Full wwPDB X-ray Structure Validation Report ⓘ

Nov 22, 2023 – 02:17 PM JST

PDB ID	:	7XWA
Title	:	Crystal structure of the receptor binding domain of SARS-CoV-2 Omicron BA.4/5 variant spike protein in complex with its receptor ACE2
Authors	:	Suzuki, T.; Kimura, K.; Hashiguchi, T.
Deposited on	:	2022-05-26
Resolution	:	3.36 Å(reported)

The following versions of software and data (see references ⓘ) were used in the production of this report:

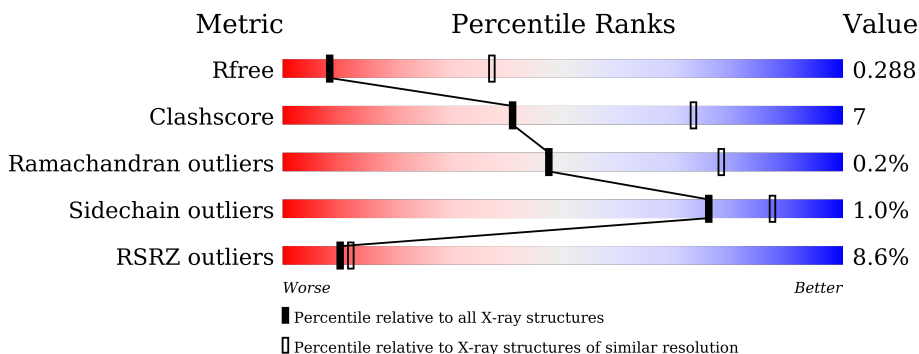|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.36 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	Percentile Ranks	Value
Rfree		0.288
Clashscore		7
Ramachandran outliers		0.2%
Sidechain outliers		1.0%
RSRZ outliers		8.6%

Worse   *Better*

▮ Percentile relative to all X-ray structures
⧠ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1558 (3.42-3.30)
Clashscore	141614	1627 (3.42-3.30)
Ramachandran outliers	138981	1599 (3.42-3.30)
Sidechain outliers	138945	1598 (3.42-3.30)
RSRZ outliers	127900	1507 (3.42-3.30)

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	608	6% / 80% / 17% / ..
1	C	608	4% / 80% / 17% / .
2	B	234	17% / 70% / 13% / 17%
2	D	234	15% / 69% / 14% / 17%
3	E	2	100%
3	G	2	100%

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	M	2	100%
4	F	3	67% 33%
4	I	3	33% 33% 33%
4	J	3	100%
5	K	4	100%
6	O	4	50% 50%

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
3	NAG	E	2	-	-	-	X
3	NAG	G	2	-	-	-	X
6	MAN	O	4	-	-	-	X

2 Entry composition ⓘ

There are 8 unique types of molecules in this entry. The entry contains 13177 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 Processed angiotensin-converting enzyme 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	596	Total 4862	C 3111	N 805	O 917	S 29	0	0	0
1	C	596	Total 4862	C 3111	N 805	O 917	S 29	0	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	618	GLY	-	expression tag	UNP Q9BYF1
A	619	THR	-	expression tag	UNP Q9BYF1
A	620	LYS	-	expression tag	UNP Q9BYF1
A	621	HIS	-	expression tag	UNP Q9BYF1
A	622	HIS	-	expression tag	UNP Q9BYF1
A	623	HIS	-	expression tag	UNP Q9BYF1
A	624	HIS	-	expression tag	UNP Q9BYF1
A	625	HIS	-	expression tag	UNP Q9BYF1
A	626	HIS	-	expression tag	UNP Q9BYF1
C	618	GLY	-	expression tag	UNP Q9BYF1
C	619	THR	-	expression tag	UNP Q9BYF1
C	620	LYS	-	expression tag	UNP Q9BYF1
C	621	HIS	-	expression tag	UNP Q9BYF1
C	622	HIS	-	expression tag	UNP Q9BYF1
C	623	HIS	-	expression tag	UNP Q9BYF1
C	624	HIS	-	expression tag	UNP Q9BYF1
C	625	HIS	-	expression tag	UNP Q9BYF1
C	626	HIS	-	expression tag	UNP Q9BYF1

- Molecule 2 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	195	Total 1554	C 1001	N 263	O 282	S 8	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	D	195	1554	1001	263	282	8	0	0	0

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	312	LEU	-	expression tag	UNP P0DTC2
B	313	LEU	-	expression tag	UNP P0DTC2
B	314	MET	-	expression tag	UNP P0DTC2
B	315	GLY	-	expression tag	UNP P0DTC2
B	316	CYS	-	expression tag	UNP P0DTC2
B	317	VAL	-	expression tag	UNP P0DTC2
B	318	ALA	-	expression tag	UNP P0DTC2
B	319	GLU	-	expression tag	UNP P0DTC2
B	320	THR	-	expression tag	UNP P0DTC2
B	321	GLY	-	expression tag	UNP P0DTC2
B	339	ASP	GLY	engineered mutation	UNP P0DTC2
B	371	PHE	SER	engineered mutation	UNP P0DTC2
B	373	PRO	SER	engineered mutation	UNP P0DTC2
B	375	PHE	SER	engineered mutation	UNP P0DTC2
B	376	ALA	THR	engineered mutation	UNP P0DTC2
B	405	ASN	ASP	engineered mutation	UNP P0DTC2
B	408	SER	ARG	engineered mutation	UNP P0DTC2
B	417	ASN	LYS	engineered mutation	UNP P0DTC2
B	440	LYS	ASN	engineered mutation	UNP P0DTC2
B	452	ARG	LEU	engineered mutation	UNP P0DTC2
B	477	ASN	SER	engineered mutation	UNP P0DTC2
B	478	LYS	THR	engineered mutation	UNP P0DTC2
B	484	ALA	GLU	engineered mutation	UNP P0DTC2
B	486	VAL	PHE	engineered mutation	UNP P0DTC2
B	498	ARG	GLN	engineered mutation	UNP P0DTC2
B	501	TYR	ASN	engineered mutation	UNP P0DTC2
B	505	HIS	TYR	engineered mutation	UNP P0DTC2
B	537	GLY	-	expression tag	UNP P0DTC2
B	538	THR	-	expression tag	UNP P0DTC2
B	539	LYS	-	expression tag	UNP P0DTC2
B	540	HIS	-	expression tag	UNP P0DTC2
B	541	HIS	-	expression tag	UNP P0DTC2
B	542	HIS	-	expression tag	UNP P0DTC2
B	543	HIS	-	expression tag	UNP P0DTC2
B	544	HIS	-	expression tag	UNP P0DTC2
B	545	HIS	-	expression tag	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	312	LEU	-	expression tag	UNP P0DTC2
D	313	LEU	-	expression tag	UNP P0DTC2
D	314	MET	-	expression tag	UNP P0DTC2
D	315	GLY	-	expression tag	UNP P0DTC2
D	316	CYS	-	expression tag	UNP P0DTC2
D	317	VAL	-	expression tag	UNP P0DTC2
D	318	ALA	-	expression tag	UNP P0DTC2
D	319	GLU	-	expression tag	UNP P0DTC2
D	320	THR	-	expression tag	UNP P0DTC2
D	321	GLY	-	expression tag	UNP P0DTC2
D	339	ASP	GLY	engineered mutation	UNP P0DTC2
D	371	PHE	SER	engineered mutation	UNP P0DTC2
D	373	PRO	SER	engineered mutation	UNP P0DTC2
D	375	PHE	SER	engineered mutation	UNP P0DTC2
D	376	ALA	THR	engineered mutation	UNP P0DTC2
D	405	ASN	ASP	engineered mutation	UNP P0DTC2
D	408	SER	ARG	engineered mutation	UNP P0DTC2
D	417	ASN	LYS	engineered mutation	UNP P0DTC2
D	440	LYS	ASN	engineered mutation	UNP P0DTC2
D	452	ARG	LEU	engineered mutation	UNP P0DTC2
D	477	ASN	SER	engineered mutation	UNP P0DTC2
D	478	LYS	THR	engineered mutation	UNP P0DTC2
D	484	ALA	GLU	engineered mutation	UNP P0DTC2
D	486	VAL	PHE	engineered mutation	UNP P0DTC2
D	498	ARG	GLN	engineered mutation	UNP P0DTC2
D	501	TYR	ASN	engineered mutation	UNP P0DTC2
D	505	HIS	TYR	engineered mutation	UNP P0DTC2
D	537	GLY	-	expression tag	UNP P0DTC2
D	538	THR	-	expression tag	UNP P0DTC2
D	539	LYS	-	expression tag	UNP P0DTC2
D	540	HIS	-	expression tag	UNP P0DTC2
D	541	HIS	-	expression tag	UNP P0DTC2
D	542	HIS	-	expression tag	UNP P0DTC2
D	543	HIS	-	expression tag	UNP P0DTC2
D	544	HIS	-	expression tag	UNP P0DTC2
D	545	HIS	-	expression tag	UNP P0DTC2

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a cetamido-2-deoxy-beta-D-glucopyranose.
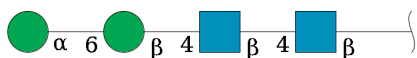
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	2	Total 28	C 16	N 2	O 10	0	0	0
3	G	2	Total 28	C 16	N 2	O 10	0	0	0
3	M	2	Total 28	C 16	N 2	O 10	0	0	0

- Molecule 4 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.
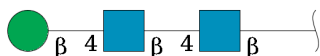
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	F	3	Total 39	C 22	N 2	O 15	0	0	0
4	I	3	Total 39	C 22	N 2	O 15	0	0	0
4	J	3	Total 39	C 22	N 2	O 15	0	0	0

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.
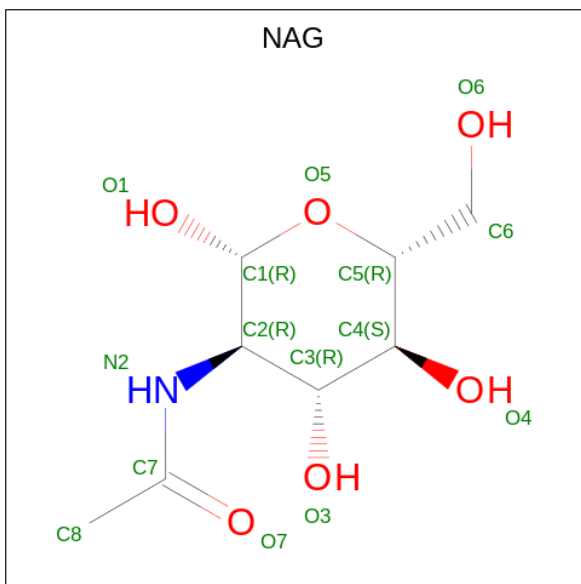

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	K	4	Total 50	C 28	N 2	O 20	0	0	0

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	O	4	Total 50	C 28	N 2	O 20	0	0	0

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total 1	Zn 1	1	0
7	C	1	Total 1	Zn 1	1	0

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).

