



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:54 PM UTC

PDB ID : 5A3I / pdb_00005a3i
Title : Crystal Structure of a Complex formed between FLD194 Fab and Transmissible Mutant H5 Haemagglutinin
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Deposited on : 2015-06-01
Resolution : 2.89 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)

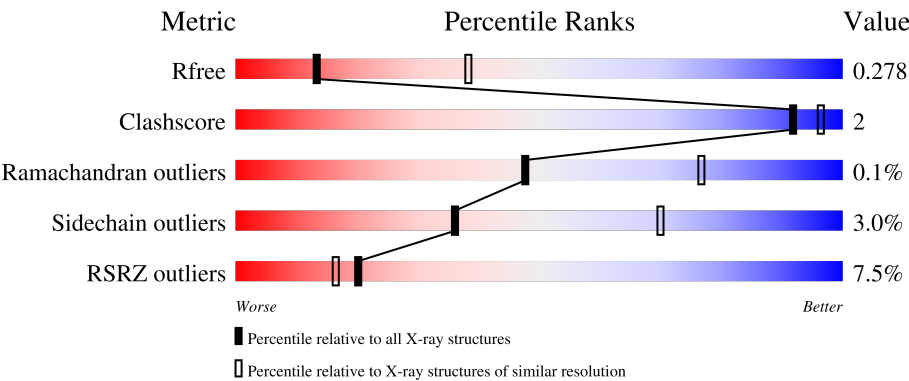
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.89 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	328	8% 94% ...
1	E	328	5% 92% 6% ..
2	B	166	22% 94% 5% .
3	C	230	3% 95% ..

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Mol	Chain	Length	Quality of chain
3	G	230	8% 90% 7% ••
4	D	219	% 93% 6%
4	H	219	8% 95% 5%
5	F	166	10% 94% 5% •
6	I	2	100%
6	J	2	100%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 14561 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 HEMAGGLUTININ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	323	Total	C	N	O	S	0	0	0
			2555	1617	437	486	15			
1	E	323	Total	C	N	O	S	0	0	0
			2563	1623	439	486	15			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ASP	-	expression tag	UNP A5A5M5
A	0	PRO	-	expression tag	UNP A5A5M5
A	325	THR	-	expression tag	UNP A5A5M5
A	326	ARG	-	expression tag	UNP A5A5M5
A	154	ASP	ASN	conflict	UNP A5A5M5
A	220	LYS	ASN	conflict	UNP A5A5M5
A	222	LEU	GLN	conflict	UNP A5A5M5
A	315	ILE	THR	conflict	UNP A5A5M5
E	-1	ASP	-	expression tag	UNP A5A5M5
E	0	PRO	-	expression tag	UNP A5A5M5
E	325	THR	-	expression tag	UNP A5A5M5
E	326	ARG	-	expression tag	UNP A5A5M5
E	154	ASP	ASN	conflict	UNP A5A5M5
E	220	LYS	ASN	conflict	UNP A5A5M5
E	222	LEU	GLN	conflict	UNP A5A5M5
E	315	ILE	THR	conflict	UNP A5A5M5

- Molecule 2 is a protein called HEMAGGLUTININ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	166	Total	C	N	O	S	0	0	0
			1331	830	227	266	8			

- Molecule 3 is a protein called ANTI-HAEMAGGLUTININ HA1 FAB HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	226	Total	C	N	O	S	0	0	0
			1695	1075	280	332	8			
3	G	226	Total	C	N	O	S	0	0	0
			1695	1075	280	332	8			

- Molecule 4 is a protein called ANTI-HAEMAGGLUTININ HA1 FAB LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	218	Total	C	N	O	S	0	0	0
			1667	1044	282	335	6			
4	H	218	Total	C	N	O	S	0	0	0
			1663	1041	281	335	6			

- Molecule 5 is a protein called HEMAGGLUTININ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	166	Total	C	N	O	S	0	0	0
			1322	822	228	264	8			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	68	LYS	ARG	conflict	UNP A5A5M5

- Molecule 6 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	J	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

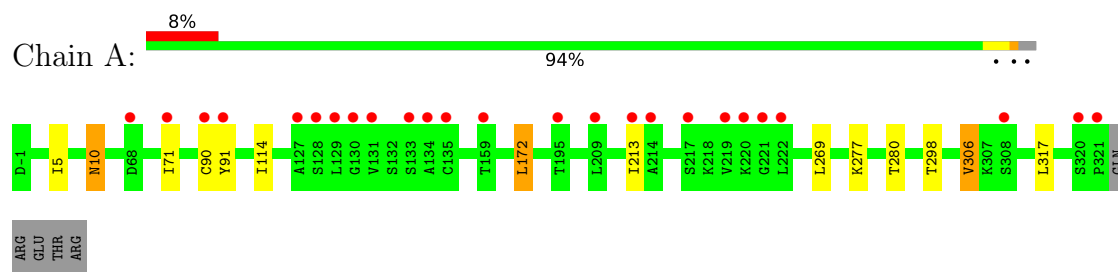


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
7	E	1	14	8	1	5	0	0

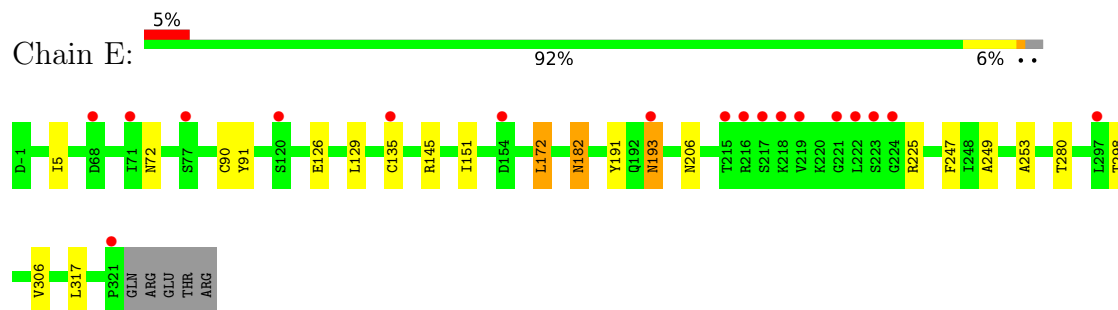
3 Residue-property plots [i](#)

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.

