wwPDB X-ray Structure Validation Summary Report (i)

Jun 25, 2024 – 11:45 PM EDT

PDB ID	:	6T9M
Title	:	Crystal structure of the Chitinase Domain of the Spore Coat Protein CotE from Clostridium difficile
Authors	:	Whittingham, J.L.; Dodson, E.J.; Wilkinson, A.J.
Deposited on	:	2019-10-28
Resolution	:	1.30 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

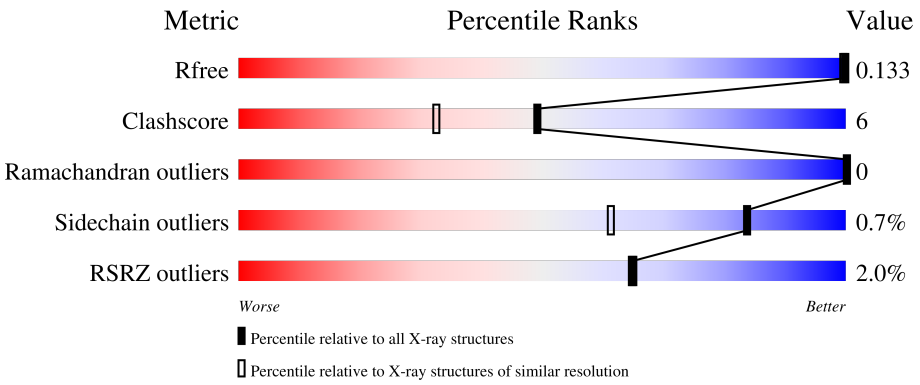
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

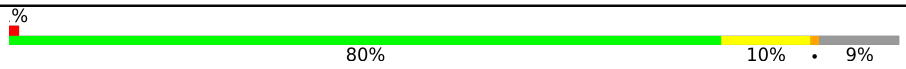
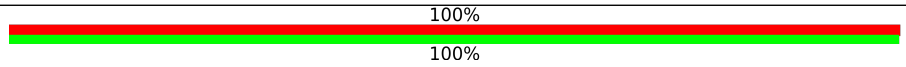
The reported resolution of this entry is 1.30 Å.

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	1058 (1.30-1.30)
Clashscore	141614	1101 (1.30-1.30)
Ramachandran outliers	138981	1058 (1.30-1.30)
Sidechain outliers	138945	1058 (1.30-1.30)
RSRZ outliers	127900	1029 (1.30-1.30)

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 <=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	AAA	386	
2	BBB	5	

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
3	1PE	AAA	801	-	X	-	-
4	PEG	AAA	804	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 6277 atoms, of which 2858 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 Peroxiredoxin.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	AAA	350	5588	1806	2745	469	558	10	136	12	0

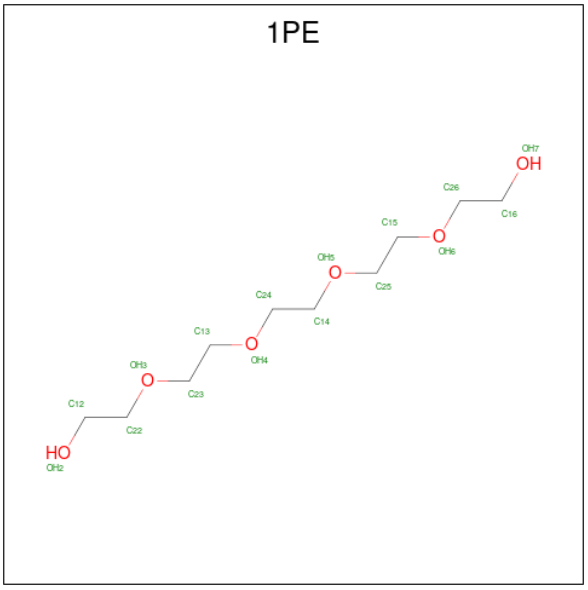
There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	327	MET	-	initiating methionine	UNP Q18BV5
AAA	328	GLY	-	expression tag	UNP Q18BV5
AAA	329	SER	-	expression tag	UNP Q18BV5
AAA	330	SER	-	expression tag	UNP Q18BV5
AAA	331	HIS	-	expression tag	UNP Q18BV5
AAA	332	HIS	-	expression tag	UNP Q18BV5
AAA	333	HIS	-	expression tag	UNP Q18BV5
AAA	334	HIS	-	expression tag	UNP Q18BV5
AAA	335	HIS	-	expression tag	UNP Q18BV5
AAA	336	HIS	-	expression tag	UNP Q18BV5
AAA	337	SER	-	expression tag	UNP Q18BV5
AAA	338	SER	-	expression tag	UNP Q18BV5
AAA	339	GLY	-	expression tag	UNP Q18BV5
AAA	340	LEU	-	expression tag	UNP Q18BV5
AAA	341	GLU	-	expression tag	UNP Q18BV5
AAA	342	VAL	-	expression tag	UNP Q18BV5
AAA	343	LEU	-	expression tag	UNP Q18BV5
AAA	344	PHE	-	expression tag	UNP Q18BV5
AAA	345	GLN	-	expression tag	UNP Q18BV5
AAA	346	GLY	-	expression tag	UNP Q18BV5
AAA	347	PRO	-	expression tag	UNP Q18BV5

- Molecule 2 is a protein called Peptide in active site.

