



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 04:48 am BST

PDB ID : 3K7C  
Title : Crystal structure of Putative NTF2-like transpeptidase (NP\_281412.1) from CAMPYLOBACTER JEJUNI at 2.00 Å resolution  
Authors : Joint Center for Structural Genomics (JCSG)  
Deposited on : 2009-10-12  
Resolution : 2.00 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  
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

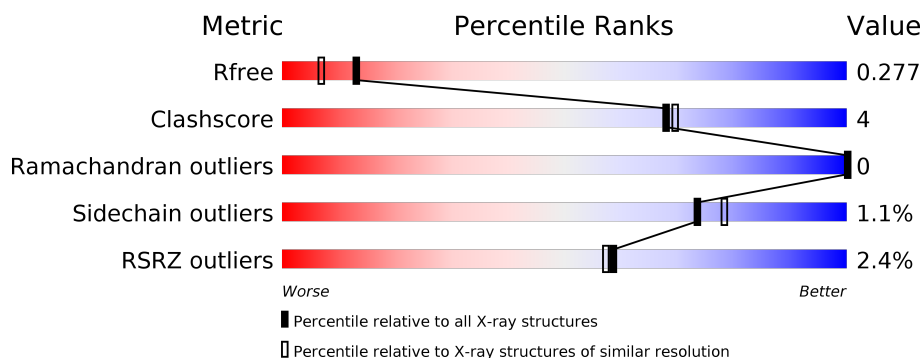
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	114	<div> <div>2%</div> <div> <div></div> <div>86%</div> <div>8%</div> <div>5%</div> </div> </div>
1	B	114	<div> <div>4%</div> <div> <div></div> <div>88%</div> <div>5%</div> <div>5%</div> </div> </div>
1	C	114	<div> <div>2%</div> <div> <div></div> <div>87%</div> <div>8%</div> <div>5%</div> </div> </div>
1	D	114	<div> <div>2%</div> <div> <div></div> <div>82%</div> <div>11%</div> <div>5%</div> </div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3664 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 Putative NTF2-like transpeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	108	Total	C	N	O	Se	0	4	0
			863	542	145	174	2			
1	B	108	Total	C	N	O	Se	0	1	0
			848	530	146	170	2			
1	C	108	Total	C	N	O	Se	0	2	0
			828	522	136	168	2			
1	D	108	Total	C	N	O	Se	0	3	0
			850	535	140	173	2			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	leader sequence	UNP Q0PBT7
B	0	GLY	-	leader sequence	UNP Q0PBT7
C	0	GLY	-	leader sequence	UNP Q0PBT7
D	0	GLY	-	leader sequence	UNP Q0PBT7

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cl	0	0
			1	1		

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			5	3	2		
3	B	1	Total	C	O	0	0
			7	4	3		
3	C	1	Total	C	O	0	0
			5	3	2		
3	C	1	Total	C	O	0	0
			6	4	2		
3	C	1	Total	C	O	0	0
			7	4	3		
3	C	1	Total	C	O	0	0
			6	4	2		
3	C	1	Total	C	O	0	0
			5	3	2		
3	C	1	Total	C	O	0	0
			7	4	3		
3	C	1	Total	C	O	0	0
			7	4	3		
3	D	1	Total	C	O	0	0
			7	4	3		

- Molecule 4 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			9	6	3		
4	B	1	Total	C	O	0	0
			8	5	3		
4	B	1	Total	C	O	0	0
			10	6	4		
4	B	1	Total	C	O	0	0
			10	6	4		
4	D	1	Total	C	O	0	0
			10	6	4		
4	D	1	Total	C	O	0	0
			10	6	4		

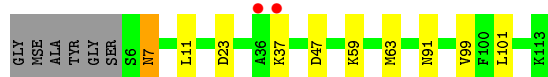
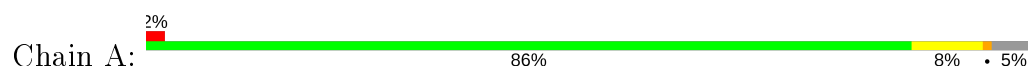
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	38	Total	O	0	1
			38	38		
5	B	38	Total	O	0	0
			38	38		
5	C	24	Total	O	0	0
			24	24		
5	D	34	Total	O	0	0
			34	34		

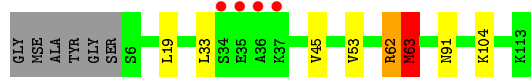
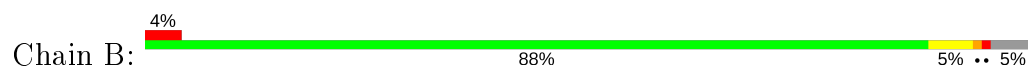
### 3 Residue-property plots [i](#)

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.

