



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 02:22 AM UTC

PDB ID : 7ZWF / pdb_00007zwf
Title : Pfs48/45 bound to scFv fragment of monoclonal antibody 32F3
Authors : Ko, K.T.; Lennartz, F.L.; Higgins, M.K.
Deposited on : 2022-05-19
Resolution : 2.13 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

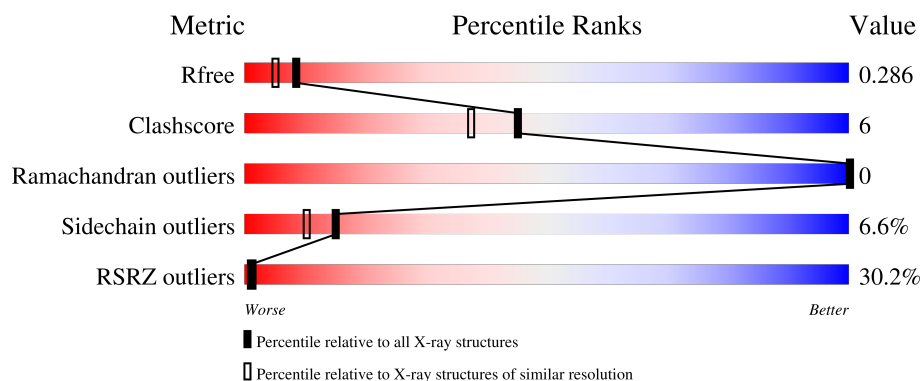
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.13 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	3689 (2.16-2.12)
Clashscore	190562	3812 (2.16-2.12)
Ramachandran outliers	187476	3773 (2.16-2.12)
Sidechain outliers	187428	3772 (2.16-2.12)
RSRZ outliers	180081	3691 (2.16-2.12)

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	428	28% 45% 13% • 40%
2	B	283	11% 77% 6% • 16%
3	C	2	100%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3983 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 Gametocyte surface protein P45/48.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	258	Total	C	N	O	S	0	0	0
			2074	1335	328	399	12			

- Molecule 2 is a protein called 32F3scFv.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	239	Total	C	N	O	S	0	0	0
			1791	1122	304	358	7			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	2	Total	C	N	O	0	0	0
			24	14	1	9			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	41	Total	O	0	0
			41	41		
4	B	53	Total	O	0	0
			53	53		

HIS

- Molecule 3: α -L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:

100%

MOL
FUC2

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	81.83Å 126.11Å 146.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.91 – 2.13 40.91 – 2.13	Depositor EDS
% Data completeness (in resolution range)	95.6 (40.91-2.13) 95.6 (40.91-2.13)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 2.14Å)	Xtriage
Refinement program	BUSTER 2.10.4 (20-OCT-2021)	Depositor
R, R_{free}	0.276 , 0.286 (Not available) , 0.286	Depositor DCC
R_{free} test set	1964 reflections (4.60%)	wwPDB-VP
Wilson B-factor (Å ²)	57.2	Xtriage
Anisotropy	0.458	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 76.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3983	wwPDB-VP
Average B, all atoms (Å ²)	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.96% 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: FUC, 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	0.74	0/2117	0.97	0/2860
2	B	0.80	2/1831 (0.1%)	1.04	4/2480 (0.2%)
All	All	0.77	2/3948 (0.1%)	1.00	4/5340 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	200	ILE	CA-C	5.56	1.59	1.52
2	B	195	SER	CA-C	5.12	1.58	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	137	PHE	CA-CB-CG	7.20	121.00	113.80
2	B	59	THR	CA-C-N	6.27	128.98	120.38
2	B	59	THR	C-N-CA	6.27	128.98	120.38
2	B	58	PHE	CA-CB-CG	5.44	119.24	113.80

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	2074	0	2040	38	0
2	B	1791	0	1728	9	0
3	C	24	0	22	0	0
4	A	41	0	0	2	0
4	B	53	0	0	0	0
All	All	3983	0	3790	45	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 6.

