

wwPDB X-ray Structure Validation Summary Report (i)

May 22, 2020 – 07:26 pm BST

PDB ID : 5C8W

Title: PKG II's Amino Terminal Cyclic Nucleotide Binding Domain (CNB-A) in a

complex with cGMP

Authors: Campbell, J.C.; Reger, A.S.; Huang, G.Y.; Sankaran, B.; Kim, J.J.; Kim,

C.W.

Deposited on : 2015-06-26

Resolution : 1.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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)

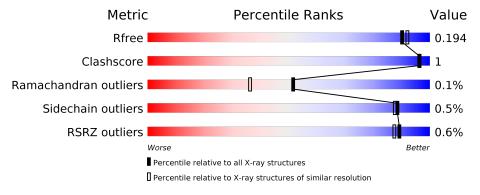
Validation Pipeline (wwPDB-VP) : 2.11

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 1.80 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	$\begin{array}{c} \text{Whole archive} \\ (\#\text{Entries}) \end{array}$	$egin{aligned} ext{Similar resolution} \ (\# ext{Entries, resolution range}(ext{Å})) \end{aligned}$
R_{free}	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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		
1	A	143	82%		16%
1	В	143	81%		15%
1	С	143	83%	•	15%
1	D	143	81%		17%
1	Е	143	82%		17%
1	F	143	78%		17%



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 12209 atoms, of which 5634 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 cGMP-dependent protein kinase 2.

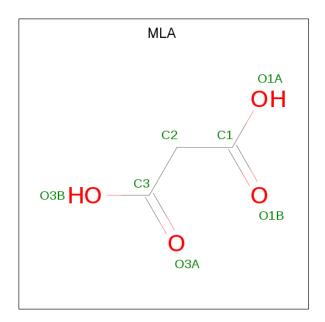
Mol	Chain	Residues			Aton	ıs			ZeroOcc	AltConf	Trace
1	A	120	Total	С	Н	N	О	S	0	0	0
1	A	120	1936	613	971	168	178	6	0	U	
1	В	121	Total	С	Н	N	О	S	0	0	0
1	D	121	1897	609	943	161	178	6	0	0	
1	С	121	Total	С	Н	N	О	S	0	0	0
1		121	1914	611	953	165	179	6		0	
1	D	119	Total	С	Н	N	О	S	0	0	0
1	D	119	1896	603	951	162	174	6	0	U	U
1	Е	119	Total	С	Н	N	О	S	0	0	0
1	15	119	1908	606	954	166	176	6	U	0	
1	F	118	Total	С	Н	N	О	S	0	0	0
1	1'	110	1742	576	848	148	164	6		0	

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	135	GLY	-	expression tag	UNP Q13237
A	136	SER	_	expression tag	UNP Q13237
В	135	GLY	-	expression tag	UNP Q13237
В	136	SER	-	expression tag	UNP Q13237
С	135	GLY	_	expression tag	UNP Q13237
С	136	SER	-	expression tag	UNP Q13237
D	135	GLY	_	expression tag	UNP Q13237
D	136	SER	-	expression tag	UNP Q13237
Е	135	GLY	_	expression tag	UNP Q13237
Е	136	SER	=	expression tag	UNP Q13237
F	135	GLY	_	expression tag	UNP Q13237
F	136	SER	-	expression tag	UNP Q13237

• Molecule 2 is MALONIC ACID (three-letter code: MLA) (formula: $C_3H_4O_4$).

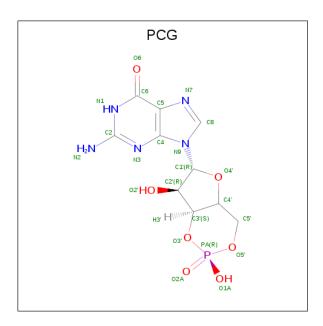




Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C H O 9 3 2 4	0	0
2	В	1	Total C H O 9 3 2 4	0	0
2	В	1	Total C H O 9 3 2 4	0	0
2	С	1	Total C H O 9 3 2 4	0	0
2	D	1	Total C H O 9 3 2 4	0	0
2	Е	1	Total C H O 9 3 2 4	0	0
2	F	1	Total C H O 9 3 2 4	0	0

 \bullet Molecule 3 is CYCLIC GUANOSINE MONOPHOSPHATE (three-letter code: PCG) (formula: $\rm C_{10}H_{12}N_5O_7P$).





