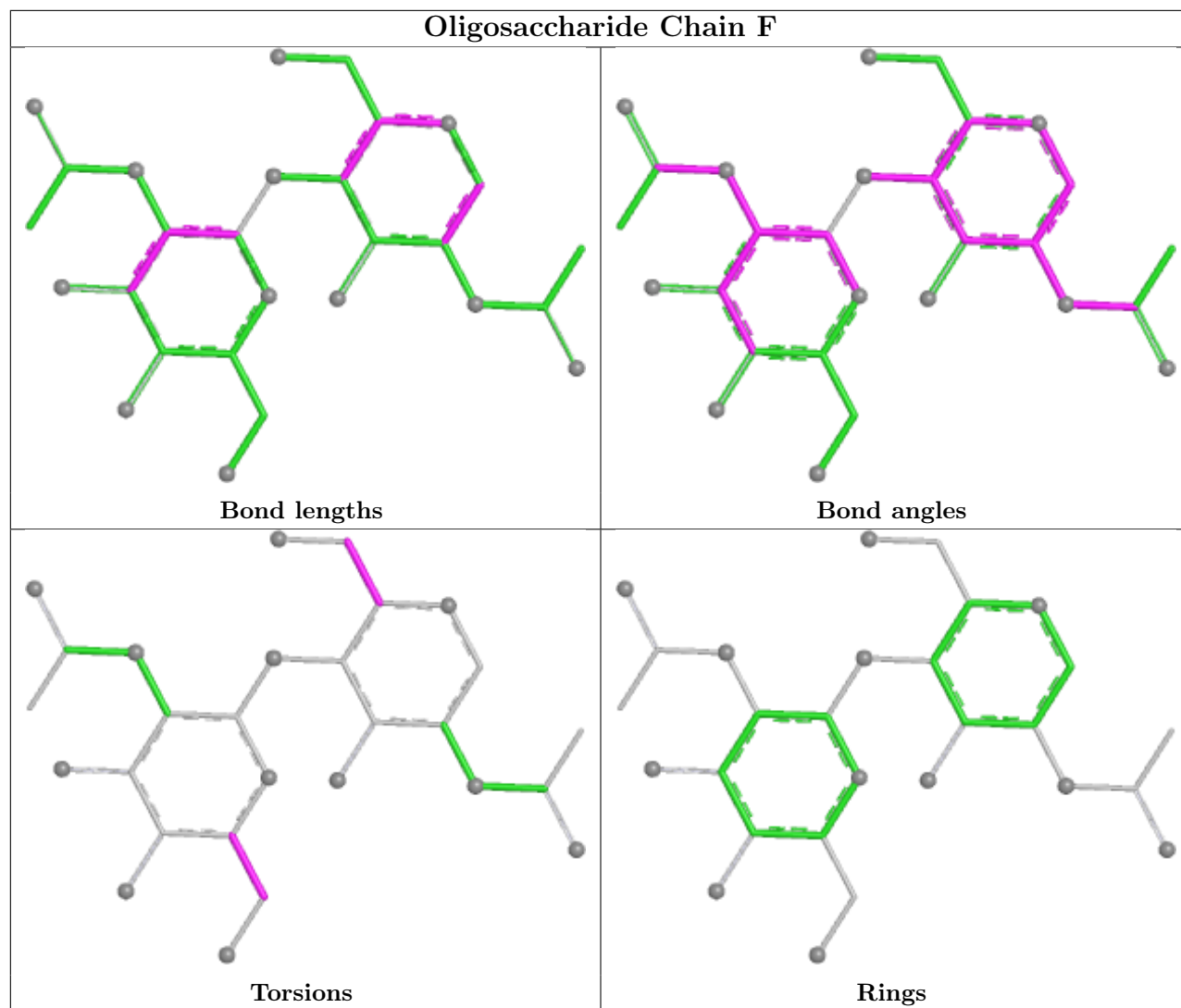
No monomer is involved in short contacts.

