



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 8, 2024 – 01:47 pm GMT

PDB ID : 5MTH  
Title : Structure of DC8E8 Fab at pH 6.5 crystallized in spacegroup P21  
Authors : Skrabana, R.; Novak, M.; Cehlar, O.; Kontsekova, E.  
Deposited on : 2017-01-09  
Resolution : 1.73 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtrriage (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

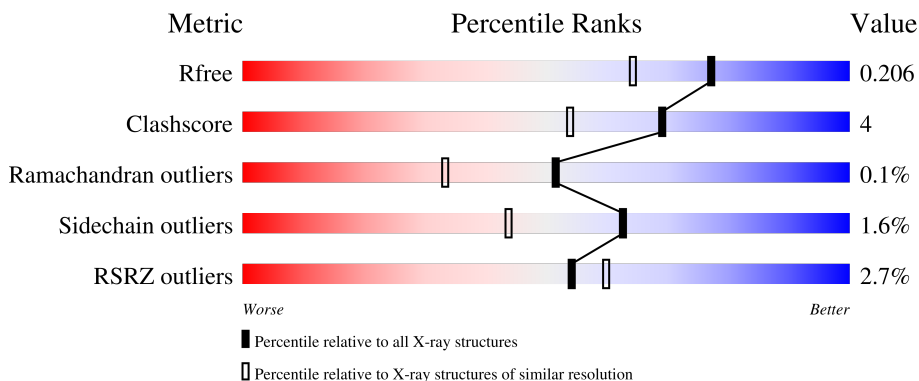
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.73 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.




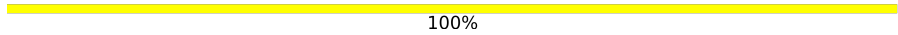
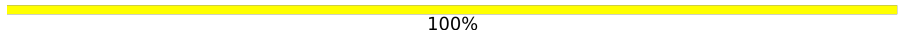
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3764 (1.76-1.72)
Clashscore	141614	3923 (1.76-1.72)
Ramachandran outliers	138981	3878 (1.76-1.72)
Sidechain outliers	138945	3878 (1.76-1.72)
RSRZ outliers	127900	3705 (1.76-1.72)

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  $\geq 3$ , 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	221	 3% 90% 9%
1	H	221	 3% 92% 7%
2	B	219	 3% 92% 7%
2	L	219	 2% 87% 11%
3	C	2	 50% 50%

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Mol	Chain	Length	Quality of chain
3	D	2	 50% 50%
3	E	2	 100%
3	F	2	 100%

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	ACT	A	301	-	-	-	X

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7524 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.

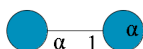
- Molecule 1 is a protein called antibody Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	H	221	1702	1078	276	338	10	0	6	0
1	A	221	1682	1068	272	332	10	0	4	0

- Molecule 2 is a protein called antibody Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	L	219	1740	1082	295	353	10	0	6	0
2	B	218	1712	1064	292	349	7	0	3	0

- Molecule 3 is an oligosaccharide called alpha-D-glucopyranose-(1-1)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
			Total	C	O			
3	C	2	23	12	11	0	0	0
3	D	2	23	12	11	0	0	0
3	E	2	23	12	11	0	0	0
3	F	2	23	12	11	0	0	0

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	H	1	Total C O 4 2 2	0	0
4	H	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0

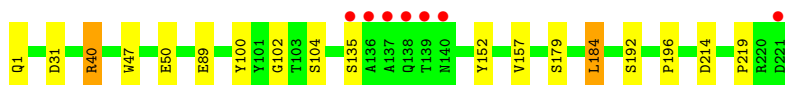
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	H	176	Total O 176 176	0	0
5	L	137	Total O 137 137	0	0
5	A	145	Total O 145 145	0	0
5	B	118	Total O 118 118	0	0

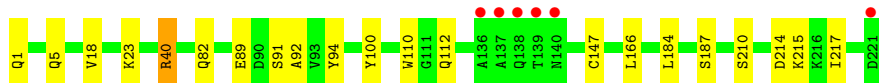
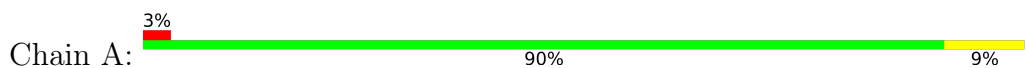
### 3 Residue-property plots [i](#)

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.

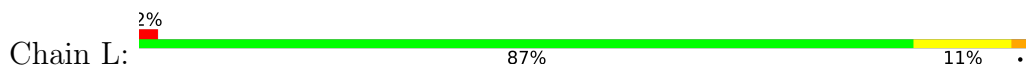
- Molecule 1: antibody Fab heavy chain



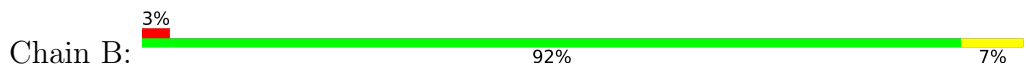
- Molecule 1: antibody Fab heavy chain



- Molecule 2: antibody Fab light chain



- Molecule 2: antibody Fab light chain



- Molecule 3: alpha-D-glucopyranose-(1-1)-alpha-D-glucopyranose



- Molecule 3: alpha-D-glucopyranose-(1-1)-alpha-D-glucopyranose

Chain D:  50% 50%

GLC1  
GLC2

- Molecule 3: alpha-D-glucopyranose-(1-1)-alpha-D-glucopyranose

Chain E:  100%

GLC1  
GLC2

- Molecule 3: alpha-D-glucopyranose-(1-1)-alpha-D-glucopyranose

Chain F:  100%

GLC1  
GLC2

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	41.45Å 111.77Å 95.64Å 90.00° 90.56° 90.00°	Depositor
Resolution (Å)	38.86 – 1.73 38.86 – 1.71	Depositor EDS
% Data completeness (in resolution range)	95.3 (38.86-1.73) 96.9 (38.86-1.71)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.13 (at 1.72Å)	Xtriage
Refinement program	REFMAC 5.8.0151	Depositor
R, $R_{free}$	0.185 , 0.235 0.168 , 0.206	Depositor DCC
$R_{free}$ test set	4506 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.4	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 39.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.116 for h,-k,-l	Xtriage
Reported twinning fraction	0.909 for H, K, L 0.091 for -h,-k,l	Depositor
Outliers	0 of 90399 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7524	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.48% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: GLC, PCA, ACT

