WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 09:38 am GMT

PDB ID : 4CLT
Title : Crystal structure of human soluble Adenylyl Cyclase with adenosine-3', 5'-cy clic-monophosphate and pyrophosphate
Authors : Kleinboelting, S.; Weyand, M.; Steegborn, C.
Deposited on : 2014-01-15
Resolution : 1.95 Å(reported)

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 1.95 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	Percentile Ranks	Value
Rfree		0.226
Clashscore		6
Ramachandran outliers		0.2%
Sidechain outliers		5.5%
RSRZ outliers		8.2%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
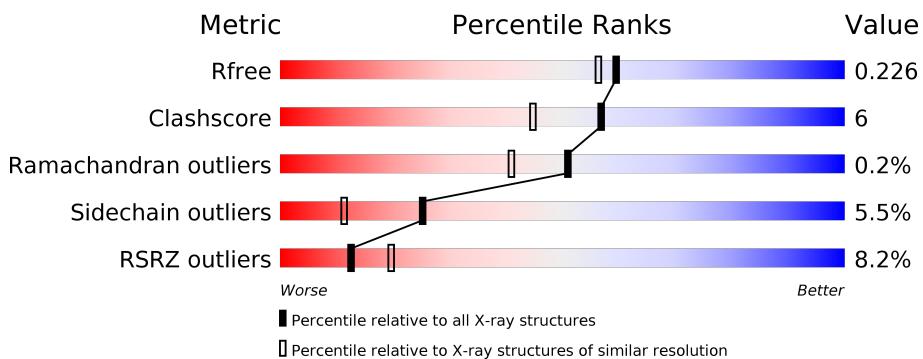
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	2004 (1.96-1.96)
Clashscore	112137	2136 (1.96-1.96)
Ramachandran outliers	110173	2117 (1.96-1.96)
Sidechain outliers	110143	2117 (1.96-1.96)
RSRZ outliers	101464	2018 (1.96-1.96)

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 >=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 <=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	8% 84% 13% • •
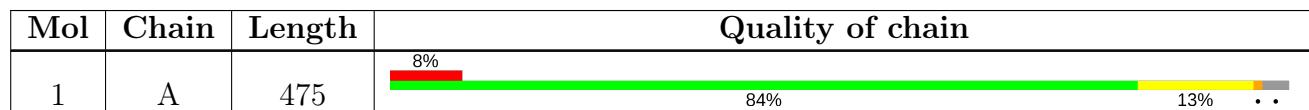
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CMP	A	1473	-	-	X	X
4	POP	A	1474	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	EDO	A	1476	-	-	-	X

2 Entry composition ⓘ

There are 7 unique types of molecules in this entry. The entry contains 3838 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
1	A	462	Total 3673	C 2380	N 596	O 663	S 34	0	3	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 (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is ADENOSINE-3',5'-CYCLIC-MONOPHOSPHATE (three-letter code: CMP) (formula: $C_{10}H_{12}N_5O_6P$).
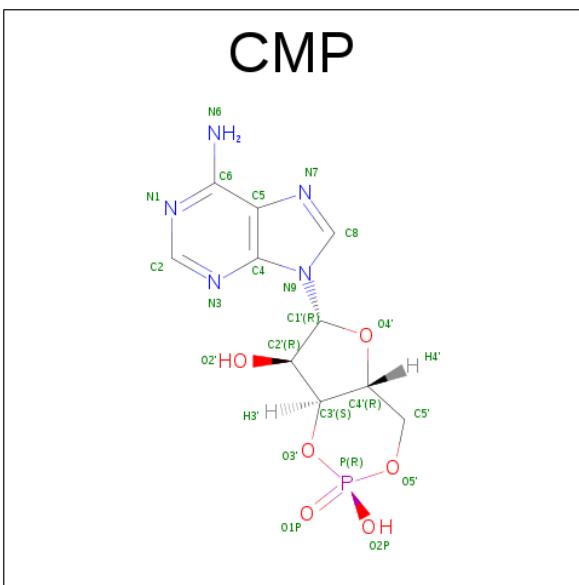
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
3	A	1	Total	C	N	O	P	0	0
			22	10	5	6	1		