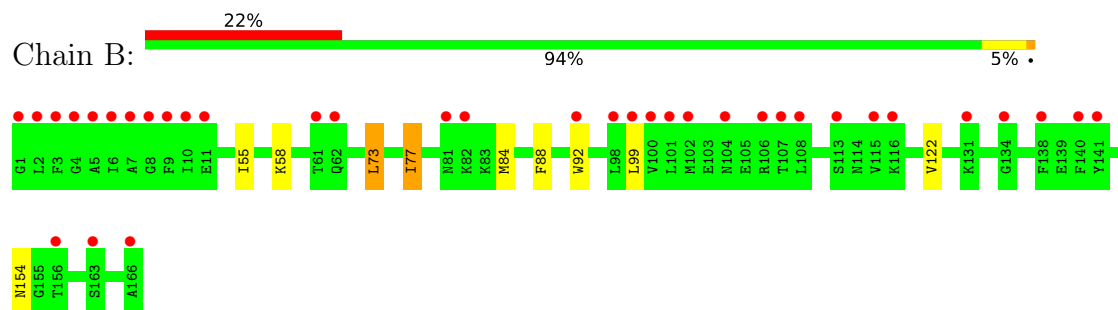
• Molecule 1: HEMAGGLUTININ



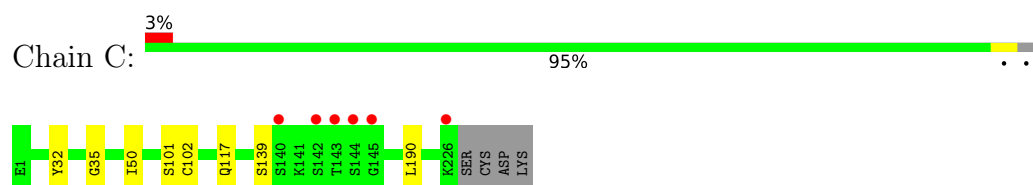
• Molecule 1: HEMAGGLUTININ



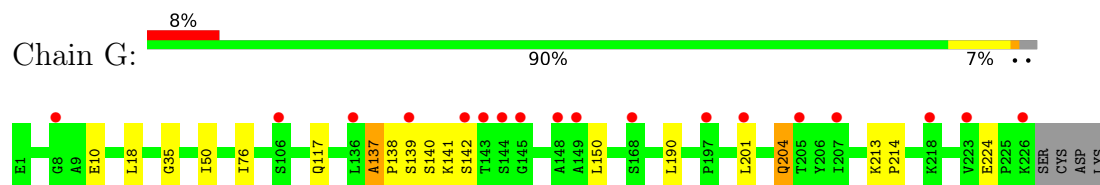
• Molecule 2: HEMAGGLUTININ



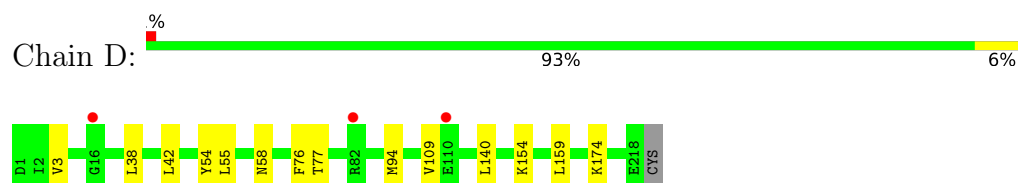
• Molecule 3: ANTI-HAEMAGGLUTININ HA1 FAB HEAVY CHAIN



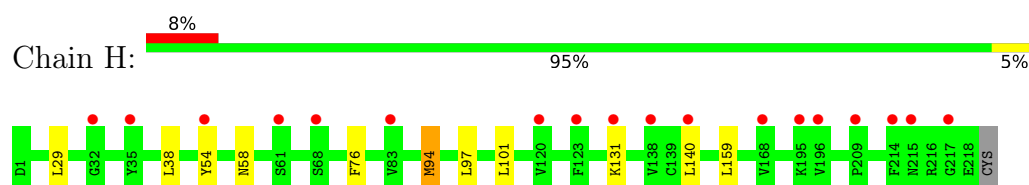
- Molecule 3: ANTI-HAEMAGGLUTININ HA1 FAB HEAVY CHAIN



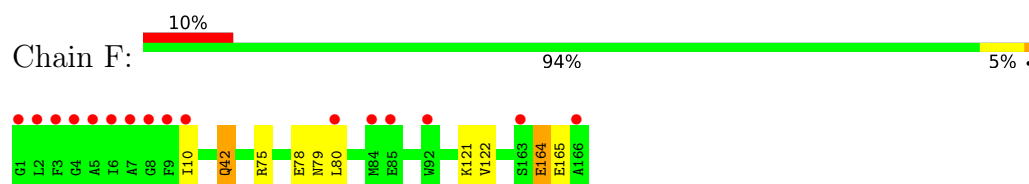
- Molecule 4: ANTI-HAEMAGGLUTININ HA1 FAB LIGHT CHAIN



