



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 26, 2023 – 12:03 PM EDT

PDB ID : 6C5K  
Title : S25-23 Fab in complex with Chlamydiaceae LPS (Crystal form 2)  
Authors : Haji-Ghassemi, O.; Evans, S.V.  
Deposited on : 2018-01-16  
Resolution : 1.75 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>.

---

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 : 2.35.1  
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) : 2.35.1

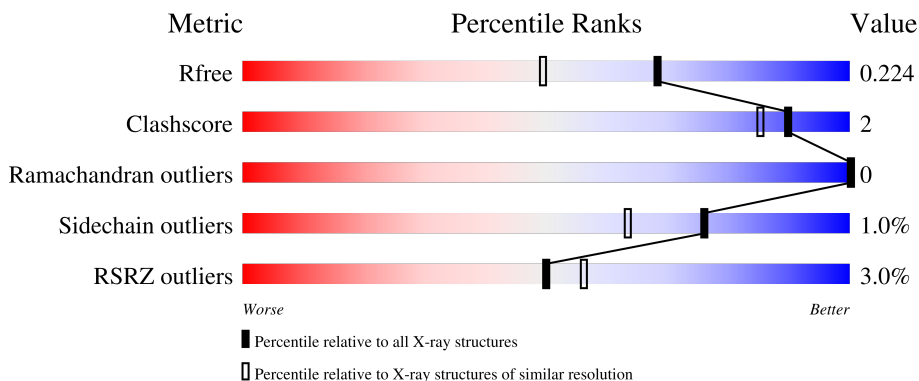
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.75 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.




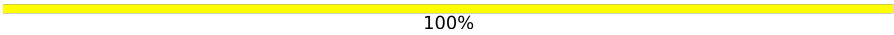
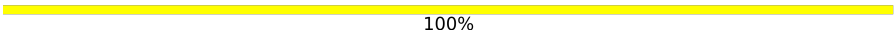
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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	218	 5% 93% 6%
1	H	218	 3% 95% 5%
2	B	219	 2% 97%
2	L	219	 2% 97%
3	C	3	 33% 67%

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
3	E	3	 33% 67%
4	D	5	 100%
4	F	5	 100%

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 7842 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.

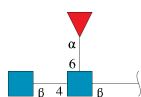
- Molecule 1 is a protein called IgG1 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	H	218	Total	C	N	O	S	0	1	0
			1662	1063	273	319	7			
1	A	216	Total	C	N	O	S	0	0	0
			1641	1047	270	317	7			

- Molecule 2 is a protein called IgG1 Fab Light Chain (Kappa).

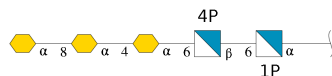
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	L	219	Total	C	N	O	S	0	0	0
			1699	1064	288	340	7			
2	B	219	Total	C	N	O	S	0	0	0
			1699	1064	288	340	7			

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



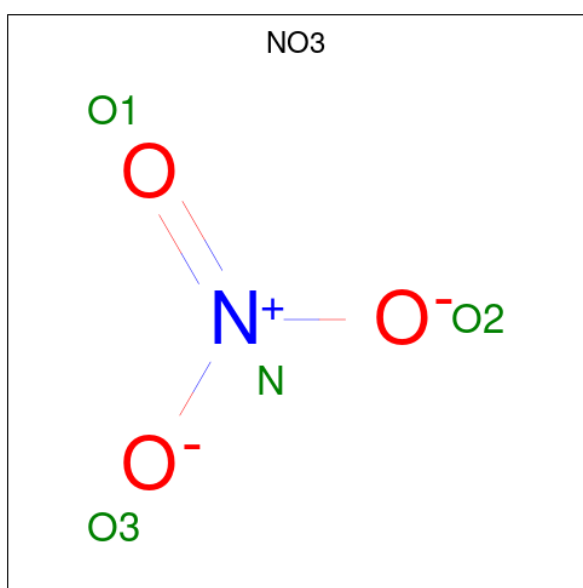
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	3	Total	C	N	O	0	0	0
			38	22	2	14			
3	E	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 4 is an oligosaccharide called 3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-8)-3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-4)-3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-6)-2-amino-2-deoxy-4-O-phosphono-beta-D-glucopyranose-(1-6)-2-amino-2-deoxy-1-O-phosphono-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
			Total	C	N	O				P
4	D	5	76	36	2	36	2	0	0	0
4	F	5	76	36	2	36	2	0	0	0

- Molecule 5 is NITRATE ION (three-letter code: NO3) (formula: NO<sub>3</sub>).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	N O		
5	B	1	4	1 3	0	0

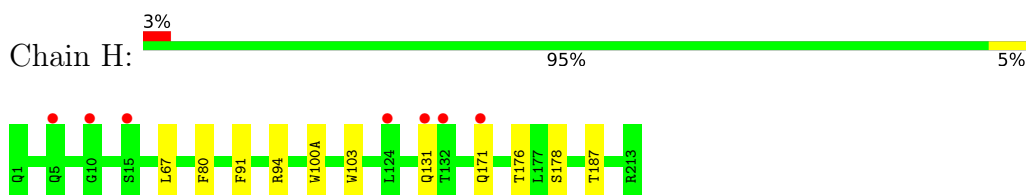
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	H	216	Total O 216 216	0	0
6	A	245	Total O 245 245	0	0
6	L	209	Total O 209 209	0	0
6	B	239	Total O 239 239	0	0

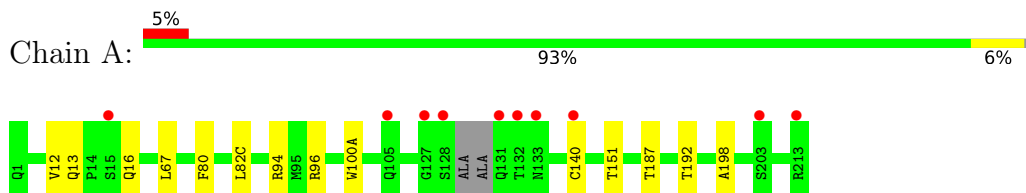
### 3 Residue-property plots [i](#)

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.

