



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 12:32 PM UTC

PDB ID : 6S2I / pdb_00006s2i
Title : Anti-tumor antibody 14F7-derived scFv in complex with NeuGc Gm3
Authors : Bjerregaard-Andersen, K.; Heggelund, J.E.; Krengel, U.
Deposited on : 2019-06-20
Resolution : 2.29 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

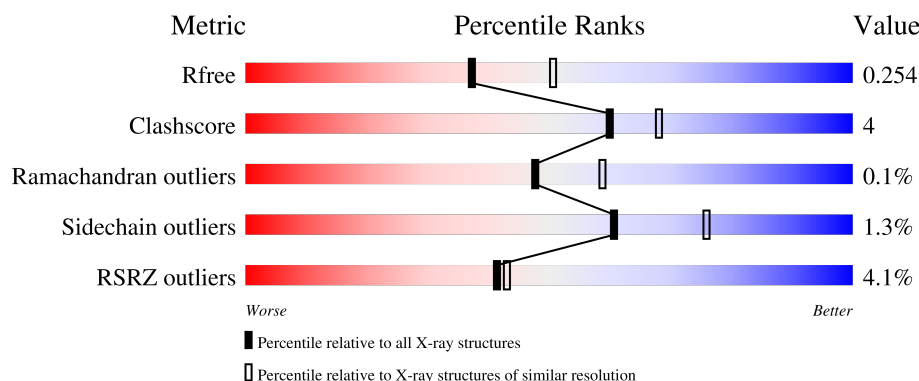
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.29 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	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (2.30-2.26)

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	253	44% 6% 51%
1	B	253	37% 5% 58%
1	C	253	40% 9% 51%
1	D	253	38% 5% 57%
1	E	253	41% 7% 52%

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Mol	Chain	Length	Quality of chain
1	F	253	40% 57%
1	G	253	8% 42% 6% 52%
1	H	253	% 36% 7% 57%
2	J	3	100%

2 Entry composition [i](#)

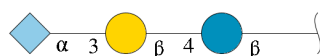
There are 3 unique types of molecules in this entry. The entry contains 7397 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 scFv C1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	125	Total	C	N	O	S	0	0	0
			1000	632	169	193	6			
1	B	106	Total	C	N	O	S	0	1	0
			817	509	136	169	3			
1	C	125	Total	C	N	O	S	0	1	0
			1003	634	169	194	6			
1	D	108	Total	C	N	O	S	0	0	0
			831	518	139	171	3			
1	E	121	Total	C	N	O	S	0	0	0
			966	612	159	189	6			
1	F	108	Total	C	N	O	S	0	0	0
			831	518	139	171	3			
1	G	121	Total	C	N	O	S	0	1	0
			971	615	160	190	6			
1	H	108	Total	C	N	O	S	0	0	0
			830	518	139	170	3			

- Molecule 2 is an oligosaccharide called N-glycolyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	J	3	Total	C	N	O	0	0	0
			44	23	1	20			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	27	Total 27	O 27	0	0
3	B	13	Total 13	O 13	0	0
3	C	22	Total 22	O 22	0	0
3	D	8	Total 8	O 8	0	0
3	E	11	Total 11	O 11	0	0
3	F	13	Total 13	O 13	0	0
3	G	2	Total 2	O 2	0	0
3	H	8	Total 8	O 8	0	0

- Molecule 1: scFv C1



Chain H:

Amino Acid	Percentage (%)
GLN	36%
VAL	36%
GLN	36%
LEU	36%
GLN	36%
GLY	36%
ALA	36%
LEU	36%
ALA	36%
LYS	36%
PRO	36%
GLY	36%
ALA	36%
SER	36%
MET	36%
LYS	36%
MET	36%
SER	36%
CYS	36%
ARG	36%
ALA	36%
SER	36%
GLY	36%
TYR	36%
PHE	36%
THR	36%
SER	36%
TRP	36%
ILE	36%
HIS	36%
TRP	36%
GLN	36%
LYS	36%
LEU	36%
ARG	36%
PRO	36%
ASP	36%
GLN	36%
GLY	36%
LEU	36%
GLY	36%
TRP	36%
ILE	36%
GLY	36%
TYR	36%
ILE	36%
ASP	36%
PRO	36%
ALA	36%
THR	36%
ALA	36%
TYR	36%
GLY	36%
THR	36%
GLI	36%
SER	36%