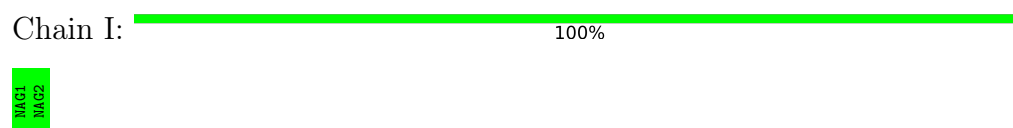
- Molecule 4: ANTI-HAEMAGGLUTININ HA1 FAB LIGHT CHAIN



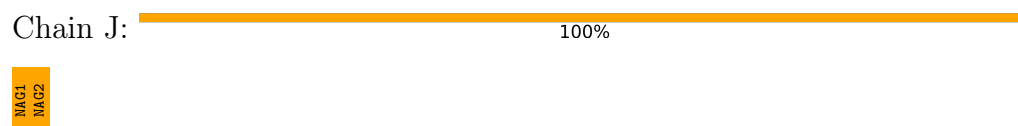
- Molecule 5: HEMAGGLUTININ



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	86.75Å 87.70Å 100.90Å 78.67° 84.66° 73.91°	Depositor
Resolution (Å)	83.33 – 2.89 83.33 – 2.89	Depositor EDS
% Data completeness (in resolution range)	91.4 (83.33-2.89) 91.4 (83.33-2.89)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.32 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.244 , 0.277 0.246 , 0.278	Depositor DCC
R_{free} test set	2901 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	50.7	Xtriage
Anisotropy	0.003	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 27.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	14561	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG

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	0.38	0/2618	0.59	0/3560
1	E	0.38	0/2626	0.60	0/3568
2	B	0.39	0/1358	0.69	0/1829
3	C	0.38	0/1741	0.63	0/2374
3	G	0.39	0/1741	0.64	0/2374
4	D	0.38	0/1703	0.61	0/2312
4	H	0.38	0/1699	0.57	0/2308
5	F	0.40	0/1348	0.72	1/1815 (0.1%)
All	All	0.38	0/14834	0.63	1/20140 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	164	GLU	N-CA-C	7.53	119.57	111.36

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	2555	0	2491	7	0
1	E	2563	0	2514	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1331	0	1226	6	0
3	C	1695	0	1653	3	0
3	G	1695	0	1653	12	0
4	D	1667	0	1629	2	0
4	H	1663	0	1618	4	0
5	F	1322	0	1217	6	0
6	I	28	0	25	0	0
6	J	28	0	25	1	0
7	E	14	0	13	0	0
All	All	14561	0	14064	46	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 (46) 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)
3:G:137:ALA:HB1	3:G:138:PRO:CD	2.20	0.70
1:E:90:CYS:SG	1:E:91:TYR:N	2.65	0.70
1:A:306:VAL:HG13	2:B:92:TRP:CZ3	2.28	0.69
1:E:5:ILE:HD11	5:F:122:VAL:HG21	1.81	0.62
5:F:42:GLN:HA	5:F:42:GLN:HE21	1.61	0.62
3:G:137:ALA:HB1	3:G:138:PRO:HD2	1.82	0.61
2:B:73:LEU:CD2	2:B:77:ILE:HD13	2.33	0.59
6:J:1:NAG:H61	6:J:2:NAG:H2	1.86	0.58
4:H:38:LEU:HD22	4:H:76:PHE:CG	2.43	0.54
3:G:139:SER:HA	3:G:140:SER:CB	2.39	0.52
3:C:32:TYR:CD2	3:C:101:SER:HB2	2.45	0.52
4:H:54:TYR:O	4:H:58:ASN:HB2	2.10	0.52
5:F:78:GLU:C	5:F:80:LEU:HB3	2.37	0.50
5:F:79:ASN:N	5:F:80:LEU:HB3	2.26	0.50
3:G:137:ALA:CB	3:G:138:PRO:CD	2.90	0.49
1:E:280:THR:HG22	1:E:298:THR:HG22	1.95	0.48
3:G:138:PRO:HG3	3:G:150:LEU:HB3	1.96	0.48
5:F:164:GLU:N	5:F:165:GLU:HA	2.30	0.46
3:C:35:GLY:HA3	3:C:50:ILE:HG22	1.97	0.46
1:A:280:THR:HG22	1:A:298:THR:HG22	1.98	0.45
3:G:204:GLN:HE21	3:G:204:GLN:HA	1.79	0.45
1:E:172:LEU:HD12	1:E:253:ALA:HB1	1.97	0.45
3:C:190:LEU:HD12	3:C:190:LEU:C	2.42	0.45
1:A:114:ILE:HD11	1:A:172:LEU:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:54:TYR:O	4:D:58:ASN:HB2	2.16	0.44
3:G:190:LEU:HD12	3:G:190:LEU:C	2.42	0.44
1:E:247:PHE:CE2	1:E:249:ALA:HB2	2.52	0.44
4:H:94:MET:HE1	4:H:101:LEU:HD23	2.00	0.44
3:G:10:GLU:HG3	3:G:18:LEU:HD11	1.99	0.43
2:B:55:ILE:HD11	2:B:99:LEU:HG	2.00	0.43
4:D:38:LEU:HD22	4:D:76:PHE:CG	2.54	0.43
1:A:5:ILE:HD11	2:B:122:VAL:HG21	2.00	0.43
1:A:10:ASN:HD22	1:A:10:ASN:N	2.16	0.42
2:B:84:MET:HE3	2:B:84:MET:HA	2.02	0.42
2:B:73:LEU:HD12	2:B:88:PHE:CZ	2.55	0.42
3:G:213:LYS:N	3:G:214:PRO:HD2	2.35	0.41
1:E:182:ASN:OD1	1:E:182:ASN:N	2.54	0.41
1:E:193:ASN:HD22	1:E:193:ASN:N	2.19	0.41
1:A:213:ILE:HD12	1:A:213:ILE:N	2.36	0.41
5:F:42:GLN:HE21	5:F:42:GLN:CA	2.27	0.41
3:G:139:SER:HA	3:G:140:SER:HB3	2.01	0.41
3:G:141:LYS:HA	3:G:142:SER:HA	1.88	0.40
3:G:35:GLY:HA3	3:G:50:ILE:HG22	2.01	0.40
1:A:90:CYS:SG	1:A:91:TYR:N	2.95	0.40
1:E:126:GLU:HG2	1:E:129:LEU:HD22	2.02	0.40
4:H:29:LEU:HA	4:H:97:LEU:HD22	2.02	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	321/328 (98%)	308 (96%)	13 (4%)	0	100	100
1	E	321/328 (98%)	305 (95%)	16 (5%)	0	100	100
2	B	164/166 (99%)	155 (94%)	9 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	224/230 (97%)	213 (95%)	11 (5%)	0	100	100
3	G	224/230 (97%)	209 (93%)	14 (6%)	1 (0%)	30	59
4	D	216/219 (99%)	208 (96%)	8 (4%)	0	100	100
4	H	216/219 (99%)	209 (97%)	7 (3%)	0	100	100
5	F	164/166 (99%)	156 (95%)	8 (5%)	0	100	100
All	All	1850/1886 (98%)	1763 (95%)	86 (5%)	1 (0%)	48	77

