



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 12:33 am GMT

PDB ID : 5AZP  
Title : Crystal structure of a membrane protein from *Pseudomonas aeruginosa*  
Authors : Yonehara, R.; Yamashita, E.; Nakagawa, A.  
Deposited on : 2015-10-21  
Resolution : 1.69 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

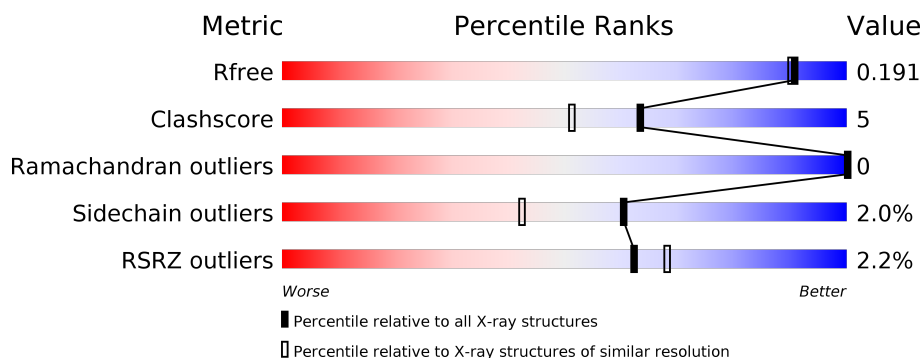
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.69 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))
$R_{free}$	100719	3453 (1.70-1.70)
Clashscore	112137	3876 (1.70-1.70)
Ramachandran outliers	110173	3815 (1.70-1.70)
Sidechain outliers	110143	3815 (1.70-1.70)
RSRZ outliers	101464	3491 (1.70-1.70)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	455	<div> <div>2%</div> <div> <div></div> <div>85%</div> <div>12%</div> <div>••</div> </div> </div>
1	B	455	<div> <div>2%</div> <div> <div></div> <div>86%</div> <div>10%</div> <div>••</div> </div> </div>
1	C	455	<div> <div>2%</div> <div> <div></div> <div>88%</div> <div>9%</div> <div>••</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	3PK	A	501	-	-	-	X
2	3PK	C	501	-	-	-	X
3	OYA	A	502	-	-	-	X
3	OYA	C	502	-	-	-	X
4	BOG	A	503	-	-	-	X
4	BOG	A	504	-	-	-	X
4	BOG	A	505	-	-	-	X
4	BOG	B	501	-	-	-	X
4	BOG	C	503	-	-	-	X
4	BOG	C	504	-	-	-	X
4	BOG	C	505	-	-	-	X
4	BOG	C	506	-	-	-	X
5	GOL	A	506	-	-	-	X
5	GOL	A	507	-	-	-	X
5	GOL	A	508	-	-	-	X
5	GOL	A	509	-	-	-	X
5	GOL	B	502	-	-	-	X
5	GOL	B	503	-	-	-	X
5	GOL	B	505	-	-	X	X
5	GOL	C	507	-	-	-	X
5	GOL	C	509	-	-	-	X
6	FMT	A	510	-	-	-	X
6	FMT	A	514	-	-	-	X
6	FMT	A	515	-	-	-	X
6	FMT	B	507	-	-	-	X
6	FMT	B	508	-	-	-	X
6	FMT	B	509	-	-	-	X
6	FMT	B	511	-	-	-	X
6	FMT	B	512	-	-	-	X
6	FMT	C	511	-	-	X	X
7	NA	B	513	-	-	-	X
8	ACT	A	517	-	-	-	X
8	ACT	B	514	-	-	-	X
8	ACT	B	515	-	-	X	X
8	ACT	B	516	-	-	X	-
8	ACT	C	517	-	-	-	X
8	ACT	C	518	-	-	-	X
8	ACT	C	519	-	-	X	X
8	ACT	C	520	-	-	-	X

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 13057 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 Multidrug efflux outer membrane protein OprN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	446	Total	C	N	O	S	0	30	0
			3584	2216	672	695	1			
1	B	450	Total	C	N	O	S	0	30	0
			3620	2244	673	702	1			
1	C	444	Total	C	N	O	S	0	34	0
			3589	2229	666	693	1			

There are 24 discrepancies between the modelled and reference sequences:

