



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:40 PM UTC

PDB ID : 6YN0 / pdb_00006yn0
Title : Structure of E. coli PBP1b with a FtsN peptide activating transglycosylase activity
Authors : Kerff, F.; Terrak, M.; Boes, A.; Herman, H.; Charlier, P.
Deposited on : 2020-04-10
Resolution : 2.40 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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

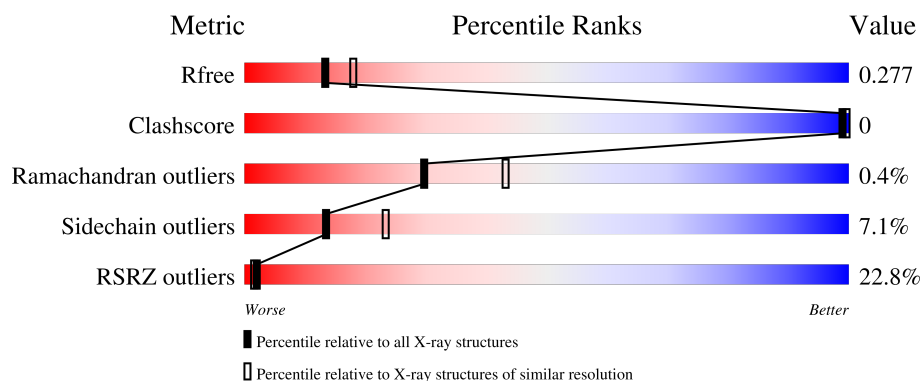
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	747	21% 85% 7% 8%
2	B	19	26% 63% 5% 32%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 11288 atoms, of which 5631 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.

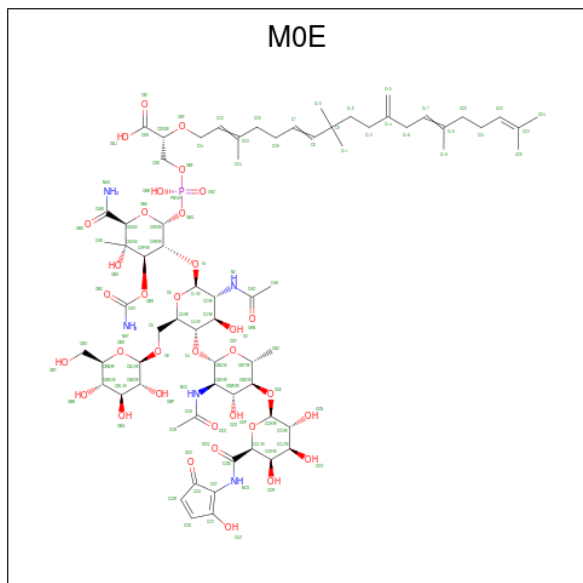
- Molecule 1 is a protein called Penicillin-binding protein 1B.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	689	Total	C	H	N	O	S	7	0	0
			10857	3423	5454	953	1001	26			

- Molecule 2 is a protein called Cell division protein FtsN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	13	Total	C	H	N	O	2	0	0
			239	78	117	21	23			

- Molecule 3 is MOENOMYCIN (CCD ID: M0E) (formula: $C_{69}H_{106}N_5O_{34}P$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	P	0	0
			137	39	60	5	32	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	55	Total	O	0	0
			55	55		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	63.14Å 283.02Å 62.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.17 – 2.40 47.17 – 2.40	Depositor EDS
% Data completeness (in resolution range)	57.3 (47.17-2.40) 57.3 (47.17-2.40)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 2.39Å)	Xtriage
Refinement program	BUSTER	Depositor
R, R_{free}	0.225 , 0.256 0.243 , 0.277	Depositor DCC
R_{free} test set	1320 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	46.0	Xtriage
Anisotropy	0.198	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 46.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.067 for l,-k,h	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	11288	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.70% 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: M0E

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	0.72	0/5510	1.01	3/7475 (0.0%)
2	B	0.73	0/125	0.84	0/166
All	All	0.72	0/5635	1.00	3/7641 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	792	SER	N-CA-C	-5.97	104.35	111.69
1	A	554	ASP	CA-CB-CG	5.95	118.55	112.60
1	A	714	ASP	CA-CB-CG	5.87	118.47	112.60

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	5403	5454	5446	4	0
2	B	122	117	116	0	0
3	A	77	60	59	0	0
4	A	55	0	0	0	0
All	All	5657	5631	5621	4	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 0.

