Full wwPDB X-ray Structure Validation Report (i)

Jun 16, 2024 – 11:07 PM EDT

PDB ID	:	2XQY
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 (i) 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 (i)) were used in the production of this report:

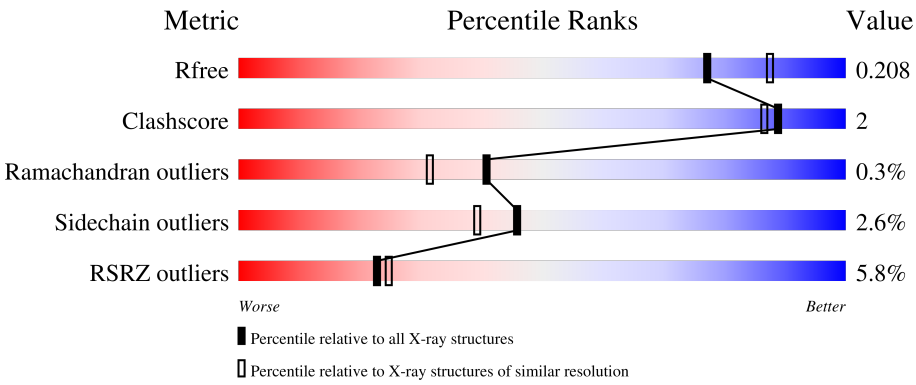
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	572	9% 74% 7% • 19%
1	E	572	6% 74% 6% • 19%
2	G	261	2% 80% • 17%
2	J	261	2% 80% • 17%
3	K	220	2% 95% • •

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Mol	Chain	Length	Quality of chain
3	L	220	2% 95% 5%
4	B	2	100%
4	C	2	100%
4	D	2	100%
4	F	2	100%
4	H	2	100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	C	1	-	-	-	X
4	NAG	C	2	-	-	-	X

2 Entry composition (i)

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
			Total	C	N	O	S			
1	A	464	3475	2195	624	637	19	0	0	0
1	E	464	3475	2195	624	637	19	0	0	0

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
			Total	C	N	O	S			
2	G	216	1648	1044	270	327	7	0	0	0
2	J	216	1648	1044	270	327	7	0	0	0

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

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

- 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
			Total	C	N	O			
4	B	2	28	16	2	10	0	0	0
4	C	2	28	16	2	10	0	0	0

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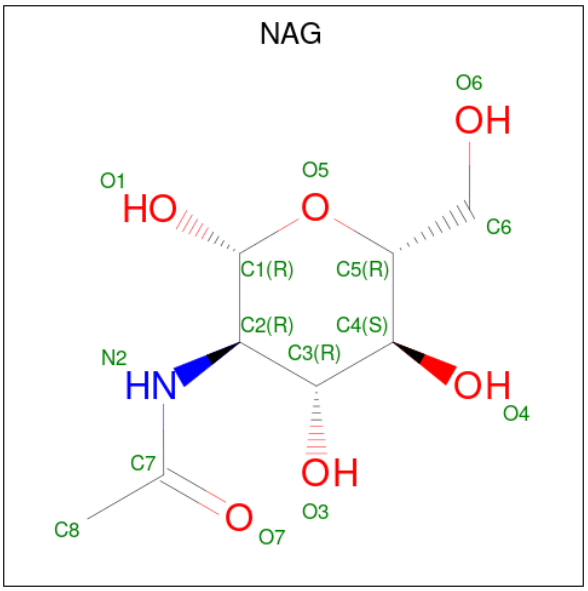
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	D	2	28	16	2	10	0	0	0
			Total	C	N	O			
4	F	2	28	16	2	10	0	0	0
			Total	C	N	O			
4	H	2	28	16	2	10	0	0	0

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



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

- Molecule 6 is water.

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

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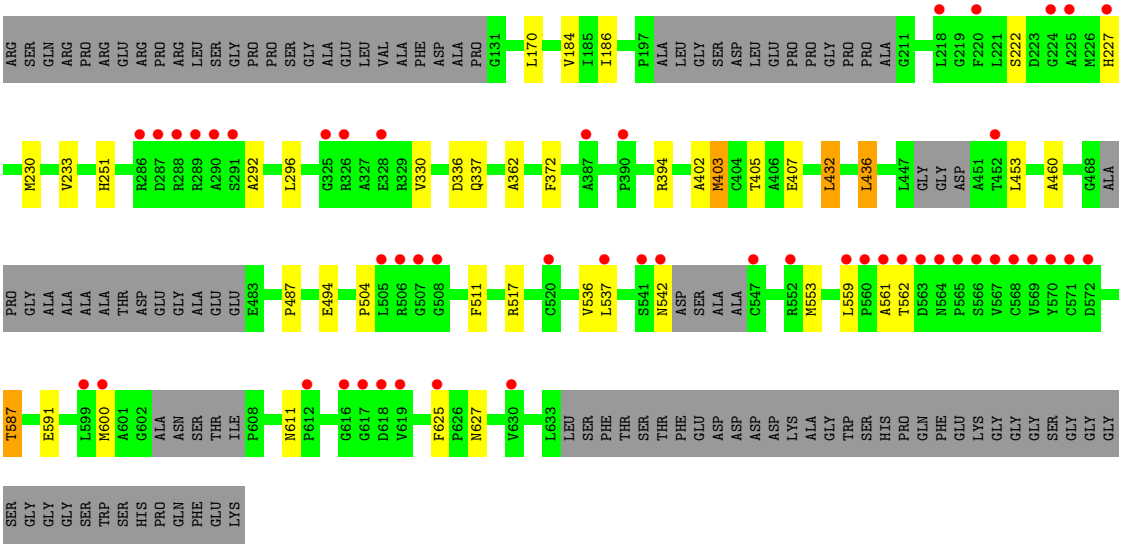
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	L	165	165	165	0	0

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.