NAG

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total 14	C 8	N 1	O 5	14	0
8	C	1	Total 14	C 8	N 1	O 5	0	0
8	C	1	Total 14	C 8	N 1	O 5	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.
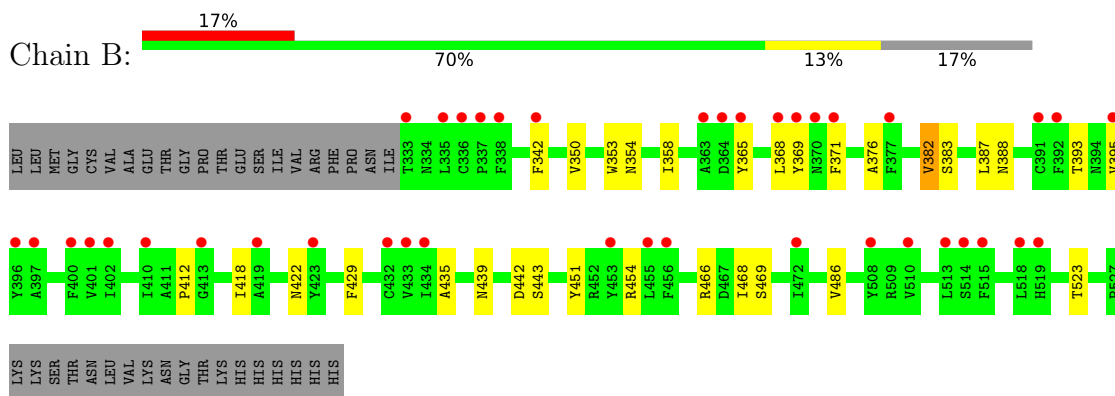
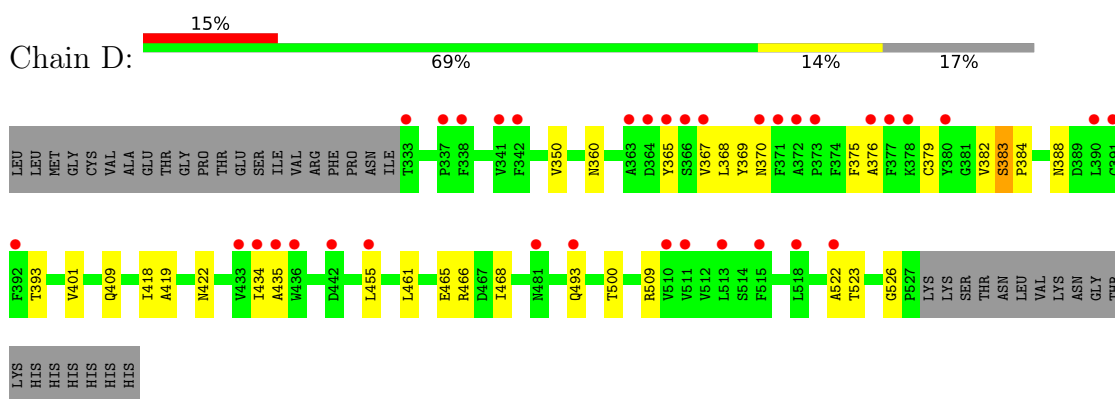• Molecule 1: Processed angiotensin-converting enzyme 2
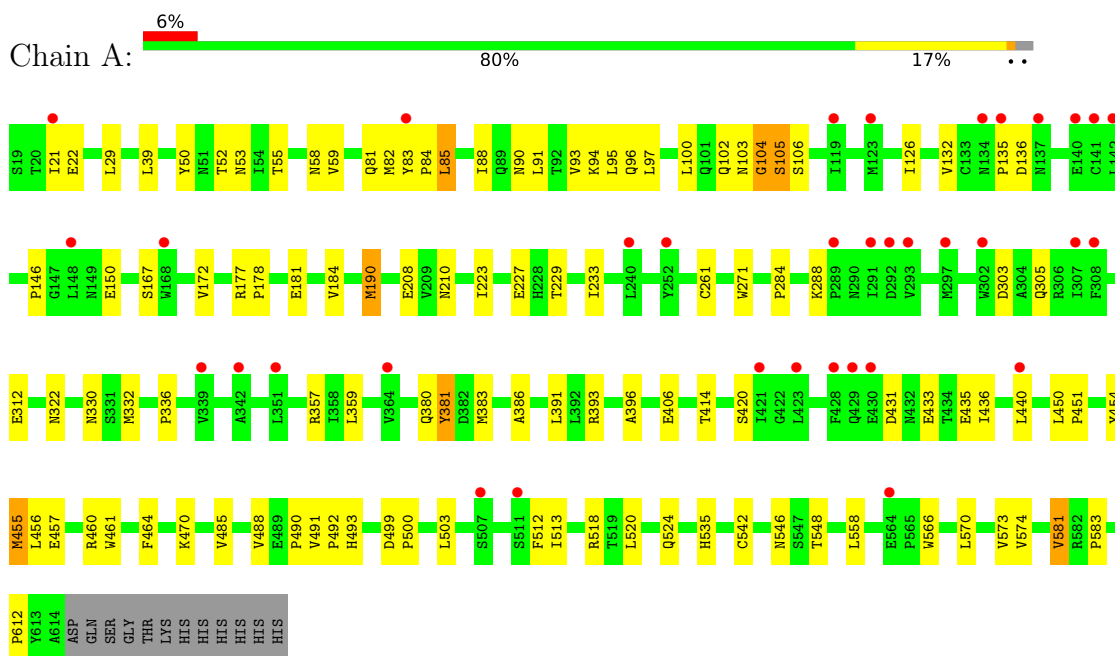
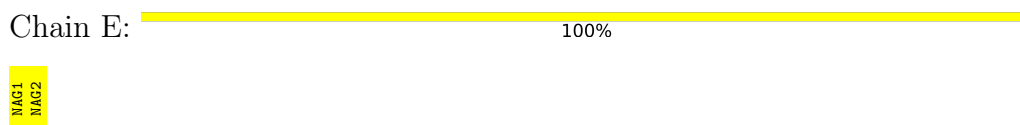• Molecule 1: Processed angiotensin-converting enzyme 2
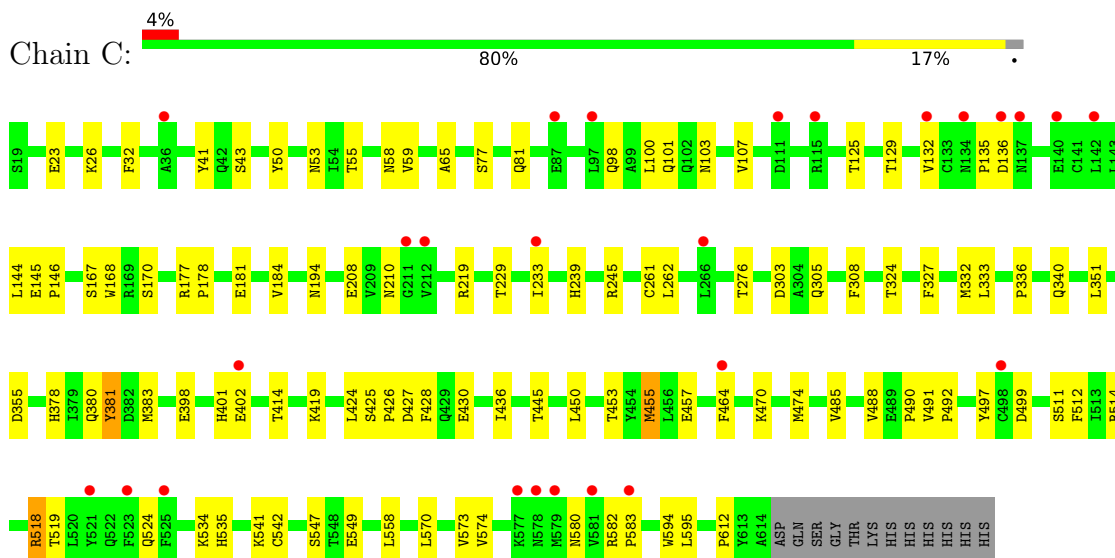
• Molecule 2: Spike protein S1

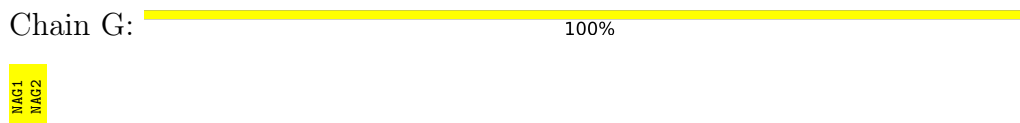Chain B:

• Molecule 2: Spike protein S1

Chain D:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-gluc opyranose

Chain E:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-gluc opyranose

Chain G:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-gluc opyranose
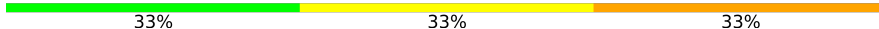
Chain M:

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

Chain F:

67%   33%

NAG1 NAG2 BMA3

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

Chain I:

33%   33%   33%

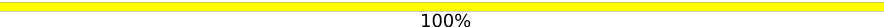NAG1 NAG2 BMA3

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

Chain J:

100%

NAG1 NAG2 BMA3

• Molecule 5: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:

100%

NAG1 NAG2 BMA3 MAN4

• Molecule 6: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:

50%   50%

NAG1 NAG2 BMA3 MAN4

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	85.51Å 130.01Å 101.88Å 90.00° 92.64° 90.00°	Depositor
Resolution (Å)	47.39 – 3.36 47.39 – 3.36	Depositor EDS
% Data completeness (in resolution range)	97.6 (47.39-3.36) 98.6 (47.39-3.36)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.48 (at 3.40Å)	Xtriage
Refinement program	BUSTER 2.10.4., PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.231 , 0.287 0.232 , 0.288	Depositor DCC
R_{free} test set	1573 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	97.3	Xtriage
Anisotropy	0.771	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 46.9	EDS
L-test for twinning[2]	$< |L| > = 0.45, < L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.036 for h,-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	13177	wwPDB-VP
Average B, all atoms (Å^2)	130.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.87% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[1]Intensities estimated from amplitudes.