All (4) 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:776:CYS:HA	1:A:793:LEU:HD13	1.90	0.53
1:A:113:LEU:HD11	1:A:124:MET:HE1	1.92	0.51
1:A:776:CYS:HB3	1:A:793:LEU:HD13	1.98	0.45
1:A:386:ILE:HG23	1:A:390:LEU:HD11	2.02	0.41

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	681/747 (91%)	641 (94%)	37 (5%)	3 (0%)	30	43
2	B	11/19 (58%)	11 (100%)	0	0	100	100
All	All	692/766 (90%)	652 (94%)	37 (5%)	3 (0%)	30	43

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	385	ILE
1	A	545	GLY
1	A	430	VAL

5.3.2 Protein sidechains [i](#)

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	581/627 (93%)	540 (93%)	41 (7%)	13	23
2	B	13/19 (68%)	12 (92%)	1 (8%)	12	20
All	All	594/646 (92%)	552 (93%)	42 (7%)	13	23

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	PHE
1	A	110	MET
1	A	118	THR
1	A	121	LYS
1	A	174	THR
1	A	186	MET
1	A	207	SER
1	A	212	GLN
1	A	219	SER
1	A	234	ASP
1	A	271	GLN
1	A	277	PHE
1	A	321	ASP
1	A	365	ASN
1	A	372	ARG
1	A	380	LEU
1	A	402	GLN
1	A	404	ARG
1	A	437	LYS
1	A	452	LYS
1	A	485	ARG
1	A	518	LEU
1	A	526	ILE
1	A	531	THR
1	A	546	GLN
1	A	556	ARG
1	A	586	LEU
1	A	598	VAL
1	A	609	MET
1	A	659	GLU
1	A	695	LEU
1	A	732	LYS
1	A	733	LEU

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Mol	Chain	Res	Type
1	A	751	THR
1	A	765	ASP
1	A	776	CYS
1	A	777	SER
1	A	785	VAL
1	A	787	THR
1	A	788	SER
1	A	791	GLN
2	B	81	GLU

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	122	ASN
1	A	346	GLN
1	A	347	GLN
1	A	383	GLN
1	A	633	ASN
1	A	676	GLN
1	A	704	ASN
1	A	728	ASN
1	A	729	GLN
1	A	744	GLN
1	A	796	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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$
3	M0E	A	901	-	79,81,114	2.26	23 (29%)	112,122,166	1.37	10 (8%)

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	M0E	A	901	-	-	12/52/158/206	0/5/5/6

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	901	M0E	CAV-NAT	7.48	1.47	1.33
3	A	901	M0E	CCM-NCS	7.01	1.49	1.32
3	A	901	M0E	CAW-NAU	6.08	1.47	1.32
3	A	901	M0E	CAG-N2	4.24	1.48	1.34
3	A	901	M0E	CCA-NCC	4.23	1.48	1.34
3	A	901	M0E	CAS-CAO	3.81	1.59	1.52
3	A	901	M0E	OCP-CCH	3.70	1.51	1.41
3	A	901	M0E	OBH-CAV	3.68	1.42	1.35
3	A	901	M0E	C2-N2	3.66	1.51	1.45
3	A	901	M0E	PBI-OBG	3.50	1.69	1.59
3	A	901	M0E	CBV-NCC	3.28	1.51	1.45
3	A	901	M0E	OCF-CBU	3.20	1.50	1.41
3	A	901	M0E	OBE-CAQ	2.90	1.48	1.44
3	A	901	M0E	OBS-CBJ	2.74	1.48	1.41
3	A	901	M0E	OBE-CAX	2.72	1.48	1.41
3	A	901	M0E	OCQ-CCM	-2.70	1.18	1.23
3	A	901	M0E	OCP-CCL	2.59	1.48	1.43
3	A	901	M0E	PBI-OBF	2.47	1.69	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	901	M0E	OBD-CAW	-2.37	1.19	1.23
3	A	901	M0E	O5-C1	2.23	1.47	1.41
3	A	901	M0E	CCB-CCA	2.12	1.54	1.50
3	A	901	M0E	O3-C3	2.09	1.48	1.43
3	A	901	M0E	CAO-CAP	-2.08	1.50	1.54