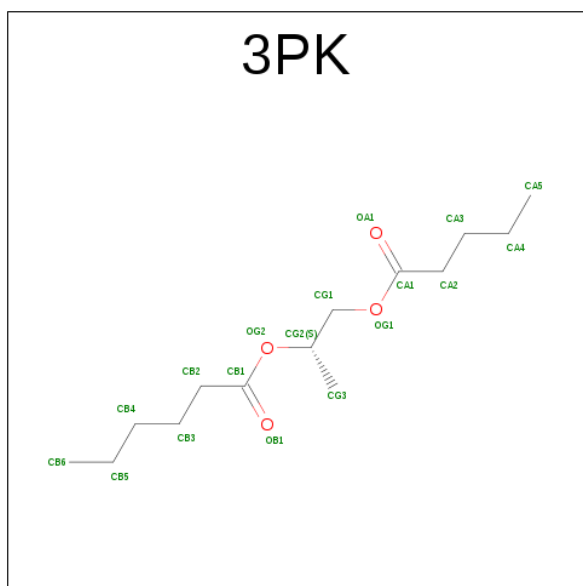
Chain	Residue	Modelled	Actual	Comment	Reference
A	448	GLY	-	expression tag	UNP Q9I0Y7
A	449	SER	-	expression tag	UNP Q9I0Y7
A	450	HIS	-	expression tag	UNP Q9I0Y7
A	451	HIS	-	expression tag	UNP Q9I0Y7
A	452	HIS	-	expression tag	UNP Q9I0Y7
A	453	HIS	-	expression tag	UNP Q9I0Y7
A	454	HIS	-	expression tag	UNP Q9I0Y7
A	455	HIS	-	expression tag	UNP Q9I0Y7
B	448	GLY	-	expression tag	UNP Q9I0Y7
B	449	SER	-	expression tag	UNP Q9I0Y7
B	450	HIS	-	expression tag	UNP Q9I0Y7
B	451	HIS	-	expression tag	UNP Q9I0Y7
B	452	HIS	-	expression tag	UNP Q9I0Y7
B	453	HIS	-	expression tag	UNP Q9I0Y7
B	454	HIS	-	expression tag	UNP Q9I0Y7
B	455	HIS	-	expression tag	UNP Q9I0Y7
C	448	GLY	-	expression tag	UNP Q9I0Y7
C	449	SER	-	expression tag	UNP Q9I0Y7
C	450	HIS	-	expression tag	UNP Q9I0Y7
C	451	HIS	-	expression tag	UNP Q9I0Y7
C	452	HIS	-	expression tag	UNP Q9I0Y7
C	453	HIS	-	expression tag	UNP Q9I0Y7
C	454	HIS	-	expression tag	UNP Q9I0Y7

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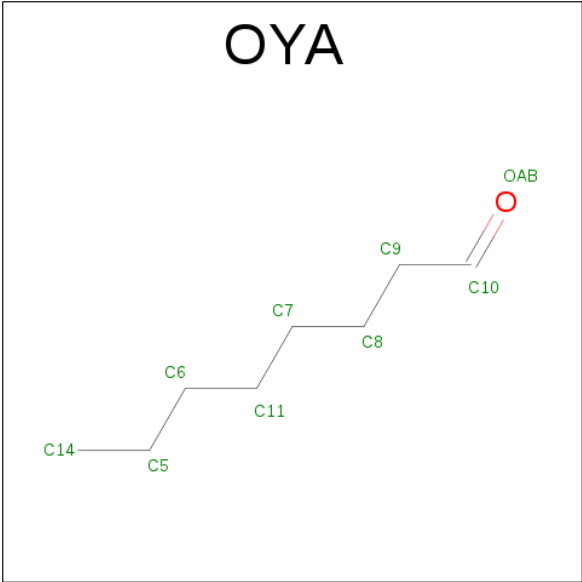
Chain	Residue	Modelled	Actual	Comment	Reference
C	455	HIS	-	expression tag	UNP Q9I0Y7

- Molecule 2 is (2S)-1-(pentanoyloxy)propan-2-yl hexanoate (three-letter code: 3PK) (formula:  $C_{14}H_{26}O_4$ ).



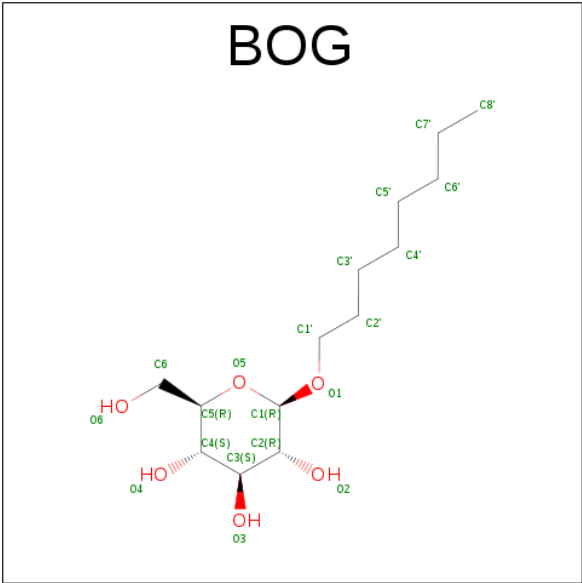
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			18	14	4		
2	C	1	Total	C	O	0	0
			18	14	4		

- Molecule 3 is OCTANAL (three-letter code: OYA) (formula:  $C_8H_{16}O$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			9	8	1		
3	C	1	Total	C	O	0	0
			9	8	1		

- Molecule 4 is B-OCTYLGLUCOSIDE (three-letter code: BOG) (formula: C<sub>14</sub>H<sub>28</sub>O<sub>6</sub>).