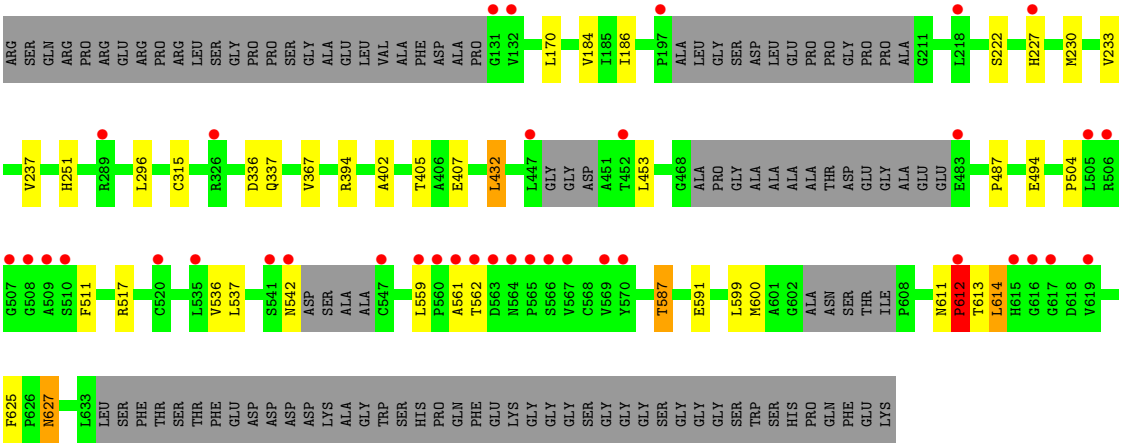
• Molecule 1: ENVELOPE GLYCOPROTEIN H

Chain A: 9% 74% 7% • 19%



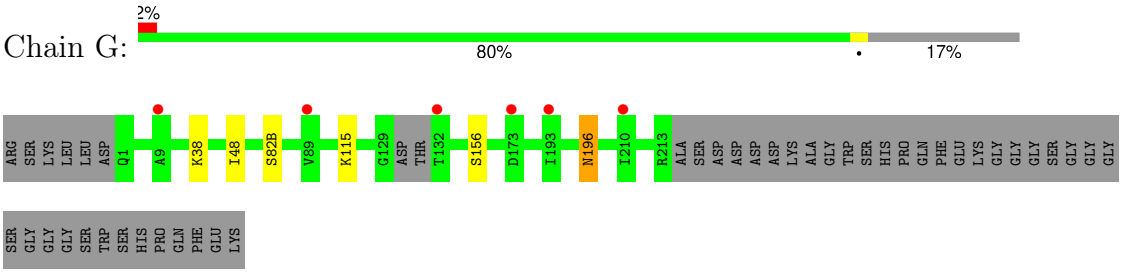
• Molecule 1: ENVELOPE GLYCOPROTEIN H

Chain E: 6% 74% 6% • 19%



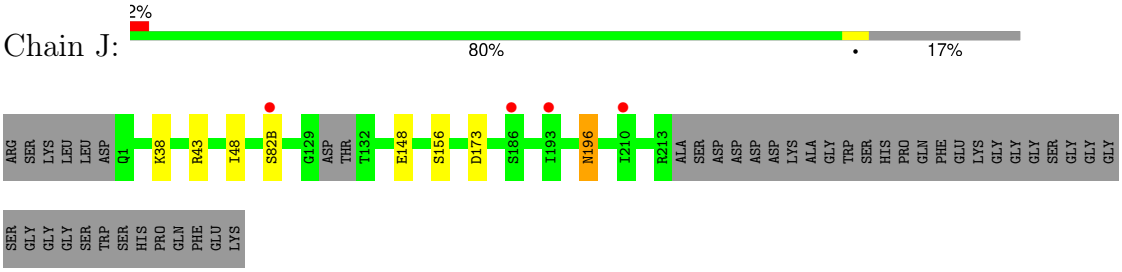
• Molecule 2: A13-D6.3 MONOCLONAL ANTIBODY

Chain G:



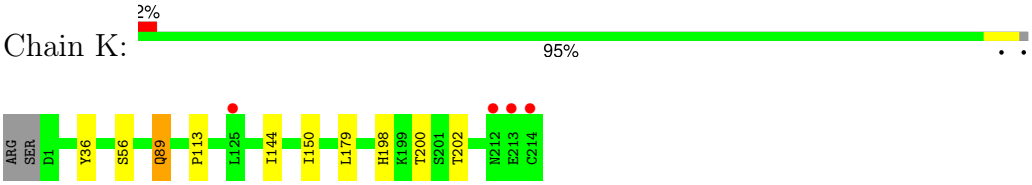
• Molecule 2: A13-D6.3 MONOCLONAL ANTIBODY

Chain J:



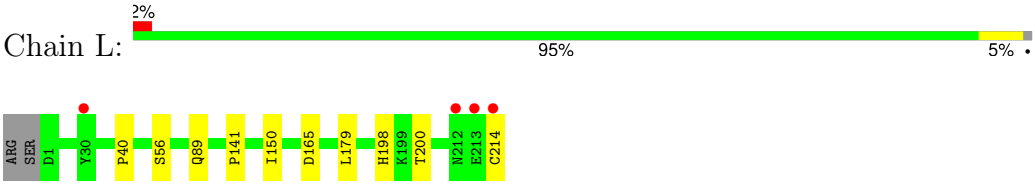
• Molecule 3: A13-D6.3 MONOCLONAL ANTIBODY

Chain K:



• Molecule 3: A13-D6.3 MONOCLONAL ANTIBODY

Chain L:

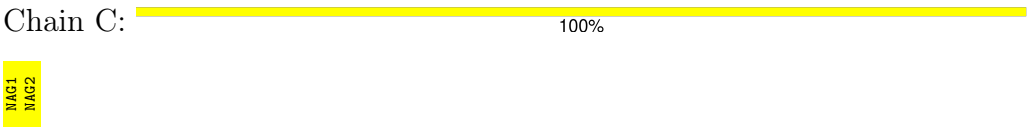


• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B:

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

Chain C:



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

Chain D: 100%

NAG1
NAG2

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

Chain F: 100%

NAG1
NAG2

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

Chain H: 100%

NAG1
NAG2

4 Data and refinement statistics (i)

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 55.64 – 2.05	Depositor EDS
% Data completeness (in resolution range)	91.8 (58.12-2.05) 92.1 (55.64-2.05)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.09 (at 2.05Å)	Xtriage
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	Xtriage
Anisotropy	0.308	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 60.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	14739	wwPDB-VP
Average B, all atoms (Å^2)	70.0	wwPDB-VP

Xtriage'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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (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	0.48	1/3544 (0.0%)	0.63	0/4826
1	E	0.48	0/3544	0.64	1/4826 (0.0%)
2	G	0.49	0/1691	0.59	0/2309
2	J	0.54	0/1691	0.60	0/2309
3	K	0.52	0/1742	0.62	0/2367
3	L	0.53	0/1730	0.62	0/2353
All	All	0.50	1/13942 (0.0%)	0.62	1/18990 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	403	MET	SD-CE	-5.96	1.44	1.77

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	612	PRO	C-N-CA	5.61	135.72	121.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:A:625:PHE:C	1:A:627:ASN:H	2.18	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
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
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
3:L:40:PRO:HG2	3:L:165:ASP:CG	2.40	0.41
1:A:372:PHE:CZ	1:A:403:MET:HE2	2.56	0.41
1:E:625:PHE:C	1:E:627:ASN:H	2.24	0.41
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:362:ALA:HB1	1:A:403:MET:HE1	2.03	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 (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	452/572 (79%)	434 (96%)	17 (4%)	1 (0%)	47	39
1	E	452/572 (79%)	433 (96%)	15 (3%)	4 (1%)	17	8
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%)	41	31