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	901	M0E	OBH-CAV-NAT	5.80	119.90	110.92
3	A	901	M0E	CAQ-CAW-NAU	5.34	120.48	117.34
3	A	901	M0E	OBC-CAV-NAT	-3.96	119.33	125.58
3	A	901	M0E	ODJ-CDH-CDG	3.41	119.96	112.74
3	A	901	M0E	CCL-CCM-NCS	2.79	120.54	116.64
3	A	901	M0E	OCQ-CCM-NCS	-2.34	118.91	123.04
3	A	901	M0E	C4-C3-C2	2.29	115.93	110.31
3	A	901	M0E	OBD-CAW-NAU	-2.14	119.25	123.04
3	A	901	M0E	CBK-CBL-CBM	2.14	114.58	110.83
3	A	901	M0E	CAH-CAG-N2	2.06	119.53	116.12

There are no chirality outliers.

All (12) torsion outliers are listed below:

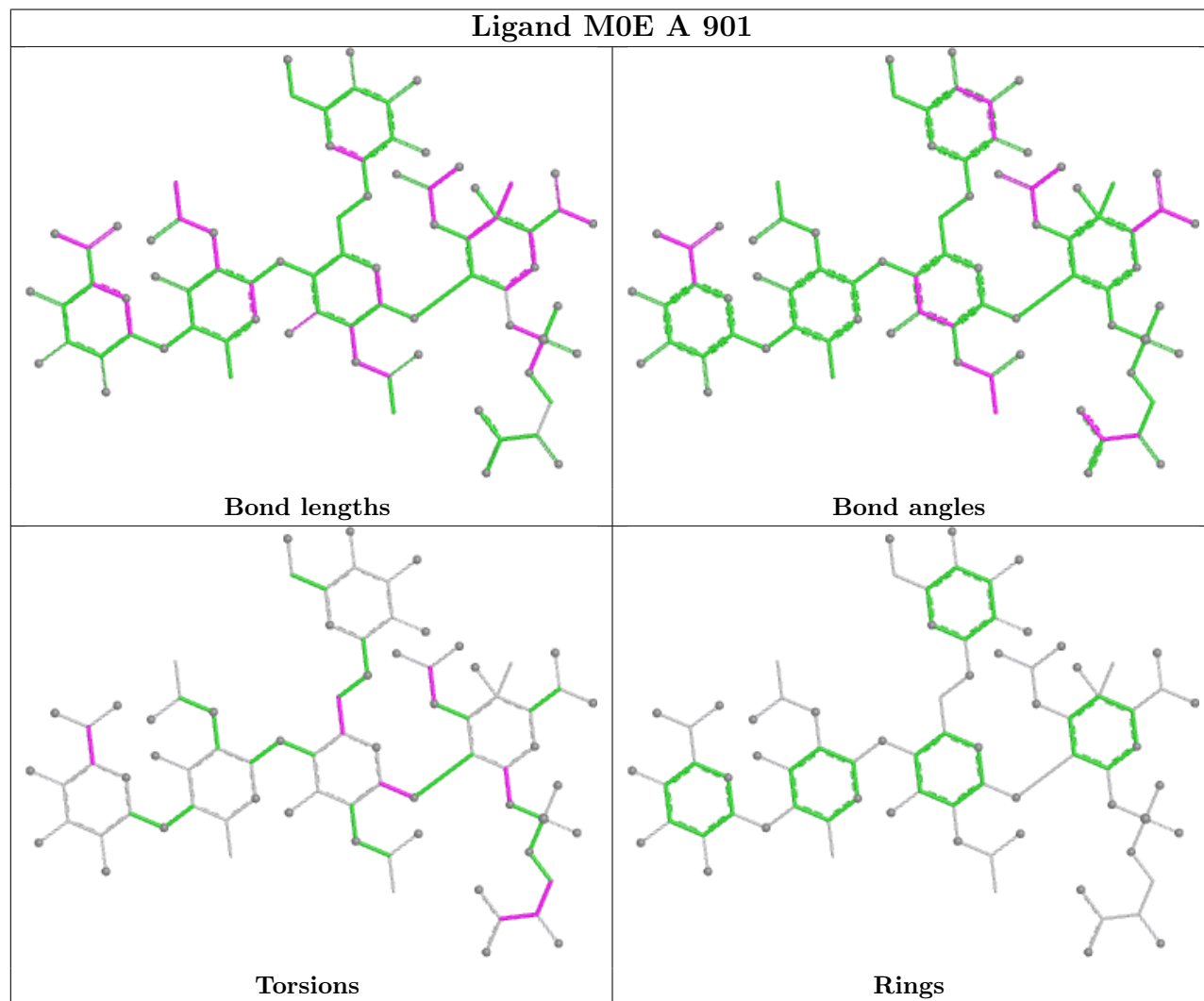
Mol	Chain	Res	Type	Atoms
3	A	901	M0E	ODF-CDG-CDK-OBF
3	A	901	M0E	CDH-CDG-CDK-OBF
3	A	901	M0E	OBC-CAV-OBH-CAP
3	A	901	M0E	NAT-CAV-OBH-CAP
3	A	901	M0E	CCK-CCL-CCM-OCQ
3	A	901	M0E	CCK-CCL-CCM-NCS
3	A	901	M0E	O5-C5-C6-O6
3	A	901	M0E	O5-C1-O1-CAR
3	A	901	M0E	C4-C5-C6-O6
3	A	901	M0E	CAR-CAX-OBG-PBI
3	A	901	M0E	ODF-CDG-CDH-ODI
3	A	901	M0E	ODF-CDG-CDH-ODJ

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 all instances of the Ligand of Interest. In

addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	689/747 (92%)	1.15	155 (22%) 2 2	26, 60, 152, 170	0
2	B	13/19 (68%)	2.08	5 (38%) 1 0	107, 117, 138, 144	0
All	All	702/766 (91%)	1.17	160 (22%) 2 1	26, 62, 152, 170	0