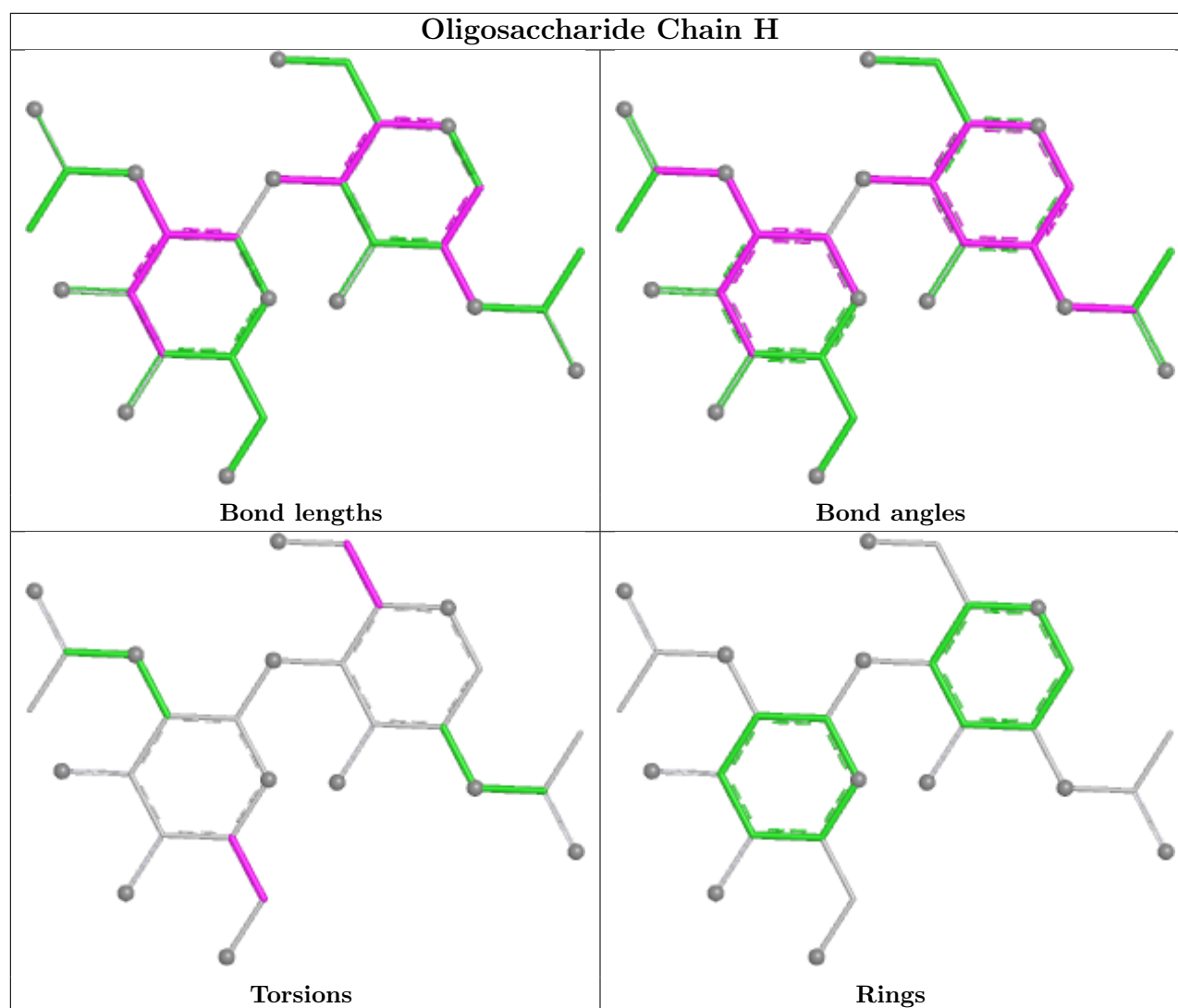
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	NAG	E	1103	1	14,14,15	1.53	2 (14%)	17,19,21	1.22	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	E	1103	1	-	1/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	1103	NAG	C1-C2	2.54	1.55	1.52
5	E	1103	NAG	O5-C5	2.47	1.48	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	1103	NAG	C1-C2-N2	3.73	116.31	110.43