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	1.05	4/1729 (0.2%)	0.97	3/2361 (0.1%)
1	H	1.05	0/1746	0.99	3/2384 (0.1%)
2	B	0.93	0/1751	0.94	4/2372 (0.2%)
2	L	0.90	0/1783	0.98	4/2414 (0.2%)
All	All	0.98	4/7009 (0.1%)	0.97	14/9531 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	94	TYR	CE1-CZ	7.75	1.48	1.38
1	A	110	TRP	C-O	5.49	1.33	1.23
1	A	110	TRP	CE3-CZ3	5.26	1.47	1.38
1	A	94	TYR	CG-CD2	5.07	1.45	1.39

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	40[A]	ARG	NE-CZ-NH1	8.81	124.70	120.30
1	H	40[B]	ARG	NE-CZ-NH1	8.81	124.70	120.30
2	B	101	ARG	NE-CZ-NH1	7.76	124.18	120.30
2	L	113	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	A	214	ASP	CB-CG-OD1	6.20	123.88	118.30
2	B	101	ARG	NE-CZ-NH2	-6.15	117.22	120.30
2	B	180	MET	CG-SD-CE	-5.56	91.31	100.20
1	A	40[A]	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	A	40[B]	ARG	NE-CZ-NH1	5.52	123.06	120.30
2	L	60	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	H	184	LEU	CA-CB-CG	5.49	127.94	115.30
2	B	193	ARG	NE-CZ-NH2	5.22	122.91	120.30
2	L	100	LEU	CB-CG-CD1	5.18	119.81	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	180	MET	CG-SD-CE	-5.08	92.06	100.20

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	1682	0	1629	11	0
1	H	1702	0	1643	13	1
2	B	1712	0	1656	10	1
2	L	1740	0	1678	22	0
3	C	23	0	21	0	0
3	D	23	0	21	0	0
3	E	23	0	21	0	0
3	F	23	0	21	0	0
4	A	8	0	6	0	0
4	B	4	0	3	0	0
4	H	8	0	6	0	0
5	A	145	0	0	0	1
5	B	118	0	0	5	0
5	H	176	0	0	3	0
5	L	137	0	0	7	1
All	All	7524	0	6705	50	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.

All (50) 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:L:31:ASN:HB3	2:L:34:THR:OG1	1.45	1.14
2:L:60:ARG:NH1	2:L:68:PHE:O	2.09	0.85
5:H:467:HOH:O	1:A:215:LYS:HE2	1.80	0.80
2:L:202:THR:HG23	5:L:520:HOH:O	1.82	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:89:LEU:HD11	5:L:495:HOH:O	1.83	0.78
2:L:31:ASN:CB	2:L:34:THR:OG1	2.34	0.70
2:B:33:ARG:NH2	5:B:401:HOH:O	1.77	0.69
1:A:40[B]:ARG:NE	1:A:91:SER:O	2.26	0.68
1:H:31:ASP:OD1	5:H:401:HOH:O	2.14	0.65
2:B:143:ASN:ND2	5:B:402:HOH:O	2.29	0.65
2:L:31:ASN:HB3	2:L:34:THR:HG1	1.58	0.65
2:L:195:ASN:HB2	5:L:409:HOH:O	1.98	0.63
2:L:89:LEU:HD21	2:L:111:ILE:HG12	1.83	0.61
2:B:89:LEU:HD11	5:B:405:HOH:O	2.01	0.60
2:L:141:LEU:HD21	2:L:151:VAL:HG22	1.84	0.58
1:H:157:VAL:HG22	1:H:184:LEU:HD21	1.85	0.57
1:H:89:GLU:HG2	5:H:533:HOH:O	2.07	0.55
2:L:89:LEU:CD1	5:L:495:HOH:O	2.49	0.55
2:L:11:LEU:HD13	2:L:19:VAL:HG21	1.87	0.54
2:B:42:TYR:CE1	2:B:95:LYS:HE3	2.43	0.54
1:A:187:SER:HB3	2:B:140:PHE:CE2	2.43	0.53
1:A:40[A]:ARG:NH1	1:A:89:GLU:O	2.41	0.51
1:H:135:SER:HB3	2:L:219:CYS:HA	1.93	0.50
2:L:89:LEU:CD2	2:L:111:ILE:HG12	2.41	0.49
1:H:100:TYR:HB3	1:H:104:SER:OG	2.13	0.48
1:H:152:TYR:CE2	1:H:157:VAL:HG13	2.48	0.48
2:B:95:LYS:HD3	2:B:103:PHE:CZ	2.49	0.48
2:B:60:ARG:NH1	2:B:68:PHE:O	2.46	0.47
2:L:78[A]:THR:HG22	5:L:420:HOH:O	2.15	0.47
1:H:40[A]:ARG:NH2	1:H:89:GLU:OE1	2.49	0.46
1:A:40[B]:ARG:CD	1:A:91:SER:O	2.64	0.46
1:A:18:VAL:O	1:A:82:GLN:HA	2.15	0.46
2:L:86:ALA:HB1	5:L:495:HOH:O	2.15	0.46
2:L:195:ASN:ND2	5:L:409:HOH:O	2.49	0.46
1:H:196:PRO:HB3	1:H:219:PRO:HG3	1.99	0.45
1:H:135:SER:CB	2:L:219:CYS:HA	2.47	0.44
2:L:32:SER:OG	2:L:33:ARG:N	2.51	0.44
1:H:214:ASP:O	1:A:210:SER:HB2	2.18	0.43
1:H:47:TRP:CZ3	2:L:100:LEU:HB3	2.53	0.43
1:A:40[B]:ARG:HD2	1:A:92:ALA:HB2	2.01	0.43
2:B:86:ALA:HB1	5:B:405:HOH:O	2.19	0.42
2:L:139[B]:CYS:SG	2:L:153:TRP:CH2	3.13	0.41
1:A:147[A]:CYS:SG	1:A:217:ILE:HD11	2.59	0.41
1:H:50:GLU:OE2	2:L:101:ARG:NH2	2.54	0.41
2:B:45:LYS:NZ	5:B:403:HOH:O	2.37	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:LEU:HD12	1:A:184:LEU:C	2.41	0.41
1:H:152:TYR:CZ	1:H:157:VAL:HG13	2.55	0.41
2:L:92:TYR:O	2:L:106:GLY:HA2	2.21	0.41
2:B:11:LEU:HD13	2:B:19:VAL:CG2	2.51	0.41
1:A:5[B]:GLN:NE2	1:A:112:GLN:HE22	2.20	0.40