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	G	137	ALA

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	289/296 (98%)	282 (98%)	7 (2%)	43	75
1	E	291/296 (98%)	279 (96%)	12 (4%)	27	61
2	B	139/141 (99%)	135 (97%)	4 (3%)	37	71
3	C	191/196 (97%)	188 (98%)	3 (2%)	55	83
3	G	191/196 (97%)	186 (97%)	5 (3%)	40	73
4	D	190/191 (100%)	180 (95%)	10 (5%)	20	52
4	H	189/191 (99%)	185 (98%)	4 (2%)	47	77
5	F	137/141 (97%)	133 (97%)	4 (3%)	37	71
All	All	1617/1648 (98%)	1568 (97%)	49 (3%)	36	70

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	71	ILE

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Mol	Chain	Res	Type
1	A	172	LEU
1	A	269	LEU
1	A	277	LYS
1	A	306	VAL
1	A	317	LEU
2	B	58	LYS
2	B	73	LEU
2	B	77	ILE
2	B	154	ASN
3	C	102	CYS
3	C	117	GLN
3	C	139	SER
4	D	3	VAL
4	D	42	LEU
4	D	55	LEU
4	D	77	THR
4	D	94	MET
4	D	109	VAL
4	D	140	LEU
4	D	154	LYS
4	D	159	LEU
4	D	174	LYS
1	E	72	ASN
1	E	135	CYS
1	E	145	ARG
1	E	151	ILE
1	E	172	LEU
1	E	182	ASN
1	E	191	TYR
1	E	193	ASN
1	E	206	ASN
1	E	225	ARG
1	E	306	VAL
1	E	317	LEU
5	F	10	ILE
5	F	42	GLN
5	F	75	ARG
5	F	121	LYS
3	G	76	ILE
3	G	117	GLN
3	G	201	LEU
3	G	204	GLN

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Mol	Chain	Res	Type
3	G	224	GLU
4	H	94	MET
4	H	131	LYS
4	H	140	LEU
4	H	159	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	15	GLN
1	A	84	ASN
1	A	103	HIS
1	A	146	ASN
1	A	187	GLN
1	A	295	HIS
2	B	42	GLN
2	B	53	ASN
2	B	60	ASN
2	B	72	ASN
2	B	125	GLN
2	B	154	ASN
3	C	3	GLN
3	C	176	HIS
3	C	216	ASN
4	D	47	GLN
4	D	142	ASN
4	D	165	GLN
4	D	203	HIS
1	E	2	GLN
1	E	28	HIS
1	E	84	ASN
1	E	125	HIS
1	E	180	HIS
1	E	206	ASN
1	E	207	GLN
5	F	15	GLN
5	F	26	HIS
5	F	42	GLN
5	F	53	ASN
5	F	60	ASN
5	F	72	ASN

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Mol	Chain	Res	Type
3	G	183	GLN
3	G	204	GLN
3	G	211	ASN
3	G	216	ASN
4	H	58	ASN
4	H	143	ASN
4	H	152	GLN
4	H	204	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