All (160) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	329	LEU	8.2
1	A	734	TYR	7.3
1	A	236	HIS	6.3
2	B	85	TYR	6.1
1	A	280	SER	6.1
1	A	100	TRP	5.8
1	A	269	THR	5.7
1	A	93	SER	5.7
1	A	410	PRO	5.6
1	A	213	ARG	5.3
1	A	408	ILE	5.2
1	A	735	GLY	5.1
1	A	273	VAL	5.1
1	A	407	VAL	5.1
1	A	306	ILE	5.0
1	A	736	ALA	5.0
1	A	221	PHE	4.9
1	A	206	SER	4.9
1	A	97	GLY	4.8
1	A	339	VAL	4.8
1	A	202	ILE	4.6
1	A	332	LEU	4.5
1	A	494	GLN	4.4
1	A	272	LEU	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	399	LEU	4.4
1	A	190	ARG	4.2
1	A	324	ILE	4.1
1	A	230	LEU	4.0
1	A	368	LEU	4.0
1	A	703	ASN	4.0
1	A	226	VAL	4.0
1	A	288	ALA	3.9
1	A	220	GLY	3.8
1	A	200	ARG	3.7
1	A	359	ILE	3.7
1	A	74	ILE	3.7
1	A	369	ALA	3.6
1	A	704	ASN	3.6
1	A	203	THR	3.6
1	A	90	LYS	3.6
1	A	276	LEU	3.6
1	A	214	LEU	3.5
1	A	99	VAL	3.5
1	A	270	GLN	3.5
1	A	349	LEU	3.5
1	A	495	PHE	3.5
1	A	402	GLN	3.4
1	A	795	GLN	3.4
1	A	393	MET	3.4
1	A	201	LEU	3.4
2	B	91	SER	3.3
1	A	385	ILE	3.3
1	A	94	ARG	3.3
2	B	89	LEU	3.3
1	A	284	TYR	3.2
1	A	375	LEU	3.2
1	A	223	ASP	3.2
1	A	392	ASP	3.2
1	A	553	ASP	3.2
1	A	548	TRP	3.2
1	A	277	PHE	3.2
1	A	333	TYR	3.2
1	A	302	SER	3.2
1	A	310	TYR	3.1
1	A	309	LEU	3.1
1	A	391	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	303	LYS	3.1
1	A	432	ASP	3.1
1	A	386	ILE	3.0
1	A	295	LEU	3.0
1	A	550	PRO	3.0
1	A	387	ASP	3.0
1	A	285	TRP	2.9
1	A	380	LEU	2.9
1	A	224	LEU	2.9
1	A	293	MET	2.9
1	A	76	PHE	2.8
1	A	365	ASN	2.8
1	A	526	ILE	2.8
1	A	271	GLN	2.8
1	A	689	LYS	2.8
1	A	307	LEU	2.8
1	A	86	TYR	2.7
1	A	130	ALA	2.7
1	A	311	MET	2.7
1	A	379	LEU	2.7
1	A	433	LEU	2.7
1	A	335	PHE	2.7
1	A	314	VAL	2.7
1	A	797	SER	2.7
1	A	301	TYR	2.7
1	A	313	GLU	2.7
1	A	363	TRP	2.7
1	A	297	MET	2.6
1	A	278	LEU	2.6
1	A	799	MET	2.6
1	A	793	LEU	2.6
1	A	308	GLU	2.6
1	A	538	ILE	2.6
1	A	340	GLU	2.6
1	A	212	GLN	2.6
1	A	232	THR	2.6
1	A	291	ALA	2.6
1	A	286	ARG	2.5
1	A	102	LEU	2.5
1	A	470	LEU	2.5
1	A	542	GLN	2.5
1	A	796	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	228	THR	2.5
1	A	493	PRO	2.5
1	A	730	PRO	2.5
1	A	290	GLU	2.5
1	A	376	VAL	2.5
1	A	729	GLN	2.4
1	A	275	ASN	2.4
1	A	320	GLY	2.4
1	A	390	LEU	2.4
1	A	215	PHE	2.4
1	A	406	GLY	2.4
1	A	234	ASP	2.4
1	A	83	TYR	2.4
1	A	358	SER	2.4
1	A	287	LYS	2.4
1	A	403	PRO	2.3
1	A	684	ARG	2.3
1	A	409	SER	2.3
1	A	732	LYS	2.3
1	A	394	LEU	2.3
1	A	448	ASP	2.3
1	A	98	LYS	2.3
1	A	354	VAL	2.3
1	A	77	ALA	2.3
1	A	496	ALA	2.3
2	B	79	PRO	2.3
1	A	721	THR	2.3
1	A	298	ASP	2.3
1	A	537	PRO	2.3
1	A	205	ILE	2.2
1	A	80	ILE	2.2
1	A	95	ILE	2.2
1	A	222	PRO	2.2
1	A	327	PHE	2.2
1	A	383	GLN	2.1
1	A	501	ALA	2.1
1	A	395	SER	2.1
1	A	469	ASP	2.1
1	A	622	ALA	2.1
1	A	554	ASP	2.1
1	A	351	VAL	2.1
1	A	547	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	86	ILE	2.1
1	A	120	SER	2.1
1	A	545	GLY	2.1
1	A	115	PRO	2.1
1	A	353	MET	2.1
1	A	450	ALA	2.0
1	A	437	LYS	2.0
1	A	204	MET	2.0
1	A	430	VAL	2.0
1	A	328	PRO	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](#)