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	1103	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	1103	NAG	1	0

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	464/572 (81%)	0.79	65 (14%) 6 5	47, 72, 135, 168	0
1	E	464/572 (81%)	0.72	62 (13%) 7 6	45, 70, 124, 160	0
2	G	216/261 (82%)	0.28	6 (2%) 55 57	43, 61, 93, 130	1 (0%)
2	J	216/261 (82%)	0.11	7 (3%) 50 50	38, 53, 88, 141	1 (0%)
3	K	218/220 (99%)	0.09	4 (1%) 67 69	41, 57, 84, 123	1 (0%)
3	L	218/220 (99%)	0.03	3 (1%) 73 75	40, 54, 87, 120	0
All	All	1796/2106 (85%)	0.45	147 (8%) 17 18	38, 63, 118, 168	3 (0%)

All (147) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	602	GLY	6.1
1	A	453	LEU	6.1
2	J	129	GLY	5.7
1	E	602	GLY	5.3
2	J	128	CYS	5.0
1	E	608	PRO	4.7
1	E	453	LEU	4.7
1	E	505	LEU	4.7
1	E	447	LEU	4.6
1	E	559	LEU	4.6
1	A	608	PRO	4.2
1	A	218	LEU	4.2
1	E	507	GLY	4.1
1	A	447	LEU	4.1
2	G	128	CYS	4.0
1	A	633	LEU	4.0
1	E	452	THR	3.9
1	A	220	PHE	3.9
1	E	509	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
2	G	129	GLY	3.9
3	K	194	CYS	3.8
1	E	633	LEU	3.8
1	E	227	HIS	3.7
1	E	550	THR	3.7
1	E	612	PRO	3.7
1	A	611	ASN	3.7
1	E	619	VAL	3.6
1	A	521	GLY	3.6
1	E	451	ALA	3.5
1	E	521	GLY	3.5
1	A	452	THR	3.5
1	A	451	ALA	3.4
1	E	562	THR	3.3
1	A	627	ASN	3.3
1	E	522	PRO	3.3
3	L	30	TYR	3.3
1	E	610	PHE	3.3
1	E	218	LEU	3.3
1	E	520	CYS	3.2
1	A	468	GLY	3.2
1	E	197	PRO	3.2
1	A	628	GLY	3.1
1	A	612	PRO	3.1
1	A	531	ILE	3.1
1	A	540	VAL	3.1
3	K	30	TYR	3.1
1	A	291	SER	3.1
1	A	227	HIS	3.0
1	A	505	LEU	3.0
1	A	539	ILE	3.0
1	E	387	ALA	3.0
2	G	42	GLY	2.9
1	A	426	TRP	2.9
1	A	520	CYS	2.9
1	A	532	ALA	2.9
1	E	391	GLY	2.9
1	A	554	PRO	2.8
1	E	549	TYR	2.8
1	A	559	LEU	2.8
1	E	468	GLY	2.8
1	E	547	CYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	567	VAL	2.7
1	E	539	ILE	2.7
1	A	292	ALA	2.7
1	E	510	SER	2.7
1	E	541	SER	2.7
1	E	517	ARG	2.7
1	A	562	THR	2.6
1	A	197	PRO	2.6
1	A	522	PRO	2.6
1	E	506	ARG	2.6
1	A	390	PRO	2.6
1	E	551	ASP	2.6
1	A	614	LEU	2.6
3	L	214	CYS	2.5
1	A	506	ARG	2.5
1	A	509	ALA	2.5
1	A	525	THR	2.5
1	E	192	ARG	2.5
1	E	560	PRO	2.5
1	E	614	LEU	2.5
1	A	387	ALA	2.5
1	A	518	PRO	2.5
1	E	426	TRP	2.5
1	E	540	VAL	2.4
1	E	223	ASP	2.4
1	E	432	LEU	2.4
2	G	43	ARG	2.4
1	A	192	ARG	2.4
1	A	327	ALA	2.4
1	E	320	ALA	2.4
1	E	601	ALA	2.4
1	A	542	ASN	2.4
1	A	598	GLN	2.4
2	J	132	THR	2.4
1	A	225	ALA	2.3
1	E	561	ALA	2.3
1	A	224	GLY	2.3
1	E	388	GLY	2.3
2	J	127	VAL	2.3
1	A	601	ALA	2.3
1	A	517	ARG	2.3
1	E	390	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	561	ALA	2.3
3	K	156	GLN	2.3
1	A	630	VAL	2.3
1	A	631	VAL	2.3
1	E	630	VAL	2.3
1	A	550	THR	2.3
2	G	41	PRO	2.3
3	L	126	THR	2.3
1	E	131	GLY	2.3
1	E	628	GLY	2.3
1	A	294	ALA	2.2
1	A	320	ALA	2.2
3	K	214	CYS	2.2
1	E	609	SER	2.2
1	E	417	ARG	2.2
1	E	569	VAL	2.2
1	A	572	ASP	2.2
1	E	403	MET	2.2
1	E	627	ASN	2.2
1	A	138	THR	2.2
1	A	553	MET	2.2
1	A	565	PRO	2.2
1	E	525	THR	2.2
2	J	41	PRO	2.1
1	A	388	GLY	2.1
1	E	220	PHE	2.1
1	E	531	ILE	2.1
1	E	291	SER	2.1
1	E	542	ASN	2.1
1	A	570	TYR	2.1
1	A	137	THR	2.1
2	G	132	THR	2.1
1	A	599	LEU	2.1
2	J	138	LEU	2.1
2	J	159	LEU	2.1
1	A	549	TYR	2.1
1	A	567	VAL	2.1
1	E	225	ALA	2.1
1	E	572	ASP	2.0
1	A	610	PHE	2.0
1	A	619	VAL	2.0
1	A	193	MET	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	454	ALA	2.0
1	E	548	ASP	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](#)

