



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:59 PM UTC

PDB ID : 5MTH / pdb_00005mth
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

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>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

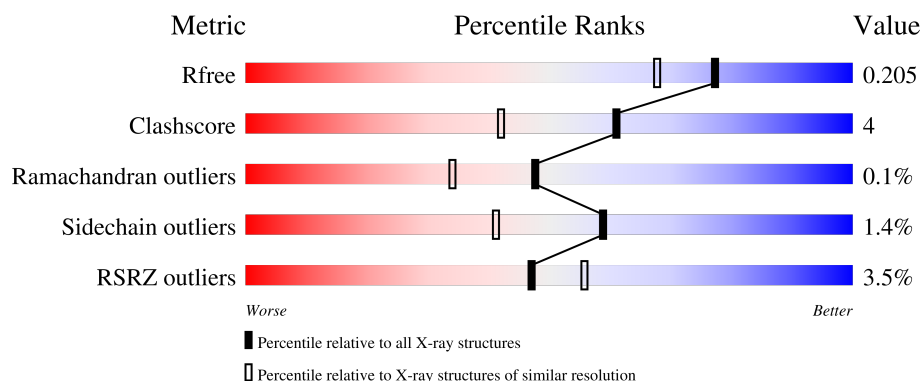
1 Overall quality at a glance

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.



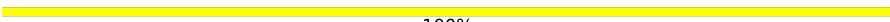
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1187 (1.74-1.74)
Clashscore	190562	1207 (1.74-1.74)
Ramachandran outliers	187476	1200 (1.74-1.74)
Sidechain outliers	187428	1200 (1.74-1.74)
RSRZ outliers	180081	1188 (1.74-1.74)

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 $\leq 5\%$. 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	4% 90% 10%
1	H	221	4% 90% 10%
2	B	219	3% 90% 9%
2	L	219	3% 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%

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.

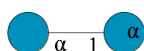
- Molecule 1 is a protein called antibody Fab heavy chain.

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

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

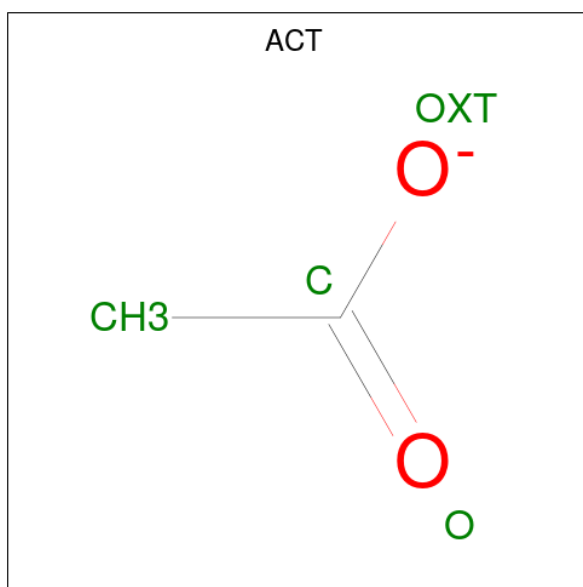
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	219	Total	C	N	O	S	0	6	0
			1740	1082	295	353	10			
2	B	218	Total	C	N	O	S	0	3	0
			1712	1064	292	349	7			

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



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

- Molecule 4 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



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

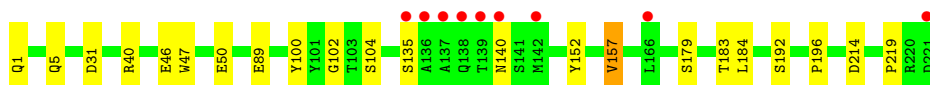
- Molecule 5 is water.

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

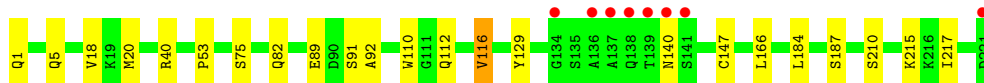
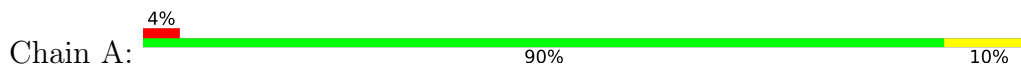
3 Residue-property plots

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.

