WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 1, 2023 – 04:59 PM JST

PDB ID	:	5WPZ
Title	:	Crystal structure of MNDA PYD with MBP tag
Authors	:	Jin, T.C.; Xiao, T.S.
Deposited on	:	2016-11-22
Resolution	:	2.00 Å(reported)

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

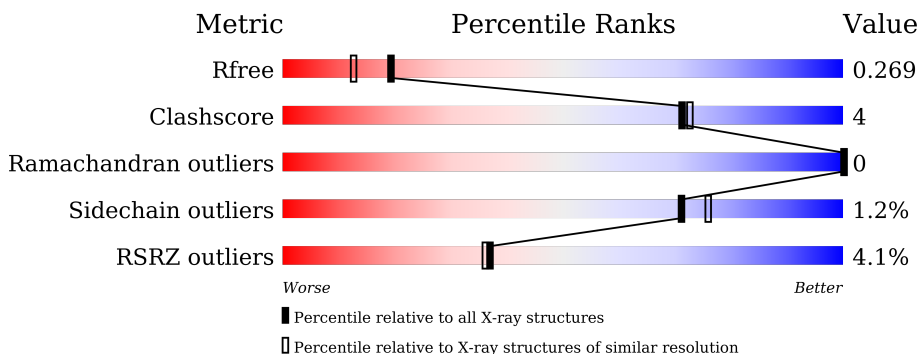|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 2.00 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.
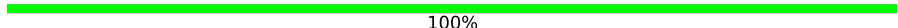
Metric	Percentile Ranks	Value
Rfree		0.269
Clashscore		4
Ramachandran outliers		0
Sidechain outliers		1.2%
RSRZ outliers		4.1%

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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	477	.% 88% 8% •
1	B	477	2% 89% 7% • •
1	C	477	3% 89% 8% •
1	D	477	3% 86% 10% •
1	E	477	5% 87% 9% •
1	F	477	9% 84% 11% •

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Mol	Chain	Length	Quality of chain
2	G	2	100%
2	H	2	100%
2	I	2	50% 50%
2	J	2	50% 50%
2	K	2	50% 50%
2	L	2	50% 50%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 22797 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 MBP-hMNDA-PYD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	460	Total 3576	C 2304	N 585	O 676	S 11	0	1	0
1	B	462	Total 3585	C 2311	N 587	O 676	S 11	0	0	0
1	C	461	Total 3599	C 2319	N 591	O 678	S 11	0	3	0
1	D	459	Total 3579	C 2306	N 587	O 675	S 11	0	2	0
1	E	463	Total 3599	C 2319	N 590	O 679	S 11	0	1	0
1	F	459	Total 3579	C 2306	N 587	O 675	S 11	0	2	0

- Molecule 2 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	G	2	Total 23	C 12	O 11	0	0	0
2	H	2	Total 23	C 12	O 11	0	0	0
2	I	2	Total 23	C 12	O 11	0	0	0
2	J	2	Total 23	C 12	O 11	0	0	0
2	K	2	Total 23	C 12	O 11	0	0	0
2	L	2	Total 23	C 12	O 11	0	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	240	Total 240	O 240	0	0
3	B	239	Total 239	O 239	0	0
3	C	189	Total 189	O 189	0	0
3	D	173	Total 173	O 173	0	0
3	E	159	Total 159	O 159	0	0
3	F	142	Total 142	O 142	0	0