4 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	$\# Z > 2$
6	NAG	I	1	1,6	14,14,15	0.47	0	17,19,21	0.70	0
6	NAG	I	2	6	14,14,15	0.49	0	17,19,21	0.70	0
6	NAG	J	1	1,6	14,14,15	0.60	0	17,19,21	1.89	6 (35%)
6	NAG	J	2	6	14,14,15	0.65	0	17,19,21	0.96	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
6	NAG	I	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	I	2	6	-	2/6/23/26	0/1/1/1
6	NAG	J	1	1,6	-	4/6/23/26	0/1/1/1
6	NAG	J	2	6	-	4/6/23/26	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(°)
6	J	1	NAG	O4-C4-C3	-3.62	101.84	110.38
6	J	1	NAG	C1-O5-C5	3.31	116.62	112.19
6	J	1	NAG	C4-C3-C2	2.68	114.95	111.02
6	J	1	NAG	O4-C4-C5	2.55	115.62	109.32
6	J	1	NAG	C8-C7-N2	2.46	120.20	116.12
6	J	2	NAG	C1-C2-N2	2.21	113.92	110.43
6	J	1	NAG	O5-C5-C6	-2.15	103.47	107.66

There are no chirality outliers.

All (10) torsion outliers are listed below:

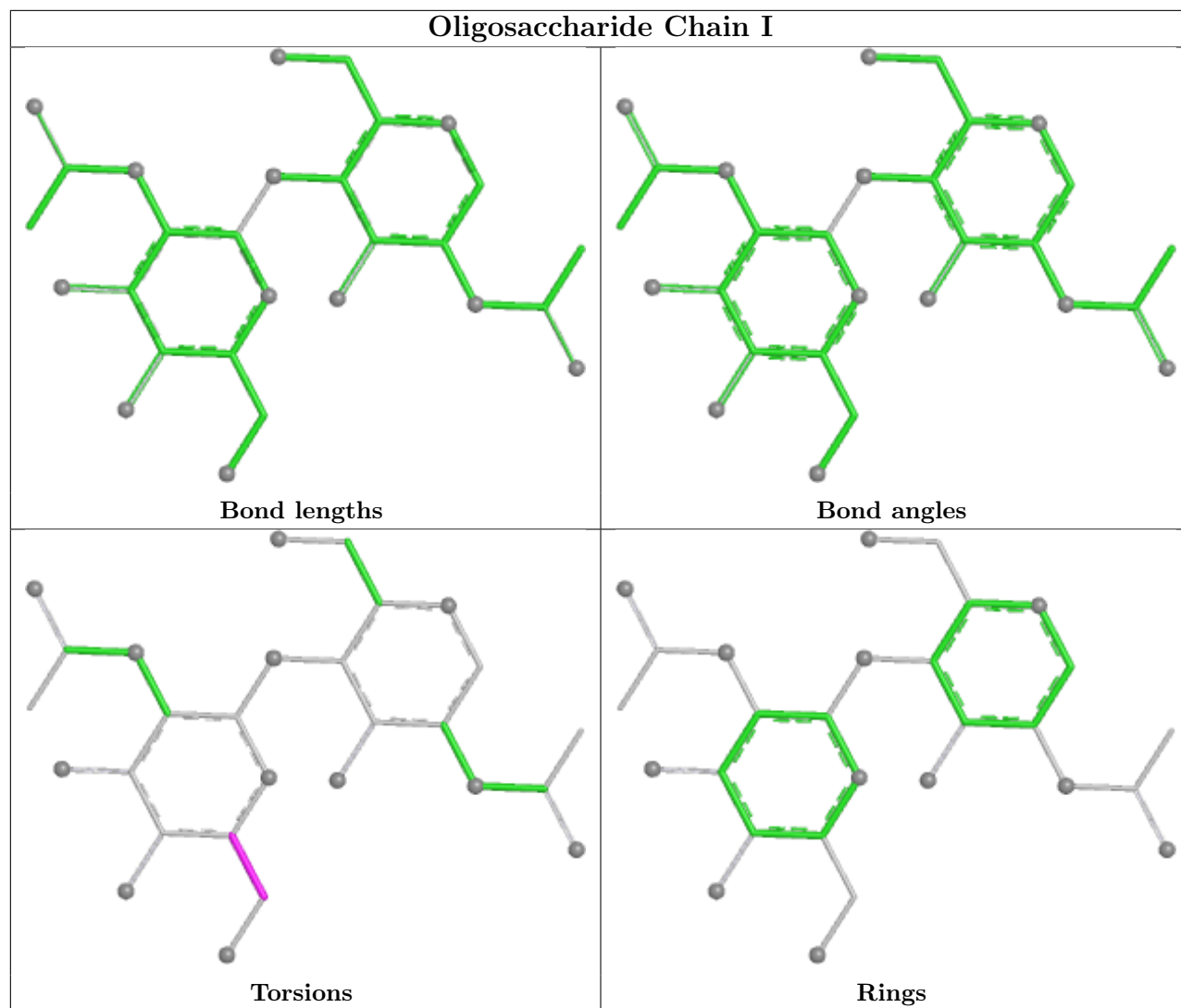
Mol	Chain	Res	Type	Atoms
6	J	1	NAG	O5-C5-C6-O6
6	J	1	NAG	C4-C5-C6-O6
6	I	2	NAG	O5-C5-C6-O6
6	J	2	NAG	O5-C5-C6-O6
6	J	1	NAG	C8-C7-N2-C2
6	J	1	NAG	O7-C7-N2-C2
6	I	2	NAG	C4-C5-C6-O6
6	J	2	NAG	C4-C5-C6-O6
6	J	2	NAG	C1-C2-N2-C7
6	J	2	NAG	C3-C2-N2-C7