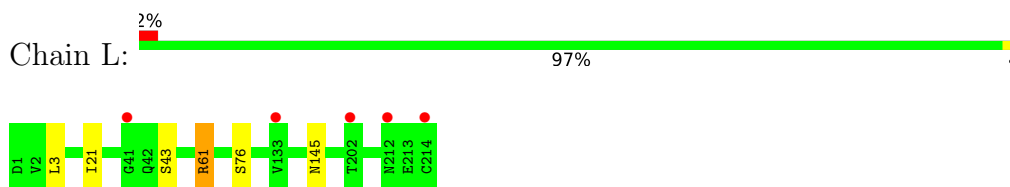
- Molecule 1: IgG1 Fab Heavy Chain



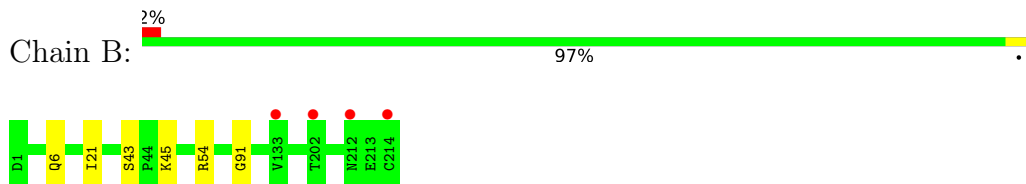
- Molecule 1: IgG1 Fab Heavy Chain



- Molecule 2: IgG1 Fab Light Chain (Kappa)



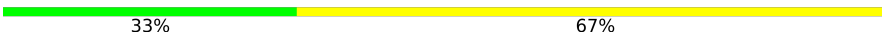
- Molecule 2: IgG1 Fab Light Chain (Kappa)



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  33% 67%

MAG1  
MAG2  
FUC3

- Molecule 4: 3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-8)-3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-4)-3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-6)-2-amino-2-deoxy-4-O-phosphono-beta-D-glucopyranose-(1-6)-2-amino-2-deoxy-1-O-phosphono-alpha-D-glucopyranose

Chain D:  100%

GP11  
Z9M2  
KD03  
KD04  
KD05

- Molecule 4: 3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-8)-3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-4)-3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-6)-2-amino-2-deoxy-4-O-phosphono-beta-D-glucopyranose-(1-6)-2-amino-2-deoxy-1-O-phosphono-alpha-D-glucopyranose

Chain F:  100%

GP11  
Z9M2  
KD03  
KD04  
KD05

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	171.65Å 62.71Å 107.07Å 90.00° 116.09° 90.00°	Depositor
Resolution (Å)	25.00 – 1.75 24.61 – 1.75	Depositor EDS
% Data completeness (in resolution range)	99.7 (25.00-1.75) 99.7 (24.61-1.75)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.81 (at 1.75Å)	Xtrriage
Refinement program	REFMAC 5.8.0155	Depositor
R, $R_{free}$	0.188 , 0.218 0.196 , 0.224	Depositor DCC
$R_{free}$ test set	5326 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	21.8	Xtrriage
Anisotropy	0.621	Xtrriage
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>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7842	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 32.24 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.7022e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: Z9M, NAG, FUC, PCA, NO3, KDO, GP1

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	0.51	0/1678	0.72	1/2299 (0.0%)
1	H	0.52	0/1705	0.71	0/2339
2	B	0.47	0/1738	0.65	0/2358
2	L	0.49	0/1738	0.67	0/2358
All	All	0.50	0/6859	0.69	1/9354 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	140	CYS	CA-CB-SG	-5.31	104.44	114.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	1641	0	1613	9	0
1	H	1662	0	1634	8	0
2	B	1699	0	1645	5	0
2	L	1699	0	1645	6	0
3	C	38	0	34	0	0
3	E	38	0	34	0	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	76	0	40	0	0
4	F	76	0	40	0	0
5	B	4	0	0	0	0
6	A	245	0	0	1	0
6	B	239	0	0	4	0
6	H	216	0	0	2	0
6	L	209	0	0	7	0
All	All	7842	0	6685	25	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 2.

All (25) 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:H:91:PHE:CE1	6:L:301:HOH:O	2.29	0.85
2:L:43:SER:OG	6:L:301:HOH:O	2.04	0.74
1:A:12:VAL:HG11	1:A:82(C):LEU:HD12	1.71	0.70
1:H:103[A]:TRP:CD1	6:L:301:HOH:O	2.44	0.70
2:L:43:SER:CB	6:L:301:HOH:O	2.41	0.68
2:L:21:ILE:HG22	6:L:318:HOH:O	2.02	0.60
1:A:12:VAL:HG11	1:A:82(C):LEU:CD1	2.32	0.59
1:H:67:LEU:HD11	1:H:80:PHE:CE2	2.39	0.58
2:B:21:ILE:CG2	6:B:409:HOH:O	2.54	0.55
1:H:187:THR:HG21	1:A:100(A):TRP:CH2	2.44	0.53
1:A:67:LEU:HD11	1:A:80:PHE:CE2	2.46	0.51
2:L:61:ARG:HD2	2:L:76:SER:O	2.10	0.51
2:L:43:SER:HB3	6:L:301:HOH:O	2.09	0.50
2:L:61:ARG:CD	2:L:76:SER:O	2.61	0.49
2:B:45:LYS:HB2	6:B:401:HOH:O	2.14	0.48
1:H:176:THR:HB	6:H:657:HOH:O	2.16	0.46
1:H:100(A):TRP:CH2	1:A:187:THR:HG21	2.52	0.44
1:A:151:THR:OG1	1:A:198:ALA:HB3	2.18	0.43
1:A:192:THR:HG22	6:A:709:HOH:O	2.18	0.42
2:B:43:SER:O	6:B:401:HOH:O	2.21	0.42
1:A:96:ARG:HD2	2:B:91:GLY:O	2.20	0.42
2:B:6:GLN:HB3	6:B:409:HOH:O	2.20	0.41
1:H:103[A]:TRP:HD1	6:L:301:HOH:O	1.97	0.40
1:H:178:SER:HB3	6:H:706:HOH:O	2.21	0.40
1:A:13:GLN:HB2	1:A:16:GLN:HG3	2.04	0.40

There are no symmetry-related clashes.

