



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2020 – 12:01 pm BST

PDB ID : 4R3J  
Title : Structure of a putative peptidoglycan glycosyltransferase from *Atopobium parvulum* in complex with cefapirin  
Authors : Filippova, E.V.; Minasov, G.; Kiryukhina, O.; Clancy, S.; Joachimiak, A.; Anderson, W.F.; Midwest Center for Structural Genomics (MCSG)  
Deposited on : 2014-08-15  
Resolution : 2.44 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](mailto: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.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

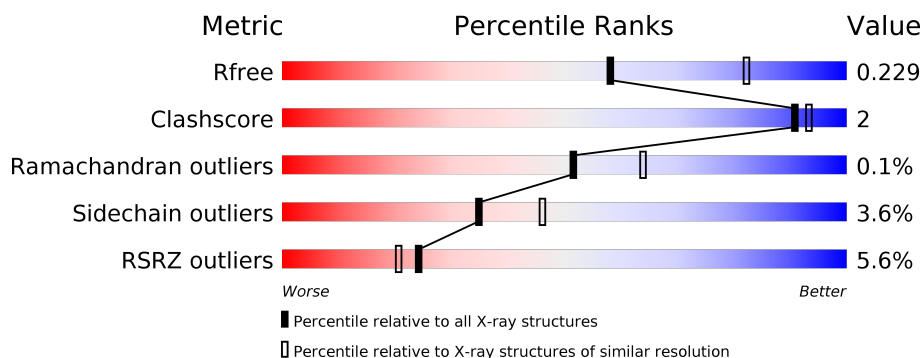
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.44 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))
$R_{free}$	130704	1564 (2.46-2.42)
Clashscore	141614	1631 (2.46-2.42)
Ramachandran outliers	138981	1617 (2.46-2.42)
Sidechain outliers	138945	1617 (2.46-2.42)
RSRZ outliers	127900	1547 (2.46-2.42)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	482	<div> <div>4%</div> <div> <div></div> <div>78%</div> <div>5%</div> <div>16%</div> </div> </div>
1	B	482	<div> <div>5%</div> <div> <div></div> <div>78%</div> <div>6%</div> <div>16%</div> </div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6073 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 Peptidoglycan glycosyltransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	407	Total	C	N	O	S	Se	0	0	0
			2910	1805	494	597	2	12			
1	B	407	Total	C	N	O	S	Se	0	0	0
			2916	1810	494	598	2	12			

There are 64 discrepancies between the modelled and reference sequences:

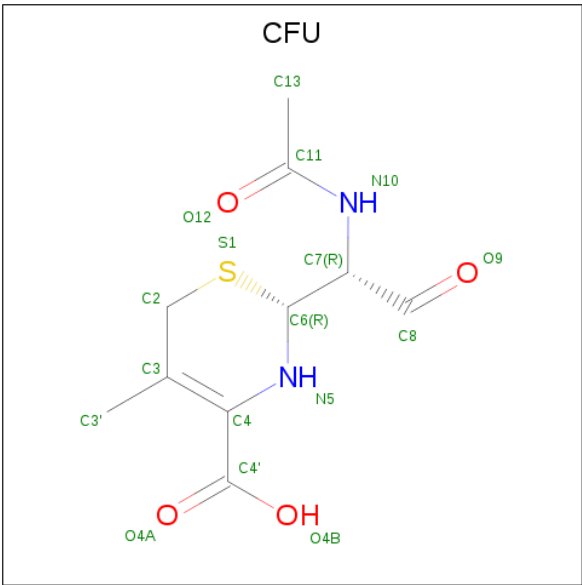
Chain	Residue	Modelled	Actual	Comment	Reference
A	473	MSE	-	EXPRESSION TAG	UNP C8W8H7
A	474	HIS	-	EXPRESSION TAG	UNP C8W8H7
A	475	HIS	-	EXPRESSION TAG	UNP C8W8H7
A	476	HIS	-	EXPRESSION TAG	UNP C8W8H7
A	477	HIS	-	EXPRESSION TAG	UNP C8W8H7
A	478	HIS	-	EXPRESSION TAG	UNP C8W8H7
A	479	HIS	-	EXPRESSION TAG	UNP C8W8H7
A	480	SER	-	EXPRESSION TAG	UNP C8W8H7
A	481	SER	-	EXPRESSION TAG	UNP C8W8H7
A	482	GLY	-	EXPRESSION TAG	UNP C8W8H7
A	483	VAL	-	EXPRESSION TAG	UNP C8W8H7
A	484	ASP	-	EXPRESSION TAG	UNP C8W8H7
A	485	LEU	-	EXPRESSION TAG	UNP C8W8H7
A	486	TRP	-	EXPRESSION TAG	UNP C8W8H7
A	487	SER	-	EXPRESSION TAG	UNP C8W8H7
A	488	HIS	-	EXPRESSION TAG	UNP C8W8H7
A	489	PRO	-	EXPRESSION TAG	UNP C8W8H7
A	490	GLN	-	EXPRESSION TAG	UNP C8W8H7
A	491	PHE	-	EXPRESSION TAG	UNP C8W8H7
A	492	GLU	-	EXPRESSION TAG	UNP C8W8H7
A	493	LYS	-	EXPRESSION TAG	UNP C8W8H7
A	494	GLY	-	EXPRESSION TAG	UNP C8W8H7
A	495	THR	-	EXPRESSION TAG	UNP C8W8H7
A	496	GLU	-	EXPRESSION TAG	UNP C8W8H7
A	497	ASN	-	EXPRESSION TAG	UNP C8W8H7

