



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 12:12 pm BST

PDB ID : 6NUF  
Title : Structure of Calcineurin in complex with NHE1 peptide  
Authors : Wang, X.; Page, R.; Peti, W.  
Deposited on : 2019-01-31  
Resolution : 1.90 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

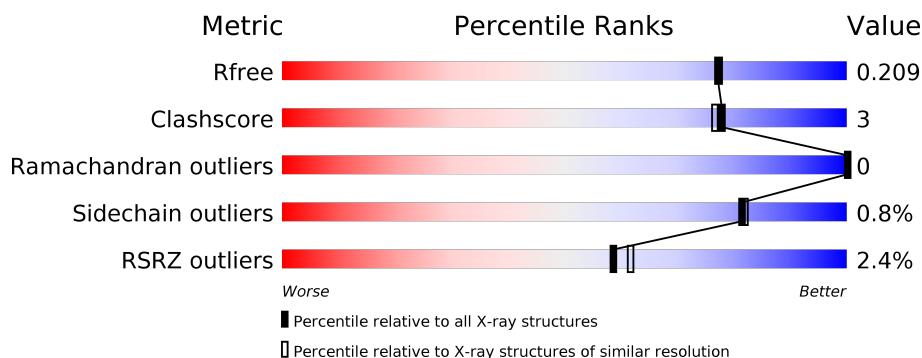
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	372	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 98%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 2px;"> <span>%</span> <span>90%</span> <span>7%</span> </div> </div>
2	B	156	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 3%, orange 1%, yellow 1%, green 95%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 2px;"> <span>3%</span> <span>97%</span> </div> </div>
3	C	48	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 10%, orange 1%, yellow 1%, green 35%, grey 53%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 2px;"> <span>10%</span> <span>35%</span> <span>60%</span> </div> </div>

## 2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 9109 atoms, of which 4272 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 Serine/threonine-protein phosphatase 2B catalytic subunit alpha isoform.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	360	Total	C	H	N	O	S	0	5	0
			5817	1896	2872	492	537	20			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q08209
A	0	HIS	-	expression tag	UNP Q08209

- Molecule 2 is a protein called Calcineurin subunit B type 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	156	Total	C	H	N	O	S	0	0	0
			2463	781	1223	206	246	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	15	MET	-	expression tag	UNP P63098

- Molecule 3 is a protein called Sodium/hydrogen exchanger 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	19	Total	C	H	N	O		0	0	0
			281	91	139	21	30				

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	676	GLY	-	expression tag	UNP P19634

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Chain	Residue	Modelled	Actual	Comment	Reference
C	677	HIS	-	expression tag	UNP P19634
C	678	MET	-	expression tag	UNP P19634
C	698	ALA	ARG	engineered mutation	UNP P19634
C	700	ALA	ARG	engineered mutation	UNP P19634

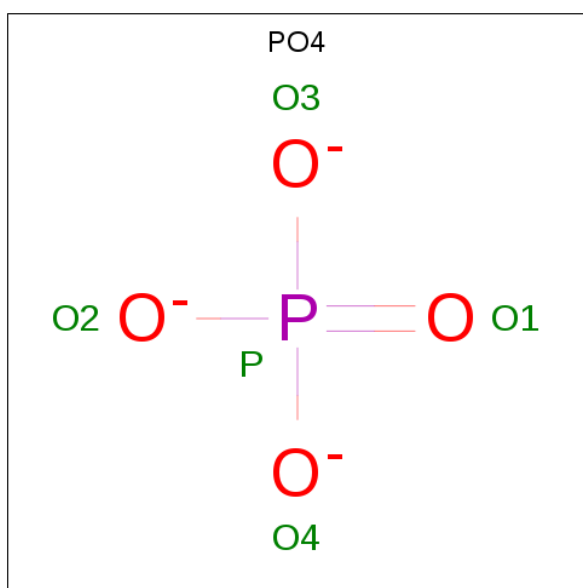
- Molecule 4 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Fe 1 1	0	0

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Zn 1 1	0	0

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



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

- Molecule 7 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
7	A	1	Total	C	H	O	0	0
			24	6	14	4		
7	A	1	Total	C	H	O	0	0
			24	6	14	4		

- Molecule 8 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).