## 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	212/218 (97%)	210 (99%)	2 (1%)	0	100	100
1	H	217/218 (100%)	214 (99%)	3 (1%)	0	100	100
2	B	217/219 (99%)	214 (99%)	3 (1%)	0	100	100
2	L	217/219 (99%)	214 (99%)	3 (1%)	0	100	100
All	All	863/874 (99%)	852 (99%)	11 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 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	189/189 (100%)	188 (100%)	1 (0%)	88	83
1	H	190/189 (100%)	187 (98%)	3 (2%)	62	45
2	B	195/195 (100%)	194 (100%)	1 (0%)	88	83
2	L	195/195 (100%)	192 (98%)	3 (2%)	65	49
All	All	769/768 (100%)	761 (99%)	8 (1%)	76	63

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	94	ARG
1	H	131	GLN
1	H	171	GLN
1	A	94	ARG
2	L	3	LEU
2	L	61	ARG
2	L	145	ASN
2	B	54	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	3	GLN
1	H	164	HIS
1	H	171	GLN
1	A	16	GLN
1	A	105	GLN
2	L	42	GLN
2	L	138	ASN
2	B	42	GLN
2	B	138	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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	A	1	1	7,8,9	0.59	0	9,10,12	0.86	0
1	PCA	H	1	1	7,8,9	0.52	0	9,10,12	0.90	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PCA	A	1	1	-	0/0/11/13	0/1/1/1
1	PCA	H	1	1	-	0/0/11/13	0/1/1/1

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.

## 5.5 Carbohydrates [i](#)

16 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	C	1	3,1	14,14,15	0.44	0	17,19,21	0.97	1 (5%)
3	NAG	C	2	3	14,14,15	0.40	0	17,19,21	1.27	1 (5%)
3	FUC	C	3	3	10,10,11	0.30	0	14,14,16	0.63	0
4	GP1	D	1	4	15,16,16	1.24	1 (6%)	23,24,24	0.99	1 (4%)
4	Z9M	D	2	4	15,15,16	1.43	3 (20%)	18,22,24	1.12	1 (5%)
4	KDO	D	3	4	15,15,16	0.69	0	19,21,24	1.46	3 (15%)
4	KDO	D	4	4	15,15,16	1.63	3 (20%)	19,21,24	1.16	3 (15%)
4	KDO	D	5	4	15,15,16	1.30	1 (6%)	19,21,24	1.21	1 (5%)
3	NAG	E	1	3,1	14,14,15	1.10	2 (14%)	17,19,21	0.96	1 (5%)
3	NAG	E	2	3	14,14,15	0.51	0	17,19,21	1.35	1 (5%)
3	FUC	E	3	3	10,10,11	0.29	0	14,14,16	0.63	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	GP1	F	1	4	15,16,16	1.30	1 (6%)	23,24,24	1.12	2 (8%)
4	Z9M	F	2	4	15,15,16	0.97	1 (6%)	18,22,24	1.29	4 (22%)
4	KDO	F	3	4	15,15,16	1.20	1 (6%)	19,21,24	1.35	5 (26%)
4	KDO	F	4	4	15,15,16	1.37	1 (6%)	19,21,24	1.23	2 (10%)
4	KDO	F	5	4	15,15,16	1.33	3 (20%)	19,21,24	1.16	2 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	C	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	0/6/23/26	0/1/1/1
3	FUC	C	3	3	-	-	0/1/1/1
4	GP1	D	1	4	-	2/6/27/27	0/1/1/1
4	Z9M	D	2	4	-	0/7/24/27	0/1/1/1
4	KDO	D	3	4	-	1/10/26/30	0/1/1/1
4	KDO	D	4	4	-	1/10/26/30	0/1/1/1
4	KDO	D	5	4	-	2/10/26/30	0/1/1/1
3	NAG	E	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
3	FUC	E	3	3	-	-	0/1/1/1
4	GP1	F	1	4	-	1/6/27/27	0/1/1/1
4	Z9M	F	2	4	-	1/7/24/27	0/1/1/1
4	KDO	F	3	4	-	1/10/26/30	0/1/1/1
4	KDO	F	4	4	-	1/10/26/30	0/1/1/1
4	KDO	F	5	4	-	2/10/26/30	0/1/1/1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	4	KDO	C2-C1	4.59	1.56	1.52
4	F	4	KDO	C2-C1	3.96	1.55	1.52
4	D	5	KDO	C2-C1	3.85	1.55	1.52
4	D	2	Z9M	P1-O9	3.37	1.61	1.50
4	F	3	KDO	O4-C4	3.32	1.50	1.43
4	F	1	GP1	P4B-O1	3.31	1.65	1.59
4	D	1	GP1	P4B-O1	3.26	1.65	1.59
4	F	5	KDO	O6-C6	2.69	1.48	1.44

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	2	Z9M	C1-C2	2.68	1.55	1.52
3	E	1	NAG	C2-N2	-2.61	1.41	1.46
4	F	5	KDO	O4-C4	2.42	1.48	1.43
4	D	4	KDO	C3-C4	2.33	1.56	1.52
4	F	5	KDO	C2-C1	2.33	1.54	1.52
3	E	1	NAG	O5-C1	-2.20	1.40	1.43
4	F	2	Z9M	P1-O7	2.15	1.63	1.54
4	D	4	KDO	O1B-C1	-2.11	1.23	1.30
4	D	2	Z9M	P1-O8	-2.07	1.46	1.54

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	2	NAG	C2-N2-C7	4.18	128.86	122.90
4	F	4	KDO	C6-O6-C2	3.60	119.04	111.34
3	C	2	NAG	C1-O5-C5	3.50	116.94	112.19
4	D	2	Z9M	O8-P1-O7	3.31	120.29	107.64
4	D	3	KDO	O1A-C1-C2	-3.16	115.11	122.57
4	F	3	KDO	O1A-C1-C2	-3.02	115.43	122.57
4	F	5	KDO	O1A-C1-C2	-2.92	115.67	122.57
4	D	3	KDO	C7-C6-C5	-2.83	109.33	114.03
4	F	1	GP1	O5-C1-O1	-2.73	107.79	111.36
4	D	3	KDO	O8-C8-C7	-2.61	105.39	111.07
4	F	3	KDO	O8-C8-C7	-2.58	105.46	111.07
4	D	4	KDO	C6-O6-C2	2.56	116.81	111.34
4	F	2	Z9M	O5-C5-C6	-2.43	103.40	107.20
4	F	2	Z9M	C1-O5-C5	-2.35	109.00	112.19
4	F	3	KDO	C7-C6-C5	-2.34	110.16	114.03
3	C	1	NAG	C1-O5-C5	2.25	115.24	112.19
4	F	2	Z9M	O7-P1-O4	-2.25	95.92	105.99
4	D	5	KDO	O1A-C1-C2	-2.24	117.28	122.57
4	D	4	KDO	O6-C6-C5	2.23	111.01	107.87
4	D	4	KDO	O1A-C1-C2	-2.18	117.41	122.57
4	F	3	KDO	C6-O6-C2	2.12	115.88	111.34
4	F	4	KDO	O1A-C1-C2	-2.11	117.60	122.57
4	F	5	KDO	O6-C2-C3	2.06	113.30	110.46
3	E	1	NAG	C4-C3-C2	-2.06	108.00	111.02
4	D	1	GP1	O9B-P4B-O8B	2.05	118.71	110.68
4	F	2	Z9M	O6-C6-C5	-2.05	104.27	111.29
4	F	3	KDO	O1B-C1-C2	2.02	118.80	113.03
4	F	1	GP1	C4-C3-C2	-2.01	107.61	111.07

