



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 12:34 AM UTC

PDB ID : 4UST / pdb\_00004ust  
Title : Crystal structure of human soluble Adenylyl Cyclase with pyrophosphate resulting from soaking with GTP and Magnesium  
Authors : Kleinboelting, S.; Steegborn, C.  
Deposited on : 2014-07-13  
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.

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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (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

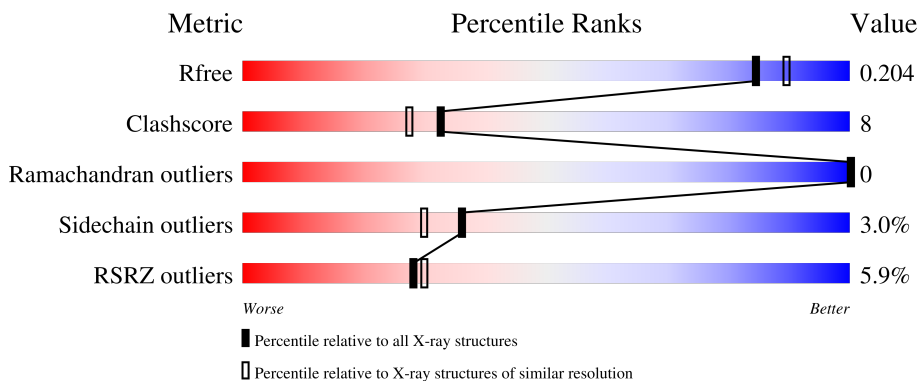
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


The reported resolution of this entry is 1.90 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))
$R_{free}$	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (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 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	475	

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 3905 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 ADENYLATE CYCLASE TYPE 10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	457	3654	2372	591	658	33	0	5	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	470	HIS	-	expression tag	UNP Q96PN6
A	471	HIS	-	expression tag	UNP Q96PN6
A	472	HIS	-	expression tag	UNP Q96PN6
A	473	HIS	-	expression tag	UNP Q96PN6
A	474	HIS	-	expression tag	UNP Q96PN6
A	475	HIS	-	expression tag	UNP Q96PN6

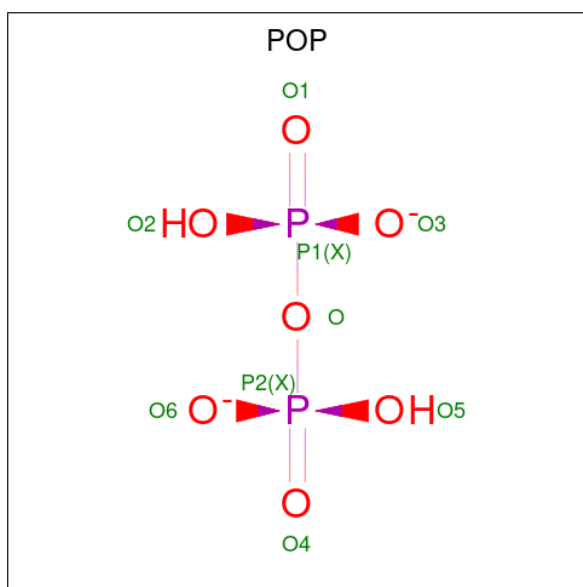
- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 4 is PYROPHOSPHATE 2- (CCD ID: POP) (formula: H<sub>2</sub>O<sub>7</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O P 9 7 2	0	0

- Molecule 5 is ACETATE ION (CCD ID: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



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

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula:  $C_3H_8O_3$ ).



