



wwPDB X-ray Structure Validation Summary Report i

Feb 27, 2014 – 04:23 AM GMT

PDB ID : 4F9G
Title : Crystal structure of STING complex with Cyclic di-GMP.
Authors : Kabaleeswaran, V.; Wu, H.
Deposited on : 2012-05-18
Resolution : 2.95 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

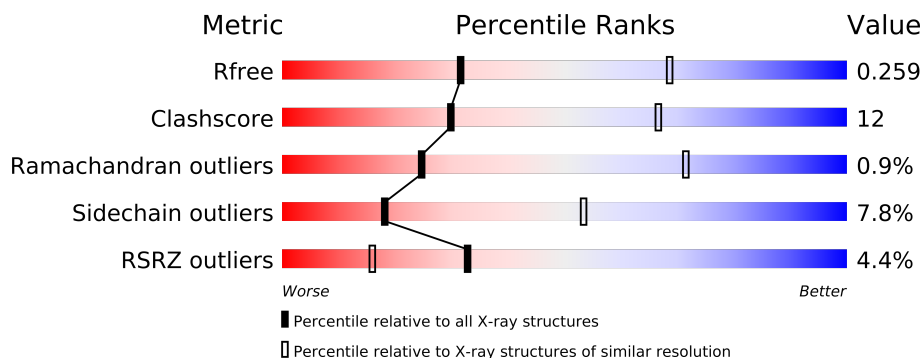
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance



The reported resolution of this entry is 2.95 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1587 (3.00-2.92)
Clashscore	79885	2029 (3.00-2.92)
Ramachandran outliers	78287	1955 (3.00-2.92)
Sidechain outliers	78261	1958 (3.00-2.92)
RSRZ outliers	66119	1588 (3.00-2.92)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	265	
1	C	265	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2720 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Transmembrane protein 173.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	170	Total	C	N	O	S	3	0	0
			1346	852	233	256	5			
1	C	169	Total	C	N	O	S	4	0	0
			1328	841	230	252	5			

There are 48 discrepancies between the modelled and reference sequences:

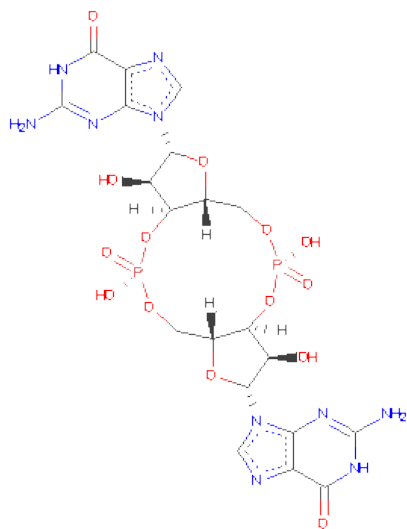
Chain	Residue	Modelled	Actual	Comment	Reference
A	115	MET	-	INITIATING METHIONINE	UNP Q86WV6
A	116	HIS	-	EXPRESSION TAG	UNP Q86WV6
A	117	HIS	-	EXPRESSION TAG	UNP Q86WV6
A	118	HIS	-	EXPRESSION TAG	UNP Q86WV6
A	119	HIS	-	EXPRESSION TAG	UNP Q86WV6
A	120	HIS	-	EXPRESSION TAG	UNP Q86WV6
A	121	HIS	-	EXPRESSION TAG	UNP Q86WV6
A	122	SER	-	EXPRESSION TAG	UNP Q86WV6
A	123	SER	-	EXPRESSION TAG	UNP Q86WV6
A	124	GLY	-	EXPRESSION TAG	UNP Q86WV6
A	125	VAL	-	EXPRESSION TAG	UNP Q86WV6
A	126	ASP	-	EXPRESSION TAG	UNP Q86WV6
A	127	LEU	-	EXPRESSION TAG	UNP Q86WV6
A	128	GLY	-	EXPRESSION TAG	UNP Q86WV6
A	129	THR	-	EXPRESSION TAG	UNP Q86WV6
A	130	GLU	-	EXPRESSION TAG	UNP Q86WV6
A	131	ASN	-	EXPRESSION TAG	UNP Q86WV6
A	132	LEU	-	EXPRESSION TAG	UNP Q86WV6
A	133	TYR	-	EXPRESSION TAG	UNP Q86WV6
A	134	PHE	-	EXPRESSION TAG	UNP Q86WV6
A	135	GLN	-	EXPRESSION TAG	UNP Q86WV6
A	136	SER	-	EXPRESSION TAG	UNP Q86WV6
A	137	ASN	-	EXPRESSION TAG	UNP Q86WV6
A	138	ALA	-	EXPRESSION TAG	UNP Q86WV6
C	115	MET	-	INITIATING METHIONINE	UNP Q86WV6

