



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:22 AM UTC

PDB ID : 2E33 / pdb_00002e33
Title : Structural basis for selection of glycosylated substrate by SCFFbs1 ubiquitin ligase
Authors : Mizushima, T.; Yoshida, Y.; Kumanomidou, T.; Hasegawa, Y.; Yamane, T.; Tanaka, K.
Deposited on : 2006-11-20
Resolution : 2.70 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

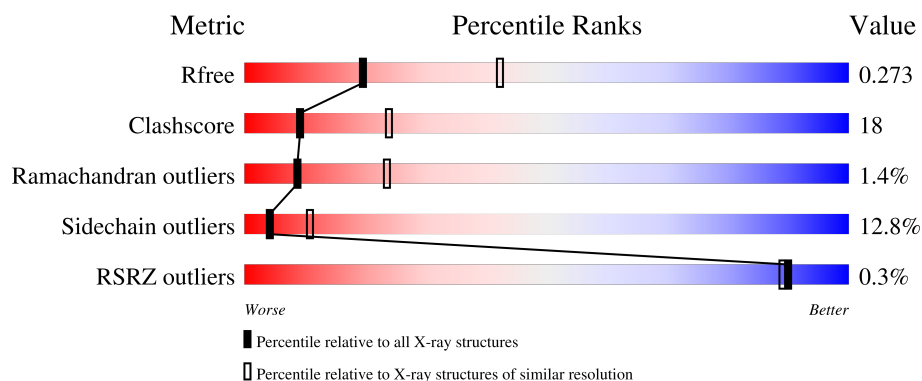
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	197	
2	B	124	
3	C	5	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 2423 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 F-box only protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	175	Total	C	N	O	S	0	0	0
			1412	893	237	279	3			

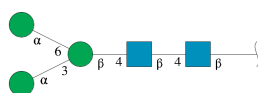
There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	101	GLY	-	cloning artifact	UNP Q80UW2
A	102	SER	-	cloning artifact	UNP Q80UW2
A	103	HIS	-	cloning artifact	UNP Q80UW2
A	104	MET	-	initiating methionine	UNP Q80UW2
A	151	LYS	ARG	SEE REMARK 999	UNP Q80UW2

- Molecule 2 is a protein called Ribonuclease pancreatic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	124	Total	C	N	O	S	0	0	0
			950	575	171	192	12			

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

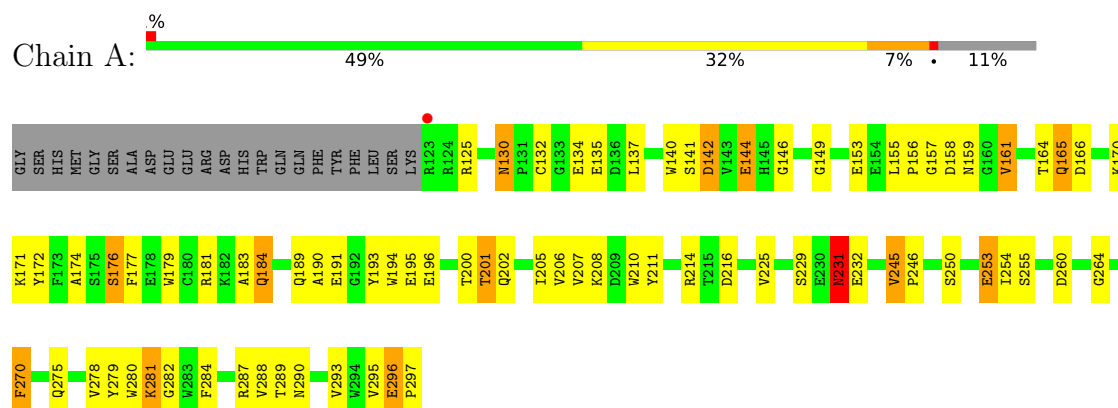


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	5	Total	C	N	O	0	0	0
			61	34	2	25			