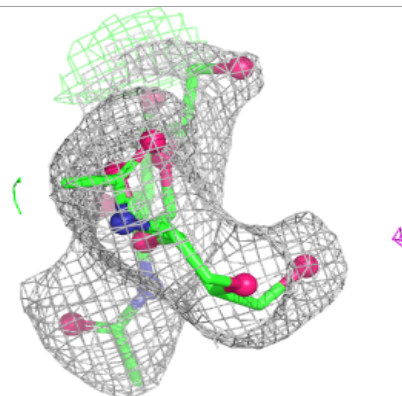
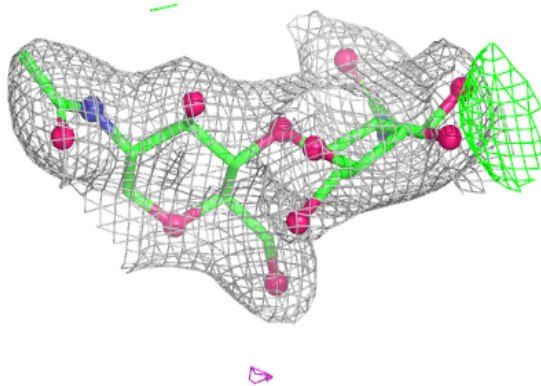
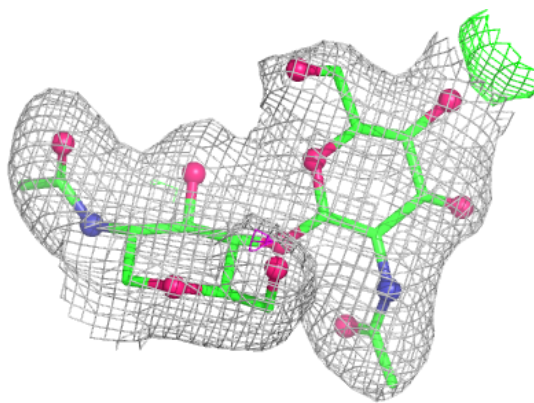
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	B	1	14/15	-	-	66,71,75,75	0
4	NAG	B	2	14/15	-	-	77,82,85,88	0
4	NAG	C	1	14/15	-	-	169,172,179,183	0
4	NAG	C	2	14/15	-	-	179,183,189,192	0
4	NAG	D	1	14/15	-	-	72,77,81,81	0
4	NAG	D	2	14/15	-	-	81,86,90,92	0
4	NAG	F	1	14/15	-	-	98,104,108,108	0
4	NAG	F	2	14/15	-	-	112,117,123,123	0
4	NAG	H	1	14/15	0.72	0.17	86,91,95,97	0
4	NAG	H	2	14/15	0.76	0.13	102,108,112,112	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.