There are no chirality outliers.

All (14) torsion outliers are listed below:

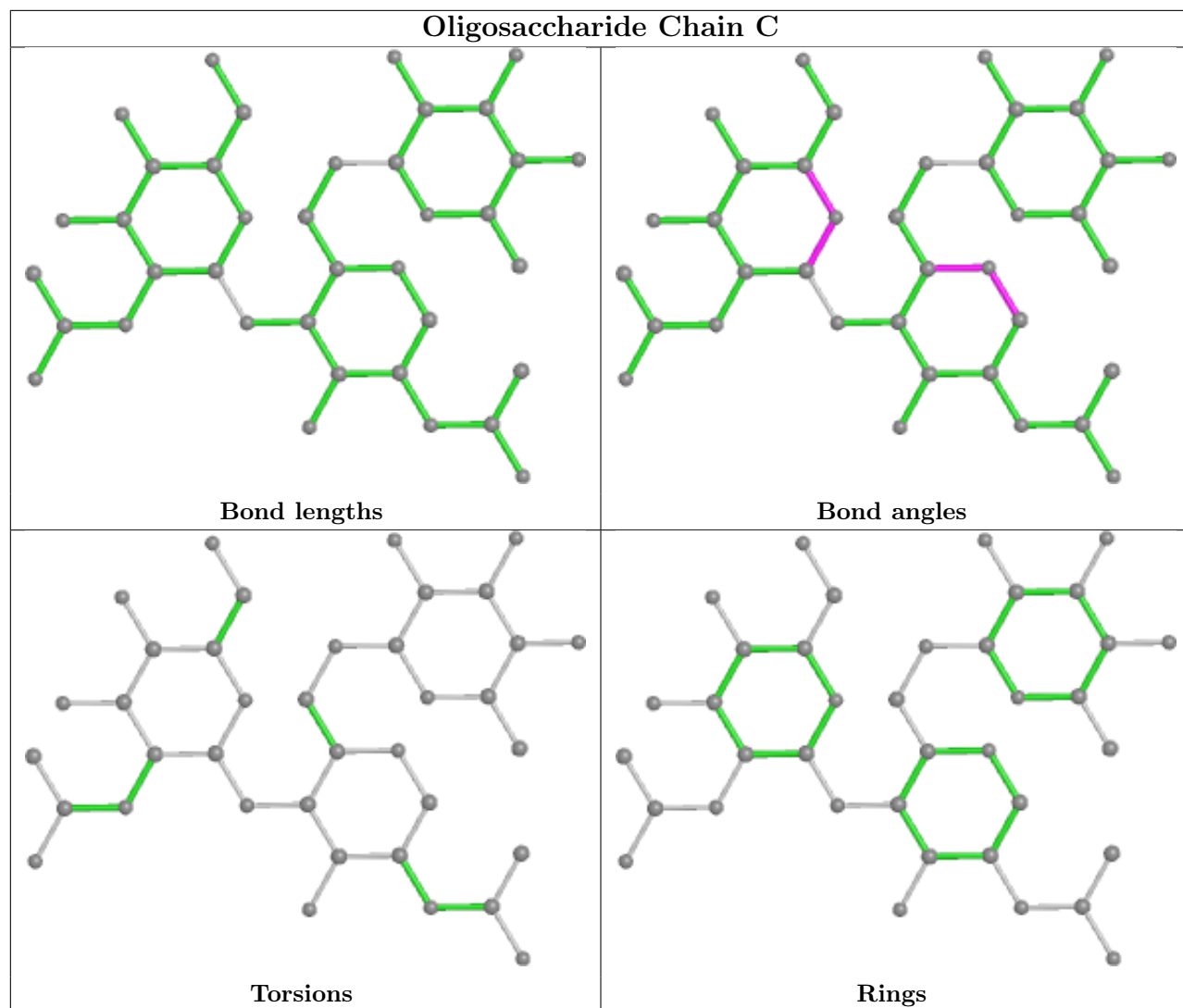
Mol	Chain	Res	Type	Atoms
3	E	2	NAG	C3-C2-N2-C7
4	F	2	Z9M	C4-O4-P1-O7
3	E	2	NAG	O5-C5-C6-O6
4	F	1	GP1	C1-O1-P4B-O8B
4	D	4	KDO	C5-C6-C7-C8
4	F	4	KDO	C5-C6-C7-C8
4	D	1	GP1	C1-O1-P4B-O7B
4	D	3	KDO	O1B-C1-C2-C3
4	D	5	KDO	O1A-C1-C2-C3
4	D	5	KDO	O1B-C1-C2-C3
4	F	3	KDO	O1B-C1-C2-C3
4	F	5	KDO	O1A-C1-C2-C3
4	F	5	KDO	O1B-C1-C2-C3
4	D	1	GP1	C1-O1-P4B-O8B