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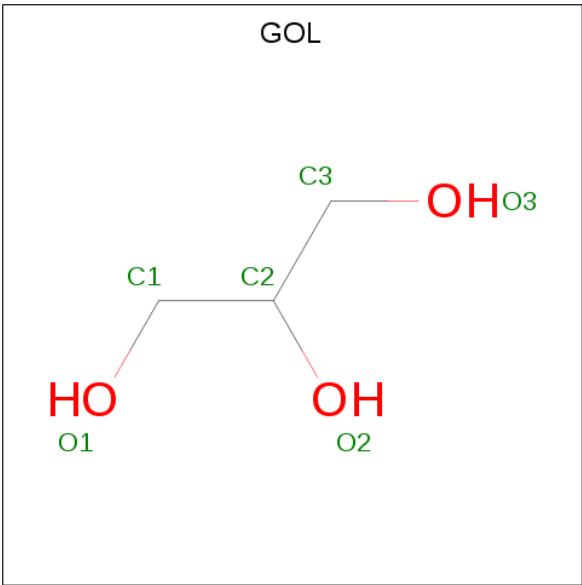
Chain	Residue	Modelled	Actual	Comment	Reference
A	498	LEU	-	EXPRESSION TAG	UNP C8W8H7
A	499	TYR	-	EXPRESSION TAG	UNP C8W8H7
A	500	PHE	-	EXPRESSION TAG	UNP C8W8H7
A	501	GLN	-	EXPRESSION TAG	UNP C8W8H7
A	502	SER	-	EXPRESSION TAG	UNP C8W8H7
A	503	ASN	-	EXPRESSION TAG	UNP C8W8H7
A	504	ALA	-	EXPRESSION TAG	UNP C8W8H7
B	473	MSE	-	EXPRESSION TAG	UNP C8W8H7
B	474	HIS	-	EXPRESSION TAG	UNP C8W8H7
B	475	HIS	-	EXPRESSION TAG	UNP C8W8H7
B	476	HIS	-	EXPRESSION TAG	UNP C8W8H7
B	477	HIS	-	EXPRESSION TAG	UNP C8W8H7
B	478	HIS	-	EXPRESSION TAG	UNP C8W8H7
B	479	HIS	-	EXPRESSION TAG	UNP C8W8H7
B	480	SER	-	EXPRESSION TAG	UNP C8W8H7
B	481	SER	-	EXPRESSION TAG	UNP C8W8H7
B	482	GLY	-	EXPRESSION TAG	UNP C8W8H7
B	483	VAL	-	EXPRESSION TAG	UNP C8W8H7
B	484	ASP	-	EXPRESSION TAG	UNP C8W8H7
B	485	LEU	-	EXPRESSION TAG	UNP C8W8H7
B	486	TRP	-	EXPRESSION TAG	UNP C8W8H7
B	487	SER	-	EXPRESSION TAG	UNP C8W8H7
B	488	HIS	-	EXPRESSION TAG	UNP C8W8H7
B	489	PRO	-	EXPRESSION TAG	UNP C8W8H7
B	490	GLN	-	EXPRESSION TAG	UNP C8W8H7
B	491	PHE	-	EXPRESSION TAG	UNP C8W8H7
B	492	GLU	-	EXPRESSION TAG	UNP C8W8H7
B	493	LYS	-	EXPRESSION TAG	UNP C8W8H7
B	494	GLY	-	EXPRESSION TAG	UNP C8W8H7
B	495	THR	-	EXPRESSION TAG	UNP C8W8H7
B	496	GLU	-	EXPRESSION TAG	UNP C8W8H7
B	497	ASN	-	EXPRESSION TAG	UNP C8W8H7
B	498	LEU	-	EXPRESSION TAG	UNP C8W8H7
B	499	TYR	-	EXPRESSION TAG	UNP C8W8H7
B	500	PHE	-	EXPRESSION TAG	UNP C8W8H7
B	501	GLN	-	EXPRESSION TAG	UNP C8W8H7
B	502	SER	-	EXPRESSION TAG	UNP C8W8H7
B	503	ASN	-	EXPRESSION TAG	UNP C8W8H7
B	504	ALA	-	EXPRESSION TAG	UNP C8W8H7