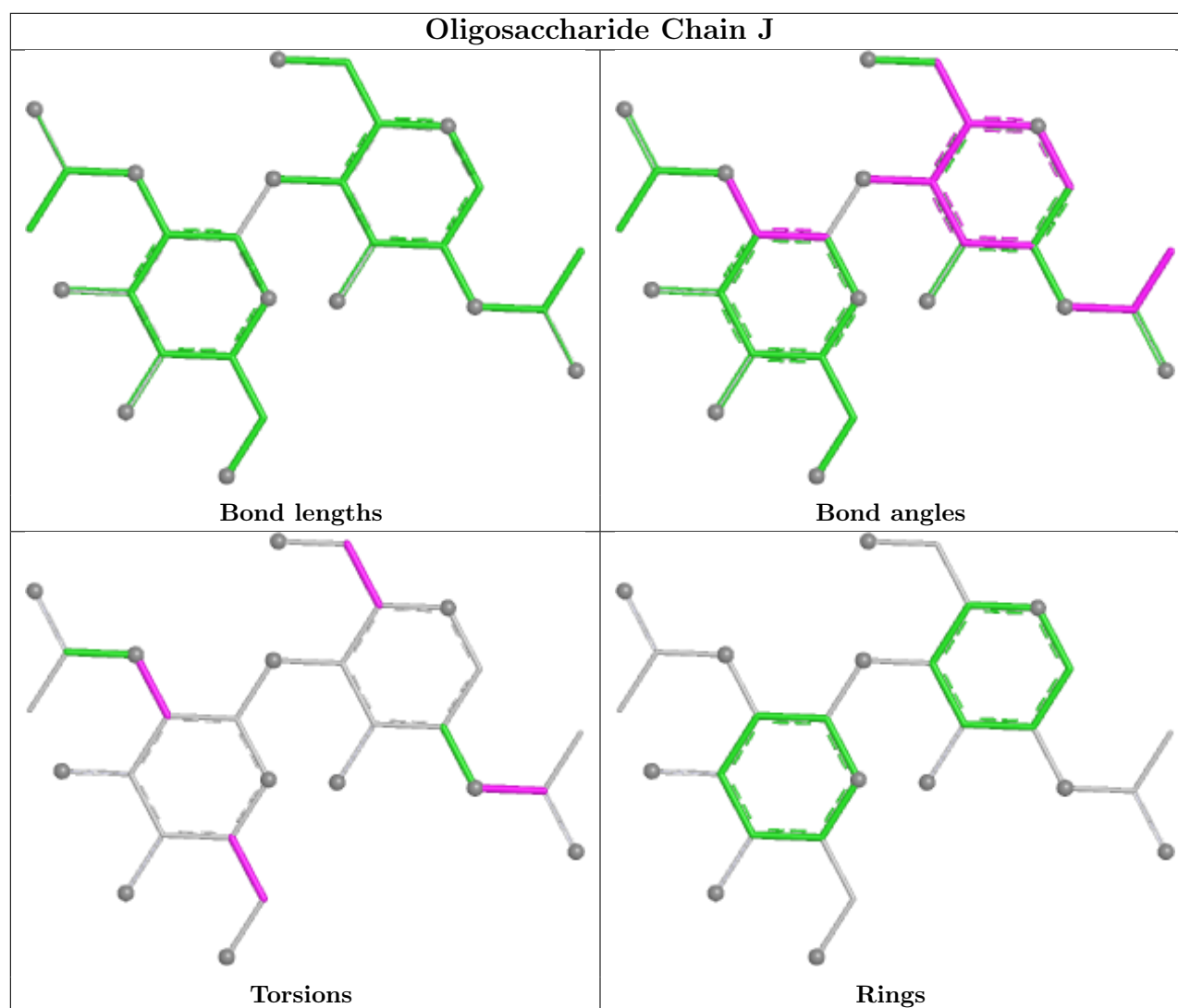
There are no ring outliers.

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	J	1	NAG	1	0
6	J	2	NAG	1	0

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





5.6 Ligand geometry [i](#)

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	$\# Z > 2$
7	NAG	E	1168	1	14,14,15	0.48	0	17,19,21	1.19	2 (11%)

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

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	E	1168	1	-	4/6/23/26	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(°)
7	E	1168	NAG	C1-O5-C5	2.44	115.45	112.19
7	E	1168	NAG	C8-C7-N2	2.24	119.83	116.12

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	E	1168	NAG	C8-C7-N2-C2
7	E	1168	NAG	O7-C7-N2-C2
7	E	1168	NAG	C4-C5-C6-O6
7	E	1168	NAG	O5-C5-C6-O6

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	323/328 (98%)	0.61	25 (7%)	19	16	35, 54, 108, 178	0
1	E	323/328 (98%)	0.69	18 (5%)	30	23	31, 61, 84, 127	0
2	B	166/166 (100%)	1.34	36 (21%)	2	2	38, 81, 125, 159	0
3	C	226/230 (98%)	0.30	6 (2%)	56	47	33, 44, 67, 90	0
3	G	226/230 (98%)	0.78	18 (7%)	18	15	47, 64, 102, 126	0
4	D	218/219 (99%)	0.32	3 (1%)	73	65	29, 47, 59, 84	0
4	H	218/219 (99%)	0.85	18 (8%)	17	14	47, 68, 92, 111	0
5	F	166/166 (100%)	0.60	16 (9%)	13	11	30, 49, 102, 150	0
All	All	1866/1886 (98%)	0.66	140 (7%)	20	16	29, 57, 102, 178	0