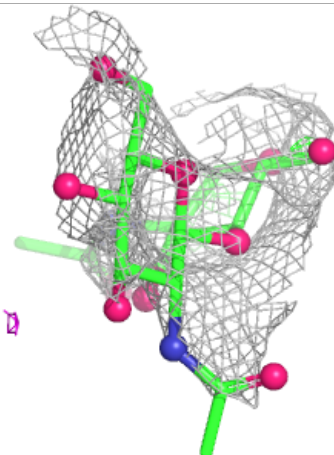
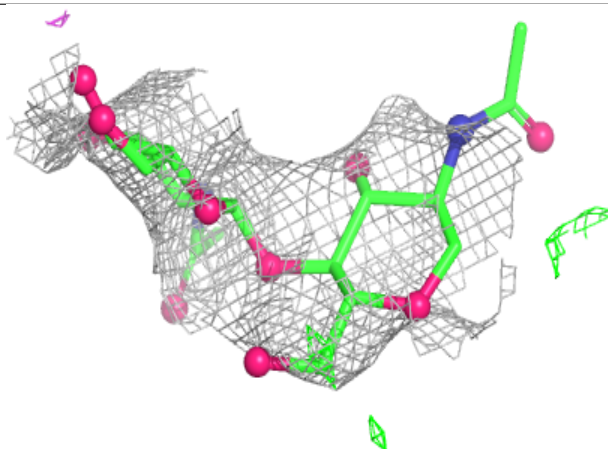
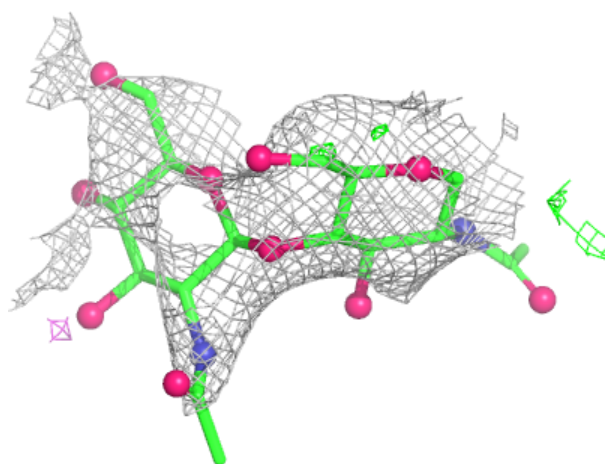
Electron density around Chain B:

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



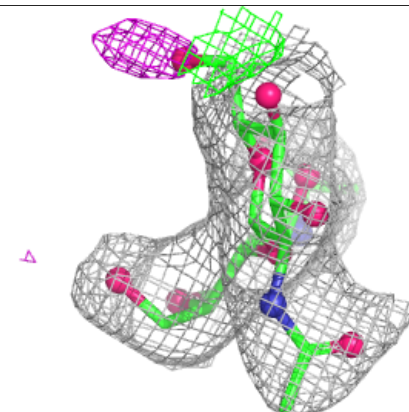
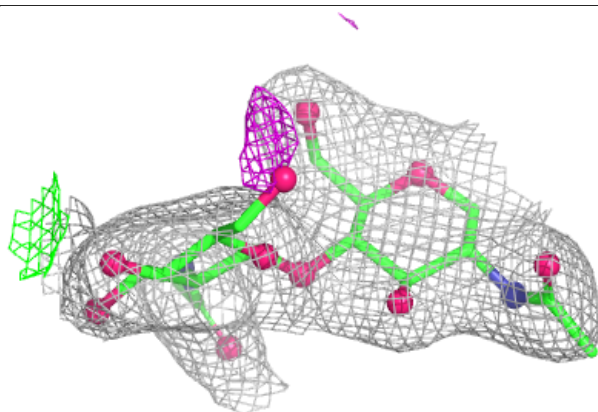
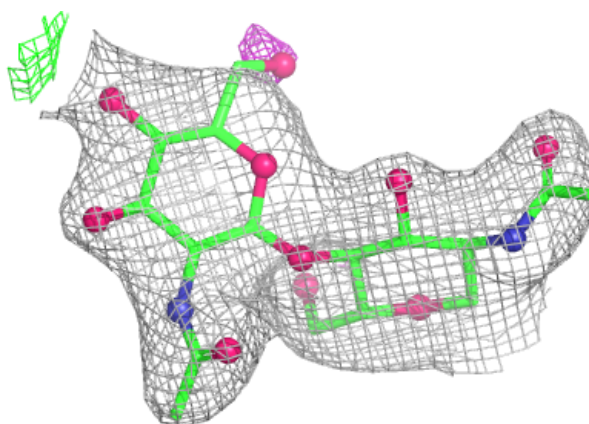
Electron density around Chain C:

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

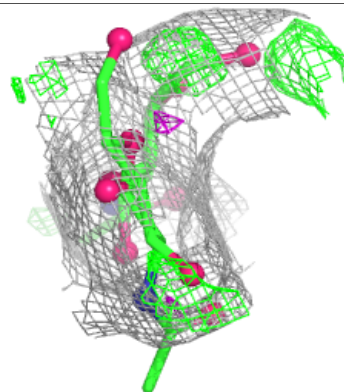
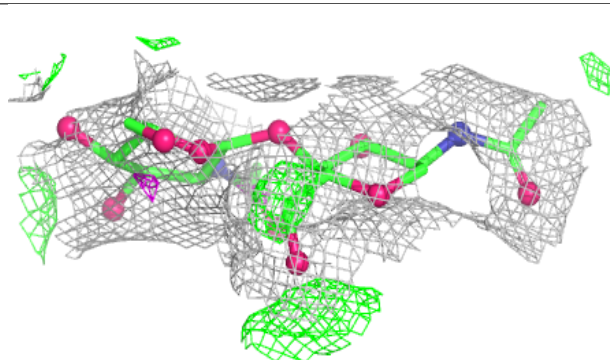
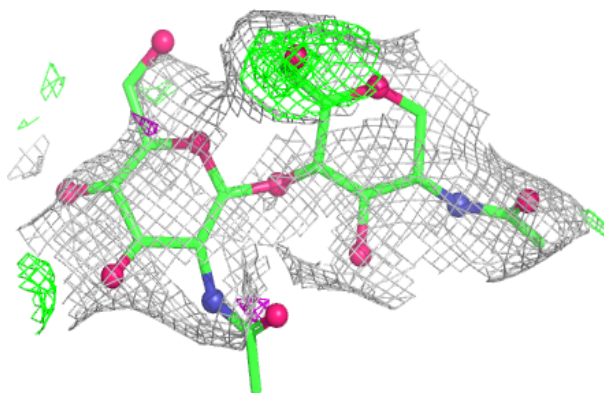