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

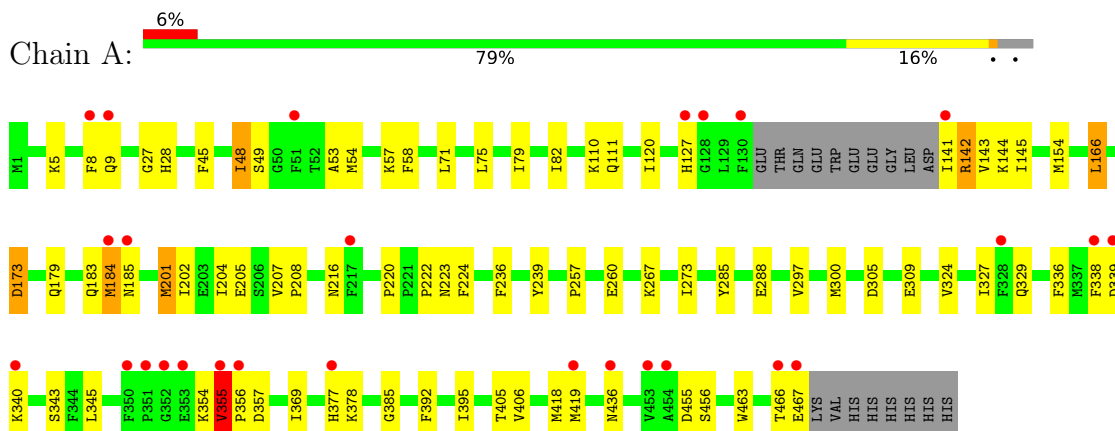
- Molecule 8 is water.

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
8	A	221	Total 221	O 221	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: ADENYLATE CYCLASE TYPE 10



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	100.34Å 100.34Å 97.42Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	86.90 – 1.90 86.90 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (86.90-1.90) 99.9 (86.90-1.90)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.94 (at 1.90Å)	Xtrriage
Refinement program	REFMAC 5.8.0073	Depositor
R, $R_{free}$	0.161 , 0.202 0.171 , 0.204	Depositor DCC
$R_{free}$ test set	2201 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.4	Xtrriage
Anisotropy	0.242	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 38.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.050 for h,-h-k,-l	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	3905	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.83% 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: GOL, EDO, CL, MG, ACT, POP, CME

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	1.27	6/3745 (0.2%)	1.17	12/5070 (0.2%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	285	TYR	C-O	-5.85	1.17	1.24
1	A	288	GLU	CA-C	-5.45	1.45	1.52
1	A	173	ASP	N-CA	5.28	1.52	1.46
1	A	385	GLY	CA-C	-5.22	1.48	1.52
1	A	405	THR	CA-C	5.19	1.59	1.52
1	A	145	ILE	CA-C	-5.07	1.46	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	220	PRO	O-C-N	7.96	124.97	121.31
1	A	355	VAL	CA-C-N	-7.21	113.38	120.52
1	A	355	VAL	C-N-CA	-7.21	113.38	120.52
1	A	327	ILE	N-CA-C	6.80	117.59	110.72
1	A	8	PHE	CA-C-N	-6.32	114.20	123.05
1	A	8	PHE	C-N-CA	-6.32	114.20	123.05
1	A	329	GLN	N-CA-C	5.87	119.34	111.24
1	A	48	ILE	CB-CA-C	-5.86	103.81	111.25
1	A	418	MET	CG-SD-CE	-5.81	88.11	100.90
1	A	53	ALA	N-CA-C	5.26	117.02	111.28
1	A	166	LEU	CB-CA-C	-5.12	99.04	109.94
1	A	220	PRO	CA-C-O	-5.07	117.25	120.90

There are no chirality outliers.

There are no planarity outliers.

## 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	3654	0	3621	57	0
2	A	1	0	0	0	0
3	A	2	0	0	0	0
4	A	9	0	0	0	0
5	A	4	0	3	0	0
6	A	8	0	12	0	0
7	A	6	0	8	2	0
8	A	221	0	0	10	0
All	All	3905	0	3644	58	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 8.