All (140) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	6	ILE	7.1
2	B	8	GLY	7.0
3	G	142	SER	5.9
1	E	219	VAL	5.8
1	E	221	GLY	5.6
5	F	10	ILE	5.5
5	F	163	SER	5.5
5	F	8	GLY	5.3
3	C	142	SER	5.2
5	F	6	ILE	5.1
1	E	321	PRO	5.1
2	B	9	PHE	5.0
1	A	220	LYS	4.9
3	G	226	LYS	4.8
2	B	3	PHE	4.6
4	H	35	TYR	4.6

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Mol	Chain	Res	Type	RSRZ
2	B	99	LEU	4.5
1	A	222	LEU	4.3
1	E	215	THR	4.2
2	B	163	SER	4.2
1	A	129	LEU	4.1
1	A	219	VAL	4.1
2	B	7	ALA	4.0
5	F	1	GLY	4.0
5	F	5	ALA	4.0
3	C	143	THR	4.0
2	B	104	ASN	4.0
5	F	9	PHE	3.9
1	E	222	LEU	3.8
2	B	2	LEU	3.8
1	A	213	ILE	3.8
5	F	7	ALA	3.8
2	B	62	GLN	3.7
5	F	3	PHE	3.7
3	G	143	THR	3.7
1	A	134	ALA	3.7
2	B	101	LEU	3.7
1	A	68	ASP	3.7
5	F	84	MET	3.7
5	F	4	GLY	3.7
5	F	92	TRP	3.6
2	B	5	ALA	3.6
1	A	127	ALA	3.6
3	G	136	LEU	3.6
1	A	221	GLY	3.5
1	A	321	PRO	3.5
3	G	8	GLY	3.5
5	F	2	LEU	3.4
2	B	98	LEU	3.4
1	A	135	CYS	3.4
3	C	145	GLY	3.3
3	G	144	SER	3.3
5	F	80	LEU	3.2
1	E	154	ASP	3.2
2	B	4	GLY	3.2
1	E	217	SER	3.2
1	A	195	THR	3.1
1	E	223	SER	3.1

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Mol	Chain	Res	Type	RSRZ
2	B	102	MET	3.1
1	A	128	SER	3.1
3	G	148	ALA	3.1
3	C	226	LYS	3.1
2	B	108	LEU	2.9
1	E	71	ILE	2.9
3	G	145	GLY	2.9
1	E	218	LYS	2.9
2	B	131	LYS	2.9
1	E	68	ASP	2.8
3	G	207	ILE	2.8
2	B	134	GLY	2.8
3	G	197	PRO	2.7
2	B	10	ILE	2.7
4	H	123	PHE	2.7
4	D	16	GLY	2.7
1	A	308	SER	2.7
2	B	1	GLY	2.7
2	B	100	VAL	2.7
2	B	92	TRP	2.6
4	H	196	VAL	2.6
3	G	201	LEU	2.6
3	C	140	SER	2.6
2	B	166	ALA	2.5
2	B	82	LYS	2.5
4	H	32	GLY	2.5
4	H	217	GLY	2.5
2	B	115	VAL	2.4
1	A	217	SER	2.4
2	B	113	SER	2.4
4	H	168	VAL	2.4
3	C	144	SER	2.4
1	A	130	GLY	2.4
1	E	224	GLY	2.4
2	B	116	LYS	2.4
4	H	61	SER	2.4
1	A	91	TYR	2.3
1	A	131	VAL	2.3
4	H	54	TYR	2.3
4	H	83	VAL	2.3
1	A	133	SER	2.3
4	H	195	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
4	D	82	ARG	2.3
2	B	138	PHE	2.3
3	G	218	LYS	2.3
1	A	320	SER	2.3
4	H	68	SER	2.3
4	H	120	VAL	2.3
5	F	166	ALA	2.2
1	E	135	CYS	2.2
3	G	139	SER	2.2
2	B	61	THR	2.2
3	G	106	SER	2.2
5	F	85	GLU	2.2
1	A	90	CYS	2.2
4	H	214	PHE	2.2
2	B	11	GLU	2.2
3	G	149	ALA	2.2
2	B	107	THR	2.2
2	B	156	THR	2.2
1	A	209	LEU	2.2
1	E	77	SER	2.2
4	H	140	LEU	2.2
1	A	71	ILE	2.1
1	E	193	ASN	2.1
3	G	223	VAL	2.1
2	B	81	ASN	2.1
4	H	209	PRO	2.1
3	G	205	THR	2.1
1	A	159	THR	2.1
1	E	216	ARG	2.1
2	B	106	ARG	2.1
2	B	141	TYR	2.1
4	D	110	GLU	2.1
3	G	168	SER	2.1
2	B	140	PHE	2.1
1	E	120	SER	2.0
4	H	138	VAL	2.0
1	E	297	LEU	2.0
1	A	214	ALA	2.0
4	H	215	ASN	2.0
4	H	131	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