- Molecule 2 is (2R)-2-[(1R)-1-(acetylamino)-2-oxoethyl]-5-methyl-3,6-dihydro-2H-1,3-thiazin e-4-carboxylic acid (three-letter code: CFU) (formula: C<sub>10</sub>H<sub>14</sub>N<sub>2</sub>O<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			17	10	2	4	1		
2	B	1	Total	C	N	O	S	0	0
			17	10	2	4	1		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		
4	A	1	Total	O	P	0	0
			5	4	1		
4	B	1	Total	O	P	0	0
			5	4	1		

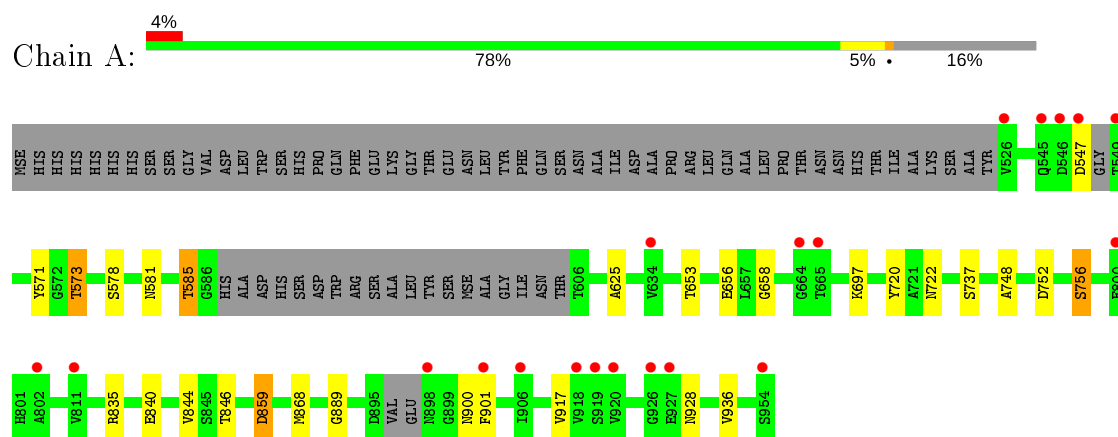
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	95	Total	O	0	2
			97	97		
5	B	83	Total	O	0	0
			83	83		

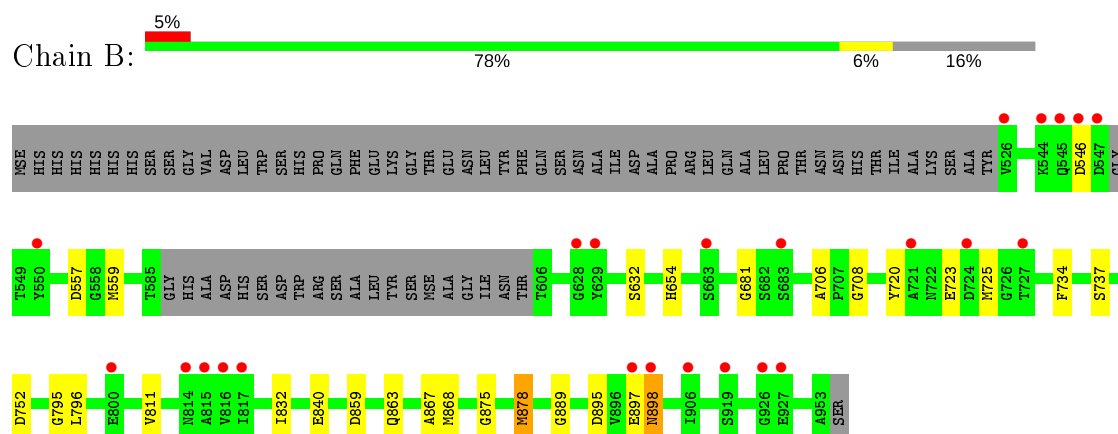
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: Peptidoglycan glycosyltransferase