Mol	Chain	Residues		Ato	ms			ZeroOcc	AltConf	
3	A	1	Total	С	N	О	Р	0	0	
) 	А	1	23	10	5	7	1	0	U	
3	В	1	Total	С	Ν	О	Р	0	0	
J	D	1	23	10	5	7	1	0	0	
3	C	1	Total	С	Ν	О	Р	0	0	
	3 0	1	23	10	5	7	1	U		
3	D	1	Total	С	Ν	О	Р	0	0	
	D	1	23	10	5	7	1	U	U	
3	E	1	Total	С	Ν	Ο	Р	0	0	
		1	23	10	5	7	1	U	U	
3	F	1	Total	С	Ν	Ο	Р	0	0	
3 F	1	23	10	5	7	1				

• Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	${f Atoms}$	ZeroOcc	AltConf
4	A	1	Total Na 1 1	0	0
4	С	1	Total Na 1 1	0	0
4	F	1	Total Na 1 1	0	0

• Molecule 5 is water.



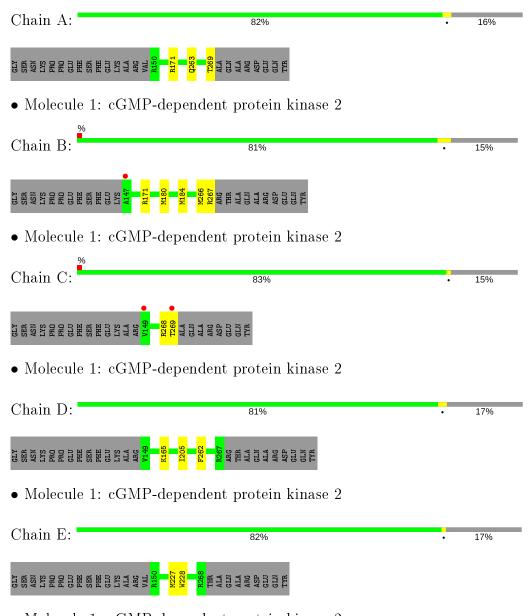
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	162	Total O 162 162	0	0
5	В	155	Total O 155 155	0	0
5	С	139	Total O 139 139	0	0
5	D	98	Total O 98 98	0	0
5	Е	91	Total O 91 91	0	0
5	F	67	Total O 67 67	0	0



3 Residue-property plots (i)

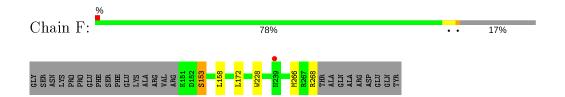
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: cGMP-dependent protein kinase 2



• Molecule 1: cGMP-dependent protein kinase 2







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	46.71Å 103.45Å 176.41Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	51.73 - 1.80	Depositor
Resolution (A)	51.73 - 1.80	EDS
% Data completeness	99.6 (51.73-1.80)	Depositor
(in resolution range)	99.6 (51.73-1.80)	EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	4.29 (at 1.79Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
P. P.	0.162 , 0.196	Depositor
R, R_{free}	0.163 , 0.194	DCC
R_{free} test set	2000 reflections (2.50%)	wwPDB-VP
Wilson B-factor (Å ²)	20.0	Xtriage
Anisotropy	0.524	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.38, 52.3	EDS
L-test for twinning ²	$ < L > = 0.48, < L^2> = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12209	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 9.96% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities 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: NA, MLA, PCG

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		
MIOI		RMSZ	# Z >5	RMSZ	# Z > 5	
1	A	0.53	0/981	0.65	0/1320	
1	В	0.55	0/970	0.66	0/1308	
1	С	0.53	0/977	0.67	0/1317	
1	D	0.55	0/961	0.64	0/1295	
1	Е	0.42	0/970	0.59	0/1306	
1	F	0.42	0/910	0.57	0/1235	
All	All	0.50	0/5769	0.63	0/7781	

There are no bond length outliers.

There are no bond angle outliers.

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	965	971	971	3	0
1	В	954	943	952	3	0
1	С	961	953	953	1	0
1	D	945	951	950	1	0
1	Е	954	954	953	1	0
1	F	894	848	849	3	0
2	A	7	2	2	0	0

Continued on next page...



Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	В	14	4	4	0	0
2	С	7	2	2	0	0
2	D	7	2	2	0	0
2	Ε	7	2	2	0	0
2	F	7	2	2	0	0
3	A	23	0	11	0	0
3	В	23	0	11	0	0
3	С	23	0	11	0	0
3	D	23	0	11	0	0
3	Ε	23	0	11	0	0
3	F	23	0	11	0	0
4	A	1	0	0	0	0
4	$^{\mathrm{C}}$	1	0	0	0	0
4	F	1	0	0	0	0
5	Α	162	0	0	3	3
5	В	155	0	0	2	5
5	С	139	0	0	0	1
5	D	98	0	0	0	2
5	Ε	91	0	0	0	2
5	F	67	0	0	1	1
All	All	6575	5634	5708	12	7

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 1.