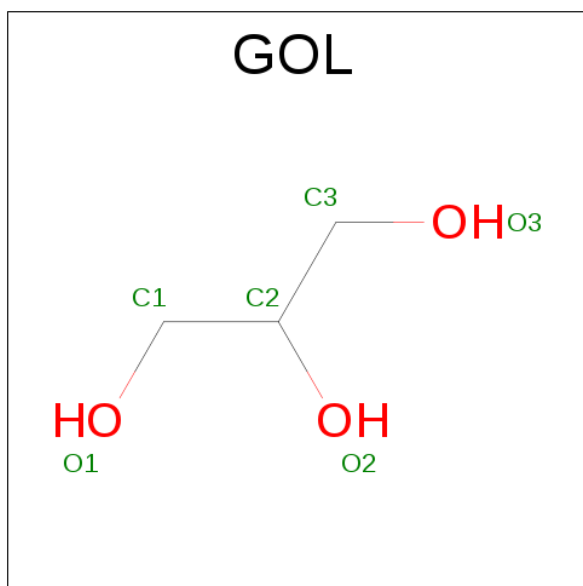
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			20	14	6		
4	A	1	Total	C	O	0	0
			20	14	6		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			20	14	6		
4	B	1	Total	C	O	0	0
			20	14	6		
4	C	1	Total	C	O	0	0
			20	14	6		
4	C	1	Total	C	O	0	0
			20	14	6		
4	C	1	Total	C	O	0	0
			20	14	6		
4	C	1	Total	C	O	0	0
			20	14	6		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



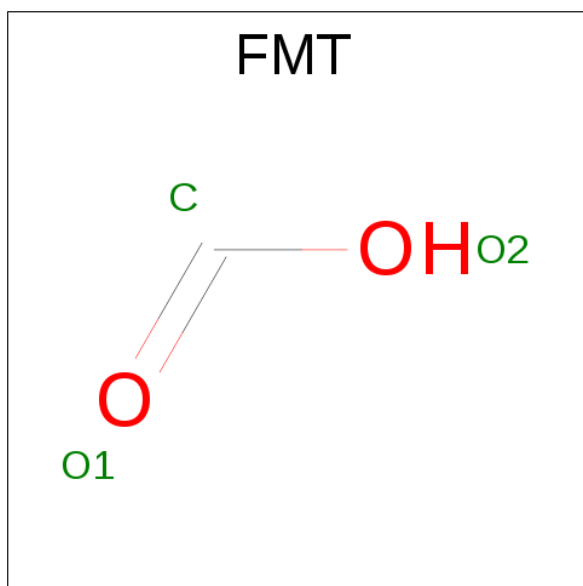
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		

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

- Molecule 6 is FORMIC ACID (three-letter code: FMT) (formula: CH<sub>2</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			3	1	2		
6	A	1	Total	C	O	0	0
			3	1	2		
6	A	1	Total	C	O	0	0
			3	1	2		
6	A	1	Total	C	O	0	0
			3	1	2		

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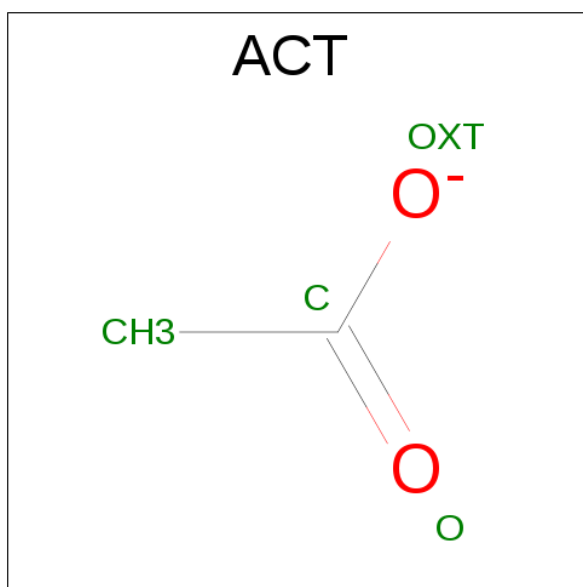
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			3	1	2		
6	A	1	Total	C	O	0	0
			3	1	2		
6	B	1	Total	C	O	0	0
			3	1	2		
6	B	1	Total	C	O	0	0
			3	1	2		
6	B	1	Total	C	O	0	0
			3	1	2		
6	B	1	Total	C	O	0	0
			3	1	2		
6	B	1	Total	C	O	0	0
			3	1	2		
6	B	1	Total	C	O	0	0
			3	1	2		
6	C	1	Total	C	O	0	0
			3	1	2		
6	C	1	Total	C	O	0	0
			3	1	2		
6	C	1	Total	C	O	0	0
			3	1	2		
6	C	1	Total	C	O	0	0
			3	1	2		

- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Na	0	0
			1	1		
7	A	1	Total	Na	0	0
			1	1		
7	C	1	Total	Na	0	0
			1	1		