- Molecule 1: Peptidoglycan glycosyltransferase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	99.63Å 119.84Å 82.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.44 29.84 – 2.44	Depositor EDS
% Data completeness (in resolution range)	99.7 (30.00-2.44) 99.8 (29.84-2.44)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.56 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.8.0069	Depositor
R, $R_{free}$	0.171 , 0.231 0.177 , 0.229	Depositor DCC
$R_{free}$ test set	1858 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	44.1	Xtriage
Anisotropy	0.070	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 41.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	6073	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.61% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: GOL, PO4, CFU

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	0.70	0/2945	0.82	1/3996 (0.0%)
1	B	0.68	0/2952	0.78	2/4008 (0.0%)
All	All	0.69	0/5897	0.80	3/8004 (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	B	878	MSE	CA-CB-CG	-5.76	103.50	113.30
1	B	559	MSE	CA-CB-CG	-5.76	103.51	113.30
1	A	859	ASP	CB-CG-OD1	-5.19	113.63	118.30

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	2910	0	2840	10	0
1	B	2916	0	2848	10	0
2	A	17	0	11	1	0
2	B	17	0	11	1	0
3	A	6	0	8	0	0
3	B	12	0	16	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	10	0	0	0	0
4	B	5	0	0	0	0
5	A	97	0	0	0	0
5	B	83	0	0	0	0
All	All	6073	0	5734	20	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 (20) 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:868:MSE:HE2	1:A:889:GLY:HA2	1.76	0.68
1:A:571:TYR:CE1	1:A:658:GLY:HA2	2.38	0.59
1:B:708:GLY:HA2	1:B:723:GLU:O	2.05	0.56
1:A:720:TYR:HB2	2:A:1001:CFU:S1	2.50	0.51
1:A:573:THR:HG23	1:A:578:SER:HB2	1.93	0.50
1:A:581:ASN:O	1:A:585:THR:HB	2.12	0.49
1:A:697:LYS:HE3	1:A:748:ALA:O	2.13	0.49
1:A:653:THR:OG1	1:A:656:GLU:HG3	2.12	0.49
1:B:720:TYR:HB2	2:B:1001:CFU:S1	2.53	0.48
1:B:632:SER:OG	1:B:811:VAL:HG21	2.13	0.48
1:B:868:MSE:HE2	1:B:889:GLY:HA2	1.97	0.47
1:B:875:GLY:O	1:B:878:MSE:HG3	2.14	0.47
1:B:706:ALA:HB3	1:B:725:MSE:HB2	1.98	0.46
1:A:752:ASP:O	1:A:756:SER:HB3	2.16	0.46
1:B:897:GLU:O	1:B:898:ASN:CB	2.65	0.45
1:B:681:GLY:O	1:B:795:GLY:HA3	2.18	0.42
1:B:734:PHE:CD2	1:B:867:ALA:HB1	2.55	0.42
1:A:625:ALA:HB1	1:A:936:VAL:HG13	2.01	0.41
1:A:901:PHE:HZ	1:A:928:ASN:OD1	2.02	0.40
1:B:557:ASP:OD1	1:B:654:HIS:N	2.49	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	399/482 (83%)	387 (97%)	12 (3%)	0	100	100
1	B	401/482 (83%)	386 (96%)	14 (4%)	1 (0%)	47	57
All	All	800/964 (83%)	773 (97%)	26 (3%)	1 (0%)	51	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	546	ASP

### 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	307/356 (86%)	294 (96%)	13 (4%)	30	39
1	B	308/356 (86%)	299 (97%)	9 (3%)	42	54
All	All	615/712 (86%)	593 (96%)	22 (4%)	35	46

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	547	ASP
1	A	573	THR
1	A	585	THR
1	A	722	ASN
1	A	737	SER

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Mol	Chain	Res	Type
1	A	756	SER
1	A	835	ARG
1	A	840	GLU
1	A	844	VAL
1	A	846	THR
1	A	859	ASP
1	A	900	ASN
1	A	917	VAL
1	B	737	SER
1	B	752	ASP
1	B	796	LEU
1	B	832	ILE
1	B	840	GLU
1	B	859	ASP
1	B	863	GLN
1	B	895	ASP
1	B	898	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	722	ASN
1	B	556	HIS