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

5   Model quality ⓘ

5.1   Standard geometry ⓘ

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

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	0.31	0/4999	0.54	0/6792
1	C	0.32	0/4999	0.55	0/6792
2	B	0.30	0/1601	0.53	0/2180
2	D	0.31	0/1601	0.52	0/2180
All	All	0.31	0/13200	0.54	0/17944

There are no bond length outliers.

There are no bond angle outliers.

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	4862	0	4634	76	0
1	C	4862	0	4633	71	0
2	B	1554	0	1477	20	0
2	D	1554	0	1477	20	0
3	E	28	0	25	0	0
3	G	28	0	25	0	0
3	M	28	0	25	0	0
4	F	39	0	34	0	0
4	I	39	0	34	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	J	39	0	34	0	0
5	K	50	0	43	1	0
6	O	50	0	43	1	0
7	A	1	0	0	0	0
7	C	1	0	0	0	0
8	A	14	0	13	0	0
8	C	28	0	26	3	0
All	All	13177	0	12523	183	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 7.

All (183) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:398:GLU:OE2	1:C:511:SER:OG	1.73	1.05
2:B:454:ARG:HH22	2:B:469:SER:H	1.15	0.89
1:A:208:GLU:OE2	1:A:210:ASN:ND2	2.10	0.84
1:C:208:GLU:OE2	1:C:210:ASN:ND2	2.13	0.81
1:A:524:GLN:HG3	1:A:583:PRO:HG2	1.65	0.78
1:C:132:VAL:HG11	1:C:167:SER:HB3	1.67	0.74
1:A:132:VAL:HG11	1:A:167:SER:HB3	1.70	0.72
1:C:103:ASN:HD21	8:C:702:NAG:H83	1.58	0.68
1:A:50:TYR:CE1	1:A:59:VAL:HG22	2.30	0.67
1:C:103:ASN:OD1	1:C:194:ASN:ND2	2.28	0.66
1:A:55:THR:O	1:A:59:VAL:HG23	1.95	0.66
1:A:284:PRO:HD3	1:A:440:LEU:HD22	1.77	0.65
1:A:420:SER:HB2	4:I:1:NAG:H62	1.78	0.64
1:C:276:THR:HG1	1:C:445:THR:HG1	1.41	0.64
1:C:524:GLN:HG3	1:C:583:PRO:HG2	1.81	0.63
1:C:50:TYR:CE1	1:C:59:VAL:HG22	2.34	0.63
1:C:55:THR:O	1:C:59:VAL:HG23	1.99	0.63
1:C:41:TYR:OH	2:D:500:THR:O	2.18	0.61
1:C:573:VAL:HG13	1:C:574:VAL:HG13	1.83	0.61
1:C:594:TRP:CD1	8:C:703:NAG:H81	2.35	0.61
1:C:332:MET:HE3	1:C:336:PRO:HD3	1.82	0.60
1:C:425:SER:OG	1:C:427:ASP:OD1	2.15	0.60
1:C:170:SER:HB2	1:C:497:TYR:HE2	1.66	0.60
1:A:406:GLU:HG3	1:A:518:ARG:NH1	2.18	0.58
1:C:53:ASN:O	1:C:58:ASN:ND2	2.30	0.58
1:C:402:GLU:HB3	1:C:518:ARG:HD2	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:548:THR:HB	1:C:534:LYS:HE2	1.86	0.58
1:C:430:GLU:OE1	1:C:541:LYS:NZ	2.34	0.57
2:D:466:ARG:HH21	2:D:468:ILE:HD11	1.68	0.57
1:A:83:TYR:HB2	1:A:97:LEU:HD21	1.87	0.56
5:K:1:NAG:H61	5:K:2:NAG:N2	2.20	0.56
1:A:105:SER:HA	1:A:190:MET:HG3	1.87	0.56
1:A:229:THR:O	1:A:233:ILE:HG13	2.06	0.56
2:B:412:PRO:HG3	2:B:429:PHE:HB3	1.88	0.56
1:C:378:HIS:CE1	1:C:401:HIS:HB3	2.41	0.56
1:A:457:GLU:HG2	1:A:513:ILE:HB	1.87	0.56
1:C:303:ASP:OD2	1:C:305:GLN:HB2	2.06	0.56
1:A:535:HIS:CE1	1:A:542:CYS:HA	2.41	0.55
2:B:393:THR:O	2:B:523:THR:OG1	2.24	0.55
2:B:382:VAL:HG22	2:B:387:LEU:HD21	1.88	0.54
1:C:547:SER:HA	4:I:1:NAG:H83	1.88	0.54
1:A:491:VAL:HG13	1:A:492:PRO:HD2	1.89	0.54
1:A:284:PRO:HG3	1:A:440:LEU:HD13	1.90	0.53
1:A:102:GLN:C	1:A:104:GLY:H	2.12	0.53
1:A:524:GLN:HB3	1:A:574:VAL:HG11	1.90	0.53
2:B:454:ARG:HH22	2:B:469:SER:N	1.97	0.53
1:A:177:ARG:HB3	1:A:178:PRO:HD3	1.90	0.53
1:A:455:MET:HG2	1:A:485:VAL:CG2	2.38	0.53
1:A:406:GLU:HG3	1:A:518:ARG:HH11	1.74	0.53
1:A:126:ILE:HG22	1:A:172:VAL:HG13	1.91	0.52
1:A:81:GLN:NE2	1:A:103:ASN:OD1	2.41	0.52
1:C:570:LEU:O	1:C:574:VAL:HG22	2.10	0.52
1:A:233:ILE:HD13	1:A:450:LEU:HD13	1.92	0.52
1:C:424:LEU:HD11	1:C:428:PHE:CD2	2.44	0.52
2:B:418:ILE:HA	2:B:422:ASN:HB2	1.92	0.51
1:C:351:LEU:HB2	1:C:355:ASP:HB3	1.93	0.51
2:B:365:TYR:HB2	2:B:388:ASN:HB3	1.92	0.51
1:C:32:PHE:CZ	1:C:100:LEU:HD21	2.45	0.51
1:C:229:THR:O	1:C:233:ILE:HG13	2.11	0.51
1:C:184:VAL:HG22	1:C:464:PHE:HE1	1.75	0.50
1:C:491:VAL:HG13	1:C:492:PRO:HD2	1.93	0.50
2:B:368:LEU:HD12	2:B:369:TYR:HB3	1.92	0.50
1:C:170:SER:HB2	1:C:497:TYR:CE2	2.45	0.50
1:C:177:ARG:HB3	1:C:178:PRO:HD3	1.94	0.49
1:C:535:HIS:CE1	1:C:542:CYS:HA	2.47	0.49
1:C:208:GLU:OE1	1:C:219:ARG:NH1	2.45	0.49
1:A:181:GLU:OE2	1:A:470:LYS:HE3	2.10	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:TYR:CD1	1:A:558:LEU:HD22	2.47	0.49
2:D:393:THR:O	2:D:523:THR:OG1	2.29	0.49
1:C:535:HIS:CD2	1:C:542:CYS:HB2	2.48	0.48
1:C:43:SER:HA	1:C:65:ALA:HB1	1.95	0.48
1:A:227:GLU:HG2	1:A:454:TYR:OH	2.13	0.48
1:A:288:LYS:NZ	1:A:431:ASP:OD2	2.46	0.48
1:C:81:GLN:HE22	1:C:101:GLN:HG2	1.79	0.48
1:A:261:CYS:HB2	1:A:488:VAL:HB	1.95	0.48
1:C:135:PRO:O	1:C:136:ASP:HB2	2.14	0.48
1:A:460:ARG:NH2	1:A:512:PHE:HB2	2.29	0.47
1:A:312:GLU:OE2	1:A:322:ASN:HB2	2.14	0.47
1:A:96:GLN:HB3	1:A:391:LEU:HD12	1.95	0.47
1:A:573:VAL:HG23	1:A:574:VAL:HG13	1.97	0.47
1:C:580:ASN:HD21	1:C:582:ARG:NH1	2.12	0.47
2:B:383:SER:H	2:B:387:LEU:HD22	1.80	0.46
1:A:85:LEU:HD21	1:A:94:LYS:HE3	1.97	0.46
2:D:367:VAL:O	2:D:370:ASN:HB2	2.15	0.46
2:D:379:CYS:HB3	2:D:383:SER:HA	1.98	0.46
1:A:29:LEU:HD12	1:A:93:VAL:HG13	1.97	0.46
1:A:431:ASP:O	1:A:435:GLU:HG3	2.16	0.46
1:A:103:ASN:O	1:A:106:SER:OG	2.23	0.46
2:B:442:ASP:OD2	2:B:451:TYR:OH	2.25	0.46
1:C:549:GLU:OE1	4:I:1:NAG:H82	2.15	0.46
2:B:376:ALA:HB3	2:B:435:ALA:HB3	1.97	0.46
1:A:380:GLN:HA	1:A:383:MET:HE2	1.97	0.46
1:C:414:THR:HG21	1:C:542:CYS:O	2.16	0.46
1:A:396:ALA:HB1	1:A:566:TRP:HA	1.99	0.45
1:A:414:THR:HG21	1:A:542:CYS:O	2.16	0.45
2:B:383:SER:H	2:B:387:LEU:CD2	2.30	0.45
1:C:125:THR:O	1:C:129:THR:OG1	2.19	0.45
1:A:386:ALA:HA	1:A:393:ARG:HD2	1.99	0.45
1:A:21:ILE:H	1:A:21:ILE:HD12	1.82	0.45
1:A:50:TYR:CD1	1:A:59:VAL:HG22	2.52	0.45
2:D:461:LEU:HB3	2:D:465:GLU:HB3	1.99	0.45
1:A:303:ASP:OD2	1:A:305:GLN:HB2	2.16	0.44
1:A:431:ASP:OD2	1:A:433:GLU:HB2	2.17	0.44
1:C:77:SER:O	1:C:81:GLN:HG2	2.18	0.44
2:D:409:GLN:HB3	2:D:419:ALA:HB2	1.99	0.44
1:A:82:MET:HE3	2:B:486:VAL:HG13	2.00	0.44
2:B:350:VAL:HG21	2:B:418:ILE:HD12	1.99	0.44
2:D:401:VAL:HG22	2:D:509:ARG:HG2	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:520:LEU:HD21	1:A:581:VAL:HG13	2.00	0.44
1:C:261:CYS:HB2	1:C:488:VAL:HB	1.98	0.44
1:C:419:LYS:HD3	1:C:426:PRO:HA	1.99	0.44
2:D:360:ASN:H	2:D:523:THR:HB	1.82	0.44
2:D:365:TYR:CD2	2:D:388:ASN:HA	2.52	0.44
1:A:21:ILE:HG21	1:A:84:PRO:HD2	1.99	0.44
1:A:52:THR:HG22	1:A:359:LEU:HD13	1.98	0.44
1:A:100:LEU:HD23	1:A:100:LEU:HA	1.76	0.44
1:C:23:GLU:HA	1:C:26:LYS:NZ	2.33	0.44
1:C:455:MET:HE2	1:C:485:VAL:HG21	1.99	0.44
2:D:368:LEU:HD23	2:D:369:TYR:N	2.33	0.44
2:D:393:THR:HA	2:D:522:ALA:HA	1.99	0.44
2:D:375:PHE:HA	2:D:435:ALA:O	2.18	0.44
1:A:82:MET:HE1	2:B:486:VAL:HG22	1.99	0.44
1:A:493:HIS:ND1	1:A:499:ASP:OD2	2.51	0.44
1:A:184:VAL:HG22	1:A:464:PHE:HE1	1.82	0.44
1:C:336:PRO:HG2	1:C:340:GLN:O	2.18	0.44
1:C:594:TRP:HD1	8:C:703:NAG:H81	1.79	0.44
2:D:376:ALA:O	2:D:434:ILE:HA	2.17	0.44
1:A:548:THR:HB	1:C:534:LYS:CE	2.48	0.43
1:A:53:ASN:O	1:A:58:ASN:ND2	2.39	0.43
1:C:453:THR:HG23	1:C:512:PHE:CD2	2.53	0.43
1:C:100:LEU:HD23	1:C:100:LEU:HA	1.72	0.43
1:A:490:PRO:HA	1:A:612:PRO:HG2	2.00	0.43
2:B:342:PHE:HB3	2:B:371:PHE:CE1	2.53	0.43
1:C:181:GLU:OE2	1:C:470:LYS:HE3	2.18	0.43
1:C:450:LEU:HD21	1:C:519:THR:HG21	2.00	0.43
1:A:135:PRO:O	1:A:136:ASP:OD1	2.37	0.43
2:B:358:ILE:HB	2:B:395:VAL:HB	1.99	0.43
1:C:103:ASN:O	1:C:107:VAL:N	2.52	0.43
1:A:223:ILE:HG12	1:A:461:TRP:CZ3	2.54	0.43
1:A:455:MET:HG2	1:A:485:VAL:HG21	2.00	0.43
1:A:535:HIS:CD2	1:A:542:CYS:HB2	2.53	0.43
1:C:381:TYR:CD1	1:C:558:LEU:HD22	2.54	0.43
1:C:474:MET:HE1	1:C:499:ASP:HB2	2.01	0.42
1:A:22:GLU:OE2	1:A:90:ASN:HB2	2.19	0.42
2:B:439:ASN:O	2:B:443:SER:HB2	2.19	0.42
1:C:98:GLN:O	1:C:101:GLN:HB2	2.19	0.42
2:B:350:VAL:HG22	2:B:422:ASN:HB3	2.02	0.42
1:C:490:PRO:HA	1:C:612:PRO:HG2	2.00	0.42
1:A:499:ASP:N	1:A:500:PRO:HD2	2.34	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:ASN:O	1:A:357:ARG:HG2	2.20	0.42
1:C:490:PRO:HA	1:C:612:PRO:CG	2.50	0.42
1:A:91:LEU:O	1:A:95:LEU:HG	2.20	0.42
1:A:104:GLY:C	1:A:106:SER:H	2.23	0.41
1:A:570:LEU:O	1:A:574:VAL:HG22	2.20	0.41
2:D:379:CYS:CB	2:D:384:PRO:HD3	2.50	0.41
1:A:39:LEU:HD23	1:A:39:LEU:HA	1.85	0.41
1:C:245:ARG:HB2	1:C:262:LEU:HD21	2.01	0.41
1:C:457:GLU:HG2	1:C:512:PHE:HB3	2.02	0.41
1:C:145:GLU:HA	1:C:146:PRO:HA	1.80	0.41
1:C:184:VAL:HG22	1:C:464:PHE:CE1	2.55	0.41
1:A:50:TYR:HE1	1:A:59:VAL:HG22	1.81	0.41
2:B:353:TRP:NE1	2:B:466:ARG:HG3	2.34	0.41
1:A:85:LEU:HA	1:A:88:ILE:HD13	2.03	0.41
1:A:271:TRP:CD2	1:A:503:LEU:HD13	2.56	0.41
2:D:365:TYR:CE2	2:D:388:ASN:HA	2.55	0.41
1:C:239:HIS:HB3	1:C:595:LEU:HB3	2.02	0.41
1:C:324:THR:O	1:C:327:PHE:HB3	2.20	0.41
1:C:380:GLN:HA	1:C:383:MET:HE2	2.03	0.41
1:C:308:PHE:CZ	1:C:333:LEU:HD22	2.56	0.41
2:D:418:ILE:HA	2:D:422:ASN:HB2	2.01	0.41
1:A:332:MET:HE3	1:A:336:PRO:HD3	2.02	0.40
1:A:455:MET:HG3	1:A:456:LEU:N	2.36	0.40
1:C:398:GLU:HG2	1:C:514:ARG:HB3	2.02	0.40
2:D:350:VAL:HG21	2:D:418:ILE:HD12	2.02	0.40
2:D:455:LEU:HD22	2:D:493:GLN:OE1	2.21	0.40
1:C:50:TYR:HE1	1:C:59:VAL:HG22	1.83	0.40
1:A:146:PRO:O	1:A:150:GLU:HB2	2.22	0.40
1:A:420:SER:HB2	4:I:2:NAG:H82	2.03	0.40
1:A:546:ASN:HB3	1:C:549:GLU:OE2	2.21	0.40
1:C:144:LEU:HB2	1:C:168:TRP:CH2	2.56	0.40
2:D:388:ASN:OD1	2:D:526:GLY:HA3	2.20	0.40
1:A:450:LEU:HB2	1:A:451:PRO:HD3	2.03	0.40
6:O:3:BMA:H3	6:O:4:MAN:H2	1.67	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	594/608 (98%)	573 (96%)	19 (3%)	2 (0%)	41	73
1	C	594/608 (98%)	575 (97%)	19 (3%)	0	100	100
2	B	193/234 (82%)	179 (93%)	14 (7%)	0	100	100
2	D	193/234 (82%)	175 (91%)	17 (9%)	1 (0%)	29	63
All	All	1574/1684 (94%)	1502 (95%)	69 (4%)	3 (0%)	47	78