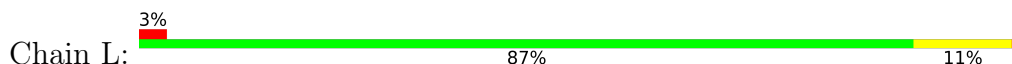
- Molecule 1: antibody Fab heavy chain



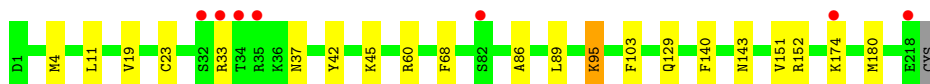
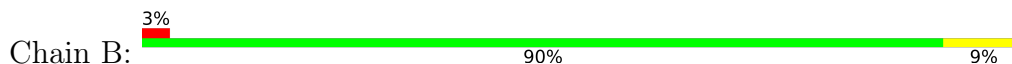
- Molecule 1: antibody Fab heavy chain



- 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, α , β , γ	41.45Å 111.77Å 95.64Å 90.00° 90.56° 90.00°	Depositor
Resolution (Å)	38.86 – 1.73 38.86 – 1.73	Depositor EDS
% Data completeness (in resolution range)	95.3 (38.86-1.73) 99.1 (38.86-1.73)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.13 (at 1.72Å)	Xtriage
Refinement program	REFMAC 5.8.0151	Depositor
R, R_{free}	0.185 , 0.235 0.168 , 0.205	Depositor DCC
R_{free} test set	4506 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	23.4	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 30.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	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	0.97	EDS
Total number of atoms	7524	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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: PCA, ACT, 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	1.28	3/1729 (0.2%)	1.11	3/2361 (0.1%)
1	H	1.31	2/1746 (0.1%)	1.11	1/2384 (0.0%)
2	B	1.16	2/1751 (0.1%)	1.05	0/2372
2	L	1.15	2/1783 (0.1%)	1.06	0/2414
All	All	1.23	9/7009 (0.1%)	1.08	4/9531 (0.0%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	110	TRP	C-O	7.67	1.33	1.24
1	H	183	THR	N-CA	6.38	1.53	1.46
1	A	116	VAL	CA-CB	5.83	1.61	1.54
1	H	46	GLU	C-O	5.73	1.30	1.24
2	L	101	ARG	C-O	5.56	1.30	1.23
2	L	196	SER	C-O	-5.34	1.17	1.24
2	B	129	GLN	C-O	-5.32	1.17	1.24
1	A	53	PRO	CA-C	5.14	1.60	1.52
2	B	37	ASN	C-O	5.09	1.30	1.24

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	140	ASN	N-CA-C	6.02	121.68	113.37
1	H	140	ASN	N-CA-C	5.77	119.65	110.70
1	A	129	TYR	CA-C-N	5.12	124.88	119.76
1	A	129	TYR	C-N-CA	5.12	124.88	119.76

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	13	0
1	H	1702	0	1643	13	1
2	B	1712	0	1656	13	1
2	L	1740	0	1678	25	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	1	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	58	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 (58) 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
2:L:31:ASN:HB3	2:L:34:THR:HG1	1.40	0.82
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
2:L:89:LEU:HD11	5:L:495:HOH:O	1.83	0.78
2:L:151:VAL:HG21	2:L:180:MET:HE1	1.69	0.74
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
2:B:151:VAL:HG21	2:B:180:MET:HE1	1.76	0.68
1:H:31:ASP:OD1	5:H:401:HOH:O	2.14	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:143:ASN:ND2	5:B:402:HOH:O	2.29	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
1:A:20:MET:HE1	1:A:116:VAL:HG21	1.95	0.47
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:A:184:LEU:HD12	1:A:184:LEU:C	2.41	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
2:L:31:ASN:CB	2:L:34:THR:HG1	2.21	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:B:4:MET:HE3	2:B:23:CYS:SG	2.60	0.42
1:A:75:SER:C	5:A:401:HOH:O	2.63	0.42
2:B:151:VAL:CG2	2:B:180:MET:HE1	2.48	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: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:L:97[A]:SER:O	2:L:97[A]:SER:OG	2.35	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

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	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%)	30	16
All	All	890/880 (101%)	865 (97%)	24 (3%)	1 (0%)	48	34

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	32	SER

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	190/190 (100%)	189 (100%)	1 (0%)	81	75
1	H	193/190 (102%)	188 (97%)	5 (3%)	40	17
2	B	197/195 (101%)	194 (98%)	3 (2%)	57	38
2	L	201/195 (103%)	197 (98%)	4 (2%)	48	26
All	All	781/770 (101%)	768 (98%)	13 (2%)	59	32

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

Mol	Chain	Res	Type
1	H	5[A]	GLN
1	H	5[B]	GLN
1	H	157	VAL
1	H	179	SER
1	H	192	SER
2	L	19	VAL
2	L	95	LYS
2	L	199[A]	CYS
2	L	199[B]	CYS
1	A	166	LEU
2	B	95	LYS
2	B	152	ARG
2	B	174	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	39	GLN
2	L	44	GLN
2	L	195	ASN
1	A	3	GLN
1	A	39	GLN
2	B	44	GLN