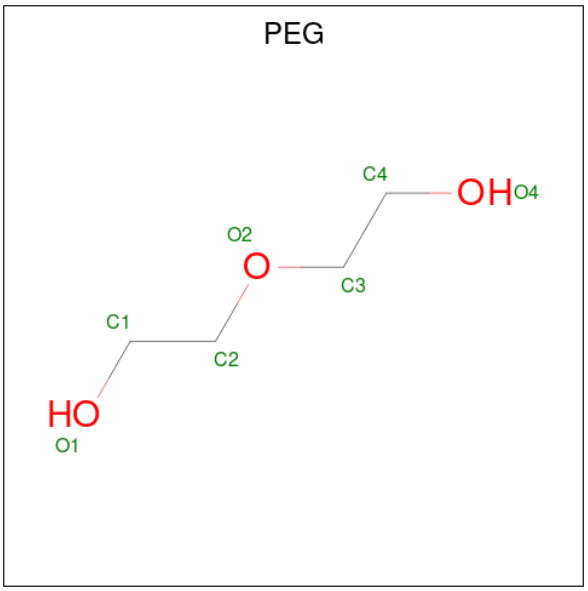
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	BBB	5	72	21	39	6	5	1	0	0	0

- Molecule 3 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
3	AAA	1	38	10	22	6	1	0
3	AAA	1	38	10	22	6	1	0

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
4	AAA	1	17	4	10	3	1	0
			Total	C	H	O		
4	AAA	1	17	4	10	3	1	0
			Total	C	H	O		
4	AAA	1	17	4	10	3	1	0

- Molecule 5 is water.

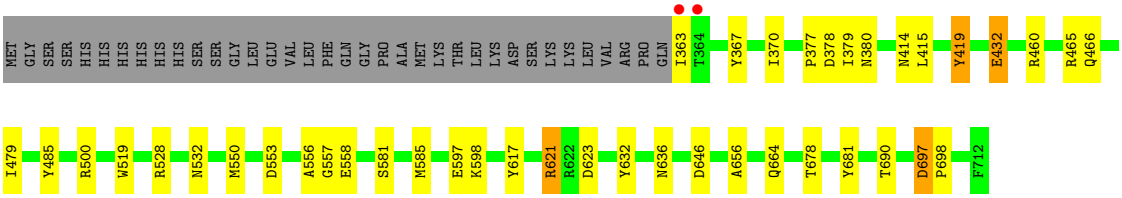
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	AAA	488	488	488	0	0
			Total	O		
5	BBB	2	2	2	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

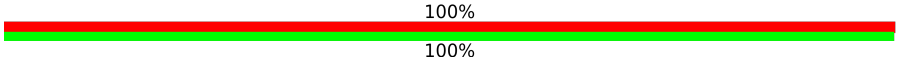
- Molecule 1: Peroxiredoxin

Chain AAA:



- Molecule 2: Peptide in active site

Chain BBB:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	45.89Å 54.90Å 80.31Å 90.00° 101.04° 90.00°	Depositor
Resolution (Å)	45.09 – 1.30 45.05 – 1.30	Depositor EDS
% Data completeness (in resolution range)	97.9 (45.09-1.30) 97.9 (45.05-1.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	6.12 (at 1.30Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.105 , 0.133 0.106 , 0.133	Depositor DCC
R_{free} test set	4557 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å^2)	11.4	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 47.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	6277	wwPDB-VP
Average B, all atoms (Å^2)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.95% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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, 1PE

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	AAA	0.93	7/2907 (0.2%)	1.09	16/3954 (0.4%)
2	BBB	0.95	0/33	0.96	0/42
All	All	0.93	7/2940 (0.2%)	1.09	16/3996 (0.4%)

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AAA	557	GLY	N-CA	8.51	1.58	1.46
1	AAA	432	GLU	CD-OE2	-7.29	1.17	1.25
1	AAA	597	GLU	CD-OE1	6.34	1.32	1.25
1	AAA	528	ARG	CD-NE	-5.84	1.36	1.46
1	AAA	557	GLY	CA-C	5.47	1.60	1.51

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AAA	556	ALA	C-N-CA	-9.72	101.88	122.30
1	AAA	485	TYR	CB-CG-CD2	-7.84	116.29	121.00
1	AAA	697	ASP	CB-CG-OD2	-6.25	112.67	118.30
1	AAA	500	ARG	NE-CZ-NH1	-6.07	117.27	120.30
1	AAA	621[A]	ARG	NE-CZ-NH2	-6.03	117.29	120.30

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	AAA	2843	2745	2733	28	1
2	BBB	33	39	39	0	0
3	AAA	32	44	44	7	0
4	AAA	21	30	30	9	0
5	AAA	488	0	0	8	2
5	BBB	2	0	0	1	0
All	All	3419	2858	2846	34	2

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 6.

