W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

Sep 17, 2023 – 07:19 AM EDT

PDB ID	:	4WA1
Title	:	The crystal structure of hemagglutinin from a H3N8 influenza virus isolated from New England harbor seals
Authors	:	Yang, H.; Villanueva, J.M.; Gubareva, L.V.; Stevens, J.
Deposited on	:	2014-08-28
Resolution	:	1.90 Å(reported)

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

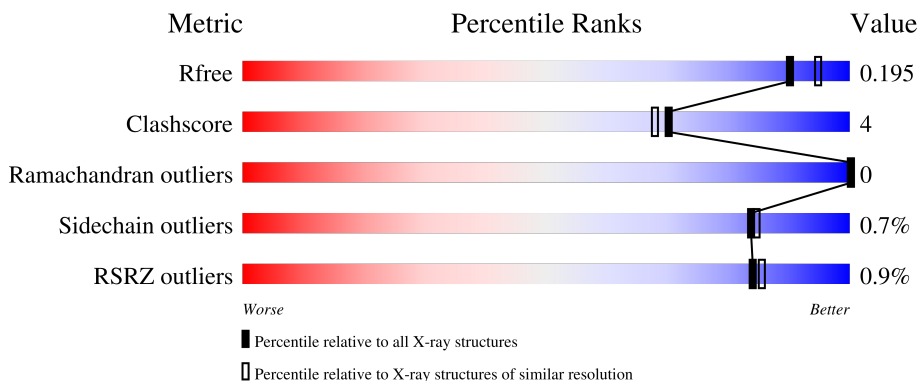|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 1.90 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		0.195
Clashscore		4
Ramachandran outliers		0
Sidechain outliers		0.7%
RSRZ outliers		0.9%

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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	496	93% 6% •
1	B	496	91% 7% •
1	C	496	91% 8% •
1	D	496	92% 7% •
1	E	496	92% 7% •

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Mol	Chain	Length	Quality of chain
1	F	496	93% 5%
2	G	2	50% 50%
2	H	2	100%
2	I	2	100%
2	J	2	50% 50%
2	L	2	50% 50%
2	M	2	100%
2	N	2	100%
2	P	2	100%
3	K	3	67% 33%
3	O	3	67% 33%

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 26664 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 Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	491	Total	C	N	O	S	0	0	0
			3860	2404	683	752	21			
1	B	491	Total	C	N	O	S	0	0	0
			3860	2404	683	752	21			
1	C	491	Total	C	N	O	S	0	0	0
			3860	2404	683	752	21			
1	D	491	Total	C	N	O	S	0	0	0
			3860	2404	683	752	21			
1	E	491	Total	C	N	O	S	0	0	0
			3860	2404	683	752	21			
1	F	491	Total	C	N	O	S	0	0	0
			3860	2404	683	752	21			

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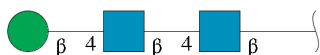

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	L	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	M	2	Total	C	N	O	0	0	0
			28	16	2	10			

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

- Molecule 3 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
3	K	3	Total 39	C 22	N 2	O 15	0	0	0
3	O	3	Total 39	C 22	N 2	O 15	0	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

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

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	527	Total 527	O 527	0	0
5	B	543	Total 543	O 543	0	0
5	C	499	Total 499	O 499	0	0
5	D	517	Total 517	O 517	0	0
5	E	501	Total 501	O 501	0	0
5	F	503	Total 503	O 503	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.
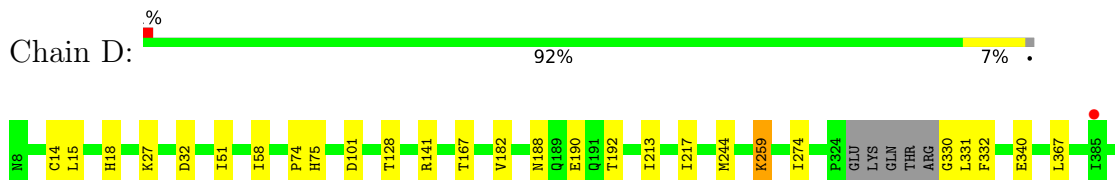
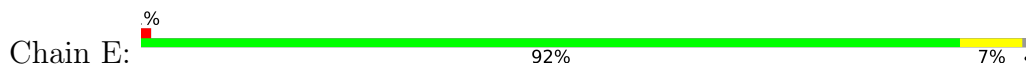- Molecule 1: Hemagglutinin
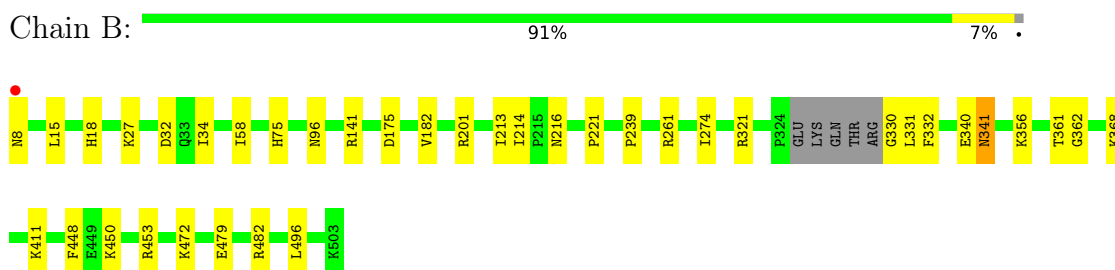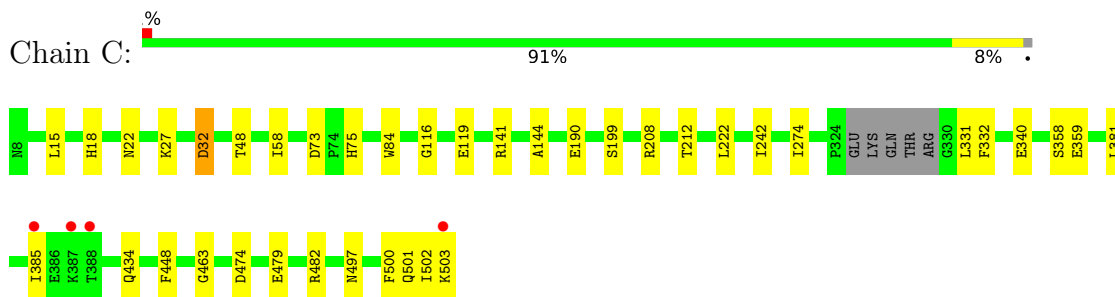
Chain A:

