WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Mar 5, 2024 – 02:56 AM EST

PDB ID	:	8V06
Title	:	Crystal structure of mouse PLD3 co-crystallized with 5'Pi-ssDNA for 9 days
Authors	:	Yuan, M.; Wilson, I.A.
Deposited on	:	2023-11-17
Resolution	:	2.73 Å(reported)

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

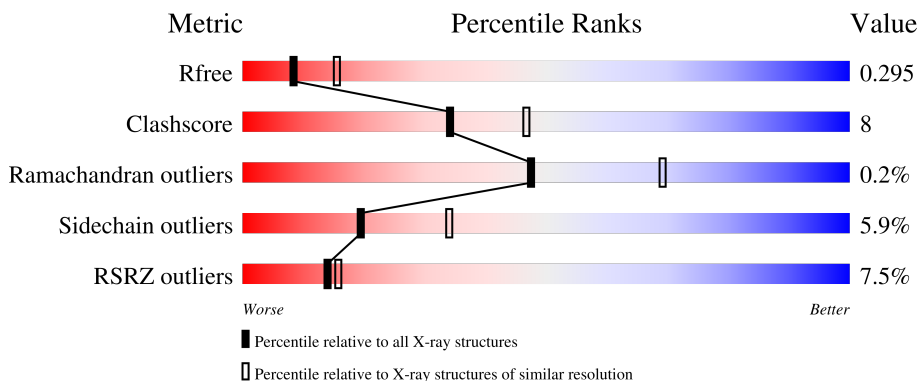|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 2.73 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.
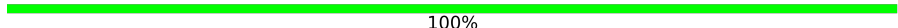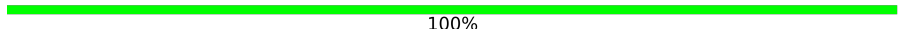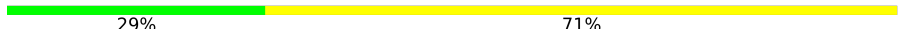
Metric	Percentile Ranks	Value
Rfree		0.295
Clashscore		8
Ramachandran outliers		0.2%
Sidechain outliers		5.9%
RSRZ outliers		7.5%

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	1271 (2.76-2.72)
Clashscore	141614	1322 (2.76-2.72)
Ramachandran outliers	138981	1297 (2.76-2.72)
Sidechain outliers	138945	1298 (2.76-2.72)
RSRZ outliers	127900	1243 (2.76-2.72)

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	467	2% / 69% 18% · 12%
1	C	467	9% / 67% 20% · 12%
2	B	467	2% / 70% 18% · 11%
2	D	467	13% / 68% 19% · 12%
3	E	2	100%

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Mol	Chain	Length	Quality of chain
3	I	2	100%
4	F	3	67% 33%
4	G	3	100%
5	H	7	29% 71%

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	F	2	-	-	-	X
4	BMA	F	3	-	-	-	X
6	NAG	D	501	-	-	-	X

2 Entry composition ⓘ

There are 8 unique types of molecules in this entry. The entry contains 13397 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 5'-3' exonuclease PLD3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	412	Total	C	N	O	P	S	0	0	0
			3229	2040	562	609	1	17			
1	C	412	Total	C	N	O	P	S	0	0	0
			3227	2039	561	609	1	17			

There are 82 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	HIS	-	expression tag	UNP O35405
A	23	HIS	-	expression tag	UNP O35405
A	24	HIS	-	expression tag	UNP O35405
A	25	HIS	-	expression tag	UNP O35405
A	26	HIS	-	expression tag	UNP O35405
A	27	HIS	-	expression tag	UNP O35405
A	28	GLY	-	expression tag	UNP O35405
A	29	PRO	-	expression tag	UNP O35405
A	30	LEU	-	expression tag	UNP O35405
A	31	VAL	-	expression tag	UNP O35405
A	32	ASP	-	expression tag	UNP O35405
A	33	VAL	-	expression tag	UNP O35405
A	34	ALA	-	expression tag	UNP O35405
A	35	SER	-	expression tag	UNP O35405
A	36	ASN	-	expression tag	UNP O35405
A	37	GLU	-	expression tag	UNP O35405
A	38	GLN	-	expression tag	UNP O35405
A	39	LYS	-	expression tag	UNP O35405
A	40	LEU	-	expression tag	UNP O35405
A	41	ILE	-	expression tag	UNP O35405
A	42	SER	-	expression tag	UNP O35405
A	43	GLU	-	expression tag	UNP O35405
A	44	GLU	-	expression tag	UNP O35405
A	45	ASP	-	expression tag	UNP O35405
A	46	LEU	-	expression tag	UNP O35405

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PROTEIN DATA BANK

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Chain	Residue	Modelled	Actual	Comment	Reference
A	47	ALA	-	expression tag	UNP O35405
A	48	SER	-	expression tag	UNP O35405
A	49	MET	-	expression tag	UNP O35405
A	50	THR	-	expression tag	UNP O35405
A	51	GLY	-	expression tag	UNP O35405
A	52	GLY	-	expression tag	UNP O35405
A	53	GLN	-	expression tag	UNP O35405
A	54	GLN	-	expression tag	UNP O35405
A	55	MET	-	expression tag	UNP O35405
A	56	GLY	-	expression tag	UNP O35405
A	57	ARG	-	expression tag	UNP O35405
A	58	ASP	-	expression tag	UNP O35405
A	59	ILE	-	expression tag	UNP O35405
A	60	GLU	-	expression tag	UNP O35405
A	61	GLY	-	expression tag	UNP O35405
A	62	ARG	-	expression tag	UNP O35405
C	22	HIS	-	expression tag	UNP O35405
C	23	HIS	-	expression tag	UNP O35405
C	24	HIS	-	expression tag	UNP O35405
C	25	HIS	-	expression tag	UNP O35405
C	26	HIS	-	expression tag	UNP O35405
C	27	HIS	-	expression tag	UNP O35405
C	28	GLY	-	expression tag	UNP O35405
C	29	PRO	-	expression tag	UNP O35405
C	30	LEU	-	expression tag	UNP O35405
C	31	VAL	-	expression tag	UNP O35405
C	32	ASP	-	expression tag	UNP O35405
C	33	VAL	-	expression tag	UNP O35405
C	34	ALA	-	expression tag	UNP O35405
C	35	SER	-	expression tag	UNP O35405
C	36	ASN	-	expression tag	UNP O35405
C	37	GLU	-	expression tag	UNP O35405
C	38	GLN	-	expression tag	UNP O35405
C	39	LYS	-	expression tag	UNP O35405
C	40	LEU	-	expression tag	UNP O35405
C	41	ILE	-	expression tag	UNP O35405
C	42	SER	-	expression tag	UNP O35405
C	43	GLU	-	expression tag	UNP O35405
C	44	GLU	-	expression tag	UNP O35405
C	45	ASP	-	expression tag	UNP O35405
C	46	LEU	-	expression tag	UNP O35405
C	47	ALA	-	expression tag	UNP O35405

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Chain	Residue	Modelled	Actual	Comment	Reference
C	48	SER	-	expression tag	UNP O35405
C	49	MET	-	expression tag	UNP O35405
C	50	THR	-	expression tag	UNP O35405
C	51	GLY	-	expression tag	UNP O35405
C	52	GLY	-	expression tag	UNP O35405
C	53	GLN	-	expression tag	UNP O35405
C	54	GLN	-	expression tag	UNP O35405
C	55	MET	-	expression tag	UNP O35405
C	56	GLY	-	expression tag	UNP O35405
C	57	ARG	-	expression tag	UNP O35405
C	58	ASP	-	expression tag	UNP O35405
C	59	ILE	-	expression tag	UNP O35405
C	60	GLU	-	expression tag	UNP O35405
C	61	GLY	-	expression tag	UNP O35405
C	62	ARG	-	expression tag	UNP O35405

- Molecule 2 is a protein called 5'-3' exonuclease PLD3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	416	Total 3252	C 2055	N 567	O 613	S 17	0	0	0
2	D	413	Total 3233	C 2045	N 564	O 607	S 17	0	0	0

There are 82 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	22	HIS	-	expression tag	UNP O35405
B	23	HIS	-	expression tag	UNP O35405
B	24	HIS	-	expression tag	UNP O35405
B	25	HIS	-	expression tag	UNP O35405
B	26	HIS	-	expression tag	UNP O35405
B	27	HIS	-	expression tag	UNP O35405
B	28	GLY	-	expression tag	UNP O35405
B	29	PRO	-	expression tag	UNP O35405
B	30	LEU	-	expression tag	UNP O35405
B	31	VAL	-	expression tag	UNP O35405
B	32	ASP	-	expression tag	UNP O35405
B	33	VAL	-	expression tag	UNP O35405
B	34	ALA	-	expression tag	UNP O35405
B	35	SER	-	expression tag	UNP O35405
B	36	ASN	-	expression tag	UNP O35405

