



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 03:12 PM UTC

PDB ID : 7KNF / pdb\_00007knf  
Title : 1.80A resolution structure of independent Phosphoglycerate mutase from *C. elegans* in complex with a macrocyclic peptide inhibitor (Ce-1 NHOH)  
Authors : Lovell, S.; Kashipathy, M.M.; Battaile, K.P.; Weidmann, M.; Dranchak, P.; Aitha, M.; Queme, B.; Collmus, C.D.; Kanter, L.; Lamy, L.; Tao, D.; Rai, G.; Suga, H.; Inglese, J.  
Deposited on : 2020-11-04  
Resolution : 1.80 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

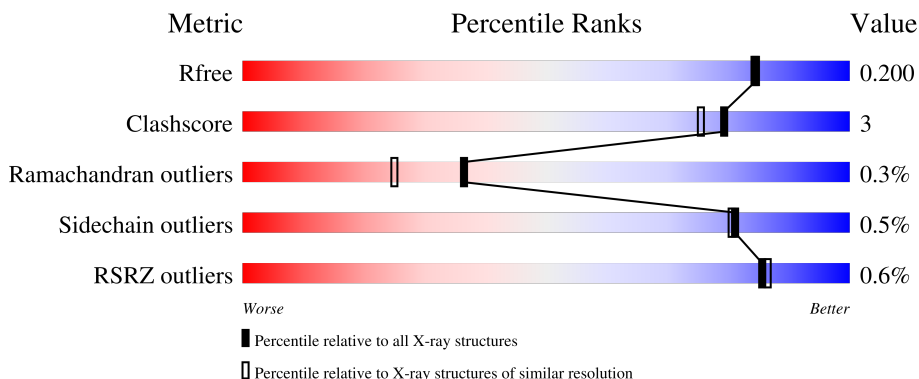
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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  $\geq 3$ , 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	538	 88% 6% 6%
1	B	538	 88% 6% 6%
2	C	15	 93% 7%
2	D	15	 93% 7%

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 8698 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 2,3-bisphosphoglycerate-independent phosphoglycerate mutase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	506	3869	2456	659	726	28	0	5	0
1	B	505	3826	2435	646	718	27	0	4	0

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	540	LYS	-	expression tag	UNP G5EFZ1
A	541	LEU	-	expression tag	UNP G5EFZ1
A	542	ALA	-	expression tag	UNP G5EFZ1
A	543	ALA	-	expression tag	UNP G5EFZ1
A	544	ALA	-	expression tag	UNP G5EFZ1
A	545	LEU	-	expression tag	UNP G5EFZ1
A	546	GLU	-	expression tag	UNP G5EFZ1
A	547	HIS	-	expression tag	UNP G5EFZ1
A	548	HIS	-	expression tag	UNP G5EFZ1
A	549	HIS	-	expression tag	UNP G5EFZ1
A	550	HIS	-	expression tag	UNP G5EFZ1
A	551	HIS	-	expression tag	UNP G5EFZ1
A	552	HIS	-	expression tag	UNP G5EFZ1
A	553	HIS	-	expression tag	UNP G5EFZ1
A	554	HIS	-	expression tag	UNP G5EFZ1
A	555	HIS	-	expression tag	UNP G5EFZ1
A	556	HIS	-	expression tag	UNP G5EFZ1
B	540	LYS	-	expression tag	UNP G5EFZ1
B	541	LEU	-	expression tag	UNP G5EFZ1
B	542	ALA	-	expression tag	UNP G5EFZ1
B	543	ALA	-	expression tag	UNP G5EFZ1
B	544	ALA	-	expression tag	UNP G5EFZ1
B	545	LEU	-	expression tag	UNP G5EFZ1
B	546	GLU	-	expression tag	UNP G5EFZ1
B	547	HIS	-	expression tag	UNP G5EFZ1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	548	HIS	-	expression tag	UNP G5EFZ1
B	549	HIS	-	expression tag	UNP G5EFZ1
B	550	HIS	-	expression tag	UNP G5EFZ1
B	551	HIS	-	expression tag	UNP G5EFZ1
B	552	HIS	-	expression tag	UNP G5EFZ1
B	553	HIS	-	expression tag	UNP G5EFZ1
B	554	HIS	-	expression tag	UNP G5EFZ1
B	555	HIS	-	expression tag	UNP G5EFZ1
B	556	HIS	-	expression tag	UNP G5EFZ1

