



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 09:37 am GMT

PDB ID : 4CLK  
Title : Crystal structure of human soluble Adenylyl Cyclase in complex with alpha,b eta-methyleneadenosine-5'-triphosphate  
Authors : Kleinboelting, S.; Weyand, M.; Steegborn, C.  
Deposited on : 2014-01-15  
Resolution : 2.20 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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

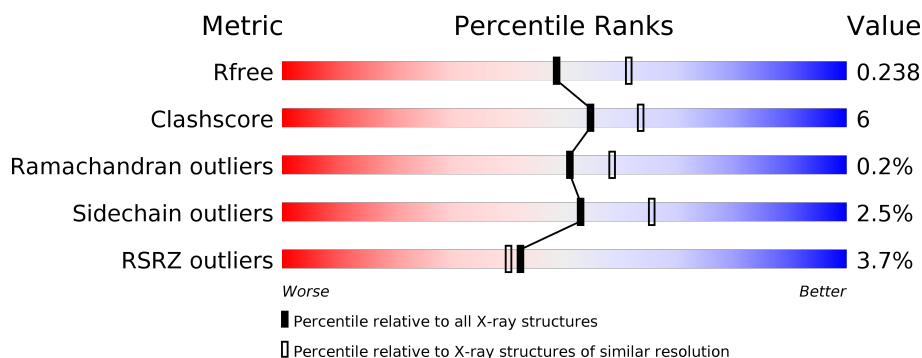
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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))
$R_{free}$	100719	4002 (2.20-2.20)
Clashscore	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (2.20-2.20)
RSRZ outliers	101464	4033 (2.20-2.20)

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. 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	<div> <div>4%</div> <div>83%</div> <div>14%</div> <div>.</div> </div>

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
5	EDO	A	1472	-	-	-	X
6	GOL	A	1473	-	-	-	X

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 3882 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.

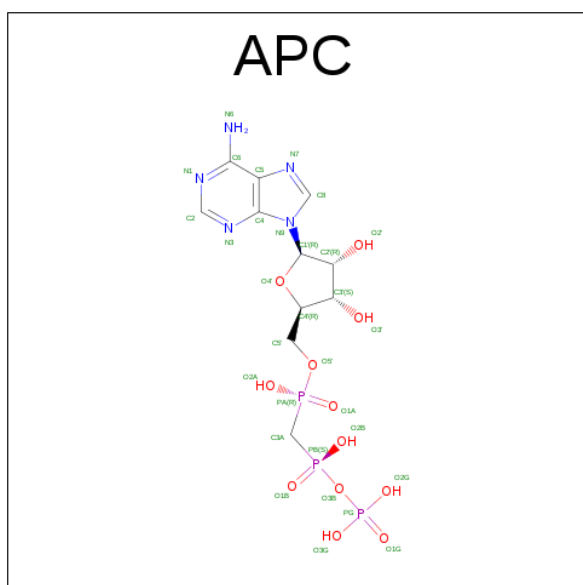
- Molecule 1 is a protein called ADENYLATE CYCLASE TYPE 10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	460	3661	2371	591	665	34	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 DIPHOSPHOMETHYLPHOSPHONIC ACID ADENOSYL ESTER (three-letter code: APC) (formula:  $C_{11}H_{18}N_5O_{12}P_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

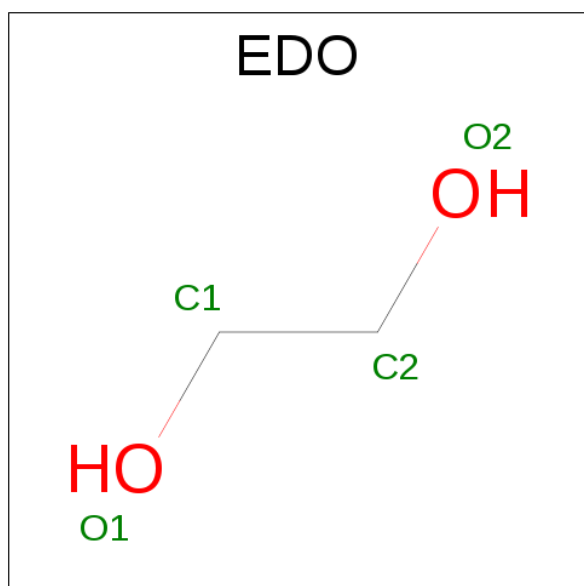
- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