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Chain	Residue	Modelled	Actual	Comment	Reference
B	37	GLU	-	expression tag	UNP O35405
B	38	GLN	-	expression tag	UNP O35405
B	39	LYS	-	expression tag	UNP O35405
B	40	LEU	-	expression tag	UNP O35405
B	41	ILE	-	expression tag	UNP O35405
B	42	SER	-	expression tag	UNP O35405
B	43	GLU	-	expression tag	UNP O35405
B	44	GLU	-	expression tag	UNP O35405
B	45	ASP	-	expression tag	UNP O35405
B	46	LEU	-	expression tag	UNP O35405
B	47	ALA	-	expression tag	UNP O35405
B	48	SER	-	expression tag	UNP O35405
B	49	MET	-	expression tag	UNP O35405
B	50	THR	-	expression tag	UNP O35405
B	51	GLY	-	expression tag	UNP O35405
B	52	GLY	-	expression tag	UNP O35405
B	53	GLN	-	expression tag	UNP O35405
B	54	GLN	-	expression tag	UNP O35405
B	55	MET	-	expression tag	UNP O35405
B	56	GLY	-	expression tag	UNP O35405
B	57	ARG	-	expression tag	UNP O35405
B	58	ASP	-	expression tag	UNP O35405
B	59	ILE	-	expression tag	UNP O35405
B	60	GLU	-	expression tag	UNP O35405
B	61	GLY	-	expression tag	UNP O35405
B	62	ARG	-	expression tag	UNP O35405
D	22	HIS	-	expression tag	UNP O35405
D	23	HIS	-	expression tag	UNP O35405
D	24	HIS	-	expression tag	UNP O35405
D	25	HIS	-	expression tag	UNP O35405
D	26	HIS	-	expression tag	UNP O35405
D	27	HIS	-	expression tag	UNP O35405
D	28	GLY	-	expression tag	UNP O35405
D	29	PRO	-	expression tag	UNP O35405
D	30	LEU	-	expression tag	UNP O35405
D	31	VAL	-	expression tag	UNP O35405
D	32	ASP	-	expression tag	UNP O35405
D	33	VAL	-	expression tag	UNP O35405
D	34	ALA	-	expression tag	UNP O35405
D	35	SER	-	expression tag	UNP O35405
D	36	ASN	-	expression tag	UNP O35405
D	37	GLU	-	expression tag	UNP O35405

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| Chain	Residue	Modelled	Actual	Comment	Reference
D	38	GLN	-	expression tag	UNP O35405
D	39	LYS	-	expression tag	UNP O35405
D	40	LEU	-	expression tag	UNP O35405
D	41	ILE	-	expression tag	UNP O35405
D	42	SER	-	expression tag	UNP O35405
D	43	GLU	-	expression tag	UNP O35405
D	44	GLU	-	expression tag	UNP O35405
D	45	ASP	-	expression tag	UNP O35405
D	46	LEU	-	expression tag	UNP O35405
D	47	ALA	-	expression tag	UNP O35405
D	48	SER	-	expression tag	UNP O35405
D	49	MET	-	expression tag	UNP O35405
D	50	THR	-	expression tag	UNP O35405
D	51	GLY	-	expression tag	UNP O35405
D	52	GLY	-	expression tag	UNP O35405
D	53	GLN	-	expression tag	UNP O35405
D	54	GLN	-	expression tag	UNP O35405
D	55	MET	-	expression tag	UNP O35405
D	56	GLY	-	expression tag	UNP O35405
D	57	ARG	-	expression tag	UNP O35405
D	58	ASP	-	expression tag	UNP O35405
D	59	ILE	-	expression tag	UNP O35405
D	60	GLU	-	expression tag	UNP O35405
D	61	GLY	-	expression tag	UNP O35405
D	62	ARG	-	expression tag	UNP O35405

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

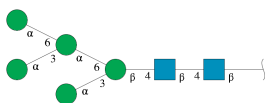| Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	I	2	Total	C	N	O	0	0	0
			28	16	2	10			

- 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.
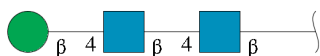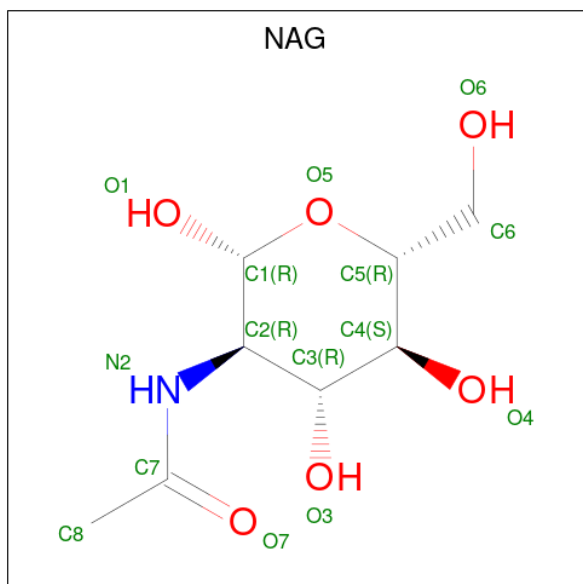
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	F	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	G	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyran ose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyran ose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glu copyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	H	7	Total	C	N	O	0	0	0
			83	46	2	35			

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

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

- Molecule 7 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).
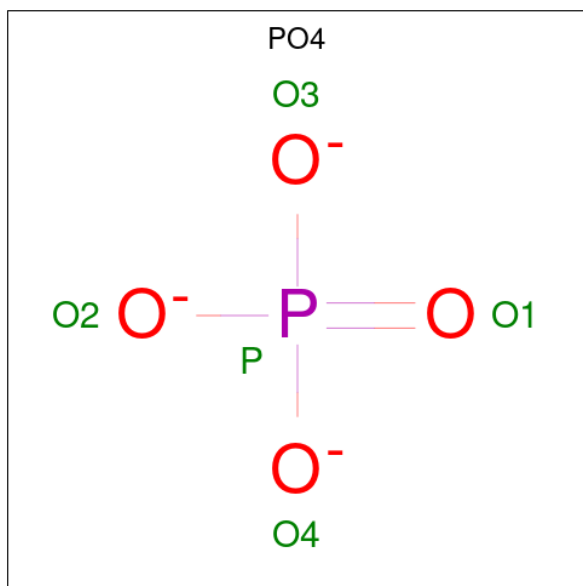
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	O	P	0	0
			5	4	1		
7	D	1	Total	O	P	0	0
			5	4	1		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	44	Total	O	0	0
			44	44		
8	B	50	Total	O	0	0
			50	50		
8	C	47	Total	O	0	0
			47	47		
8	D	46	Total	O	0	0
			46	46		

