



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 25, 2026 – 03:25 PM UTC

PDB ID : 2J6E / pdb_00002j6e
Title : Crystal Structure of an Autoimmune Complex between a Human IgM Rheumatoid Factor and IgG1 Fc reveals a Novel Fc Epitope and Evidence for Affinity Maturation
Authors : Duquerroy, S.; Stura, E.A.; Bressanelli, S.; Browne, H.; Beale, D.; Hamon, M.; Casali, P.; Vaney, M.C.; Rey, F.A.; Sutton, B.J.; Taussig, M.J.
Deposited on : 2006-09-28
Resolution : 3.00 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	:	FAILED
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

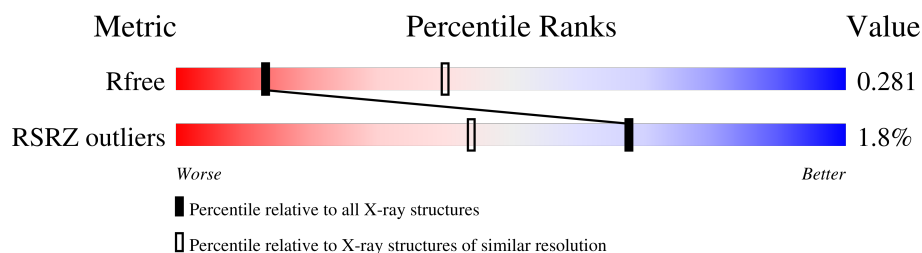
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

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
7	CAC	A	503	-	X	-	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 10195 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 IG GAMMA-1 CHAIN C REGION.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	210	Total	C	N	O	S	0	0	1
			1670	1062	282	320	6			
1	B	209	Total	C	N	O	S	0	0	1
			1667	1061	281	319	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	270	GLU	ASP	conflict	UNP P01857
B	270	GLU	ASP	conflict	UNP P01857

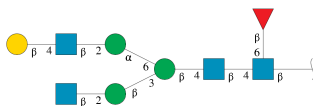
- Molecule 2 is a protein called IGM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	216	Total	C	N	O	S	0	0	0
			1633	1029	275	323	6			
2	I	220	Total	C	N	O	S	0	0	0
			1660	1043	279	331	7			

- Molecule 3 is a protein called IGM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	214	Total	C	N	O	S	0	0	1
			1587	993	270	320	4			
3	M	215	Total	C	N	O	S	0	0	0
			1602	1001	271	325	5			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	C	9	Total	C	N	O	0	0	0
			110	62	4	44			
4	D	9	Total	C	N	O	0	0	0
			110	62	4	44			

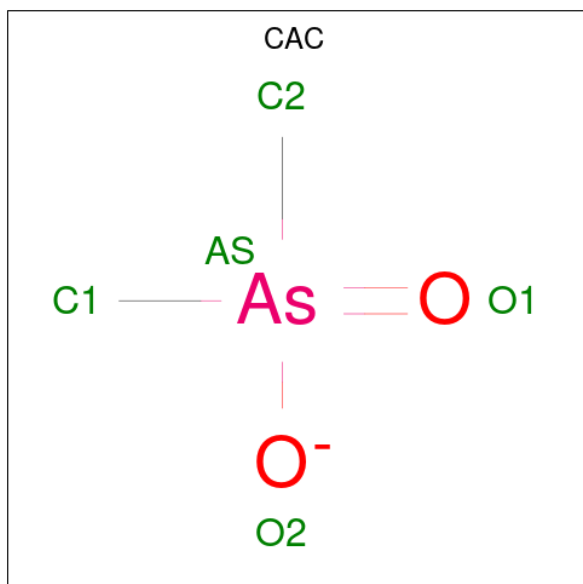
- Molecule 5 is CADMIUM ION (CCD ID: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Cd	0	0
			1	1		

- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Zn	0	0
			1	1		
6	B	1	Total	Zn	0	0
			1	1		

- Molecule 7 is CACODYLATE ION (CCD ID: CAC) (formula: C₂H₆AsO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	As	C	O	0	0
			5	1	2	2		