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

- Molecule 9 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total Na 1 1	0	0

- Molecule 10 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	4	Total Ca 4 4	0	0

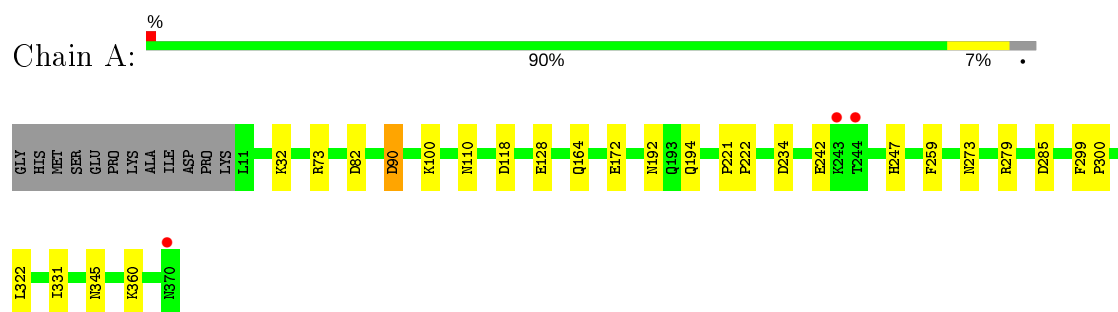
- Molecule 11 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	351	Total O 351 351	0	0
11	B	105	Total O 105 105	0	0
11	C	15	Total O 15 15	0	0

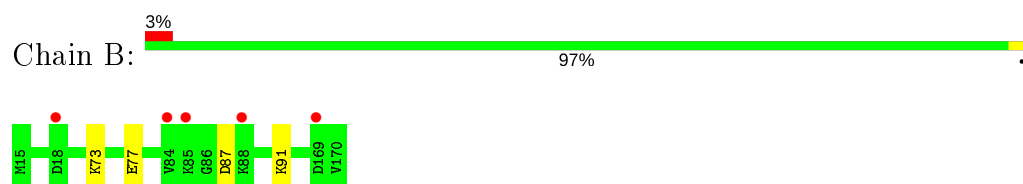
### 3 Residue-property plots [i](#)

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.

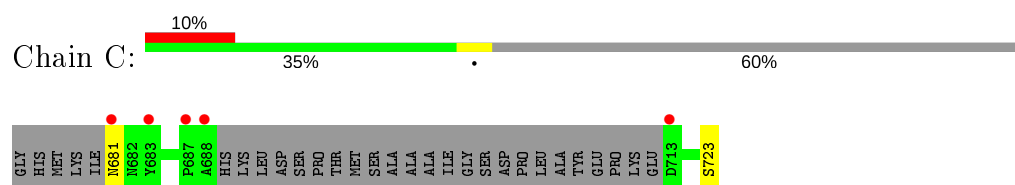
- Molecule 1: Serine/threonine-protein phosphatase 2B catalytic subunit alpha isoform



- Molecule 2: Calcineurin subunit B type 1



- Molecule 3: Sodium/hydrogen exchanger 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	79.48Å 126.81Å 127.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	16.13 – 1.90 16.13 – 1.90	Depositor EDS
% Data completeness (in resolution range)	97.5 (16.13-1.90) 85.1 (16.13-1.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.64 (at 1.90Å)	Xtriage
Refinement program	PHENIX (1.11.1 _2575: ???)	Depositor
R, $R_{free}$	0.169 , 0.209 0.169 , 0.209	Depositor DCC
$R_{free}$ test set	2494 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	15.9	Xtriage
Anisotropy	0.283	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.43 , 54.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	9109	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.35% 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: ZN, PGE, NA, PO4, FE, PEG, CA

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	0.56	0/3028	0.69	3/4110 (0.1%)
2	B	0.49	0/1255	0.62	0/1678
3	C	0.41	0/144	0.60	0/198
All	All	0.53	0/4427	0.67	3/5986 (0.1%)

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

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	118	ASP	CB-CG-OD2	7.11	124.70	118.30
1	A	73	ARG	NE-CZ-NH2	5.57	123.08	120.30
1	A	90	ASP	CB-CG-OD1	5.40	123.16	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	242	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	2945	2872	2858	21	0
2	B	1240	1223	1223	2	0
3	C	142	139	139	2	0
4	A	1	0	0	0	0
5	A	1	0	0	0	0
6	A	5	0	0	0	0
7	A	20	28	28	0	0
8	A	7	10	10	3	0
9	A	1	0	0	0	0
10	B	4	0	0	0	0
11	A	351	0	0	10	3
11	B	105	0	0	0	2
11	C	15	0	0	1	0
All	All	4837	4272	4258	25	3

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.