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: 5'-3' exonuclease PLD3
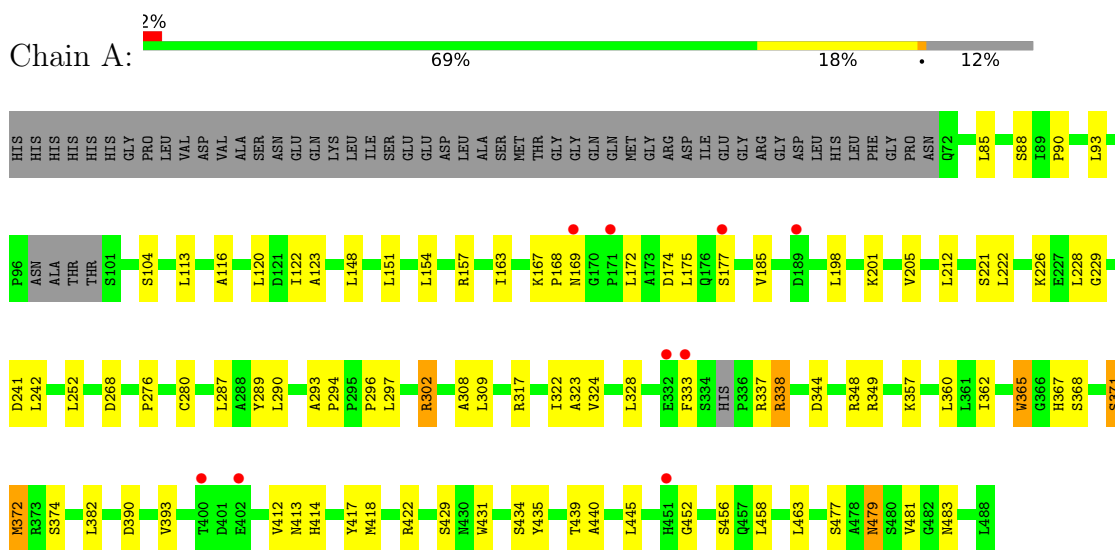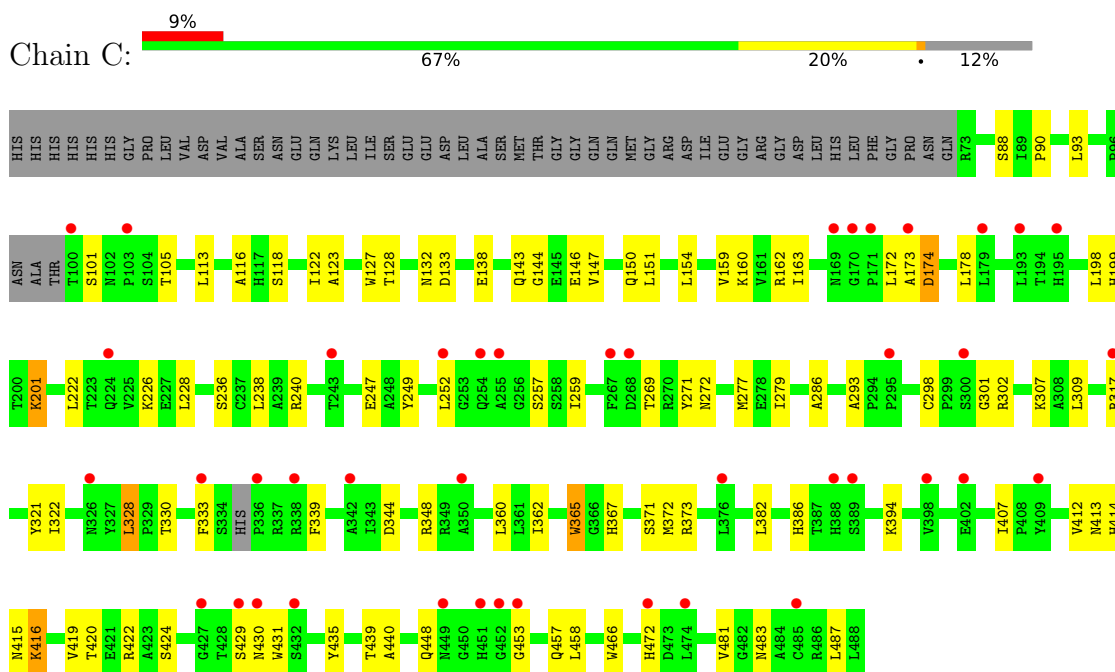
Chain A:

• Molecule 1: 5'-3' exonuclease PLD3

Chain C:

- Molecule 2: 5'-3' exonuclease PLD3

Chain B:
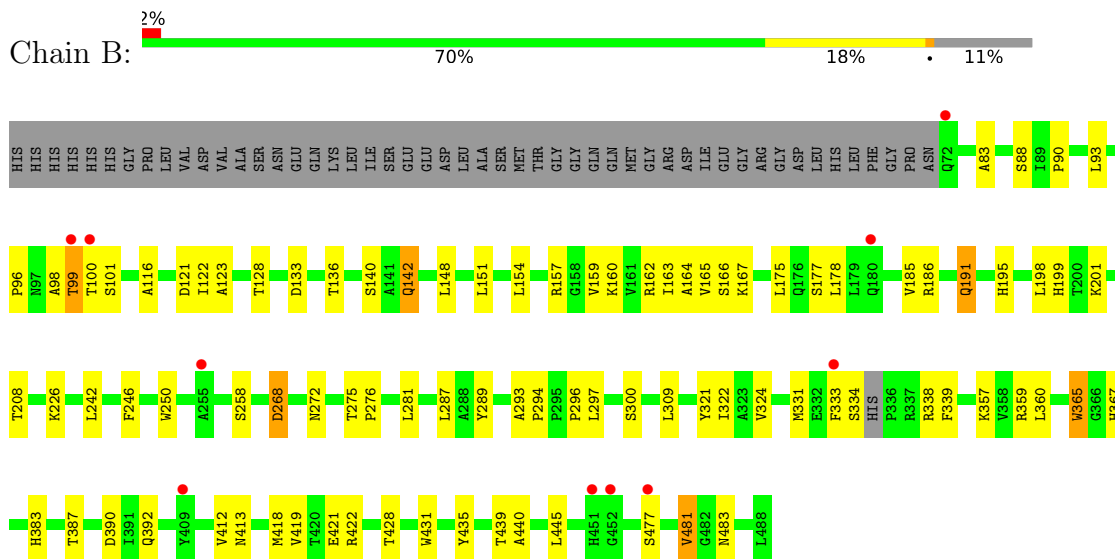
- Molecule 2: 5'-3' exonuclease PLD3
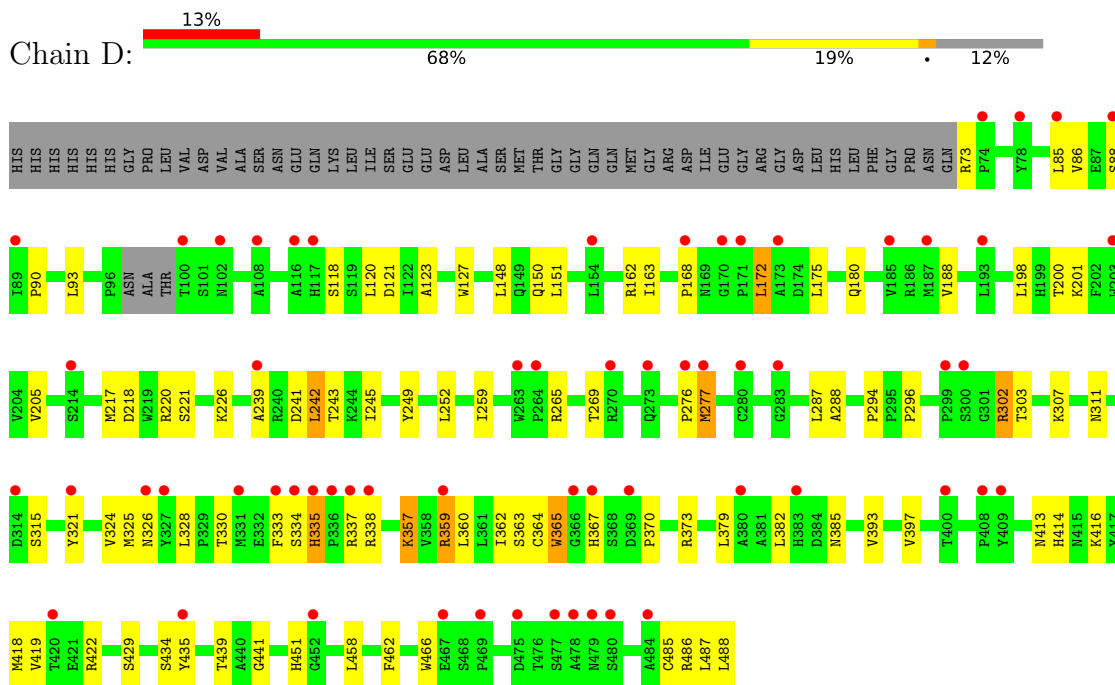
Chain D:

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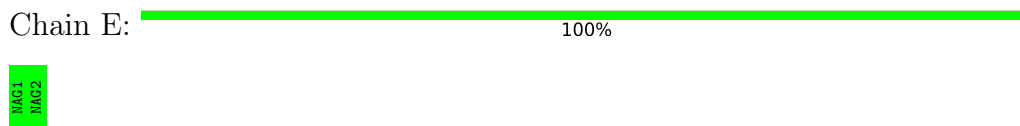
Chain E:

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

Chain I:

100%

NAG1 NAG2

• 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 G:

100%

NAG1 NAG2 BMA3

• Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[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 H:

29%   71%

NAG1 NAG2 BMA3 MAN4 MAN5 MAN6 MAN7

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	54.16Å 54.19Å 202.77Å 96.61° 89.16° 90.10°	Depositor
Resolution (Å)	49.92 – 2.73 49.92 – 2.73	Depositor EDS
% Data completeness (in resolution range)	93.8 (49.92-2.73) 88.0 (49.92-2.73)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.27 (at 2.73Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.255 , 0.295 0.257 , 0.295	Depositor DCC
R_{free} test set	2641 reflections (4.62%)	wwPDB-VP
Wilson B-factor (Å^2)	37.2	Xtriage
Anisotropy	0.189	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 18.9	EDS
L-test for twinning [2]	$< |L| > = 0.39, < L^2 > = 0.22$	Xtriage
Estimated twinning fraction	0.159 for h,-k,-l 0.139 for -h,k,-k-l 0.110 for -h,-k,k+l	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	13397	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.64% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, NEP, MAN, 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	0.25	0/3297	0.49	0/4491
1	C	0.28	0/3295	0.51	0/4489
2	B	0.27	0/3337	0.52	1/4550 (0.0%)
2	D	0.29	0/3319	0.54	1/4526 (0.0%)
All	All	0.27	0/13248	0.52	2/18056 (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
2	D	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	142	GLN	CA-CB-CG	5.76	126.07	113.40
2	D	359	ARG	CB-CG-CD	-5.15	98.21	111.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	486	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3229	0	3129	49	0
1	C	3227	0	3129	63	0
2	B	3252	0	3156	51	0
2	D	3233	0	3137	58	0
3	E	28	0	25	0	0
3	I	28	0	25	0	0
4	F	39	0	34	0	0
4	G	39	0	32	0	0
5	H	83	0	70	0	0
6	A	14	0	13	0	0
6	B	14	0	13	0	0
6	D	14	0	13	0	0
7	B	5	0	0	1	0
7	D	5	0	0	0	0
8	A	44	0	0	0	0
8	B	50	0	0	4	0
8	C	47	0	0	6	0
8	D	46	0	0	5	0
All	All	13397	0	12776	218	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 8.

