

# Full wwPDB X-ray Structure Validation Report (i)

#### May 14, 2020 – 10:06 pm BST

PDB ID : 5O3Q

Title : Carbon regulatory PII-like protein SbtB from Synechocystis sp. 6803 in com-

plex with cyclic AMP (cAMP)

Authors: Selim, K.A.; Albrecht, R.; Forchhammer, K.; Hartmann, M.D.

Deposited on : 2017-05-24

Resolution : 1.75 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
A user guide is available at

https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) 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

buster-report : 1.1.7 (2018)

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)

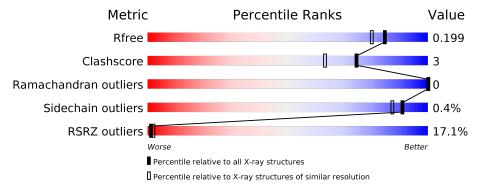
Validation Pipeline (wwPDB-VP) : 2.11

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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	Similar resolution
Metric	$(\# { m Entries})$	$(\#  ext{Entries},  ext{resolution range}( ext{Å}))$
$R_{free}$	130704	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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 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 <=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		
			19%		
1	Α	120	78%	•	18%
			10%		
1	В	120	78%	6%	16%
			13%		
1	$\mathbf{C}$	120	76%	6% •	18%



# 2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 2536 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 Membrane-associated protein slr1513.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	Λ	98	Total	С	N	О	S	0	2	0
1	A	90	746	480	118	143	5	0	J	
1	D	101	Total	С	N	О	S	0	4	0
1	Б	101	789	509	126	149	5	0	<del>4</del>	0
1	С	99	Total	С	N	О	S	0	2	0
1		99	764	495	121	142	6	0	)	0

There are 30 discrepancies between the modelled and reference sequences:

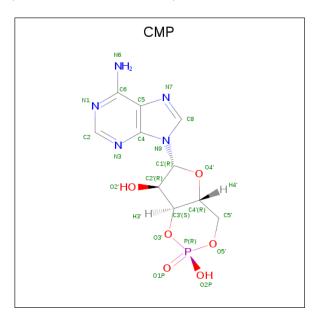
Chain	Residue	Modelled	Actual	Comment	Reference
A	111	SER	-	expression tag	UNP P73954
A	112	ALA	-	expression tag	UNP P73954
A	113	TRP	-	expression tag	UNP P73954
A	114	SER	-	expression tag	UNP P73954
A	115	HIS	-	expression tag	UNP P73954
A	116	PRO	_	expression tag	UNP P73954
A	117	GLN	-	expression tag	UNP P73954
A	118	PHE	-	expression tag	UNP P73954
A	119	GLU	-	expression tag	UNP P73954
A	120	LYS	-	expression tag	UNP P73954
В	111	SER	=	expression tag	UNP P73954
В	112	ALA	-	expression tag	UNP P73954
В	113	TRP	-	expression tag	UNP P73954
В	114	SER	-	expression tag	UNP P73954
В	115	HIS	-	expression tag	UNP P73954
В	116	PRO	-	expression tag	UNP P73954
В	117	GLN	-	expression tag	UNP P73954
В	118	PHE	-	expression tag	UNP P73954
В	119	GLU	-	expression tag	UNP P73954
В	120	LYS	-	expression tag	UNP P73954
С	111	SER	-	expression tag	UNP P73954
С	112	ALA	-	expression tag	UNP P73954
С	113	TRP	-	expression tag	UNP P73954



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Chain	Residue	Modelled	Actual	Comment	Reference
С	114	SER	_	expression tag	UNP P73954
С	115	HIS	-	expression tag	UNP P73954
С	116	PRO	-	expression tag	UNP P73954
С	117	GLN	-	expression tag	UNP P73954
С	118	PHE	-	expression tag	UNP P73954
С	119	GLU	_	expression tag	UNP P73954
С	120	LYS	=	expression tag	UNP P73954

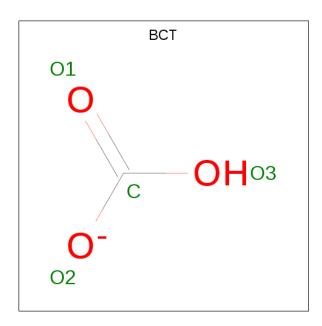
• Molecule 2 is ADENOSINE-3',5'-CYCLIC-MONOPHOSPHATE (three-letter code: CMP) (formula:  $C_{10}H_{12}N_5O_6P$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf		
2	Λ	1	Total	С	N	О	Р	0	0	
	Λ	1	22	10	5	6	1	0		
9	B	1	Total	С	N	О	Р	0	0	
	D	1	22	10	5	6	1	0	0	
9	D	1	Total	С	N	О	Р	0	0	
2	Ъ	1	22	10	5	6	1	U	0	