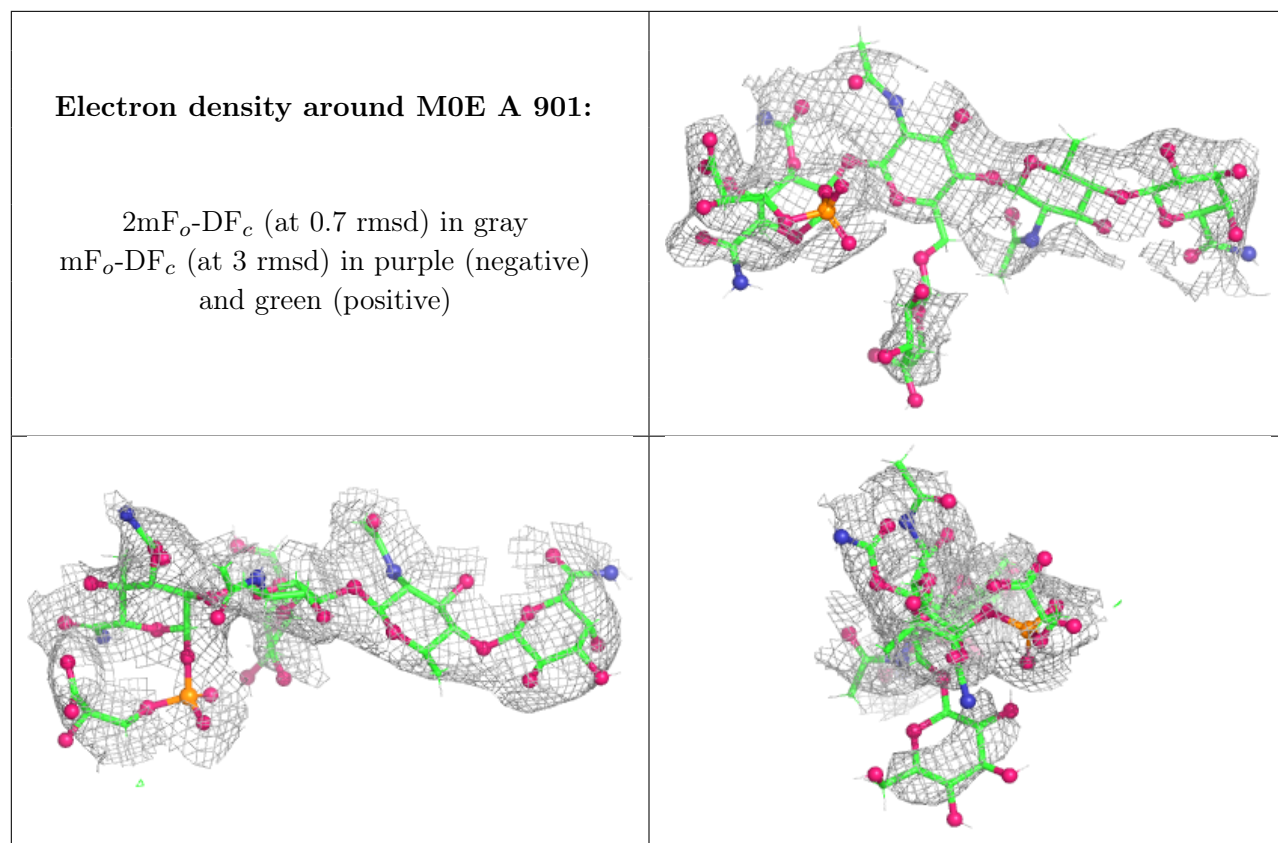
There are no oligosaccharides in this entry.

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
3	M0E	A	901	77/109	0.63	0.15	142,152,156,156	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.