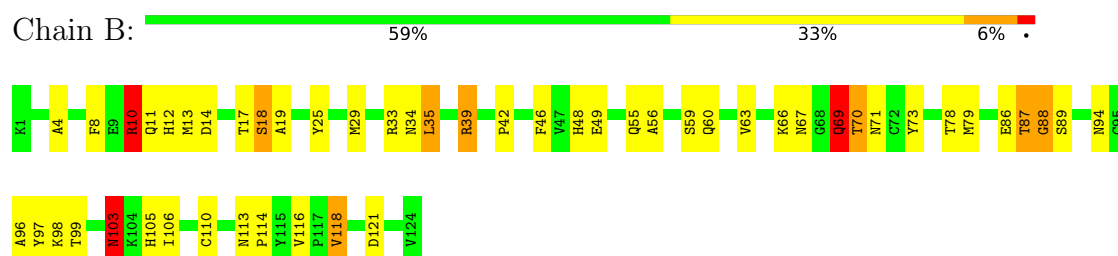
3 Residue-property plots

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: F-box only protein 2



- Molecule 2: Ribonuclease pancreatic



- Molecule 3: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-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 4 3 2	Depositor
Cell constants a, b, c, α , β , γ	148.31 Å 148.31 Å 148.31 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.70 50.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.4 (50.00-2.70) 99.4 (50.00-2.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.24 (at 2.69 Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.216 , 0.288 (Not available) , 0.273	Depositor DCC
R_{free} test set	790 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	56.3	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 26.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	2423	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.58% 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

5.1 Standard geometry

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

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	1.47	7/1452 (0.5%)	1.48	15/1973 (0.8%)
2	B	1.50	6/966 (0.6%)	1.57	11/1304 (0.8%)
All	All	1.48	13/2418 (0.5%)	1.52	26/3277 (0.8%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	190	ALA	CA-CB	8.94	1.68	1.53
1	A	253	GLU	C-O	-6.74	1.15	1.23
1	A	164	THR	CA-CB	6.01	1.63	1.53
2	B	94	ASN	CA-C	-5.94	1.45	1.53
2	B	99	THR	C-O	-5.94	1.16	1.23
1	A	295	VAL	CA-CB	-5.88	1.47	1.54
1	A	141	SER	CA-C	5.79	1.61	1.53
1	A	130	ASN	C-O	5.62	1.26	1.23
2	B	103	ASN	N-CA	-5.52	1.39	1.46
2	B	13	MET	CA-C	-5.24	1.46	1.52
2	B	97	TYR	CA-C	-5.12	1.46	1.52
1	A	174	ALA	CA-CB	-5.11	1.45	1.53
2	B	96	ALA	C-O	5.01	1.29	1.23

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	161	VAL	N-CA-C	7.67	118.87	110.21
1	A	281	LYS	N-CA-C	-7.46	99.45	110.48
1	A	184	GLN	N-CA-C	-7.05	96.70	108.75
2	B	88	GLY	N-CA-C	-6.78	101.54	111.03
1	A	125	ARG	N-CA-C	6.23	119.40	109.24
2	B	12	HIS	CA-C-N	-6.23	114.41	123.00
2	B	12	HIS	C-N-CA	-6.23	114.41	123.00
2	B	19	ALA	N-CA-C	-6.06	99.75	108.60
1	A	165	GLN	N-CA-C	6.05	118.18	110.61
1	A	201	THR	CA-C-N	-6.00	116.34	122.83
1	A	201	THR	C-N-CA	-6.00	116.34	122.83
1	A	156	PRO	CA-C-N	-5.97	113.14	121.67
1	A	156	PRO	C-N-CA	-5.97	113.14	121.67
1	A	296	GLU	N-CA-C	5.79	114.97	108.25
1	A	191	GLU	CA-C-N	-5.73	114.55	122.63
1	A	191	GLU	C-N-CA	-5.73	114.55	122.63
2	B	35	LEU	CA-C-N	-5.63	113.74	123.25
2	B	35	LEU	C-N-CA	-5.63	113.74	123.25
2	B	18	SER	N-CA-C	5.58	118.56	111.69
2	B	73	TYR	N-CA-C	5.44	117.27	108.34
2	B	18	SER	CA-CB-OG	-5.44	100.21	111.10
2	B	87	THR	N-CA-CB	-5.15	102.47	110.29
1	A	146	GLY	N-CA-C	-5.12	105.76	112.82
1	A	231	ASN	N-CA-C	-5.10	106.89	113.01
1	A	164	THR	N-CA-CB	5.09	118.70	110.40
2	B	10	ARG	N-CA-C	-5.02	105.90	112.23

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	69	GLN	Peptide

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	1412	0	1297	45	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	950	0	904	39	0
3	C	61	0	52	7	0
All	All	2423	0	2253	84	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 18.