- Molecule 8 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			4	2	2		
8	A	1	Total	C	O	0	0
			4	2	2		
8	B	1	Total	C	O	0	0
			4	2	2		
8	B	1	Total	C	O	0	0
			4	2	2		
8	B	1	Total	C	O	0	0
			4	2	2		
8	C	1	Total	C	O	0	0
			4	2	2		
8	C	1	Total	C	O	0	0
			4	2	2		
8	C	1	Total	C	O	0	0
			4	2	2		
8	C	1	Total	C	O	0	0
			4	2	2		

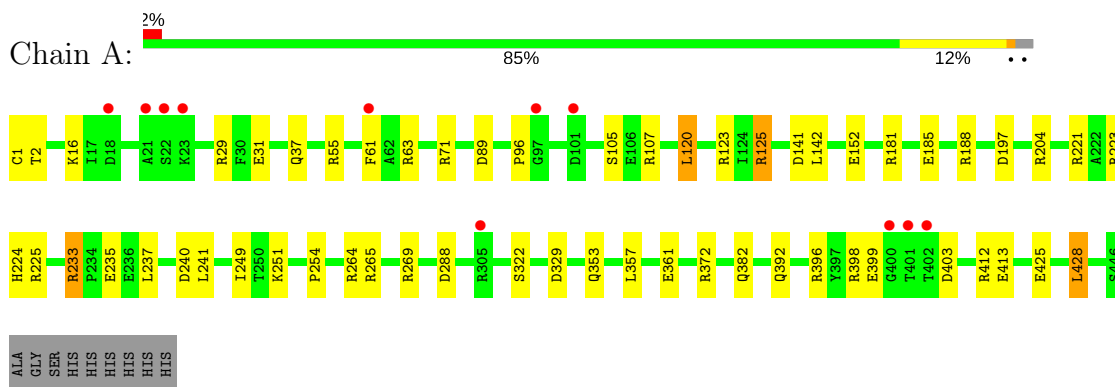
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	660	Total	O	0	0
			660	660		
9	B	627	Total	O	0	0
			627	627		
9	C	598	Total	O	0	0
			598	598		

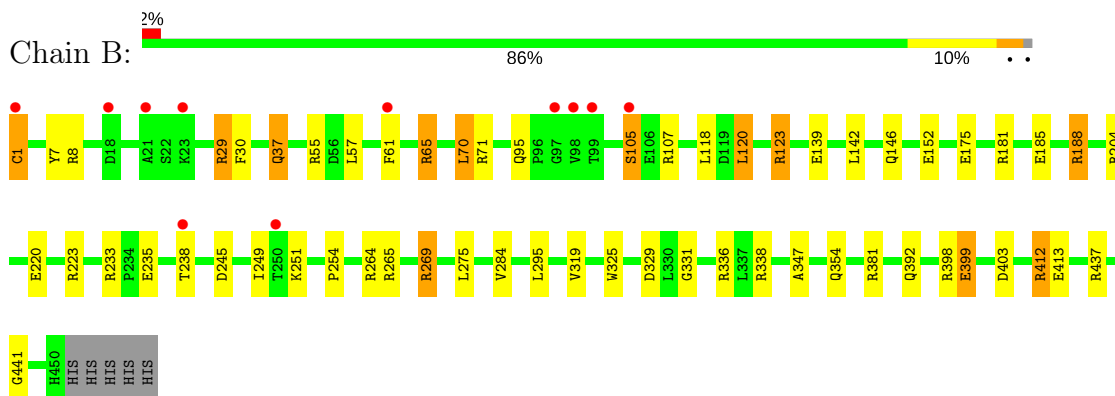
### 3 Residue-property plots [i](#)

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.

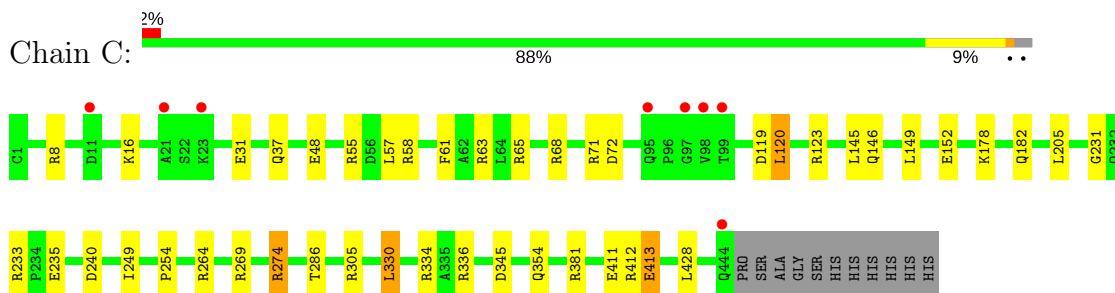
- Molecule 1: Multidrug efflux outer membrane protein OprN