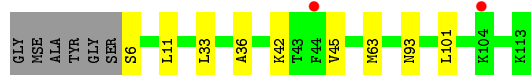
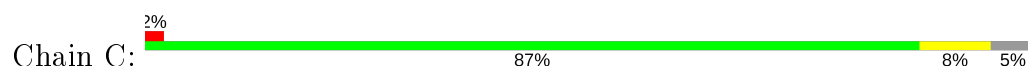
- Molecule 1: Putative NTF2-like transpeptidase



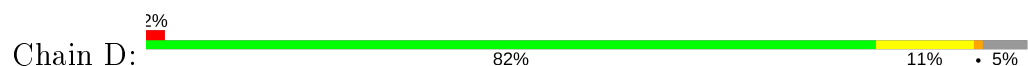
- Molecule 1: Putative NTF2-like transpeptidase



- Molecule 1: Putative NTF2-like transpeptidase



- Molecule 1: Putative NTF2-like transpeptidase



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	94.44Å 89.81Å 59.66Å 90.00° 110.50° 90.00°	Depositor
Resolution (Å)	28.57 – 2.00 28.57 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.3 (28.57-2.00) 99.3 (28.57-2.00)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.66 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0102, PHENIX	Depositor
R, $R_{free}$	0.214 , 0.256 0.230 , 0.277	Depositor DCC
$R_{free}$ test set	1576 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.7	Xtriage
Anisotropy	0.589	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 53.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	3664	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.51% 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: PEG, PGE, CL

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	0.79	0/877	0.84	2/1173 (0.2%)
1	B	0.78	0/854	0.88	5/1141 (0.4%)
1	C	0.76	0/840	0.82	0/1128
1	D	0.81	0/865	0.88	1/1159 (0.1%)
All	All	0.79	0/3436	0.86	8/4601 (0.2%)

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	B	0	1
1	D	0	1
All	All	0	2

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	62[A]	ARG	NE-CZ-NH1	6.53	123.57	120.30
1	B	62[B]	ARG	NE-CZ-NH1	6.53	123.57	120.30
1	D	62	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	B	63	MSE	CG-SE-CE	-5.86	86.02	98.90
1	A	23	ASP	CB-CG-OD2	-5.53	113.32	118.30
1	A	47	ASP	CB-CG-OD1	5.50	123.25	118.30
1	B	62[A]	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	B	62[B]	ARG	NE-CZ-NH2	-5.22	117.69	120.30

There are no chirality outliers.



All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	104	LYS	Peptide
1	D	6	SER	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	863	0	866	7	0
1	B	848	0	850	8	0
1	C	828	0	808	4	0
1	D	850	0	846	8	0
2	A	1	0	0	0	0
3	A	14	0	20	0	0
3	B	19	0	25	0	0
3	C	43	0	54	0	0
3	D	7	0	10	0	0
4	A	9	0	11	1	0
4	B	28	0	37	0	0
4	D	20	0	28	0	0
5	A	38	0	0	1	0
5	B	38	0	0	0	0
5	C	24	0	0	0	0
5	D	34	0	0	1	0
All	All	3664	0	3555	27	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 4.