All (84) 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:179:TRP:HB3	1:A:181:ARG:NH1	1.58	1.17
1:A:179:TRP:CB	1:A:181:ARG:HH12	1.60	1.12
1:A:179:TRP:HB3	1:A:181:ARG:HH12	0.99	1.10
1:A:179:TRP:CD1	1:A:275:GLN:HE21	1.73	1.06
2:B:49:GLU:HG3	2:B:79:MET:HG2	1.52	0.92
2:B:39:ARG:HB2	2:B:39:ARG:HH11	1.32	0.91
2:B:34:ASN:CG	3:C:1:NAG:C1	2.46	0.88
2:B:39:ARG:HH11	2:B:39:ARG:CB	1.88	0.85
2:B:39:ARG:HB2	2:B:39:ARG:NH1	1.93	0.82
1:A:279:TYR:CD2	3:C:1:NAG:H82	2.23	0.72
1:A:179:TRP:NE1	1:A:275:GLN:HE21	1.89	0.71
2:B:49:GLU:HG3	2:B:79:MET:CG	2.22	0.70
1:A:179:TRP:CD1	1:A:275:GLN:NE2	2.56	0.70
2:B:113:ASN:HA	2:B:114:PRO:C	2.16	0.69
1:A:207:VAL:HG21	1:A:225:VAL:HG11	1.75	0.68
1:A:210:TRP:CD1	1:A:290:ASN:HB3	2.30	0.67
1:A:158:ASP:HB3	1:A:214:ARG:HH12	1.61	0.64
2:B:103:ASN:C	2:B:103:ASN:HD22	2.05	0.61
1:A:207:VAL:HG11	1:A:225:VAL:HG21	1.83	0.61
2:B:88:GLY:O	2:B:89:SER:CB	2.50	0.59
2:B:42:PRO:HA	2:B:86:GLU:HG3	1.83	0.59
1:A:245:VAL:O	1:A:246:PRO:C	2.45	0.59
2:B:78:THR:HG22	2:B:105:HIS:CE1	2.37	0.59
1:A:279:TYR:CE2	3:C:1:NAG:H82	2.39	0.58
1:A:153:GLU:HB2	1:A:172:TYR:CZ	2.39	0.58
2:B:11:GLN:HG2	2:B:35:LEU:CD2	2.34	0.57
1:A:130:ASN:ND2	1:A:135:GLU:H	2.04	0.56
2:B:39:ARG:CB	2:B:39:ARG:NH1	2.62	0.55
1:A:214:ARG:HD3	1:A:284:PHE:HA	1.89	0.55
1:A:172:TYR:HA	1:A:289:THR:HB	1.89	0.54
2:B:25:TYR:CZ	2:B:29:MET:HG3	2.42	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:78:THR:CG2	2:B:105:HIS:CE1	2.89	0.54
2:B:106:ILE:O	2:B:106:ILE:HG13	2.03	0.54
1:A:189:GLN:HA	1:A:193:TYR:O	2.08	0.54
2:B:4:ALA:O	2:B:118:VAL:CG2	2.56	0.53
2:B:79:MET:O	2:B:103:ASN:HA	2.09	0.53
1:A:296:GLU:HB2	1:A:297:PRO:HD2	1.91	0.52
1:A:132:CYS:HB3	1:A:171:LYS:O	2.10	0.52
1:A:159:ASN:HB2	1:A:214:ARG:NH2	2.24	0.51
1:A:181:ARG:HG3	1:A:181:ARG:HH11	1.74	0.51
2:B:29:MET:HB3	2:B:46:PHE:CZ	2.46	0.51
1:A:157:GLY:HA3	1:A:172:TYR:OH	2.10	0.51
1:A:144:GLU:OE2	1:A:181:ARG:HD2	2.10	0.50
2:B:103:ASN:C	2:B:103:ASN:ND2	2.68	0.50
1:A:142:ASP:N	1:A:142:ASP:OD1	2.44	0.50
2:B:11:GLN:HG2	2:B:35:LEU:HD22	1.94	0.50
2:B:4:ALA:O	2:B:118:VAL:HG23	2.12	0.49
1:A:210:TRP:HD1	1:A:290:ASN:HB3	1.77	0.49
2:B:34:ASN:OD1	3:C:1:NAG:C1	2.59	0.49
2:B:49:GLU:CG	2:B:79:MET:HG2	2.34	0.49
2:B:56:ALA:O	2:B:60:GLN:HG3	2.13	0.49
1:A:229:SER:HA	1:A:264:GLY:O	2.13	0.48
1:A:270:PHE:C	1:A:270:PHE:CD2	2.91	0.48
1:A:158:ASP:OD2	3:C:4:MAN:H62	2.14	0.47
1:A:176:SER:OG	1:A:282:GLY:O	2.32	0.47
2:B:67:ASN:HD21	2:B:69:GLN:NE2	2.13	0.47
2:B:69:GLN:HB3	2:B:70:THR:H	1.48	0.47
2:B:66:LYS:HE3	2:B:121:ASP:O	2.15	0.46
1:A:214:ARG:HH21	1:A:216:ASP:CG	2.23	0.46
2:B:11:GLN:HG2	2:B:35:LEU:HD21	1.96	0.46
1:A:211:TYR:HA	1:A:287:ARG:O	2.15	0.46
2:B:8:PHE:C	2:B:8:PHE:CD2	2.94	0.46
2:B:33:ARG:HH11	2:B:33:ARG:HG3	1.81	0.46
1:A:177:PHE:HB3	1:A:280:TRP:O	2.16	0.45
2:B:69:GLN:HE21	2:B:69:GLN:HB2	1.63	0.44
1:A:208:LYS:HD2	1:A:253:GLU:OE2	2.17	0.44
2:B:17:THR:O	2:B:48:HIS:HB3	2.18	0.44
2:B:34:ASN:ND2	3:C:1:NAG:O5	2.43	0.43
1:A:288:VAL:O	1:A:289:THR:HB	2.19	0.43
1:A:206:VAL:O	1:A:293:VAL:HA	2.18	0.42
1:A:130:ASN:HD21	1:A:135:GLU:H	1.68	0.42
1:A:158:ASP:HB3	1:A:214:ARG:NH1	2.29	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:ALA:HA	1:A:270:PHE:O	2.21	0.41
1:A:280:TRP:HA	3:C:1:NAG:HN2	1.84	0.41
2:B:4:ALA:O	2:B:118:VAL:HG22	2.20	0.41
1:A:140:TRP:CE3	1:A:184:GLN:HG3	2.55	0.41
1:A:134:GLU:OE1	1:A:134:GLU:HA	2.21	0.41
2:B:10:ARG:O	2:B:33:ARG:HG3	2.21	0.41
2:B:29:MET:HA	2:B:29:MET:HE2	2.02	0.41
2:B:14:ASP:OD1	2:B:14:ASP:C	2.62	0.40
1:A:201:THR:O	1:A:202:GLN:C	2.60	0.40
1:A:210:TRP:CH2	1:A:253:GLU:HB2	2.56	0.40
1:A:231:ASN:O	1:A:232:GLU:HB2	2.20	0.40
2:B:71:ASN:ND2	2:B:110:CYS:O	2.51	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	173/197 (88%)	156 (90%)	13 (8%)	4 (2%)	5	13
2	B	122/124 (98%)	106 (87%)	16 (13%)	0	100	100
All	All	295/321 (92%)	262 (89%)	29 (10%)	4 (1%)	9	23