- Molecule 1: Multidrug efflux outer membrane protein OprN



- Molecule 1: Multidrug efflux outer membrane protein OprN



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	257.51Å 257.51Å 81.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.69 39.92 – 1.69	Depositor EDS
% Data completeness (in resolution range)	99.4 (50.00-1.69) 99.4 (39.92-1.69)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.94 (at 1.69Å)	Xtriage
Refinement program	REFMAC 5.8.0131	Depositor
R, $R_{free}$	0.160 , 0.180 0.173 , 0.191	Depositor DCC
$R_{free}$ test set	15011 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	20.8	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 58.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.010 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	13057	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.89% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, NA, FMT, 3PK, ACT, OYA, BOG

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	1.01	5/3720 (0.1%)	1.12	36/5030 (0.7%)
1	B	1.07	7/3760 (0.2%)	1.30	36/5084 (0.7%)
1	C	1.02	7/3739 (0.2%)	1.12	29/5056 (0.6%)
All	All	1.03	19/11219 (0.2%)	1.19	101/15170 (0.7%)

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
1	A	0	1

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	399	GLU	CD-OE1	7.28	1.33	1.25
1	B	399	GLU	CB-CG	-6.68	1.39	1.52
1	A	31	GLU	CD-OE1	6.64	1.32	1.25
1	A	235	GLU	CD-OE2	6.39	1.32	1.25
1	B	152	GLU	CD-OE1	6.31	1.32	1.25

The worst 5 of 101 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	65[A]	ARG	NE-CZ-NH1	-21.97	109.31	120.30
1	B	65[B]	ARG	NE-CZ-NH1	-21.97	109.31	120.30
1	B	65[A]	ARG	NE-CZ-NH2	19.70	130.15	120.30
1	B	65[B]	ARG	NE-CZ-NH2	19.70	130.15	120.30
1	C	123[A]	ARG	NE-CZ-NH2	-12.92	113.84	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	399	GLU	Peptide

## 5.2 Too-close contacts ⓘ

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	3584	0	3636	26	0
1	B	3620	0	3677	53	0
1	C	3589	0	3662	26	0
2	A	18	0	25	0	0
2	C	18	0	25	0	0
3	A	9	0	15	0	0
3	C	9	0	15	0	0
4	A	60	0	84	0	0
4	B	20	0	28	0	0
4	C	80	0	112	1	0
5	A	24	0	32	3	0
5	B	24	0	32	10	0
5	C	24	0	32	3	0
6	A	18	0	8	0	0
6	B	21	0	8	1	0
6	C	15	0	6	3	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
8	A	8	0	6	1	0
8	B	12	0	9	7	0
8	C	16	0	12	3	0
9	A	660	0	0	6	4
9	B	627	0	0	16	3
9	C	598	0	0	10	0
All	All	13057	0	11424	111	4

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 5.

The worst 5 of 111 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:181[A]:ARG:NH2	1:A:185:GLU:OE1	1.87	1.05
1:B:29[A]:ARG:NH1	9:B:601:HOH:O	2.03	0.91
1:B:37[B]:GLN:HE22	1:B:254:PRO:HG2	1.36	0.90
1:B:37[B]:GLN:HE22	1:B:254:PRO:CG	1.85	0.89
1:B:57[A]:LEU:HD12	1:B:142[A]:LEU:CD1	2.04	0.87

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:1055:HOH:O	9:B:1089:HOH:O[8_445]	1.74	0.46
9:A:672:HOH:O	9:B:1089:HOH:O[8_445]	2.01	0.19
9:A:922:HOH:O	9:A:1078:HOH:O[8_445]	2.07	0.13
9:A:1055:HOH:O	9:B:844:HOH:O[8_445]	2.16	0.04

## 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	474/455 (104%)	468 (99%)	6 (1%)	0	100	100
1	B	479/455 (105%)	472 (98%)	7 (2%)	0	100	100
1	C	476/455 (105%)	467 (98%)	9 (2%)	0	100	100
All	All	1429/1365 (105%)	1407 (98%)	22 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	376/353 (106%)	368 (98%)	8 (2%)	59	40
1	B	379/353 (107%)	368 (97%)	11 (3%)	48	26
1	C	378/353 (107%)	373 (99%)	5 (1%)	73	60
All	All	1133/1059 (107%)	1109 (98%)	24 (2%)	60	40

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	37[A]	GLN
1	B	70[B]	LEU
1	C	120	LEU
1	B	37[B]	GLN
1	B	70[A]	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	76	ASN
1	B	95	GLN
1	C	176	ASN
1	B	45	GLN
1	C	159	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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



## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 54 ligands modelled in this entry, 3 are monoatomic - leaving 51 for Mogul analysis.

