



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 6, 2020 – 09:56 AM BST

PDB ID : 3ABG
Title : X-ray Crystal Analysis of Bilirubin Oxidase from *Myrothecium verrucaria* at 2.3 angstrom Resolution using a Twin Crystal
Authors : Mizutani, K.; Toyoda, M.; Sagara, K.; Takahashi, N.; Sato, A.; Kamitaka, Y.; Tsujimura, S.; Nakanishi, Y.; Sugiura, T.; Yamaguchi, S.; Kano, K.; Mikami, B.
Deposited on : 2009-12-10
Resolution : 2.30 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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	:	2.13.1
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)	:	2.13.1

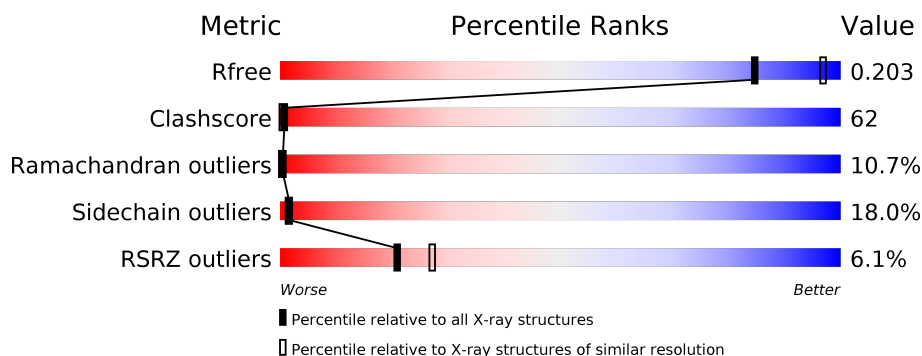
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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 $\leq 5\%$. 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	534	
1	B	534	
2	C	3	
2	E	3	
3	D	2	
3	F	2	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	D	1	X	-	-	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 8616 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 Bilirubin oxidase.

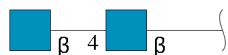
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	508	Total	C	N	O	S	0	1	0
			4045	2587	686	759	13			
1	B	518	Total	C	N	O	S	0	1	0
			4112	2628	698	773	13			

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

- 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	D	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	F	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	4	Total 4	Cu 4	0	0
4	A	4	Total 4	Cu 4	0	0

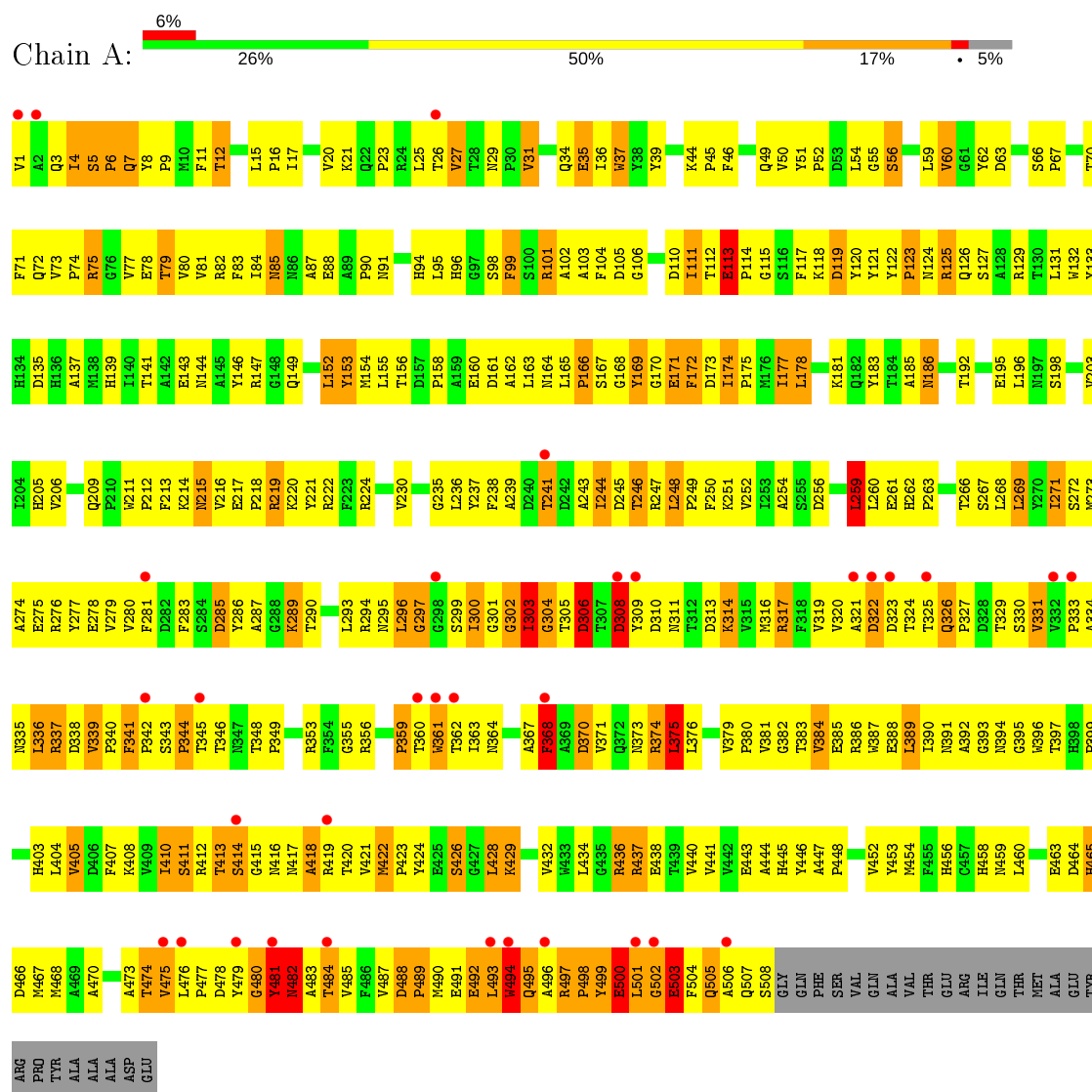
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	147	Total 147	O 147	0	0
5	B	170	Total 170	O 170	0	0