- Molecule 8 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			8	6	2		
8	A	1	Total	C	O	0	0
			8	6	2		
8	A	1	Total	C	O	0	0
			8	6	2		
8	B	1	Total	C	O	0	0
			8	6	2		
8	B	1	Total	C	O	0	0
			8	6	2		
8	M	1	Total	C	O	0	0
			8	6	2		

- Molecule 9 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



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

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	32	Total	O	0	0
			32	32		
10	B	16	Total	O	0	0
			16	16		
10	H	9	Total	O	0	0
			9	9		
10	I	20	Total	O	0	0
			20	20		
10	L	4	Total	O	0	0
			4	4		
10	M	3	Total	O	0	0
			3	3		

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3 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	241.98Å 75.61Å 102.40Å 90.00° 91.13° 90.00°	Depositor
Resolution (Å)	25.00 – 3.00 25.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	95.3 (25.00-3.00) 97.7 (25.00-3.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.59 (at 2.99Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.223 , 0.288 0.218 , 0.281	Depositor DCC
R_{free} test set	2601 reflections (7.12%)	wwPDB-VP
Wilson B-factor (Å ²)	69.3	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 53.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.010 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	10195	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.94% 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.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

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4.2 Too-close contacts [i](#)

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4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

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

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

4.5 Carbohydrates [i](#)

18 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
4	NAG	C	1	1,4	14,14,15	0.61	0	17,19,21	1.01	1 (5%)
4	NAG	C	2	4	14,14,15	0.55	0	17,19,21	0.96	0
4	BMA	C	3	4	11,11,12	0.66	0	15,15,17	0.71	0
4	MAN	C	4	4	11,11,12	0.46	0	15,15,17	0.54	0
4	NAG	C	5	4	14,14,15	0.68	0	17,19,21	1.12	1 (5%)
4	GAL	C	6	4	11,11,12	0.42	0	15,15,17	0.50	0
4	BMA	C	7	4	11,11,12	0.70	0	15,15,17	0.89	1 (6%)
4	NAG	C	8	4	14,14,15	0.73	0	17,19,21	0.95	1 (5%)
4	FUL	C	9	4	10,10,11	0.45	0	14,14,16	0.86	0
4	NAG	D	1	1,4	14,14,15	0.67	0	17,19,21	0.76	0
4	NAG	D	2	4	14,14,15	0.70	0	17,19,21	0.69	0
4	BMA	D	3	4	11,11,12	0.57	0	15,15,17	0.41	0
4	MAN	D	4	4	11,11,12	0.57	0	15,15,17	0.82	1 (6%)
4	NAG	D	5	4	14,14,15	0.55	0	17,19,21	1.02	2 (11%)
4	GAL	D	6	4	11,11,12	0.49	0	15,15,17	0.35	0
4	BMA	D	7	4	11,11,12	0.72	0	15,15,17	0.71	0
4	NAG	D	8	4	14,14,15	0.60	0	17,19,21	0.65	0
4	FUL	D	9	4	10,10,11	0.44	0	14,14,16	0.52	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
4	NAG	C	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	C	2	4	-	3/6/23/26	0/1/1/1
4	BMA	C	3	4	-	0/2/19/22	0/1/1/1
4	MAN	C	4	4	-	1/2/19/22	1/1/1/1
4	NAG	C	5	4	1/1/5/7	5/6/23/26	0/1/1/1
4	GAL	C	6	4	-	1/2/19/22	0/1/1/1
4	BMA	C	7	4	-	2/2/19/22	0/1/1/1
4	NAG	C	8	4	-	4/6/23/26	0/1/1/1
4	FUL	C	9	4	-	-	0/1/1/1
4	NAG	D	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	D	2	4	-	4/6/23/26	0/1/1/1
4	BMA	D	3	4	-	2/2/19/22	0/1/1/1
4	MAN	D	4	4	-	1/2/19/22	1/1/1/1
4	NAG	D	5	4	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GAL	D	6	4	-	2/2/19/22	0/1/1/1
4	BMA	D	7	4	-	2/2/19/22	0/1/1/1
4	NAG	D	8	4	-	4/6/23/26	0/1/1/1
4	FUL	D	9	4	-	-	0/1/1/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	5	NAG	C2-N2-C7	-3.04	118.83	122.90
4	D	4	MAN	C1-O5-C5	2.71	115.82	112.19
4	C	8	NAG	C2-N2-C7	-2.52	119.52	122.90
4	D	5	NAG	C4-C3-C2	-2.51	107.34	111.02
4	D	5	NAG	C2-N2-C7	-2.42	119.65	122.90
4	C	7	BMA	C3-C4-C5	-2.16	106.31	110.23
4	C	1	NAG	C2-N2-C7	-2.13	120.05	122.90