• Molecule 3 is BICARBONATE ION (three-letter code: BCT) (formula: CHO<sub>3</sub>).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	С	1	Total 4	C 1	O 3	0	0

#### • Molecule 4 is water.

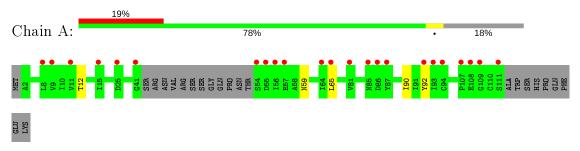
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	49	Total O 49 49	0	0
4	В	57	Total O 57 57	0	0
4	С	61	Total O 61 61	0	0



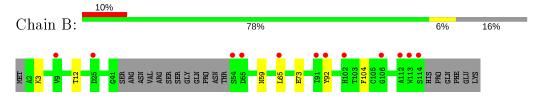
# 3 Residue-property plots (i)

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.

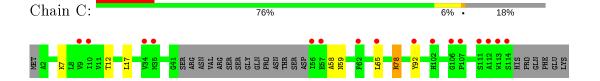
• Molecule 1: Membrane-associated protein slr1513



• Molecule 1: Membrane-associated protein slr1513



• Molecule 1: Membrane-associated protein slr1513





# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32	Depositor
Cell constants	64.39Å 64.39Å 81.46Å	Danasitan
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $120.00^{\circ}$	Depositor
Resolution (Å)	32.89 - 1.75	Depositor
Resolution (A)	32.89 - 1.75	EDS
% Data completeness	99.9 (32.89-1.75)	Depositor
(in resolution range)	99.9 (32.89-1.75)	EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.52 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
$R, R_{free}$	0.170 , $0.193$	Depositor
	0.181 , $0.199$	DCC
$R_{free}$ test set	1901 reflections $(4.99\%)$	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	35.8	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	$0.38 \; ,  51.5$	EDS
L-test for twinning <sup>2</sup>	$< L >=0.49, < L^2>=0.32$	Xtriage
	0.013  for -h,-k,l	
Estimated twinning fraction	0.045  for h,-h-k,-l	Xtriage
	0.024  for -k,-h,-l	
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	2536	wwPDB-VP
Average B, all atoms $(\mathring{A}^2)$	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.59% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 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: BCT, 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).

Mal	Mol Chain		lengths	Bond angles		
MIOI	Chain	RMSZ	# Z >5	RMSZ	# Z  > 5	
1	A	0.83	0/764	0.89	0/1030	
1	В	0.98	0/809	0.94	0/1089	
1	С	1.02	0/784	1.02	2/1055~(0.2%)	
All	All	0.95	0/2357	0.95	$2/3174 \ (0.1\%)$	

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	${f Res}$	Type	Atoms Z		$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^o)$
1	С	78	ARG	NE-CZ-NH2	8.11	124.35	120.30
1	С	78	ARG	NE-CZ-NH1	-5.40	117.60	120.30

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	746	0	751	4	0
1	В	789	0	805	6	0
1	С	764	0	780	6	0
2	A	22	0	11	1	0
2	В	44	0	22	2	0
3	С	4	0	0	0	0



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Mol	Chain	Non-H	H(model)	$\mathbf{H}(\mathbf{added})$	Clashes	Symm-Clashes
4	A	49	0	0	0	0
4	В	57	0	0	1	0
4	С	61	0	0	2	0
All	All	2536	0	2369	15	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.