3 Residue-property plots

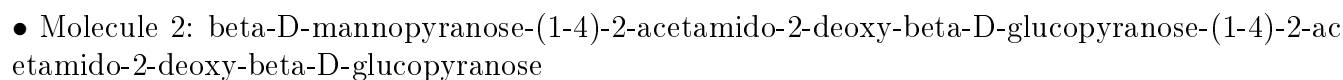
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Bilirubin oxidase

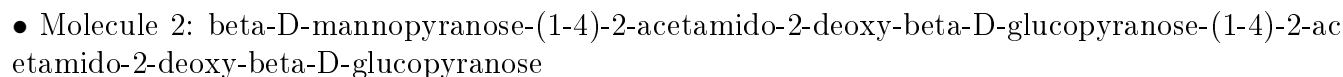


• Molecule 1: Bilirubin oxidase

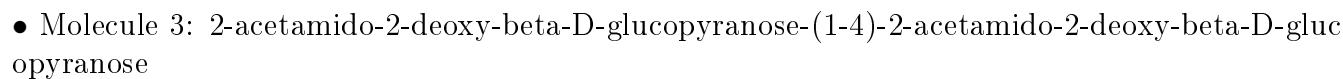




100%



100%



Frequency	Percentage
Daily	50%
Weekly	50%

MAG1
MAG2

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

Chain F:

100%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	139.74Å 139.74Å 135.56Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	33.56 – 2.30 48.65 – 2.30	Depositor EDS
% Data completeness (in resolution range)	96.7 (33.56-2.30) 96.7 (48.65-2.30)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.51 (at 2.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.203 , 0.263 0.208 , 0.203	Depositor DCC
R_{free} test set	3361 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	42.7	Xtriage
Anisotropy	0.273	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 76.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.469 for h,-h-k,-l	Xtriage
Reported twinning fraction	0.487 for h,-h-k,-l	Depositor
Outliers	0 of 66357 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8616	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.03% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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, CU

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	0/4175	0.66	0/5712
1	B	0.37	0/4243	0.65	0/5805
All	All	0.37	0/8418	0.65	0/11517

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	4
1	B	0	4
All	All	0	8

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	119	ASP	Peptide
1	A	304	GLY	Peptide
1	A	465	HIS	Peptide
1	A	484	THR	Peptide
1	B	119	ASP	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	4045	0	3842	505	0
1	B	4112	0	3897	502	0
2	C	39	0	34	1	0
2	E	39	0	34	4	0
3	D	28	0	25	1	0
3	F	28	0	25	2	0
4	A	4	0	0	0	0
4	B	4	0	0	0	0
5	A	147	0	0	23	0
5	B	170	0	0	29	0
All	All	8616	0	7857	1004	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 62.

The worst 5 of 1004 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:495:GLN:HB3	3:F:1:NAG:H62	1.23	1.14
1:A:317:ARG:HH11	1:A:317:ARG:HG2	1.02	1.14
1:A:17:ILE:HG21	1:A:172:PHE:HA	1.32	1.12
1:A:247:ARG:HD3	1:A:267:SER:HB3	1.15	1.11
1:B:158:PRO:HA	1:B:161:ASP:HB3	1.31	1.11

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	507/534 (95%)	349 (69%)	106 (21%)	52 (10%)	0	0
1	B	517/534 (97%)	365 (71%)	95 (18%)	57 (11%)	0	0
All	All	1024/1068 (96%)	714 (70%)	201 (20%)	109 (11%)	0	0

5 of 109 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	113	GLU
1	A	166	PRO
1	A	169	TYR
1	A	244	ILE

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	434/453 (96%)	356 (82%)	78 (18%)	1	1
1	B	440/453 (97%)	360 (82%)	80 (18%)	1	1
All	All	874/906 (96%)	716 (82%)	158 (18%)	1	1