The worst 5 of 12 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$egin{aligned} & ext{Interatomic} \ & ext{distance} \ & ext{(Å)} \end{aligned}$	$egin{array}{c} ext{Clash} \ ext{overlap } (ext{Å}) \end{array}$
1:A:263:GLN:NE2	5:A:402:HOH:O	2.24	0.68
1:B:267:ARG:O	5:B:401:HOH:O	2.14	0.65
1:A:171:ARG:NH2	5:A:406:HOH:O	2.31	0.55
1:A:269:THR:O	5:A:401:HOH:O	2.17	0.50
1:F:172:LEU:HD21	1:F:266:MET:HE1	1.95	0.48

The worst 5 of 7 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	$egin{aligned} ext{Interatomic} \ ext{distance} \ (ext{Å}) \end{aligned}$	Clash overlap (Å)
5:B:461:HOH:O	5:E:476:HOH:O[2_555]	2.12	0.08
5:A:537:HOH:O	5:B:497:HOH:O[4_545]	2.12	0.08

Continued on next page...



Continued from previous page...

Atom-1	Atom-2	$egin{aligned} ext{Interatomic} \ ext{distance} & (ext{Å}) \end{aligned}$	Clash overlap (Å)
5:B:406:HOH:O	5:D:406:HOH:O[1_455]	2.16	0.04
5:B:498:HOH:O	5:D:461:HOH:O[1_455]	2.17	0.03
5:E:481:HOH:O	5:F:437:HOH:O[3_654]	2.18	0.02

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	$118/143 \ (82\%)$	117 (99%)	1 (1%)	0	100 100
1	В	119/143 (83%)	117 (98%)	2 (2%)	0	100 100
1	С	119/143 (83%)	118 (99%)	1 (1%)	0	100 100
1	D	117/143 (82%)	116 (99%)	1 (1%)	0	100 100
1	Е	117/143 (82%)	115 (98%)	2 (2%)	0	100 100
1	F	116/143 (81%)	113 (97%)	2 (2%)	1 (1%)	17 6
All	All	706/858 (82%)	696 (99%)	9 (1%)	1 (0%)	51 36

All (1) Ramachandran outliers are listed below:

Mol	Chain	${f Res}$	Type
1	F	153	SER

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	104/126~(82%)	104 (100%)	0	100 100
1	В	102/126 (81%)	101 (99%)	1 (1%)	76 71
1	С	102/126 (81%)	102 (100%)	0	100 100
1	D	102/126 (81%)	101 (99%)	1 (1%)	76 71
1	E	102/126~(81%)	102 (100%)	0	100 100
1	F	87/126 (69%)	86 (99%)	1 (1%)	73 68
All	All	599/756 (79%)	596 (100%)	3 (0%)	88 87

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	В	266	MET
1	D	165	LYS
1	F	153	SER

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)

Of 16 ligands modelled in this entry, 3 are monoatomic - leaving 13 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	Tuno	Chain	Dog	Res Link Bo		Bond lengths			ond ang	gles
IVIOI	Type	Chain	nes	LIIIK	Counts	RMSZ	$\mid \# Z > 2$	Counts	RMSZ	# Z > 2
2	MLA	В	301	_	0,6,6	0.00	-	0,7,7	0.00	-
3	PCG	D	302	_	22,26,26	2.45	7 (31%)	26,41,41	2.26	11 (42%)
2	MLA	D	301	-	0,6,6	0.00	-	0,7,7	0.00	-
2	MLA	F	301	_	0,6,6	0.00	-	0,7,7	0.00	-
2	MLA	A	301	_	0,6,6	0.00	-	0,7,7	0.00	-
2	MLA	Е	301	_	0,6,6	0.00	-	0,7,7	0.00	-
3	PCG	A	302	_	22,26,26	2.38	7 (31%)	26,41,41	2.54	12 (46%)
3	PCG	С	302	-	22,26,26	2.13	6 (27%)	26,41,41	2.43	10 (38%)
3	PCG	F	302	-	22,26,26	1.85	6 (27%)	26,41,41	2.82	10 (38%)
3	PCG	В	303	-	22,26,26	2.22	7 (31%)	26,41,41	2.66	13 (50%)
2	MLA	В	302	-	0,6,6	0.00	-	0,7,7	0.00	-
3	PCG	Е	302	_	22,26,26	1.99	6 (27%)	26,41,41	2.67	11 (42%)
2	MLA	С	301	_	0,6,6	0.00	_	0,7,7	0.00	-