### 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 carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

8 ligands 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	GOL	B	1003	-	5,5,5	0.30	0	5,5,5	0.84	0
4	PO4	A	1004	-	4,4,4	0.98	0	6,6,6	0.95	0
2	CFU	A	1001	1	11,17,17	5.85	5 (45%)	12,23,23	2.71	7 (58%)
2	CFU	B	1001	1	11,17,17	5.77	3 (27%)	12,23,23	3.23	6 (50%)
4	PO4	A	1003	-	4,4,4	0.49	0	6,6,6	0.96	0
4	PO4	B	1004	-	4,4,4	1.20	1 (25%)	6,6,6	1.25	1 (16%)
3	GOL	B	1002	-	5,5,5	0.50	0	5,5,5	0.97	0
3	GOL	A	1002	-	5,5,5	0.40	0	5,5,5	0.69	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
2	CFU	A	1001	1	-	0/4/27/27	0/0/1/1
2	CFU	B	1001	1	-	0/4/27/27	0/0/1/1
3	GOL	B	1002	-	-	4/4/4/4	-
3	GOL	A	1002	-	-	2/4/4/4	-
3	GOL	B	1003	-	-	4/4/4/4	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	CFU	C4'-C4	-11.65	1.34	1.52
2	B	1001	CFU	C4'-C4	-11.43	1.34	1.52
2	A	1001	CFU	C3'-C3	-10.96	1.32	1.50
2	B	1001	CFU	C3-C4	10.66	1.47	1.34
2	B	1001	CFU	C3'-C3	-10.54	1.33	1.50
2	A	1001	CFU	C3-C4	10.29	1.47	1.34
2	A	1001	CFU	C4-N5	-2.34	1.26	1.33
2	A	1001	CFU	C2-S1	-2.11	1.77	1.82
4	B	1004	PO4	P-O3	-2.00	1.48	1.54

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1001	CFU	C6-N5-C4	5.48	131.22	118.32
2	B	1001	CFU	C2-S1-C6	4.81	103.90	94.47
2	B	1001	CFU	C2-C3-C4	-4.69	115.76	123.48
2	A	1001	CFU	C3-C2-S1	-4.53	110.55	116.98
2	B	1001	CFU	C3'-C3-C2	4.35	120.29	113.23
2	A	1001	CFU	C3'-C3-C2	3.81	119.41	113.23
2	B	1001	CFU	C3-C2-S1	-3.78	111.61	116.98
2	A	1001	CFU	C2-S1-C6	3.61	101.54	94.47
2	B	1001	CFU	C7-N10-C11	3.34	126.77	123.12
2	A	1001	CFU	C6-N5-C4	2.98	125.33	118.32
2	A	1001	CFU	C6-C7-N10	-2.79	103.88	109.98
2	A	1001	CFU	C2-C3-C4	-2.58	119.23	123.48
2	A	1001	CFU	C7-N10-C11	2.29	125.63	123.12
4	B	1004	PO4	O4-P-O2	2.10	114.72	107.97

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1003	GOL	O1-C1-C2-C3
3	B	1003	GOL	C1-C2-C3-O3
3	B	1002	GOL	O1-C1-C2-C3
3	B	1003	GOL	O1-C1-C2-O2
3	A	1002	GOL	O2-C2-C3-O3
3	B	1002	GOL	C1-C2-C3-O3
3	A	1002	GOL	C1-C2-C3-O3
3	B	1002	GOL	O1-C1-C2-O2
3	B	1003	GOL	O2-C2-C3-O3
3	B	1002	GOL	O2-C2-C3-O3