All (58) 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:222:PRO:O	1:A:223:ASN:HB2	1.67	0.92
1:A:357:ASP:OD1	1:A:436:ASN:ND2	2.06	0.88
1:A:28[A]:HIS:HE1	8:A:2029:HOH:O	1.62	0.80
1:A:377:HIS:CD2	8:A:2192:HOH:O	2.42	0.73
1:A:205:GLU:HG3	1:A:216:ASN:HD21	1.55	0.70
1:A:467:GLU:C	8:A:2221:HOH:O	2.35	0.69
1:A:205:GLU:CG	1:A:216:ASN:HD21	2.06	0.69
7:A:1474:GOL:C1	8:A:2076:HOH:O	2.43	0.65
1:A:28[A]:HIS:CE1	8:A:2029:HOH:O	2.45	0.63
1:A:377:HIS:O	1:A:378:LYS:HB2	1.96	0.62
1:A:309:GLU:OE1	1:A:378:LYS:HE2	2.00	0.61
1:A:239:TYR:HB2	7:A:1474:GOL:H2	1.85	0.59
1:A:75:LEU:HD11	1:A:79:ILE:HD11	1.85	0.58
1:A:204:ILE:C	1:A:204:ILE:HD12	2.29	0.58
1:A:166:LEU:CD2	1:A:336:PHE:HA	2.35	0.57
1:A:48:ILE:HD13	1:A:143:VAL:HG22	1.89	0.55
1:A:58:PHE:CD2	1:A:71[A]:LEU:HD13	2.42	0.55
1:A:183:GLN:O	1:A:184:MET:C	2.51	0.54
1:A:338:PHE:O	1:A:339:ASP:C	2.51	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:GLU:HG3	1:A:216:ASN:ND2	2.23	0.53
1:A:377:HIS:HD2	8:A:2192:HOH:O	1.88	0.52
1:A:120:ILE:HD12	1:A:202:ILE:HD13	1.93	0.51
1:A:201:MET:HE1	1:A:224:PHE:CE1	2.45	0.51
1:A:355:VAL:HG12	1:A:356:PRO:HD2	1.91	0.51
1:A:54:MET:O	1:A:58:PHE:HD2	1.94	0.51
1:A:455:ASP:OD1	1:A:456:SER:O	2.29	0.50
1:A:222:PRO:O	1:A:223:ASN:CB	2.41	0.50
1:A:466:THR:HG22	1:A:467:GLU:N	2.26	0.50
1:A:173:ASP:OD2	1:A:305:ASP:OD1	2.29	0.50
1:A:75:LEU:HD11	1:A:79:ILE:CD1	2.42	0.49
1:A:49:SER:HB2	1:A:144:LYS:NZ	2.28	0.48
1:A:54:MET:HB3	1:A:58:PHE:HE2	1.78	0.48
1:A:355:VAL:HG12	1:A:356:PRO:CD	2.44	0.48
1:A:120:ILE:CD1	1:A:202:ILE:HD13	2.44	0.47
1:A:324:VAL:HG21	1:A:369:ILE:HG13	1.97	0.47
1:A:463:TRP:HE1	1:A:467:GLU:CB	2.29	0.46
1:A:260:GLU:HG3	8:A:2146:HOH:O	2.15	0.46
1:A:27:GLY:O	1:A:28[B]:HIS:CG	2.69	0.45
1:A:357:ASP:HA	8:A:2186:HOH:O	2.16	0.45
1:A:48:ILE:HD11	1:A:82:ILE:HD11	1.99	0.45
1:A:339:ASP:O	1:A:340:LYS:C	2.58	0.45
1:A:110:LYS:HG2	8:A:2089:HOH:O	2.17	0.44
1:A:75:LEU:HG	1:A:79:ILE:HD12	1.99	0.44
1:A:339:ASP:CB	1:A:419:MET:HG2	2.47	0.44
1:A:143:VAL:O	1:A:185:ASN:HA	2.18	0.43
1:A:45[A]:PHE:CD1	1:A:179:GLN:HG3	2.53	0.43
1:A:392:PHE:O	1:A:406:VAL:HA	2.19	0.43
1:A:48:ILE:HD11	1:A:82:ILE:CD1	2.49	0.43
1:A:207:VAL:HG13	1:A:208:PRO:HD2	2.01	0.43
1:A:111:GLN:HG3	1:A:236:PHE:CG	2.54	0.42
1:A:273:ILE:CD1	1:A:395:ILE:HD11	2.49	0.42
1:A:297:VAL:O	1:A:343:SER:HA	2.19	0.42
1:A:142:ARG:HD3	1:A:184:MET:HB3	2.02	0.42
1:A:466:THR:CG2	1:A:467:GLU:N	2.83	0.42
1:A:345:LEU:C	1:A:345:LEU:HD23	2.46	0.41
1:A:300:MET:HE2	8:A:2173:HOH:O	2.20	0.40