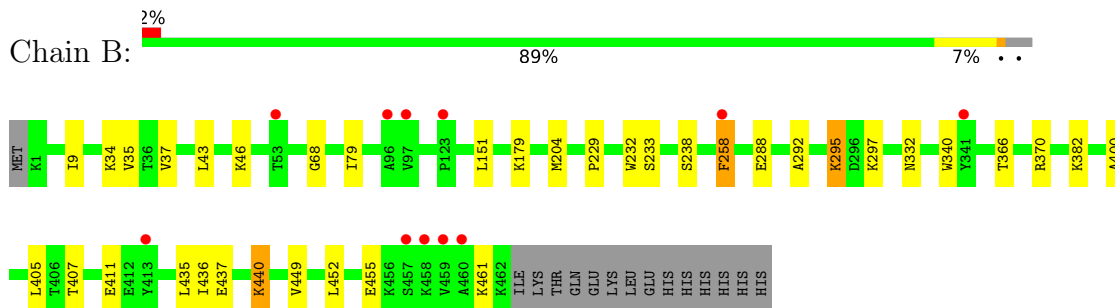# 3 Residue-property plots ⓘ

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.
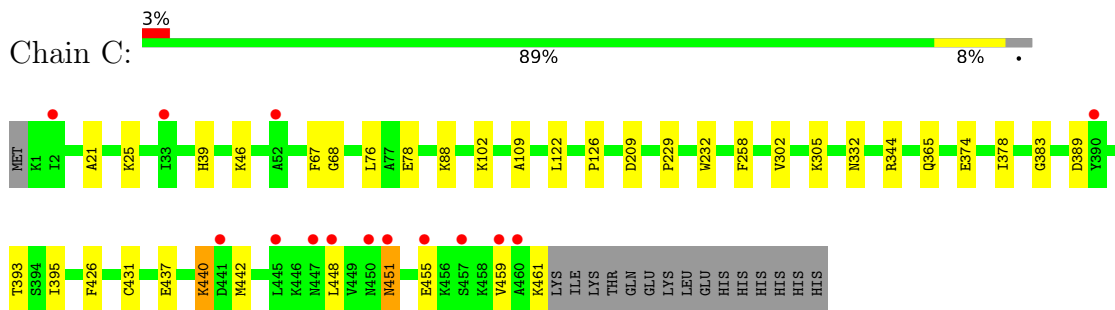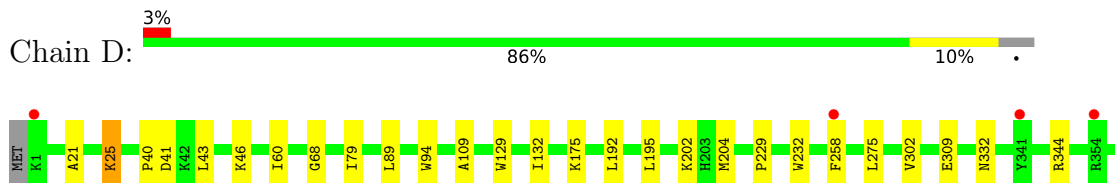
- Molecule 1: MBP-hMNDA-PYD
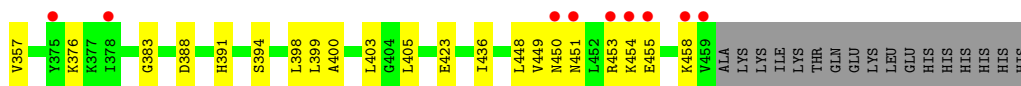

- Molecule 1: MBP-hMNDA-PYD

- Molecule 1: MBP-hMNDA-PYD

- Molecule 1: MBP-hMNDA-PYD

V357 Y375 K376 K377 I378 G383 D388 H391 S394 L398 L399 A400 L403 G404 L405 E423 I436 L448 V449 N450 N451 L452 R453 K454 E455 K458 V459 ALA LYS LYS ILE LYS THR GLN GLU LYS LEU GLU HIS HIS HIS HIS HIS

• Molecule 1: MBP-hMNDA-PYD

Chain E:

5%

87%   9%   •

MET K1 I2 W10 I11 N12 G13 D14 K34 E38 L43 E44 V50 A51 D55 W62 R66 F67 G68 G74 K119 D120 L121 L122 P123 N124 P125 P126 W129 E130 P133 A134 L135 D136 K137 E138 L139 K144 S145 A146 Q152 K179 P229 W230

A231 W232 I235 N241 P248 F258 E288 G289 L290 E291 K295 N332 I348 N349 R354 E374 I378 S397 Y401 D402 E423 K424 K425 F426 Q427 L435 D441 L452 E455 K456 S457 A458 V459 A460 K461 K462 I463 LYS THR GLN GLU LYS
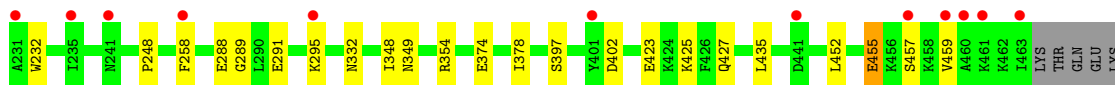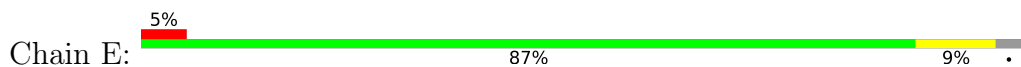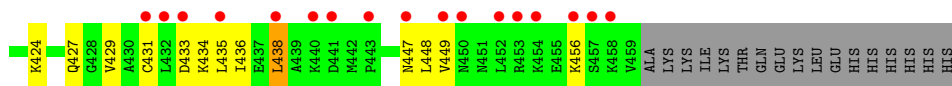
LEU GLU HIS HIS HIS HIS HIS

• Molecule 1: MBP-hMNDA-PYD

Chain F:

9%

84%   11%   •

MET K1 K6 W10 K15 G16 Y17 G24 K34 V35 L43 E44 R66 F67 G68 I79 T80 P81 E111 Y117 N118 K119 D120 L121 L122 P123 N124 P125 A141 Q152 E153 P154 K202 N218 T222 A223 N227 G228 P229 W232 I235

S238 A239 Q253 F258 A269 E278 N282 E288 E310 K313 N332 Y341 R344 A363 N367 A371 E374 Y375 L379 L380 L381 F384 E385 L386 M387 Y390 H391 S397 A400 L405 T406 T407 K408 M409 Q410 Y413 D420

K424 Q427 G428 V429 A430 C431 L432 D433 K434 L435 I436 E437 L438 A439 K440 D441 M442 P443 N447 L448 V449 N450 N451 L452 R453 K454 E455 K456 S457 K458 V459 ALA LYS ILE LYS THR GLN LYS LEU GLU HIS HIS HIS HIS HIS

• Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain G:

100%

GLC1 GLC2

• Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain H:

100%

GLC1 GLC2

• Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain I:

50%   50%

GLC1 GLC2

• Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain J: 50% 50%

GLC1 GLC2

• Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain K: 50% 50%

GLC1 GLC2

• Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain L: 50% 50%

GLC1 GLC2

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	192.15Å 235.61Å 73.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.36 – 2.00 48.36 – 2.00	Depositor EDS
% Data completeness (in resolution range)	89.0 (48.36-2.00) 89.0 (48.36-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.91 (at 2.00Å)	Xtriage
Refinement program	PHENIX (dev_2481: ???)	Depositor
R, R_{free}	0.221 , 0.269 0.221 , 0.269	Depositor DCC
R_{free} test set	10016 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	30.3	Xtriage
Anisotropy	0.853	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 38.5	EDS
L-test for twinning[2]	$< |L| > = 0.46, < L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	22797	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.75% 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: GLC

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	0.26	0/3654	0.43	0/4950
1	B	0.27	0/3663	0.43	0/4960
1	C	0.27	0/3683	0.43	0/4988
1	D	0.26	0/3660	0.43	0/4957
1	E	0.26	0/3677	0.43	0/4979
1	F	0.27	0/3660	0.43	0/4957
All	All	0.26	0/21997	0.43	0/29791

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	3576	0	3597	27	0
1	B	3585	0	3616	21	0
1	C	3599	0	3631	23	0
1	D	3579	0	3605	26	0
1	E	3599	0	3625	27	0
1	F	3579	0	3605	32	0
2	G	23	0	21	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	23	0	21	0	0
2	I	23	0	21	1	0
2	J	23	0	21	0	0
2	K	23	0	21	0	0
2	L	23	0	21	0	0
3	A	240	0	0	7	0
3	B	239	0	0	5	0
3	C	189	0	0	2	0
3	D	173	0	0	1	0
3	E	159	0	0	1	0
3	F	142	0	0	3	0
All	All	22797	0	21805	154	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 4.

The worst 5 of 154 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:437:GLU:O	1:C:440:LYS:HE3	1.77	0.83
1:F:436:ILE:HG12	1:F:449:VAL:HG13	1.67	0.74
1:B:295:LYS:NZ	3:B:601:HOH:O	2.20	0.72
1:D:399:LEU:HB3	1:D:403:LEU:HD12	1.71	0.72
1:F:407:THR:HA	1:F:410:GLN:HB2	1.72	0.71

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	459/477 (96%)	452 (98%)	7 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	460/477 (96%)	453 (98%)	7 (2%)	0	100	100
1	C	462/477 (97%)	452 (98%)	10 (2%)	0	100	100
1	D	459/477 (96%)	449 (98%)	10 (2%)	0	100	100
1	E	462/477 (97%)	450 (97%)	12 (3%)	0	100	100
1	F	459/477 (96%)	446 (97%)	13 (3%)	0	100	100
All	All	2761/2862 (96%)	2702 (98%)	59 (2%)	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	368/384 (96%)	367 (100%)	1 (0%)	92	95
1	B	369/384 (96%)	363 (98%)	6 (2%)	62	67
1	C	371/384 (97%)	367 (99%)	4 (1%)	73	78
1	D	369/384 (96%)	364 (99%)	5 (1%)	67	72
1	E	370/384 (96%)	364 (98%)	6 (2%)	62	67
1	F	369/384 (96%)	363 (98%)	6 (2%)	62	67
All	All	2216/2304 (96%)	2188 (99%)	28 (1%)	71	74

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	344[A]	ARG
1	F	438	LEU
1	E	55	ASP
1	F	344[A]	ARG
1	E	34	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	450	ASN
1	F	152	GLN
1	F	253	GLN
1	B	253	GLN
1	B	72	GLN

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 ⓘ

12 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	GLC	G	1	2	12,12,12	0.50	0	17,17,17	0.48	0
2	GLC	G	2	2	11,11,12	0.60	0	15,15,17	0.79	0
2	GLC	H	1	2	12,12,12	0.52	0	17,17,17	0.60	0
2	GLC	H	2	2	11,11,12	0.62	0	15,15,17	0.65	0
2	GLC	I	1	2	12,12,12	0.47	0	17,17,17	0.53	0
2	GLC	I	2	2	11,11,12	0.59	0	15,15,17	0.87	1 (6%)
2	GLC	J	1	2	12,12,12	0.51	0	17,17,17	0.41	0
2	GLC	J	2	2	11,11,12	0.58	0	15,15,17	1.08	1 (6%)
2	GLC	K	1	2	12,12,12	0.52	0	17,17,17	0.70	0
2	GLC	K	2	2	11,11,12	0.58	0	15,15,17	0.90	1 (6%)
2	GLC	L	1	2	12,12,12	0.51	0	17,17,17	0.48	0
2	GLC	L	2	2	11,11,12	0.58	0	15,15,17	0.94	1 (6%)