- Molecule 1: Hemagglutinin

Chain B:

- Molecule 1: Hemagglutinin

Chain C:

- Molecule 1: Hemagglutinin

Chain D:

T388 F448 R453 C466 D493 L496 N497 F500 Q501 I502 K503

• Molecule 1: Hemagglutinin

Chain E:

%

92%   7% •

N8 L15 H18 D32 T48 G49 I58 D73 P74 H75 W84 G116 E119 E135 A144 E190 S199 G200 R201 R208 L222 K259 I274 I278 N285 P324 GLU LYS GLN THR ARG G330 L331 E340 I347 E359

L381 I385 E386 K387 T388 F448 E449 D474 N483 F500 Q501 I502 K503

• Molecule 1: Hemagglutinin

Chain F:

%

93%   5% •

N8 L15 H18 K27 D32 I51 I58 P74 R141 T167 N188 T192 M244 I274 P324 GLU LYS GLN THR ARG G330 L331 F332 E340 E359 N382 E386 K387 T388 E401 F448 D474 D493 E494 N497 F500

Q501 I502 K503

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

Chain G: 50%   50%

NAG1 NAG2

• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose
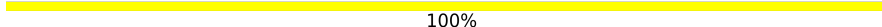
Chain H: 100%

NAG1 NAG2

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

Chain I: 100%

NAG1 NAG2

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

Chain J:

50%   50%

NAG1 NAG2

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

Chain L:

50%   50%

NAG1 NAG2

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

Chain M:

100%

NAG1 NAG2

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

Chain N:

100%

NAG1 NAG2

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

Chain P:

100%

NAG1 NAG2

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

Chain K:

67%   33%

NAG1 NAG2 BMA3

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

Chain O:

67%   33%

NAG1 NAG2 BMA3

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	80.06Å 103.16Å 110.86Å 89.95° 90.00° 90.28°	Depositor
Resolution (Å)	46.78 – 1.90 46.78 – 1.90	Depositor EDS
% Data completeness (in resolution range)	96.9 (46.78-1.90) 91.0 (46.78-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.42 (at 1.90Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.170 , 0.195 0.170 , 0.195	Depositor DCC
R_{free} test set	13742 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	19.0	Xtriage
Anisotropy	0.145	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 35.0	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.018 for h,-k,-l 0.019 for -h,k,-l 0.440 for -h,-k,l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	26664	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: BMA, 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	0.37	0/3937	0.56	0/5333
1	B	0.38	0/3937	0.56	1/5333 (0.0%)
1	C	0.37	0/3937	0.56	0/5333
1	D	0.38	0/3937	0.57	0/5333
1	E	0.37	0/3937	0.55	0/5333
1	F	0.38	0/3937	0.56	1/5333 (0.0%)
All	All	0.37	0/23622	0.56	2/31998 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
All	All	0	6

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	497	ASN	CB-CA-C	-6.66	97.08	110.40
1	B	341	ASN	N-CA-CB	-5.17	101.29	110.60

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	340	GLU	Peptide
1	B	340	GLU	Peptide
1	C	340	GLU	Peptide
1	D	340	GLU	Peptide
1	E	340	GLU	Peptide

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	3860	0	3739	23	0
1	B	3860	0	3739	37	0
1	C	3860	0	3739	31	0
1	D	3860	0	3739	39	0
1	E	3860	0	3739	26	0
1	F	3860	0	3739	25	0
2	G	28	0	25	1	0
2	H	28	0	25	0	0
2	I	28	0	25	0	0
2	J	28	0	25	1	0
2	L	28	0	25	3	0
2	M	28	0	25	0	0
2	N	28	0	25	0	0
2	P	28	0	25	2	0
3	K	39	0	34	1	0
3	O	39	0	34	0	0
4	A	28	0	26	1	0
4	B	28	0	26	0	0
4	C	14	0	13	0	0
4	D	14	0	13	0	0
4	E	14	0	13	0	0
4	F	14	0	13	0	0
5	A	527	0	0	16	1
5	B	543	0	0	18	1
5	C	499	0	0	12	0
5	D	517	0	0	7	0
5	E	501	0	0	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	503	0	0	1	2
All	All	26664	0	22806	166	2

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 4.

The worst 5 of 166 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:B:8:ASN:ND2	5:B:1136:HOH:O	1.92	1.02
1:B:201:ARG:NE	5:B:868:HOH:O	1.96	0.97
1:B:27:LYS:NZ	5:B:1236:HOH:O	1.99	0.96
1:D:500:PHE:HB2	1:D:502:ILE:HG13	1.52	0.91
1:C:141:ARG:NH2	5:C:1084:HOH:O	2.02	0.91

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:711:HOH:O	5:F:772:HOH:O[1_565]	1.99	0.21
5:A:849:HOH:O	5:F:785:HOH:O[1_556]	2.16	0.04