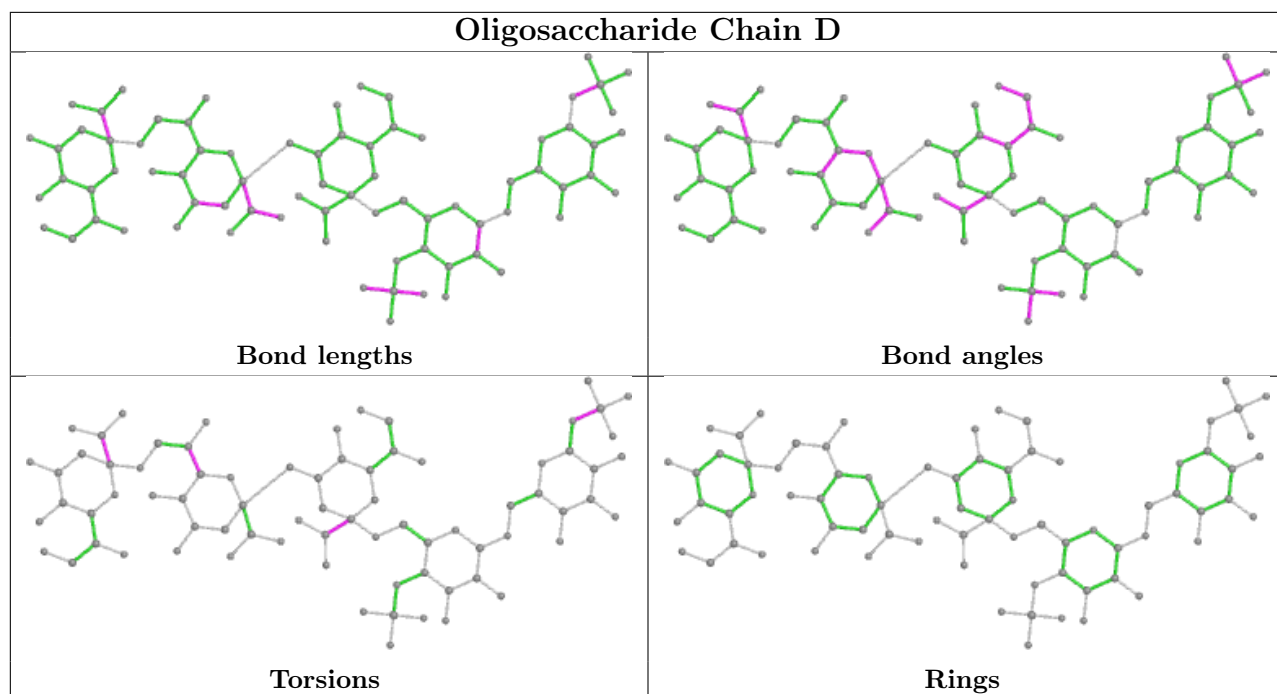
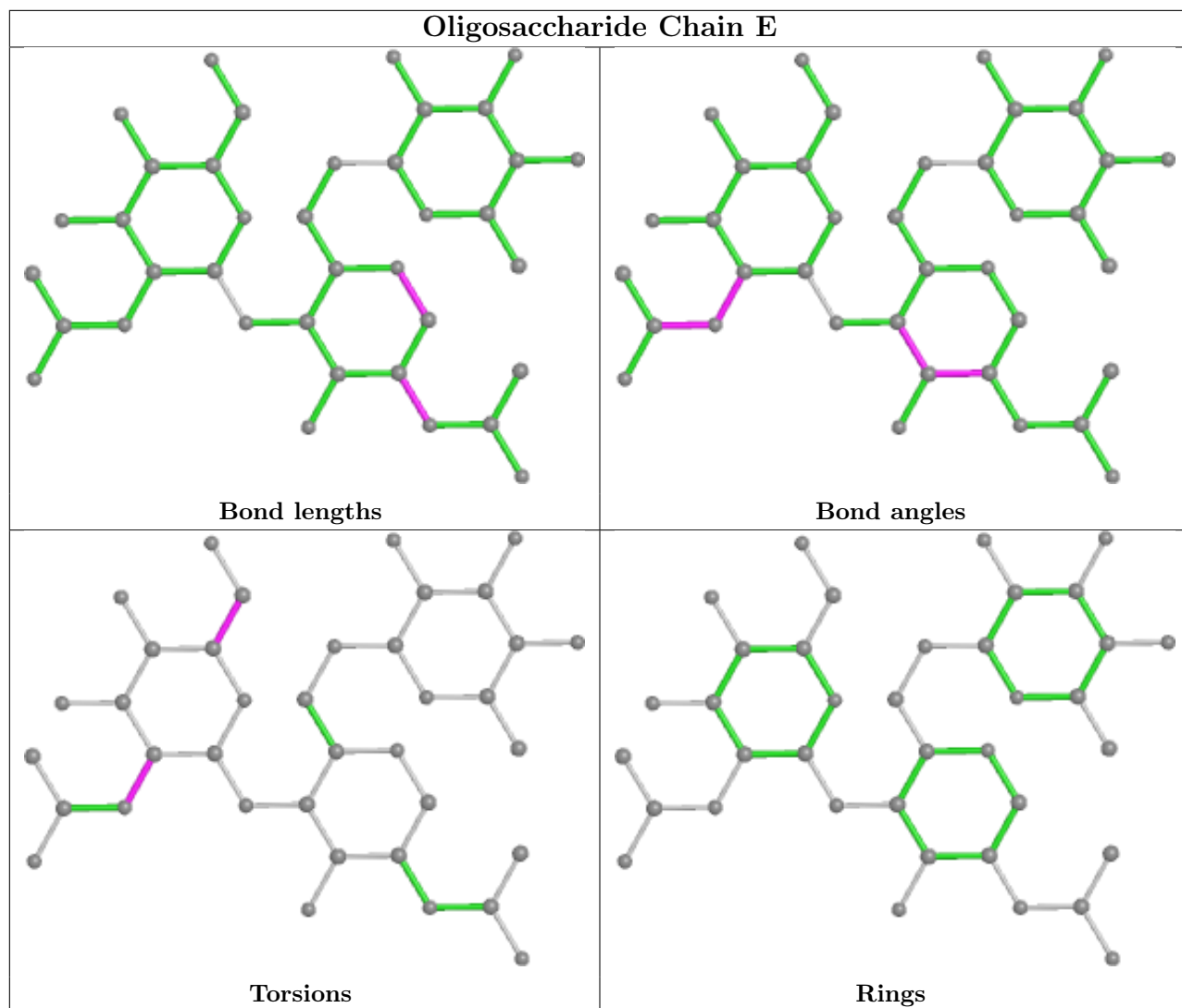
There are no ring outliers.