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	GLC	G	1	2	-	0/2/22/22	0/1/1/1
2	GLC	G	2	2	-	0/2/19/22	0/1/1/1
2	GLC	H	1	2	-	1/2/22/22	0/1/1/1
2	GLC	H	2	2	-	0/2/19/22	0/1/1/1
2	GLC	I	1	2	-	0/2/22/22	0/1/1/1
2	GLC	I	2	2	-	0/2/19/22	0/1/1/1
2	GLC	J	1	2	-	0/2/22/22	0/1/1/1
2	GLC	J	2	2	-	0/2/19/22	0/1/1/1
2	GLC	K	1	2	-	0/2/22/22	0/1/1/1
2	GLC	K	2	2	-	0/2/19/22	0/1/1/1
2	GLC	L	1	2	-	1/2/22/22	0/1/1/1
2	GLC	L	2	2	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	2	GLC	C1-O5-C5	3.35	116.74	112.19
2	L	2	GLC	C1-O5-C5	2.82	116.02	112.19
2	I	2	GLC	C1-O5-C5	2.43	115.49	112.19
2	K	2	GLC	C1-O5-C5	2.17	115.13	112.19

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	L	1	GLC	C4-C5-C6-O6
2	H	1	GLC	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

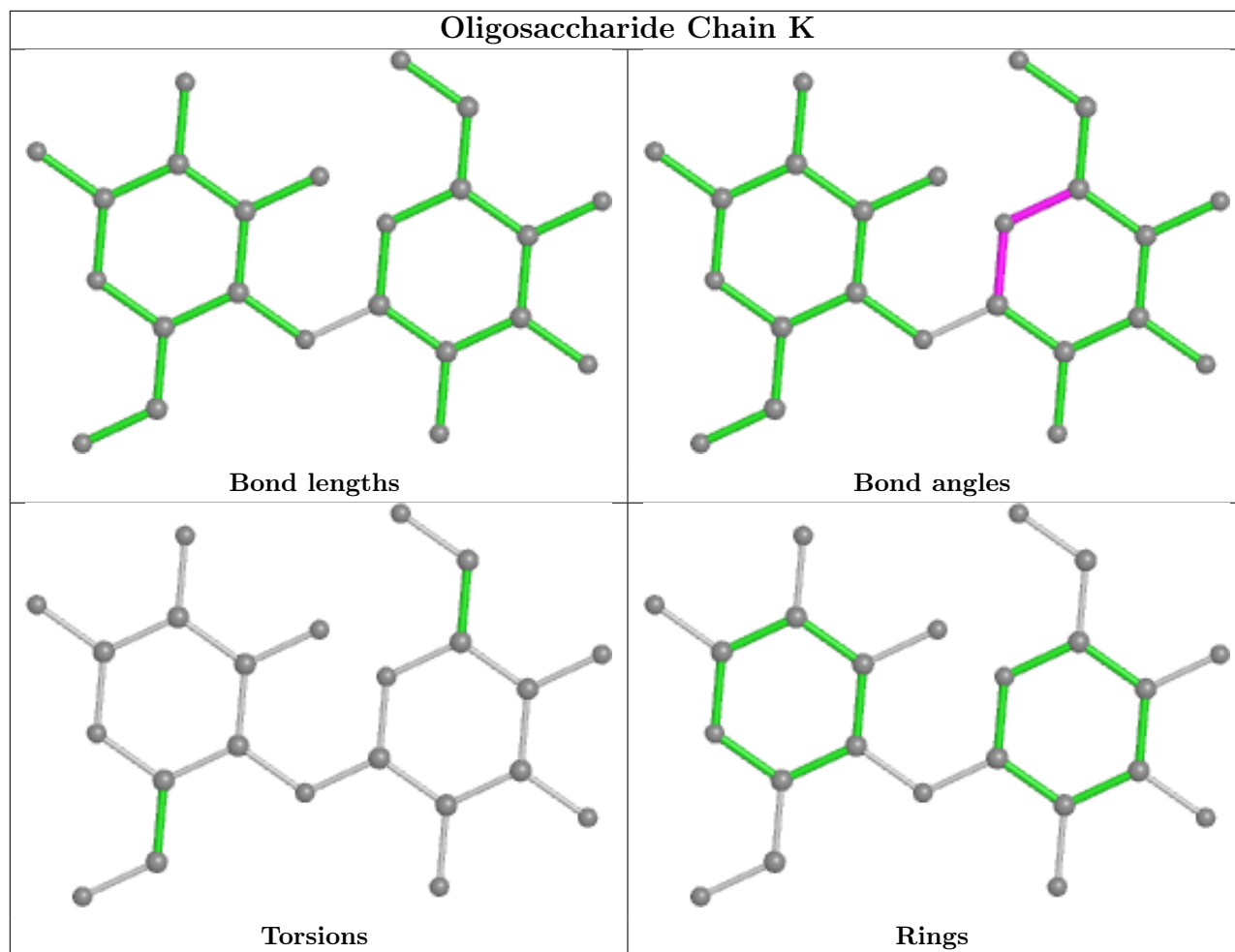| Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	2	GLC	1	0