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	104	GLY
2	D	382	VAL
1	A	105	SER

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	526/537 (98%)	520 (99%)	6 (1%)	73	86
1	C	526/537 (98%)	522 (99%)	4 (1%)	81	91
2	B	167/202 (83%)	164 (98%)	3 (2%)	59	80
2	D	167/202 (83%)	166 (99%)	1 (1%)	86	93
All	All	1386/1478 (94%)	1372 (99%)	14 (1%)	76	87

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	85	LEU
1	A	190	MET
1	A	381	TYR
1	A	436	ILE
1	A	455	MET
1	A	581	VAL
2	B	354	ASN
2	B	382	VAL
2	B	468	ILE
1	C	381	TYR
1	C	436	ILE
1	C	455	MET
1	C	518	ARG
2	D	383	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	GLN
1	A	535	HIS
1	C	535	HIS

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 ⓘ

23 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
3	NAG	E	1	3,1	14,14,15	0.47	0	17,19,21	1.01	1 (5%)
3	NAG	E	2	3	14,14,15	0.91	1 (7%)	17,19,21	1.20	1 (5%)
4	NAG	F	1	4,1	14,14,15	0.33	0	17,19,21	0.48	0
4	NAG	F	2	4	14,14,15	0.28	0	17,19,21	0.54	0
4	BMA	F	3	4	11,11,12	0.88	1 (9%)	15,15,17	0.60	0
3	NAG	G	1	3,1	14,14,15	0.67	1 (7%)	17,19,21	1.07	1 (5%)
3	NAG	G	2	3	14,14,15	1.65	2 (14%)	17,19,21	1.15	1 (5%)
4	NAG	I	1	4,1	14,14,15	0.45	0	17,19,21	0.75	1 (5%)
4	NAG	I	2	4	14,14,15	0.27	0	17,19,21	0.48	0
4	BMA	I	3	4	11,11,12	0.76	0	15,15,17	0.71	0
4	NAG	J	1	4,1	14,14,15	0.48	0	17,19,21	0.88	1 (5%)
4	NAG	J	2	4	14,14,15	0.36	0	17,19,21	1.10	1 (5%)
4	BMA	J	3	4	11,11,12	0.85	1 (9%)	15,15,17	0.76	0
5	NAG	K	1	1,5	14,14,15	0.45	0	17,19,21	0.56	0
5	NAG	K	2	5	14,14,15	0.24	0	17,19,21	0.50	0
5	BMA	K	3	5	11,11,12	1.01	0	15,15,17	1.03	1 (6%)
5	MAN	K	4	5	11,11,12	1.12	1 (9%)	15,15,17	2.41	5 (33%)
3	NAG	M	1	3,1	14,14,15	0.46	0	17,19,21	0.55	0
3	NAG	M	2	3	14,14,15	0.30	0	17,19,21	0.40	0
6	NAG	O	1	6,1	14,14,15	0.33	0	17,19,21	0.54	0
6	NAG	O	2	6	14,14,15	0.31	0	17,19,21	0.44	0
6	BMA	O	3	6	11,11,12	0.90	0	15,15,17	0.98	1 (6%)
6	MAN	O	4	6	11,11,12	1.25	1 (9%)	15,15,17	1.74	5 (33%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	E	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
4	NAG	F	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	F	2	4	-	0/6/23/26	0/1/1/1
4	BMA	F	3	4	-	2/2/19/22	0/1/1/1
3	NAG	G	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
4	NAG	I	1	4,1	-	2/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	I	2	4	-	0/6/23/26	0/1/1/1
4	BMA	I	3	4	-	0/2/19/22	0/1/1/1
4	NAG	J	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	J	2	4	-	3/6/23/26	0/1/1/1
4	BMA	J	3	4	-	0/2/19/22	0/1/1/1
5	NAG	K	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	K	2	5	-	1/6/23/26	0/1/1/1
5	BMA	K	3	5	-	2/2/19/22	0/1/1/1
5	MAN	K	4	5	-	0/2/19/22	0/1/1/1
3	NAG	M	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	M	2	3	-	0/6/23/26	0/1/1/1
6	NAG	O	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	O	2	6	-	0/6/23/26	0/1/1/1
6	BMA	O	3	6	-	2/2/19/22	0/1/1/1
6	MAN	O	4	6	-	1/2/19/22	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	2	NAG	O5-C1	5.63	1.52	1.43
3	E	2	NAG	O5-C1	3.14	1.48	1.43
6	O	4	MAN	C4-C3	2.60	1.58	1.52
3	G	2	NAG	C1-C2	2.45	1.56	1.52
5	K	4	MAN	C1-C2	2.29	1.57	1.52
4	J	3	BMA	C1-C2	2.17	1.57	1.52
3	G	1	NAG	O5-C1	2.09	1.47	1.43
4	F	3	BMA	C1-C2	2.00	1.56	1.52