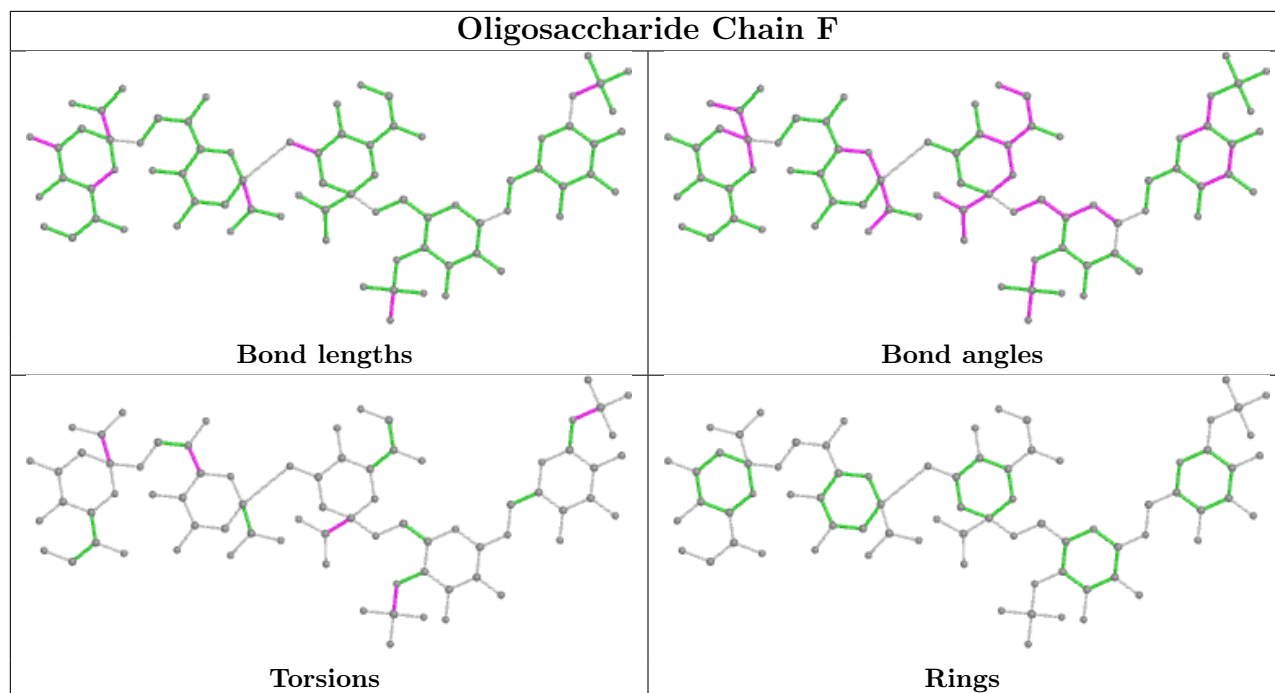
No monomer is involved in short contacts.

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](#)

1 ligand is 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	$\# Z  > 2$
5	NO3	B	301	-	1,3,3	0.35	0	0,3,3	-	-

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 [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, 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	215/218 (98%)	0.14	10 (4%) 31 37	12, 22, 40, 58	0
1	H	217/218 (99%)	0.20	7 (3%) 47 54	13, 23, 42, 62	0
2	B	219/219 (100%)	0.13	4 (1%) 68 76	13, 23, 39, 76	0
2	L	219/219 (100%)	0.21	5 (2%) 60 67	14, 26, 41, 57	0
All	All	870/874 (99%)	0.17	26 (2%) 50 56	12, 23, 40, 76	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	214	CYS	6.6
1	H	132	THR	5.4
2	B	212	ASN	4.8
2	B	202	THR	4.2
2	L	214	CYS	4.0
1	A	128	SER	3.6
2	L	212	ASN	2.8
2	L	202	THR	2.6
1	H	131	GLN	2.6
2	L	133	VAL	2.5
1	A	132	THR	2.5
2	L	41	GLY	2.4
2	B	133	VAL	2.3
1	A	133	ASN	2.3
1	A	140	CYS	2.3
1	A	127	GLY	2.3
1	H	15	SER	2.3
1	H	171	GLN	2.2
1	A	15	SER	2.2
1	A	105	GLN	2.1
1	A	131	GLN	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	H	5	GLN	2.1
1	H	124	LEU	2.1
1	H	10	GLY	2.0
1	A	213	ARG	2.0
1	A	203	SER	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.