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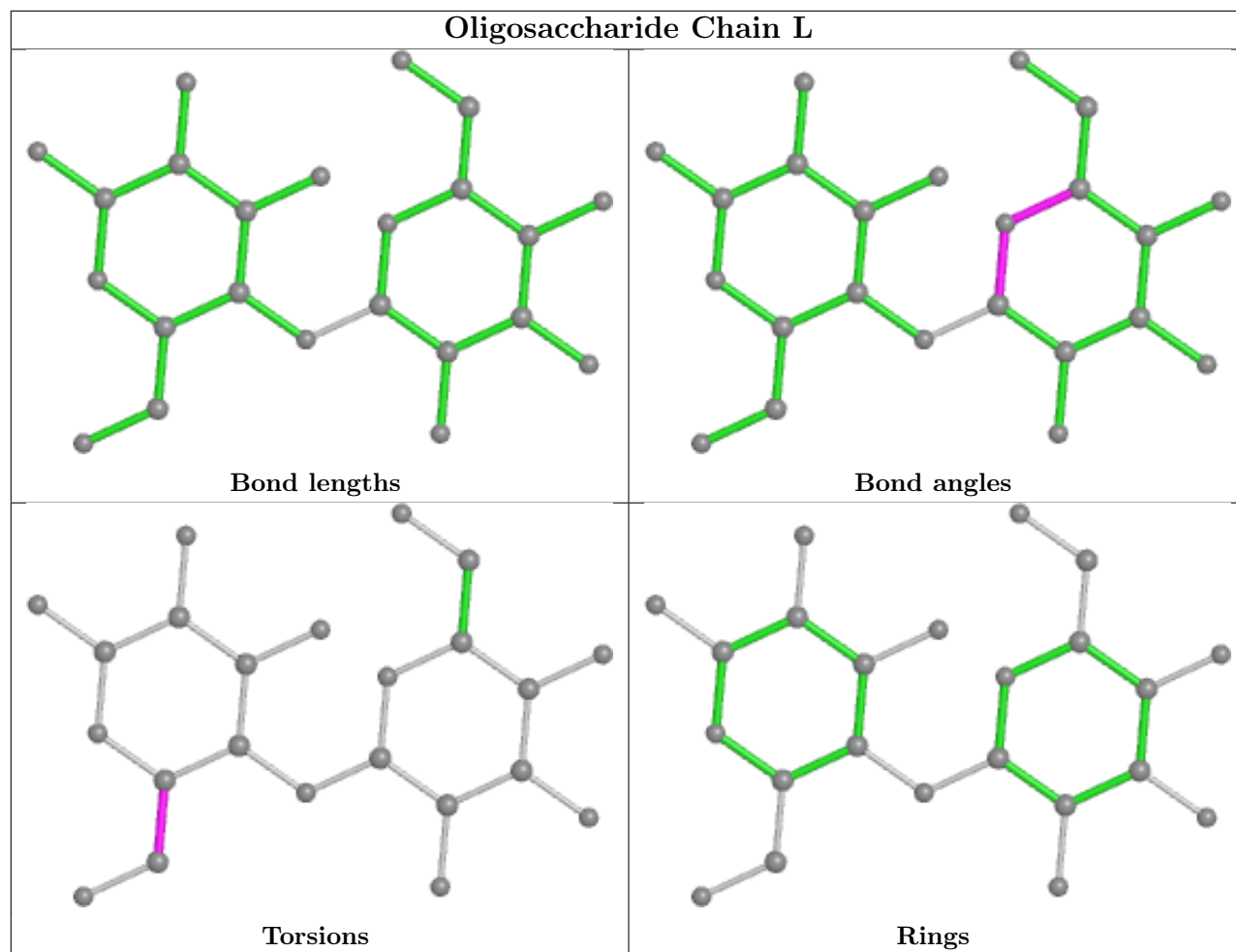
Oligosaccharide Chain G

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 K

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain L

Bond lengths

Bond angles

Torsions

Rings

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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(Å^2)	Q<0.9
1	A	460/477 (96%)	0.30	6 (1%)	77	76	22, 31, 47, 62	0
1	B	462/477 (96%)	0.47	11 (2%)	59	57	20, 31, 60, 75	0
1	C	461/477 (96%)	0.43	14 (3%)	50	49	24, 33, 54, 74	0
1	D	459/477 (96%)	0.44	13 (2%)	53	51	23, 35, 56, 84	0
1	E	463/477 (97%)	0.59	25 (5%)	25	24	23, 38, 56, 77	0
1	F	459/477 (96%)	0.87	44 (9%)	8	7	26, 42, 76, 90	0
All	All	2764/2862 (96%)	0.52	113 (4%)	37	36	20, 35, 59, 90	0

The worst 5 of 113 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	459	VAL	5.6
1	F	239	ALA	5.5
1	F	453	ARG	5.2
1	F	443	PRO	4.7
1	F	375	TYR	4.5

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

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

6.3 Carbohydrates (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GLC	K	1	12/12	0.89	0.15	32,34,36,39	0
2	GLC	L	1	12/12	0.90	0.12	33,38,41,46	0
2	GLC	G	1	12/12	0.91	0.12	28,32,33,35	0
2	GLC	L	2	11/12	0.91	0.16	28,32,35,36	0
2	GLC	J	1	12/12	0.93	0.11	25,33,36,38	0
2	GLC	I	1	12/12	0.94	0.11	28,31,35,36	0
2	GLC	K	2	11/12	0.94	0.11	28,31,34,35	0
2	GLC	I	2	11/12	0.94	0.12	23,27,30,32	0
2	GLC	H	1	12/12	0.94	0.12	26,30,31,32	0
2	GLC	G	2	11/12	0.95	0.14	23,25,30,30	0
2	GLC	J	2	11/12	0.95	0.15	23,29,32,32	0
2	GLC	H	2	11/12	0.96	0.11	20,24,26,27	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.
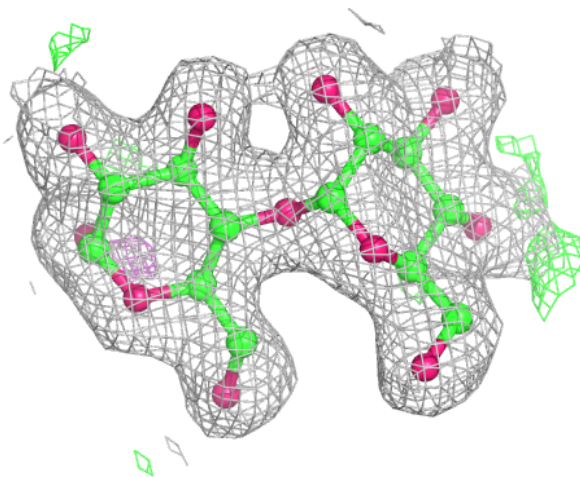