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	C	5	NAG	C1

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	2	NAG	C8-C7-N2-C2
4	C	2	NAG	O7-C7-N2-C2
4	C	5	NAG	C8-C7-N2-C2
4	C	5	NAG	O7-C7-N2-C2
4	C	8	NAG	C8-C7-N2-C2
4	C	8	NAG	O7-C7-N2-C2
4	D	1	NAG	C8-C7-N2-C2
4	D	1	NAG	O7-C7-N2-C2
4	D	2	NAG	C8-C7-N2-C2
4	D	2	NAG	O7-C7-N2-C2
4	D	5	NAG	C8-C7-N2-C2
4	D	5	NAG	O7-C7-N2-C2
4	D	8	NAG	C8-C7-N2-C2
4	D	8	NAG	O7-C7-N2-C2
4	C	8	NAG	C4-C5-C6-O6
4	C	1	NAG	C8-C7-N2-C2

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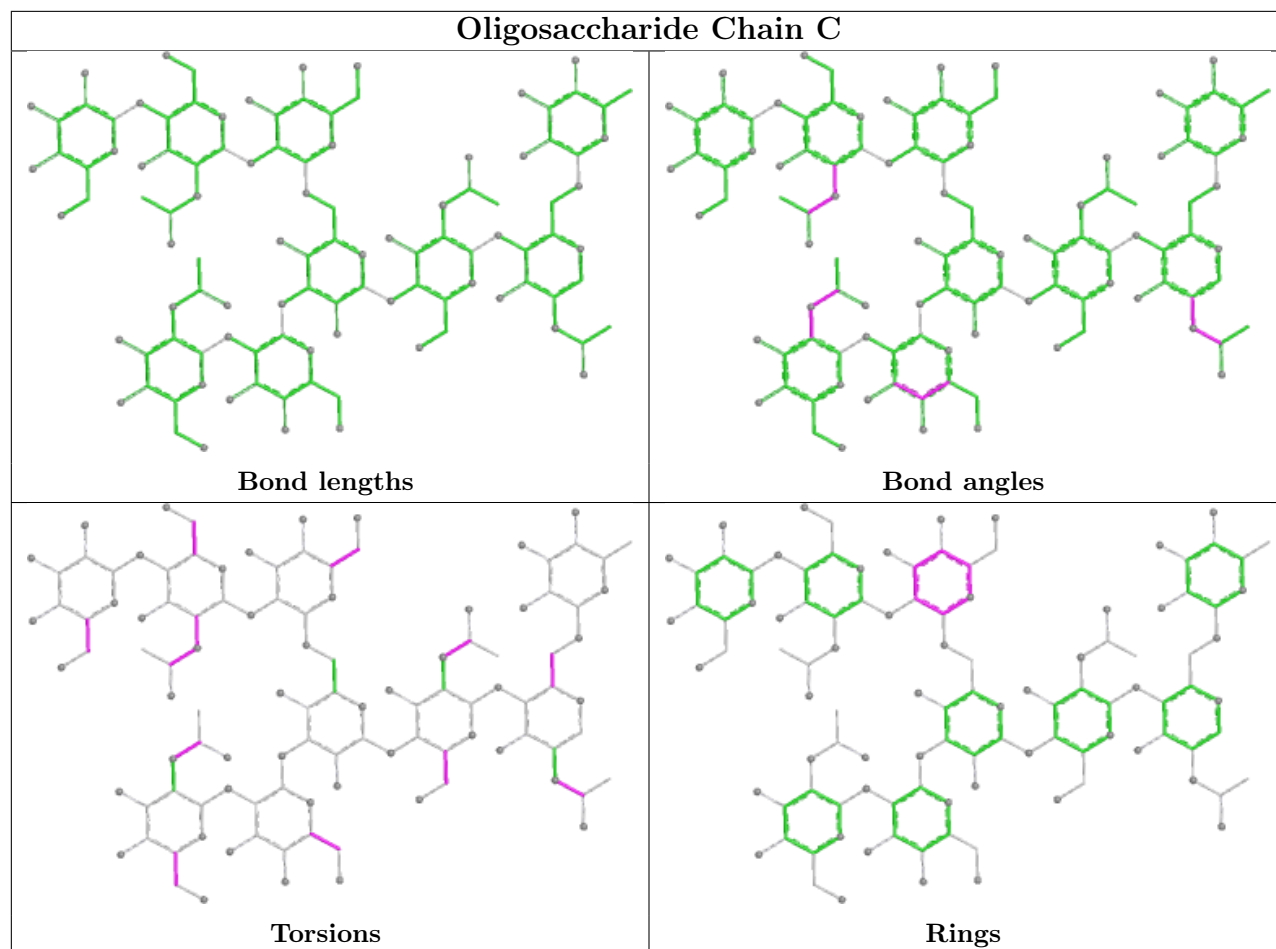
Mol	Chain	Res	Type	Atoms
4	C	1	NAG	O7-C7-N2-C2
4	D	7	BMA	O5-C5-C6-O6
4	D	1	NAG	O5-C5-C6-O6
4	D	6	GAL	O5-C5-C6-O6
4	C	1	NAG	O5-C5-C6-O6
4	C	8	NAG	O5-C5-C6-O6
4	C	7	BMA	C4-C5-C6-O6
4	D	7	BMA	C4-C5-C6-O6
4	D	8	NAG	O5-C5-C6-O6
4	D	1	NAG	C4-C5-C6-O6
4	C	5	NAG	O5-C5-C6-O6
4	C	1	NAG	C4-C5-C6-O6
4	D	8	NAG	C4-C5-C6-O6
4	C	7	BMA	O5-C5-C6-O6
4	D	6	GAL	C4-C5-C6-O6
4	C	6	GAL	O5-C5-C6-O6
4	C	5	NAG	C4-C5-C6-O6
4	D	3	BMA	C4-C5-C6-O6
4	C	4	MAN	C4-C5-C6-O6
4	D	2	NAG	C4-C5-C6-O6
4	D	2	NAG	O5-C5-C6-O6
4	D	3	BMA	O5-C5-C6-O6
4	C	5	NAG	C1-C2-N2-C7
4	D	4	MAN	O5-C5-C6-O6
4	C	2	NAG	O5-C5-C6-O6