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	116	HIS	-	EXPRESSION TAG	UNP Q86WV6
C	117	HIS	-	EXPRESSION TAG	UNP Q86WV6
C	118	HIS	-	EXPRESSION TAG	UNP Q86WV6
C	119	HIS	-	EXPRESSION TAG	UNP Q86WV6
C	120	HIS	-	EXPRESSION TAG	UNP Q86WV6
C	121	HIS	-	EXPRESSION TAG	UNP Q86WV6
C	122	SER	-	EXPRESSION TAG	UNP Q86WV6
C	123	SER	-	EXPRESSION TAG	UNP Q86WV6
C	124	GLY	-	EXPRESSION TAG	UNP Q86WV6
C	125	VAL	-	EXPRESSION TAG	UNP Q86WV6
C	126	ASP	-	EXPRESSION TAG	UNP Q86WV6
C	127	LEU	-	EXPRESSION TAG	UNP Q86WV6
C	128	GLY	-	EXPRESSION TAG	UNP Q86WV6
C	129	THR	-	EXPRESSION TAG	UNP Q86WV6
C	130	GLU	-	EXPRESSION TAG	UNP Q86WV6
C	131	ASN	-	EXPRESSION TAG	UNP Q86WV6
C	132	LEU	-	EXPRESSION TAG	UNP Q86WV6
C	133	TYR	-	EXPRESSION TAG	UNP Q86WV6
C	134	PHE	-	EXPRESSION TAG	UNP Q86WV6
C	135	GLN	-	EXPRESSION TAG	UNP Q86WV6
C	136	SER	-	EXPRESSION TAG	UNP Q86WV6
C	137	ASN	-	EXPRESSION TAG	UNP Q86WV6
C	138	ALA	-	EXPRESSION TAG	UNP Q86WV6

- Molecule 2 is 9,9'-[(2R,3R,3AS,5S,7AR,9R,10R,10AS,12S,14AR)-3,5,10,12-TETRAHYDRO XY-5,12-DIOXIDOOCTAHYDRO-2H,7H-DIFURO[3,2-D:3',2'-J][1,3,7,9,2,8]TETRAOXA DIPHOSPHACYCLODODECINE-2,9-DIYL]BIS(2-AMINO-1,9-DIHYDRO-6H-PURIN-6-ONE) (three-letter code: C2E) (formula: C₂₀H₂₄N₁₀O₁₄P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	46	20	10	14	2	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	60.03Å 74.20Å 60.01Å 90.00° 96.32° 90.00°	Depositor
Resolution (Å)	38.30 – 2.95 38.30 – 2.94	Depositor EDS
% Data completeness (in resolution range)	98.5 (38.30-2.95) 98.6 (38.30-2.94)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.25 (at 2.95Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.205 , 0.255 0.208 , 0.259	Depositor DCC
R_{free} test set	1089 reflections (9.83%)	DCC
Wilson B-factor (Å ²)	80.5	Xtriage
Anisotropy	0.433	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 59.5	EDS
Estimated twinning fraction	0.479 for l,-k,h	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 11107 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	2720	wwPDB-VP
Average B, all atoms (Å ²)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.64% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: C2E

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	0.55	0/1369	0.71	1/1858 (0.1%)
1	C	0.52	0/1350	0.70	0/1832
All	All	0.54	0/2719	0.70	1/3690 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	340	GLU	OE1-CD-OE2	-5.75	116.39	123.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1346	0	1294	33	0
1	C	1328	0	1281	36	0
2	A	46	0	22	1	0
All	All	2720	0	2597	64	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including

hydrogens) of the entry. The overall clashscore for this entry is 12.

The worst 5 of 64 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:189:LEU:C	1:A:191:ARG:N	2.15	0.99
1:C:212:LEU:HD13	1:C:261:TYR:CE1	2.19	0.78
1:A:212:LEU:HD13	1:A:261:TYR:CE1	2.23	0.74
2:A:401:C2E:H512	2:A:401:C2E:H5'2	1.73	0.69
1:C:212:LEU:HD13	1:C:261:TYR:HE1	1.61	0.64

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	160/265 (60%)	141 (88%)	17 (11%)	2 (1%)	18	60
1	C	159/265 (60%)	139 (87%)	19 (12%)	1 (1%)	33	79
All	All	319/530 (60%)	280 (88%)	36 (11%)	3 (1%)	25	71

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	175	LEU
1	C	175	LEU
1	A	262	ALA

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	142/231 (62%)	131 (92%)	11 (8%)	18	54
1	C	140/231 (61%)	129 (92%)	11 (8%)	18	52
All	All	282/462 (61%)	260 (92%)	22 (8%)	18	53

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	331	ARG
1	C	170	LEU
1	C	331	ARG
1	A	342	THR
1	C	169	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

1 ligand 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
2	C2E	A	401	-	52,52,52	2.34	14 (26%)	76,82,82	2.66	19 (25%)

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	C2E	A	401	-	-	0/30/62/62	0/0/7/7

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	C2E	C2-N2	6.83	1.43	1.32
2	A	401	C2E	C21-N21	6.62	1.42	1.32
2	A	401	C2E	O6-C6	5.69	1.35	1.24
2	A	401	C2E	C2'-C3'	-5.16	1.40	1.53
2	A	401	C2E	C2A-C3A	-5.03	1.41	1.53

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	C2E	C61-C51-N71	-12.54	132.45	134.14
2	A	401	C2E	C6-C5-N7	-9.94	132.80	134.14
2	A	401	C2E	N31-C41-N91	5.68	135.23	126.91
2	A	401	C2E	C51-C41-N31	-5.57	117.87	125.94
2	A	401	C2E	N3-C4-N9	5.18	134.50	126.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	170/265 (64%)	0.60	7 (4%)	35 17	69, 89, 120, 140	2 (1%)
1	C	169/265 (63%)	0.59	8 (4%)	30 15	68, 89, 120, 133	2 (1%)
All	All	339/530 (63%)	0.59	15 (4%)	33 16	68, 89, 120, 140	4 (1%)

The worst 5 of 15 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	240	TYR	6.1
1	A	225	LEU	3.2
1	C	343	VAL	2.8
1	A	317	PRO	2.6
1	A	212	LEU	2.5

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

There are no non-standard protein/DNA/RNA residues in this entry.

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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	C2E	A	401	46/46	0.17	-0.71	72,89,98,101	0

6.5 Other polymers ⓘ

There are no such residues in this entry.