Electron density around Chain G:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
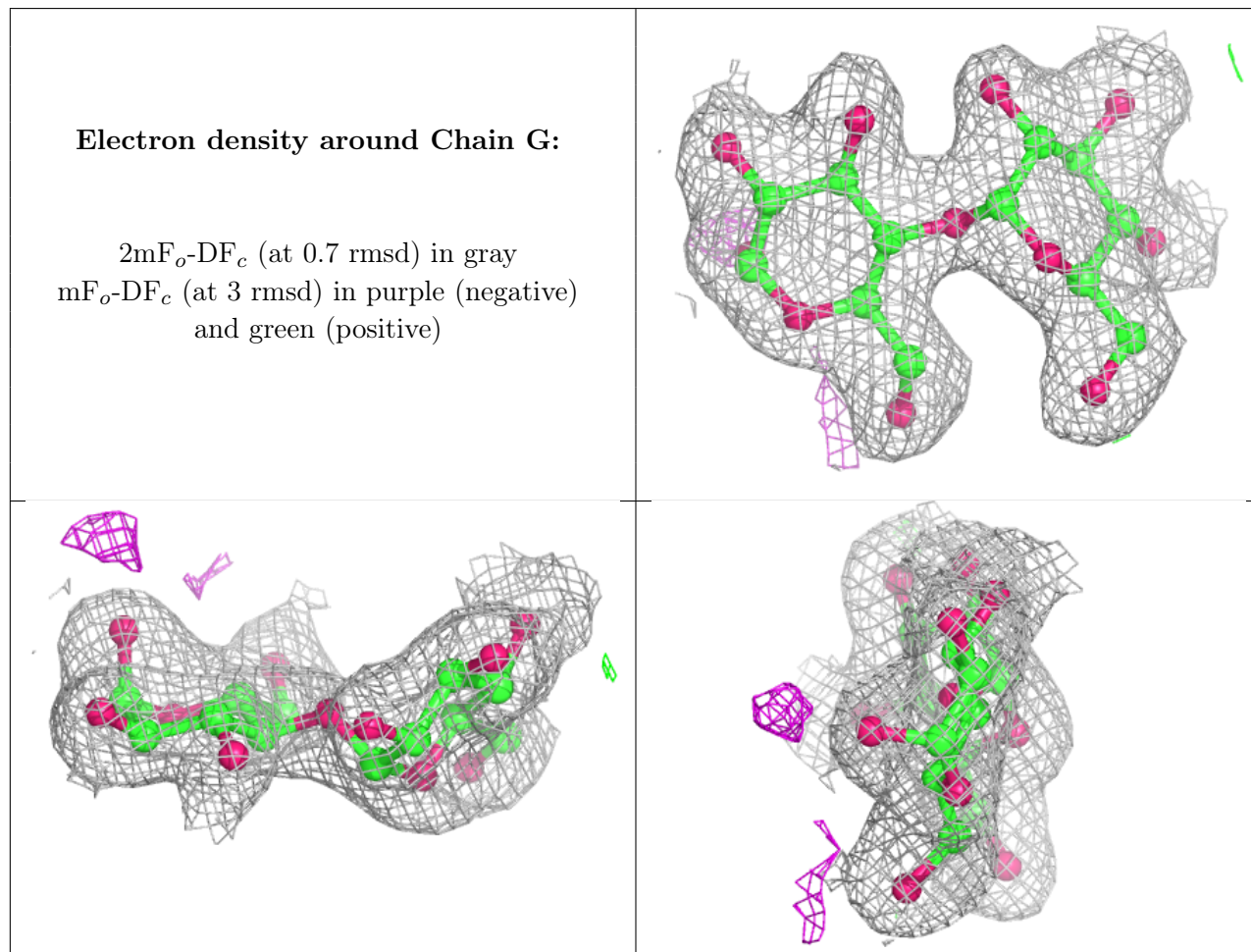
Electron density around Chain H:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
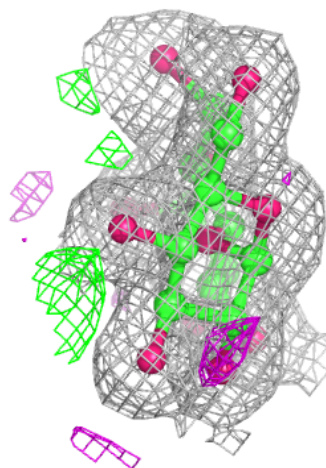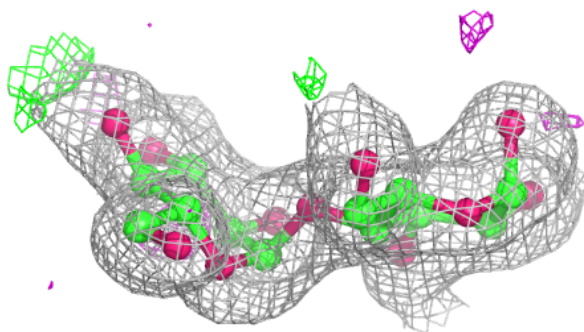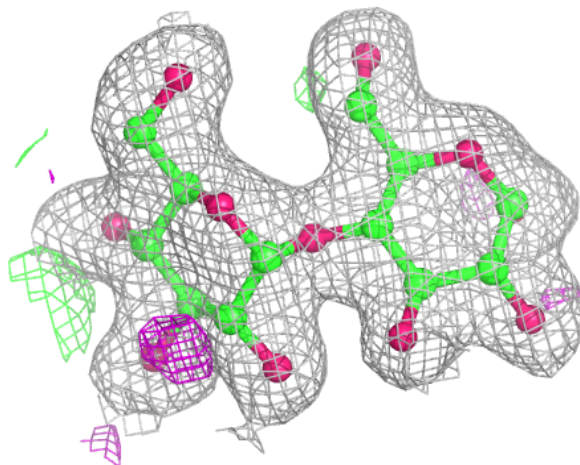
Electron density around Chain I:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