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	487/496 (98%)	472 (97%)	15 (3%)	0	100	100
1	B	487/496 (98%)	472 (97%)	15 (3%)	0	100	100
1	C	487/496 (98%)	470 (96%)	17 (4%)	0	100	100
1	D	487/496 (98%)	472 (97%)	15 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	487/496 (98%)	471 (97%)	16 (3%)	0	100	100
1	F	487/496 (98%)	472 (97%)	15 (3%)	0	100	100
All	All	2922/2976 (98%)	2829 (97%)	93 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	427/432 (99%)	425 (100%)	2 (0%)	88	89
1	B	427/432 (99%)	426 (100%)	1 (0%)	93	94
1	C	427/432 (99%)	423 (99%)	4 (1%)	78	79
1	D	427/432 (99%)	422 (99%)	5 (1%)	71	70
1	E	427/432 (99%)	423 (99%)	4 (1%)	78	79
1	F	427/432 (99%)	425 (100%)	2 (0%)	88	89
All	All	2562/2592 (99%)	2544 (99%)	18 (1%)	84	84

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	201	ARG
1	F	502	ILE
1	F	18	HIS
1	D	75	HIS
1	E	32	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	75	HIS
1	D	197	GLN

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Mol	Chain	Res	Type
1	E	18	HIS
1	F	355	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 ⓘ

22 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
2	NAG	G	1	1,2	14,14,15	0.47	0	17,19,21	0.57	0
2	NAG	G	2	2	14,14,15	0.43	0	17,19,21	0.43	0
2	NAG	H	1	1,2	14,14,15	0.50	0	17,19,21	0.48	0
2	NAG	H	2	2	14,14,15	0.33	0	17,19,21	0.44	0
2	NAG	I	1	1,2	14,14,15	0.22	0	17,19,21	0.46	0
2	NAG	I	2	2	14,14,15	0.40	0	17,19,21	0.39	0
2	NAG	J	1	1,2	14,14,15	0.53	0	17,19,21	0.41	0
2	NAG	J	2	2	14,14,15	0.43	0	17,19,21	0.52	0
3	NAG	K	1	1,3	14,14,15	0.25	0	17,19,21	0.54	0
3	NAG	K	2	3	14,14,15	0.22	0	17,19,21	0.48	0
3	BMA	K	3	3	11,11,12	0.59	0	15,15,17	1.15	2 (13%)
2	NAG	L	1	1,2	14,14,15	0.52	0	17,19,21	0.45	0
2	NAG	L	2	2	14,14,15	0.30	0	17,19,21	0.59	0
2	NAG	M	1	1,2	14,14,15	0.29	0	17,19,21	0.55	0
2	NAG	M	2	2	14,14,15	0.53	0	17,19,21	0.36	0
2	NAG	N	1	1,2	14,14,15	0.39	0	17,19,21	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
2	NAG	N	2	2	14,14,15	0.39	0	17,19,21	0.57	0
3	NAG	O	1	1,3	14,14,15	0.21	0	17,19,21	0.62	0
3	NAG	O	2	3	14,14,15	0.45	0	17,19,21	0.44	0
3	BMA	O	3	3	11,11,12	0.66	0	15,15,17	1.18	2 (13%)
2	NAG	P	1	1,2	14,14,15	0.31	0	17,19,21	0.53	0
2	NAG	P	2	2	14,14,15	0.42	0	17,19,21	0.68	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
2	NAG	G	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	2/6/23/26	0/1/1/1
2	NAG	H	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	0/6/23/26	0/1/1/1
2	NAG	I	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	I	2	2	-	0/6/23/26	0/1/1/1
2	NAG	J	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	J	2	2	-	0/6/23/26	0/1/1/1
3	NAG	K	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	K	2	3	-	2/6/23/26	0/1/1/1
3	BMA	K	3	3	-	0/2/19/22	0/1/1/1
2	NAG	L	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	L	2	2	-	0/6/23/26	0/1/1/1
2	NAG	M	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	M	2	2	-	0/6/23/26	0/1/1/1
2	NAG	N	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	N	2	2	-	0/6/23/26	0/1/1/1
3	NAG	O	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	O	2	3	-	0/6/23/26	0/1/1/1
3	BMA	O	3	3	-	2/2/19/22	0/1/1/1
2	NAG	P	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	P	2	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	K	3	BMA	C1-O5-C5	3.32	116.69	112.19
3	O	3	BMA	C1-O5-C5	2.83	116.03	112.19
3	O	3	BMA	O2-C2-C3	-2.42	105.29	110.14
2	P	2	NAG	C1-O5-C5	2.11	115.05	112.19
3	K	3	BMA	O2-C2-C3	-2.08	105.97	110.14

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	P	2	NAG	O5-C5-C6-O6
2	G	2	NAG	O5-C5-C6-O6
2	P	2	NAG	C4-C5-C6-O6
2	G	2	NAG	C4-C5-C6-O6
3	O	3	BMA	C4-C5-C6-O6

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L	1	NAG	3	0
2	G	2	NAG	1	0
3	K	3	BMA	1	0
2	J	2	NAG	1	0
2	P	1	NAG	2	0

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

Oligosaccharide Chain G

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain H

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 L

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain M

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain N

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain P

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain K

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain O

Bond lengths

Bond angles

Torsions

Rings

5.6 Ligand geometry ⓘ

8 ligands 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	C	605	1	14,14,15	0.46	0	17,19,21	0.70	1 (5%)
4	NAG	B	601	1	14,14,15	0.37	0	17,19,21	0.72	1 (5%)
4	NAG	A	601	1	14,14,15	0.31	0	17,19,21	0.71	0
4	NAG	B	604	1	14,14,15	0.25	0	17,19,21	0.63	0
4	NAG	A	604	1	14,14,15	0.31	0	17,19,21	0.62	0
4	NAG	D	606	1	14,14,15	0.62	1 (7%)	17,19,21	0.52	0
4	NAG	F	606	1	14,14,15	0.47	0	17,19,21	0.44	0
4	NAG	E	605	1	14,14,15	0.25	0	17,19,21	0.50	0