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	K	4	MAN	C1-O5-C5	5.96	120.26	112.19
3	G	2	NAG	C1-O5-C5	4.48	118.27	112.19
3	E	2	NAG	C1-O5-C5	4.45	118.23	112.19
5	K	4	MAN	C1-C2-C3	4.22	114.85	109.67
4	J	2	NAG	C1-O5-C5	4.02	117.64	112.19
6	O	4	MAN	C3-C4-C5	3.79	117.00	110.24
3	E	1	NAG	C1-O5-C5	3.47	116.89	112.19
3	G	1	NAG	C1-O5-C5	3.05	116.33	112.19
5	K	4	MAN	O5-C1-C2	3.04	115.46	110.77
5	K	4	MAN	O5-C5-C6	-2.83	102.77	107.20

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	K	4	MAN	C2-C3-C4	2.62	115.44	110.89
6	O	4	MAN	C1-C2-C3	2.62	112.89	109.67
6	O	4	MAN	C2-C3-C4	2.61	115.41	110.89
4	J	1	NAG	O4-C4-C5	2.36	115.16	109.30
5	K	3	BMA	C2-C3-C4	2.35	114.96	110.89
6	O	4	MAN	O5-C5-C6	2.34	110.88	107.20
4	I	1	NAG	O4-C4-C3	-2.26	105.12	110.35
6	O	3	BMA	C1-C2-C3	2.11	112.27	109.67
6	O	4	MAN	O2-C2-C3	-2.08	105.97	110.14

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	K	3	BMA	C4-C5-C6-O6
6	O	3	BMA	C4-C5-C6-O6
4	J	2	NAG	C4-C5-C6-O6
4	J	2	NAG	O5-C5-C6-O6
5	K	3	BMA	O5-C5-C6-O6
6	O	3	BMA	O5-C5-C6-O6
4	I	1	NAG	O5-C5-C6-O6
4	I	1	NAG	C4-C5-C6-O6
4	F	3	BMA	O5-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6
4	F	3	BMA	C4-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6
5	K	2	NAG	O5-C5-C6-O6
4	J	1	NAG	C4-C5-C6-O6
4	F	1	NAG	C4-C5-C6-O6
6	O	4	MAN	C4-C5-C6-O6
4	J	1	NAG	O5-C5-C6-O6
3	E	2	NAG	C3-C2-N2-C7
4	J	2	NAG	C3-C2-N2-C7
3	M	1	NAG	O5-C5-C6-O6
4	F	1	NAG	O5-C5-C6-O6

There are no ring outliers.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	I	1	NAG	3	0
5	K	2	NAG	1	0
6	O	4	MAN	1	0
6	O	3	BMA	1	0
5	K	1	NAG	1	0
4	I	2	NAG	1	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.
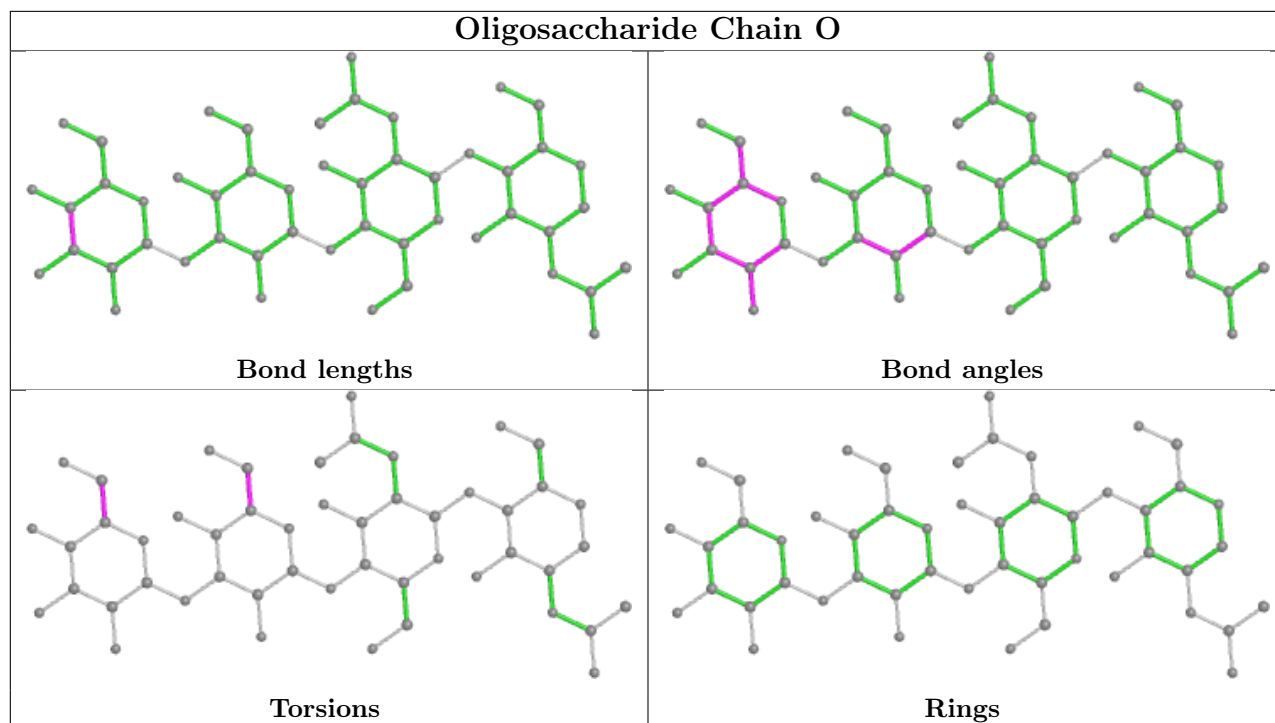

Oligosaccharide Chain E

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain G

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain M

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain F

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain I

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain J

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain K

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain O

5.6 Ligand geometry ⓘ

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 for Mogul analysis.

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	#$|Z|>2$
8	NAG	C	703	1	14,14,15	0.72	1 (7%)	17,19,21	1.06	1 (5%)
8	NAG	A	702	1	14,14,15	1.05	2 (14%)	17,19,21	1.06	1 (5%)
8	NAG	C	702	1	14,14,15	1.53	2 (14%)	17,19,21	2.08	2 (11%)

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
8	NAG	C	703	1	-	2/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	A	702	1	-	1/6/23/26	0/1/1/1
8	NAG	C	702	1	-	4/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	702	NAG	C1-C2	4.60	1.59	1.52
8	A	702	NAG	O5-C1	2.85	1.48	1.43
8	C	702	NAG	O5-C1	2.81	1.48	1.43
8	A	702	NAG	C1-C2	2.37	1.55	1.52
8	C	703	NAG	O5-C1	-2.36	1.39	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	702	NAG	C1-O5-C5	7.17	121.91	112.19
8	C	702	NAG	C4-C3-C2	4.47	117.57	111.02
8	A	702	NAG	C1-O5-C5	3.90	117.48	112.19
8	C	703	NAG	C1-O5-C5	2.88	116.10	112.19

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	C	702	NAG	C8-C7-N2-C2
8	C	702	NAG	O7-C7-N2-C2
8	C	702	NAG	O5-C5-C6-O6
8	A	702	NAG	O5-C5-C6-O6
8	C	703	NAG	C4-C5-C6-O6
8	C	703	NAG	O5-C5-C6-O6
8	C	702	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	703	NAG	2	0
8	C	702	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand NAG C 703