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Mol	Chain	Res	Type
2	B	217	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	0.57	0	9,10,12	1.48	1 (11%)
1	PCA	A	1	1	7,8,9	0.80	0	9,10,12	1.44	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 (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	1	PCA	CB-CA-C	-3.09	108.41	112.66
1	A	1	PCA	OE-CD-CG	-2.97	121.43	126.72

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	1.24	0	15,15,17	1.28	1 (6%)
3	GLC	C	2	3	12,12,12	0.97	0	17,17,17	0.80	0
3	GLC	D	1	3	11,11,12	0.38	0	15,15,17	1.18	0
3	GLC	D	2	3	12,12,12	0.36	0	17,17,17	1.10	1 (5%)
3	GLC	E	1	3	11,11,12	0.70	0	15,15,17	1.27	2 (13%)
3	GLC	E	2	3	12,12,12	0.86	0	17,17,17	1.37	3 (17%)
3	GLC	F	1	3	11,11,12	0.95	1 (9%)	15,15,17	1.62	3 (20%)
3	GLC	F	2	3	12,12,12	0.95	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	2.25	1.58	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	1	GLC	C1-O5-C5	4.59	118.34	112.19
3	E	2	GLC	O5-C1-C2	3.13	115.80	110.30
3	C	1	GLC	C1-O5-C5	2.79	115.92	112.19
3	F	1	GLC	C2-C3-C4	-2.78	105.98	110.86
3	E	2	GLC	O3-C3-C2	-2.76	103.87	110.38
3	F	2	GLC	O4-C4-C5	2.57	115.65	109.32
3	E	1	GLC	O3-C3-C4	-2.30	104.96	110.38
3	E	1	GLC	O3-C3-C2	2.13	114.41	110.05
3	D	2	GLC	C1-C2-C3	2.13	114.70	110.36
3	E	2	GLC	O3-C3-C4	2.11	115.35	110.38
3	F	1	GLC	O2-C2-C3	2.06	114.42	110.15

There are no chirality outliers.