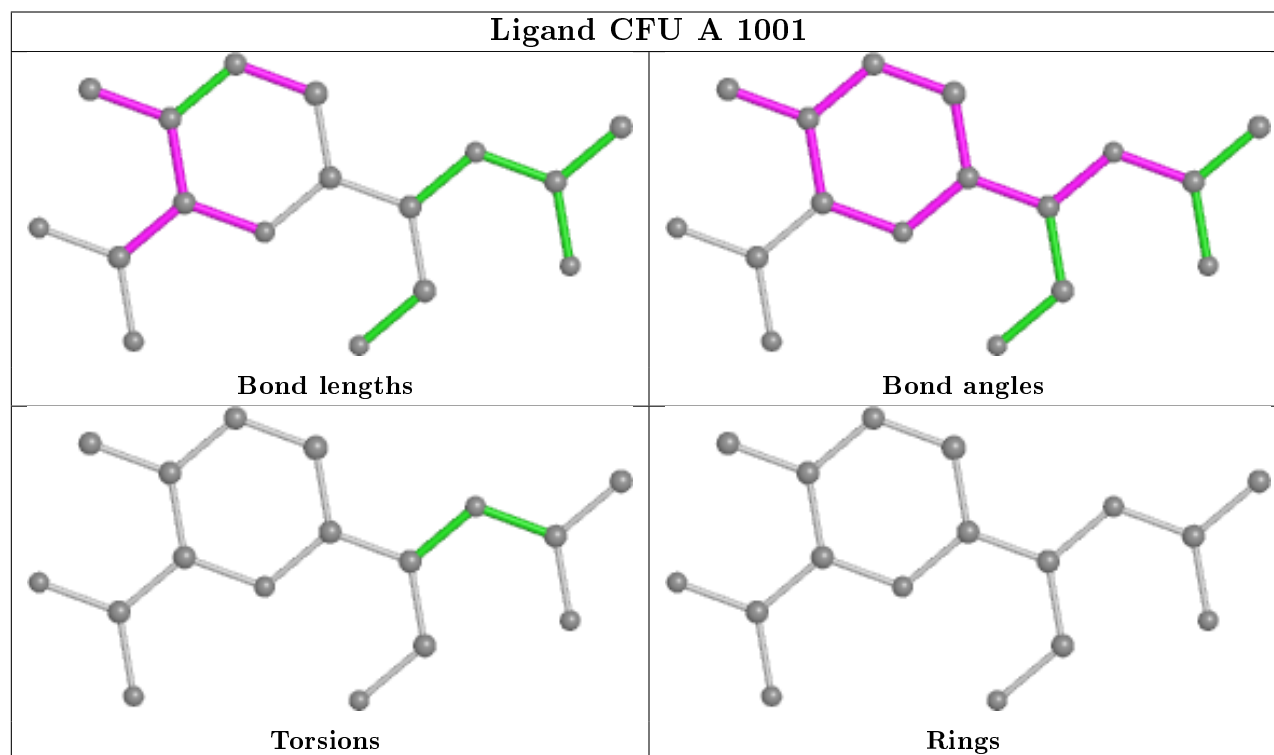
There are no ring outliers.

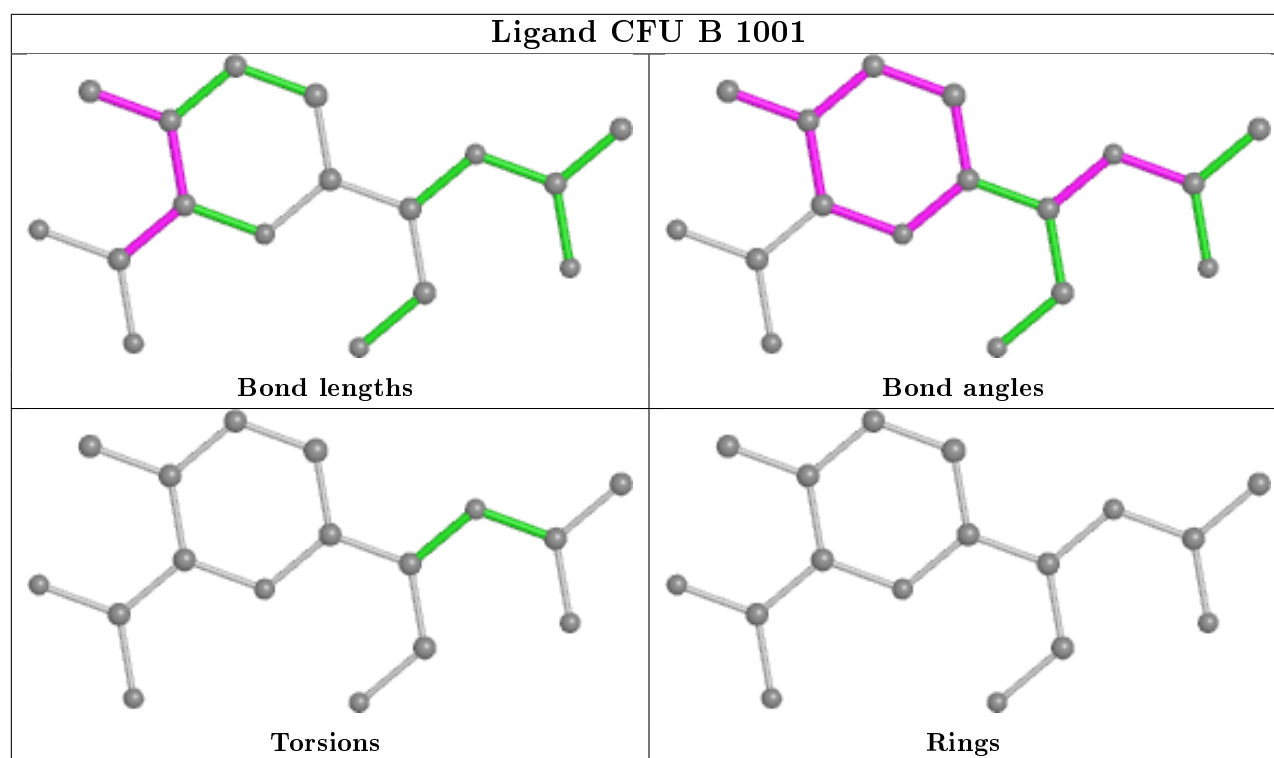
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	CFU	1	0
2	B	1001	CFU	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 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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	395/482 (81%)	-0.05	20 (5%) 28 25	27, 43, 82, 119	0
1	B	395/482 (81%)	-0.08	24 (6%) 21 17	29, 45, 77, 122	0
All	All	790/964 (81%)	-0.07	44 (5%) 24 20	27, 44, 80, 122	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	546	ASP	5.3
1	B	546	ASP	4.5
1	A	927	GLU	4.0
1	B	898	ASN	4.0
1	A	926	GLY	4.0
1	B	906	ILE	3.6
1	B	547	ASP	3.5
1	A	906	ILE	3.5
1	A	954	SER	3.3
1	A	545	GLN	3.3
1	B	526	VAL	3.2
1	B	800	GLU	3.1
1	B	897	GLU	3.0
1	A	918	VAL	2.9
1	A	665	THR	2.9
1	B	629	TYR	2.9
1	B	814	ASN	2.9
1	B	683	SER	2.9
1	A	802	ALA	2.9
1	A	664	GLY	2.8
1	B	721	ALA	2.7
1	B	724	ASP	2.7
1	B	544	LYS	2.7
1	B	545	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	901	PHE	2.6
1	B	817	ILE	2.5
1	A	898	ASN	2.4
1	B	816	VAL	2.4
1	B	926	GLY	2.3
1	A	634	VAL	2.3
1	A	547	ASP	2.3
1	B	550	TYR	2.3
1	A	919	SER	2.3
1	B	919	SER	2.3
1	B	927	GLU	2.3
1	B	663	SER	2.3
1	A	800	GLU	2.3
1	A	549	THR	2.2
1	A	526	VAL	2.2
1	B	628	GLY	2.2
1	B	727	THR	2.2
1	A	811	VAL	2.2
1	B	815	ALA	2.1
1	A	920	VAL	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 carbohydrates 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, 95<sup>th</sup> 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.