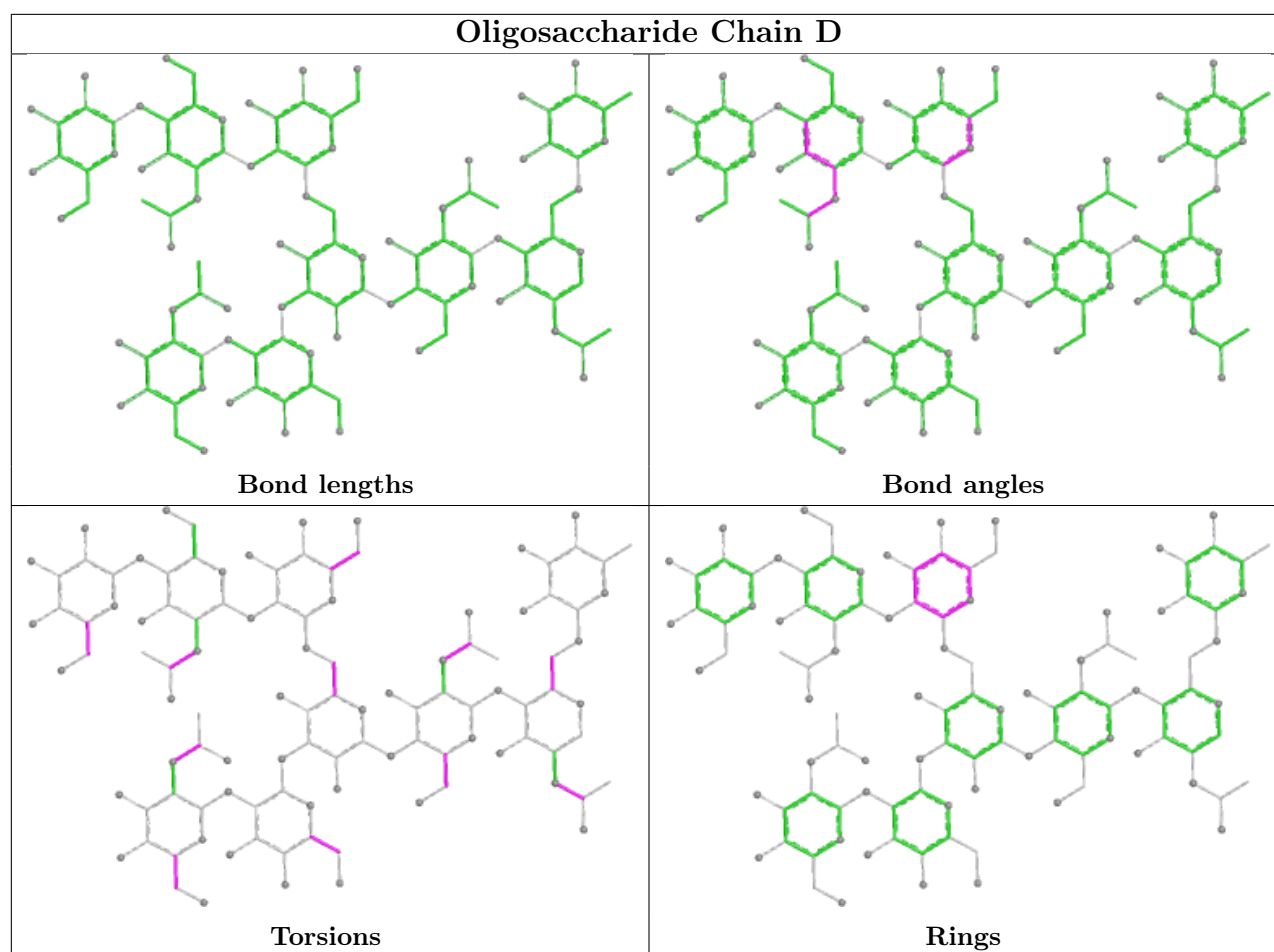
All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	4	MAN	C1-C2-C3-C4-C5-O5
4	C	4	MAN	C1-C2-C3-C4-C5-O5

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.





4.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 3 are monoatomic - leaving 11 for Mogul analysis.