Amino Acid	Count
ASN	1
GLN	1
LYS	1
PHE	1
LYS	1
ASP	1
LYS	1
ALA	1
ILE	1
LEU	1
THR	1
ALA	1
ASP	1
ARG	1
LYS	1
SER	1
SER	1
ASN	1
THR	1
ALA	1
PHE	1
MET	1
TYR	1
LEU	1
ASN	1
SER	1
LEU	1
THR	1
SER	1
GLI	1
ASP	1
ALA	1
TYR	1
VAL	1
TYR	1
CYS	1
ALA	1
GLU	1
ARG	1
GLY	1
SER	1
PRO	1
ARG	1
LEU	1
ARG	1
GLY	1
ILE	1
TYR	1
TYR	1
ALA	1
MET	1
ASP	1
TYR	1
THR	1
GLY	1
GLN	1
TYR	1
THR	1

Residue	Count
VAL	1
THR	1
VAL	1
SER	1
SER	1
LYS	1
LEU	1
SER	1
GLY	1
SER	1
ALA	1
SER	1
ALA	1
PRO	1
LYS	1
LEU	1
GLU	1
GLU	1
GLY	1
PHE	1
SER	1
SER	1
GLU	1
ALA	1
ARG	1
V0	1
D1	1
I2	1
Q3	1
Q6	1
G16	1
S26	1
L33	1
Q37	1
Q38	1
K39	1
F40	1
D41	1
L47	1
I48	1
Y49	1
R53	1
N77	1
Y86	1
Q89	1
P96	1
T97	1
F98	1

Chain J: 100%

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	62.88Å 113.69Å 66.95Å 90.00° 91.24° 90.00°	Depositor
Resolution (Å)	62.87 – 2.29 62.87 – 2.29	Depositor EDS
% Data completeness (in resolution range)	98.7 (62.87-2.29) 98.8 (62.87-2.29)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.44 (at 2.29Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.222 , 0.255 0.223 , 0.254	Depositor DCC
R_{free} test set	2152 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	36.5	Xtriage
Anisotropy	0.388	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 36.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7397	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.91% 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: NGC, BGC, GAL

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	0.10	0/1026	0.32	0/1390
1	B	0.12	0/836	0.32	0/1136
1	C	0.10	0/1032	0.31	0/1398
1	D	0.09	0/847	0.31	0/1149
1	E	0.13	0/991	0.35	0/1343
1	F	0.10	0/847	0.33	0/1149
1	G	0.15	0/999	0.36	0/1354
1	H	0.09	0/846	0.33	0/1149
All	All	0.11	0/7424	0.33	0/10068

There are no bond length outliers.

There are no bond angle outliers.

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	1000	0	953	8	0
1	B	817	0	791	8	0
1	C	1003	0	958	14	0
1	D	831	0	808	9	0
1	E	966	0	912	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	831	0	808	4	0
1	G	971	0	918	6	0
1	H	830	0	808	9	0
2	J	44	0	28	0	0
3	A	27	0	0	0	0
3	B	13	0	0	0	0
3	C	22	0	0	2	0
3	D	8	0	0	0	0
3	E	11	0	0	0	0
3	F	13	0	0	0	0
3	G	2	0	0	0	0
3	H	8	0	0	0	0
All	All	7397	0	6984	61	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 4.

The worst 5 of 61 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:B:37:GLN:HB2	1:B:47:LEU:HD11	1.79	0.64
1:A:89:VAL:HG22	1:A:108:THR:HG22	1.82	0.61
1:F:37:GLN:HB2	1:F:47:LEU:HD11	1.83	0.60
1:C:38:LYS:HB2	1:C:48:ILE:HD11	1.86	0.58
1:D:21:ILE:HD11	1:D:73:LEU:HD23	1.86	0.57

There are no symmetry-related clashes.