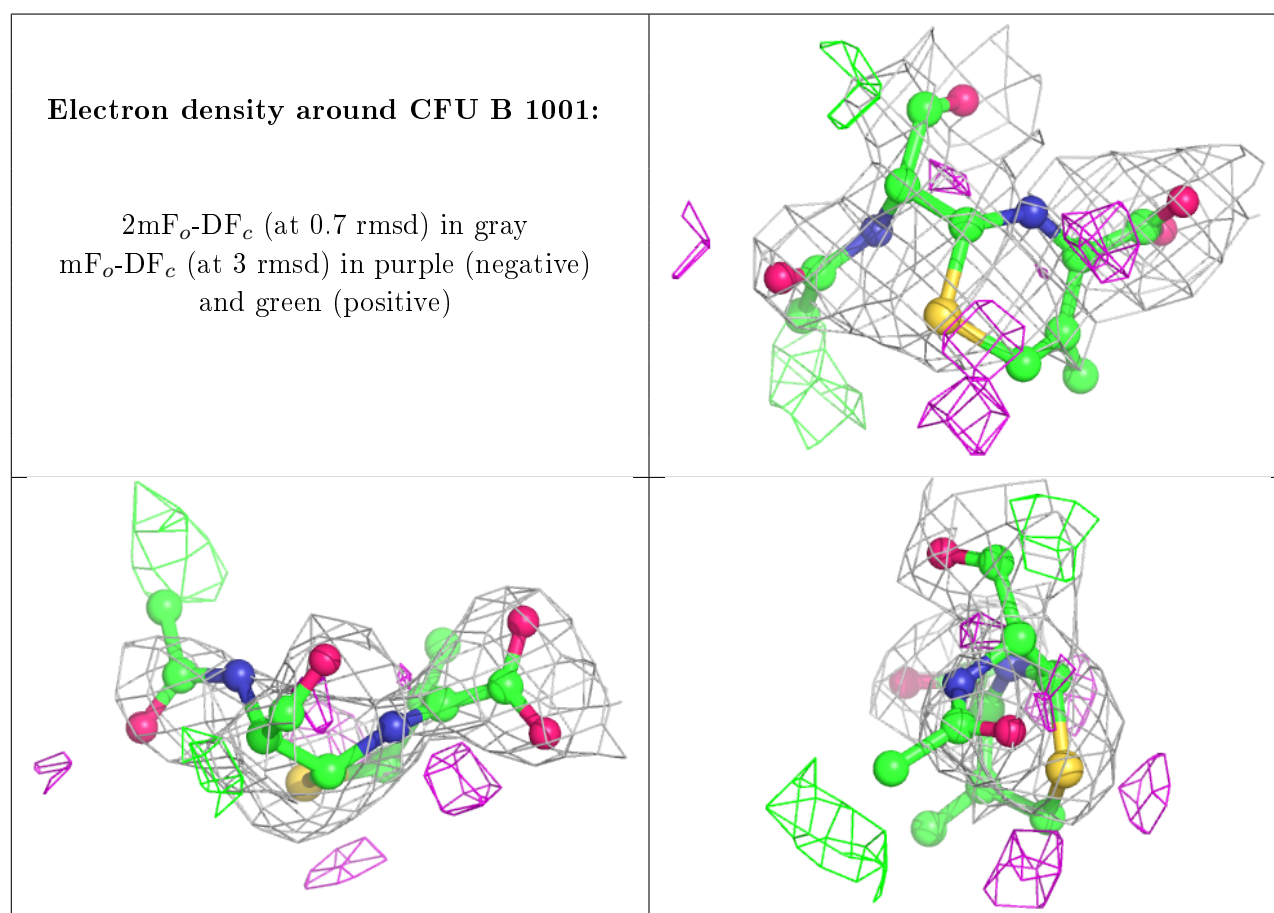
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CFU	B	1001	17/17	0.84	0.22	74,85,92,92	0
2	CFU	A	1001	17/17	0.90	0.12	60,70,75,76	0
4	PO4	A	1003	5/5	0.91	0.23	67,70,82,83	0