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	149	GLY
1	A	166	ASP
1	A	260	ASP
1	A	278	VAL

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	148/167 (89%)	128 (86%)	20 (14%)	4	9
2	B	109/109 (100%)	96 (88%)	13 (12%)	5	13
All	All	257/276 (93%)	224 (87%)	33 (13%)	4	11

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	137	LEU
1	A	142	ASP
1	A	144	GLU
1	A	155	LEU
1	A	161	VAL
1	A	165	GLN
1	A	170	LYS
1	A	176	SER
1	A	194	TRP
1	A	195	GLU
1	A	196	GLU
1	A	200	THR
1	A	205	ILE
1	A	231	ASN
1	A	245	VAL
1	A	250	SER
1	A	254	ILE
1	A	255	SER
1	A	270	PHE
1	A	281	LYS
2	B	10	ARG
2	B	18	SER
2	B	39	ARG
2	B	55	GLN
2	B	59	SER
2	B	63	VAL
2	B	69	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	70	THR
2	B	87	THR
2	B	98	LYS
2	B	103	ASN
2	B	116	VAL
2	B	118	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	130	ASN
1	A	159	ASN
1	A	242	GLN
2	B	24	ASN
2	B	55	GLN
2	B	69	GLN
2	B	103	ASN
2	B	113	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 ⓘ