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	123/253 (49%)	123 (100%)	0	0	100	100
1	B	105/253 (42%)	100 (95%)	5 (5%)	0	100	100
1	C	124/253 (49%)	123 (99%)	1 (1%)	0	100	100
1	D	106/253 (42%)	103 (97%)	3 (3%)	0	100	100
1	E	117/253 (46%)	113 (97%)	4 (3%)	0	100	100
1	F	106/253 (42%)	101 (95%)	5 (5%)	0	100	100
1	G	118/253 (47%)	112 (95%)	5 (4%)	1 (1%)	16	18
1	H	106/253 (42%)	102 (96%)	4 (4%)	0	100	100
All	All	905/2024 (45%)	877 (97%)	27 (3%)	1 (0%)	48	59

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	41	PRO

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	105/215 (49%)	105 (100%)	0	100	100
1	B	94/215 (44%)	94 (100%)	0	100	100
1	C	106/215 (49%)	102 (96%)	4 (4%)	29	42
1	D	95/215 (44%)	95 (100%)	0	100	100
1	E	102/215 (47%)	101 (99%)	1 (1%)	68	81
1	F	95/215 (44%)	94 (99%)	1 (1%)	65	79
1	G	103/215 (48%)	100 (97%)	3 (3%)	37	52
1	H	95/215 (44%)	94 (99%)	1 (1%)	65	79
All	All	795/1720 (46%)	785 (99%)	10 (1%)	61	76

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	57	THR
1	G	111	VAL
1	H	33	LEU
1	C	73	ARG
1	E	43	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	31	ASN
1	C	5	GLN
1	C	76	ASN
1	H	92	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

3 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
2	BGC	J	1	2	12,12,12	1.25	1 (8%)	17,17,17	1.09	1 (5%)
2	GAL	J	2	2	11,11,12	1.58	3 (27%)	15,15,17	1.76	3 (20%)
2	NGC	J	3	2	21,21,22	2.74	6 (28%)	22,29,32	1.76	5 (22%)

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
2	BGC	J	1	2	-	2/2/22/22	0/1/1/1
2	GAL	J	2	2	-	1/2/19/22	0/1/1/1
2	NGC	J	3	2	-	4/20/36/40	0/1/1/1

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	3	NGC	C2-C1	9.36	1.63	1.52
2	J	3	NGC	C7-C6	4.61	1.58	1.52
2	J	3	NGC	C8-C7	2.72	1.58	1.53
2	J	1	BGC	C4-C5	2.44	1.58	1.53
2	J	3	NGC	C3-C2	2.42	1.56	1.52

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	2	GAL	C1-O5-C5	4.48	118.19	112.19
2	J	3	NGC	O11-C11-C10	-4.41	105.00	113.95
2	J	3	NGC	O6-C2-C1	3.27	113.89	107.72
2	J	3	NGC	O1A-C1-C2	-3.06	116.25	122.85
2	J	3	NGC	O10-C10-C11	-2.52	117.99	119.62

There are no chirality outliers.