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	C	605	1	-	2/6/23/26	0/1/1/1
4	NAG	B	601	1	-	0/6/23/26	0/1/1/1
4	NAG	A	601	1	-	0/6/23/26	0/1/1/1
4	NAG	B	604	1	-	2/6/23/26	0/1/1/1
4	NAG	A	604	1	-	2/6/23/26	0/1/1/1
4	NAG	D	606	1	-	2/6/23/26	0/1/1/1
4	NAG	F	606	1	-	2/6/23/26	0/1/1/1
4	NAG	E	605	1	-	1/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	606	NAG	C1-C2	2.04	1.55	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	605	NAG	C1-O5-C5	2.11	115.05	112.19
4	B	601	NAG	C1-O5-C5	2.02	114.93	112.19

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	605	NAG	O5-C5-C6-O6
4	A	604	NAG	C4-C5-C6-O6
4	B	604	NAG	C4-C5-C6-O6
4	C	605	NAG	C4-C5-C6-O6
4	A	604	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
4	A	604	NAG	1	0

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 ⓘ

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(Å²)	Q<0.9
1	A	491/496 (98%)	-0.39	3 (0%)	89	90	15, 24, 40, 66	0
1	B	491/496 (98%)	-0.31	1 (0%)	95	95	14, 23, 39, 66	0
1	C	491/496 (98%)	-0.26	4 (0%)	86	87	13, 26, 43, 82	0
1	D	491/496 (98%)	-0.22	6 (1%)	79	81	14, 25, 47, 128	0
1	E	491/496 (98%)	-0.32	5 (1%)	82	84	15, 26, 45, 77	0
1	F	491/496 (98%)	-0.27	7 (1%)	75	77	15, 26, 47, 136	0
All	All	2946/2976 (98%)	-0.30	26 (0%)	84	85	13, 25, 43, 136	0

The worst 5 of 26 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	502	ILE	17.0
1	F	502	ILE	16.7
1	D	503	LYS	12.4
1	F	503	LYS	9.6
1	D	501	GLN	5.1

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

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

6.3 Carbohydrates ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	BMA	O	3	11/12	0.80	0.16	60,64,67,67	0
3	BMA	K	3	11/12	0.88	0.12	58,65,67,67	0
3	NAG	K	2	14/15	0.88	0.12	41,43,49,50	0
2	NAG	P	2	14/15	0.89	0.10	22,37,43,45	0
3	NAG	O	1	14/15	0.90	0.12	29,36,40,44	0
3	NAG	O	2	14/15	0.90	0.13	41,45,53,53	0
2	NAG	I	2	14/15	0.90	0.14	45,48,50,51	0
2	NAG	I	1	14/15	0.91	0.12	29,38,45,46	0
2	NAG	G	1	14/15	0.92	0.11	23,31,39,41	0
2	NAG	M	1	14/15	0.92	0.15	31,39,50,50	0
2	NAG	M	2	14/15	0.92	0.14	43,46,51,51	0
2	NAG	H	1	14/15	0.93	0.12	23,29,36,37	0
2	NAG	H	2	14/15	0.93	0.10	27,36,46,50	0
2	NAG	N	2	14/15	0.93	0.10	32,40,48,51	0
2	NAG	L	2	14/15	0.93	0.10	22,34,42,46	0
3	NAG	K	1	14/15	0.93	0.09	29,35,39,44	0
2	NAG	G	2	14/15	0.94	0.10	26,34,45,49	0
2	NAG	N	1	14/15	0.94	0.09	22,35,45,49	0
2	NAG	J	2	14/15	0.95	0.09	26,41,46,48	0
2	NAG	P	1	14/15	0.95	0.07	23,32,39,41	0
2	NAG	L	1	14/15	0.95	0.08	21,28,36,39	0
2	NAG	J	1	14/15	0.96	0.09	22,34,42,45	0

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

Electron density around Chain G:

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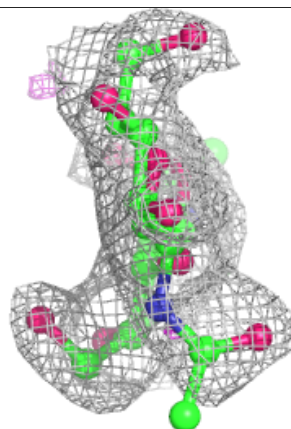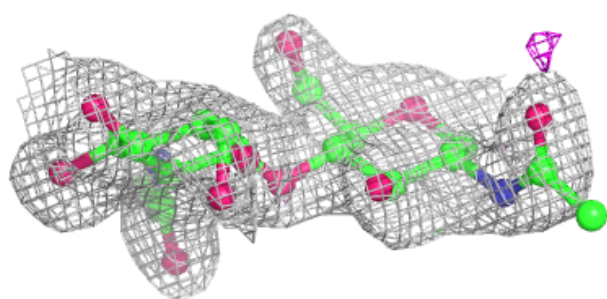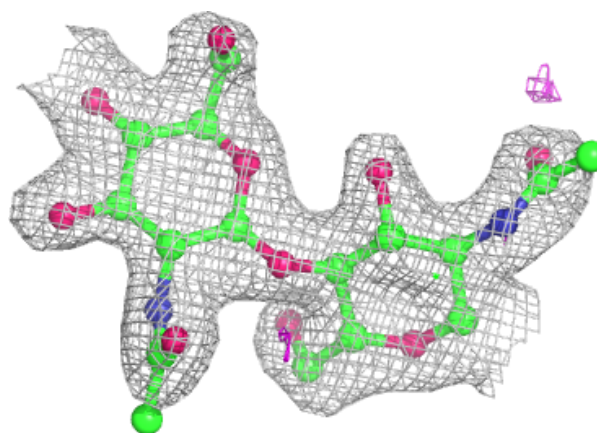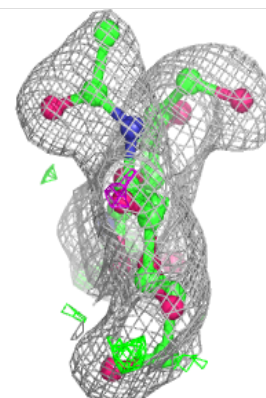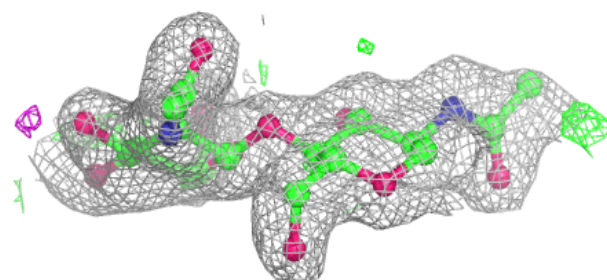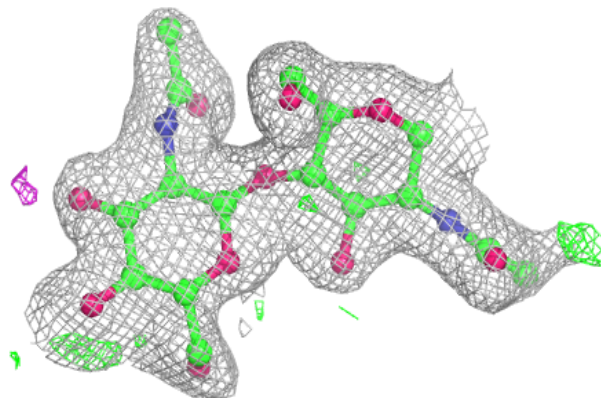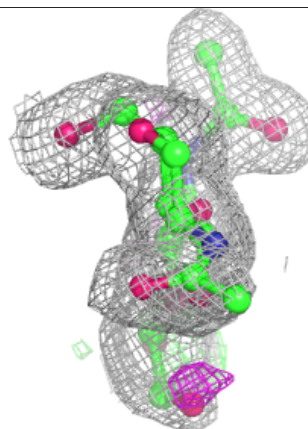mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
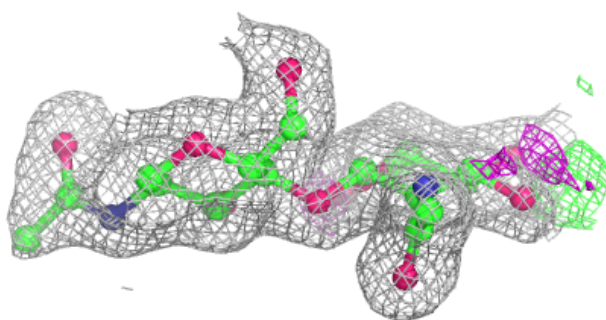and green (positive)
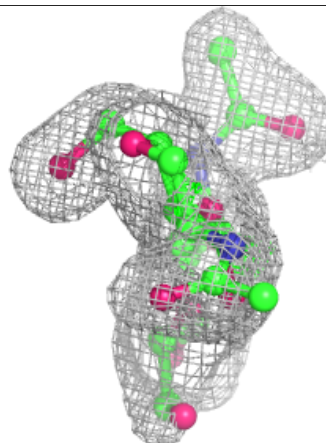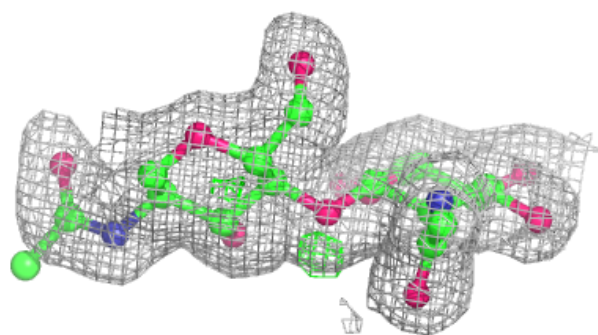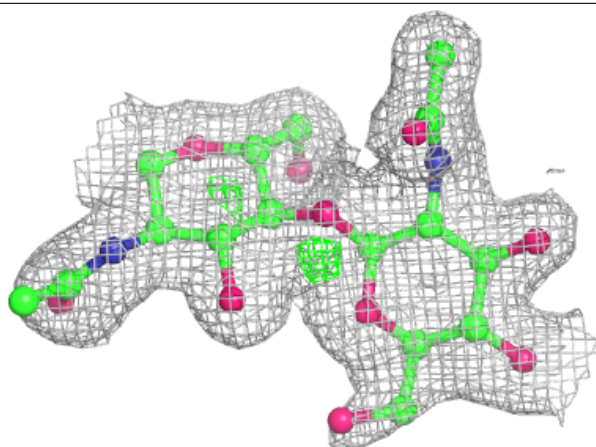
Electron density around Chain H:

$2mF_o$-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:

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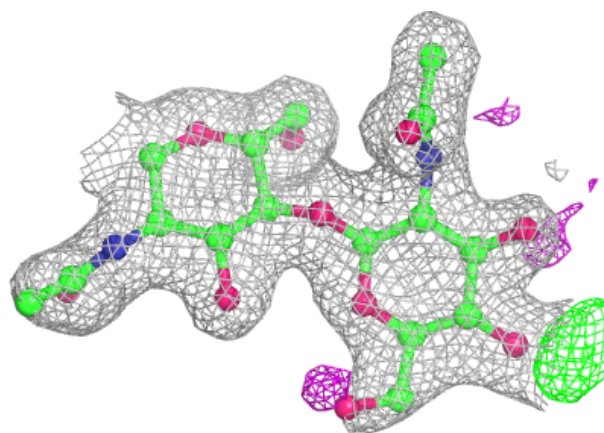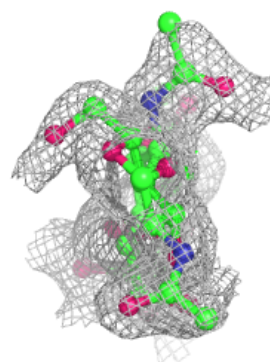and green (positive)