5 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	3,2	14,14,15	0.97	0	17,19,21	2.24	7 (41%)
3	NAG	C	2	3	14,14,15	1.01	1 (7%)	17,19,21	2.53	6 (35%)
3	BMA	C	3	3	11,11,12	1.33	2 (18%)	15,15,17	2.85	5 (33%)
3	MAN	C	4	3	11,11,12	0.87	0	15,15,17	1.95	5 (33%)
3	MAN	C	5	3	11,11,12	1.59	2 (18%)	15,15,17	2.07	5 (33%)

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	3,2	-	4/6/23/26	0/1/1/1
3	NAG	C	2	3	-	4/6/23/26	0/1/1/1
3	BMA	C	3	3	-	1/2/19/22	0/1/1/1
3	MAN	C	4	3	-	2/2/19/22	0/1/1/1
3	MAN	C	5	3	-	2/2/19/22	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	5	MAN	C2-C3	3.70	1.58	1.52
3	C	3	BMA	O5-C1	-2.86	1.38	1.43
3	C	5	MAN	C4-C3	2.63	1.59	1.52
3	C	3	BMA	O2-C2	-2.31	1.38	1.43
3	C	2	NAG	O5-C1	-2.24	1.39	1.43

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	3	BMA	O5-C5-C6	7.91	123.06	107.66
3	C	2	NAG	C2-N2-C7	-6.16	114.65	122.90
3	C	4	MAN	C1-O5-C5	4.91	118.77	112.19
3	C	2	NAG	O5-C5-C6	4.57	116.57	107.66
3	C	3	BMA	C1-C2-C3	4.03	115.51	109.64
3	C	2	NAG	O5-C1-C2	-3.98	105.13	111.29
3	C	1	NAG	O5-C1-C2	3.97	117.44	111.29
3	C	1	NAG	O6-C6-C5	-3.93	97.96	111.33
3	C	3	BMA	O4-C4-C3	-3.90	101.19	110.38
3	C	5	MAN	C2-C3-C4	3.82	117.58	110.86

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	4	MAN	C6-C5-C4	-3.80	103.70	113.02
3	C	5	MAN	C3-C4-C5	3.71	116.96	110.23
3	C	5	MAN	O2-C2-C3	3.28	116.94	110.15
3	C	2	NAG	C3-C4-C5	-3.17	104.48	110.23
3	C	1	NAG	C3-C4-C5	3.17	115.97	110.23
3	C	1	NAG	C1-O5-C5	3.16	116.42	112.19
3	C	1	NAG	O7-C7-C8	-3.13	116.47	122.05
3	C	3	BMA	C2-C3-C4	2.87	115.92	110.86
3	C	3	BMA	O2-C2-C3	-2.82	104.30	110.15
3	C	2	NAG	O4-C4-C3	2.60	116.50	110.38
3	C	5	MAN	O4-C4-C5	-2.46	103.27	109.32
3	C	1	NAG	O3-C3-C2	-2.40	104.42	109.40
3	C	4	MAN	O5-C5-C6	-2.22	103.35	107.66
3	C	2	NAG	O4-C4-C5	-2.18	103.95	109.32
3	C	1	NAG	C8-C7-N2	2.10	119.60	116.12
3	C	5	MAN	O4-C4-C3	2.05	115.21	110.38
3	C	4	MAN	O4-C4-C5	-2.02	104.35	109.32
3	C	4	MAN	C3-C4-C5	2.00	113.86	110.23

There are no chirality outliers.

All (13) torsion outliers are listed below:

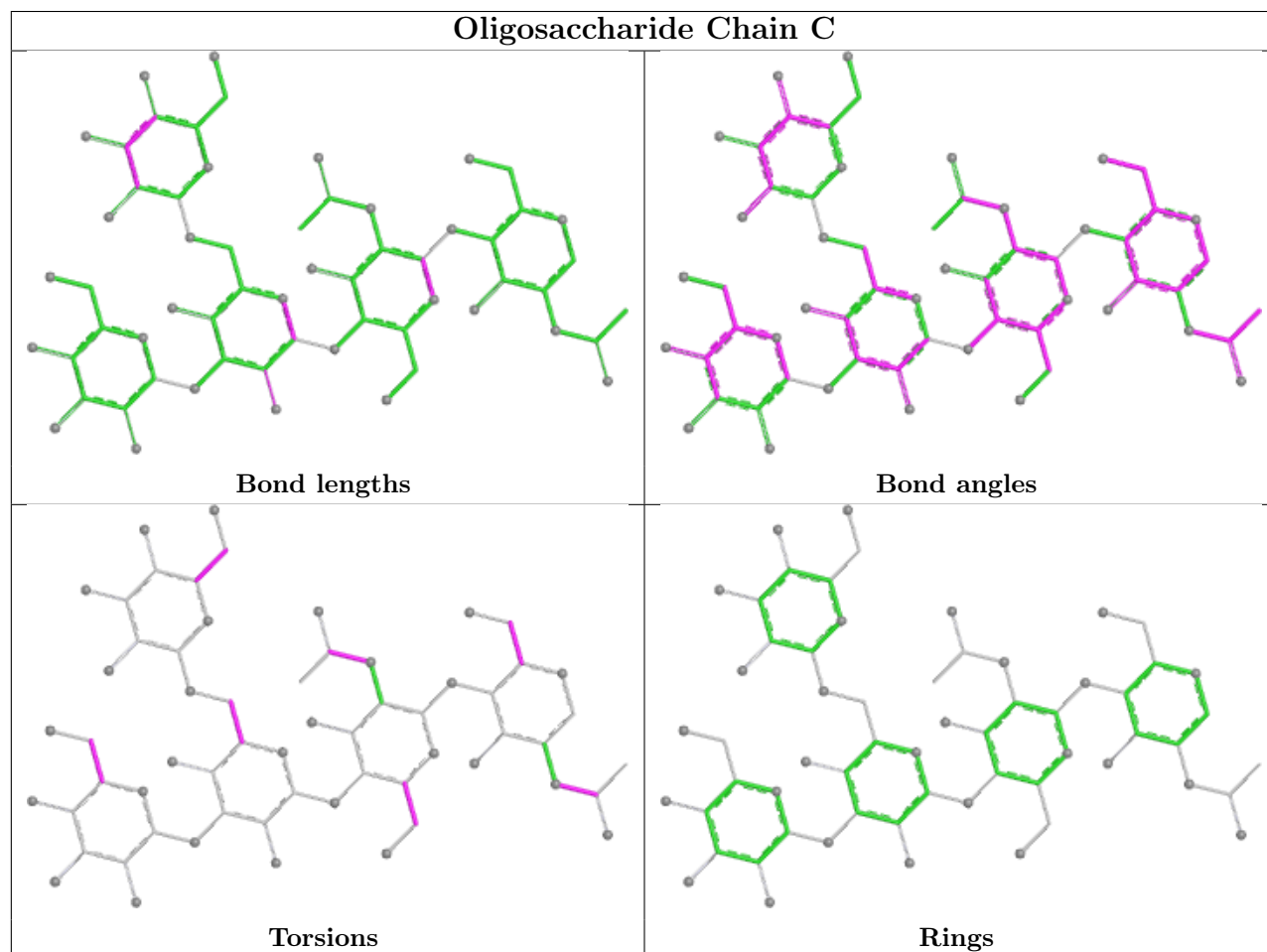
Mol	Chain	Res	Type	Atoms
3	C	2	NAG	C8-C7-N2-C2
3	C	2	NAG	O7-C7-N2-C2
3	C	5	MAN	O5-C5-C6-O6
3	C	1	NAG	O5-C5-C6-O6
3	C	4	MAN	O5-C5-C6-O6
3	C	4	MAN	C4-C5-C6-O6
3	C	2	NAG	O5-C5-C6-O6
3	C	5	MAN	C4-C5-C6-O6
3	C	2	NAG	C4-C5-C6-O6
3	C	1	NAG	C4-C5-C6-O6
3	C	1	NAG	C8-C7-N2-C2
3	C	1	NAG	O7-C7-N2-C2
3	C	3	BMA	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	4	MAN	1	0
3	C	1	NAG	6	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](#)

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	175/197 (88%)	-0.29	1 (0%) 85 85	37, 49, 66, 74	0
2	B	124/124 (100%)	0.10	0 100 100	41, 57, 78, 82	0
All	All	299/321 (93%)	-0.13	1 (0%) 90 89	37, 52, 75, 82	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	123	ARG	2.1