All (27) 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:B:62[B]:ARG:HH11	1:B:62[B]:ARG:HG2	1.15	1.08
1:B:62[B]:ARG:CG	1:B:62[B]:ARG:HH11	1.91	0.83
1:D:31:ILE:HD13	1:D:112:LEU:HD21	1.72	0.70
1:D:11:LEU:HD23	1:D:101:LEU:HD23	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62[B]:ARG:NH1	1:B:62[B]:ARG:HG2	1.97	0.63
1:B:19:LEU:HD12	1:B:53:VAL:HG22	1.80	0.63
1:D:53:VAL:HG12	5:D:128:HOH:O	2.01	0.60
1:B:62[B]:ARG:CG	1:B:62[B]:ARG:NH1	2.59	0.60
1:A:11:LEU:HD23	1:A:101:LEU:HD23	1.83	0.59
1:B:63:MSE:HE2	1:B:91:ASN:HD21	1.68	0.59
1:B:33:LEU:HD21	1:B:45:VAL:HG11	1.86	0.58
1:C:33:LEU:HD21	1:C:45:VAL:HG11	1.86	0.56
1:D:63:MSE:HE2	1:D:91:ASN:HD21	1.70	0.56
1:A:7[A]:ASN:OD1	1:A:7[A]:ASN:C	2.43	0.56
1:A:59:LYS:NZ	5:A:135:HOH:O	2.38	0.55
1:A:63:MSE:HE2	1:A:91:ASN:HD21	1.73	0.54
1:D:19:LEU:HD12	1:D:53:VAL:HG22	1.92	0.52
1:A:11:LEU:HD23	1:A:101:LEU:CD2	2.40	0.51
1:D:23:ASP:O	1:D:27:VAL:HG23	2.11	0.49
1:C:63:MSE:CE	1:C:93:ASN:HB2	2.43	0.49
1:D:8:PRO:HG2	1:D:76:ILE:HD13	1.96	0.48
1:A:99:VAL:HG22	4:A:117:PGE:H1	1.97	0.47
1:D:63:MSE:HE2	1:D:91:ASN:ND2	2.30	0.46
1:C:11:LEU:HD23	1:C:101:LEU:HD23	1.98	0.44
1:C:36:ALA:HB3	1:C:42:LYS:HE3	2.00	0.43
1:A:37[A]:LYS:HE3	1:A:37[A]:LYS:HB3	1.66	0.42
1:B:63:MSE:HE2	1:B:91:ASN:ND2	2.34	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	110/114 (96%)	109 (99%)	1 (1%)	0	100	100
1	B	107/114 (94%)	103 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	108/114 (95%)	106 (98%)	2 (2%)	0	100	100
1	D	109/114 (96%)	106 (97%)	3 (3%)	0	100	100
All	All	434/456 (95%)	424 (98%)	10 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	95/97 (98%)	93 (98%)	2 (2%)	53	57
1	B	93/97 (96%)	92 (99%)	1 (1%)	73	78
1	C	87/97 (90%)	86 (99%)	1 (1%)	73	78
1	D	93/97 (96%)	92 (99%)	1 (1%)	73	78
All	All	368/388 (95%)	363 (99%)	5 (1%)	73	72

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7[A]	ASN
1	A	7[B]	ASN
1	B	63	MSE
1	C	6	SER
1	D	63	MSE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 20 ligands modelled in this entry, 1 is monoatomic - leaving 19 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	$\# Z  > 2$
3	PEG	A	116	-	6,6,6	0.51	0	5,5,5	0.45	0
3	PEG	B	116	-	6,6,6	0.69	0	5,5,5	0.53	0
3	PEG	C	116	-	6,6,6	0.75	0	5,5,5	1.29	1 (20%)
3	PEG	C	119	-	6,6,6	0.46	0	5,5,5	0.23	0
3	PEG	C	120	-	6,6,6	0.60	0	5,5,5	0.59	0
3	PEG	B	114	-	6,6,6	0.55	0	5,5,5	0.35	0
3	PEG	B	115	-	4,4,6	0.47	0	3,3,5	0.31	0
3	PEG	C	117	-	5,5,6	0.84	0	4,4,5	0.96	0
4	PGE	D	116	-	9,9,9	0.49	0	8,8,8	0.22	0
3	PEG	D	114	-	6,6,6	0.55	0	5,5,5	0.55	0
4	PGE	D	115	-	9,9,9	0.68	0	8,8,8	0.99	0
3	PEG	C	115	-	5,5,6	0.62	0	4,4,5	0.53	0
3	PEG	C	114	-	4,4,6	0.44	0	3,3,5	0.38	0
3	PEG	C	118	-	4,4,6	0.62	0	3,3,5	0.37	0
4	PGE	A	117	-	8,8,9	0.67	0	7,7,8	0.83	0
4	PGE	B	117	-	7,7,9	0.52	0	6,6,8	0.57	0
4	PGE	B	119	-	9,9,9	0.63	0	8,8,8	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	PEG	A	115	-	6,6,6	0.49	0	5,5,5	0.39	0
4	PGE	B	118	-	9,9,9	0.56	0	8,8,8	0.59	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PEG	A	116	-	-	2/4/4/4	-
3	PEG	B	116	-	-	2/4/4/4	-
3	PEG	C	116	-	-	2/4/4/4	-
3	PEG	C	119	-	-	2/4/4/4	-
3	PEG	C	120	-	-	2/4/4/4	-
3	PEG	B	114	-	-	1/4/4/4	-
3	PEG	B	115	-	-	1/2/2/4	-
3	PEG	C	117	-	-	2/3/3/4	-
4	PGE	D	116	-	-	1/7/7/7	-
3	PEG	D	114	-	-	1/4/4/4	-
4	PGE	D	115	-	-	4/7/7/7	-
3	PEG	C	115	-	-	2/3/3/4	-
3	PEG	C	114	-	-	1/2/2/4	-
3	PEG	C	118	-	-	2/2/2/4	-
4	PGE	A	117	-	-	2/6/6/7	-
4	PGE	B	117	-	-	2/5/5/7	-
4	PGE	B	119	-	-	4/7/7/7	-
3	PEG	A	115	-	-	2/4/4/4	-
4	PGE	B	118	-	-	3/7/7/7	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	116	PEG	C3-O2-C2	2.53	124.27	113.29