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	MLA	В	301	-	-	0/0/4/4	-
3	PCG	D	302	-	-	0/0/31/31	0/4/4/4
2	MLA	D	301	-	-	0/0/4/4	_
2	MLA	F	301	_	_	0/0/4/4	-
2	MLA	A	301	_	_	0/0/4/4	-
2	MLA	Е	301	_	_	0/0/4/4	-
3	PCG	A	302	_	_	0/0/31/31	0/4/4/4
3	PCG	С	302	_	-	0/0/31/31	0/4/4/4
3	PCG	F	302	_	_	0/0/31/31	0/4/4/4
3	PCG	В	303	_	_	0/0/31/31	0/4/4/4
2	MLA	В	302	_	_	0/0/4/4	_
3	PCG	Е	302	-	-	0/0/31/31	0/4/4/4
2	MLA	С	301	-	-	0/0/4/4	-

The worst 5 of 39 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	${ m Observed}(m \AA)$	$\operatorname{Ideal}(ext{\AA})$
3	D	302	PCG	PA-O5'	-6.35	1.50	1.57

Continued on next page...



Continued from previous page...

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	${f Observed(\AA)}$	$\operatorname{Ideal}(ext{\AA})$
3	С	302	PCG	PA-O5'	-6.06	1.50	1.57
3	A	302	PCG	PA-O5'	-5.95	1.50	1.57
3	A	302	PCG	O5'-C5'	-5.40	1.38	1.46
3	В	303	PCG	O5'-C5'	-5.38	1.38	1.46

The worst 5 of 67 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\mathrm{Ideal}(^{o})$
3	F	302	PCG	O3'-C3'-C4'	-6.93	105.48	110.71
3	E	302	PCG	O3'-C3'-C4'	-6.05	106.14	110.71
3	Е	302	PCG	C2-N3-C4	5.85	122.04	115.36
3	В	303	PCG	C2-N3-C4	5.66	121.82	115.36
3	F	302	PCG	C2-N3-C4	5.51	121.64	115.36

There are no chirality outliers.

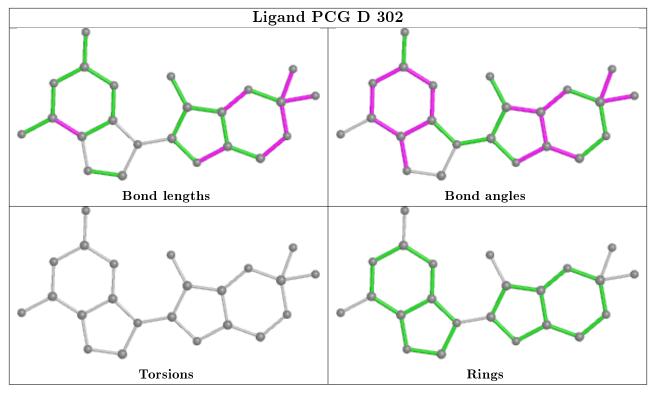
There are no torsion outliers.

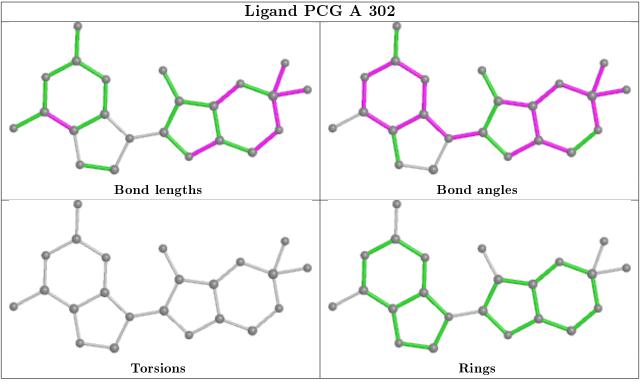
There are no ring outliers.

No monomer is involved in short contacts.

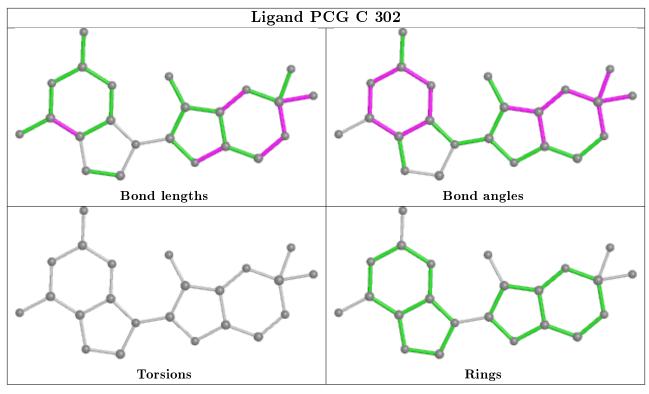
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