The worst 5 of 218 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)
2:B:122:ILE:O	8:B:601:HOH:O	1.92	0.86
2:B:331:MET:HG3	2:B:338:ARG:HD2	1.58	0.85
1:C:269:THR:HG22	1:C:271:TYR:H	1.46	0.77
2:B:123:ALA:O	2:B:201:LYS:HA	1.85	0.76
1:C:88:SER:O	1:C:226:LYS:HA	1.85	0.76

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	405/467 (87%)	389 (96%)	16 (4%)	0	100	100
1	C	405/467 (87%)	390 (96%)	15 (4%)	0	100	100
2	B	412/467 (88%)	396 (96%)	15 (4%)	1 (0%)	47	69
2	D	409/467 (88%)	393 (96%)	14 (3%)	2 (0%)	29	48
All	All	1631/1868 (87%)	1568 (96%)	60 (4%)	3 (0%)	47	69

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	335	HIS
2	B	99	THR
2	D	337	ARG

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	352/397 (89%)	330 (94%)	22 (6%)	18	31
1	C	352/397 (89%)	332 (94%)	20 (6%)	20	36
2	B	356/398 (89%)	333 (94%)	23 (6%)	17	30
2	D	354/398 (89%)	336 (95%)	18 (5%)	24	41
All	All	1414/1590 (89%)	1331 (94%)	83 (6%)	19	34

5 of 83 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	317	ARG
2	D	242	LEU
1	C	333	PHE
2	D	85	LEU
2	D	302	ARG

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

Mol	Chain	Res	Type
2	B	415	ASN
1	C	199	HIS
1	C	386	HIS

5.3.3   RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\#|Z| > 2$
1	NEP	A	414	1	10,14,15	1.85	3 (30%)	5,20,22	2.24	3 (60%)
1	NEP	C	414	1	10,14,15	5.48	4 (40%)	5,20,22	4.47	4 (80%)

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
1	NEP	A	414	1	-	4/5/12/14	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	NEP	C	414	1	-	2/5/12/14	0/1/1/1

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	414	NEP	P-O3P	16.13	1.61	1.47
1	C	414	NEP	P-O1P	-4.25	1.46	1.54
1	A	414	NEP	P-O1P	3.22	1.61	1.54
1	A	414	NEP	CD2-CG	3.05	1.40	1.36
1	C	414	NEP	CD2-CG	2.96	1.40	1.36

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	414	NEP	O2P-P-O3P	-9.00	93.98	113.44
1	A	414	NEP	O1P-P-O2P	-3.14	94.22	106.57
1	C	414	NEP	O1P-P-O2P	2.64	116.94	106.57
1	A	414	NEP	CB-CA-C	-2.52	106.74	111.47
1	A	414	NEP	O1P-P-O3P	-2.45	108.15	113.44

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	414	NEP	O-C-CA-CB
1	A	414	NEP	N-CA-CB-CG
1	A	414	NEP	C-CA-CB-CG
1	A	414	NEP	CA-CB-CG-ND1
1	C	414	NEP	N-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

17 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	0.28	0	17,19,21	0.49	0
3	NAG	E	2	3	14,14,15	0.29	0	17,19,21	0.38	0
4	NAG	F	1	4,2	14,14,15	0.44	0	17,19,21	0.88	0
4	NAG	F	2	4	14,14,15	0.42	0	17,19,21	1.08	1 (5%)
4	BMA	F	3	4	11,11,12	0.84	0	15,15,17	0.78	0
4	NAG	G	1	4,2	14,14,15	0.28	0	17,19,21	0.60	0
4	NAG	G	2	4	14,14,15	0.21	0	17,19,21	0.43	0
4	BMA	G	3	4	11,11,12	0.63	0	15,15,17	0.69	0
5	NAG	H	1	5,1	14,14,15	0.33	0	17,19,21	0.69	0
5	NAG	H	2	5	14,14,15	0.27	0	17,19,21	0.48	0
5	BMA	H	3	5	11,11,12	0.81	1 (9%)	15,15,17	1.26	3 (20%)
5	MAN	H	4	5	11,11,12	0.74	0	15,15,17	0.98	1 (6%)
5	MAN	H	5	5	11,11,12	0.65	0	15,15,17	0.92	1 (6%)
5	MAN	H	6	5	11,11,12	0.70	0	15,15,17	0.92	1 (6%)
5	MAN	H	7	5	11,11,12	0.70	0	15,15,17	1.02	2 (13%)
3	NAG	I	1	3,2	14,14,15	0.28	0	17,19,21	0.52	0
3	NAG	I	2	3	14,14,15	0.20	0	17,19,21	0.45	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
3	NAG	E	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	0/6/23/26	0/1/1/1
4	NAG	F	1	4,2	-	3/6/23/26	0/1/1/1
4	NAG	F	2	4	-	2/6/23/26	0/1/1/1
4	BMA	F	3	4	-	0/2/19/22	0/1/1/1
4	NAG	G	1	4,2	-	3/6/23/26	0/1/1/1
4	NAG	G	2	4	-	0/6/23/26	0/1/1/1
4	BMA	G	3	4	-	0/2/19/22	0/1/1/1
5	NAG	H	1	5,1	-	1/6/23/26	0/1/1/1
5	NAG	H	2	5	-	2/6/23/26	0/1/1/1
5	BMA	H	3	5	-	0/2/19/22	0/1/1/1
5	MAN	H	4	5	-	1/2/19/22	0/1/1/1
5	MAN	H	5	5	-	0/2/19/22	0/1/1/1

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W O R L D W I D E
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PROTEIN DATA BANK

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MAN	H	6	5	-	1/2/19/22	0/1/1/1
5	MAN	H	7	5	-	2/2/19/22	0/1/1/1
3	NAG	I	1	3,2	-	4/6/23/26	0/1/1/1
3	NAG	I	2	3	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	3	BMA	C1-C2	2.00	1.56	1.52

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	2	NAG	C3-C4-C5	3.39	116.28	110.24
5	H	3	BMA	C1-C2-C3	2.61	112.88	109.67
5	H	7	MAN	C1-O5-C5	2.39	115.44	112.19
5	H	5	MAN	O2-C2-C3	-2.22	105.68	110.14
5	H	3	BMA	C1-O5-C5	2.19	115.16	112.19

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

| Mol	Chain	Res	Type	Atoms
5	H	7	MAN	O5-C5-C6-O6
5	H	7	MAN	C4-C5-C6-O6
3	I	1	NAG	O5-C5-C6-O6
3	I	2	NAG	O5-C5-C6-O6
4	F	1	NAG	O5-C5-C6-O6