The worst 5 of 34 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)
3:AAA:802:1PE:OH7	4:AAA:803:PEG:O4	1.76	1.03
3:AAA:801:1PE:H251	5:AAA:1040:HOH:O	1.73	0.88
3:AAA:801:1PE:OH7	3:AAA:802:1PE:OH2	1.93	0.85
1:AAA:598:LYS:NZ	4:AAA:804:PEG:H22	1.93	0.83
1:AAA:370:ILE:H	1:AAA:664:GLN:HE22	1.29	0.80

All (2) 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)
5:AAA:949:HOH:O	5:AAA:1305:HOH:O[2_545]	1.14	1.06
1:AAA:465:ARG:HD3	5:AAA:916:HOH:O[2_546]	1.46	0.14

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	AAA	360/386 (93%)	352 (98%)	8 (2%)	0	100	100
2	BBB	3/5 (60%)	2 (67%)	1 (33%)	0	100	100
All	All	363/391 (93%)	354 (98%)	9 (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	AAA	305/325 (94%)	303 (99%)	2 (1%)	84	61
2	BBB	3/3 (100%)	3 (100%)	0	100	100
All	All	308/328 (94%)	306 (99%)	2 (1%)	84	65

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	479	ILE
1	AAA	519	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

5 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	1PE	AAA	801	-	15,15,15	1.47	3 (20%)	14,14,14	3.33	9 (64%)
3	1PE	AAA	802	-	15,15,15	0.56	0	14,14,14	1.19	1 (7%)
4	PEG	AAA	805	-	6,6,6	0.77	0	5,5,5	0.53	0
4	PEG	AAA	804	-	6,6,6	0.69	0	5,5,5	0.68	0
4	PEG	AAA	803	-	6,6,6	0.32	0	5,5,5	0.38	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	1PE	AAA	801	-	-	9/13/13/13	-
3	1PE	AAA	802	-	-	3/13/13/13	-
4	PEG	AAA	805	-	-	3/4/4/4	-
4	PEG	AAA	804	-	-	3/4/4/4	-
4	PEG	AAA	803	-	-	3/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	AAA	801	1PE	OH5-C14	3.02	1.55	1.42
3	AAA	801	1PE	C23-C13	-2.53	1.35	1.49
3	AAA	801	1PE	OH4-C24	-2.46	1.31	1.42

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	AAA	801	1PE	OH3-C23-C13	-6.68	80.28	110.39
3	AAA	801	1PE	OH4-C13-C23	4.12	128.96	110.39
3	AAA	801	1PE	OH5-C14-C24	-4.12	91.83	110.39
3	AAA	801	1PE	C23-OH3-C22	-4.09	95.58	113.29
3	AAA	801	1PE	OH5-C25-C15	3.88	127.87	110.39

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	AAA	804	PEG	C1-C2-O2-C3
3	AAA	801	1PE	OH5-C14-C24-OH4
3	AAA	801	1PE	OH6-C15-C25-OH5
3	AAA	801	1PE	C16-C26-OH6-C15
4	AAA	804	PEG	O2-C3-C4-O4

There are no ring outliers.

4 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	AAA	801	1PE	5	0
3	AAA	802	1PE	3	0
4	AAA	804	PEG	7	0
4	AAA	803	PEG	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, 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	AAA	350/386 (90%)	-0.46	2 (0%) 89 88	7, 12, 25, 54	0
2	BBB	5/5 (100%)	2.61	5 (100%) 0 0	19, 22, 24, 45	0
All	All	355/391 (90%)	-0.42	7 (1%) 65 65	7, 12, 25, 54	0

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	363	ILE	5.4
1	AAA	364	THR	3.6
2	BBB	5	LYS	3.1
2	BBB	1	GLY	3.0
2	BBB	3	ALA	2.4

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 monosaccharides 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(Å^2)	Q<0.9
4	PEG	AAA	805	7/7	0.68	0.23	29,32,37,37	1
4	PEG	AAA	804	7/7	0.90	0.25	25,36,40,40	1
4	PEG	AAA	803	7/7	0.90	0.09	34,40,48,48	1
3	1PE	AAA	802	16/16	0.93	0.12	25,33,48,48	1
3	1PE	AAA	801	16/16	0.93	0.09	20,25,31,42	1

6.5 Other polymers (i)

There are no such residues in this entry.