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	116	PEG	C1-C2-O2-C3
3	B	116	PEG	O1-C1-C2-O2
3	D	114	PEG	O1-C1-C2-O2
3	C	119	PEG	O1-C1-C2-O2
3	B	114	PEG	O1-C1-C2-O2
4	B	118	PGE	O2-C3-C4-O3
4	D	116	PGE	O3-C5-C6-O4
3	C	115	PEG	O1-C1-C2-O2
3	C	114	PEG	O1-C1-C2-O2
4	B	118	PGE	O3-C5-C6-O4
3	A	116	PEG	O2-C3-C4-O4
3	C	116	PEG	O2-C3-C4-O4
3	C	120	PEG	O1-C1-C2-O2
3	B	115	PEG	O1-C1-C2-O2
4	D	115	PGE	O3-C5-C6-O4
3	C	118	PEG	O1-C1-C2-O2
4	B	118	PGE	O1-C1-C2-O2
4	B	119	PGE	O3-C5-C6-O4
3	A	115	PEG	O1-C1-C2-O2
3	A	115	PEG	O2-C3-C4-O4
4	A	117	PGE	O2-C3-C4-O3
3	C	115	PEG	C4-C3-O2-C2
3	A	116	PEG	O1-C1-C2-O2
4	D	115	PGE	O1-C1-C2-O2
3	C	117	PEG	C1-C2-O2-C3
3	C	120	PEG	C1-C2-O2-C3
4	B	117	PGE	C3-C4-O3-C5
4	D	115	PGE	C3-C4-O3-C5
4	B	117	PGE	O2-C3-C4-O3
3	B	116	PEG	O2-C3-C4-O4
4	A	117	PGE	C3-C4-O3-C5
3	C	119	PEG	C1-C2-O2-C3
4	B	119	PGE	O2-C3-C4-O3
4	D	115	PGE	O2-C3-C4-O3
3	C	118	PEG	C1-C2-O2-C3
3	C	117	PEG	C4-C3-O2-C2
4	B	119	PGE	C4-C3-O2-C2
4	B	119	PGE	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	117	PGE	1	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	106/114 (92%)	-0.02	2 (1%) 66 65	6, 15, 24, 38	0
1	B	106/114 (92%)	0.36	4 (3%) 40 39	9, 15, 28, 38	0
1	C	106/114 (92%)	0.14	2 (1%) 66 65	10, 16, 26, 38	0
1	D	106/114 (92%)	0.09	2 (1%) 66 65	8, 16, 24, 41	0
All	All	424/456 (92%)	0.14	10 (2%) 59 57	6, 16, 25, 41	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	36	ALA	6.6
1	B	37	LYS	4.9
1	B	35	GLU	4.9
1	B	34	SER	4.2
1	C	44	PHE	4.0
1	D	6	SER	3.8
1	D	113	LYS	2.7
1	C	104	LYS	2.3
1	A	37[A]	LYS	2.0
1	A	36	ALA	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(Å <sup>2</sup> )	Q<0.9
3	PEG	C	118	5/7	0.50	0.24	51,53,59,60	0
3	PEG	B	116	7/7	0.51	0.28	68,70,72,72	0
3	PEG	B	114	7/7	0.53	0.28	63,65,67,68	0
3	PEG	C	120	7/7	0.60	0.24	47,51,51,53	7
3	PEG	A	115	7/7	0.65	0.20	70,70,71,71	0
4	PGE	B	119	10/10	0.67	0.26	54,64,65,66	0
3	PEG	B	115	5/7	0.68	0.31	64,65,67,67	0
3	PEG	C	116	7/7	0.69	0.27	53,56,58,58	0
3	PEG	C	117	6/7	0.72	0.22	43,56,59,60	0
3	PEG	A	116	7/7	0.72	0.21	71,73,76,76	0
4	PGE	D	116	10/10	0.74	0.21	59,61,67,68	0
2	CL	A	114	1/1	0.75	0.23	79,79,79,79	0
4	PGE	B	118	10/10	0.81	0.15	46,54,60,61	0
3	PEG	D	114	7/7	0.83	0.25	68,69,70,70	0
3	PEG	C	119	7/7	0.87	0.13	61,63,64,65	0
4	PGE	B	117	8/10	0.89	0.19	38,42,43,45	0
3	PEG	C	114	5/7	0.89	0.22	49,49,51,52	0
3	PEG	C	115	6/7	0.91	0.29	59,64,65,65	0
4	PGE	D	115	10/10	0.92	0.16	33,38,44,46	0
4	PGE	A	117	9/10	0.93	0.20	29,34,42,42	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.