- Molecule 2 is a protein called DTY-ASP-TYR-PRO-GLY-ASP-HIS-CYS-TYR-LEU-TYR-GLY-THR.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
2	C	15	Total	C	N	O	S	0	0	1
			108	68	16	23	1			
2	D	15	Total	C	N	O	S	0	0	1
			108	68	16	23	1			

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Zn	0	0
			2	2		
3	B	2	Total	Zn	0	0
			2	2		

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Na	0	0
			2	2		
4	B	2	Total	Na	0	0
			2	2		

- Molecule 5 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C<sub>8</sub>H<sub>18</sub>O<sub>5</sub>).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	416	Total O 416 416	0	0
6	B	307	Total O 307 307	0	0
6	C	14	Total O 14 14	0	0
6	D	12	Total O 12 12	0	0



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.67Å 75.85Å 100.42Å 90.00° 98.31° 90.00°	Depositor
Resolution (Å)	44.13 – 1.80 44.13 – 1.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (44.13-1.80) 99.9 (44.13-1.80)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.99 (at 1.79Å)	Xtrriage
Refinement program	PHENIX 1.18rc1_3769	Depositor
R, $R_{free}$	0.152 , 0.194 0.163 , 0.200	Depositor DCC
$R_{free}$ test set	5042 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.0	Xtrriage
Anisotropy	0.619	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 47.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	8698	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.46% 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: DTY, ACE, HOA, PG4, CSO, NA, ZN

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	0.44	0/3955	0.61	0/5365
1	B	0.40	0/3909	0.59	1/5309 (0.0%)
2	C	0.46	0/94	0.62	0/128
2	D	0.44	0/94	0.54	0/128
All	All	0.42	0/8052	0.60	1/10930 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	172	PHE	CA-CB-CG	5.05	118.85	113.80

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	3869	0	3734	24	0
1	B	3826	0	3655	19	0
2	C	108	0	81	1	0
2	D	108	0	81	1	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	20	0	26	1	0
5	B	10	0	13	1	0
6	A	416	0	0	1	0
6	B	307	0	0	2	0
6	C	14	0	0	0	0
6	D	12	0	0	0	0
All	All	8698	0	7590	42	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 3.

The worst 5 of 42 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:481:LYS:NZ	6:B:701:HOH:O	2.29	0.65
1:B:86:SER:OG	2:D:14:HOA:O	2.16	0.62
1:B:231[A]:ILE:HD13	1:B:272:VAL:HB	1.83	0.61
1:A:371:LEU:C	1:A:371:LEU:HD12	2.26	0.61
1:A:86:SER:HB3	1:A:362:HIS:CD2	2.40	0.56

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	505/538 (94%)	496 (98%)	7 (1%)	2 (0%)	30 19
1	B	503/538 (94%)	493 (98%)	9 (2%)	1 (0%)	43 31
2	C	12/15 (80%)	11 (92%)	1 (8%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	12/15 (80%)	11 (92%)	1 (8%)	0	100	100
All	All	1032/1106 (93%)	1011 (98%)	18 (2%)	3 (0%)	36	25

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	470	ASN
1	A	470	ASN
1	A	468	HIS

### 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	394/434 (91%)	392 (100%)	2 (0%)	81	80
1	B	381/434 (88%)	379 (100%)	2 (0%)	81	80
2	C	9/10 (90%)	9 (100%)	0	100	100
2	D	9/10 (90%)	9 (100%)	0	100	100
All	All	793/888 (89%)	789 (100%)	4 (0%)	81	80

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	269	LYS
1	A	478	ASP
1	B	180	SER
1	B	335	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	ASN
1	A	314	GLN

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Mol	Chain	Res	Type
1	A	394	GLN
1	B	29	ASN
1	B	394	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](#)