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 (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	347/423 (82%)	333 (96%)	14 (4%)	31	24
1	E	347/423 (82%)	333 (96%)	14 (4%)	31	24
2	G	189/222 (85%)	187 (99%)	2 (1%)	73	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	J	189/222 (85%)	185 (98%)	4 (2%)	53	48
3	K	192/193 (100%)	190 (99%)	2 (1%)	76	75
3	L	191/193 (99%)	189 (99%)	2 (1%)	76	75
All	All	1455/1676 (87%)	1417 (97%)	38 (3%)	46	39

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	222	SER
1	A	227	HIS
1	A	230	MET
1	A	432	LEU
1	A	436	LEU
1	A	453	LEU
1	A	487	PRO
1	A	553	MET
1	A	559	LEU
1	A	562	THR
1	A	587	THR
1	A	591	GLU
1	A	600	MET
1	A	611	ASN
1	E	222	SER
1	E	227	HIS
1	E	230	MET
1	E	237	VAL
1	E	367	VAL
1	E	432	LEU
1	E	453	LEU
1	E	487	PRO
1	E	559	LEU
1	E	562	THR
1	E	587	THR
1	E	591	GLU
1	E	600	MET
1	E	614	LEU
2	G	82(B)	SER
2	G	196	ASN
2	J	43	ARG
2	J	82(B)	SER
2	J	173	ASP

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Mol	Chain	Res	Type
2	J	196	ASN
3	K	89	GLN
3	K	202	THR
3	L	89	GLN
3	L	214	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	251	HIS
1	A	542	ASN
1	A	557	GLN
1	A	615	HIS
1	E	251	HIS
1	E	542	ASN
1	E	557	GLN
1	E	611	ASN
1	E	615	HIS
2	G	196	ASN
2	J	196	ASN
3	K	89	GLN
3	K	198	HIS
3	L	89	GLN
3	L	198	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)

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	4,1	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	4,1	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	4,1	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	4,2	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	4,2	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	4,1	-	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	4,1	-	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	4,1	-	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	4,2	-	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	4,2	-	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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
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(^{o})	Ideal(^{o})
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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:

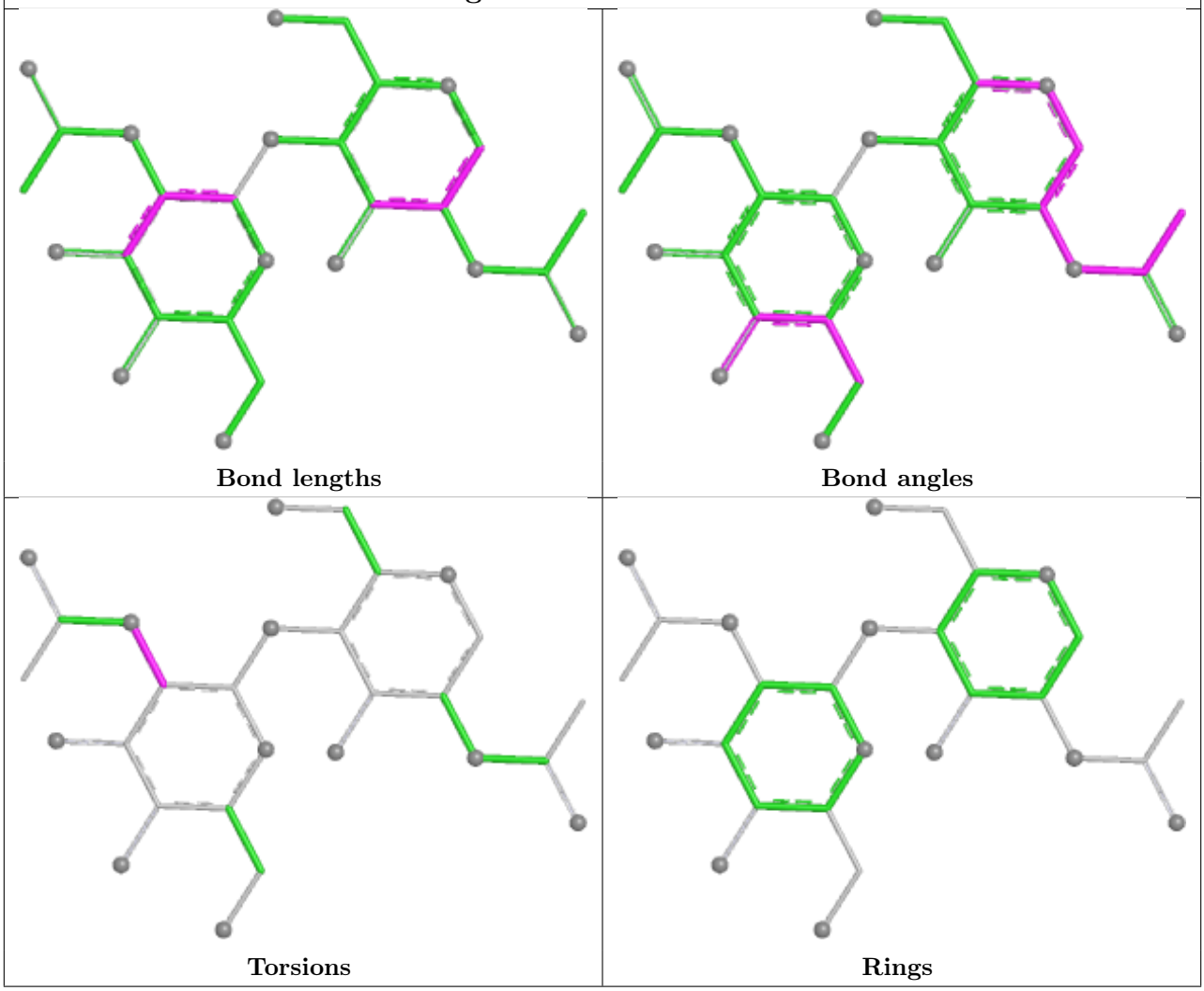
Mol	Chain	Res	Type	Atoms
4	F	2	NAG	O5-C5-C6-O6
4	H	2	NAG	O5-C5-C6-O6
4	F	2	NAG	C4-C5-C6-O6
4	H	2	NAG	C4-C5-C6-O6
4	H	1	NAG	C4-C5-C6-O6
4	F	1	NAG	C4-C5-C6-O6
4	H	1	NAG	O5-C5-C6-O6
4	F	1	NAG	O5-C5-C6-O6
4	C	1	NAG	O5-C5-C6-O6
4	C	2	NAG	O5-C5-C6-O6
4	B	2	NAG	C1-C2-N2-C7
4	D	2	NAG	C1-C2-N2-C7

There are no ring outliers.