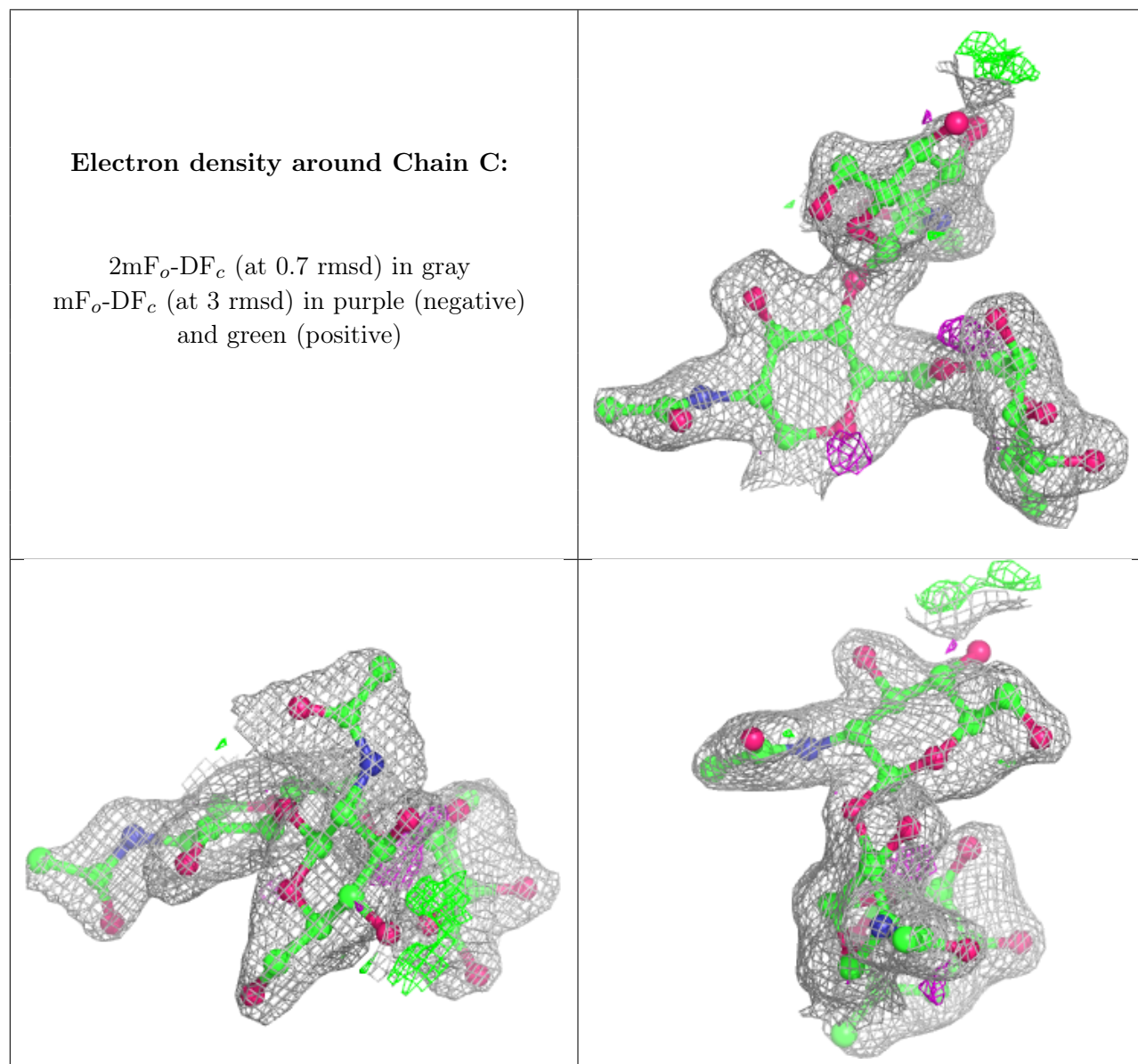
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
1	PCA	H	1	8/9	0.93	0.12	23,28,30,31	0
1	PCA	A	1	8/9	0.93	0.08	21,24,26,30	0

## 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.

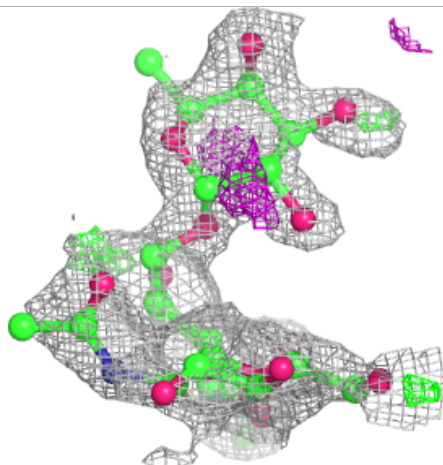
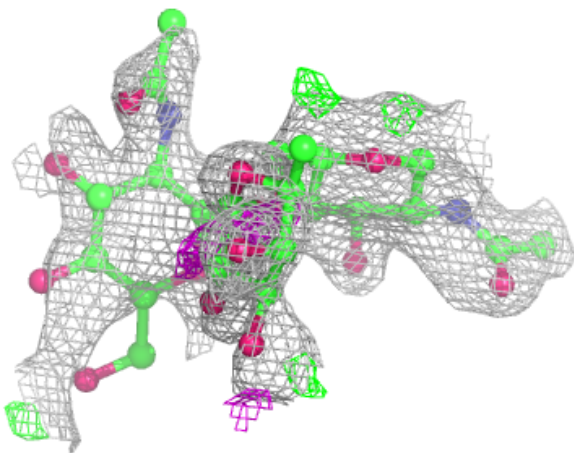
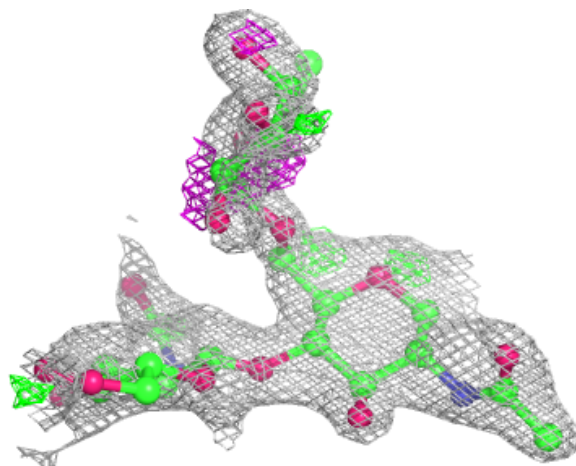
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	FUC	E	3	10/11	0.51	0.36	62,65,66,66	0
4	GP1	D	1	16/16	0.74	0.34	43,71,88,89	0
3	NAG	E	2	14/15	0.75	0.32	69,74,81,82	0
3	FUC	C	3	10/11	0.77	0.20	45,46,48,49	0
3	NAG	E	1	14/15	0.81	0.16	45,50,61,64	0
3	NAG	C	2	14/15	0.82	0.25	43,49,54,58	0
3	NAG	C	1	14/15	0.87	0.15	35,40,44,47	0
4	GP1	F	1	16/16	0.92	0.20	30,36,42,45	0
4	KDO	D	4	15/16	0.93	0.08	17,19,26,27	0
4	Z9M	F	2	15/16	0.94	0.12	21,33,37,40	0
4	KDO	F	4	15/16	0.94	0.08	16,17,21,21	0
4	Z9M	D	2	15/16	0.95	0.12	24,32,39,40	0
4	KDO	F	3	15/16	0.95	0.09	18,20,28,32	0
4	KDO	D	3	15/16	0.95	0.09	21,24,30,33	0
4	KDO	D	5	15/16	0.97	0.05	17,19,21,21	0
4	KDO	F	5	15/16	0.97	0.06	15,18,21,21	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:**