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	$\# Z > 2$
8	MPD	A	505	-	7,7,7	0.59	0	9,10,10	0.56	0
9	ACT	A	507	-	3,3,3	0.87	0	3,3,3	1.81	1 (33%)
8	MPD	A	506	-	7,7,7	0.71	0	9,10,10	0.61	0
8	MPD	B	503	-	7,7,7	0.50	0	9,10,10	0.46	0
9	ACT	B	504	-	3,3,3	0.72	0	3,3,3	1.81	1 (33%)
9	ACT	A	508	-	3,3,3	1.36	1 (33%)	3,3,3	0.72	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	MPD	A	504	-	7,7,7	0.53	0	9,10,10	0.49	0
8	MPD	M	301	-	7,7,7	0.45	0	9,10,10	0.50	0
9	ACT	H	301	-	3,3,3	0.81	0	3,3,3	1.80	1 (33%)
7	CAC	A	503	6	2,4,4	5.07	2 (100%)	4,6,6	1.92	2 (50%)
8	MPD	B	502	-	7,7,7	0.44	0	9,10,10	0.44	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
8	MPD	A	505	-	-	0/5/5/5	-
8	MPD	A	506	-	-	1/5/5/5	-
8	MPD	B	503	-	-	3/5/5/5	-
8	MPD	A	504	-	-	0/5/5/5	-
8	MPD	M	301	-	-	3/5/5/5	-
8	MPD	B	502	-	-	0/5/5/5	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	503	CAC	AS-C1	-5.07	1.78	1.90
7	A	503	CAC	AS-C2	-5.06	1.78	1.90
9	A	508	ACT	O-C	2.23	1.32	1.22

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	503	CAC	O1-AS-C1	-2.64	108.21	111.50
9	B	504	ACT	O-C-CH3	-2.50	112.28	122.53
9	A	507	ACT	O-C-CH3	-2.50	112.30	122.53
9	H	301	ACT	O-C-CH3	-2.47	112.39	122.53
7	A	503	CAC	O1-AS-C2	-2.19	108.78	111.50

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	506	MPD	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
8	B	503	MPD	C1-C2-C3-C4
8	B	503	MPD	O2-C2-C3-C4
8	M	301	MPD	O2-C2-C3-C4
8	B	503	MPD	CM-C2-C3-C4
8	M	301	MPD	C1-C2-C3-C4
8	M	301	MPD	CM-C2-C3-C4

There are no ring outliers.

No monomer is involved in short contacts.

4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	I	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	127:CYS	C	132:ASP	N	15.42

5 Fit of model and data

5.1 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	210/232 (90%)	-0.55	0	100	100	24, 39, 56, 68	0
1	B	209/232 (90%)	-0.07	9 (4%)	40	21	23, 56, 131, 140	0
2	H	216/231 (93%)	0.17	4 (1%)	66	43	32, 77, 151, 152	0
2	I	220/231 (95%)	-0.08	1 (0%)	87	72	24, 56, 133, 146	0
3	L	214/234 (91%)	0.36	7 (3%)	49	28	36, 89, 151, 152	0
3	M	215/234 (91%)	0.33	2 (0%)	81	61	45, 95, 138, 141	0
All	All	1284/1394 (92%)	0.03	23 (1%)	67	44	23, 67, 148, 152	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	323	VAL	3.8
2	I	146	LEU	3.5
2	H	146	LEU	2.8
1	B	263	VAL	2.7
3	M	62	PHE	2.6
3	L	185	TRP	2.5
1	B	238	PRO	2.5
3	L	191	TYR	2.5
2	H	184	LEU	2.5
3	L	157	ALA	2.4
3	L	120	PRO	2.4
1	B	324	SER	2.4
1	B	273	VAL	2.4
3	L	186	LYS	2.2
1	B	321	CYS	2.2
1	B	271	PRO	2.2
3	M	150	ALA	2.2
3	L	136	ILE	2.1
1	B	264	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
2	H	181	SER	2.1
2	H	125	VAL	2.1
3	L	110	PRO	2.0
1	B	266	VAL	2.0