6 non-standard protein/DNA/RNA residues 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
2	DTY	C	1	2	11,12,13	0.65	0	10,15,17	0.32	0
1	CSO	A	381	1	3,6,7	0.49	0	1,6,8	0.27	0
1	CSO	B	381	1	3,6,7	0.62	0	1,6,8	0.69	0
2	DTY	D	1	2	11,12,13	0.67	0	10,15,17	0.28	0
1	CSO	B	487	1	3,6,7	0.66	0	1,6,8	0.47	0
1	CSO	A	487	1	3,6,7	0.68	0	1,6,8	0.36	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	DTY	C	1	2	-	1/5/6/8	0/1/1/1
1	CSO	A	381	1	-	0/1/5/7	-
1	CSO	B	381	1	-	0/1/5/7	-
2	DTY	D	1	2	-	2/5/6/8	0/1/1/1
1	CSO	B	487	1	-	0/1/5/7	-
1	CSO	A	487	1	-	0/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1	DTY	O-C-CA-CB
2	D	1	DTY	CA-CB-CG-CD1
2	D	1	DTY	CA-CB-CG-CD2

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 8 are monoatomic - leaving 3 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	$\# Z  > 2$
5	PG4	A	606	-	9,9,12	0.25	0	8,8,11	0.15	0
5	PG4	B	605	-	9,9,12	0.22	0	8,8,11	0.24	0
5	PG4	A	605	-	9,9,12	0.15	0	8,8,11	0.20	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
5	PG4	A	606	-	-	3/7/7/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PG4	B	605	-	-	1/7/7/10	-
5	PG4	A	605	-	-	1/7/7/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	606	PG4	O4-C7-C8-O5
5	B	605	PG4	O2-C3-C4-O3
5	A	606	PG4	O3-C5-C6-O4
5	A	605	PG4	O2-C3-C4-O3
5	A	606	PG4	C3-C4-O3-C5

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	606	PG4	1	0
5	B	605	PG4	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	504/538 (93%)	-0.39	3 (0%) 85 86	9, 19, 32, 60	5 (0%)
1	B	503/538 (93%)	-0.14	3 (0%) 85 86	11, 24, 38, 51	4 (0%)
2	C	12/15 (80%)	-0.25	0 100 100	17, 21, 23, 29	0
2	D	12/15 (80%)	0.23	0 100 100	22, 25, 29, 34	0
All	All	1031/1106 (93%)	-0.26	6 (0%) 85 86	9, 22, 36, 60	9 (0%)

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	539	ILE	2.8
1	A	478	ASP	2.4
1	B	27	VAL	2.3
1	B	306	LYS	2.3
1	B	539	ILE	2.1

### 6.2 Non-standard residues in protein, DNA, RNA chains [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
2	DTY	D	1	12/13	0.94	0.07	19,22,27,27	0
1	CSO	B	381	7/8	0.95	0.09	18,22,26,30	0
1	CSO	A	381	7/8	0.97	0.06	17,21,26,27	0
1	CSO	B	487	7/8	0.97	0.05	18,22,26,30	0
2	DTY	C	1	12/13	0.97	0.06	15,19,22,23	0
1	CSO	A	487	7/8	0.97	0.06	13,17,20,22	0

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
5	PG4	A	606	10/13	0.81	0.14	29,33,46,51	0
5	PG4	B	605	10/13	0.85	0.13	30,36,54,54	0
5	PG4	A	605	10/13	0.92	0.10	28,35,46,48	0
4	NA	B	604	1/1	0.99	0.05	18,18,18,18	0
4	NA	A	603	1/1	0.99	0.06	19,19,19,19	0
4	NA	A	604	1/1	0.99	0.05	15,15,15,15	0
4	NA	B	603	1/1	0.99	0.04	22,22,22,22	0
3	ZN	B	602	1/1	1.00	0.03	20,20,20,20	0
3	ZN	A	601	1/1	1.00	0.01	14,14,14,14	0
3	ZN	A	602	1/1	1.00	0.01	17,17,17,17	0
3	ZN	B	601	1/1	1.00	0.01	18,18,18,18	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.