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

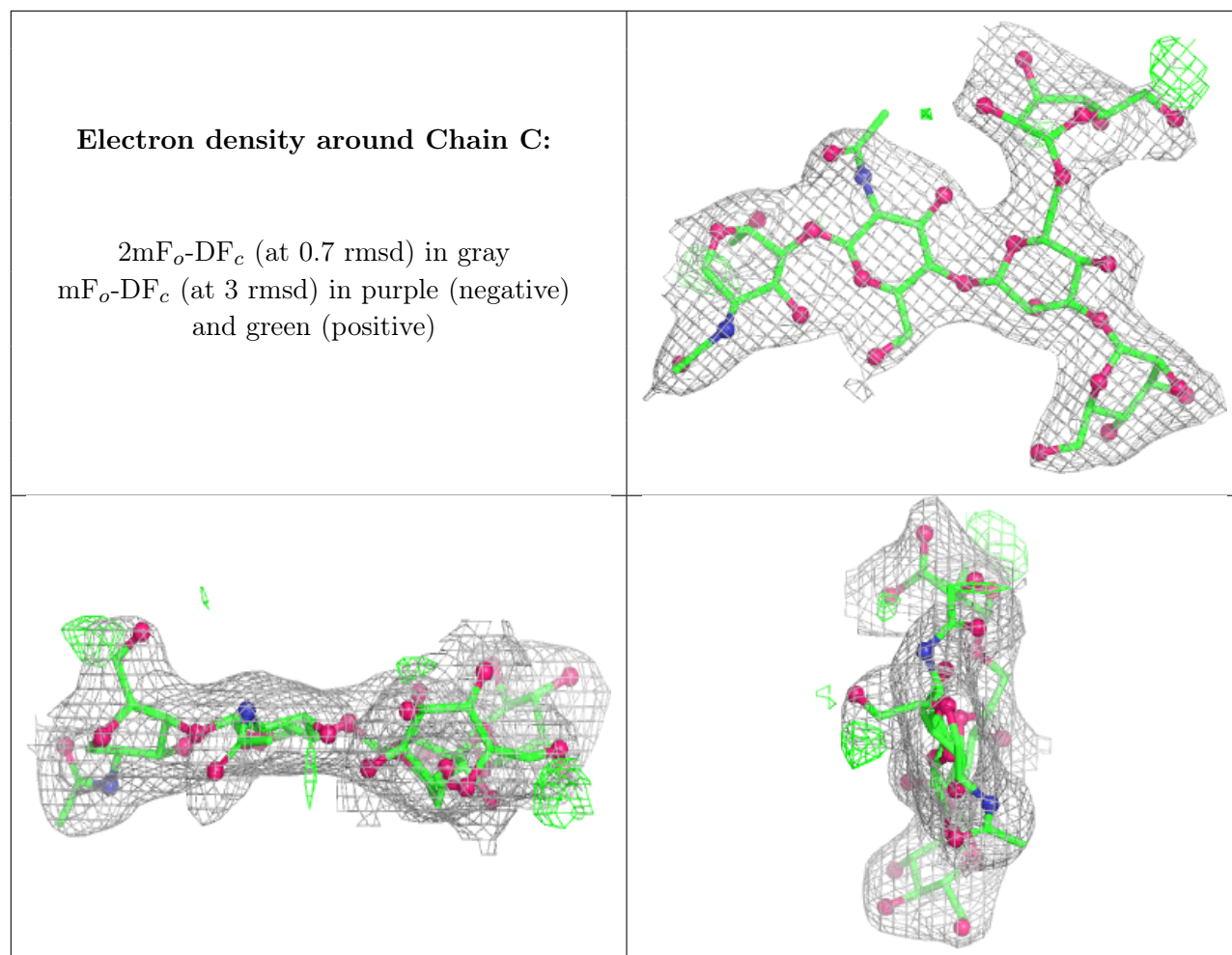
There are no non-standard protein/DNA/RNA residues in this entry.

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(Å ²)	Q<0.9
3	MAN	C	5	11/12	0.57	0.20	88,91,96,97	0
3	BMA	C	3	11/12	0.93	0.10	59,65,70,73	0
3	NAG	C	1	14/15	0.93	0.10	54,57,63,65	0
3	MAN	C	4	11/12	0.94	0.08	70,72,75,77	0
3	NAG	C	2	14/15	0.94	0.09	61,65,77,78	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.