Bond lengths

Bond angles

Torsions

Rings

Ligand NAG A 702

Bond lengths

Bond angles

Torsions

Rings

Ligand NAG C 702

Bond lengths

Bond angles

Torsions

Rings
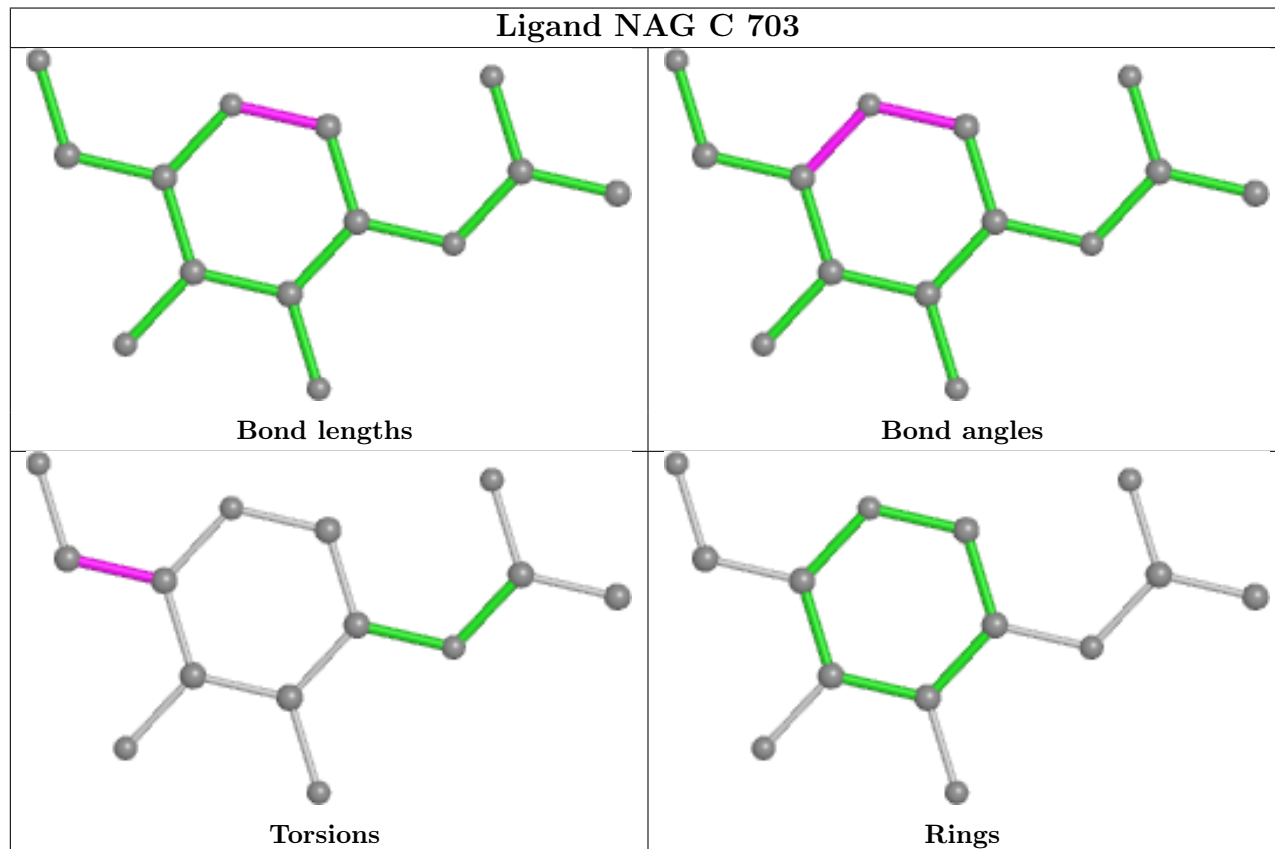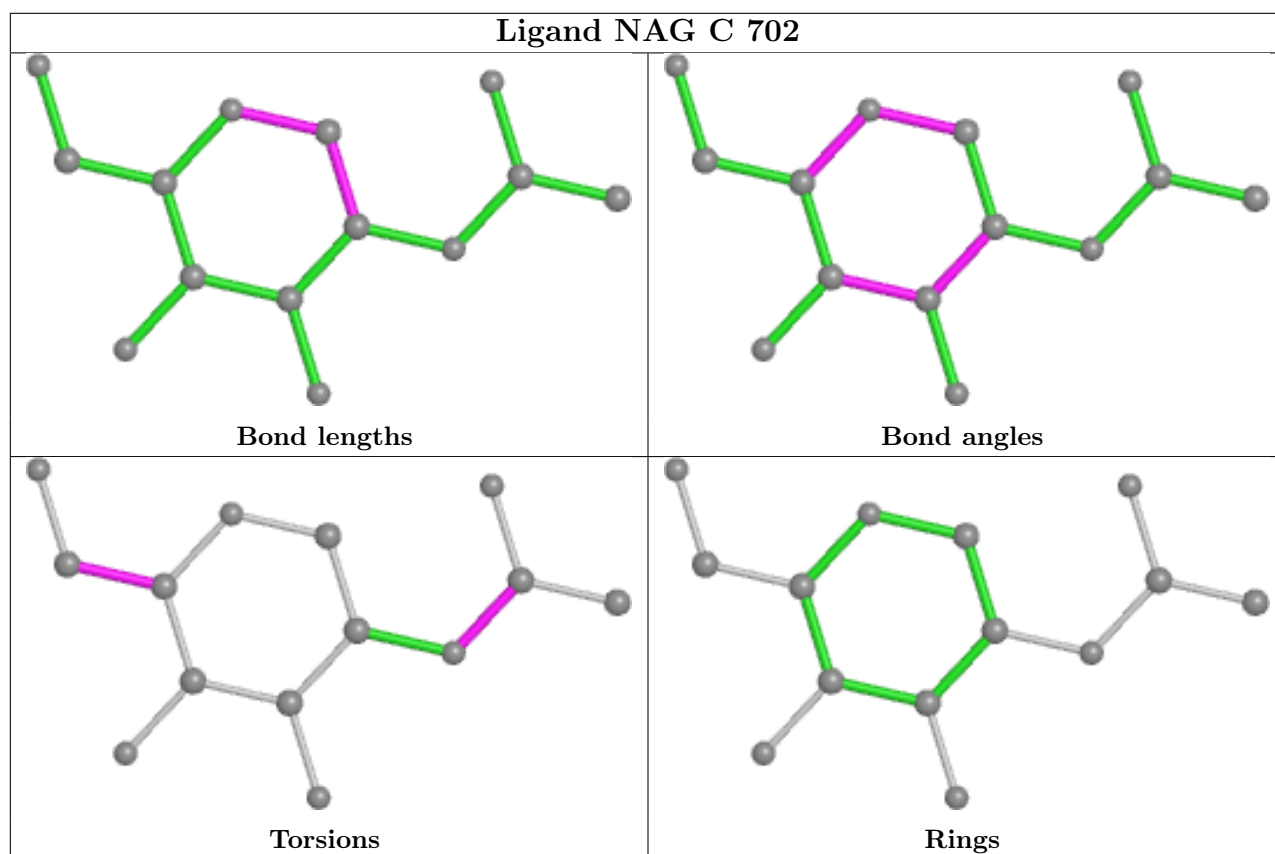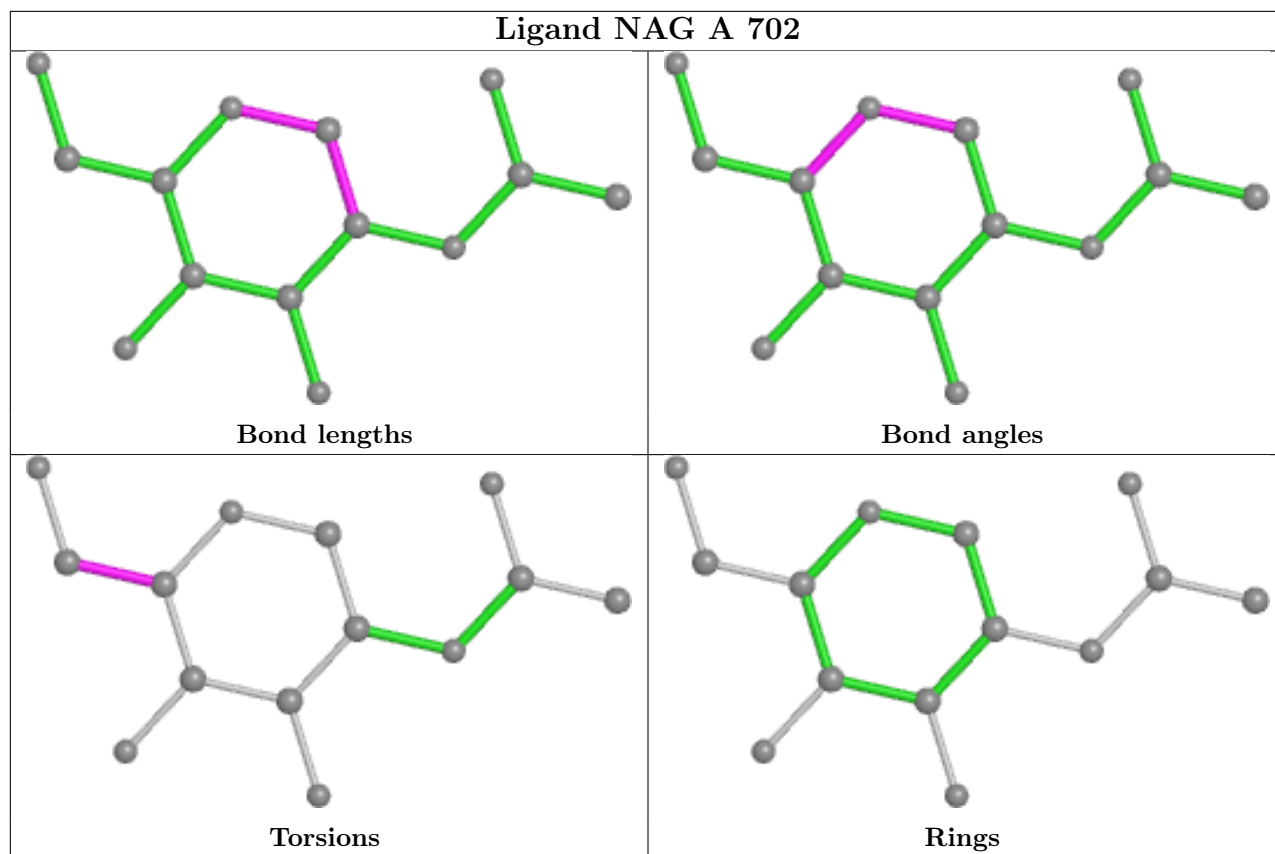
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data (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(Å²)	Q<0.9
1	A	596/608 (98%)	0.44	35 (5%)	22	25	92, 121, 173, 242	0
1	C	596/608 (98%)	0.32	26 (4%)	34	37	90, 120, 168, 252	0
2	B	195/234 (83%)	0.97	40 (20%)	1	1	108, 133, 205, 240	0
2	D	195/234 (83%)	0.94	35 (17%)	1	1	116, 132, 207, 267	0
All	All	1582/1684 (93%)	0.52	136 (8%)	10	12	90, 124, 182, 267	0