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)
1:H:102:GLY:O	2:B:33:ARG:NE 1_554	2.03	0.17
5:L:514:HOH:O	5:A:402:HOH:O 1_554	2.03	0.17

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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	223/221 (101%)	218 (98%)	5 (2%)	0	100	100
1	H	225/221 (102%)	219 (97%)	6 (3%)	0	100	100
2	B	219/219 (100%)	211 (96%)	8 (4%)	0	100	100
2	L	223/219 (102%)	217 (97%)	5 (2%)	1 (0%)	34	17
All	All	890/880 (101%)	865 (97%)	24 (3%)	1 (0%)	51	33

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	32	SER

### 5.3.2 Protein sidechains [i](#)

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	190/190 (100%)	187 (98%)	3 (2%)	62	44
1	H	193/190 (102%)	191 (99%)	2 (1%)	76	63
2	B	197/195 (101%)	195 (99%)	2 (1%)	76	63
2	L	201/195 (103%)	195 (97%)	6 (3%)	41	17
All	All	781/770 (101%)	768 (98%)	13 (2%)	62	41

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	179	SER
1	H	192	SER
2	L	19	VAL
2	L	95	LYS
2	L	162	ASN
2	L	199[A]	CYS
2	L	199[B]	CYS
2	L	219	CYS
1	A	23	LYS
1	A	100	TYR
1	A	166	LEU
2	B	95	LYS
2	B	124	PRO

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

Mol	Chain	Res	Type
2	L	195	ASN
1	A	3	GLN
2	B	143	ASN

### 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	PCA	H	1	1	7,8,9	0.55	0	9,10,12	1.48	2 (22%)
1	PCA	A	1	1	7,8,9	0.79	0	9,10,12	1.45	1 (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
1	PCA	H	1	1	-	0/0/11/13	0/1/1/1
1	PCA	A	1	1	-	0/0/11/13	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	1	PCA	CB-CA-C	-3.12	108.41	112.70
1	A	1	PCA	OE-CD-CG	-3.06	121.43	126.76
1	H	1	PCA	OE-CD-CG	-2.05	123.19	126.76

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates i

8 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	GLC	C	1	3	11,11,12	1.25	0	15,15,17	1.39	3 (20%)
3	GLC	C	2	3	12,12,12	0.99	0	17,17,17	0.81	0
3	GLC	D	1	3	11,11,12	0.39	0	15,15,17	1.30	0
3	GLC	D	2	3	12,12,12	0.36	0	17,17,17	1.11	1 (5%)
3	GLC	E	1	3	11,11,12	0.70	0	15,15,17	1.40	3 (20%)
3	GLC	E	2	3	12,12,12	0.88	0	17,17,17	1.38	3 (17%)
3	GLC	F	1	3	11,11,12	0.97	1 (9%)	15,15,17	1.66	3 (20%)
3	GLC	F	2	3	12,12,12	0.96	0	17,17,17	1.08	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
3	GLC	C	1	3	-	0/2/19/22	0/1/1/1
3	GLC	C	2	3	-	0/2/22/22	0/1/1/1
3	GLC	D	1	3	-	2/2/19/22	0/1/1/1
3	GLC	D	2	3	-	0/2/22/22	0/1/1/1
3	GLC	E	1	3	-	0/2/19/22	0/1/1/1
3	GLC	E	2	3	-	0/2/22/22	0/1/1/1
3	GLC	F	1	3	-	0/2/19/22	0/1/1/1
3	GLC	F	2	3	-	0/2/22/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	1	GLC	C4-C3	2.30	1.58	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	1	GLC	C1-O5-C5	4.54	118.34	112.19
3	E	2	GLC	O5-C1-C2	3.09	115.80	110.28
3	F	1	GLC	C2-C3-C4	-2.84	105.98	110.89
3	E	2	GLC	O3-C3-C2	-2.80	103.87	110.35
3	C	1	GLC	C1-O5-C5	2.76	115.92	112.19
3	F	2	GLC	O4-C4-C5	2.56	115.65	109.30
3	E	1	GLC	O3-C3-C4	-2.33	104.96	110.35
3	E	1	GLC	O3-C3-C2	2.31	114.41	109.99
3	E	2	GLC	O3-C3-C4	2.16	115.35	110.35
3	C	1	GLC	O5-C5-C6	2.16	110.59	107.20
3	F	1	GLC	O2-C2-C3	2.14	114.42	110.14
3	E	1	GLC	O5-C1-C2	2.12	114.05	110.77
3	D	2	GLC	C1-C2-C3	2.11	114.70	110.31
3	C	1	GLC	C1-C2-C3	-2.06	107.14	109.67

There are no chirality outliers.