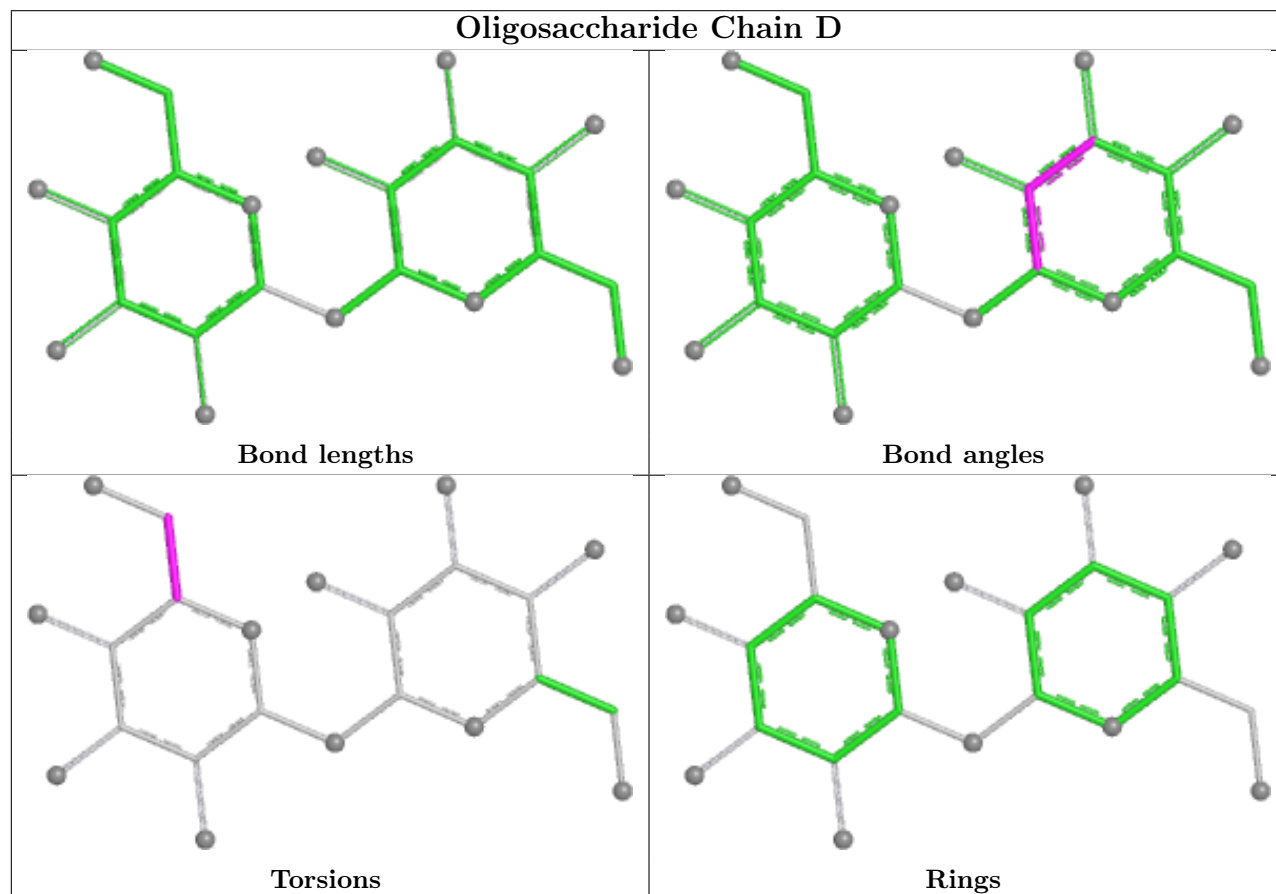
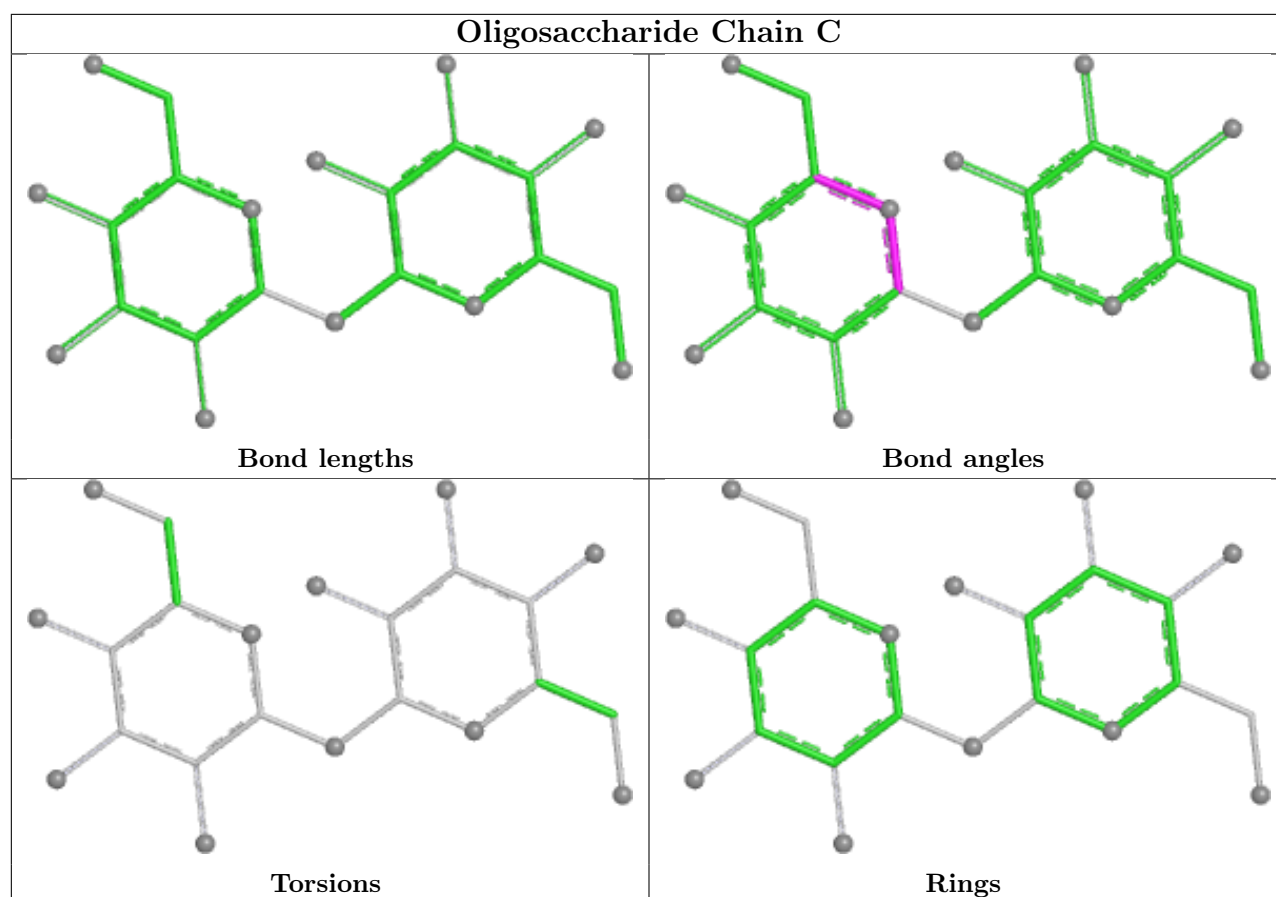
All (2) torsion outliers are listed below:

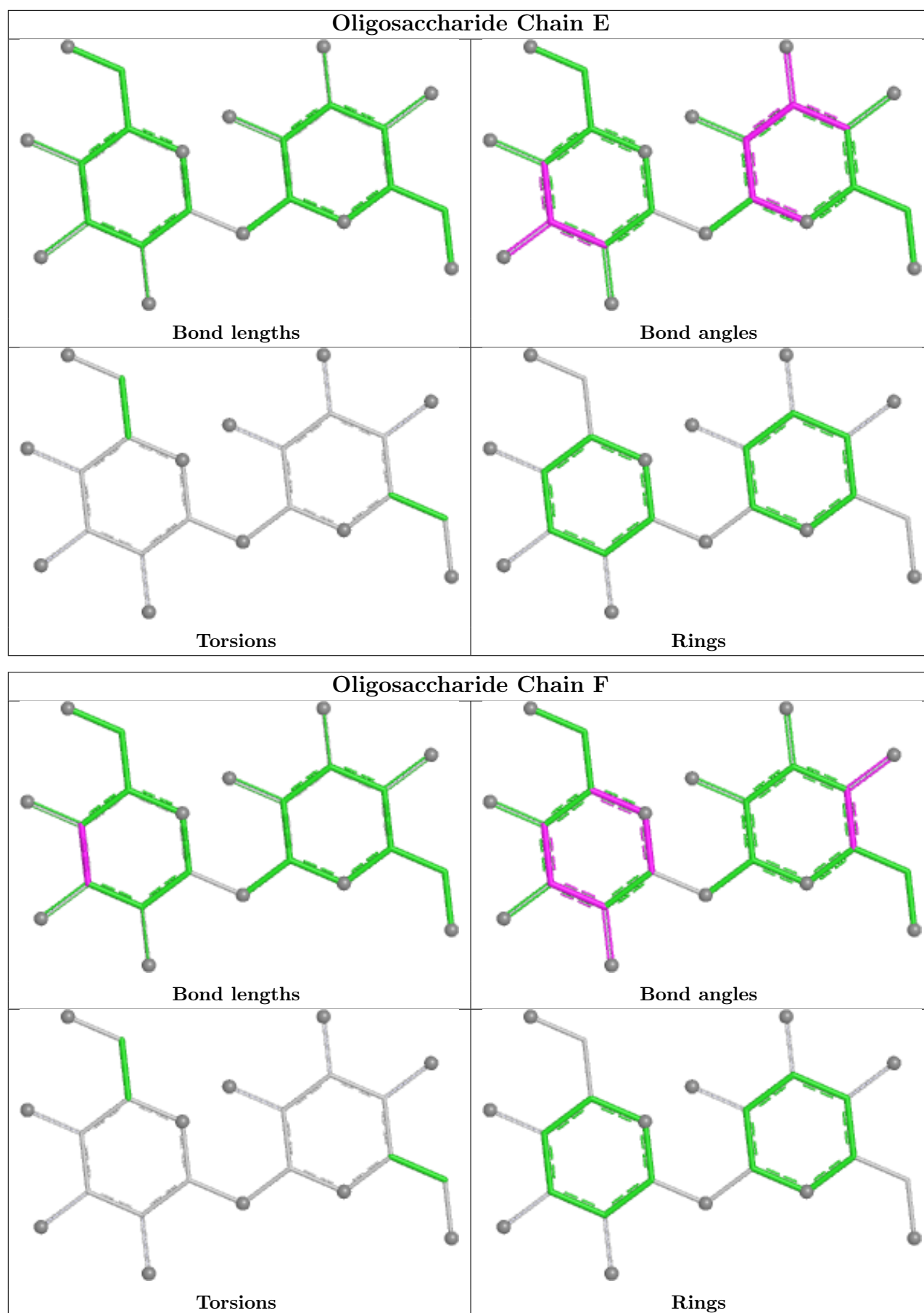
Mol	Chain	Res	Type	Atoms
3	D	1	GLC	O5-C5-C6-O6
3	D	1	GLC	C4-C5-C6-O6