5 of 158 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	482	ASN
1	B	100	SER
1	B	485	VAL
1	A	494	TRP
1	B	7	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	7	GLN
1	B	85	ASN
1	B	505	GLN
1	B	34	GLN
1	B	86	ASN

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 ⓘ

10 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	C	1	1,2	14,14,15	0.53	0	17,19,21	0.80	0
2	NAG	C	2	2	14,14,15	0.58	0	17,19,21	1.23	2 (11%)
2	BMA	C	3	2	11,11,12	0.55	0	15,15,17	1.87	3 (20%)
3	NAG	D	1	1,3	14,14,15	0.57	0	17,19,21	1.46	3 (17%)
3	NAG	D	2	3	14,14,15	0.46	0	17,19,21	1.76	3 (17%)
2	NAG	E	1	1,2	14,14,15	0.59	0	17,19,21	1.82	2 (11%)
2	NAG	E	2	2	14,14,15	0.40	0	17,19,21	2.93	7 (41%)
2	BMA	E	3	2	11,11,12	0.75	0	15,15,17	1.73	3 (20%)
3	NAG	F	1	1,3	14,14,15	0.39	0	17,19,21	1.37	3 (17%)
3	NAG	F	2	3	14,14,15	0.71	0	17,19,21	1.53	2 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	BMA	C	3	2	-	1/2/19/22	0/1/1/1
3	NAG	D	1	1,3	1/1/5/7	3/6/23/26	0/1/1/1
3	NAG	D	2	3	-	4/6/23/26	0/1/1/1
2	NAG	E	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
2	BMA	E	3	2	-	1/2/19/22	0/1/1/1
3	NAG	F	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	2	NAG	C1-O5-C5	7.72	122.66	112.19
2	E	1	NAG	C1-O5-C5	5.98	120.29	112.19
2	E	2	NAG	C2-N2-C7	-5.29	115.37	122.90
2	E	3	BMA	C1-C2-C3	5.12	115.96	109.67
2	C	3	BMA	C1-C2-C3	-4.63	103.98	109.67

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	D	1	NAG	C1

5 of 15 torsion outliers are listed below:

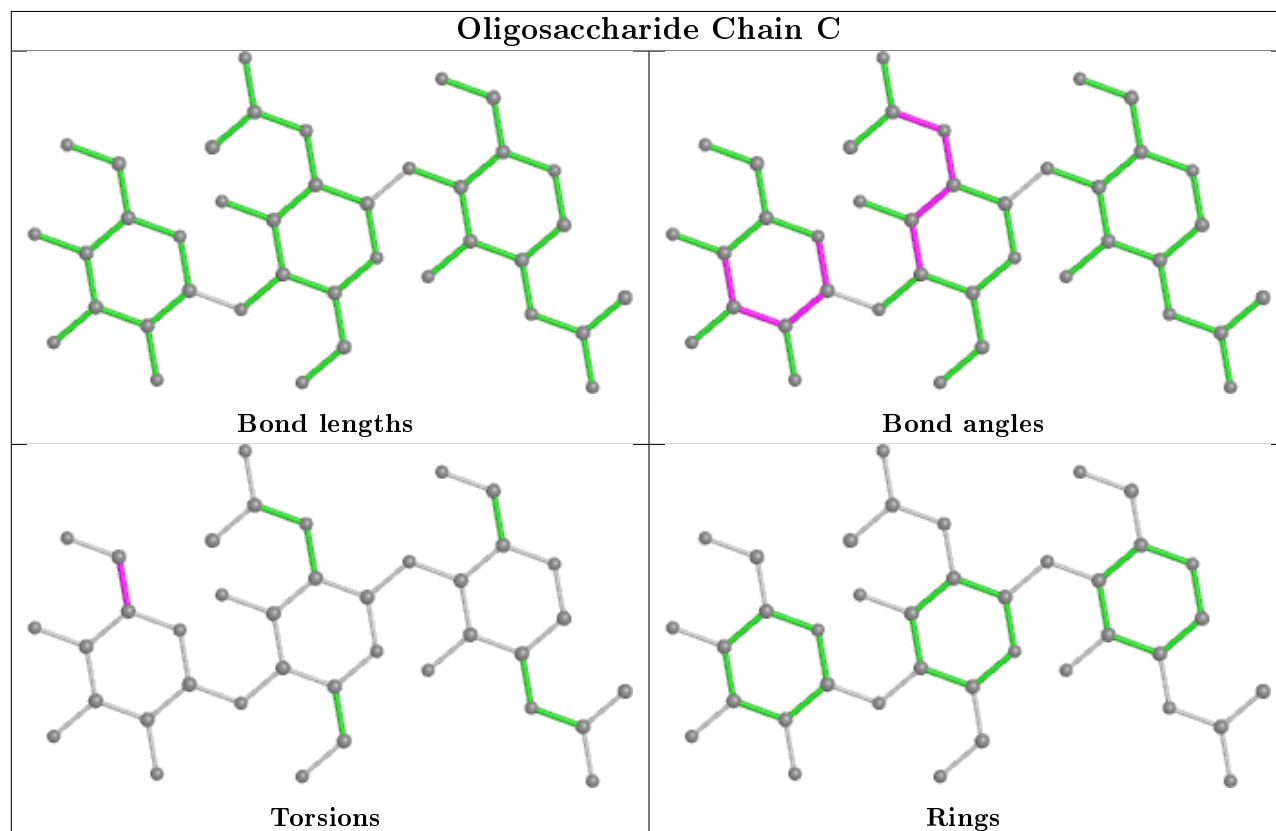
Mol	Chain	Res	Type	Atoms
2	E	1	NAG	O7-C7-N2-C2
3	D	1	NAG	C8-C7-N2-C2
3	D	1	NAG	O7-C7-N2-C2
2	E	1	NAG	C8-C7-N2-C2
3	D	2	NAG	O5-C5-C6-O6