All (2) torsion outliers are listed below:

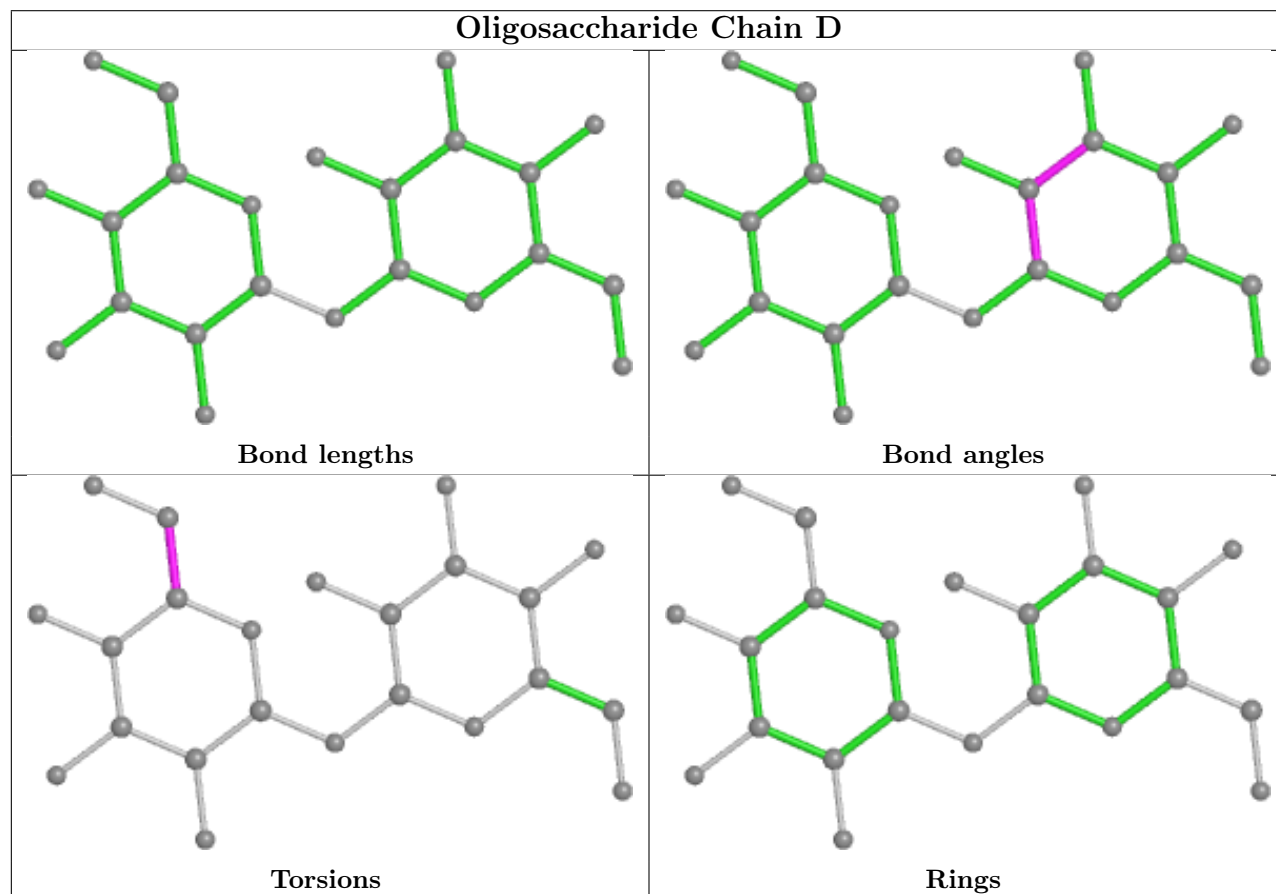
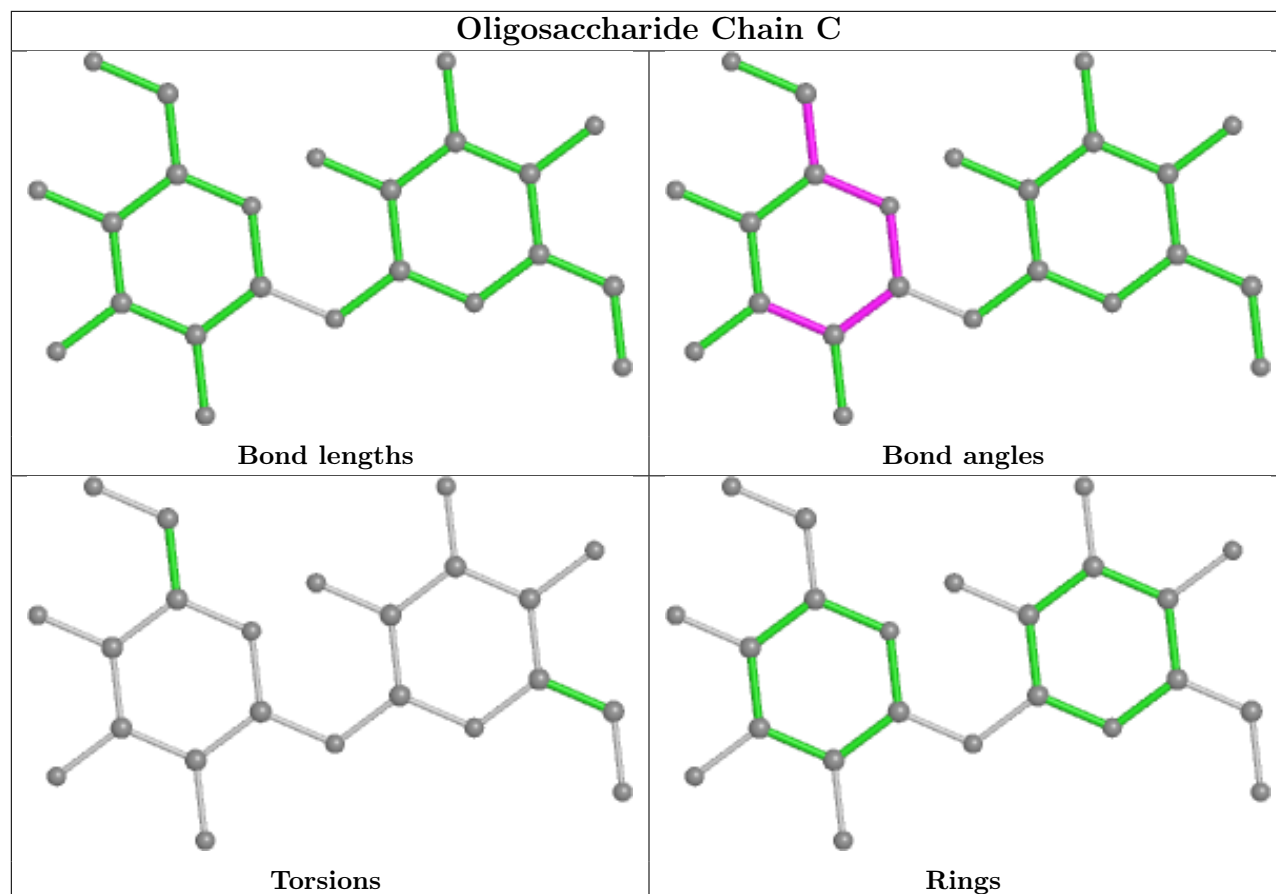
Mol	Chain	Res	Type	Atoms
3	D	1	GLC	O5-C5-C6-O6
3	D	1	GLC	C4-C5-C6-O6