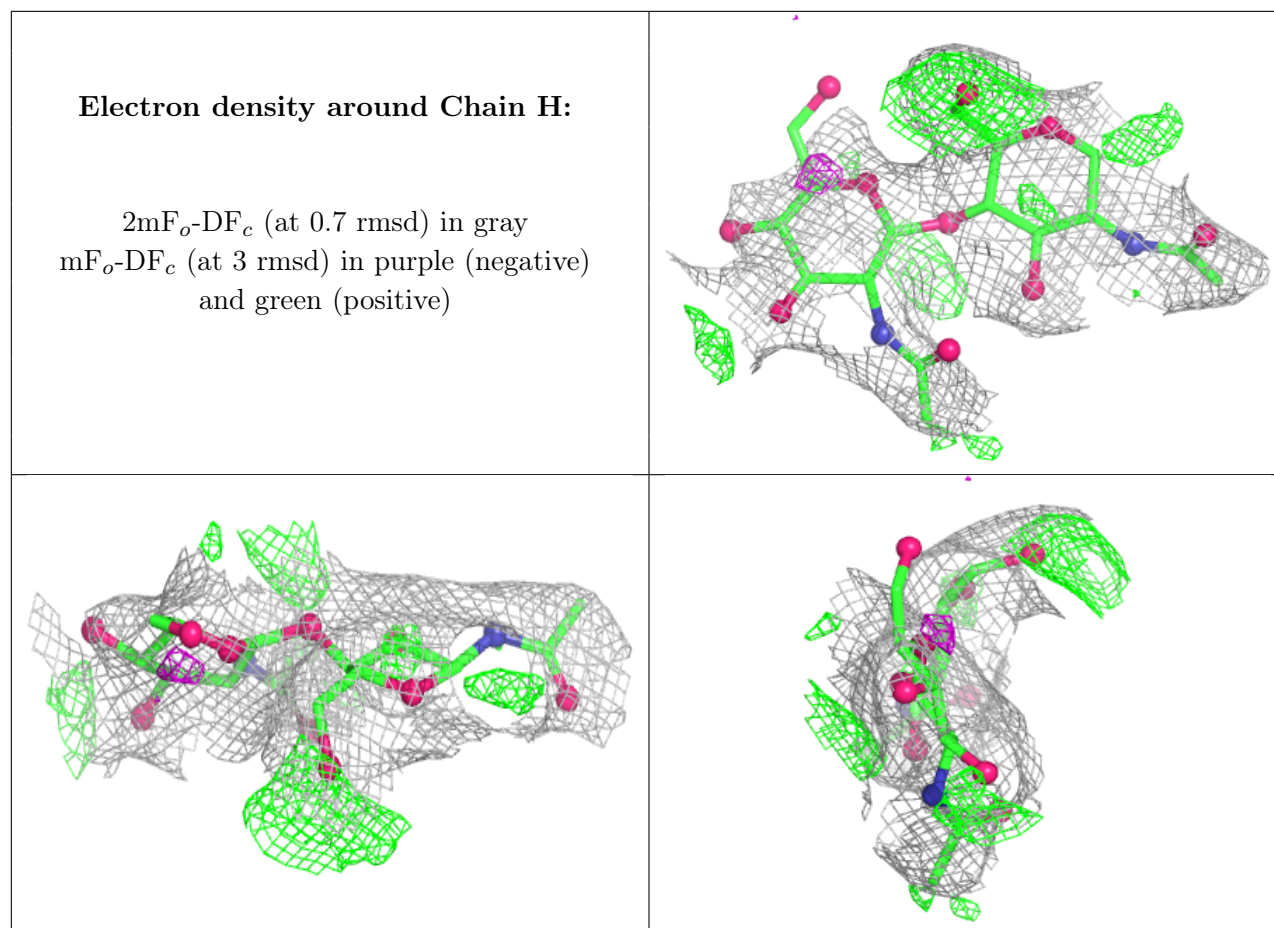
Electron density around Chain D:

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

**Electron density around Chain F:**

$2mF_o-DF_c$ (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
5	NAG	E	1103	14/15	0.65	0.15	128,133,140,141	0

6.5 Other polymers [i](#)

There are no such residues in this entry.