All (15) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	${ m distance}\;({ m \AA})$	${ m overlap}({ m \AA})$
2:A:200:CMP:C2	2:A:200:CMP:H2	0.97	1.49
2:B:201:CMP:H2	2:B:201:CMP:C2	0.97	1.48
2:B:202:CMP:C2	2:B:202:CMP:H2	0.97	1.48
1:C:12:THR:O	1:C:59:ASN:HB2	2.00	0.60
1:A:92:TYR:CD1	1:B:65[A]:LEU:HD11	2.36	0.59
1:B:12:THR:O	1:B:59[B]:ASN:HB2	2.07	0.54
1:B:92:TYR:CD1	1:C:65[A]:LEU:HD11	2.43	0.54
1:A:65[A]:LEU:HD11	1:C:92:TYR:CD1	2.43	0.54
1:C:17:LEU:C	1:C:17:LEU:HD23	2.31	0.52
1:B:73:GLU:CD	4:B:309:HOH:O	2.48	0.50
1:C:58:ALA:HB1	4:C:325:HOH:O	2.12	0.49
1:A:12:THR:O	1:A:59:ASN:HB2	2.16	0.46
1:B:3:LYS:HE3	1:B:104:PHE:CE2	2.51	0.46
1:A:90:ILE:HD13	1:B:65[A]:LEU:HD12	1.99	0.45
1:C:7:LYS:NZ	4:C:305:HOH:O	2.54	0.41

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	Perce	$\mathbf{rcentiles}$	
1	A	97/120 (81%)	96 (99%)	1 (1%)	0	100	100	
1	В	101/120 (84%)	100 (99%)	1 (1%)	0	100	100	
1	С	98/120 (82%)	93 (95%)	5 (5%)	0	100	100	
All	All	296/360 (82%)	289 (98%)	7 (2%)	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	Rotameric Outliers		Percentiles		
1	A	77/99 (78%)	77 (100%)	0	100	100		
1	В	83/99 (84%)	83 (100%)	0	100	100		
1	С	79/99 (80%)	78 (99%)	1 (1%)	69	54		
All	All	239/297 (80%)	238 (100%)	1 (0%)	91	87		

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	С	78	ARG

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)

4 ligands 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	Trme	Chain	Res	Link	Bond lengths			Bond angles		
MIOI	Type				Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	CMP	A	200	-	22,25,25	1.90	6 (27%)	24,39,39	2.58	9 (37%)
3	BCT	С	201	-	0,3,3	0.00	=	0,3,3	0.00	-
2	CMP	В	201	-	22,25,25	1.73	3 (13%)	24,39,39	2.20	9 (37%)
2	CMP	В	202	-	22,25,25	1.31	3 (13%)	24,39,39	2.57	9 (37%)

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	CMP	A	200	_	_	0/0/31/31	0/4/4/4
2	CMP	В	201	_	-	0/0/31/31	0/4/4/4
2	CMP	В	202	_	_	0/0/31/31	0/4/4/4

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	$\operatorname{Ideal}(\text{\AA})$
2	В	201	CMP	P-O3'	6.26	1.68	1.57
2	A	200	CMP	C2-N3	4.31	1.39	1.32
2	A	200	CMP	C2'-C1'	3.84	1.59	1.53
2	В	202	CMP	P-O5'	3.81	1.62	1.57
2	A	200	CMP	P-O5'	3.53	1.61	1.57
2	В	201	CMP	C2-N3	2.59	1.36	1.32
2	A	200	CMP	C4-N3	-2.49	1.32	1.35
2	A	200	CMP	C2'-C3'	-2.46	1.47	1.52



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	Mol	Chain	${f Res}$	$\mathbf{Type}$	${f Atoms}$	$\mathbf{Z}$	${ m Observed}({ m \AA})$	$\operatorname{Ideal}( ext{\AA})$
Г	2	В	202	CMP	O5'-C5'	-2.33	1.42	1.46
	2	A	200	CMP	C2-N1	2.30	1.38	1.33
	2	В	201	CMP	O4'-C1'	2.19	1.44	1.41
	2	В	202	CMP	C5-C4	2.05	1.46	1.40