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	3PK	A	501	1	17,17,17	0.57	0	19,19,19	0.39	0
3	OYA	A	502	1	8,8,8	0.94	1 (12%)	7,7,7	0.81	1 (14%)
4	BOG	A	503	-	20,20,20	0.51	0	25,25,25	0.83	1 (4%)
4	BOG	A	504	-	20,20,20	0.83	1 (5%)	25,25,25	1.53	4 (16%)
4	BOG	A	505	-	20,20,20	0.75	1 (5%)	25,25,25	1.33	3 (12%)
5	GOL	A	506	-	5,5,5	0.41	0	5,5,5	0.44	0
5	GOL	A	507	-	5,5,5	0.67	0	5,5,5	1.42	1 (20%)
5	GOL	A	508	-	5,5,5	0.14	0	5,5,5	0.99	0
5	GOL	A	509	-	5,5,5	0.46	0	5,5,5	0.58	0
6	FMT	A	510	-	0,2,2	0.00	-	0,1,1	0.00	-
6	FMT	A	511	-	0,2,2	0.00	-	0,1,1	0.00	-
6	FMT	A	512	-	0,2,2	0.00	-	0,1,1	0.00	-
6	FMT	A	513	-	0,2,2	0.00	-	0,1,1	0.00	-
6	FMT	A	514	7	0,2,2	0.00	-	0,1,1	0.00	-
6	FMT	A	515	-	0,2,2	0.00	-	0,1,1	0.00	-
8	ACT	A	517	-	1,3,3	1.05	0	0,3,3	0.00	-
8	ACT	A	518	-	1,3,3	2.03	1 (100%)	0,3,3	0.00	-
4	BOG	B	501	-	20,20,20	0.55	0	25,25,25	0.78	0
5	GOL	B	502	-	5,5,5	0.38	0	5,5,5	1.14	0
5	GOL	B	503	-	5,5,5	0.37	0	5,5,5	0.23	0
5	GOL	B	504	-	5,5,5	0.32	0	5,5,5	0.80	0
5	GOL	B	505	-	5,5,5	0.14	0	5,5,5	1.14	0
6	FMT	B	506	-	0,2,2	0.00	-	0,1,1	0.00	-
6	FMT	B	507	-	0,2,2	0.00	-	0,1,1	0.00	-
6	FMT	B	508	-	0,2,2	0.00	-	0,1,1	0.00	-
6	FMT	B	509	-	0,2,2	0.00	-	0,1,1	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	FMT	B	510	-	0,2,2	0.00	-	0,1,1	0.00	-
6	FMT	B	511	-	0,2,2	0.00	-	0,1,1	0.00	-
6	FMT	B	512	-	0,2,2	0.00	-	0,1,1	0.00	-
8	ACT	B	514	-	1,3,3	0.79	0	0,3,3	0.00	-
8	ACT	B	515	-	1,3,3	3.94	1 (100%)	0,3,3	0.00	-
8	ACT	B	516	-	1,3,3	1.22	0	0,3,3	0.00	-
2	3PK	C	501	1	17,17,17	0.55	0	19,19,19	0.84	1 (5%)
3	OYA	C	502	1	8,8,8	1.12	1 (12%)	7,7,7	0.56	0
4	BOG	C	503	-	20,20,20	0.74	1 (5%)	25,25,25	1.51	4 (16%)
4	BOG	C	504	-	20,20,20	0.54	0	25,25,25	0.91	2 (8%)
4	BOG	C	505	-	20,20,20	1.84	3 (15%)	25,25,25	2.50	13 (52%)
4	BOG	C	506	-	20,20,20	0.49	0	25,25,25	1.41	5 (20%)
5	GOL	C	507	-	5,5,5	0.33	0	5,5,5	0.44	0
5	GOL	C	508	-	5,5,5	0.41	0	5,5,5	1.08	0
5	GOL	C	509	-	5,5,5	0.36	0	5,5,5	0.49	0
5	GOL	C	510	-	5,5,5	0.40	0	5,5,5	0.28	0
6	FMT	C	511	-	0,2,2	0.00	-	0,1,1	0.00	-
6	FMT	C	512	-	0,2,2	0.00	-	0,1,1	0.00	-
6	FMT	C	513	-	0,2,2	0.00	-	0,1,1	0.00	-
6	FMT	C	514	-	0,2,2	0.00	-	0,1,1	0.00	-
6	FMT	C	515	-	0,2,2	0.00	-	0,1,1	0.00	-
8	ACT	C	517	-	1,3,3	0.77	0	0,3,3	0.00	-
8	ACT	C	518	-	1,3,3	0.56	0	0,3,3	0.00	-
8	ACT	C	519	-	1,3,3	2.51	1 (100%)	0,3,3	0.00	-
8	ACT	C	520	-	1,3,3	2.28	1 (100%)	0,3,3	0.00	-