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 E

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain I

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain F

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain G

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain H
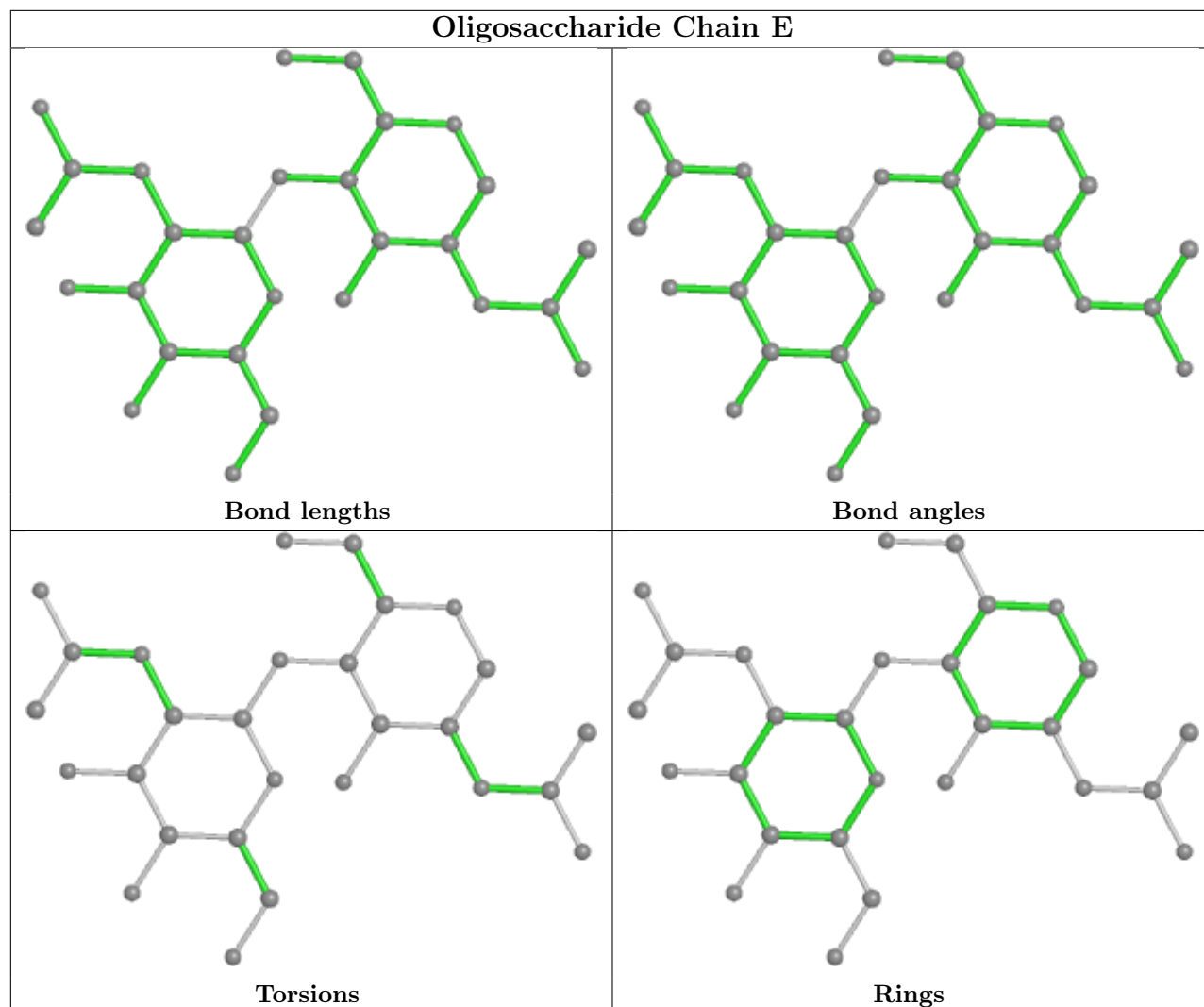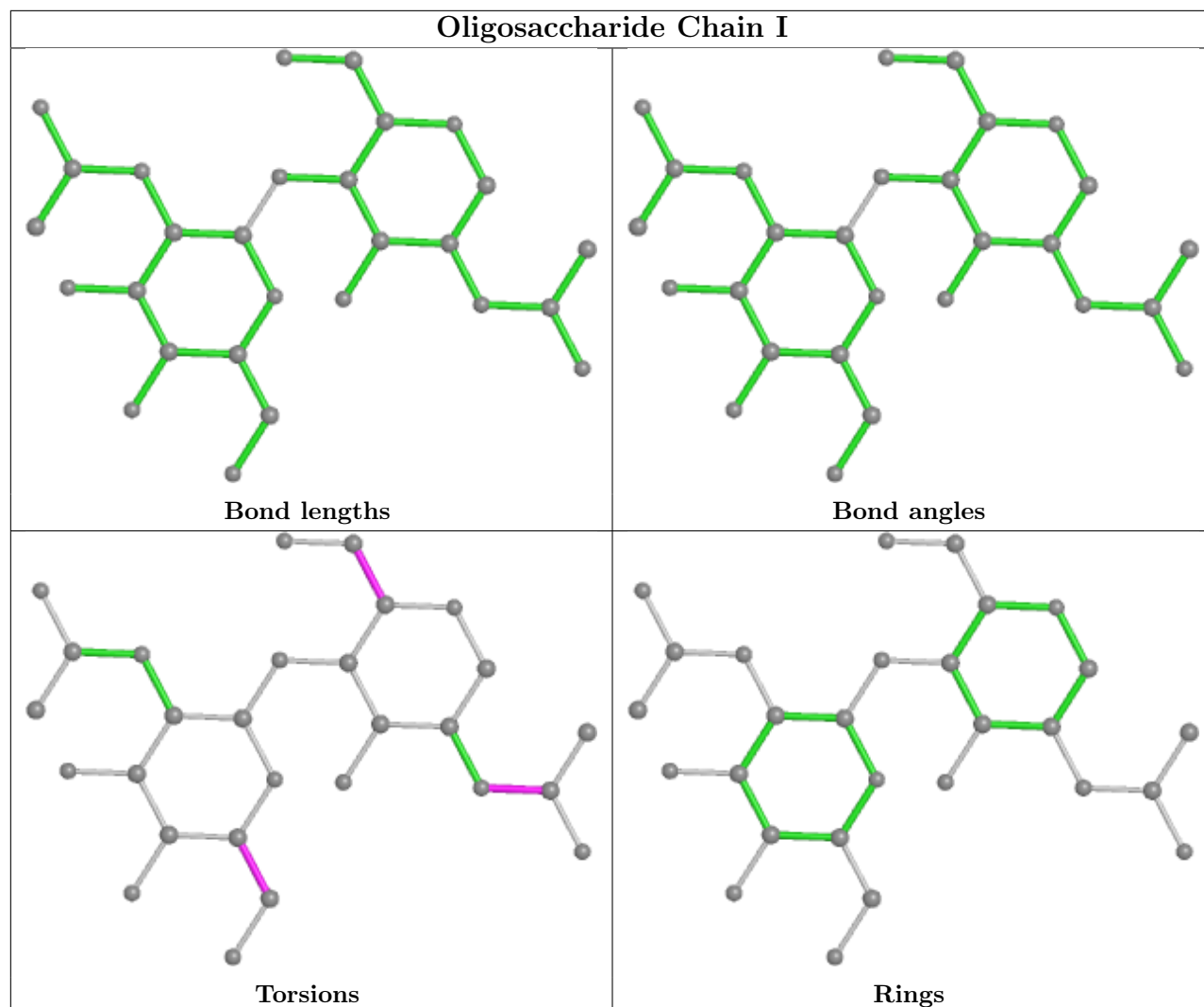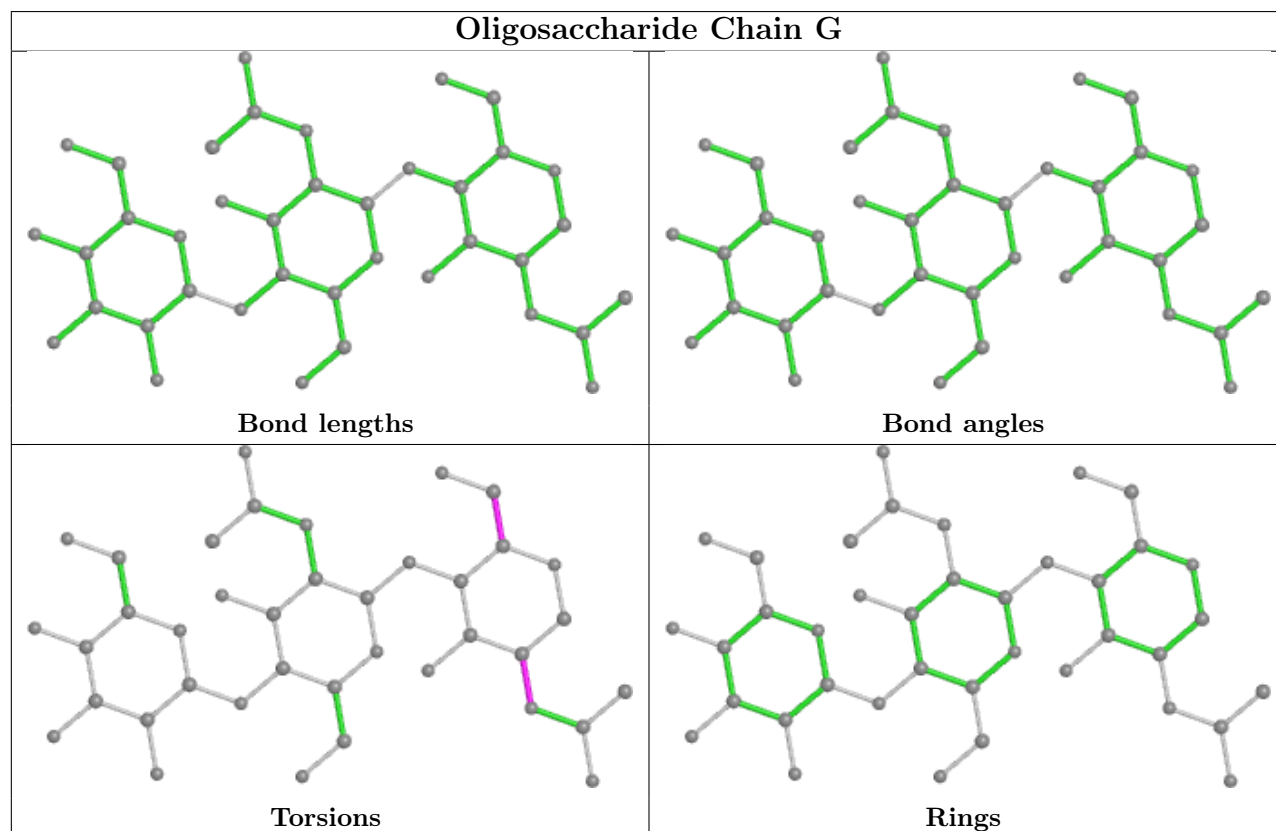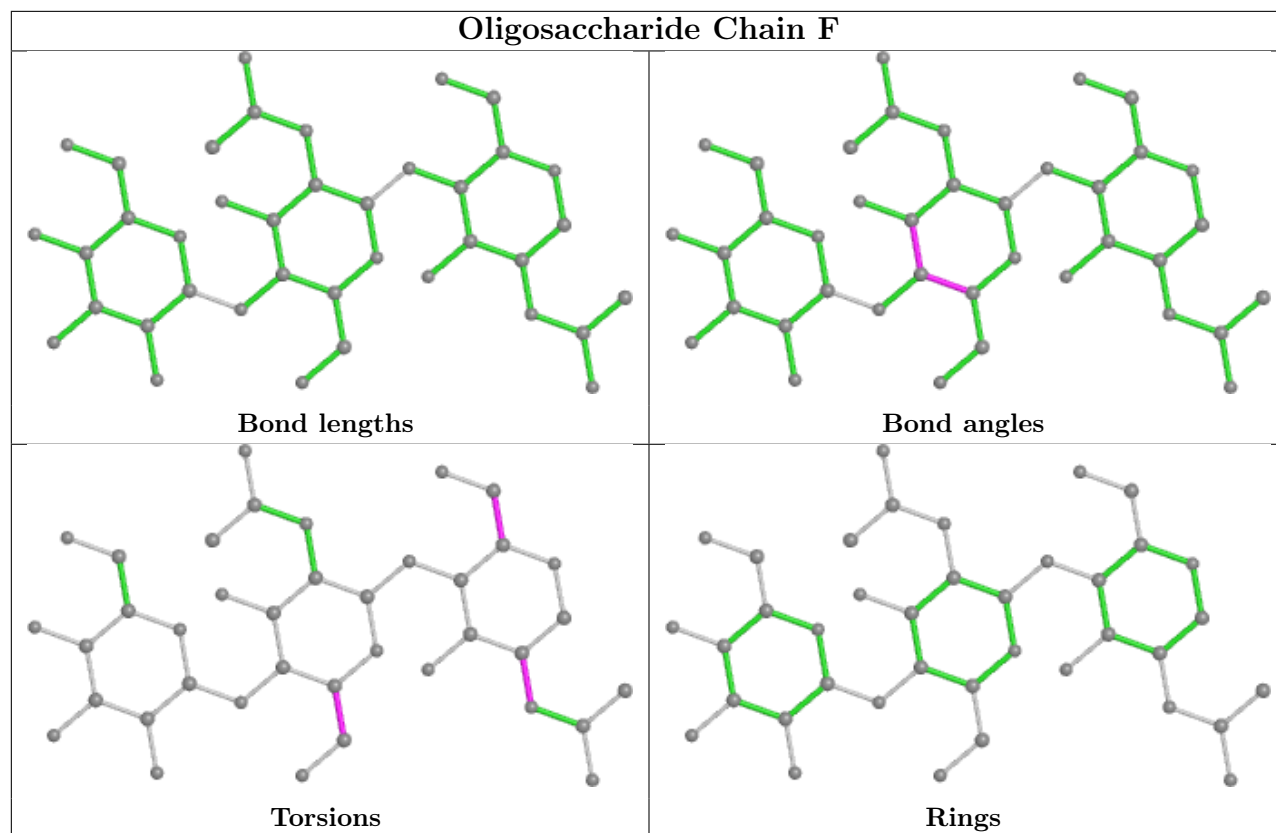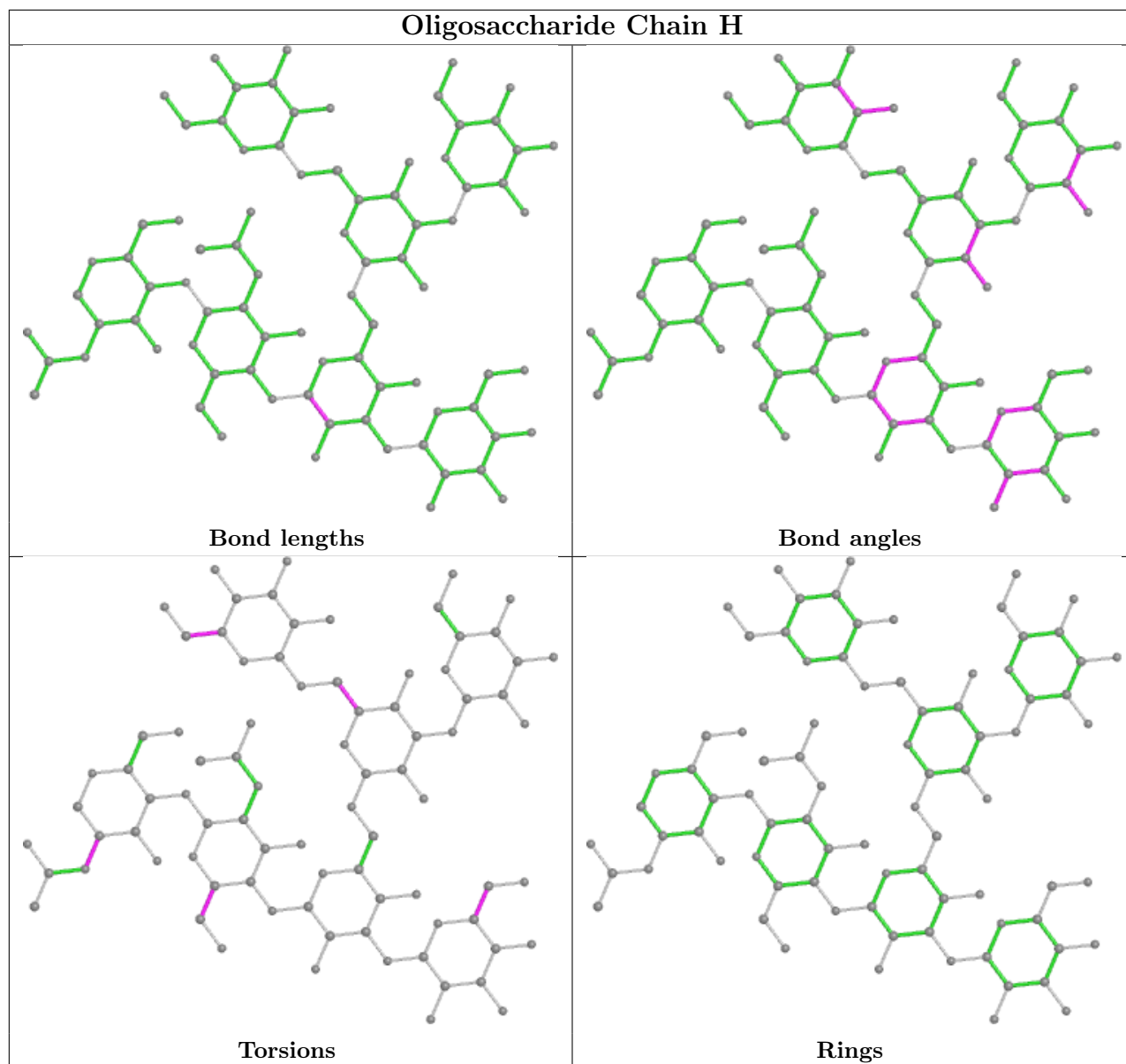
5.6 Ligand geometry ⓘ