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\mathbf{Ideal}(^{o})$
2	В	201	CMP	N3-C2-N1	-5.83	119.57	128.68
2	A	200	CMP	N3-C2-N1	-5.50	120.08	128.68
2	В	202	CMP	O3'-C3'-C2'	5.33	120.83	115.61
2	A	200	CMP	C1'-N9-C4	-4.98	117.90	126.64
2	В	202	CMP	O2P-P-O1P	4.91	124.09	108.73
2	A	200	CMP	O2P-P-O3'	4.66	117.89	107.04
2	A	200	CMP	N6-C6-N1	4.46	127.83	118.57
2	В	202	CMP	O3'-C3'-C4'	-4.16	107.57	110.71
2	В	202	CMP	N3-C2-N1	-3.90	122.58	128.68
2	A	200	CMP	O3'-P-O1P	-3.66	102.56	110.39
2	В	202	CMP	N6-C6-N1	3.55	125.94	118.57
2	В	202	CMP	C1'-N9-C4	-3.52	120.47	126.64
2	A	200	CMP	C5-C6-N6	-3.50	115.04	120.35
2	В	201	CMP	O2P-P-O5'	3.40	115.45	107.16
2	В	201	CMP	C2-N1-C6	3.29	124.38	118.75
2	В	201	CMP	N6-C6-N1	3.17	125.15	118.57
2	В	202	CMP	O2P-P-O3'	-3.14	99.72	107.04
2	В	201	CMP	O2P-P-O1P	3.11	118.46	108.73
2	В	202	CMP	C2-N1-C6	2.85	123.64	118.75
2	В	201	CMP	C1'-N9-C4	-2.84	121.65	126.64
2	A	200	CMP	C2-N1-C6	2.77	123.50	118.75
2	В	201	CMP	C5-C6-N6	-2.50	116.55	120.35
2	В	201	CMP	O4'-C1'-C2'	2.48	110.55	106.93
2	В	201	CMP	O2P-P-O3'	-2.42	101.40	107.04
2	В	202	CMP	C2'-C3'-C4'	-2.33	99.09	103.22
2	A	200	CMP	O5'-P-O1P	-2.15	105.48	110.44
2	A	200	СМР	O2P-P-O1P	2.11	115.33	108.73

There are no chirality outliers.

There are no torsion outliers.

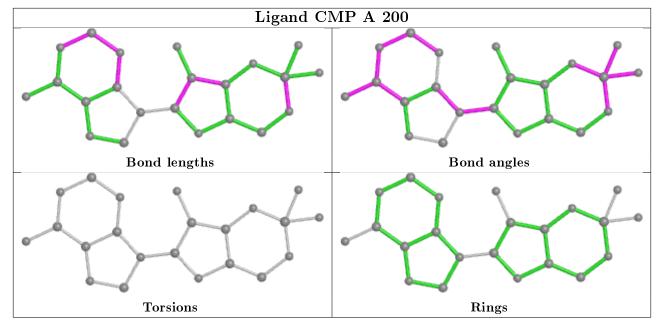
There are no ring outliers.

3 monomers are involved in 3 short contacts:

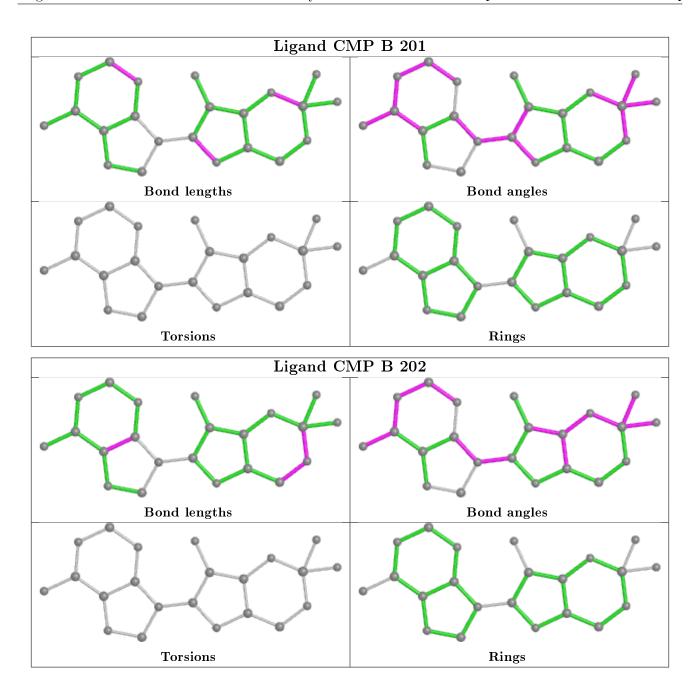


Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	200	CMP	1	0
2	В	201	CMP	1	0
2	В	202	CMP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







# 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,  $95^{th}$  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 $>$	$\#\mathrm{RSRZ}{>}2$		$OWAB(A^2)$	Q < 0.9	
1	A	98/120 (81%)	1.07	23 (23%)	0	0	28, 40, 61, 80	0
1	В	101/120 (84%)	0.71	12 (11%)	4	6	25, 37, 62, 88	0
1	С	99/120 (82%)	0.70	16 (16%)	1	2	26, 37, 64, 80	0
All	All	298/360 (82%)	0.83	51 (17%)	1	2	25, 38, 63, 88	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res Type		RSRZ	
1	A	55 ASP		5.6	
1	A	54	SER	5.6	
1	С	107	PRO	5.1	
1	A	107	PRO	4.4	
1	В	114	SER	4.4	
1	В	113 TRP		4.3	
1	В	54 SER		4.2	
1	С	35[A]	MET	4.1	
1	A	15	ILE	4.0	
1	A	111	SER	4.0	
1	С	114	SER	4.0	
1	С	106	GLY	4.0	
1	A	86	ASP	3.9	
1	A	41	GLY	3.9	
1	В	55	ASP	3.8	
1	A	85	ASN	3.5	
1	С	111	SER	3.5	
1	В	112	ALA	3.5	
1	A	109	GLY	3.2	
1	A	25	ASP	3.1	
1	С	10	ILE	3.0	
1	A	65[A]	LEU	3.0	
1	С	56	ILE	2.9	