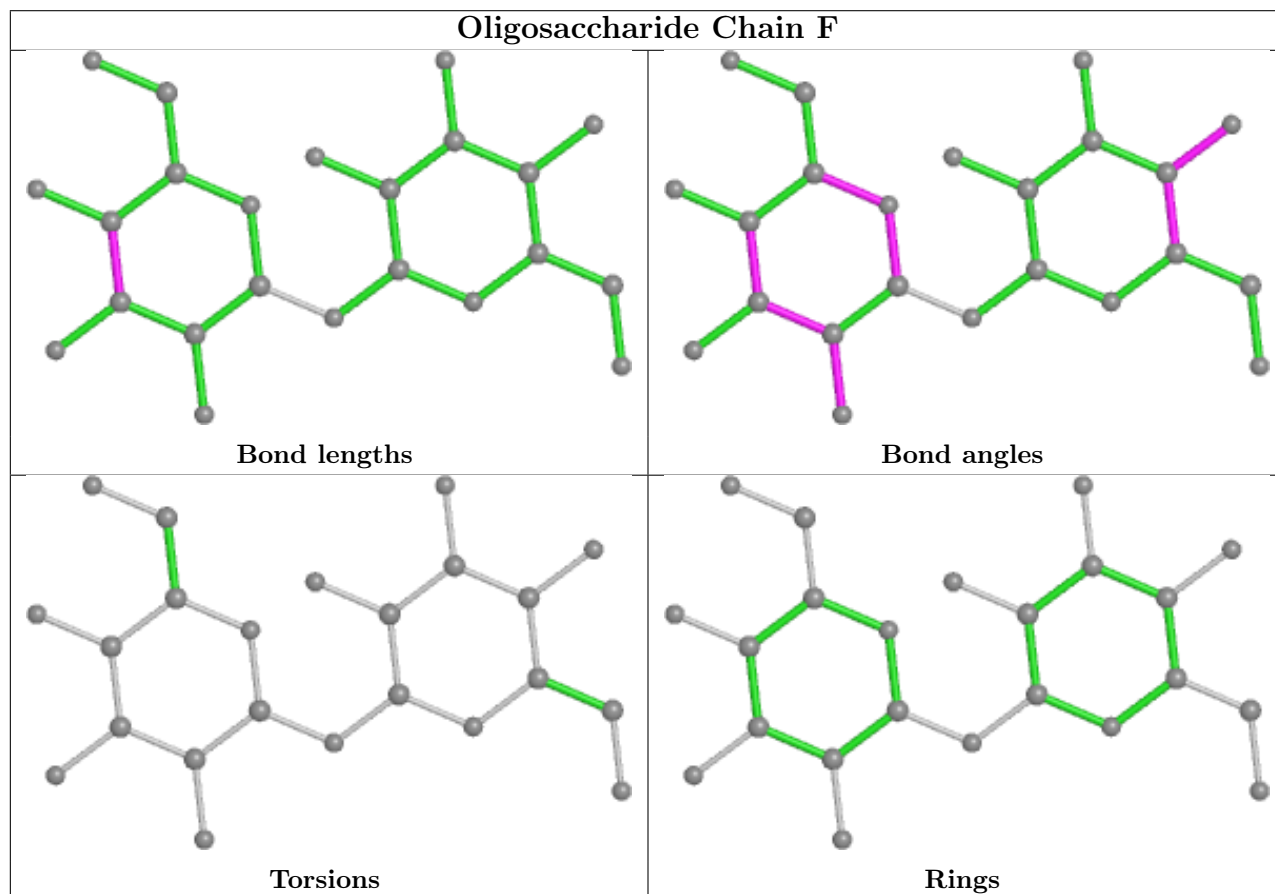
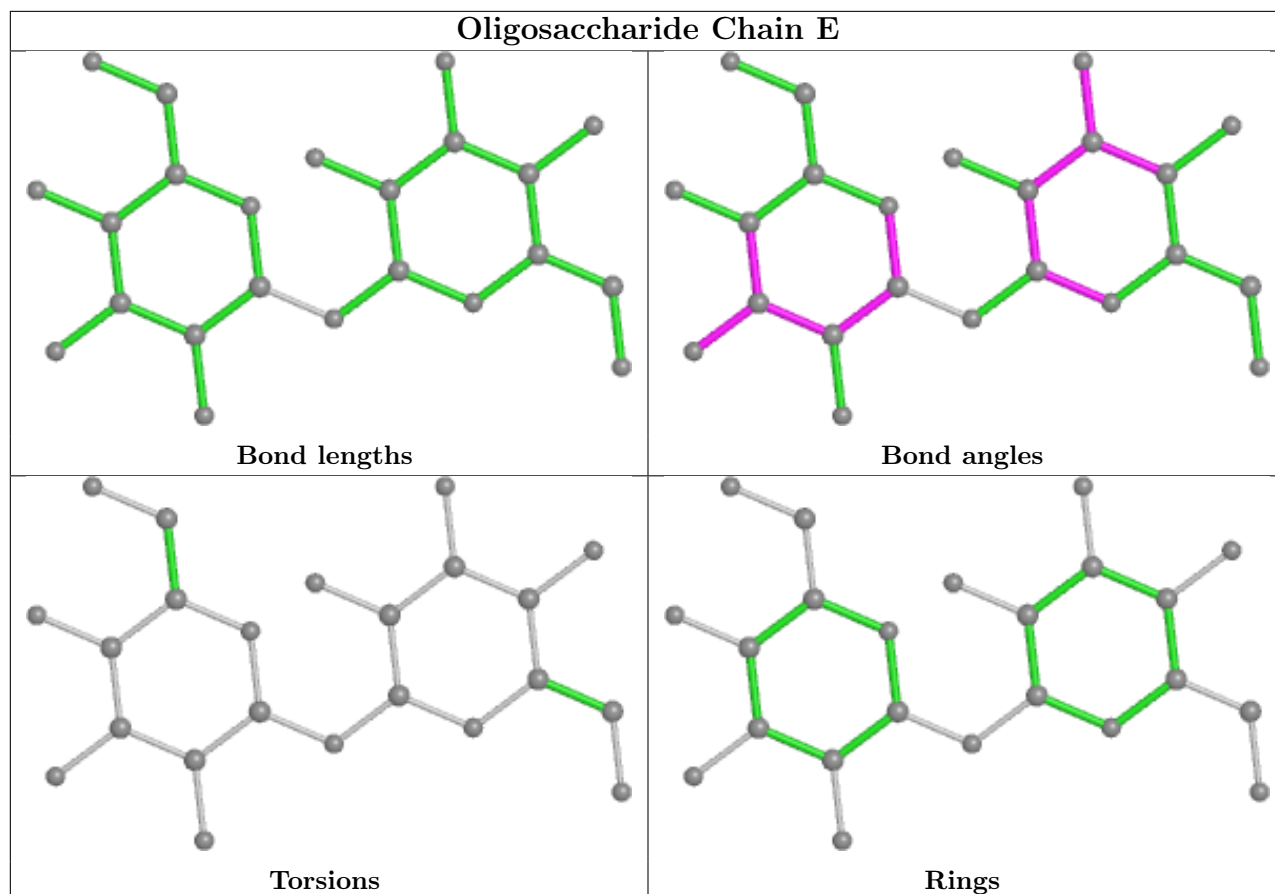
There are no ring outliers.