5 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	$\#|Z| > 2$

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
7	PO4	D	502	-	4,4,4	0.92	0	6,6,6	0.43	0
6	NAG	B	501	2	14,14,15	0.26	0	17,19,21	0.46	0
7	PO4	B	502	-	4,4,4	0.90	0	6,6,6	0.44	0
6	NAG	A	501	1	14,14,15	0.29	0	17,19,21	0.46	0
6	NAG	D	501	2	14,14,15	0.29	0	17,19,21	0.48	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
6	NAG	A	501	1	-	2/6/23/26	0/1/1/1
6	NAG	D	501	2	-	2/6/23/26	0/1/1/1
6	NAG	B	501	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	501	NAG	O5-C5-C6-O6
6	A	501	NAG	C4-C5-C6-O6
6	D	501	NAG	C8-C7-N2-C2
6	D	501	NAG	O7-C7-N2-C2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	502	PO4	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	411/467 (88%)	0.17	9 (2%)	62	69	17, 30, 53, 125	0
1	C	411/467 (88%)	0.87	42 (10%)	6	6	33, 51, 76, 159	0
2	B	416/467 (89%)	0.31	10 (2%)	59	66	19, 31, 60, 127	0
2	D	413/467 (88%)	1.08	62 (15%)	2	2	30, 56, 88, 160	0
All	All	1651/1868 (88%)	0.61	123 (7%)	14	16	17, 45, 75, 160	0

The worst 5 of 123 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	451	HIS	11.1
2	D	452	GLY	9.9
1	C	170	GLY	7.9
2	B	333	PHE	6.2
1	C	100	THR	5.9

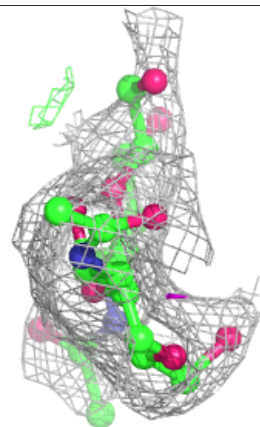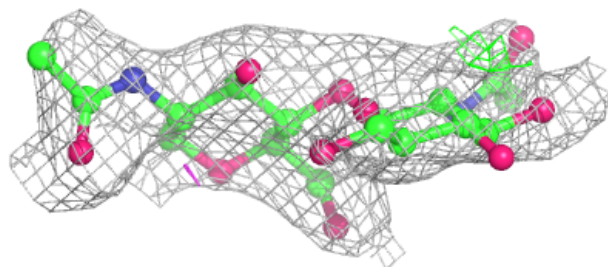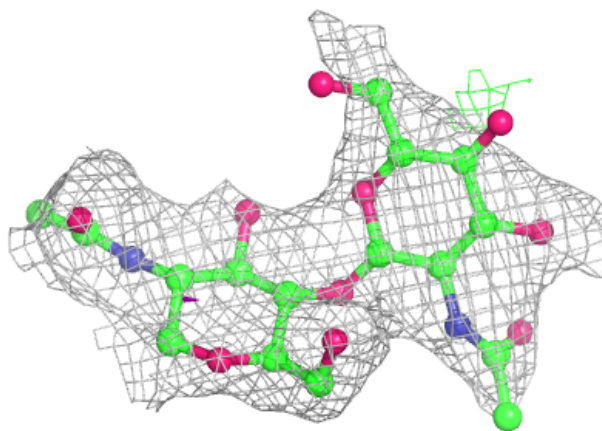## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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
1	NEP	C	414	14/15	0.82	0.25	33,51,66,74	0
1	NEP	A	414	14/15	0.90	0.17	11,32,50,53	0

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
4	BMA	F	3	11/12	0.43	0.53	63,85,109,120	0
4	NAG	F	2	14/15	0.64	0.51	48,74,108,124	0
5	MAN	H	6	11/12	0.71	0.31	49,76,89,90	0
3	NAG	I	1	14/15	0.74	0.40	54,69,86,86	0
5	MAN	H	5	11/12	0.78	0.36	46,56,68,86	0
3	NAG	I	2	14/15	0.78	0.36	37,74,97,106	0
4	NAG	G	2	14/15	0.80	0.31	40,60,82,88	0
5	BMA	H	3	11/12	0.81	0.22	41,45,50,58	0
5	MAN	H	4	11/12	0.81	0.32	41,61,73,74	0
4	BMA	G	3	11/12	0.83	0.29	48,60,71,74	0
3	NAG	E	1	14/15	0.84	0.22	40,52,59,62	0
4	NAG	G	1	14/15	0.85	0.28	38,50,60,63	0
5	NAG	H	2	14/15	0.85	0.22	44,55,65,72	0
3	NAG	E	2	14/15	0.85	0.30	47,59,72,81	0
5	NAG	H	1	14/15	0.86	0.19	35,58,70,71	0
4	NAG	F	1	14/15	0.87	0.28	30,56,73,81	0
5	MAN	H	7	11/12	0.90	0.30	32,55,69,72	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.
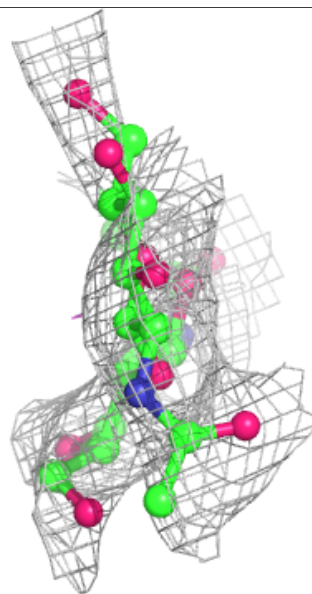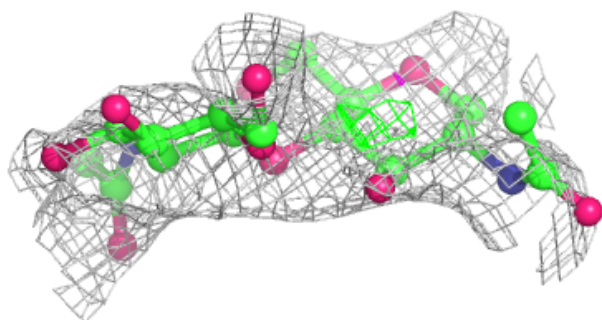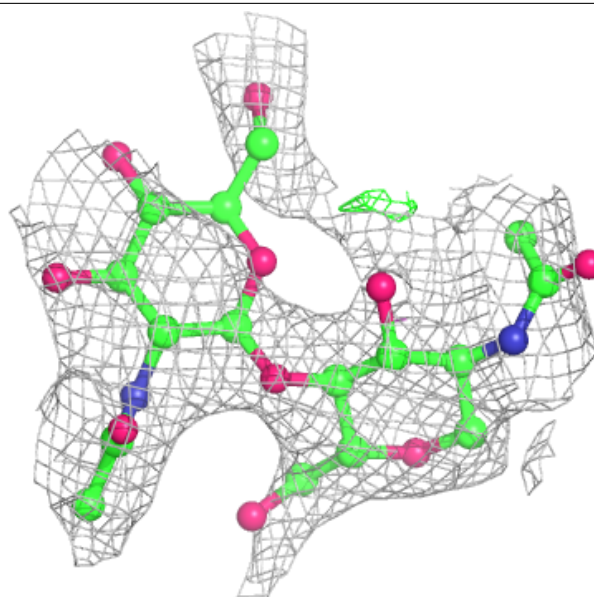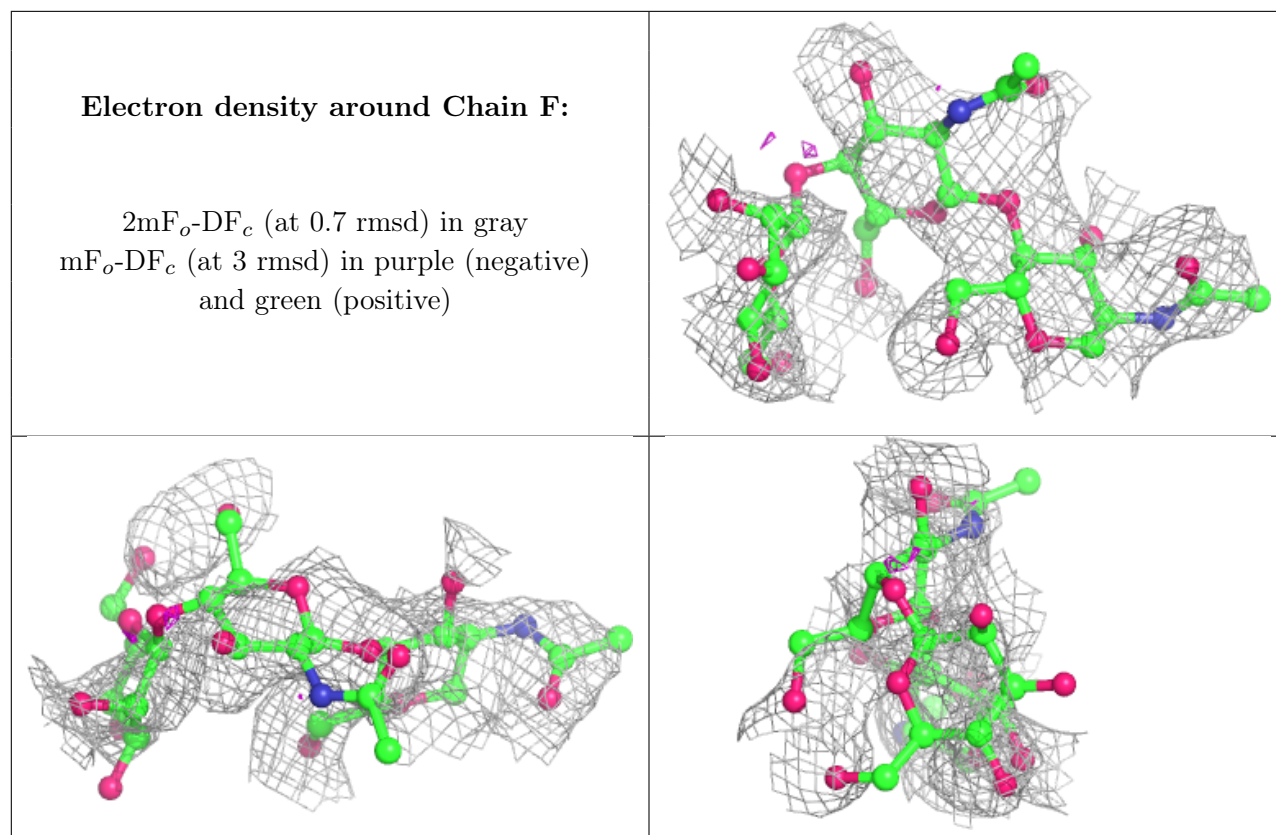
Electron density around Chain E:

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 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 F:

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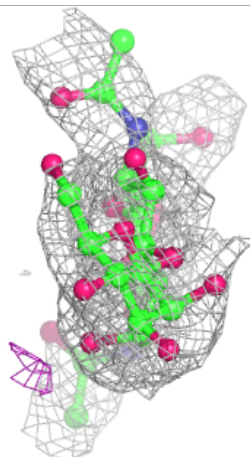mF_o-DF_c (at 3 rmsd) in purple (negative)
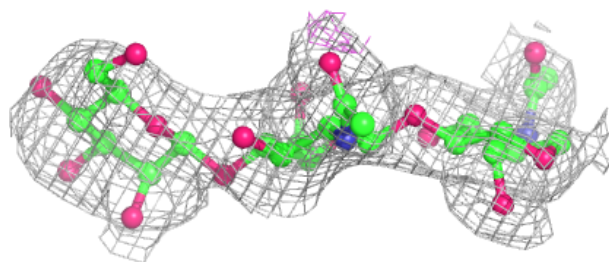and green (positive)

Electron density around Chain G:

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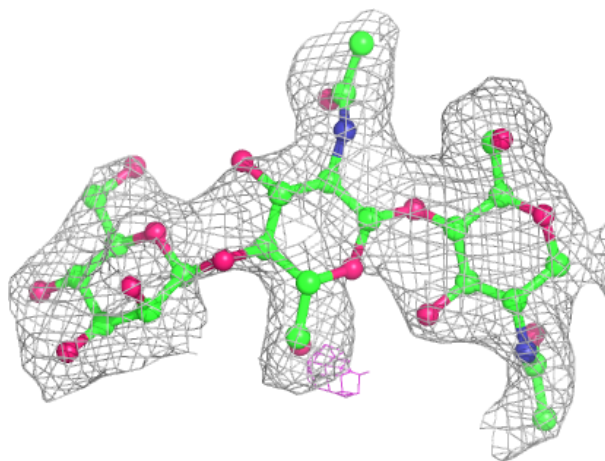and green (positive)

Electron density around Chain H:

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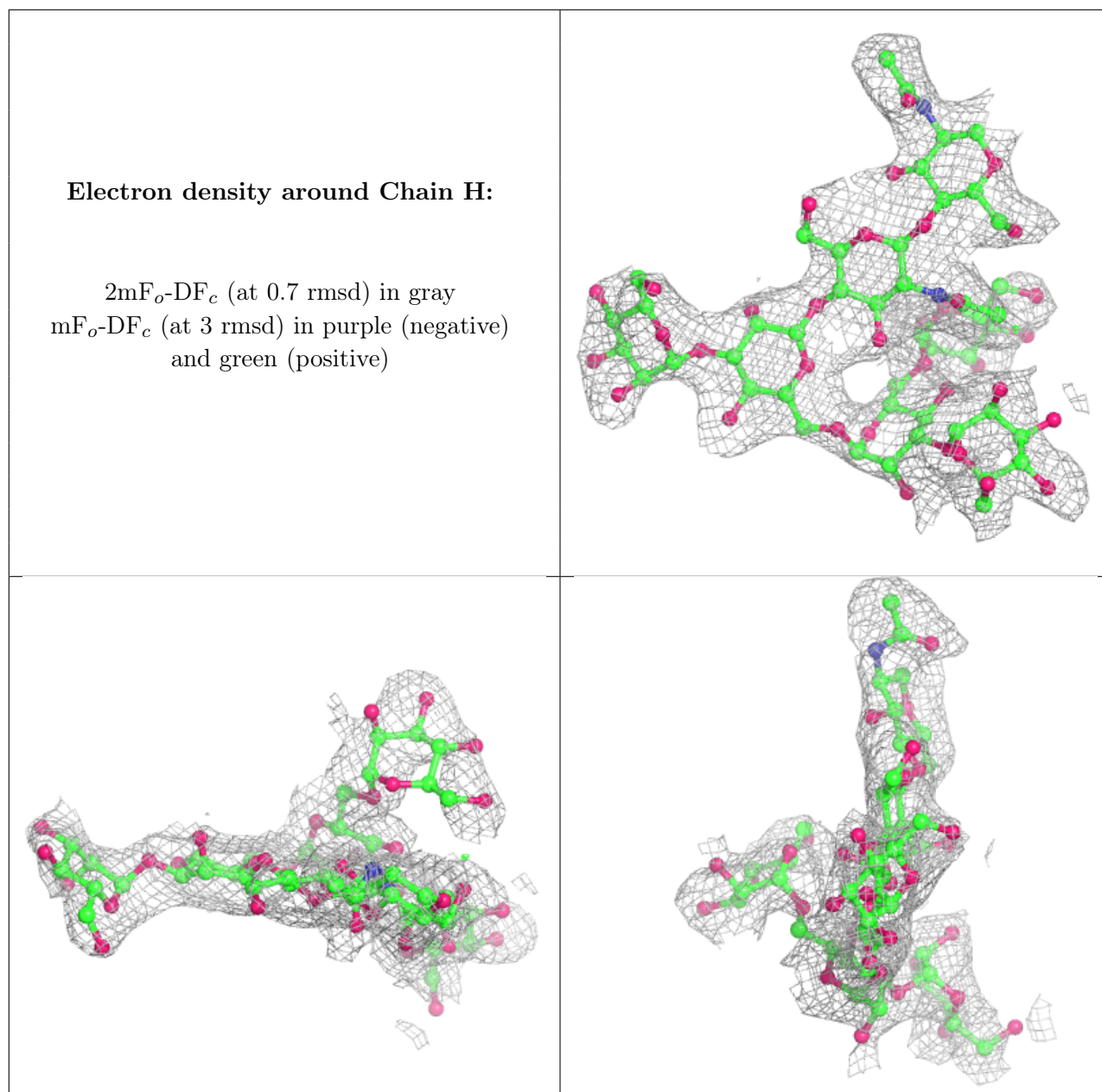mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

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
6	NAG	D	501	14/15	0.63	0.47	49,76,84,84	0
6	NAG	B	501	14/15	0.76	0.37	45,63,77,85	0
6	NAG	A	501	14/15	0.82	0.22	34,52,64,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	PO4	B	502	5/5	0.96	0.12	25,26,38,45	0
7	PO4	D	502	5/5	0.96	0.13	46,46,50,50	0

6.5 Other polymers ⓘ

There are no such residues in this entry.