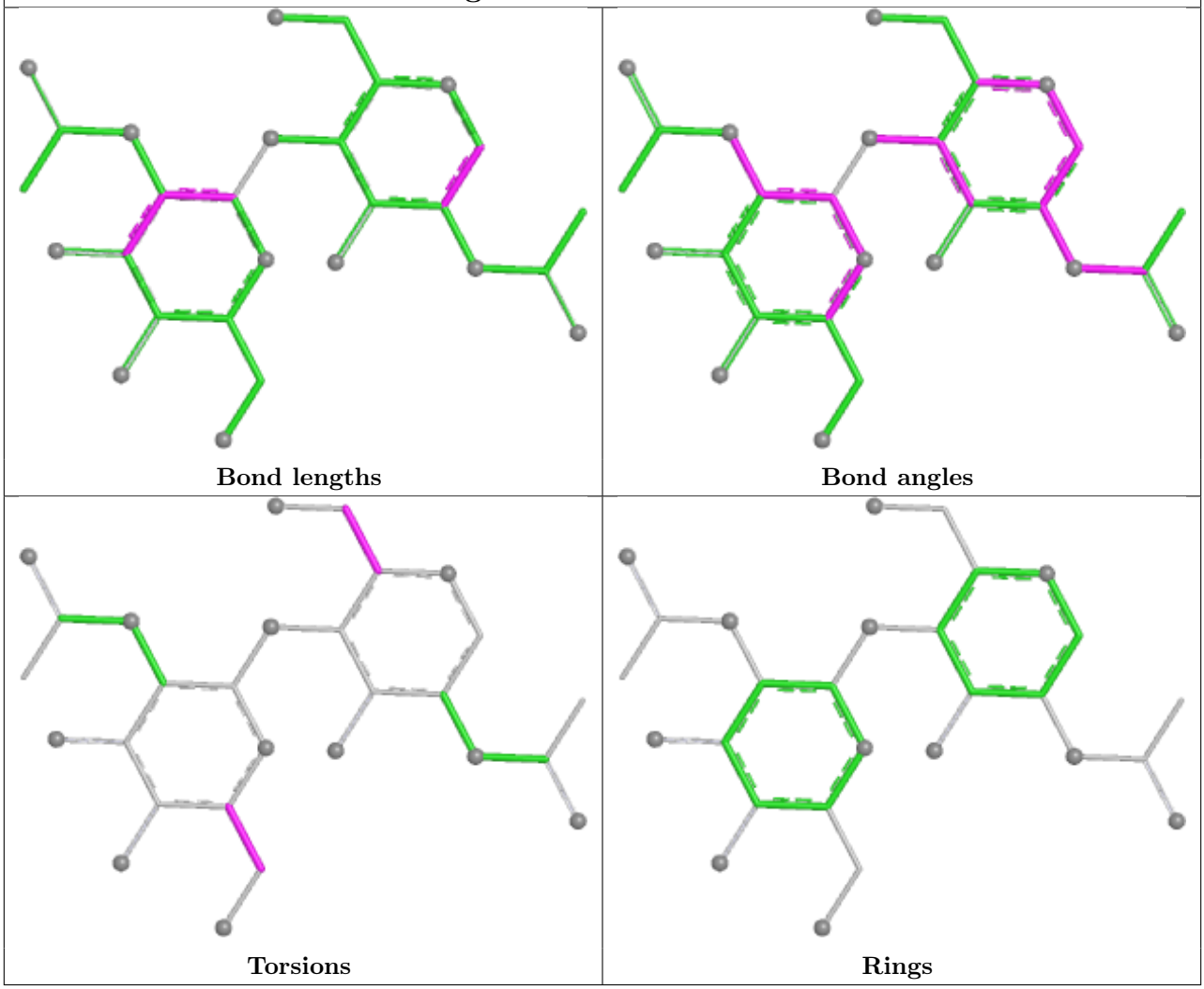
No monomer is involved in short contacts.