All (45) 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:A:242:ALA:HB1	1:A:269:VAL:HA	1.36	1.07
1:A:250:ILE:HB	1:A:257:ILE:HB	1.56	0.85
2:B:50:LYS:HE2	2:B:111:ASN:HB3	1.72	0.71
1:A:343:ASN:HD21	1:A:391:ASP:HB3	1.55	0.70
1:A:328:ASN:HB2	4:A:522:HOH:O	1.92	0.69
1:A:250:ILE:CG2	1:A:252:HIS:HD2	2.07	0.68
1:A:71:CYS:HB2	1:A:175:VAL:HG13	1.79	0.64
2:B:73:GLU:HG2	2:B:161:GLY:H	1.66	0.61
1:A:228:GLU:HA	1:A:254:ASN:HB3	1.83	0.60
1:A:385:GLU:HG2	1:A:394:LYS:HD3	1.84	0.59
2:B:135:LEU:HD22	2:B:217:ALA:HB2	1.86	0.58
2:B:114:MET:HB3	2:B:117:LEU:HD21	1.86	0.57
1:A:351:ASP:H	1:A:355:GLN:HE21	1.54	0.55
1:A:239:LYS:HB2	1:A:272:GLU:HB2	1.87	0.55
1:A:78:ILE:HG12	1:A:146:PRO:HG3	1.89	0.55
1:A:369:ILE:HD12	2:B:199:TYR:HB3	1.87	0.55
1:A:239:LYS:HE2	1:A:272:GLU:HG3	1.88	0.55
2:B:201:HIS:CE1	2:B:217:ALA:H	2.26	0.54
1:A:73:ILE:HB	1:A:177:VAL:HG13	1.89	0.54
1:A:217:LEU:HD23	1:A:221:GLU:HB3	1.89	0.54
1:A:229:LEU:HB3	1:A:276:LYS:HB2	1.89	0.53
1:A:250:ILE:CG2	1:A:252:HIS:CD2	2.90	0.51
1:A:336:TYR:HD1	1:A:338:HIS:CD2	2.30	0.49
2:B:53:CYS:HB3	2:B:110:LEU:HB3	1.94	0.49
1:A:242:ALA:CB	1:A:269:VAL:HA	2.25	0.49
1:A:77:PHE:HB3	1:A:144:ILE:HB	1.94	0.48
1:A:376:ILE:HD13	1:A:406:THR:HG21	1.95	0.48
1:A:250:ILE:HG22	1:A:252:HIS:HD2	1.75	0.48
1:A:250:ILE:O	1:A:256:THR:HA	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:PHE:CZ	1:A:399:VAL:HG21	2.50	0.46
1:A:331:LEU:HD23	1:A:338:HIS:HD2	1.81	0.46
1:A:319:VAL:O	1:A:417:LYS:HD2	2.16	0.46
1:A:319:VAL:HG22	1:A:417:LYS:HB3	1.97	0.46
1:A:364:LEU:HD23	2:B:90:TYR:HB3	1.98	0.44
1:A:250:ILE:HG23	1:A:252:HIS:CD2	2.52	0.43
1:A:264:VAL:HG21	1:A:269:VAL:HG11	2.00	0.43
1:A:186:ILE:HG23	1:A:222:LEU:HD23	2.00	0.43
1:A:352:CYS:HA	1:A:353:PHE:HA	1.84	0.43
2:B:73:GLU:HG2	2:B:161:GLY:N	2.34	0.43
1:A:331:LEU:HB3	1:A:336:TYR:CE1	2.54	0.42
1:A:249:ILE:HG23	1:A:249:ILE:O	2.20	0.41
1:A:297:GLY:HA2	1:A:329:VAL:HG21	2.02	0.41
1:A:228:GLU:HA	1:A:254:ASN:CB	2.50	0.41
1:A:392:LYS:NZ	4:A:503:HOH:O	2.53	0.41
1:A:331:LEU:HD23	1:A:338:HIS:CD2	2.56	0.40

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	248/428 (58%)	225 (91%)	23 (9%)	0	100	100
2	B	235/283 (83%)	223 (95%)	12 (5%)	0	100	100
All	All	483/711 (68%)	448 (93%)	35 (7%)	0	100	100

There are no Ramachandran outliers to report.