- Molecule 4 is PYROPHOSPHATE 2- (three-letter code: POP) (formula: $H_2O_7P_2$).
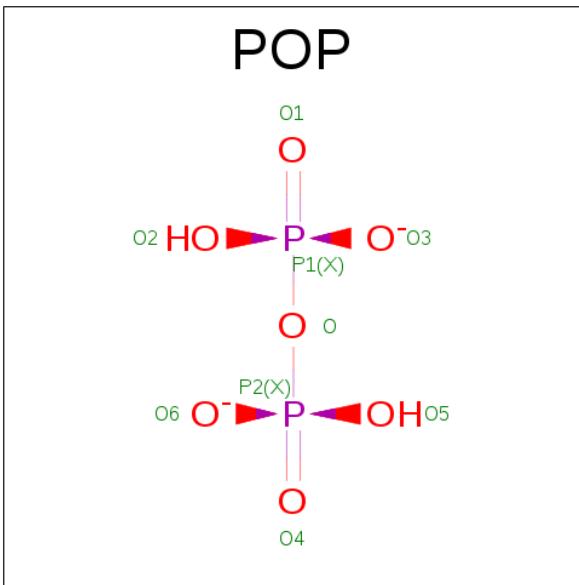
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			9	7	2		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).
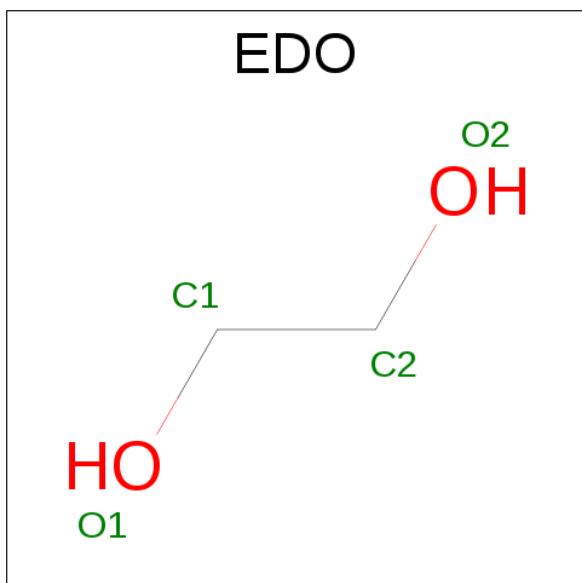
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total C O 4 2 2			0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	106	Total O 106 106		0	0

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
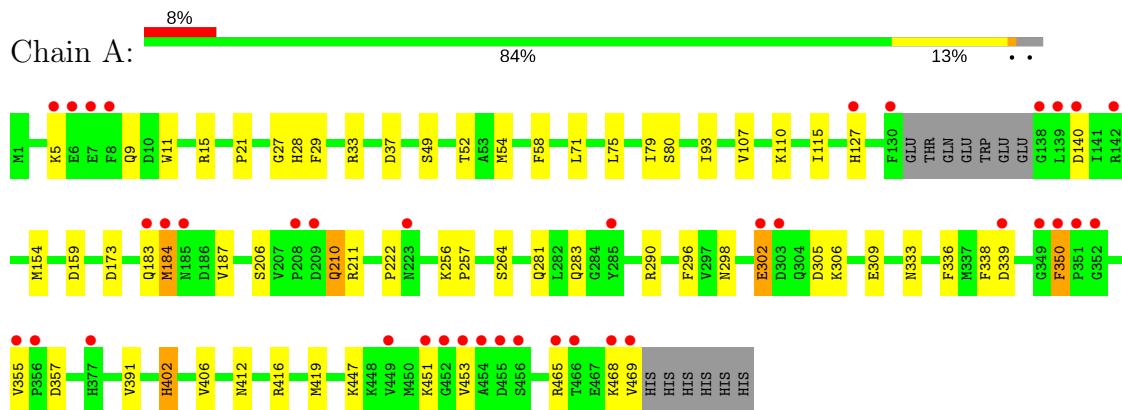
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α, β, γ	100.97Å 100.97Å 97.21Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	87.44 – 1.95 44.80 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.9 (87.44-1.95) 99.9 (44.80-1.95)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.97 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.173 , 0.220 0.183 , 0.226	Depositor DCC
R_{free} test set	2065 reflections (5.30%)	DCC
Wilson B-factor (Å^2)	23.7	Xtriage
Anisotropy	0.230	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 45.3	EDS
L-test for twinning[2]	$< |L| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.048 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	3838	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.54% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: MG, CL, CME, EDO, POP, CMP