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

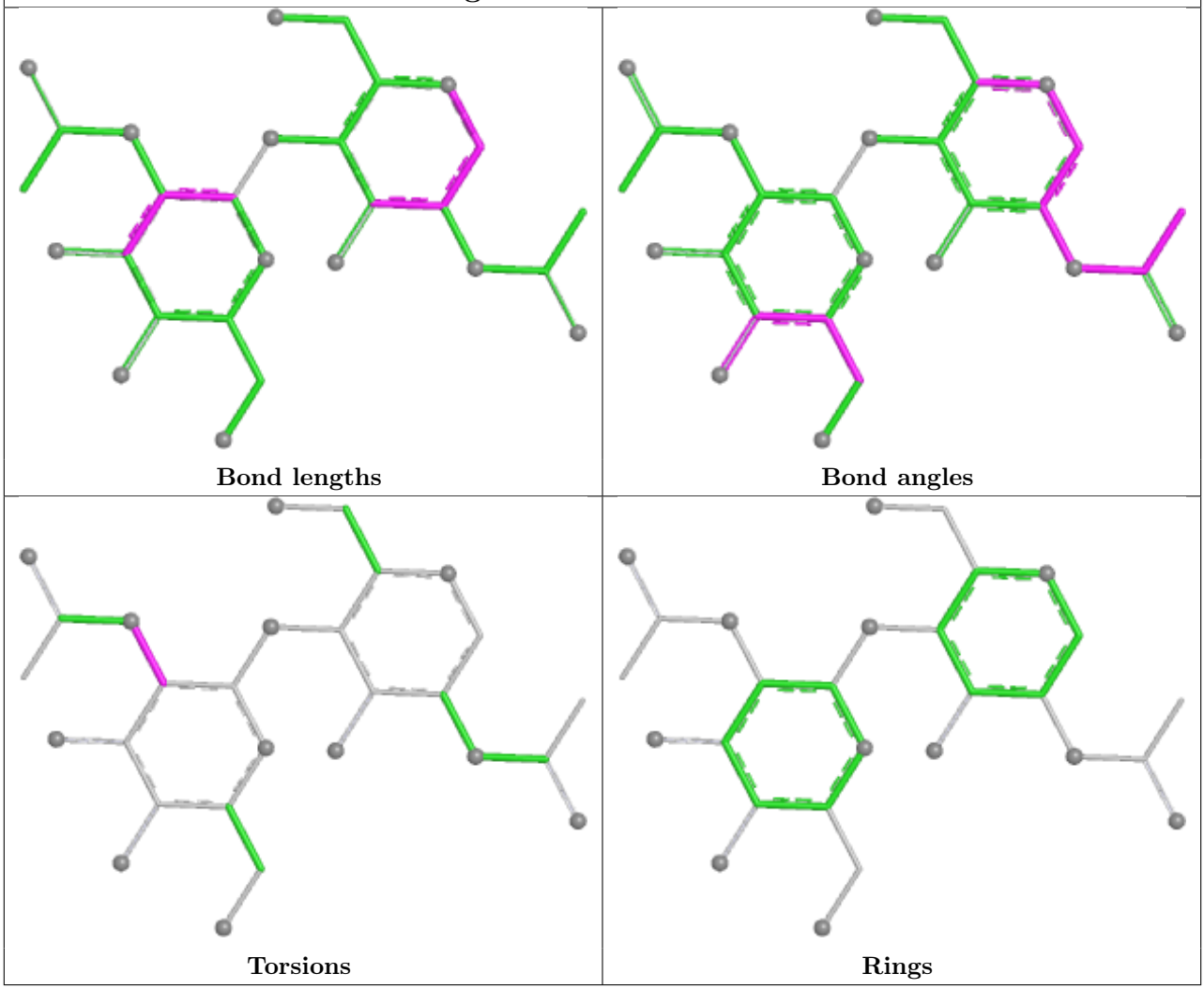
Oligosaccharide Chain B



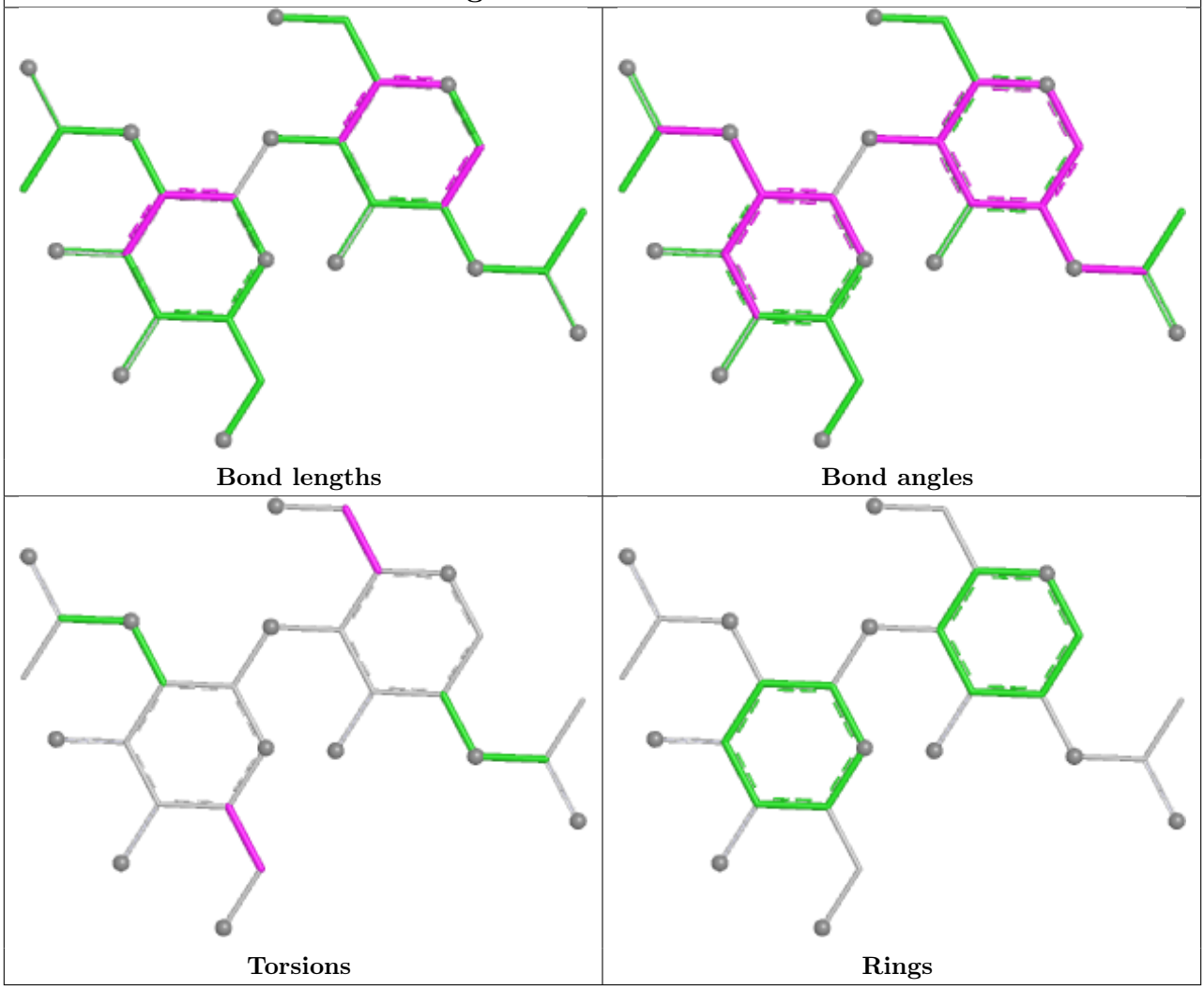
Oligosaccharide Chain C

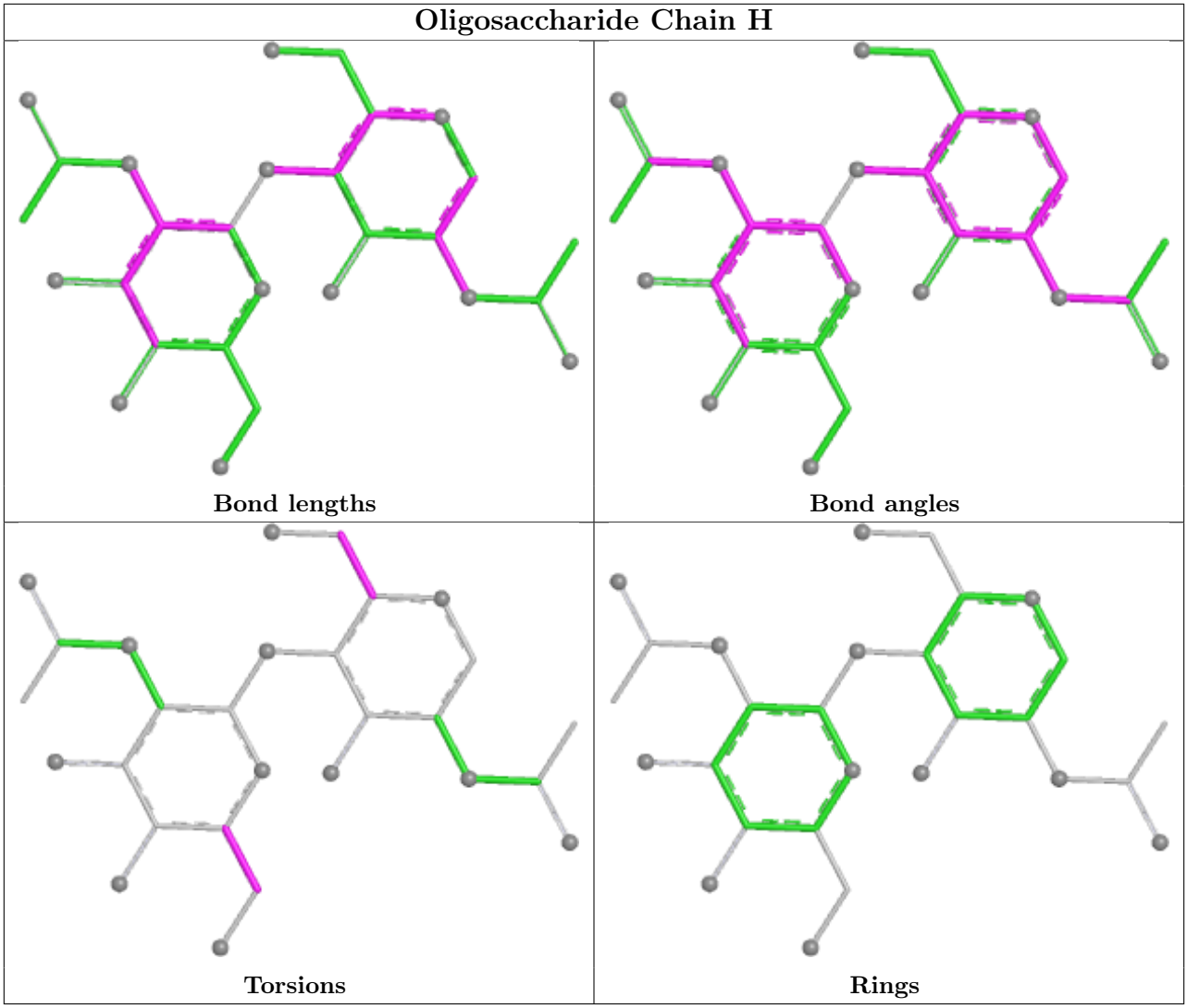


Oligosaccharide Chain D



Oligosaccharide Chain F





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(^{o})	Ideal(^{o})
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 (i)

6.1 Protein, DNA and RNA chains (i)

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%)	0.62	50 (10%) 5 6	47, 72, 135, 168	0
1	E	464/572 (81%)	0.51	37 (7%) 12 13	45, 70, 124, 160	0
2	G	216/261 (82%)	0.42	6 (2%) 53 58	43, 61, 93, 130	1 (0%)
2	J	216/261 (82%)	0.43	4 (1%) 66 71	38, 53, 89, 141	1 (0%)
3	K	218/220 (99%)	0.22	4 (1%) 68 71	41, 58, 84, 123	0
3	L	218/220 (99%)	0.36	4 (1%) 68 71	40, 54, 87, 120	0
All	All	1796/2106 (85%)	0.46	105 (5%) 23 25	38, 63, 118, 168	2 (0%)

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	561	ALA	9.8
1	A	561	ALA	9.0
1	E	612	PRO	8.6
1	A	562	THR	8.4
1	A	560	PRO	7.6
1	E	562	THR	7.6
1	E	507	GLY	7.5
1	E	541	SER	6.9
3	L	214	CYS	6.7
3	K	214	CYS	6.2
1	E	560	PRO	6.1
1	A	564	ASN	6.0
1	A	567	VAL	5.9
1	A	559	LEU	5.4
1	E	509	ALA	5.2
1	E	563	ASP	5.2
1	A	568	CYS	5.0
1	A	565	PRO	4.9
1	A	220	PHE	4.9

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Mol	Chain	Res	Type	RSRZ
1	A	570	TYR	4.9
1	E	452	THR	4.8
1	E	564	ASN	4.5
1	E	619	VAL	4.3
1	E	566	SER	4.3
1	E	542	ASN	4.3