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	243/402 (60%)	220 (90%)	23 (10%)	8	4
2	B	194/230 (84%)	188 (97%)	6 (3%)	35	35
All	All	437/632 (69%)	408 (93%)	29 (7%)	15	10

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	TYR
1	A	216	GLU
1	A	217	LEU
1	A	221	GLU
1	A	229	LEU
1	A	234	CYS
1	A	240	GLU
1	A	254	ASN
1	A	259	LYS
1	A	263	TYR
1	A	267	LYS
1	A	269	VAL
1	A	270	ASN
1	A	280	ASN
1	A	286	LEU
1	A	291	GLU
1	A	319	VAL
1	A	342	LEU
1	A	364	LEU
1	A	395	LEU
1	A	398	ILE
1	A	404	LYS
1	A	417	LYS
2	B	30	THR
2	B	45	LEU
2	B	50	LYS
2	B	52	SER

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Mol	Chain	Res	Type
2	B	73	GLU
2	B	135	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	HIS
1	A	252	HIS
1	A	280	ASN
1	A	296	HIS
1	A	343	ASN
1	A	355	GLN
2	B	70	GLN
2	B	111	ASN
2	B	143	GLN
2	B	169	GLN
2	B	205	GLN

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 ⓘ

2 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	1,3	14,14,15	0.27	0	17,19,21	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	FUC	C	2	3	10,10,11	0.35	0	14,14,16	0.59	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
3	NAG	C	1	1,3	-	0/6/23/26	0/1/1/1
3	FUC	C	2	3	-	-	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

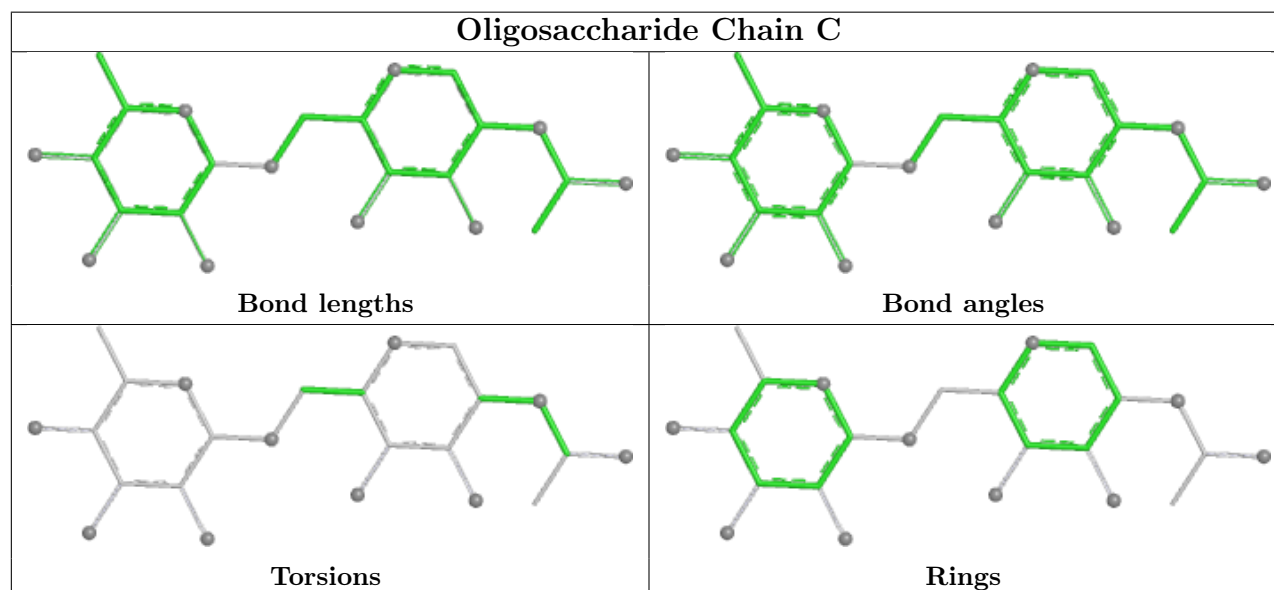
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 ⓘ

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

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	258/428 (60%)	2.19	120 (46%) 0 1	67, 109, 171, 210	0
2	B	239/283 (84%)	1.02	30 (12%) 8 9	51, 83, 116, 129	0
All	All	497/711 (69%)	1.62	150 (30%) 1 1	51, 92, 156, 210	0

All (150) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	398	ILE	8.6
1	A	230	ILE	8.5
1	A	180	LEU	7.0
1	A	82	ILE	6.6
1	A	182	TYR	6.4
1	A	243	LEU	5.8
1	A	191	LEU	5.8
1	A	249	ILE	5.7
1	A	208	PHE	5.5
2	B	162	GLY	5.5
1	A	223	PHE	5.5
1	A	146	PRO	5.5
1	A	77	PHE	5.5
1	A	177	VAL	5.1
1	A	179	VAL	5.1
1	A	215	VAL	5.1
1	A	252	HIS	5.1
1	A	76	TYR	5.1
1	A	186	ILE	5.1
1	A	181	LYS	4.9
1	A	184	HIS	4.9
1	A	378	ILE	4.9
1	A	263	TYR	4.9
1	A	209	VAL	4.9