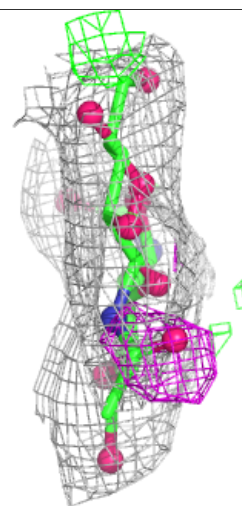
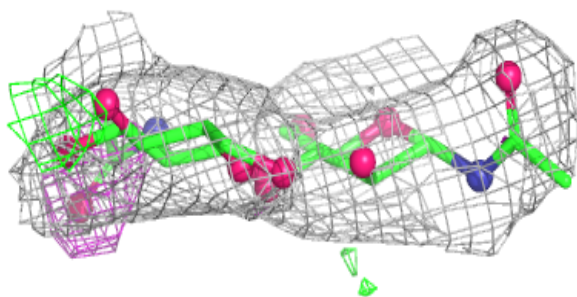
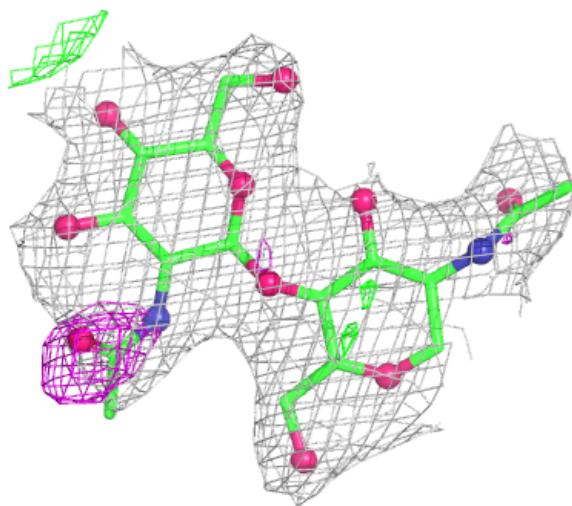
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

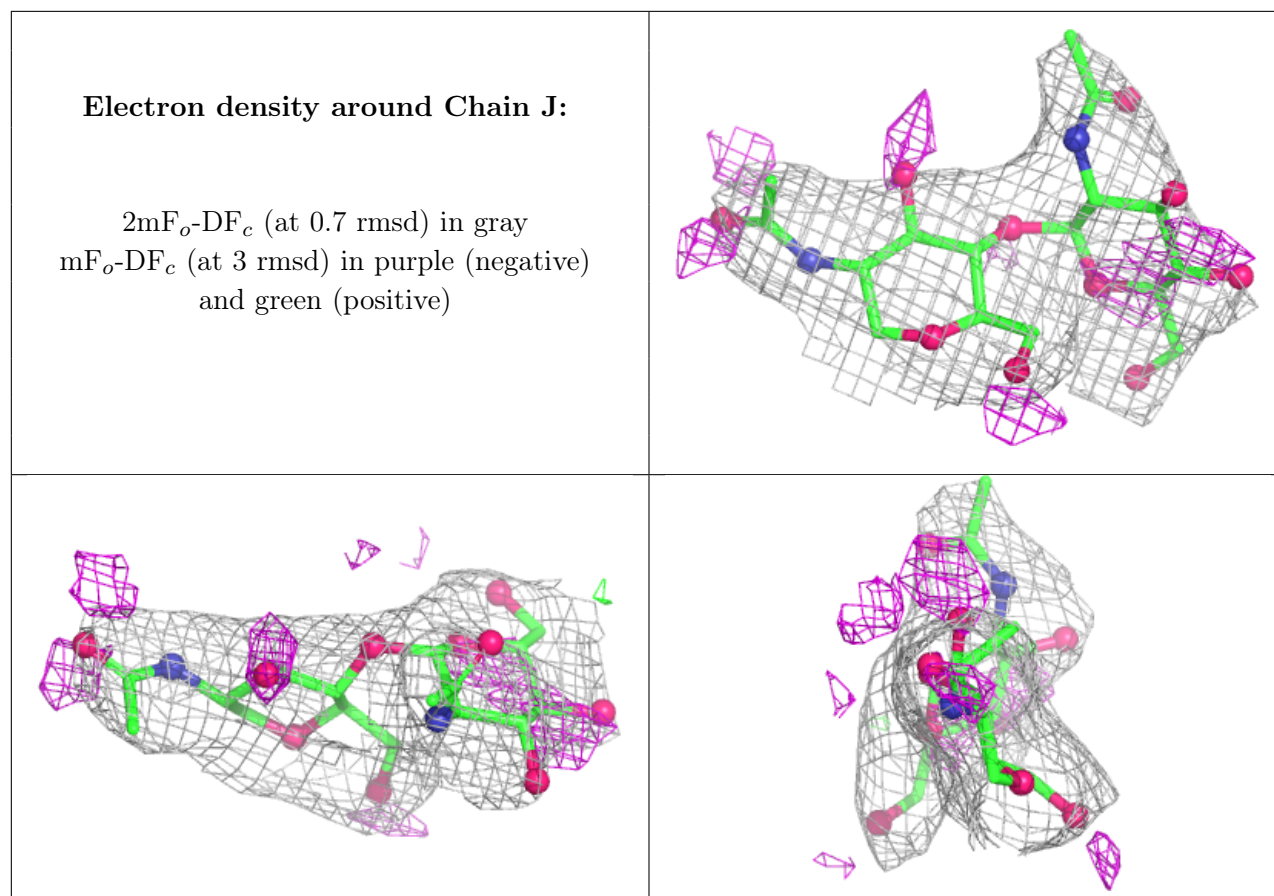
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	NAG	J	2	14/15	0.71	0.15	56,58,59,60	0
6	NAG	J	1	14/15	0.81	0.12	42,45,48,52	0
6	NAG	I	1	14/15	0.82	0.11	40,45,46,48	0
6	NAG	I	2	14/15	0.86	0.12	51,52,55,56	0

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 I:

$2mF_o-DF_c$ (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($\text{\AA}^2$)	Q<0.9
7	NAG	E	1168	14/15	0.83	0.18	31,33,34,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.