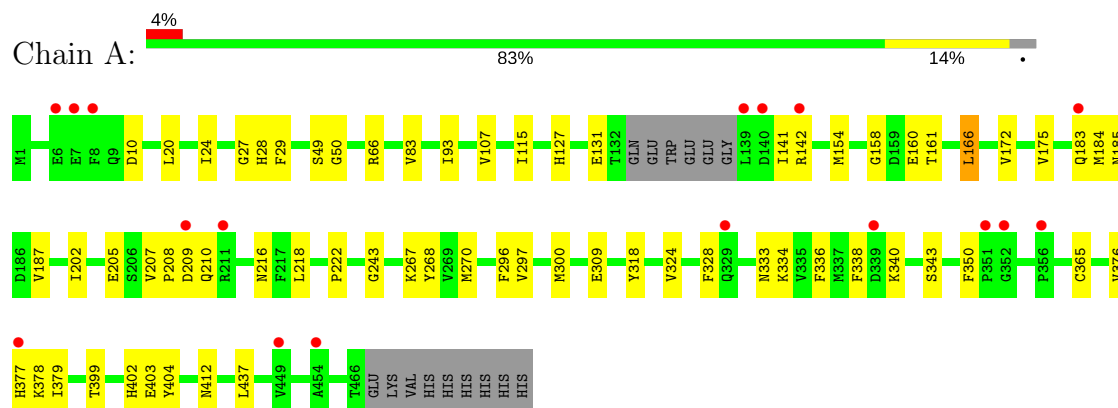
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	168	Total	O	0	0
			168	168		

### 3 Residue-property plots

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: ADENYLATE CYCLASE TYPE 10



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	100.25Å 100.25Å 97.45Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	86.82 – 2.20 48.73 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (86.82-2.20) 100.0 (48.73-2.20)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.09 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, $R_{free}$	0.176 , 0.237 0.185 , 0.238	Depositor DCC
$R_{free}$ test set	1440 reflections (5.36%)	DCC
Wilson B-factor (Å <sup>2</sup> )	27.4	Xtriage
Anisotropy	0.150	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 43.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.064 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	3882	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% 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, CL, CME, EDO, APC, 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	0.76	0/3753	0.86	3/5081 (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	10	ASP	CB-CG-OD2	-5.95	112.94	118.30
1	A	66	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	A	166	LEU	CB-CA-C	-5.21	100.29	110.20

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	3661	0	3625	44	0
2	A	31	0	14	2	0
3	A	1	0	0	0	0
4	A	1	0	0	0	0
5	A	8	0	12	1	0
6	A	12	0	16	2	0
7	A	168	0	0	6	0
All	All	3882	0	3667	44	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 6.

All (44) 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:160:GLU:HG3	7:A:2072:HOH:O	1.74	0.86
1:A:324:VAL:HG12	1:A:365[B]:CYS:SG	2.19	0.82
1:A:412:ASN:OD1	2:A:1468:APC:H8	1.84	0.77
1:A:207:VAL:HG12	1:A:210:GLN:HB2	1.70	0.71
1:A:324:VAL:CG1	1:A:365[B]:CYS:SG	2.84	0.65
1:A:328:PHE:CD2	1:A:365[A]:CYS:SG	2.91	0.64
1:A:24:ILE:O	6:A:1473:GOL:H31	1.99	0.63
1:A:166:LEU:CD2	1:A:336:PHE:HA	2.29	0.63
1:A:161:THR:HG23	7:A:2073:HOH:O	1.99	0.62
1:A:270[A]:MET:HG2	7:A:2115:HOH:O	1.99	0.62
1:A:83:VAL:HG13	1:A:93:ILE:CD1	2.30	0.61
1:A:27:GLY:O	1:A:28:HIS:C	2.37	0.61
1:A:437:LEU:O	6:A:1474:GOL:O2	2.07	0.59
1:A:399:THR:HG21	5:A:1471:EDO:H12	1.85	0.57
1:A:207:VAL:HG12	1:A:210:GLN:CB	2.34	0.57
1:A:300:MET:SD	1:A:340:LYS:CB	2.95	0.54
1:A:166:LEU:HD21	1:A:336:PHE:HA	1.90	0.53
1:A:160:GLU:O	1:A:267:LYS:HE2	2.09	0.53
1:A:202:ILE:HG22	1:A:218:LEU:HD12	1.91	0.53
1:A:328:PHE:HD2	1:A:365[A]:CYS:SG	2.32	0.53
1:A:184:MET:O	1:A:185:ASN:HB2	2.08	0.53
1:A:107:VAL:HG11	1:A:115:ILE:HG13	1.92	0.52
1:A:28:HIS:CE1	7:A:2018:HOH:O	2.63	0.51
1:A:207:VAL:HG13	1:A:208:PRO:HD2	1.93	0.50
1:A:28:HIS:HE1	7:A:2018:HOH:O	1.93	0.50
1:A:243:GLY:N	7:A:2100:HOH:O	2.45	0.48
1:A:127:HIS:CD2	1:A:187:VAL:HG23	2.48	0.48
1:A:297:VAL:O	1:A:343:SER:HA	2.13	0.48
1:A:376:VAL:HB	1:A:379:ILE:HD12	1.97	0.47
1:A:172:VAL:O	1:A:175:VAL:HG12	2.15	0.47
1:A:336:PHE:CE1	2:A:1468:APC:H2	2.50	0.47
1:A:334:LYS:NZ	1:A:403:GLU:OE1	2.49	0.46
1:A:205:GLU:HB3	1:A:216:ASN:HD21	1.82	0.44
1:A:142:ARG:HD3	1:A:185:ASN:OD1	2.17	0.43
1:A:158:GLY:HA2	1:A:318:TYR:CE1	2.54	0.43
1:A:183:GLN:OE1	1:A:183:GLN:HA	2.19	0.42
1:A:270[A]:MET:HE2	1:A:270[A]:MET:HB2	1.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:GLY:HA3	1:A:141:ILE:HG22	2.00	0.42
1:A:20:LEU:HD21	1:A:268:TYR:CB	2.49	0.42
1:A:309:GLU:OE2	1:A:378:LYS:HE3	2.20	0.41
1:A:202:ILE:O	1:A:202:ILE:HG13	2.21	0.41
1:A:270[A]:MET:HE1	1:A:404:TYR:CD2	2.55	0.41
1:A:333:ASN:OD1	1:A:334:LYS:HG2	2.21	0.40
1:A:210:GLN:OE1	1:A:210:GLN:HA	2.22	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	460/475 (97%)	434 (94%)	25 (5%)	1 (0%)	51 58