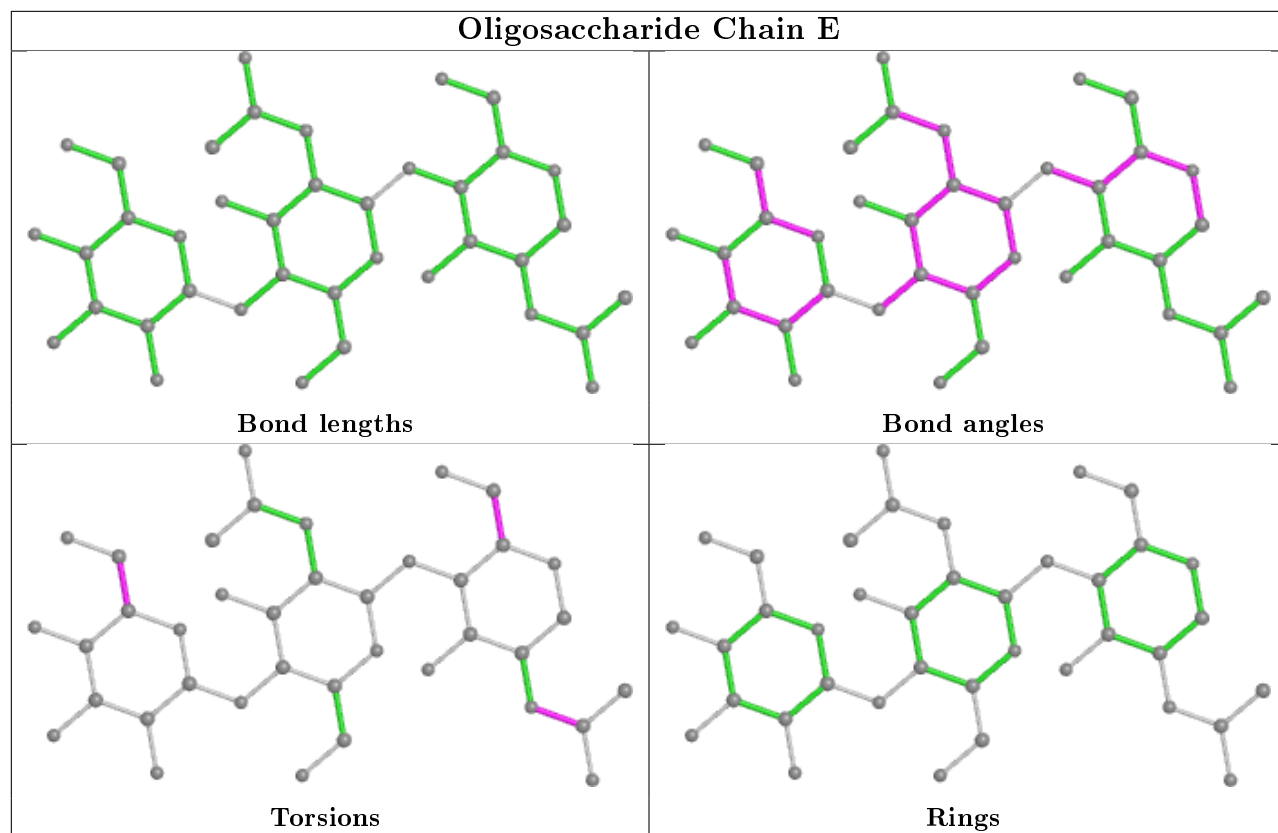
There are no ring outliers.