All (25) 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:110:ASN:ND2	11:A:501:HOH:O	1.90	1.03
3:C:723:SER:OXT	11:C:801:HOH:O	1.93	0.86
1:A:285[B]:ASP:OD1	11:A:502:HOH:O	1.99	0.81
1:A:82:ASP:OD1	11:A:503:HOH:O	2.06	0.73
1:A:172:GLU:OE2	11:A:504:HOH:O	2.08	0.71
1:A:285[B]:ASP:OD1	11:A:505:HOH:O	2.12	0.67
1:A:128:GLU:OE2	11:A:506:HOH:O	2.12	0.67
1:A:322:LEU:HD22	1:A:331:ILE:CD1	2.30	0.61
1:A:273:ASN:HB2	11:A:772:HOH:O	2.06	0.56
1:A:32:LYS:HG3	11:A:776:HOH:O	2.08	0.51
1:A:322:LEU:CD2	1:A:331:ILE:HD12	2.41	0.50
1:A:100:LYS:HE2	11:A:743:HOH:O	2.11	0.50
1:A:164:GLN:HG3	8:A:406:PEG:O4	2.14	0.47
1:A:322:LEU:CD2	1:A:331:ILE:CD1	2.93	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:73:LYS:NZ	2:B:77:GLU:OE2	2.43	0.46
1:A:234:ASP:O	1:A:259:PHE:HA	2.16	0.45
2:B:87:ASP:N	2:B:87:ASP:OD1	2.43	0.44
1:A:164:GLN:NE2	1:A:345:ASN:O	2.51	0.44
1:A:322:LEU:HD22	1:A:331:ILE:HD13	2.00	0.44
8:A:406:PEG:H22	11:A:761:HOH:O	2.18	0.42
1:A:360:LYS:NZ	3:C:681:ASN:O	2.42	0.42
1:A:299:PHE:CG	1:A:300:PRO:HD2	2.55	0.41
1:A:221:PRO:HA	1:A:222:PRO:HD3	1.98	0.41
1:A:192:ASN:O	1:A:194:GLN:HG3	2.21	0.40
1:A:164:GLN:HA	8:A:406:PEG:H32	2.03	0.40

All (3) 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)
11:A:813:HOH:O	11:B:401:HOH:O[6_544]	1.93	0.27
11:A:793:HOH:O	11:B:396:HOH:O[4_555]	1.93	0.27
11:A:624:HOH:O	11:A:799:HOH:O[4_555]	2.19	0.01

## 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	362/372 (97%)	348 (96%)	14 (4%)	0	100	100
2	B	154/156 (99%)	153 (99%)	1 (1%)	0	100	100
3	C	15/48 (31%)	15 (100%)	0	0	100	100
All	All	531/576 (92%)	516 (97%)	15 (3%)	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	324/332 (98%)	321 (99%)	3 (1%)	78	79
2	B	138/139 (99%)	137 (99%)	1 (1%)	84	84
3	C	17/40 (42%)	17 (100%)	0	100	100
All	All	479/511 (94%)	475 (99%)	4 (1%)	81	82

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

Mol	Chain	Res	Type
1	A	90	ASP
1	A	247	HIS
1	A	279	ARG
2	B	91	LYS

Some 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 7 are monoatomic - leaving 4 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
7	PGE	A	404	-	9,9,9	0.55	0	8,8,8	0.58	0
7	PGE	A	405	-	9,9,9	0.55	0	8,8,8	0.50	0
8	PEG	A	406	-	6,6,6	0.55	0	5,5,5	0.60	0
6	PO4	A	403	5,4	4,4,4	0.76	0	6,6,6	0.60	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
7	PGE	A	404	-	-	3/7/7/7	-
7	PGE	A	405	-	-	2/7/7/7	-
8	PEG	A	406	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	404	PGE	O1-C1-C2-O2
7	A	405	PGE	O2-C3-C4-O3
7	A	404	PGE	C1-C2-O2-C3
8	A	406	PEG	O1-C1-C2-O2
8	A	406	PEG	C1-C2-O2-C3
7	A	404	PGE	C3-C4-O3-C5
7	A	405	PGE	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	406	PEG	3	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	360/372 (96%)	-0.33	3 (0%) 86 87	11, 20, 38, 78	0
2	B	156/156 (100%)	0.16	5 (3%) 47 50	15, 29, 55, 67	0
3	C	19/48 (39%)	1.16	5 (26%) 0 0	17, 28, 64, 68	0
All	All	535/576 (92%)	-0.13	13 (2%) 59 62	11, 23, 49, 78	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	244	THR	7.0
3	C	681	ASN	6.8
3	C	688	ALA	6.5
2	B	85	LYS	3.7
3	C	713	ASP	3.6
2	B	84	VAL	3.4
1	A	370	ASN	3.3
3	C	683	TYR	2.6
1	A	243	LYS	2.3
2	B	169	ASP	2.3
3	C	687	PRO	2.3
2	B	18	ASP	2.1
2	B	88	LYS	2.1

### 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
7	PGE	A	404	10/10	0.67	0.20	41,56,66,69	0
8	PEG	A	406	7/7	0.70	0.40	41,56,68,71	0
7	PGE	A	405	10/10	0.71	0.24	28,48,58,61	0
10	CA	B	201	1/1	0.94	0.06	27,27,27,27	0
9	NA	A	407	1/1	0.95	0.10	35,35,35,35	0
10	CA	B	204	1/1	0.98	0.06	28,28,28,28	0
10	CA	B	202	1/1	0.98	0.06	23,23,23,23	0
6	PO4	A	403	5/5	0.99	0.06	18,20,23,23	0
10	CA	B	203	1/1	0.99	0.03	24,24,24,24	0
4	FE	A	401	1/1	0.99	0.06	14,14,14,14	1
5	ZN	A	402	1/1	1.00	0.06	13,13,13,13	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.