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	3PK	A	501	1	-	0/18/18/18	0/0/0/0
3	OYA	A	502	1	-	0/5/6/6	0/0/0/0
4	BOG	A	503	-	-	0/11/31/31	0/1/1/1
4	BOG	A	504	-	-	0/11/31/31	0/1/1/1
4	BOG	A	505	-	-	0/11/31/31	0/1/1/1
5	GOL	A	506	-	-	0/4/4/4	0/0/0/0
5	GOL	A	507	-	-	0/4/4/4	0/0/0/0
5	GOL	A	508	-	-	0/4/4/4	0/0/0/0
5	GOL	A	509	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	FMT	A	510	-	-	0/0/0/0	0/0/0/0
6	FMT	A	511	-	-	0/0/0/0	0/0/0/0
6	FMT	A	512	-	-	0/0/0/0	0/0/0/0
6	FMT	A	513	-	-	0/0/0/0	0/0/0/0
6	FMT	A	514	7	-	0/0/0/0	0/0/0/0
6	FMT	A	515	-	-	0/0/0/0	0/0/0/0
8	ACT	A	517	-	-	0/0/0/0	0/0/0/0
8	ACT	A	518	-	-	0/0/0/0	0/0/0/0
4	BOG	B	501	-	-	0/11/31/31	0/1/1/1
5	GOL	B	502	-	-	0/4/4/4	0/0/0/0
5	GOL	B	503	-	-	0/4/4/4	0/0/0/0
5	GOL	B	504	-	-	0/4/4/4	0/0/0/0
5	GOL	B	505	-	-	0/4/4/4	0/0/0/0
6	FMT	B	506	-	-	0/0/0/0	0/0/0/0
6	FMT	B	507	-	-	0/0/0/0	0/0/0/0
6	FMT	B	508	-	-	0/0/0/0	0/0/0/0
6	FMT	B	509	-	-	0/0/0/0	0/0/0/0
6	FMT	B	510	-	-	0/0/0/0	0/0/0/0
6	FMT	B	511	-	-	0/0/0/0	0/0/0/0
6	FMT	B	512	-	-	0/0/0/0	0/0/0/0
8	ACT	B	514	-	-	0/0/0/0	0/0/0/0
8	ACT	B	515	-	-	0/0/0/0	0/0/0/0
8	ACT	B	516	-	-	0/0/0/0	0/0/0/0
2	3PK	C	501	1	-	0/18/18/18	0/0/0/0
3	OYA	C	502	1	-	0/5/6/6	0/0/0/0
4	BOG	C	503	-	-	0/11/31/31	0/1/1/1
4	BOG	C	504	-	-	0/11/31/31	0/1/1/1
4	BOG	C	505	-	-	0/11/31/31	0/1/1/1
4	BOG	C	506	-	-	0/11/31/31	0/1/1/1
5	GOL	C	507	-	-	0/4/4/4	0/0/0/0
5	GOL	C	508	-	-	0/4/4/4	0/0/0/0
5	GOL	C	509	-	-	0/4/4/4	0/0/0/0
5	GOL	C	510	-	-	0/4/4/4	0/0/0/0
6	FMT	C	511	-	-	0/0/0/0	0/0/0/0
6	FMT	C	512	-	-	0/0/0/0	0/0/0/0
6	FMT	C	513	-	-	0/0/0/0	0/0/0/0
6	FMT	C	514	-	-	0/0/0/0	0/0/0/0
6	FMT	C	515	-	-	0/0/0/0	0/0/0/0
8	ACT	C	517	-	-	0/0/0/0	0/0/0/0
8	ACT	C	518	-	-	0/0/0/0	0/0/0/0
8	ACT	C	519	-	-	0/0/0/0	0/0/0/0
8	ACT	C	520	-	-	0/0/0/0	0/0/0/0

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	OYA	C9-C10	2.00	1.55	1.49
8	A	518	ACT	CH3-C	2.03	1.51	1.48
4	A	505	BOG	O1-C1	2.24	1.44	1.40
8	C	520	ACT	CH3-C	2.28	1.51	1.48
8	C	519	ACT	CH3-C	2.51	1.52	1.48

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	505	BOG	C4-C3-C2	-4.90	102.19	110.84
4	C	505	BOG	C6-C5-C4	-3.60	104.58	113.00
4	C	505	BOG	C1-C2-C3	-3.41	103.64	109.98
4	A	505	BOG	C1'-O1-C1	-2.55	109.48	113.87
4	C	506	BOG	C1'-O1-C1	-2.38	109.78	113.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

15 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	508	GOL	1	0
5	A	509	GOL	2	0
8	A	517	ACT	1	0
5	B	502	GOL	2	0
5	B	504	GOL	1	0
5	B	505	GOL	7	0
6	B	507	FMT	1	0
8	B	515	ACT	3	0
8	B	516	ACT	4	0
4	C	505	BOG	1	0
5	C	508	GOL	3	0
6	C	511	FMT	2	0
6	C	514	FMT	1	0
8	C	518	ACT	1	0
8	C	519	ACT	2	0

## 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, 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	446/455 (98%)	-0.26	11 (2%) 58 63	13, 22, 44, 62	0
1	B	450/455 (98%)	-0.31	11 (2%) 59 64	14, 21, 42, 53	0
1	C	444/455 (97%)	-0.37	8 (1%) 69 74	14, 21, 42, 64	0
All	All	1340/1365 (98%)	-0.32	30 (2%) 62 68	13, 21, 43, 64	0