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	457/475 (96%)	440 (96%)	17 (4%)	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	400/418 (96%)	388 (97%)	12 (3%)	36 30

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LYS
1	A	9	GLN
1	A	57	LYS
1	A	127	HIS
1	A	141	ILE
1	A	142	ARG
1	A	154	MET
1	A	184	MET
1	A	201	MET
1	A	257	PRO
1	A	354	LYS
1	A	355	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	114	ASN
1	A	216	ASN
1	A	223	ASN
1	A	238	HIS
1	A	304	GLN
1	A	331	GLN
1	A	380	GLN
1	A	433	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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$
1	CME	A	253	1	8,9,10	0.89	0	6,9,11	0.87	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
1	CME	A	253	1	-	2/5/8/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	253	CME	SD-CE-CZ-OH
1	A	253	CME	CZ-CE-SD-SG

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 8 ligands modelled in this entry, 3 are monoatomic - leaving 5 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	$\# Z  > 2$
4	POP	A	1471	2	6,8,8	0.78	0	12,13,13	0.91	0
7	GOL	A	1474	-	5,5,5	0.88	0	5,5,5	2.35	3 (60%)
6	EDO	A	1475	-	3,3,3	0.42	0	2,2,2	0.40	0
5	ACT	A	1472	-	3,3,3	0.87	0	3,3,3	0.12	0
6	EDO	A	1473	-	3,3,3	0.54	0	2,2,2	0.29	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
4	POP	A	1471	2	-	1/6/6/6	-
7	GOL	A	1474	-	-	0/4/4/4	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	A	1475	-	-	1/1/1/1	-
6	EDO	A	1473	-	-	0/1/1/1	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1474	GOL	C3-C2-C1	-3.36	99.46	111.80
7	A	1474	GOL	O2-C2-C3	2.92	121.25	109.18
7	A	1474	GOL	O1-C1-C2	-2.54	98.92	110.38

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1471	POP	P1-O-P2-O6
6	A	1475	EDO	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1474	GOL	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

### 6.1 Protein, DNA and RNA chains

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	456/475 (96%)	0.20	27 (5%) <span style="border: 1px solid red; padding: 2px;">28</span> <span style="border: 1px solid red; padding: 2px;">30</span>	14, 34, 73, 93	5 (1%)

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	339	ASP	5.7
1	A	351	PRO	5.5
1	A	130	PHE	4.5
1	A	466	THR	4.3
1	A	8	PHE	4.2
1	A	51	PHE	3.9
1	A	350	PHE	3.9
1	A	338	PHE	3.8
1	A	352	GLY	3.5
1	A	328	PHE	3.4
1	A	355	VAL	3.2
1	A	184	MET	3.2
1	A	356	PRO	3.0
1	A	141	ILE	2.9
1	A	340	LYS	2.9
1	A	454	ALA	2.7
1	A	377	HIS	2.7
1	A	436	ASN	2.6
1	A	467	GLU	2.5
1	A	185	ASN	2.4
1	A	128	GLY	2.4
1	A	127	HIS	2.2
1	A	419	MET	2.2
1	A	9	GLN	2.1
1	A	453	VAL	2.1
1	A	353	GLU	2.1
1	A	217	PHE	2.0

## 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
1	CME	A	253	10/11	0.98	0.06	21,25,32,32	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
6	EDO	A	1475	4/4	0.69	0.16	67,70,76,79	0
6	EDO	A	1473	4/4	0.74	0.18	76,88,89,105	0
4	POP	A	1471	9/9	0.79	0.10	86,102,121,123	0
5	ACT	A	1472	4/4	0.84	0.15	48,49,50,60	0
2	MG	A	1468	1/1	0.88	0.11	55,55,55,55	0
7	GOL	A	1474	6/6	0.89	0.13	32,35,50,55	0
3	CL	A	1470	1/1	0.93	0.13	41,41,41,41	0
3	CL	A	1469	1/1	0.99	0.03	28,28,28,28	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.