All (136) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	423	TYR	8.0
1	C	136	ASP	6.7
2	B	370	ASN	6.2
2	D	364	ASP	6.1
2	D	365	TYR	6.1
2	D	371	PHE	5.9
2	B	365	TYR	5.2
2	D	363	ALA	5.2
2	D	370	ASN	5.0
2	B	515	PHE	4.9
2	D	342	PHE	4.6
2	D	510	VAL	4.5
1	A	429	GLN	4.4
1	A	293	VAL	4.4
2	D	366	SER	4.1
2	D	515	PHE	4.0
2	B	338	PHE	4.0
1	A	289	PRO	3.9
1	A	423	LEU	3.9
2	B	392	PHE	3.8
1	A	428	PHE	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	137	ASN	3.7
1	C	137	ASN	3.7
2	D	511	VAL	3.7
1	C	211	GLY	3.6
2	B	368	LEU	3.6
2	D	372	ALA	3.5
2	B	337	PRO	3.5
2	D	513	LEU	3.5
2	B	369	TYR	3.5
2	B	395	VAL	3.4
2	B	371	PHE	3.4
2	D	435	ALA	3.4
2	D	378	LYS	3.3
1	C	464	PHE	3.3
1	C	212	VAL	3.3
2	D	377	PHE	3.3
2	D	518	LEU	3.3
1	C	115	ARG	3.2
2	B	364	ASP	3.2
1	A	21	ILE	3.2
1	A	148	LEU	3.2
2	D	390	LEU	3.2
2	B	335	LEU	3.1
2	B	410	ILE	3.1
2	B	333	THR	3.1
2	B	397	ALA	3.0
2	D	380	TYR	3.0
1	C	134	ASN	3.0
2	D	522	ALA	3.0
1	A	430	GLU	2.9
2	D	373	PRO	2.9
1	A	364	VAL	2.9
1	C	140	GLU	2.9
1	C	233	ILE	2.9
2	B	396	TYR	2.9
1	A	421	ILE	2.8
1	C	132	VAL	2.8
2	D	392	PHE	2.8
1	A	135	PRO	2.8
2	B	413	GLY	2.7
2	B	402	ILE	2.7
2	B	342	PHE	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	376	ALA	2.7
1	C	97	LEU	2.7
2	D	337	PRO	2.7
1	C	579	MET	2.6
2	D	455	LEU	2.6
1	A	140	GLU	2.6
2	B	377	PHE	2.6
2	B	401	VAL	2.5
2	D	433	VAL	2.5
1	C	266	LEU	2.5
1	C	521	TYR	2.5
1	A	297	MET	2.5
1	C	498	CYS	2.5
2	D	341	VAL	2.5
2	D	338	PHE	2.5
1	A	307	ILE	2.5
1	A	351	LEU	2.5
1	A	119	ILE	2.5
2	B	513	LEU	2.5
1	A	292	ASP	2.5
1	C	111	ASP	2.5
1	A	302	TRP	2.4
2	D	333	THR	2.4
2	B	400	PHE	2.4
1	A	564	GLU	2.4
2	B	434	ILE	2.4
1	C	578	ASN	2.4
1	A	142	LEU	2.4
2	D	367	VAL	2.4
1	C	402	GLU	2.4
1	C	36	ALA	2.4
1	A	123	MET	2.3
1	A	134	ASN	2.3
2	B	472	ILE	2.3
2	B	518	LEU	2.3
1	C	577	LYS	2.3
1	C	523	PHE	2.3
1	A	339	VAL	2.3
2	D	493	GLN	2.3
1	A	252	TYR	2.3
2	B	391	CYS	2.3
2	B	519	HIS	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	419	ALA	2.3
2	B	336	CYS	2.3
2	D	434	ILE	2.3
2	B	508	TYR	2.3
2	B	456	PHE	2.2
2	B	363	ALA	2.2
1	A	440	LEU	2.2
1	A	291	ILE	2.2
1	A	83	TYR	2.2
2	B	453	TYR	2.2
2	D	442	ASP	2.2
2	B	514	SER	2.1
1	A	168	TRP	2.1
2	D	436	TRP	2.1
1	C	87	GLU	2.1
2	B	510	VAL	2.1
1	A	342	ALA	2.1
2	D	481	ASN	2.1
2	B	455	LEU	2.1
1	C	525	PHE	2.1
1	C	581	VAL	2.1
1	A	240	LEU	2.1
1	A	507	SER	2.1
2	D	391	CYS	2.1
1	A	511	SER	2.1
2	B	433	VAL	2.0
1	A	141	CYS	2.0
1	C	583	PRO	2.0
2	B	432	CYS	2.0
1	C	142	LEU	2.0
1	A	308	PHE	2.0

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

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

6.3 Carbohydrates ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	MAN	O	4	11/12	0.52	0.54	120,153,173,174	0
5	MAN	K	4	11/12	0.54	0.38	132,152,160,164	0
3	NAG	E	2	14/15	0.60	0.40	140,168,183,186	0
5	BMA	K	3	11/12	0.68	0.32	151,169,176,178	0
6	BMA	O	3	11/12	0.69	0.35	158,170,174,178	0
3	NAG	G	2	14/15	0.76	0.50	153,165,179,183	0
3	NAG	E	1	14/15	0.77	0.23	136,158,167,171	0
4	BMA	F	3	11/12	0.77	0.17	133,142,154,159	0
4	NAG	F	1	14/15	0.79	0.26	125,148,159,160	0
4	NAG	I	1	14/15	0.80	0.25	123,146,155,158	0
6	NAG	O	1	14/15	0.80	0.25	102,144,158,159	0
4	BMA	J	3	11/12	0.81	0.20	139,155,162,164	0
4	NAG	I	2	14/15	0.83	0.22	143,159,165,173	0
4	NAG	J	2	14/15	0.83	0.28	125,160,167,168	0
6	NAG	O	2	14/15	0.85	0.19	139,155,166,169	0
4	NAG	F	2	14/15	0.88	0.18	135,150,162,163	0
3	NAG	M	1	14/15	0.88	0.18	94,124,129,136	0
4	BMA	I	3	11/12	0.89	0.12	144,162,170,177	0
3	NAG	M	2	14/15	0.91	0.18	129,141,156,156	0
5	NAG	K	2	14/15	0.91	0.16	127,133,145,158	0
4	NAG	J	1	14/15	0.92	0.12	102,121,140,146	0
5	NAG	K	1	14/15	0.92	0.25	112,119,131,132	0
3	NAG	G	1	14/15	0.92	0.24	119,153,155,160	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.
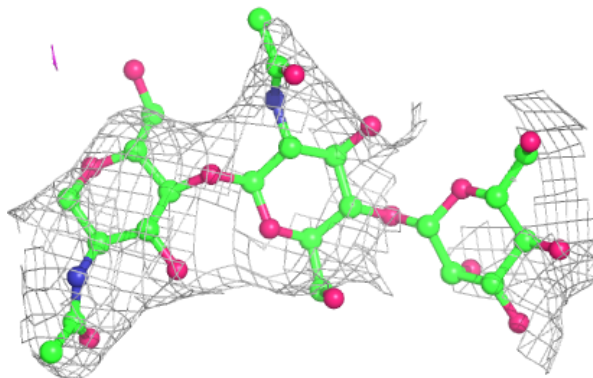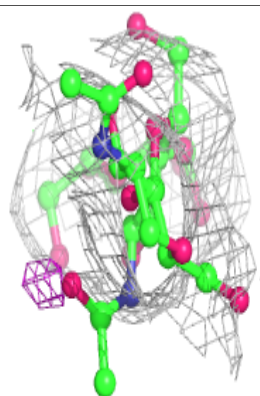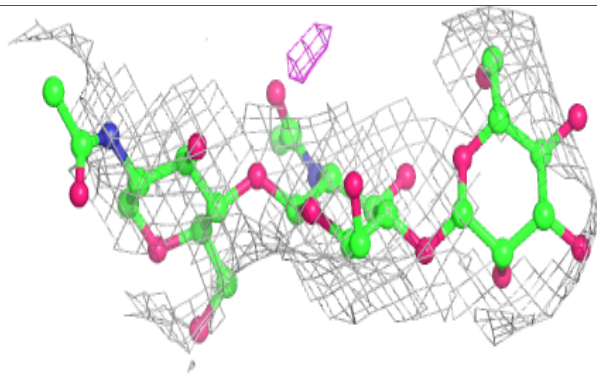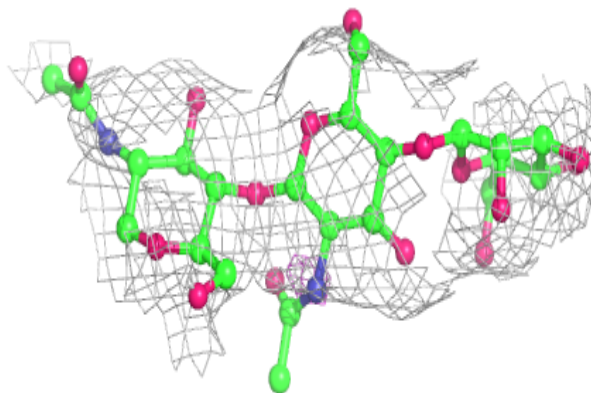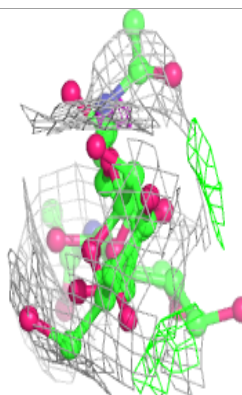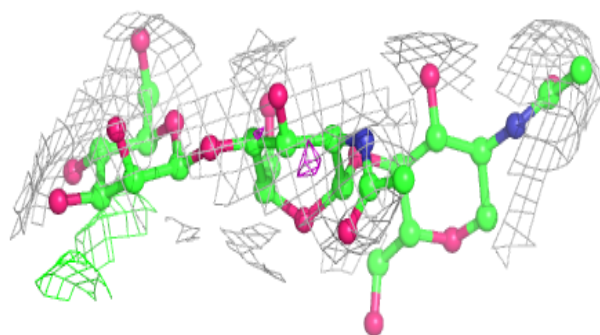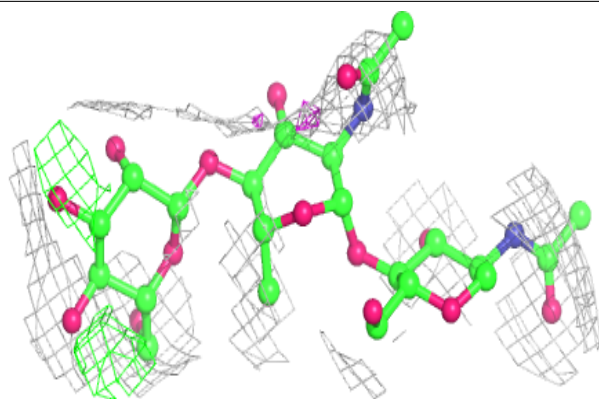
Electron density around Chain E:

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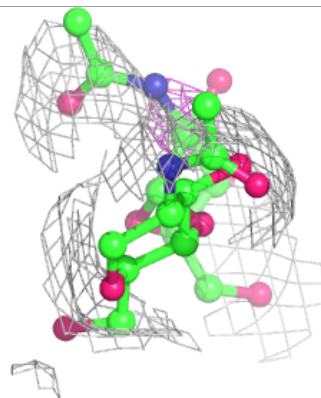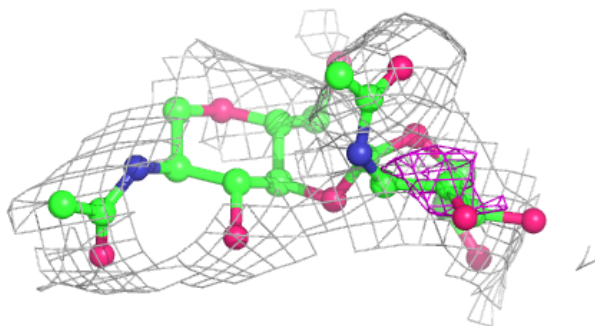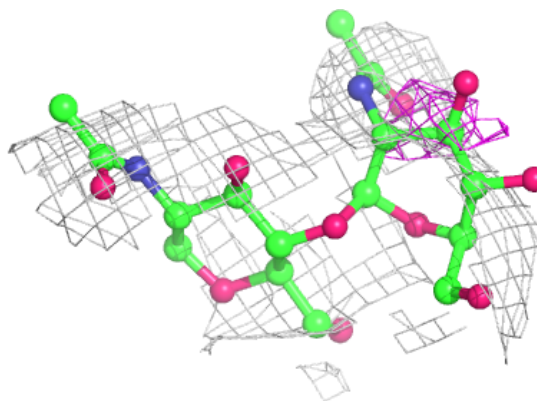