The worst 5 of 30 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	97	GLY	3.8
1	A	402[A]	THR	3.7
1	C	98	VAL	3.6
1	B	97	GLY	3.3
1	B	23	LYS	3.2

### 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
6	FMT	A	514	3/3	0.94	0.26	18.83	49,49,49,54	0
5	GOL	A	506	6/6	0.92	0.17	17.06	25,36,47,55	0
4	BOG	C	506	20/20	0.67	0.21	15.75	50,65,76,84	0
5	GOL	A	509	6/6	0.88	0.22	14.46	34,50,57,59	0
5	GOL	B	502	6/6	0.89	0.28	13.83	36,49,53,55	0
8	ACT	C	519	4/4	0.58	0.28	13.80	55,58,62,64	0
4	BOG	C	504	20/20	0.81	0.21	13.75	40,49,62,64	0
6	FMT	B	511	3/3	0.97	0.30	12.27	46,46,52,52	0
4	BOG	C	503	20/20	0.80	0.18	12.27	55,65,82,82	0
5	GOL	B	505	6/6	0.80	0.30	11.65	41,48,50,59	0
6	FMT	B	508	3/3	0.89	0.20	10.90	36,36,41,50	0
6	FMT	B	507	3/3	0.83	0.23	10.69	34,34,47,48	0
4	BOG	A	503	20/20	0.87	0.17	10.38	41,52,72,75	0
5	GOL	A	508	6/6	0.89	0.34	9.95	40,47,49,49	0
4	BOG	A	504	20/20	0.59	0.35	9.90	57,80,89,94	0
8	ACT	C	520	4/4	0.72	0.15	9.60	52,59,63,66	0
8	ACT	B	515	4/4	0.45	0.26	8.38	31,41,46,47	0
4	BOG	C	505	20/20	0.75	0.24	8.20	38,52,60,62	0
6	FMT	C	511	3/3	0.62	0.26	6.53	45,45,47,49	0
3	OYA	C	502	9/9	0.83	0.19	6.34	39,57,70,70	0
8	ACT	C	518	4/4	0.91	0.11	6.28	37,39,40,44	0
5	GOL	A	507	6/6	0.73	0.16	6.03	40,52,55,59	0
2	3PK	A	501	18/18	0.57	0.20	5.42	54,66,68,69	0
8	ACT	C	517	4/4	0.87	0.15	5.40	34,43,47,48	0
2	3PK	C	501	18/18	0.69	0.16	5.35	42,56,62,68	0
4	BOG	B	501	20/20	0.82	0.19	5.29	46,53,63,66	0
6	FMT	B	509	3/3	0.84	0.16	5.12	44,44,54,55	0
7	NA	B	513	1/1	0.99	0.10	4.94	27,27,27,27	0
6	FMT	B	512	3/3	0.64	0.17	4.84	53,53,57,61	0
6	FMT	A	515	3/3	0.68	0.16	3.97	48,48,53,59	0
6	FMT	A	510	3/3	0.82	0.22	3.86	24,24,33,39	0
8	ACT	A	517	4/4	0.89	0.10	3.81	34,35,39,45	0
3	OYA	A	502	9/9	0.78	0.15	3.62	49,54,62,62	0
5	GOL	B	503	6/6	0.57	0.21	3.35	64,71,73,77	0
5	GOL	C	507	6/6	0.88	0.12	3.00	44,45,47,48	0
4	BOG	A	505	20/20	0.69	0.23	2.89	43,56,64,66	0
5	GOL	C	509	6/6	0.74	0.18	2.64	55,60,61,61	0
8	ACT	B	514	4/4	0.84	0.13	2.08	38,38,39,45	0
6	FMT	C	515	3/3	0.93	0.08	1.62	56,56,56,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	GOL	B	504	6/6	0.89	0.11	1.07	44,45,48,53	0
7	NA	A	516	1/1	0.97	0.08	0.88	32,32,32,32	0
6	FMT	A	513	3/3	0.94	0.14	0.85	33,33,40,47	0
7	NA	C	516	1/1	0.98	0.06	-0.57	30,30,30,30	0
5	GOL	C	510	6/6	0.78	0.27	-	58,61,63,63	0
5	GOL	C	508	6/6	0.85	0.17	-	41,46,52,52	0
8	ACT	A	518	4/4	0.74	0.28	-	67,68,70,71	0
6	FMT	A	512	3/3	0.78	0.21	-	48,48,61,66	0
6	FMT	B	510	3/3	0.86	0.10	-	71,71,78,80	0
6	FMT	C	513	3/3	0.85	0.13	-	37,37,45,50	0
6	FMT	B	506	3/3	0.82	0.15	-	40,40,54,56	0
6	FMT	A	511	3/3	0.81	0.28	-	41,41,42,52	0
6	FMT	C	512	3/3	0.90	0.10	-	30,30,42,48	0
8	ACT	B	516	4/4	0.57	0.22	-	30,46,52,55	0
6	FMT	C	514	3/3	0.55	0.23	-	50,50,59,60	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.