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	H	303	-	3,3,3	0.82	0	3,3,3	0.82	0
4	ACT	A	302	-	3,3,3	0.64	0	3,3,3	1.57	1 (33%)
4	ACT	A	301	-	3,3,3	1.06	0	3,3,3	0.24	0
4	ACT	H	304	-	3,3,3	0.73	0	3,3,3	1.02	0
4	ACT	B	302	-	3,3,3	1.43	1 (33%)	3,3,3	0.59	0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	302	ACT	OXT-C	-2.35	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	-2.00	114.31	122.53

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 ⓘ

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	220/221 (99%)	0.16	8 (3%)	46	55	12, 25, 52, 100	4 (1%)
1	H	220/221 (99%)	0.06	9 (4%)	41	51	10, 22, 47, 99	6 (2%)
2	B	218/219 (99%)	0.34	7 (3%)	50	58	11, 29, 50, 119	3 (1%)
2	L	219/219 (100%)	0.35	7 (3%)	50	58	10, 29, 53, 98	6 (2%)
All	All	877/880 (99%)	0.23	31 (3%)	47	56	10, 26, 48, 119	19 (2%)

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	34	THR	5.9
2	L	33	ARG	5.3
2	B	33	ARG	5.0
1	H	137	ALA	5.0
1	A	139	THR	4.9
1	H	136	ALA	4.5
2	L	34	THR	4.1
1	H	138	GLN	3.8
2	L	32	SER	3.8
1	A	137	ALA	3.7
2	B	32	SER	3.4
1	A	140	ASN	3.3
1	H	139	THR	3.2
2	L	162	ASN	3.2
1	H	140	ASN	3.1
1	A	138	GLN	2.8
1	A	221	ASP	2.6
1	H	166	LEU	2.4
1	A	141	SER	2.4
1	H	221	ASP	2.4
2	L	158	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	136	ALA	2.3
2	L	219	CYS	2.2
1	H	135	SER	2.2
1	H	142	MET	2.2
2	L	165	LEU	2.2
1	A	134	GLY	2.2
2	B	35	ARG	2.2
2	B	218	GLU	2.1
2	B	174	LYS	2.1
2	B	82	SER	2.1

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, 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	PCA	H	1	8/9	0.94	0.07	21,22,25,28	0
1	PCA	A	1	8/9	0.98	0.05	19,27,29,33	0

6.3 Carbohydrates [i](#)

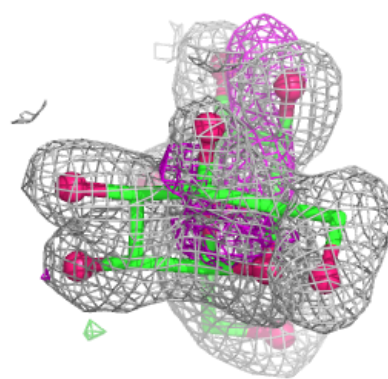
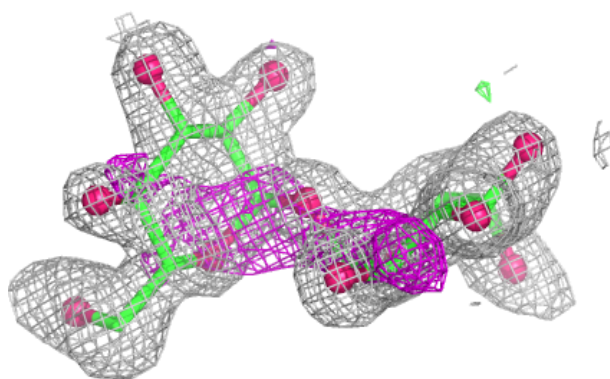
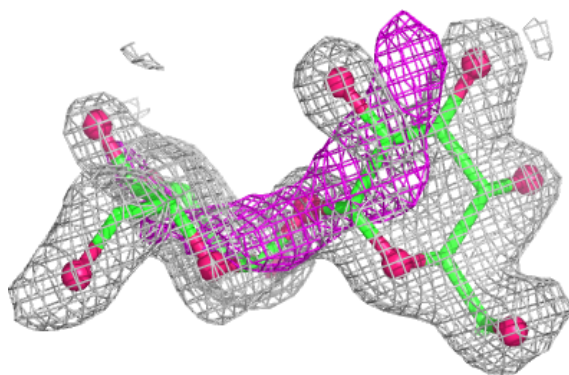
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	GLC	C	1	11/12	-	-	34,39,42,42	0
3	GLC	C	2	12/12	-	-	33,40,42,43	0
3	GLC	D	1	11/12	-	-	38,45,46,48	11
3	GLC	D	2	12/12	-	-	47,49,52,54	12
3	GLC	F	1	11/12	0.75	0.25	31,34,35,42	0
3	GLC	F	2	12/12	0.77	0.25	31,35,37,37	0
3	GLC	E	1	11/12	0.78	0.12	27,29,31,31	0
3	GLC	E	2	12/12	0.82	0.11	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.