Electron density around Chain G:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
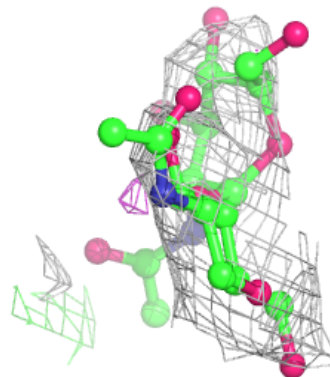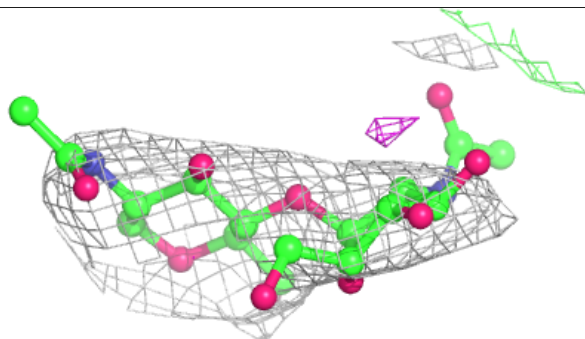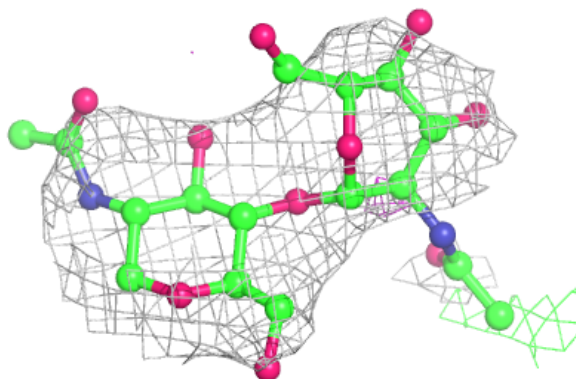
Electron density around Chain M:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
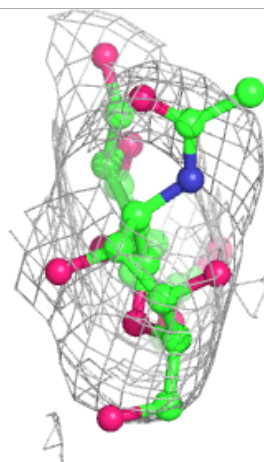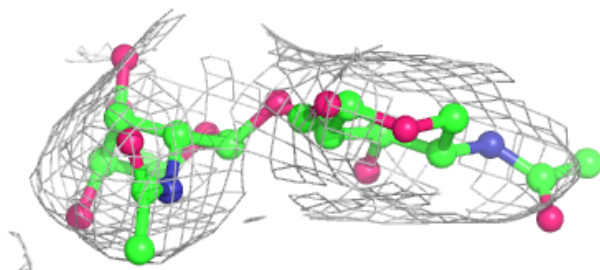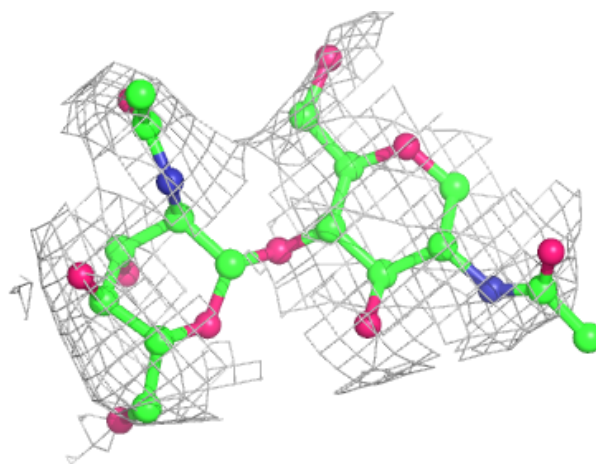
Electron density around Chain F:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
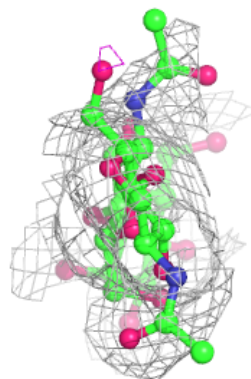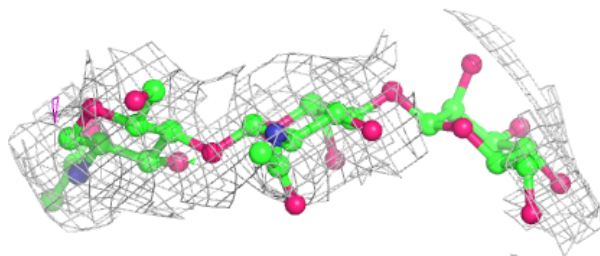
Electron density around Chain I:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
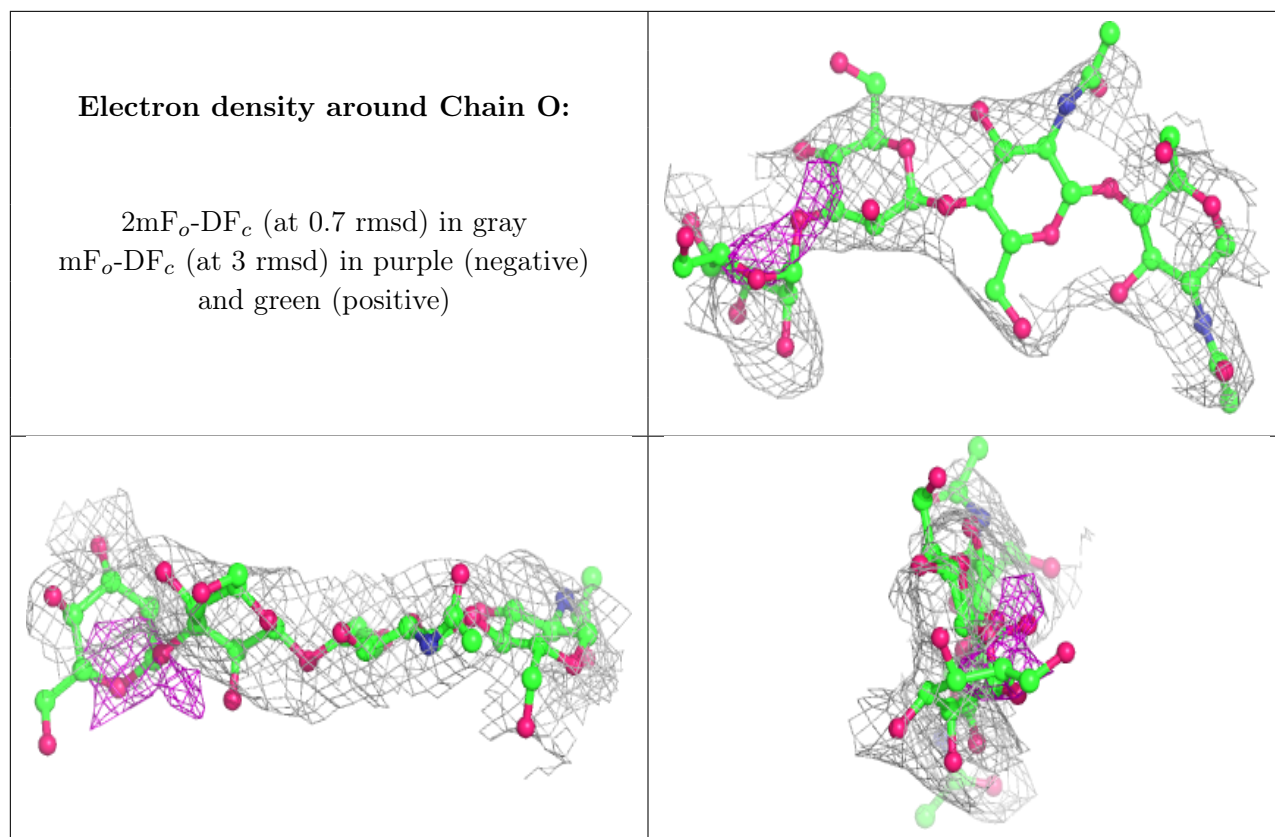and green (positive)

Electron density around Chain J:

$2mF_o$-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 K:

$2mF_o$-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 O:

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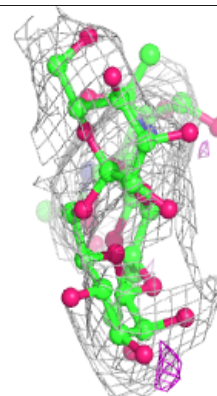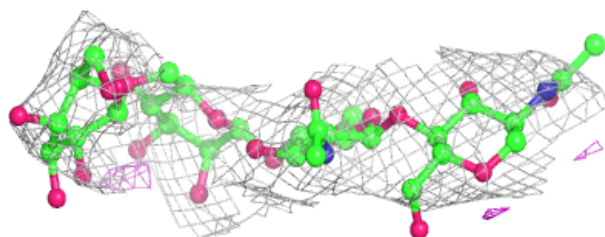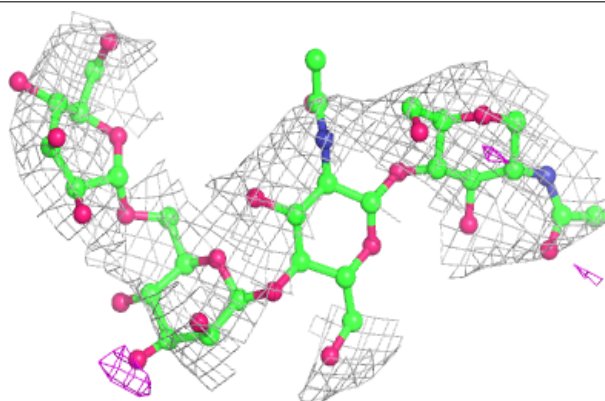
6.4 Ligands ⓘ

LIGAND-RSR INFOmissingINFO

6.5 Other polymers ⓘ

There are no such residues in this entry.