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.







## 5.6 Ligand geometry [i](#)

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
4	ACT	A	301	-	3,3,3	1.00	0	3,3,3	0.21	0
4	ACT	B	302	-	3,3,3	1.36	1 (33%)	3,3,3	0.58	0
4	ACT	H	303	-	3,3,3	0.77	0	3,3,3	0.81	0
4	ACT	H	304	-	3,3,3	0.69	0	3,3,3	1.01	0
4	ACT	A	302	-	3,3,3	0.60	0	3,3,3	1.60	1 (33%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	302	ACT	OXT-C	-2.25	1.20	1.30

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	302	ACT	O-C-CH3	-2.06	114.31	122.33

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 [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	220/221 (99%)	-0.15	6 (2%) 54 60	16, 25, 52, 100	0
1	H	220/221 (99%)	-0.18	7 (3%) 47 53	14, 23, 47, 99	0
2	B	218/219 (99%)	0.03	6 (2%) 53 58	16, 29, 50, 119	0
2	L	219/219 (100%)	-0.09	5 (2%) 60 66	18, 29, 53, 98	0
All	All	877/880 (99%)	-0.10	24 (2%) 54 60	14, 26, 48, 119	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	33	ARG	20.5
2	B	34	THR	10.7
1	A	139	THR	8.0
2	L	33	ARG	7.7
1	A	138	GLN	7.5
1	H	137	ALA	6.4
2	L	34	THR	6.4
1	H	138	GLN	6.2
1	A	137	ALA	5.9
1	H	136	ALA	5.6
2	B	32	SER	5.1
1	A	221	ASP	4.6
1	H	140	ASN	4.0
2	L	162	ASN	3.8
1	H	139	THR	3.7
2	L	32	SER	3.6
2	B	35	ARG	3.5
1	A	136	ALA	3.3
1	A	140	ASN	3.2
1	H	135	SER	2.7
2	B	189	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
2	L	219	CYS	2.3
2	B	162	ASN	2.2
1	H	221	ASP	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	PCA	H	1	8/9	0.96	0.07	21,22,25,28	0
1	PCA	A	1	8/9	0.98	0.06	19,27,29,33	0