Continued from previous page...

Mol	Chain	$ hootnote{Res}$	$\overline{\text{Type}}$	RSRZ	
1	В	65[A]	LEU	2.9	
1	Α	108 GLU		2.8	
1	С	57	GLU	2.7	
1	В	92	TYR	2.7	
1	A	9	VAL	2.7	
1	A	11	VAL	2.7	
1	A	87	TYR	2.5	
1	A	57 GLU		2.5	
1	A	8	LEU	2.4	
1	A	94 CYS		2.3	
1	С	92	TYR	2.3	
1	С	65[A]	LEU	2.3	
1	A	93	ILE	2.3	
1	A C	56	ILE	2.3	
1	С	62	PHE	2.3	
1	A	92	TYR	2.3	
1	С	112	ALA	2.2	
1	A	64	ILE	2.2	
1	В	106	GLY	2.2	
1	С	113	TRP	2.2	
1	В	25	ASP	2.1	
1	С	34	VAL	2.1	
1	С	102	HIS	2.1	
1	В	9	VAL	2.1	
1	В	91	ILE	2.1	
1	В	102	HIS	2.0	
1	A	81	VAL	2.0	
1	С	9	VAL	2.0	

## 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)

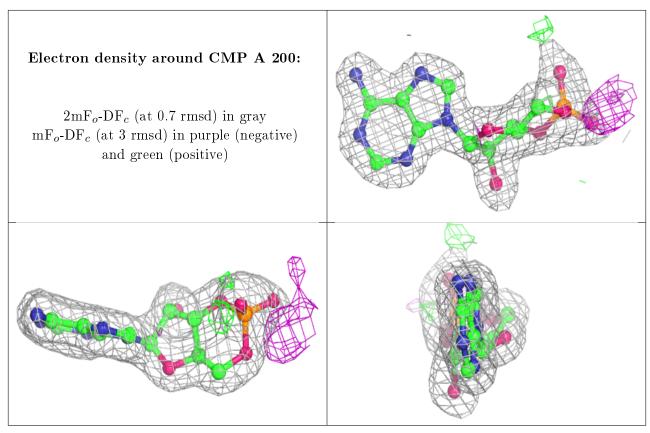
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,



median,  $95^{th}$  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.

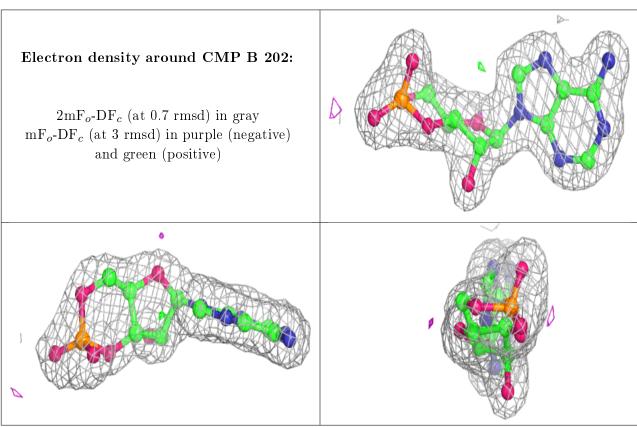
Mol	Type	Chain	$\operatorname{Res}$	Atoms	RSCC	RSR	$ig  \mathbf{B} ext{-factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
3	BCT	С	201	4/4	0.88	0.15	58,68,69,70	0
2	CMP	A	200	22/22	0.92	0.09	31,37,43,60	0
2	CMP	В	201	22/22	0.92	0.10	33,38,48,58	0
2	CMP	В	202	22/22	0.93	0.08	28,33,46,48	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





# Electron density around CMP B 201: 2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative) and green (positive) Electron density around CMP B 202:





# 6.5 Other polymers (i)

There are no such residues in this entry.