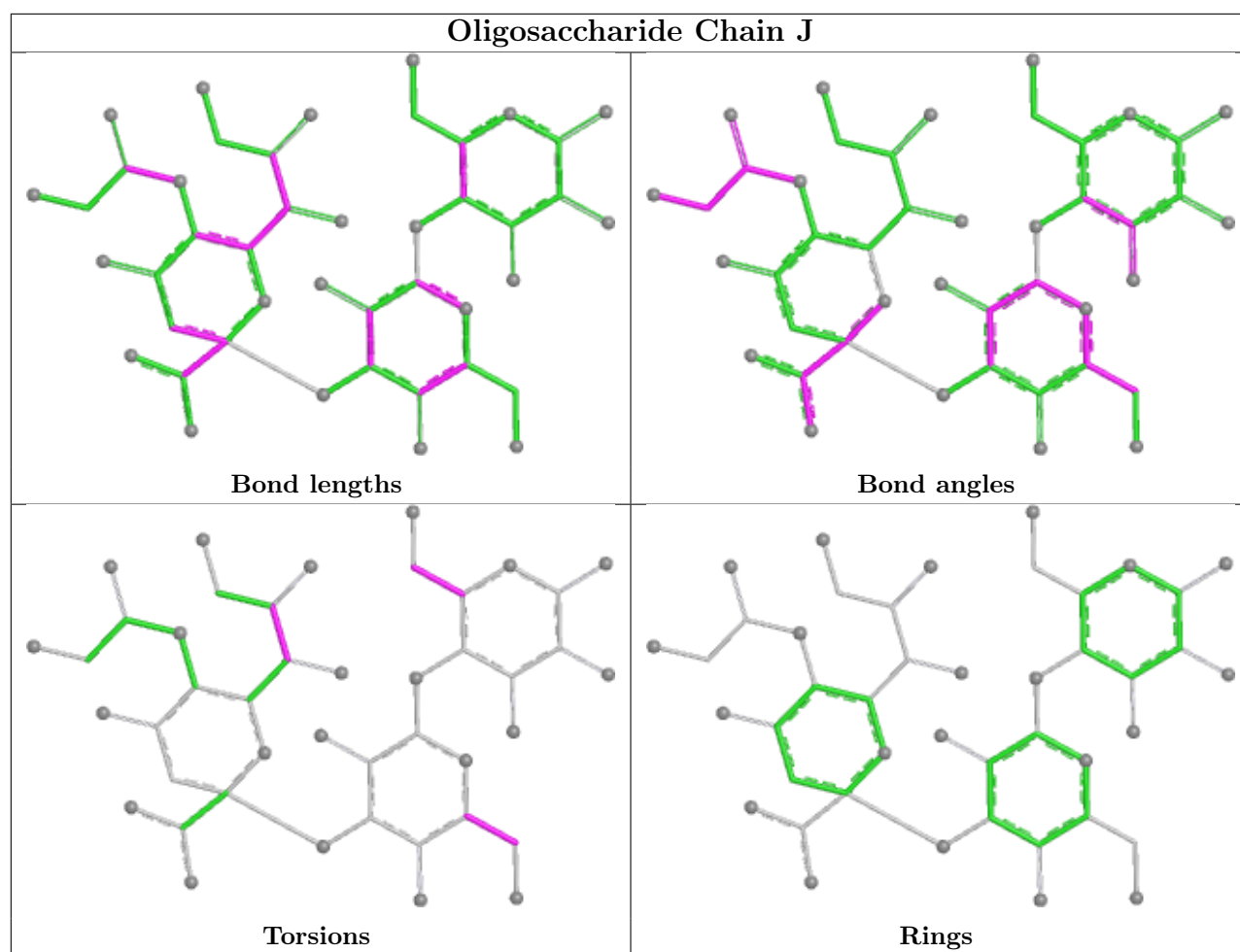
5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	J	1	BGC	C4-C5-C6-O6
2	J	1	BGC	O5-C5-C6-O6
2	J	3	NGC	O7-C7-C8-C9
2	J	3	NGC	C6-C7-C8-C9
2	J	3	NGC	C6-C7-C8-O8

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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	125/253 (49%)	0.59	3 (2%) 59 61	35, 45, 67, 88	0
1	B	106/253 (41%)	0.50	2 (1%) 66 68	32, 46, 57, 63	1 (0%)
1	C	125/253 (49%)	0.42	2 (1%) 70 72	32, 46, 63, 77	1 (0%)
1	D	108/253 (42%)	0.53	3 (2%) 55 56	37, 46, 56, 75	0
1	E	121/253 (47%)	0.63	6 (4%) 34 35	36, 47, 67, 84	0
1	F	108/253 (42%)	0.46	1 (0%) 81 82	37, 46, 60, 71	0
1	G	121/253 (47%)	1.24	19 (15%) 5 5	33, 64, 88, 100	1 (0%)
1	H	108/253 (42%)	0.70	2 (1%) 66 68	41, 54, 71, 83	0
All	All	922/2024 (45%)	0.64	38 (4%) 41 43	32, 49, 72, 100	3 (0%)