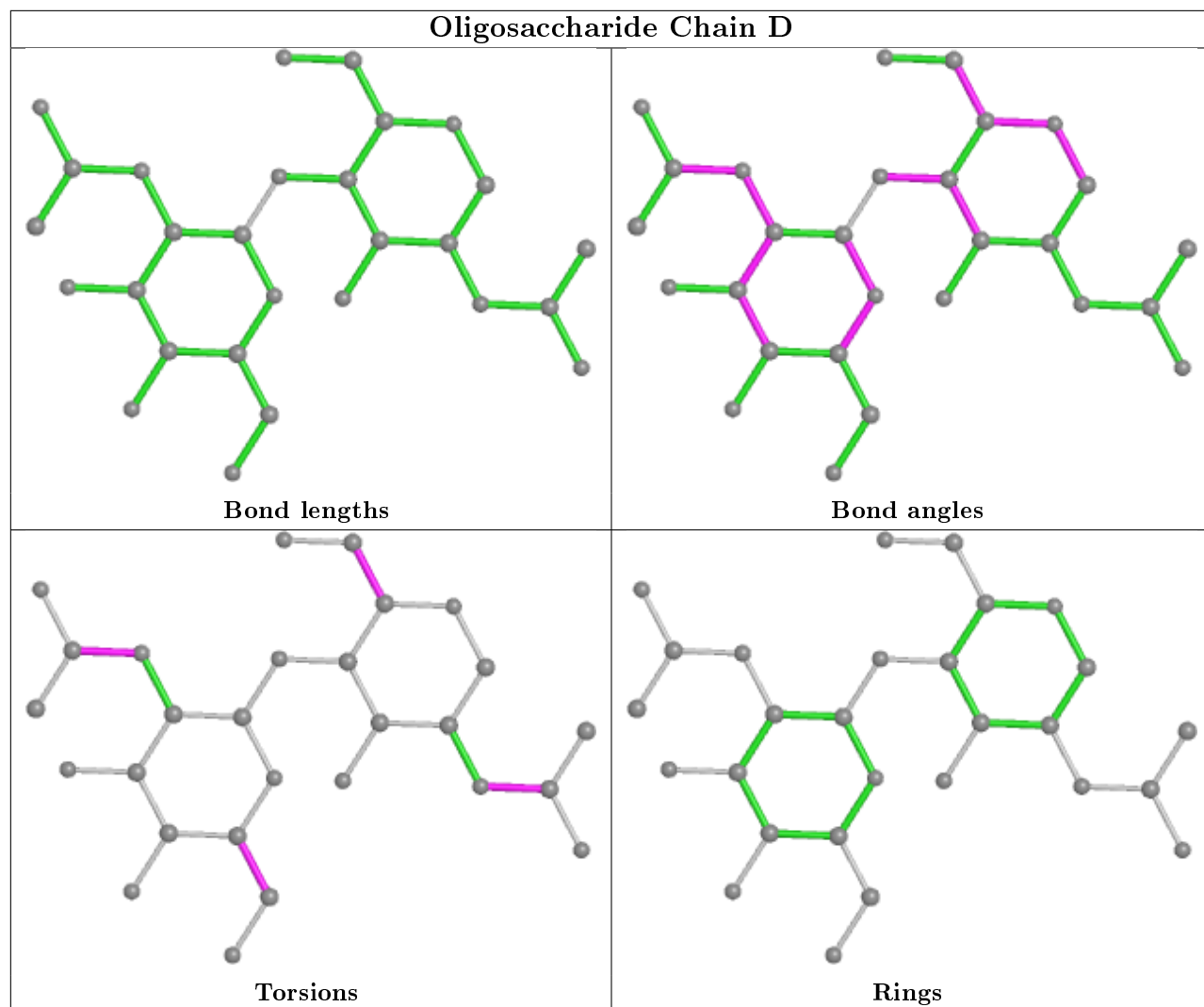
7 monomers are involved in 8 short contacts:

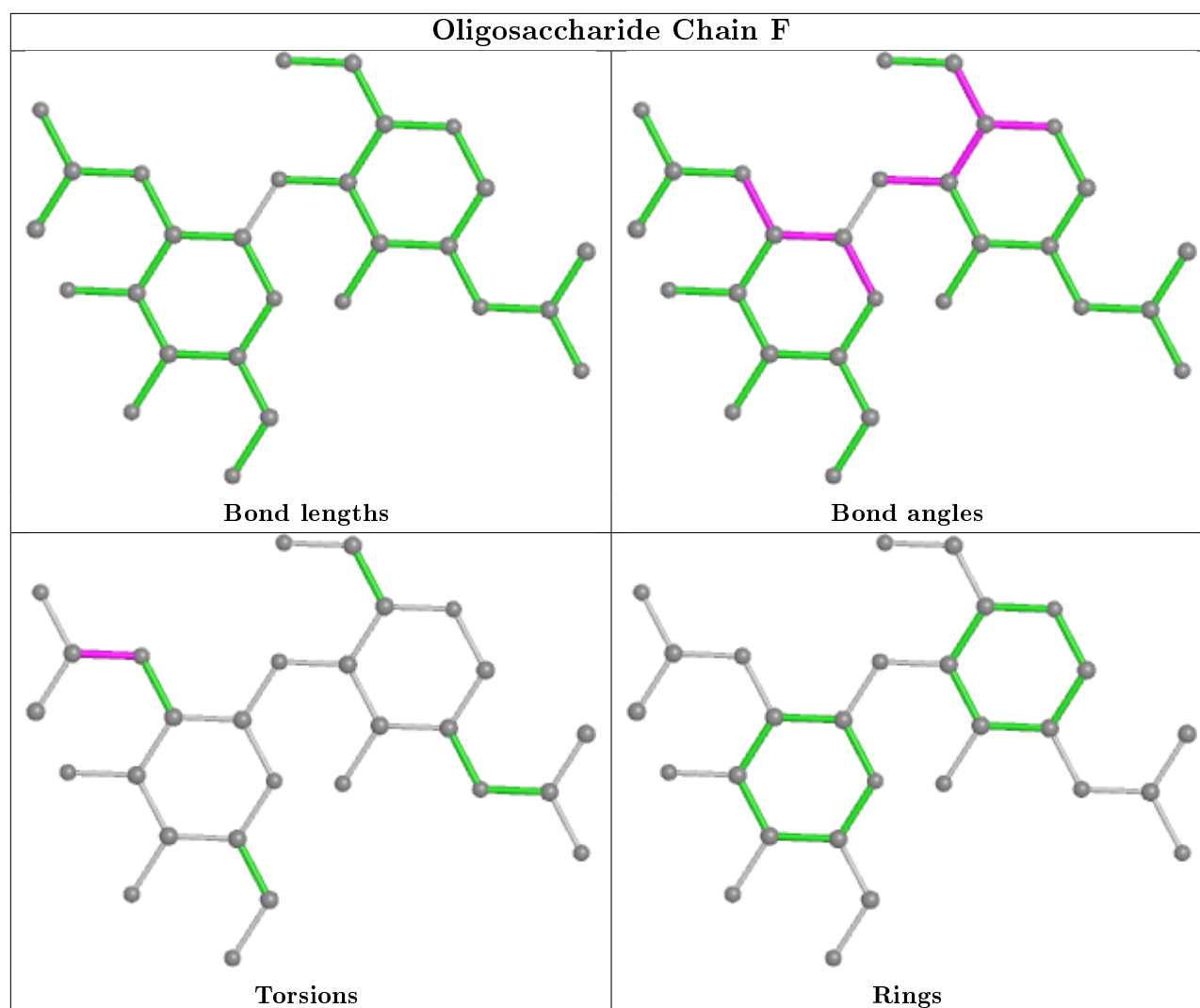
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1	NAG	1	0
2	E	3	BMA	1	0
2	E	2	NAG	4	0
2	C	1	NAG	1	0
3	F	2	NAG	1	0
3	F	1	NAG	2	0
2	E	1	NAG	2	0

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









5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

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	508/534 (95%)	0.21	33 (6%) 18 24	28, 48, 79, 125	0
1	B	518/534 (97%)	0.19	30 (5%) 23 29	28, 48, 81, 125	0
All	All	1026/1068 (96%)	0.20	63 (6%) 21 27	28, 48, 80, 125	0

The worst 5 of 63 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	501	LEU	10.1
1	A	342	PRO	8.0
1	B	322	ASP	7.4
1	B	416	ASN	6.4
1	A	476	LEU	6.3

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.

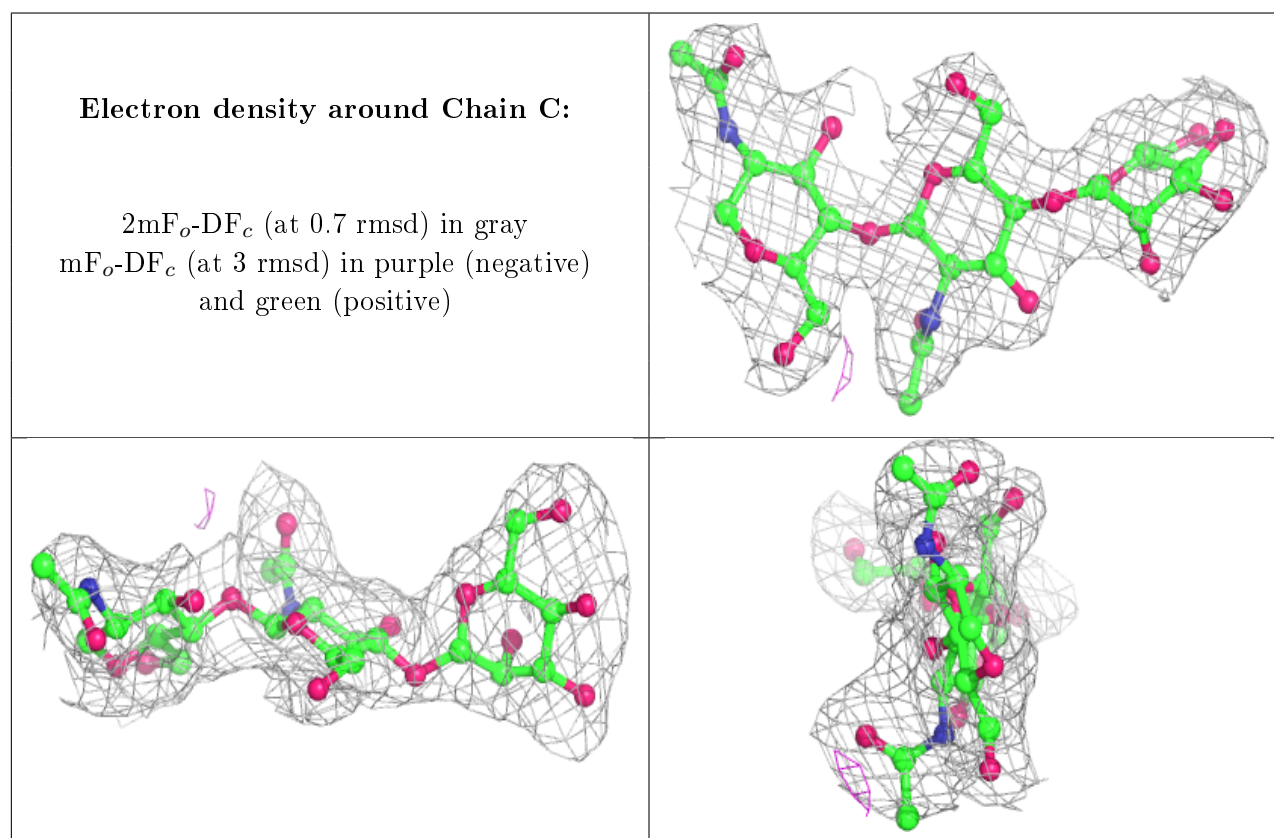
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	D	2	14/15	0.72	0.26	78,95,106,109	0
3	NAG	D	1	14/15	0.74	0.17	75,85,93,93	0
2	BMA	E	3	11/12	0.76	0.19	76,79,91,92	0
3	NAG	F	2	14/15	0.87	0.12	54,64,70,79	0
3	NAG	F	1	14/15	0.87	0.16	60,69,78,83	0