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	0.99	2/3759 (0.1%)	0.99	8/5086 (0.2%)

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	80	SER	CB-OG	-6.50	1.33	1.42
1	A	264	SER	CB-OG	-6.49	1.33	1.42

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	159	ASP	CB-CG-OD1	7.31	124.88	118.30
1	A	37	ASP	CB-CG-OD2	-5.92	112.97	118.30
1	A	159	ASP	CB-CG-OD2	-5.87	113.02	118.30
1	A	15	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	A	33	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	A	290	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	A	211	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	A	281	GLN	CA-CB-CG	5.12	124.67	113.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	355	VAL	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	3673	0	3648	40	0
2	A	1	0	0	0	0
3	A	44	0	22	8	0
4	A	9	0	0	1	0
5	A	1	0	0	0	0
6	A	4	0	6	2	0
7	A	106	0	0	3	0
All	All	3838	0	3676	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 6.

All (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)
3:A:1472:CMP:H2	3:A:1472:CMP:C2	0.97	1.48
3:A:1473:CMP:H2	3:A:1473:CMP:C2	0.97	1.47
1:A:58:PHE:CD2	1:A:71[A]:LEU:HD23	2.00	0.95
1:A:58:PHE:CE2	1:A:71[A]:LEU:HD23	2.12	0.85
1:A:52:THR:HG23	4:A:1474:POP:P2	2.27	0.74
1:A:468:LYS:O	1:A:469:VAL:CB	2.36	0.73
1:A:28:HIS:HE1	7:A:2018:HOH:O	1.76	0.69
1:A:256:LYS:H	6:A:1476:EDO:C2	2.12	0.63
1:A:412[A]:ASN:OD1	3:A:1473:CMP:H5'2	2.02	0.59
1:A:75:LEU:HD11	1:A:79:ILE:HD11	1.85	0.59
1:A:412[B]:ASN:OD1	3:A:1473:CMP:H8	2.03	0.58
1:A:58:PHE:CE2	1:A:71[A]:LEU:CD2	2.86	0.56
1:A:256:LYS:H	6:A:1476:EDO:H21	1.71	0.56
1:A:27:GLY:O	1:A:28:HIS:C	2.44	0.55
1:A:302:GLU:H	1:A:302:GLU:CD	2.10	0.54
1:A:412[A]:ASN:OD1	3:A:1473:CMP:C5'	2.55	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:VAL:HG11	1:A:115:ILE:HG13	1.87	0.54
1:A:54:MET:O	1:A:58:PHE:CD2	2.61	0.53
1:A:75:LEU:HG	1:A:79:ILE:HD12	1.91	0.53
1:A:416:ARG:CZ	3:A:1473:CMP:O5'	2.57	0.52
1:A:333:ASN:HD22	1:A:350:PHE:HZ	1.58	0.52
1:A:9:GLN:CG	1:A:11:TRP:CE2	2.93	0.52
1:A:406:VAL:O	3:A:1473:CMP:N6	2.44	0.51
1:A:9:GLN:HG3	1:A:11:TRP:CE2	2.46	0.50
1:A:28:HIS:CE1	7:A:2018:HOH:O	2.56	0.48
1:A:184:MET:SD	1:A:184:MET:N	2.88	0.47
1:A:336:PHE:CE2	3:A:1473:CMP:H2	2.50	0.46
1:A:9:GLN:HG2	1:A:11:TRP:CE2	2.51	0.46
1:A:9:GLN:HG2	1:A:11:TRP:CZ2	2.51	0.46
1:A:298:ASN:ND2	1:A:339:ASP:HB3	2.31	0.45
1:A:338:PHE:HZ	1:A:419[A]:MET:SD	2.40	0.44
1:A:338:PHE:CZ	1:A:419[A]:MET:SD	3.10	0.44
1:A:127:HIS:CD2	1:A:187:VAL:HG23	2.52	0.44
1:A:402:HIS:HD2	7:A:2096:HOH:O	2.00	0.44
1:A:173:ASP:OD2	1:A:305:ASP:OD1	2.36	0.43
1:A:210:GLN:HA	1:A:210:GLN:HE21	1.83	0.43
1:A:127:HIS:CD2	1:A:187:VAL:CG2	3.02	0.42
1:A:54:MET:O	1:A:58:PHE:HD2	2.02	0.42
1:A:75:LEU:HD11	1:A:79:ILE:CD1	2.50	0.42
1:A:21:PRO:HB3	1:A:93:ILE:O	2.21	0.40
1:A:306:LYS:HD3	1:A:309:GLU:HG3	2.03	0.40
1:A:127:HIS:HD2	1:A:187:VAL:HG23	1.86	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%)	442 (96%)	17 (4%)	1 (0%)	51	41