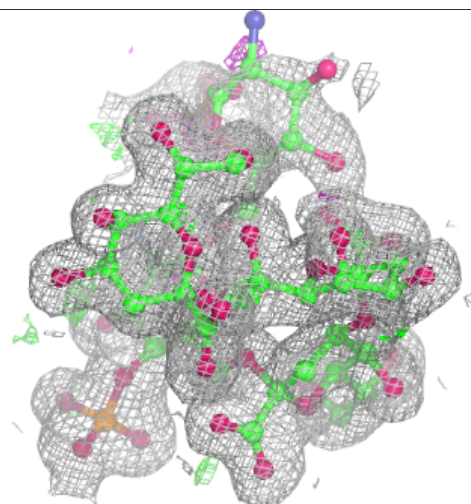
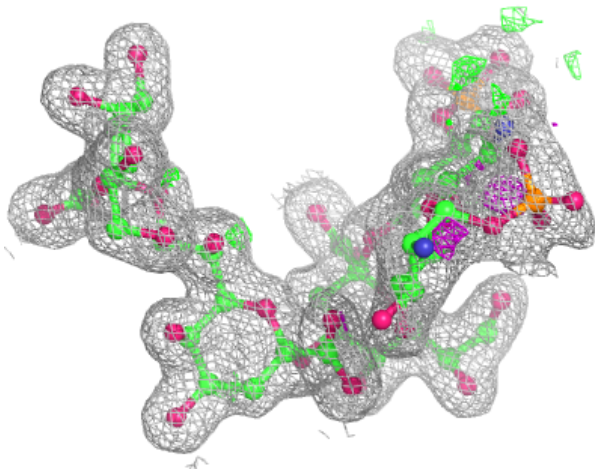
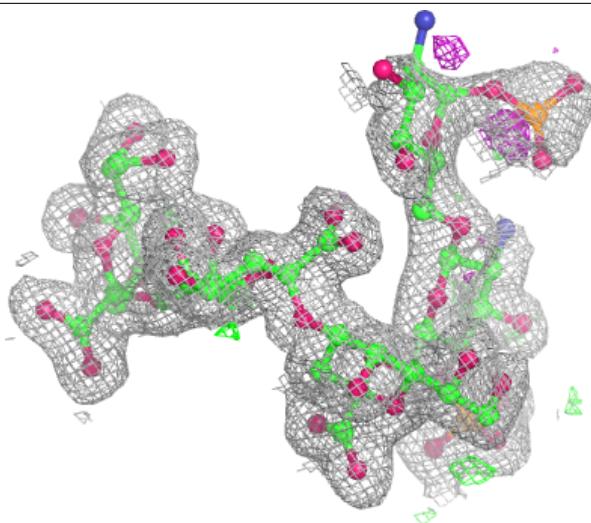
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

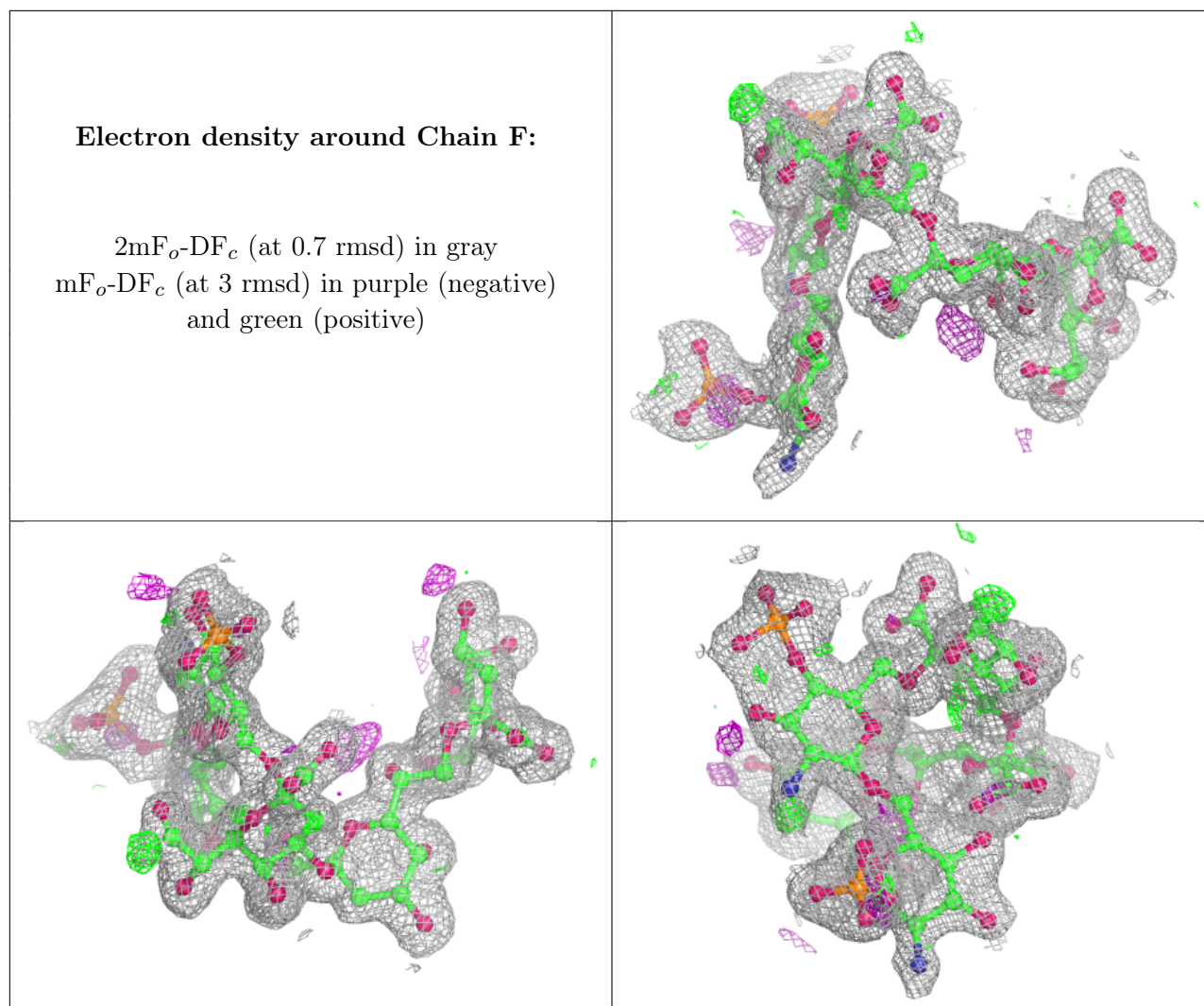




**Electron density around Chain D:**

$2mF_o-DF_c$  (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, 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
5	NO3	B	301	4/4	0.92	0.29	34,36,37,40	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.