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

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

5.3 Carbohydrates [i](#)

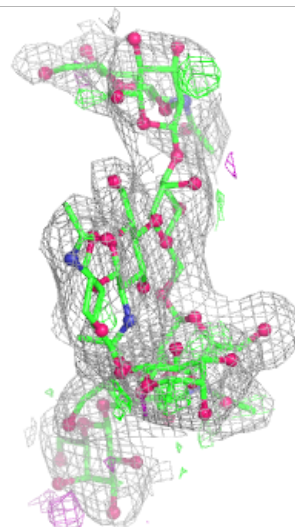
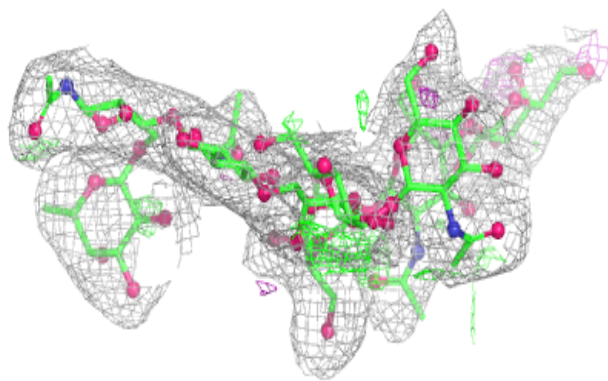
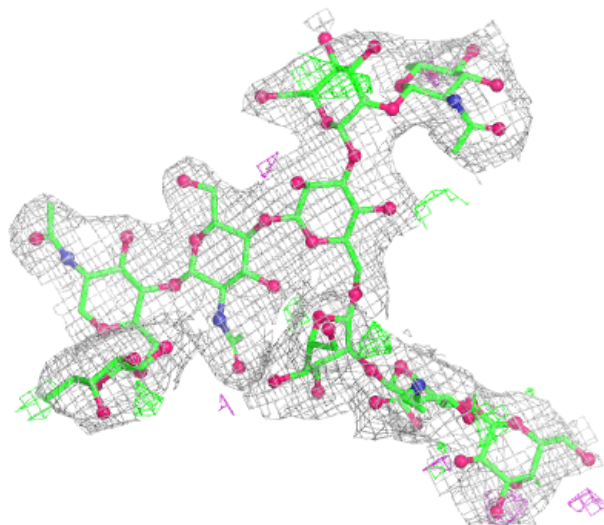
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