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Mol	Chain	Res	Type	RSRZ
1	A	277	PHE	4.9
2	B	30	THR	4.7
2	B	45	LEU	4.5
1	A	187	LEU	4.4
1	A	213	LEU	4.3
1	A	72	THR	4.2
1	A	227	CYS	4.1
1	A	142	ILE	4.1
1	A	231	ASN	4.1
1	A	144	ILE	4.1
2	B	208	GLY	4.0
1	A	78	ILE	4.0
1	A	185	ASN	4.0
1	A	217	LEU	4.0
1	A	141	THR	4.0
1	A	73	ILE	4.0
1	A	222	LEU	3.9
1	A	255	LEU	3.9
1	A	282	TYR	3.9
1	A	235	PHE	3.8
1	A	334	PRO	3.8
2	B	274	LYS	3.7
1	A	286	LEU	3.6
2	B	273	LEU	3.6
1	A	79	TYR	3.6
1	A	232	LYS	3.5
1	A	399	VAL	3.5
1	A	143	THR	3.5
1	A	189	THR	3.5
1	A	238	GLY	3.5
1	A	175	VAL	3.5
1	A	212	VAL	3.5
1	A	259	LYS	3.5
1	A	226	ALA	3.4
1	A	145	SER	3.4
1	A	400	GLY	3.4
1	A	257	ILE	3.3
1	A	225	LEU	3.2
1	A	285	VAL	3.2
2	B	161	GLY	3.2
1	A	241	LYS	3.2
1	A	229	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	251	TYR	3.1
1	A	279	ASN	3.1
1	A	224	VAL	3.1
1	A	237	GLU	3.1
2	B	164	SER	3.1
1	A	381	ILE	3.0
1	A	126	TYR	3.0
1	A	292	LYS	3.0
2	B	41	GLY	3.0
2	B	182	SER	3.0
2	B	163	GLY	3.0
1	A	278	LYS	3.0
1	A	254	ASN	2.9
1	A	239	LYS	2.9
1	A	258	PHE	2.9
1	A	242	ALA	2.9
1	A	183	PRO	2.8
1	A	81	LYS	2.8
1	A	75	SER	2.8
1	A	301	SER	2.8
2	B	150	SER	2.8
1	A	264	VAL	2.8
1	A	250	ILE	2.8
1	A	74	HIS	2.8
1	A	234	CYS	2.8
1	A	262	PHE	2.8
2	B	117	LEU	2.8
1	A	248	LYS	2.8
1	A	339	LEU	2.7
1	A	271	THR	2.7
2	B	31	GLY	2.7
1	A	176	HIS	2.6
2	B	184	GLY	2.6
1	A	336	TYR	2.6
1	A	71	CYS	2.6
1	A	188	PHE	2.6
1	A	256	THR	2.6
2	B	43	VAL	2.5
1	A	284	ILE	2.5
1	A	354	PHE	2.5
2	B	160	GLY	2.5
1	A	290	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	265	PHE	2.5
1	A	380	ASP	2.4
2	B	33	VAL	2.4
2	B	157	SER	2.4
2	B	188	THR	2.4
1	A	276	LYS	2.4
1	A	331	LEU	2.4
2	B	124	LEU	2.3
1	A	384	TYR	2.3
1	A	376	ILE	2.3
1	A	402	ILE	2.3
1	A	244	TYR	2.3
2	B	73	GLU	2.2
2	B	149	VAL	2.2
1	A	214	GLU	2.2
2	B	192	ARG	2.2
1	A	274	THR	2.2
1	A	288	PRO	2.2
1	A	395	LEU	2.2
2	B	243	SER	2.2
1	A	245	LYS	2.2
1	A	396	PHE	2.2
2	B	166	GLY	2.2
2	B	271	LEU	2.2
1	A	401	SER	2.2
1	A	253	LYS	2.2
1	A	80	ASP	2.2
1	A	261	PRO	2.1
1	A	424	THR	2.2
1	A	408	PHE	2.1
2	B	245	VAL	2.1
2	B	40	GLY	2.1
1	A	387	ALA	2.1
1	A	281	ASN	2.1
1	A	420	TYR	2.1
1	A	265	THR	2.1
1	A	221	GLU	2.1
1	A	415	ASP	2.1
1	A	266	SER	2.1
1	A	268	ASP	2.0
1	A	340	VAL	2.0
1	A	219	ASP	2.0