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)
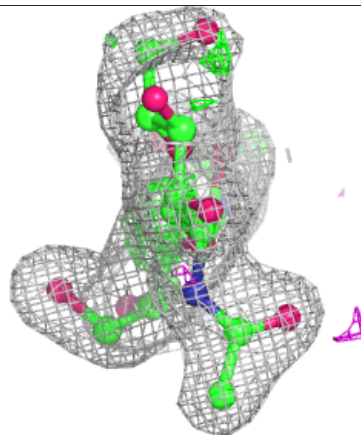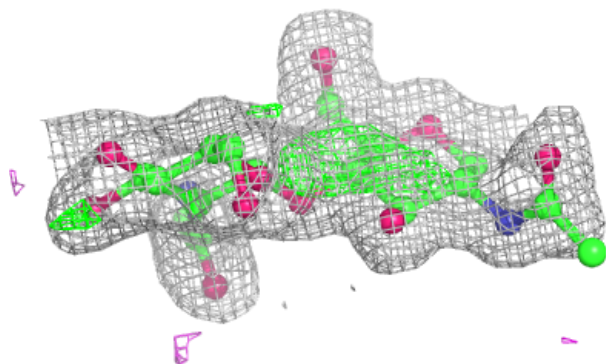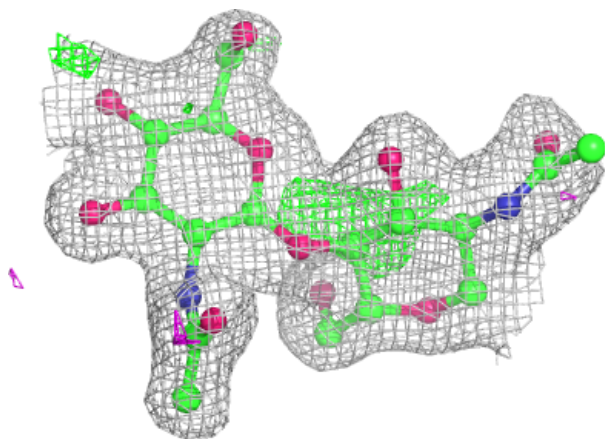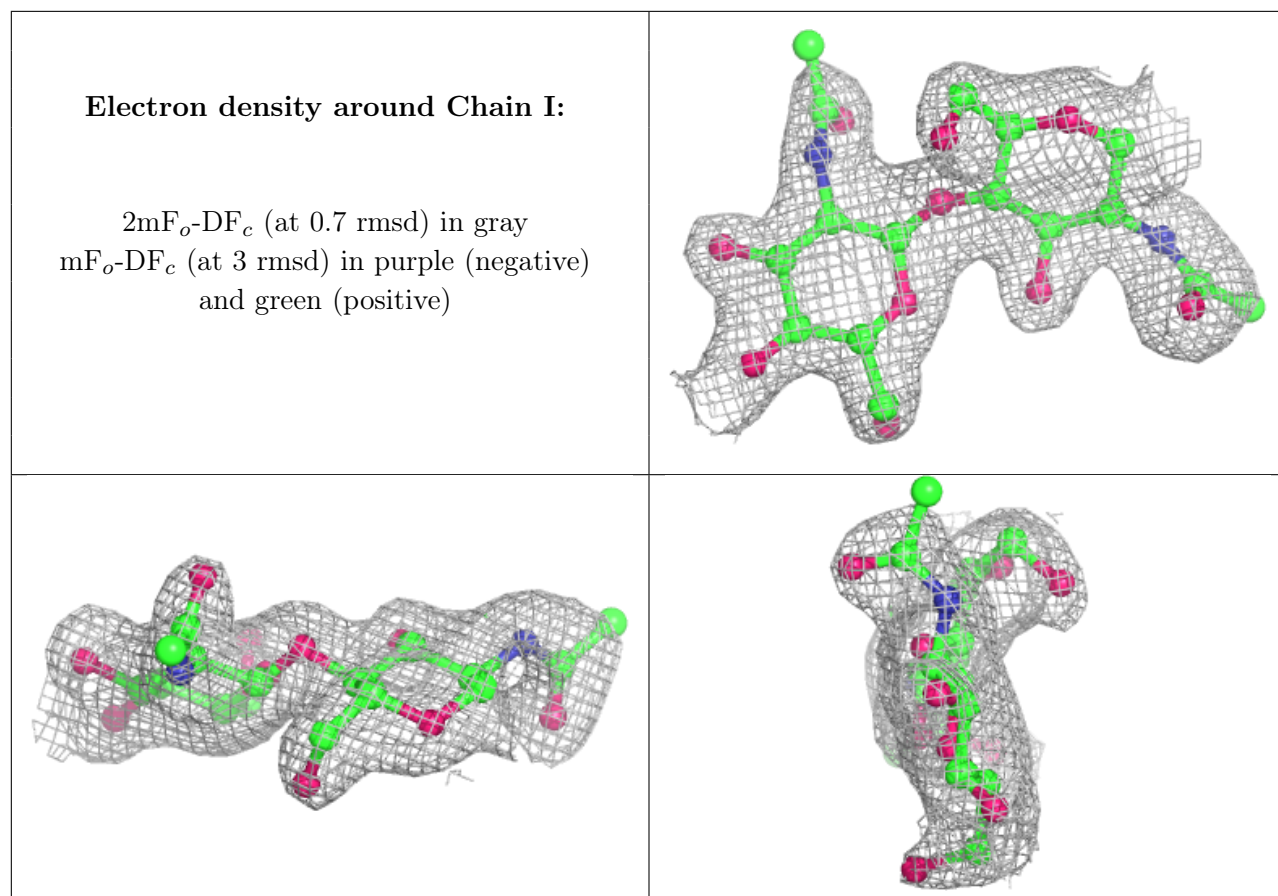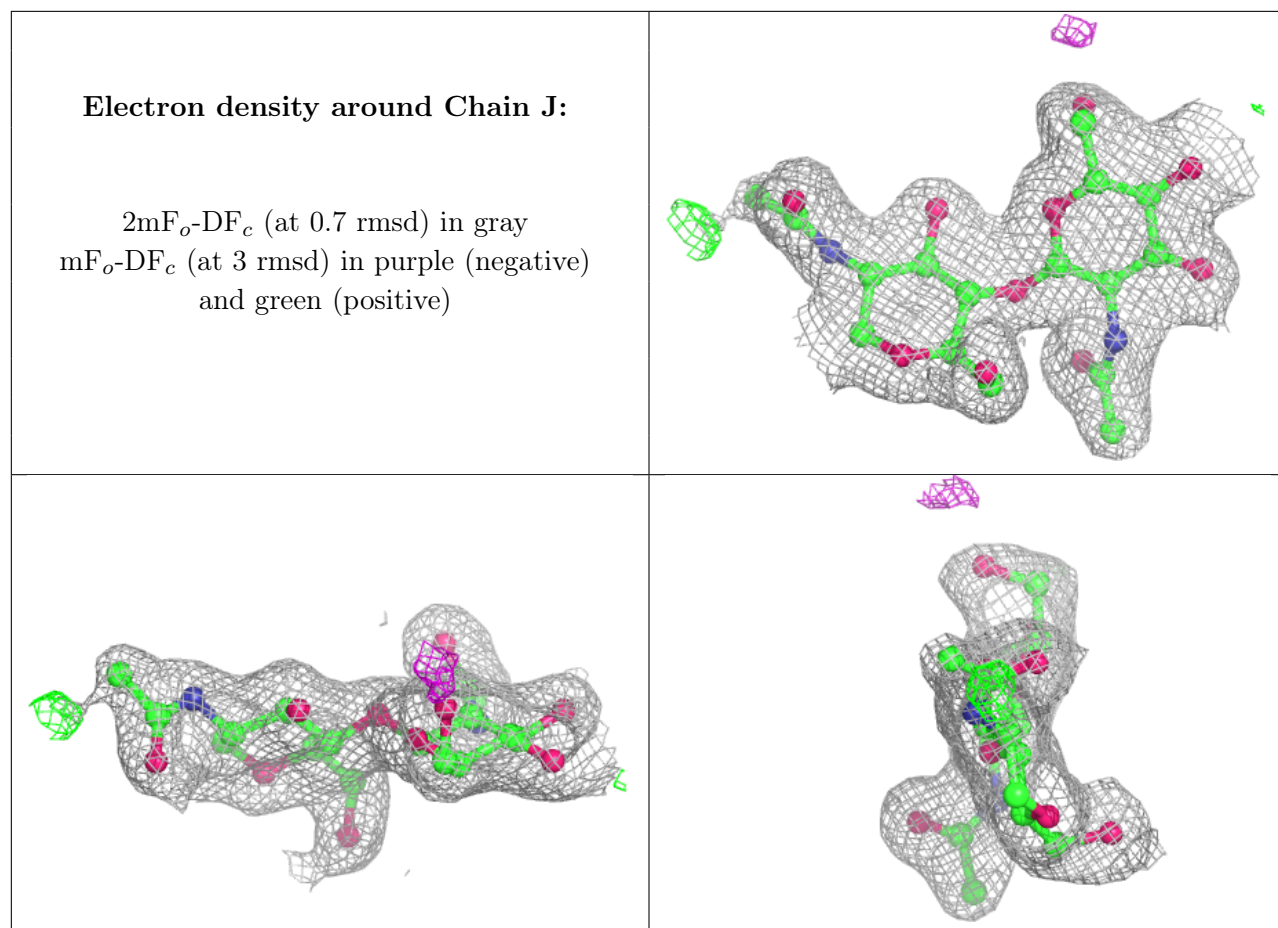
Electron density around Chain L:

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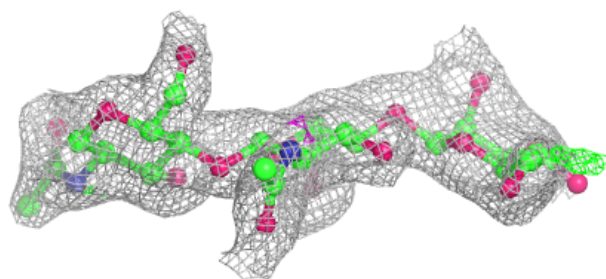and green (positive)
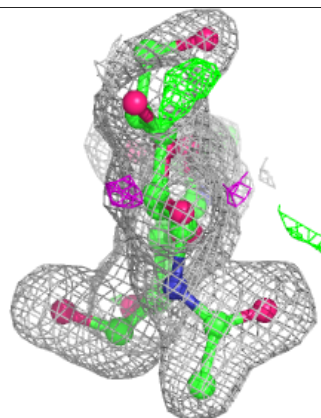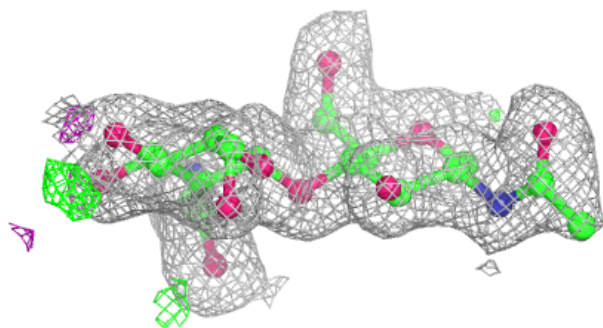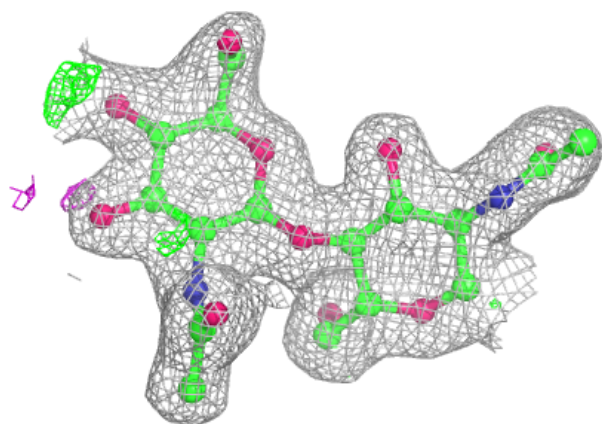
Electron density around Chain M:

$2mF_o$-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 N:

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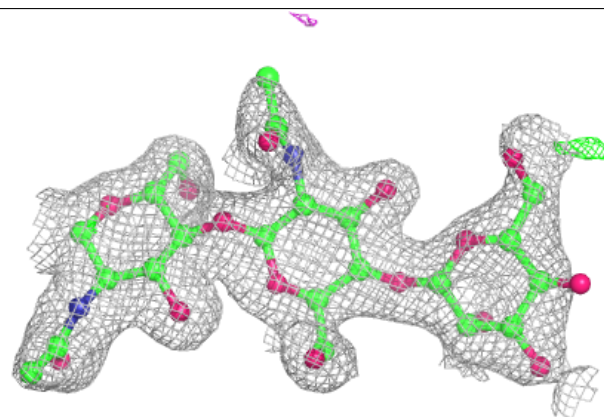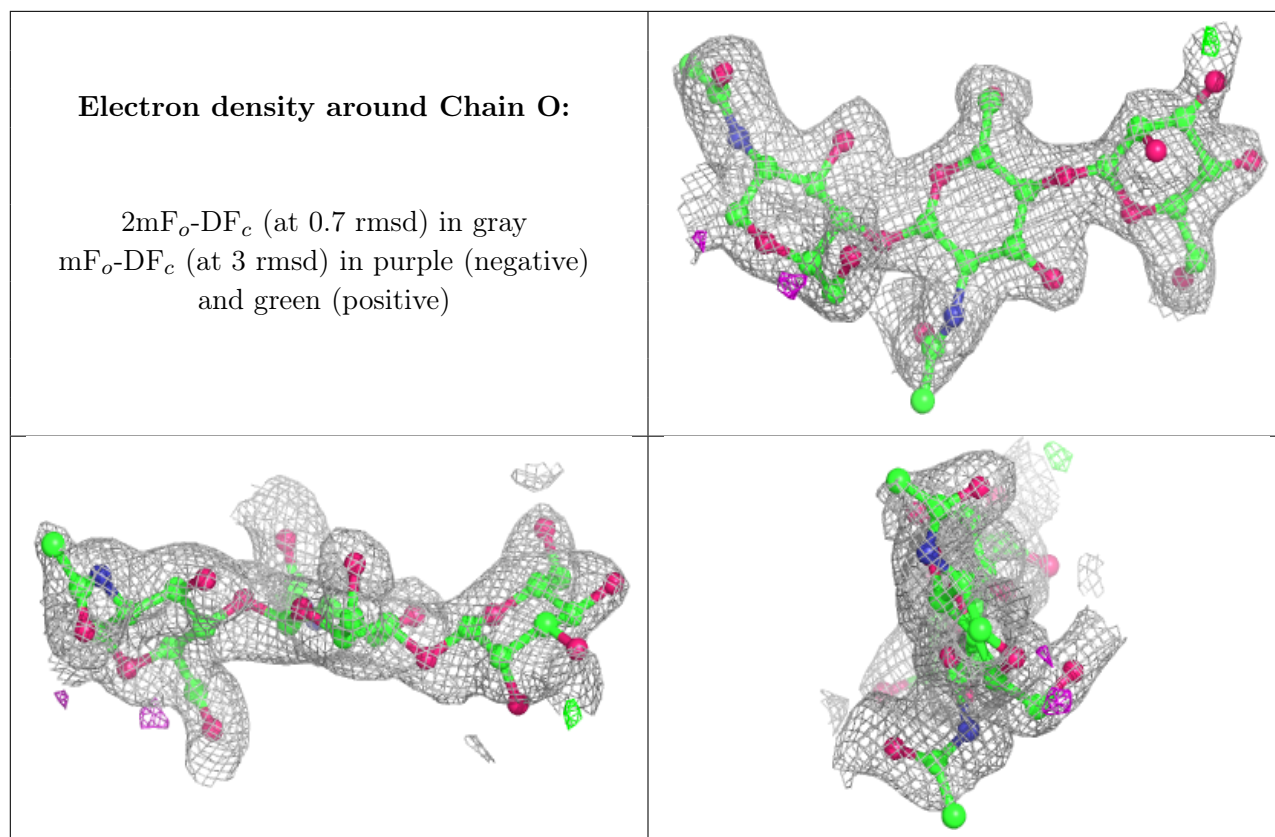and green (positive)

Electron density around Chain P:

$2mF_o-DF_c$ (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:

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

6.4 Ligands ⓘ

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	A	604	14/15	0.85	0.12	34,38,44,45	0
4	NAG	B	601	14/15	0.86	0.16	31,41,48,49	0
4	NAG	A	601	14/15	0.87	0.17	35,43,50,54	0
4	NAG	C	605	14/15	0.87	0.13	36,44,52,56	0
4	NAG	E	605	14/15	0.88	0.10	37,44,48,51	0
4	NAG	D	606	14/15	0.89	0.15	30,37,44,46	0
4	NAG	B	604	14/15	0.89	0.09	33,37,46,47	0
4	NAG	F	606	14/15	0.89	0.16	30,38,43,44	0

6.5 Other polymers ⓘ

There are no such residues in this entry.