The worst 5 of 38 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	99	LEU	4.0
1	G	51	ILE	3.3
1	D	0	VAL	3.3
1	H	0	VAL	3.2
1	E	113	SER	2.8

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

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

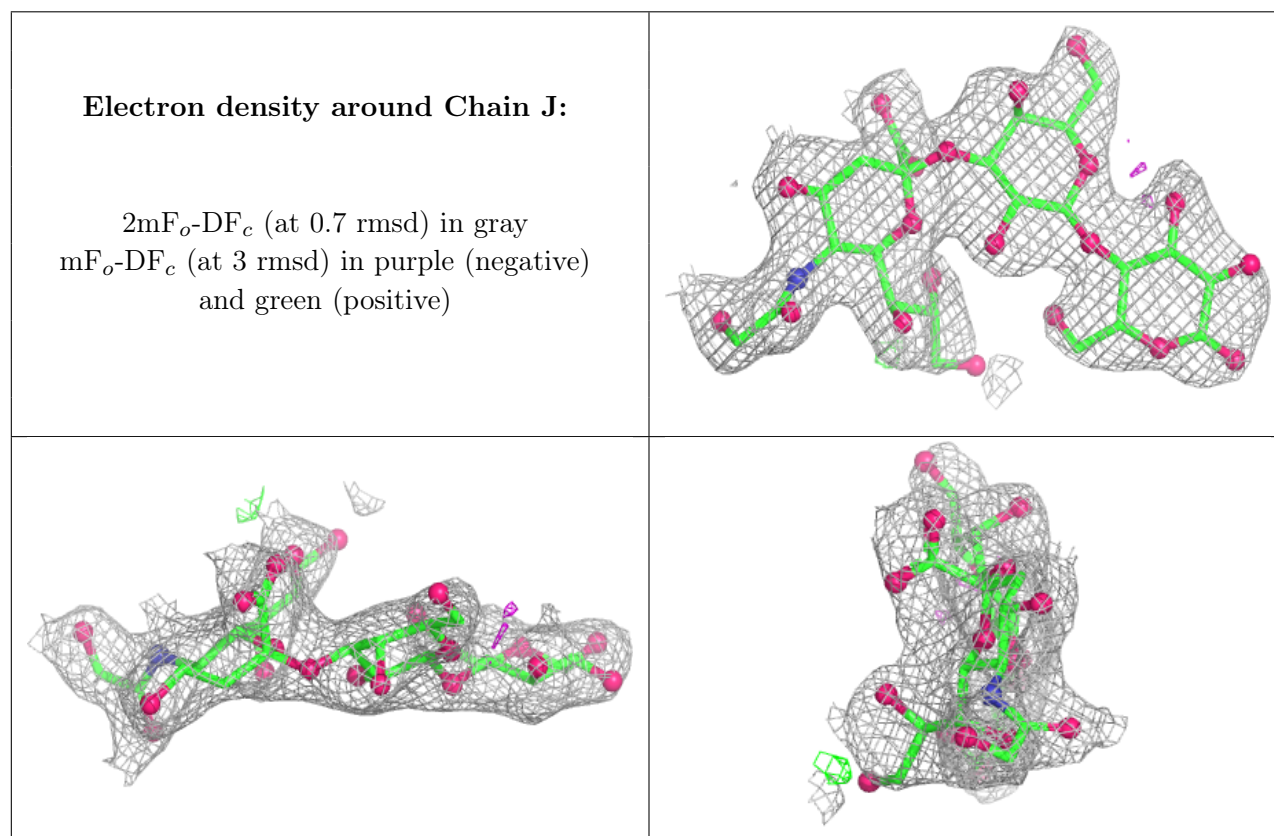
6.3 Carbohydrates [i](#)

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
2	BGC	J	1	12/12	-	-	46,53,56,59	12
2	GAL	J	2	11/12	-	-	44,50,54,56	11
2	NGC	J	3	21/22	-	-	44,52,57,67	21

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.



6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.