1	E	567	VAL	4.3
3	L	213	GLU	4.2
2	J	193	ILE	4.1
1	A	569	VAL	4.1
1	E	569	VAL	4.0
1	A	452	THR	4.0
1	A	506	ARG	3.9
1	A	541	SER	3.8
1	E	506	ARG	3.7
1	A	563	ASP	3.5
1	A	290	ALA	3.5
1	A	571	CYS	3.5
2	J	210	ILE	3.4
1	A	227	HIS	3.3
1	A	600	MET	3.3
1	A	542	ASN	3.2
1	E	570	TYR	3.2
1	A	218	LEU	3.2
1	A	287	ASP	3.2
1	A	618	ASP	3.2
1	E	289	ARG	3.2
1	A	616	GLY	3.2
1	E	508	GLY	3.1
1	A	599	LEU	3.1
1	E	616	GLY	3.1
1	A	390	PRO	3.0
1	A	289	ARG	3.0
1	A	566	SER	3.0
1	E	559	LEU	3.0
1	E	218	LEU	2.9
1	E	565	PRO	2.9
1	E	505	LEU	2.9
1	A	326	ARG	2.8
1	A	552	ARG	2.8
1	E	131	GLY	2.8
2	G	132	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	507	GLY	2.8
1	A	225	ALA	2.8
2	G	193	ILE	2.8
1	A	630	VAL	2.7
1	E	617	GLY	2.6
1	E	483	GLU	2.6
1	A	286	ARG	2.6
1	A	612	PRO	2.6
1	A	288	ARG	2.6
1	E	520	CYS	2.6
2	G	173	ASP	2.6
1	E	326	ARG	2.5
1	E	447	LEU	2.5
1	E	510	SER	2.5
1	E	535	LEU	2.4
1	E	227	HIS	2.4
1	A	508	GLY	2.4
1	A	520	CYS	2.4
1	E	615	HIS	2.3
3	K	212	ASN	2.3
1	A	387	ALA	2.3
1	A	619	VAL	2.3
3	K	125	LEU	2.2
1	A	291	SER	2.2
1	A	625	PHE	2.2
1	A	224	GLY	2.2
1	A	325	GLY	2.2
1	A	328	GLU	2.2
1	A	537	LEU	2.1
1	A	547	CYS	2.1
3	L	212	ASN	2.1
2	G	9	ALA	2.1
2	J	186	SER	2.1
1	A	572	ASP	2.1
1	A	505	LEU	2.1
2	J	82(B)	SER	2.1
1	E	132	VAL	2.1
2	G	89	VAL	2.1
1	A	617	GLY	2.1
1	E	197	PRO	2.0
1	E	547	CYS	2.0
2	G	210	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
3	L	30	TYR	2.0
3	K	213	GLU	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)