## 6.3 Carbohydrates [i](#)

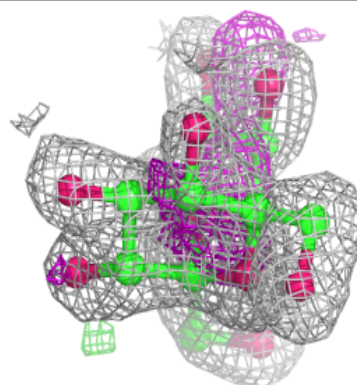
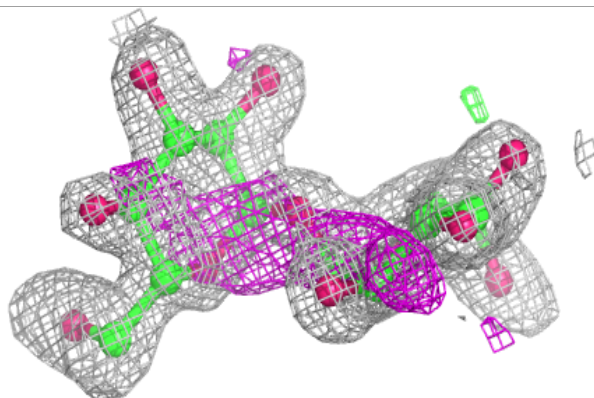
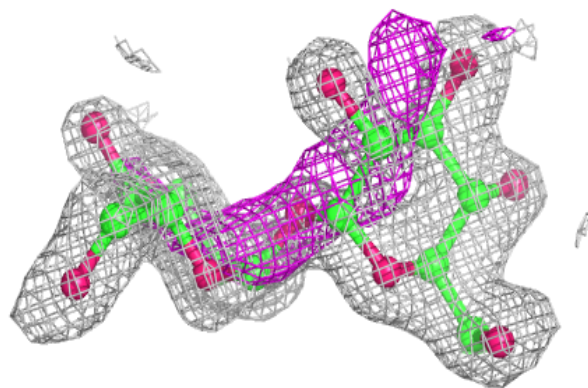
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	GLC	D	1	11/12	0.74	0.31	38,45,46,48	11
3	GLC	D	2	12/12	0.76	0.25	47,49,52,54	12
3	GLC	C	1	11/12	0.80	0.23	34,39,42,42	0
3	GLC	C	2	12/12	0.82	0.22	33,40,42,43	0
3	GLC	F	1	11/12	0.83	0.17	31,34,35,42	0
3	GLC	F	2	12/12	0.91	0.19	31,35,37,37	0
3	GLC	E	1	11/12	0.94	0.10	27,29,31,31	0
3	GLC	E	2	12/12	0.94	0.13	26,29,30,33	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.

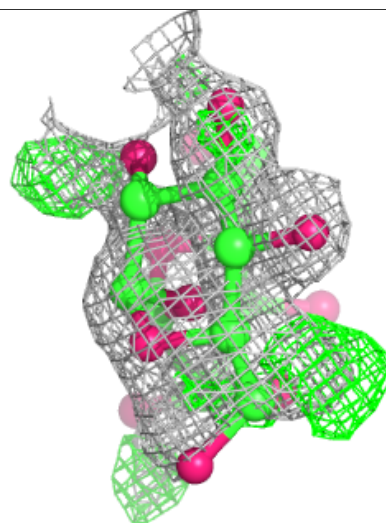
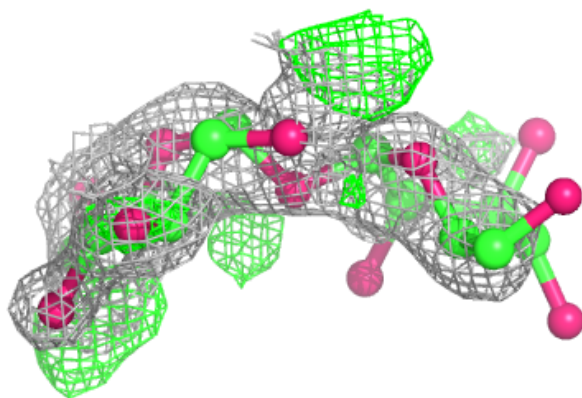
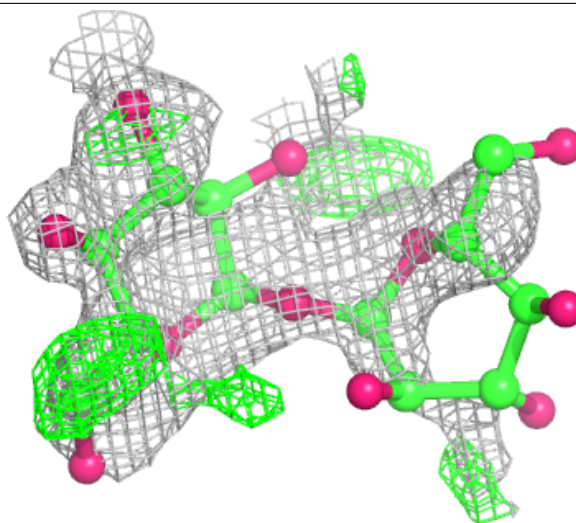
**Electron density around Chain C:**

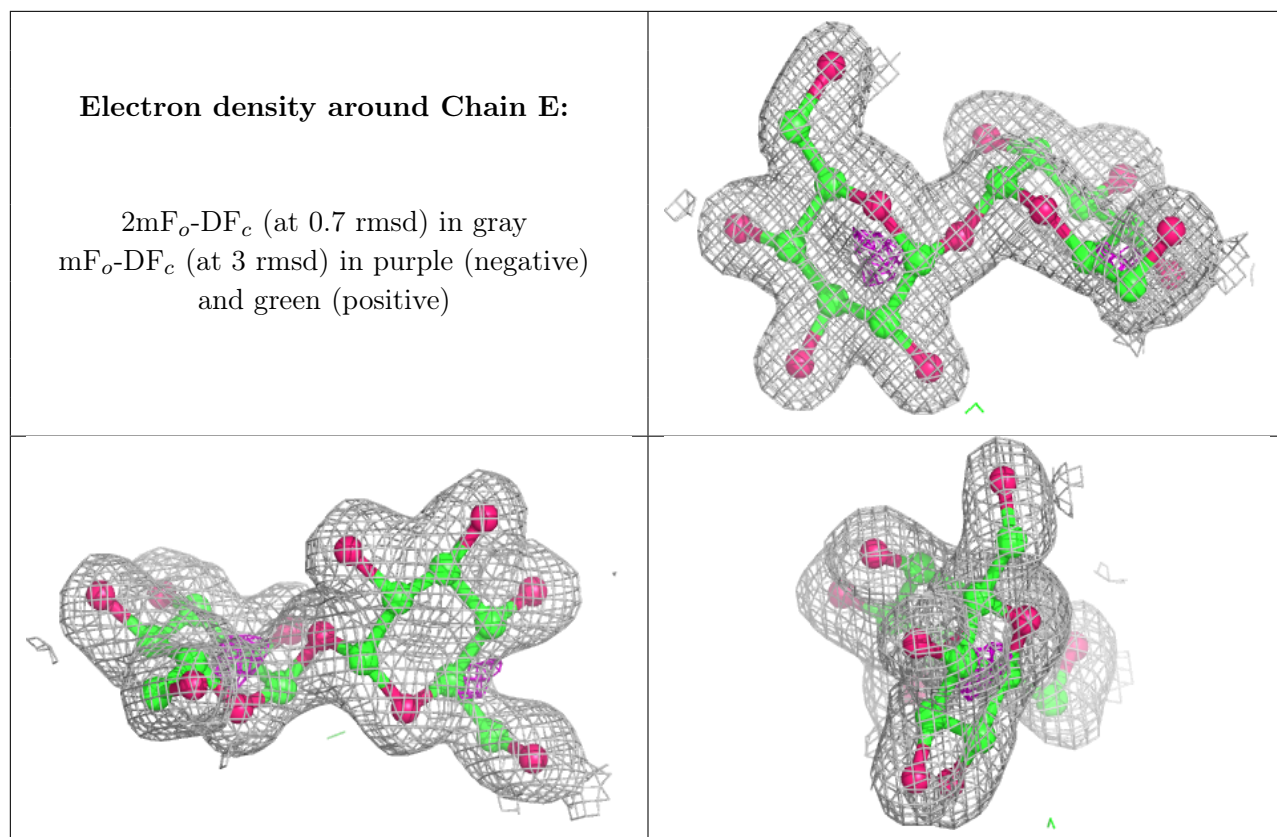
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