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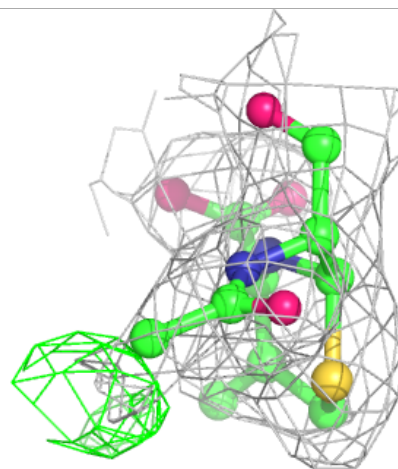
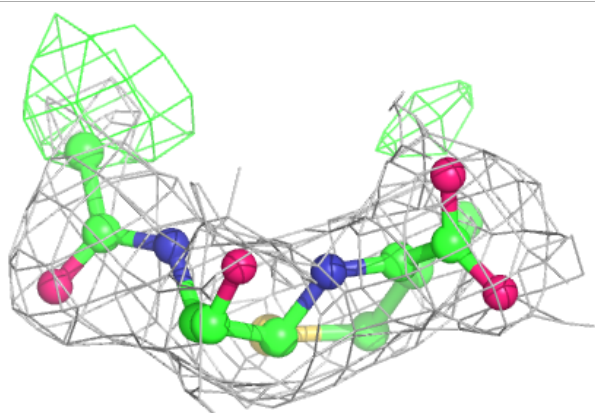
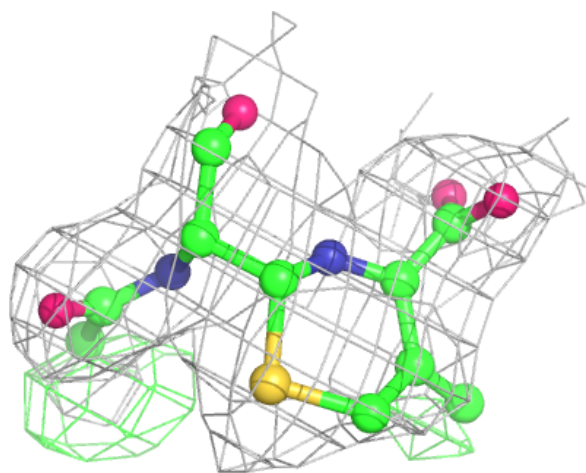
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	GOL	A	1002	6/6	0.91	0.16	48,49,53,59	0
3	GOL	B	1003	6/6	0.93	0.24	49,68,74,82	0
3	GOL	B	1002	6/6	0.95	0.13	42,42,46,50	0
4	PO4	A	1004	5/5	0.96	0.38	62,74,77,80	0
4	PO4	B	1004	5/5	0.96	0.15	52,52,62,66	0

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.



**Electron density around CFU A 1001:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.