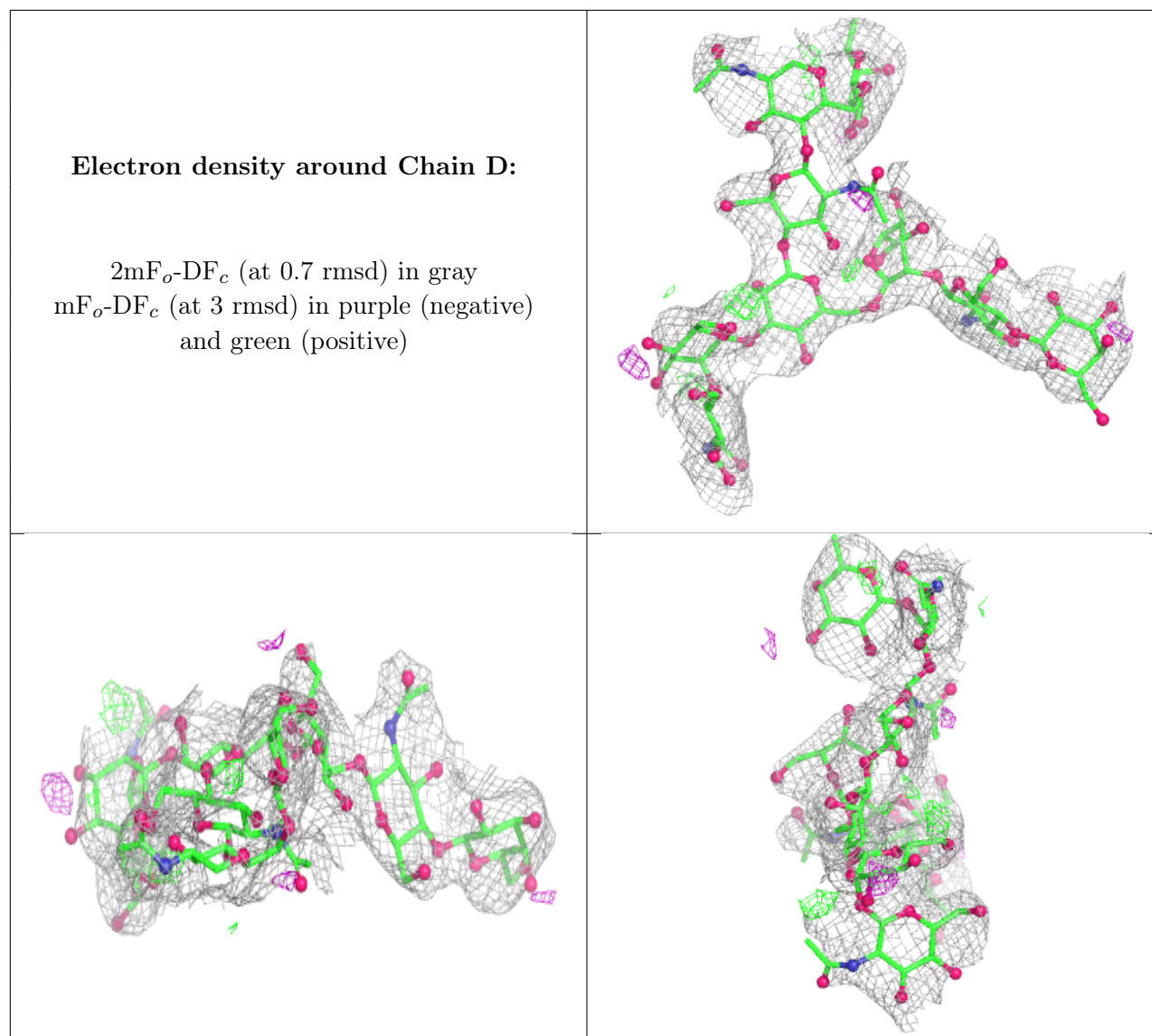
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	C	1	14/15	-	-	32,34,40,45	0
4	NAG	C	2	14/15	-	-	34,36,39,40	0
4	BMA	C	3	11/12	-	-	45,47,51,62	0
4	MAN	C	4	11/12	-	-	49,50,52,54	0
4	NAG	C	5	14/15	-	-	50,51,57,59	0
4	GAL	C	6	11/12	-	-	53,56,61,61	0
4	BMA	C	7	11/12	-	-	71,78,82,83	0
4	NAG	C	8	14/15	-	-	88,91,92,92	0
4	FUL	C	9	10/11	-	-	45,48,51,51	0
4	NAG	D	1	14/15	-	-	118,122,123,123	0
4	NAG	D	2	14/15	-	-	120,122,126,126	0
4	BMA	D	3	11/12	-	-	112,117,119,120	0
4	MAN	D	4	11/12	-	-	108,109,110,110	0
4	NAG	D	5	14/15	-	-	106,107,108,109	0
4	GAL	D	6	11/12	-	-	108,108,109,110	0
4	BMA	D	7	11/12	-	-	112,117,118,119	0
4	NAG	D	8	14/15	-	-	119,121,122,122	0
4	FUL	D	9	10/11	-	-	119,119,120,120	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)





5.4 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
8	MPD	B	502	8/8	0.56	0.24	81,83,83,84	0
9	ACT	H	301	4/4	0.70	0.19	81,81,81,81	0
8	MPD	B	503	8/8	0.74	0.23	82,83,84,84	0
8	MPD	A	505	8/8	0.77	0.33	81,83,85,86	0
9	ACT	A	508	4/4	0.79	0.26	85,85,85,85	0
8	MPD	M	301	8/8	0.80	0.14	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	MPD	A	504	8/8	0.82	0.34	92,95,96,98	0
8	MPD	A	506	8/8	0.83	0.28	81,81,81,81	0
6	ZN	B	501	1/1	0.87	0.09	143,143,143,143	0
9	ACT	B	504	4/4	0.93	0.17	81,81,81,81	0
9	ACT	A	507	4/4	0.94	0.14	64,65,65,66	0
7	CAC	A	503	5/5	0.97	0.08	83,84,84,87	0
5	CD	A	501	1/1	0.99	0.03	57,57,57,57	0
6	ZN	A	502	1/1	0.99	0.03	43,43,43,43	0

5.5 Other polymers [i](#)

There are no such residues in this entry.