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

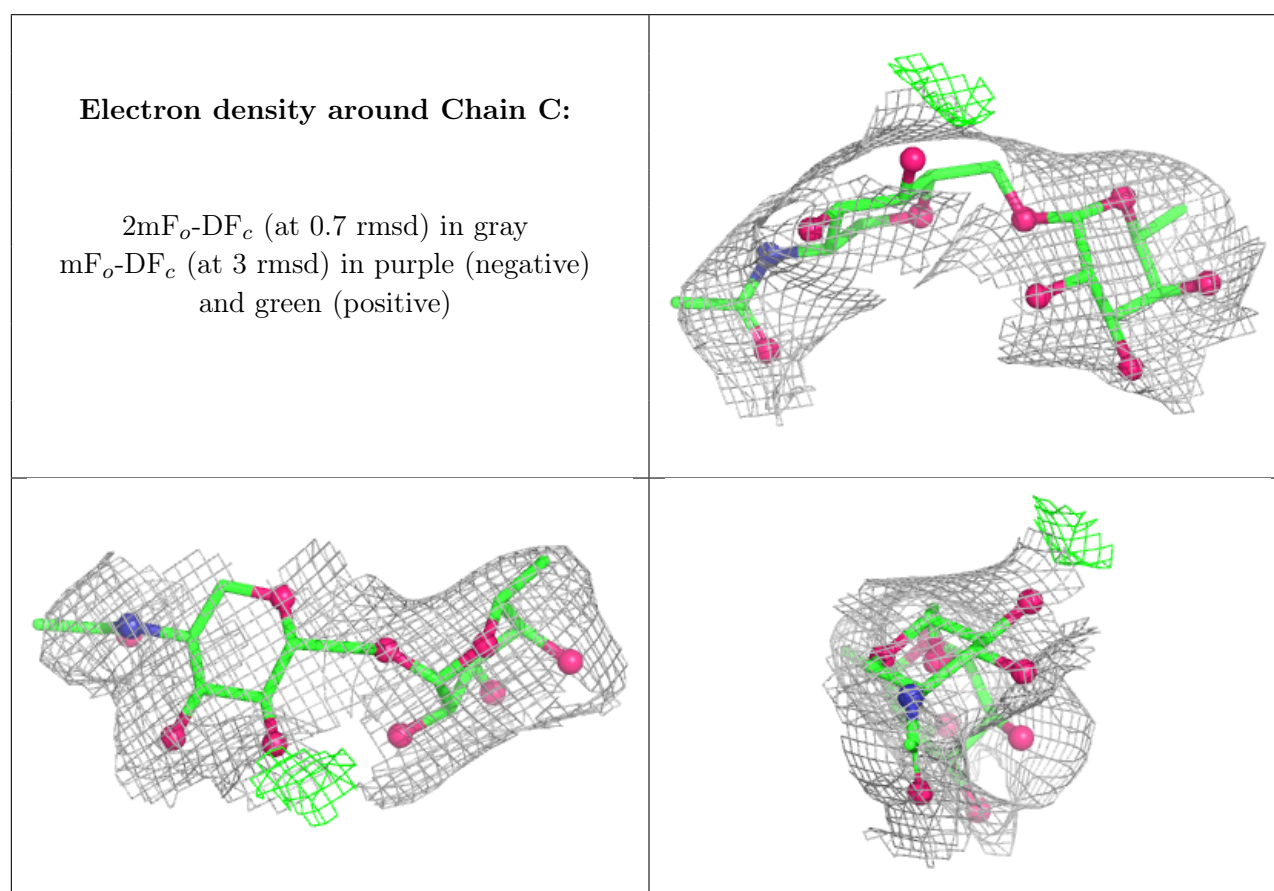
There are no non-standard protein/DNA/RNA residues in this entry.

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
3	NAG	C	1	14/15	0.86	0.11	114,115,116,117	0
3	FUC	C	2	10/11	0.87	0.14	118,118,119,119	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.



6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.