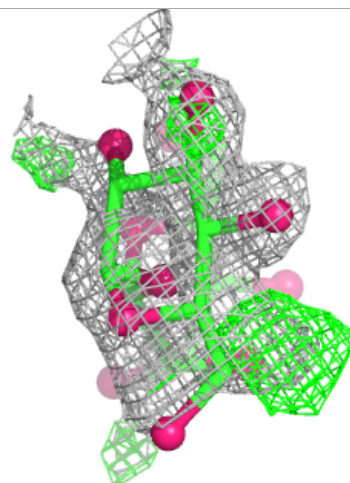
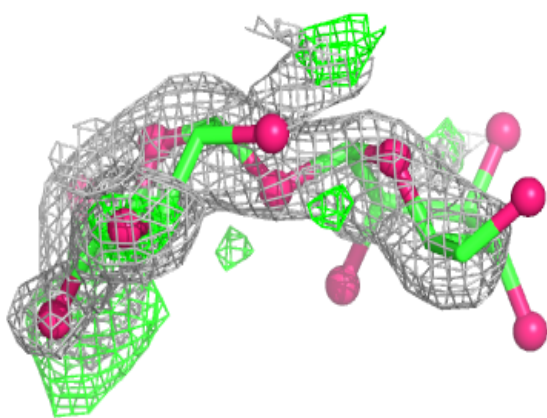
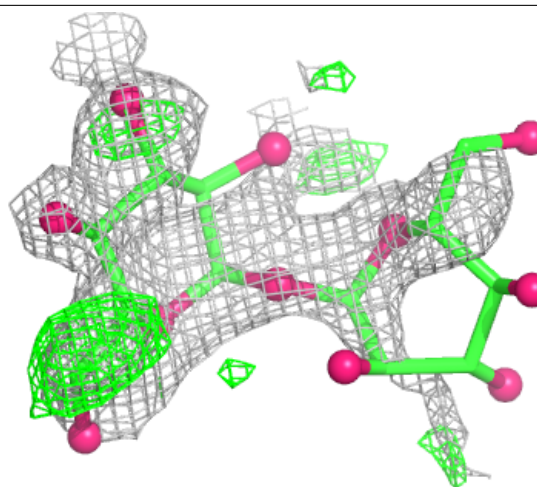
Electron density around Chain C:

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



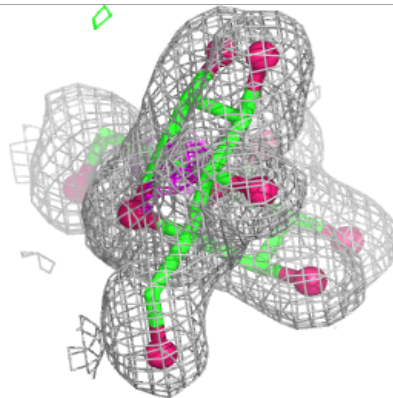
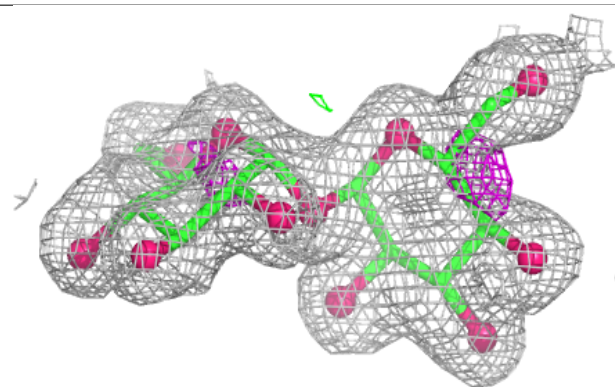
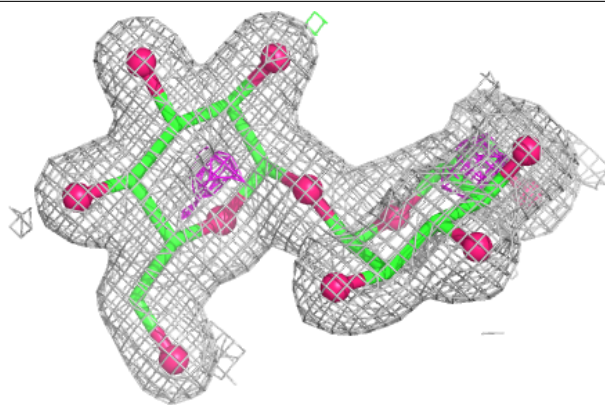
Electron density around Chain D:

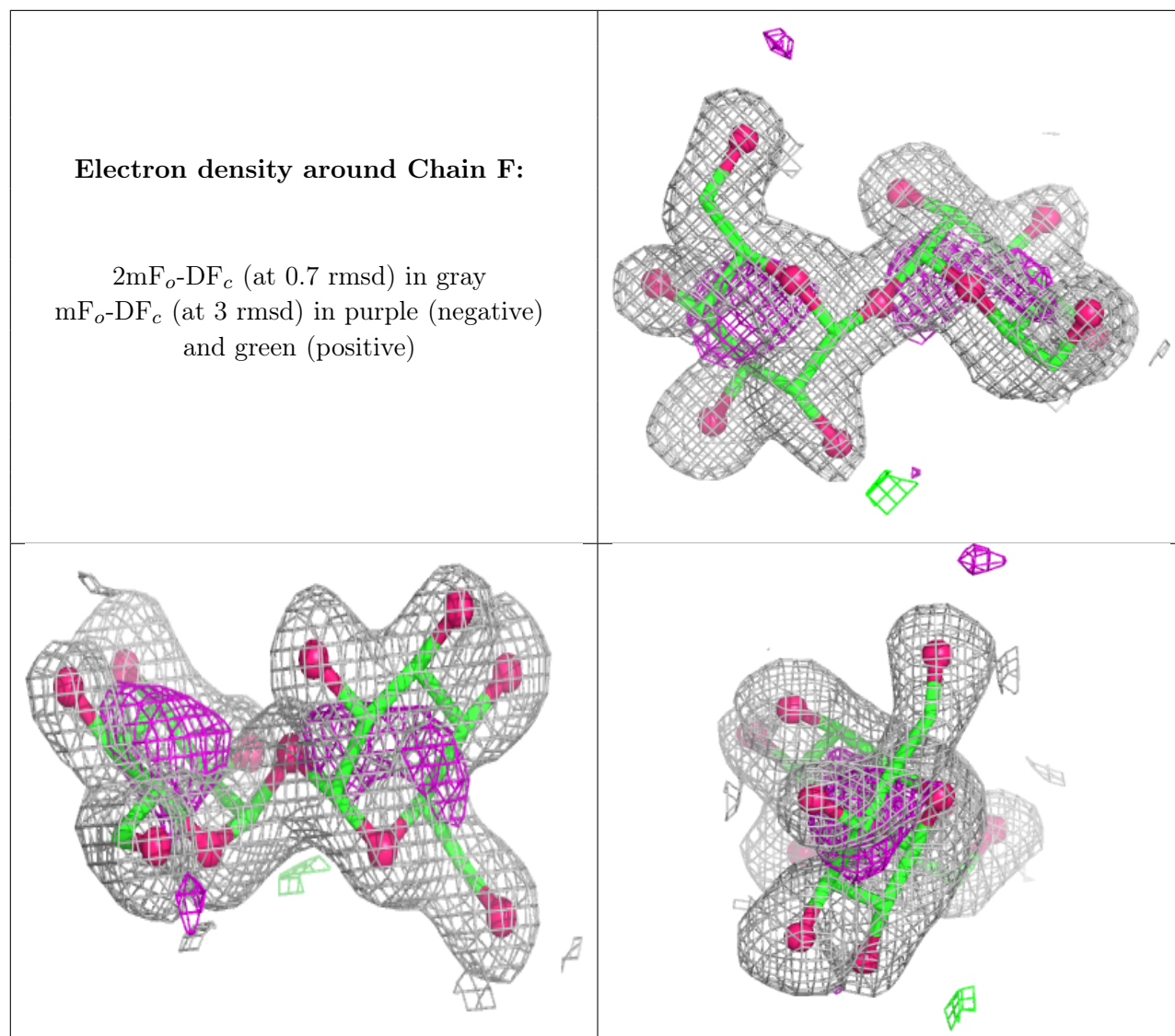
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





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(Å ²)	Q<0.9
4	ACT	H	303	4/4	0.50	0.18	46,57,61,62	0
4	ACT	A	301	4/4	0.69	0.17	43,46,48,49	0
4	ACT	A	302	4/4	0.88	0.15	34,36,37,37	0
4	ACT	B	302	4/4	0.97	0.05	20,21,22,25	0
4	ACT	H	304	4/4	0.98	0.04	24,25,27,29	0

6.5 Other polymers [i](#)

There are no such residues in this entry.