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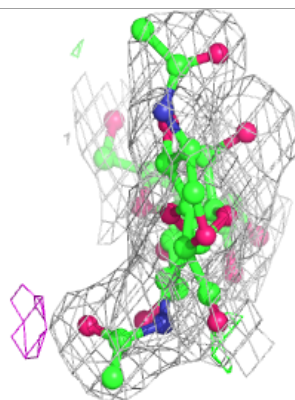
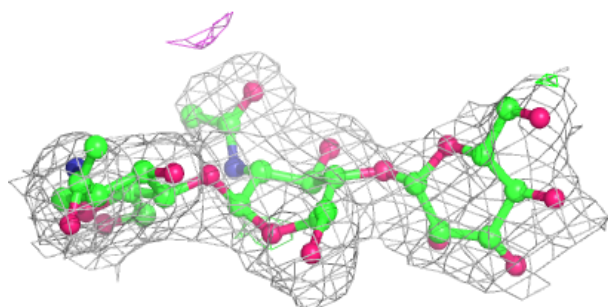
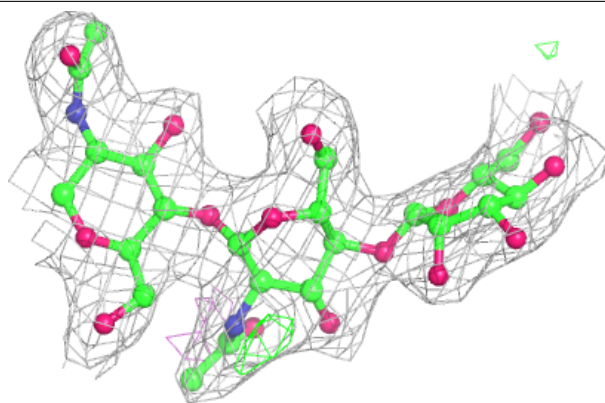
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NAG	C	2	14/15	0.89	0.12	57,63,71,72	0
2	BMA	C	3	11/12	0.90	0.10	52,72,84,84	0
2	NAG	E	2	14/15	0.94	0.10	48,59,68,74	0
2	NAG	C	1	14/15	0.94	0.12	41,47,54,57	0
2	NAG	E	1	14/15	0.96	0.13	33,43,55,57	0

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.



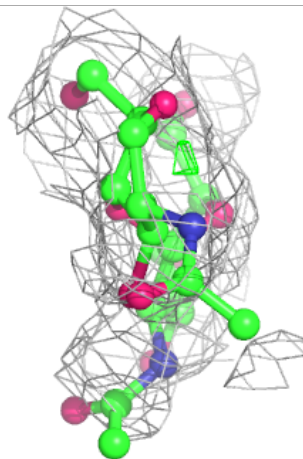
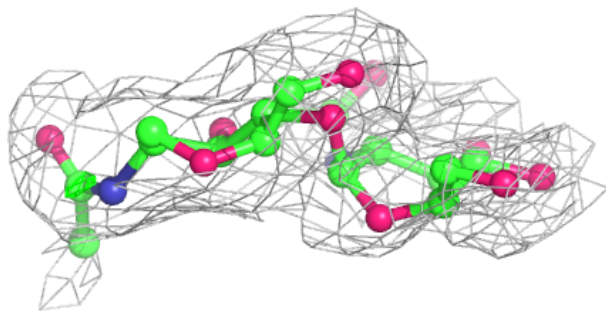
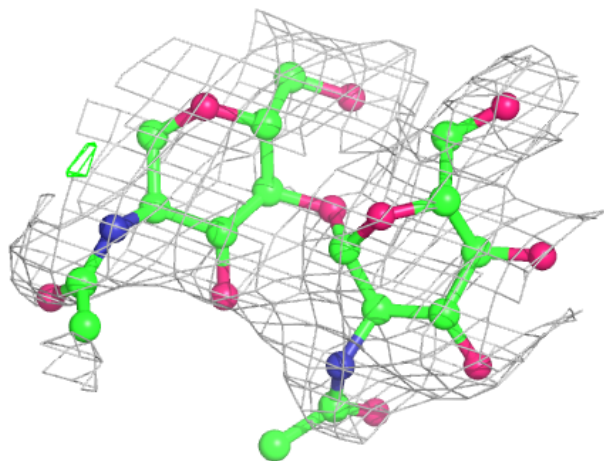
Electron density around Chain E:

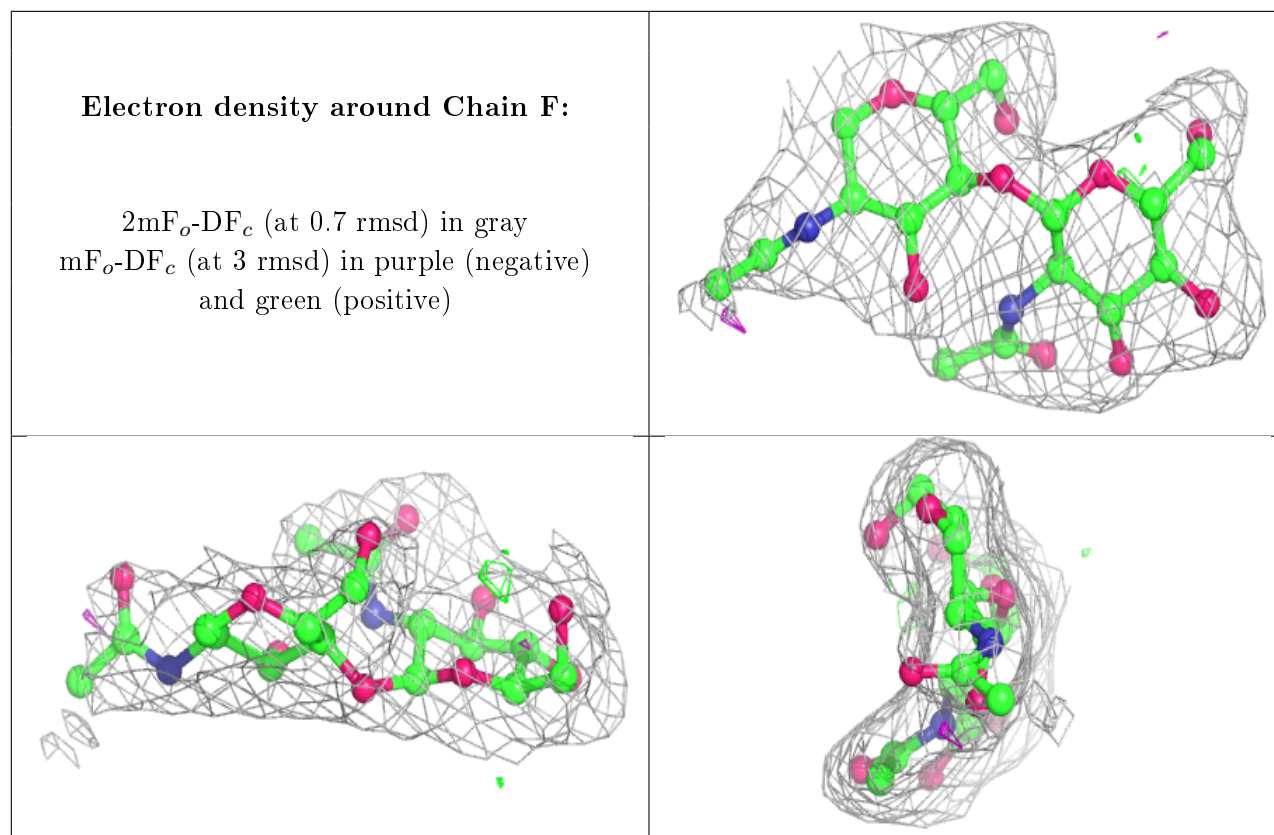
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain D:

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





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	CU	A	703	1/1	0.98	0.11	43,43,43,43	0
4	CU	B	701	1/1	0.99	0.14	37,37,37,37	0
4	CU	B	702	1/1	0.99	0.12	36,36,36,36	0
4	CU	A	701	1/1	0.99	0.14	35,35,35,35	0
4	CU	A	702	1/1	1.00	0.15	43,43,43,43	0
4	CU	B	704	1/1	1.00	0.13	32,32,32,32	0
4	CU	B	703	1/1	1.00	0.14	43,43,43,43	0
4	CU	A	704	1/1	1.00	0.10	34,34,34,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.