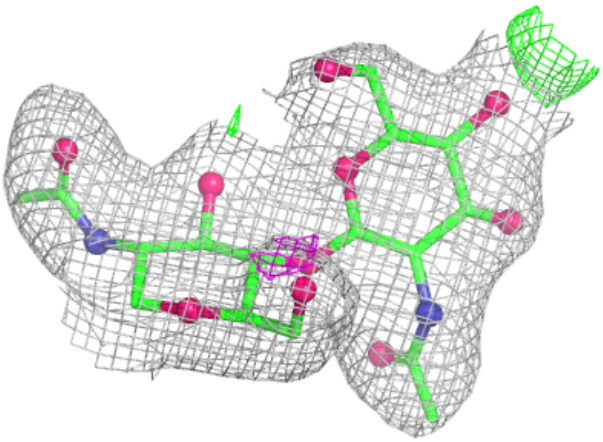
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

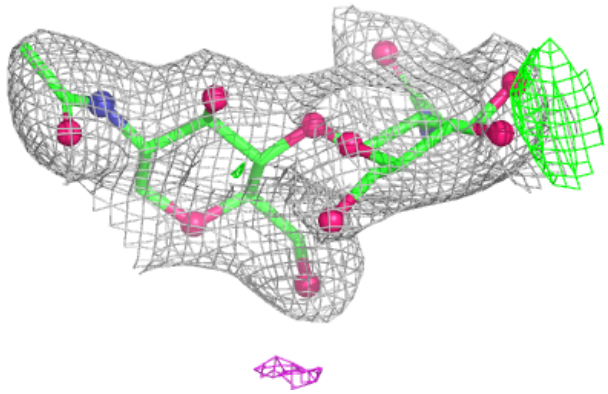
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAG	H	2	14/15	0.69	0.26	102,108,112,112	0
4	NAG	C	1	14/15	0.76	0.40	169,172,179,183	0
4	NAG	F	2	14/15	0.78	0.20	112,117,123,123	0
4	NAG	H	1	14/15	0.78	0.20	86,91,95,97	0
4	NAG	C	2	14/15	0.78	0.44	179,183,189,192	0
4	NAG	F	1	14/15	0.86	0.18	98,104,108,108	0
4	NAG	D	2	14/15	0.91	0.15	81,86,90,92	0
4	NAG	B	2	14/15	0.94	0.12	77,82,85,88	0
4	NAG	B	1	14/15	0.95	0.09	66,71,75,75	0
4	NAG	D	1	14/15	0.97	0.10	72,77,81,81	0

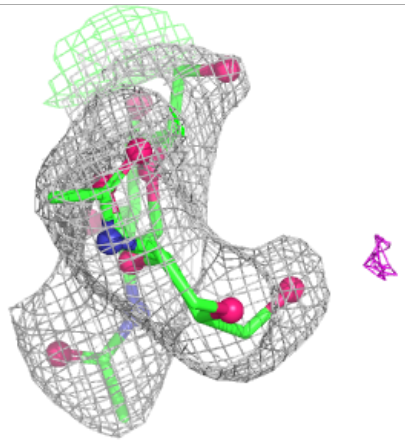
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

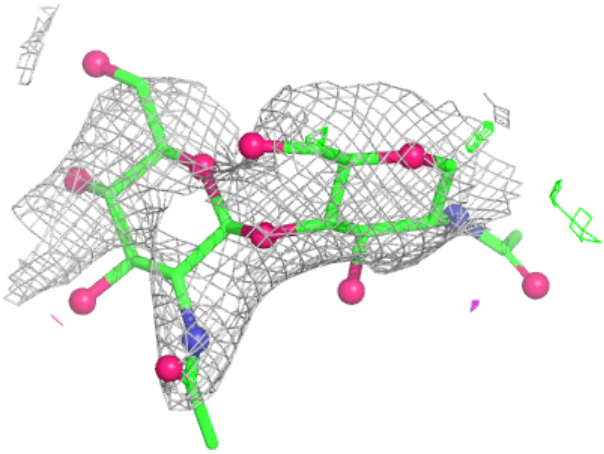


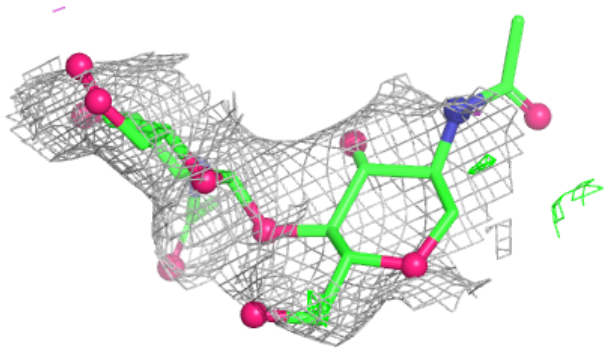


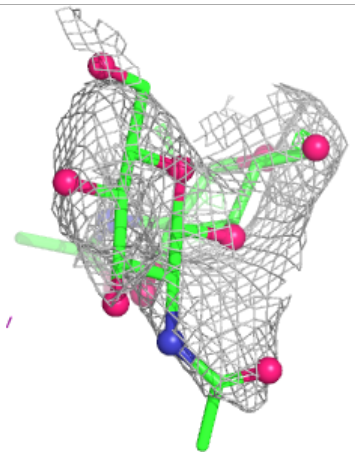


Electron density around Chain C:

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

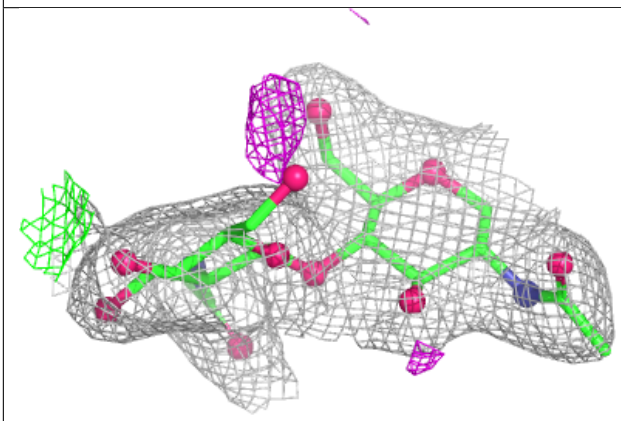


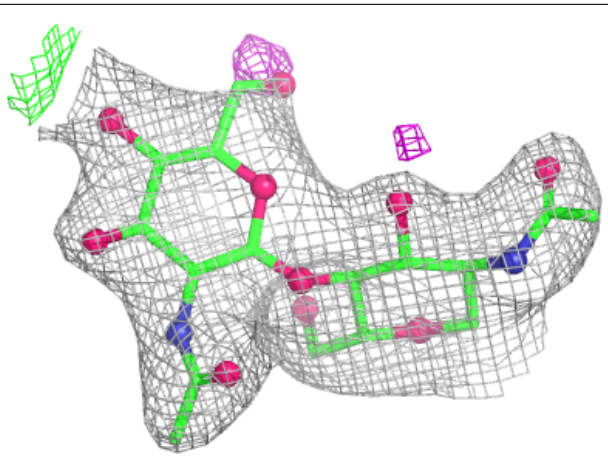


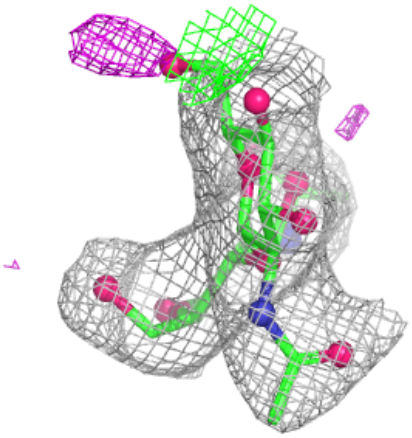


Electron density around Chain D:

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

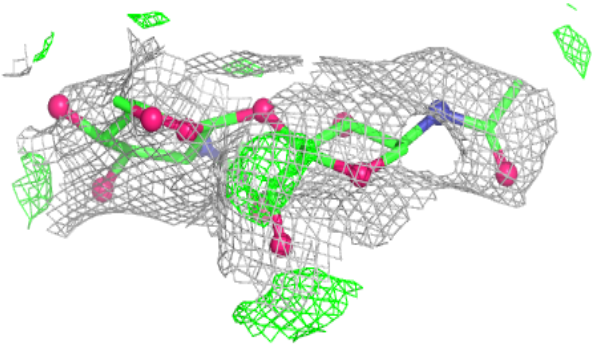


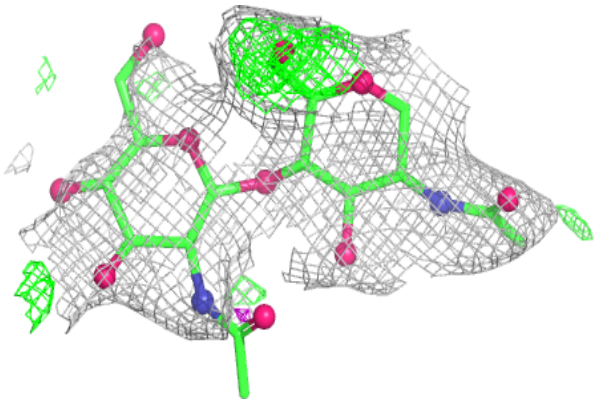


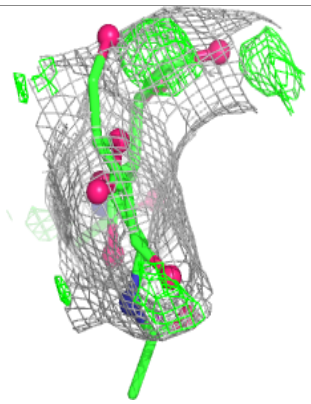


Electron density around Chain F:

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

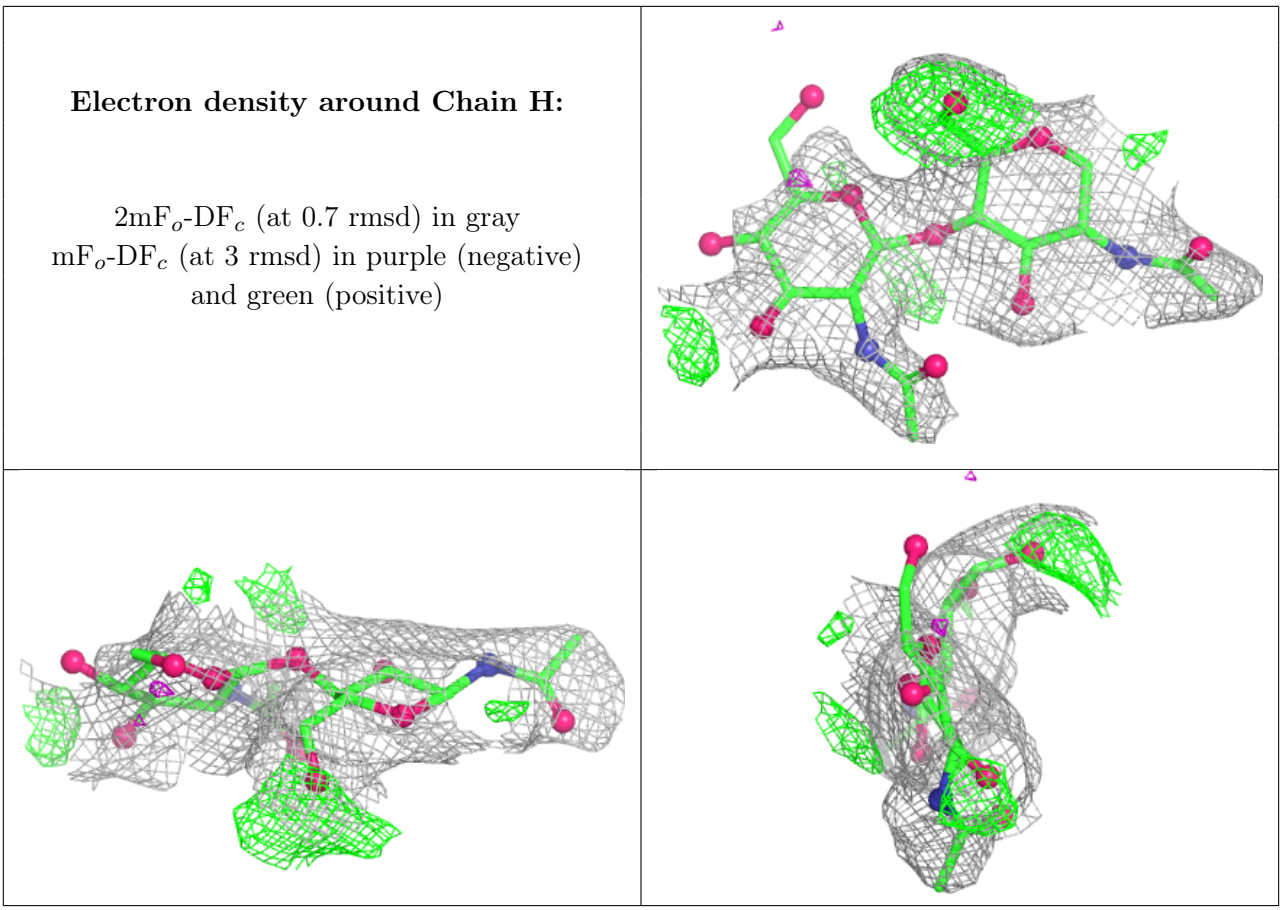






Electron density around Chain H:

$2mF_o$-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(Å^2)	Q<0.9
5	NAG	E	1103	14/15	0.65	0.26	128,133,140,141	0

6.5 Other polymers (i)

There are no such residues in this entry.