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	377	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	402/418 (96%)	392 (98%)	10 (2%)	53 65

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	PHE
1	A	49	SER
1	A	131	GLU
1	A	154	MET
1	A	209	ASP
1	A	222	PRO
1	A	296	PHE
1	A	338	PHE
1	A	350	PHE
1	A	402	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	114	ASN
1	A	127	HIS
1	A	216	ASN
1	A	238	HIS
1	A	266	GLN
1	A	377	HIS
1	A	409	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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	9,9,10	1.06	1 (11%)	6,9,11	1.31	2 (33%)

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	-	0/5/8/10	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	253	CME	CA-C	2.61	1.53	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	253	CME	CB-SG-SD	-2.09	99.77	103.83
1	A	253	CME	O-C-CA	-2.07	119.29	125.02

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 2 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
2	APC	A	1468	4	28,33,33	1.48	6 (21%)	28,52,52	1.77	4 (14%)
5	EDO	A	1471	-	3,3,3	0.62	0	2,2,2	0.25	0
5	EDO	A	1472	-	3,3,3	0.67	0	2,2,2	0.29	0
6	GOL	A	1473	-	5,5,5	0.28	0	5,5,5	0.77	0
6	GOL	A	1474	-	5,5,5	0.54	0	5,5,5	0.85	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	APC	A	1468	4	-	0/15/38/38	0/3/3/3
5	EDO	A	1471	-	-	0/1/1/1	0/0/0/0
5	EDO	A	1472	-	-	0/1/1/1	0/0/0/0
6	GOL	A	1473	-	-	0/4/4/4	0/0/0/0
6	GOL	A	1474	-	-	0/4/4/4	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1468	APC	C2-N3	2.17	1.35	1.32
2	A	1468	APC	PB-O3B	2.23	1.60	1.58
2	A	1468	APC	PA-O2A	2.32	1.62	1.56
2	A	1468	APC	O4'-C1'	2.47	1.44	1.41
2	A	1468	APC	PA-O5'	3.05	1.60	1.57
2	A	1468	APC	C5-C4	3.31	1.48	1.40

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1468	APC	N3-C2-N1	-5.91	123.71	128.86
2	A	1468	APC	PG-O3B-PB	-3.12	121.38	132.38
2	A	1468	APC	C4-C5-N7	-2.69	106.81	109.41
2	A	1468	APC	O1A-PA-C3A	2.95	116.26	108.97

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1468	APC	2	0
5	A	1471	EDO	1	0
6	A	1473	GOL	1	0
6	A	1474	GOL	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	459/475 (96%)	-0.25	17 (3%) 42 40	14, 31, 66, 88	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	352	GLY	3.1
1	A	139	LEU	2.8
1	A	377	HIS	2.8
1	A	356	PRO	2.8
1	A	449	VAL	2.8
1	A	140	ASP	2.8
1	A	8	PHE	2.7
1	A	351	PRO	2.5
1	A	209	ASP	2.3
1	A	211	ARG	2.2
1	A	329	GLN	2.2
1	A	7	GLU	2.1
1	A	454	ALA	2.1
1	A	6	GLU	2.0
1	A	183	GLN	2.0
1	A	142	ARG	2.0
1	A	339	ASP	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
1	CME	A	253	10/11	0.97	0.08	-	19,21,30,30	0

### 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	EDO	A	1472	4/4	0.81	0.20	4.21	47,47,48,51	0
6	GOL	A	1473	6/6	0.88	0.18	4.20	35,36,37,38	6
6	GOL	A	1474	6/6	0.82	0.14	1.44	41,45,45,46	0
2	APC	A	1468	31/31	0.91	0.18	1.11	26,46,55,58	31
5	EDO	A	1471	4/4	0.85	0.16	-0.05	38,41,41,45	0
3	CL	A	1469	1/1	0.99	0.11	-0.66	26,26,26,26	0
4	CA	A	1470	1/1	0.86	0.15	-	78,78,78,78	1

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

There are no such residues in this entry.