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	465	ARG

5.3.2 Protein sidechains ⓘ

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%)	380 (94%)	22 (6%)	25	11

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LYS
1	A	29	PHE
1	A	49	SER
1	A	110	LYS
1	A	140	ASP
1	A	154	MET
1	A	183	GLN
1	A	184	MET
1	A	206	SER
1	A	210	GLN
1	A	222	PRO
1	A	257	PRO
1	A	283	GLN
1	A	296	PHE
1	A	302	GLU
1	A	350	PHE
1	A	357	ASP
1	A	391	VAL
1	A	402	HIS
1	A	447	LYS

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Mol	Chain	Res	Type
1	A	451	LYS
1	A	453	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	HIS
1	A	114	ASN
1	A	127	HIS
1	A	210	GLN
1	A	223	ASN
1	A	238	HIS
1	A	304	GLN
1	A	331	GLN
1	A	402	HIS

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	0.86	0	6,9,11	2.06	3 (50%)

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

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	253	CME	OH-CZ-CE	-3.54	96.33	110.93
1	A	253	CME	O-C-CA	-2.80	117.30	125.02
1	A	253	CME	CE-SD-SG	-2.13	92.68	103.40

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 6 ligands modelled in this entry, 2 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	#$|Z| > 2$
3	CMP	A	1472	-	21,25,25	1.21	1 (4%)	22,39,39	2.61	10 (45%)
3	CMP	A	1473	-	21,25,25	1.47	3 (14%)	22,39,39	2.64	9 (40%)
4	POP	A	1474	2	8,8,8	0.93	0	8,13,13	1.47	2 (25%)
6	EDO	A	1476	-	3,3,3	0.36	0	2,2,2	0.05	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	CMP	A	1472	-	-	0/0/31/31	0/4/4/4
3	CMP	A	1473	-	-	0/0/31/31	0/4/4/4
4	POP	A	1474	2	-	0/6/6/6	0/0/0/0
6	EDO	A	1476	-	-	0/1/1/1	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1473	CMP	O5'-C5'	-2.45	1.42	1.46
3	A	1473	CMP	P-O3'	2.80	1.62	1.58
3	A	1473	CMP	C5-C4	3.15	1.47	1.40
3	A	1472	CMP	C5-C4	3.48	1.48	1.40