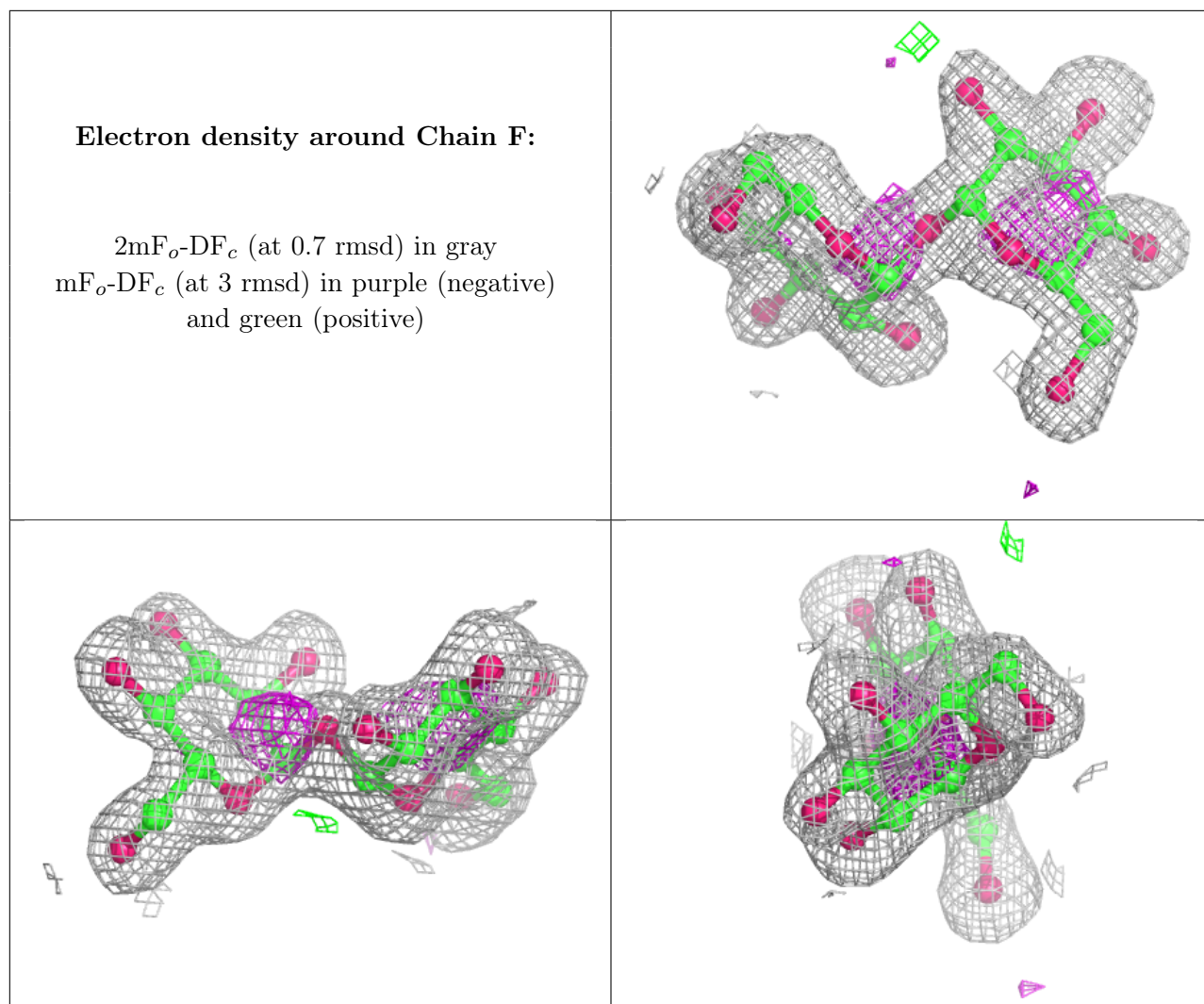
**Electron density around Chain D:**

$2mF_o-DF_c$  (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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	ACT	A	301	4/4	0.59	0.42	43,46,48,49	0
4	ACT	H	303	4/4	0.78	0.30	46,57,61,62	0
4	ACT	A	302	4/4	0.87	0.19	34,36,37,37	0
4	ACT	B	302	4/4	0.97	0.06	20,21,22,25	0
4	ACT	H	304	4/4	0.99	0.06	24,25,27,29	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.