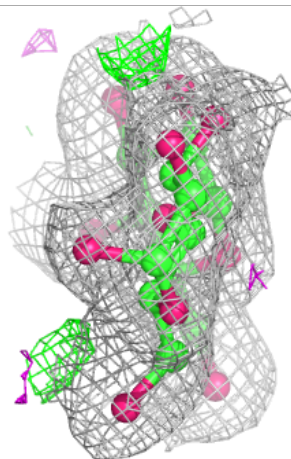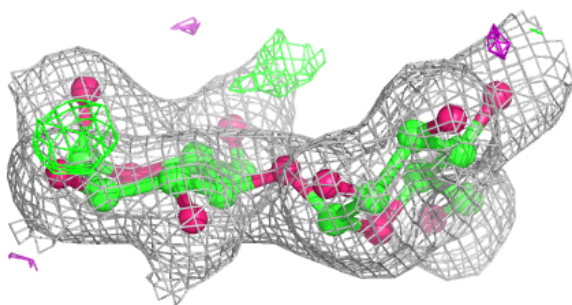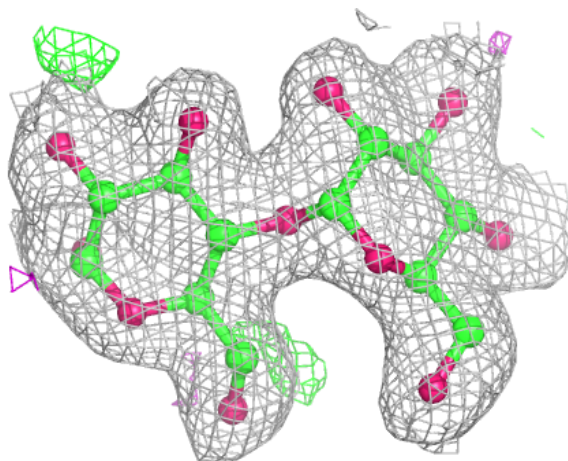$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
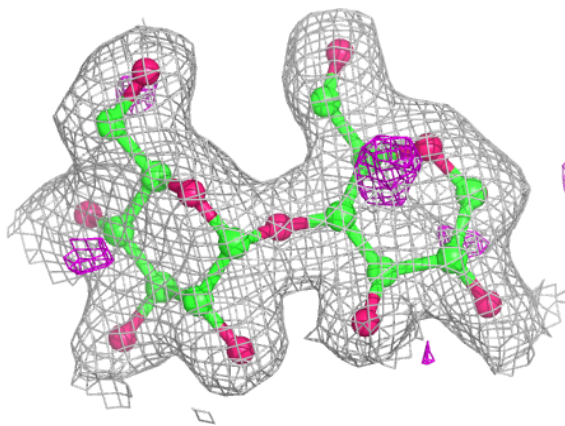and green (positive)
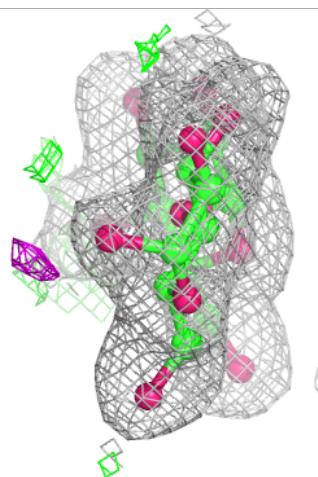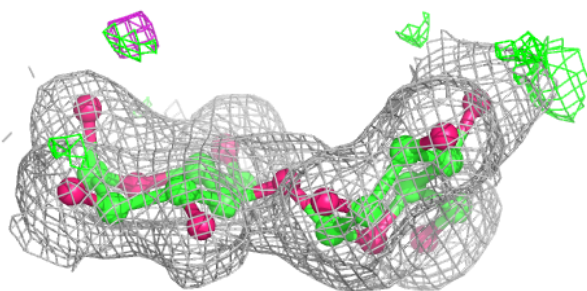
Electron density around Chain J:

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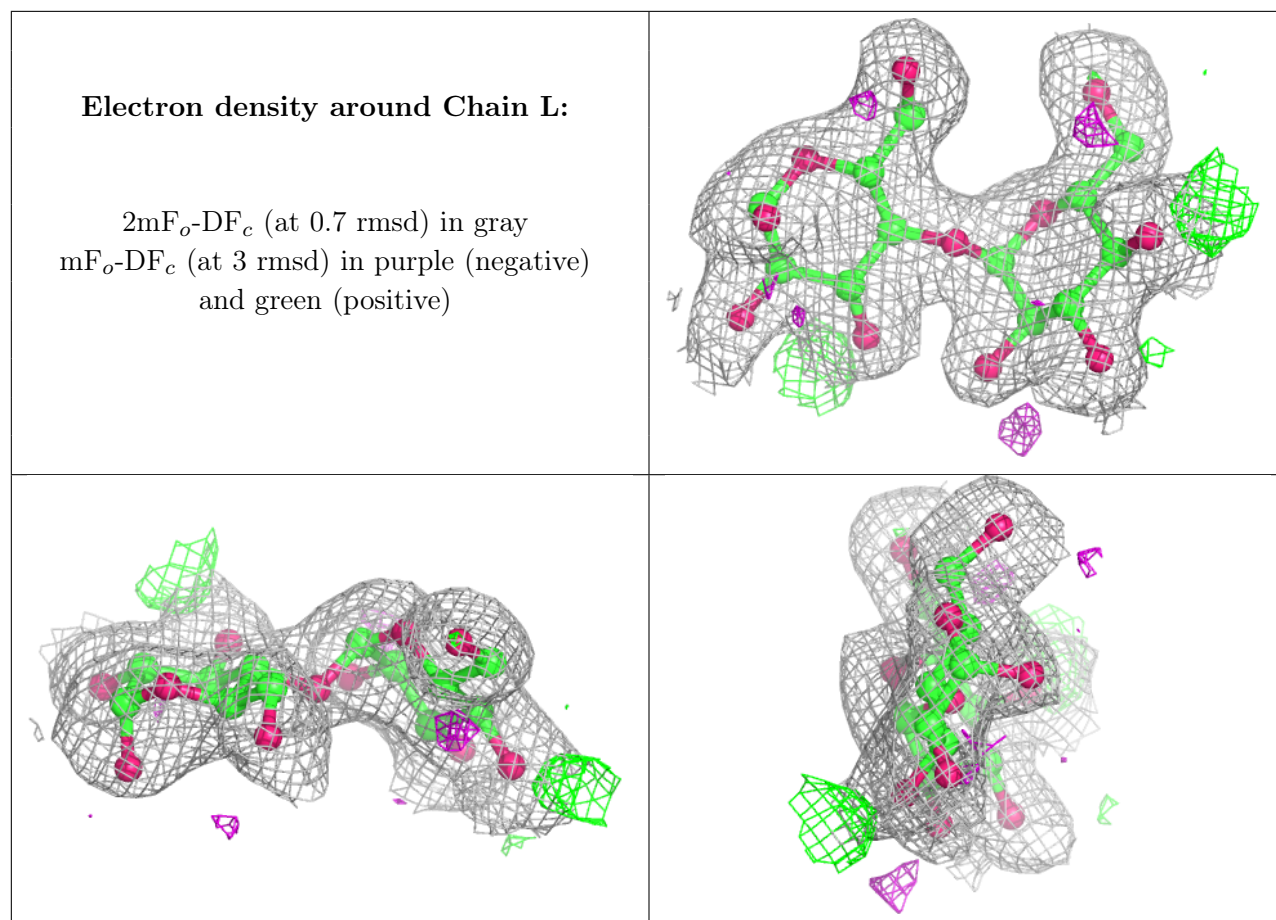and green (positive)

Electron density around Chain 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 L:

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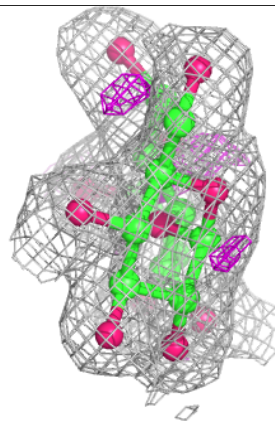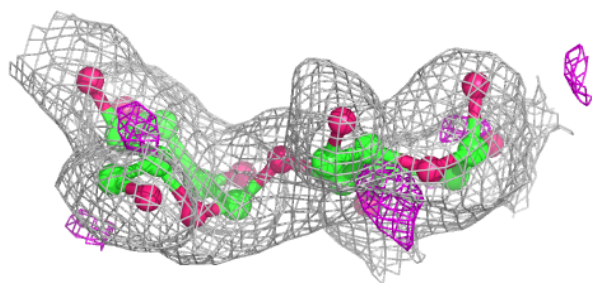
6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.