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1472	CMP	N3-C2-N1	-6.48	123.21	128.86
3	A	1473	CMP	C4'-O4'-C1'	-6.13	103.24	109.77
3	A	1473	CMP	O3'-C3'-C4'	-5.39	106.53	110.69
3	A	1472	CMP	C4'-O4'-C1'	-4.83	104.63	109.77
3	A	1473	CMP	C4-C5-N7	-4.03	105.52	109.41
3	A	1472	CMP	O2P-P-O3'	-4.00	97.61	107.23
3	A	1473	CMP	N3-C2-N1	-3.95	125.41	128.86
3	A	1472	CMP	O3'-C3'-C2'	-2.52	113.15	115.67
3	A	1472	CMP	C4-C5-N7	-2.46	107.04	109.41
3	A	1473	CMP	C1'-N9-C4	-2.14	122.93	126.64
3	A	1473	CMP	N6-C6-N1	-2.08	114.64	118.77
3	A	1472	CMP	C1'-N9-C4	-2.07	123.07	126.64
4	A	1474	POP	O2-P1-O1	2.00	118.33	110.50
4	A	1474	POP	O3-P1-O1	2.22	119.18	110.50
3	A	1473	CMP	O3'-C3'-C2'	2.27	117.94	115.67
3	A	1472	CMP	C2-N1-C6	2.45	123.05	118.77
3	A	1472	CMP	C5'-C4'-C3'	2.46	117.62	112.57
3	A	1472	CMP	O2P-P-O1P	2.54	116.89	108.63
3	A	1473	CMP	C5-C6-N6	2.94	126.46	120.47
3	A	1472	CMP	O5'-P-O3'	4.59	111.99	105.81
3	A	1473	CMP	O2P-P-O1P	5.04	125.00	108.63

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1472	CMP	1	0
3	A	1473	CMP	7	0
4	A	1474	POP	1	0
6	A	1476	EDO	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, 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	A	461/475 (97%)	0.16	38 (8%)	12	20	13, 27, 66, 96	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	139	LEU	11.5
1	A	469	VAL	7.2
1	A	352	GLY	7.1
1	A	454	ALA	5.7
1	A	8	PHE	5.5
1	A	351	PRO	5.3
1	A	138	GLY	4.7
1	A	466	THR	4.5
1	A	356	PRO	4.4
1	A	449	VAL	4.0
1	A	451	LYS	3.9
1	A	285	TYR	3.6
1	A	127	HIS	3.5
1	A	7	GLU	3.1
1	A	6	GLU	3.1
1	A	184	MET	3.0
1	A	350	PHE	3.0
1	A	453	VAL	3.0
1	A	468	LYS	2.9
1	A	142	ARG	2.9
1	A	130	PHE	2.8
1	A	455	ASP	2.8
1	A	209	ASP	2.7
1	A	5	LYS	2.7
1	A	377	HIS	2.7
1	A	140	ASP	2.6
1	A	208	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	355	VAL	2.5
1	A	185	ASN	2.5
1	A	349	GLY	2.4
1	A	456	SER	2.3
1	A	183	GLN	2.3
1	A	303	ASP	2.3
1	A	302	GLU	2.1
1	A	223	ASN	2.1
1	A	452	GLY	2.1
1	A	465	ARG	2.0
1	A	339	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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, 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	LLDF	B-factors(Å^2)	Q<0.9
1	CME	A	253	10/11	0.98	0.07	-	16,21,36,37	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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, 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	LLDF	B-factors(Å^2)	Q<0.9
6	EDO	A	1476	4/4	0.91	0.16	3.97	39,42,50,57	0
4	POP	A	1474	9/9	0.94	0.23	3.09	48,56,62,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors($Å^2$)	Q<0.9
3	CMP	A	1473	22/22	0.88	0.18	2.59	43,61,91,96	0
5	CL	A	1475	1/1	1.00	0.12	1.61	23,23,23,23	0
3	CMP	A	1472	22/22	0.95	0.13	0.41	34,40,46,49	0
2	MG	A	1471	1/1	0.87	0.09	-	40,40,40,40	0

6.5 Other polymers ⓘ

There are no such residues in this entry.