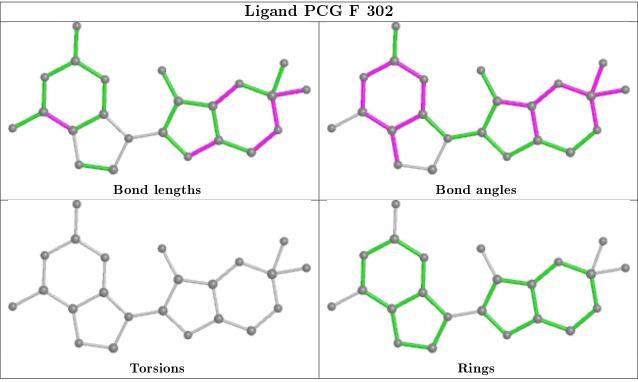




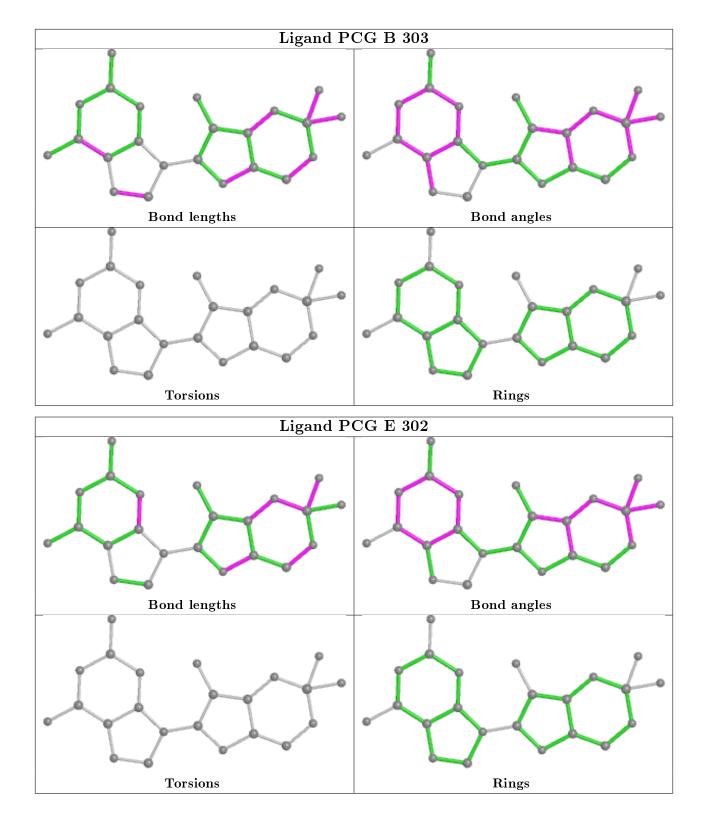












5.7 Other polymers (i)

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	$\langle { m RSRZ} \rangle$	$\# \mathrm{RSRZ} {>} 2$	$OWAB(\AA^2)$	Q < 0.9
1	A	120/143 (83%)	-0.51	0 100 100	12, 20, 45, 75	0
1	В	121/143 (84%)	-0.45	1 (0%) 86 84	12, 20, 43, 76	0
1	С	121/143 (84%)	-0.46	2 (1%) 70 66	14, 22, 49, 76	0
1	D	119/143 (83%)	-0.43	0 100 100	14, 27, 53, 58	0
1	E	119/143 (83%)	-0.25	0 100 100	21, 33, 60, 85	0
1	F	118/143 (82%)	-0.16	1 (0%) 86 84	24, 35, 63, 95	0
All	All	718/858 (83%)	-0.38	4 (0%) 89 87	12, 27, 53, 95	0

All (4) RSRZ outliers are listed below:

Mol	Chain	${f Res}$	\mathbf{Type}	RSRZ
1	С	149	VAL	3.8
1	В	147	ALA	2.9
1	С	269	THR	2.8
1	F	239	ASN	2.2

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	Res	Atoms	RSCC	RSR	${f B\text{-factors}}({f \AA}^2)$	Q < 0.9
2	MLA	В	302	7/7	0.86	0.14	36,50,59,61	0
2	MLA	Ε	301	7/7	0.89	0.14	33,42,51,51	0
4	NA	С	303	1/1	0.95	0.17	28,28,28,28	0
3	PCG	F	302	23/23	0.96	0.09	17,23,36,45	0
2	MLA	F	301	7/7	0.96	0.09	27,47,56,57	0
2	MLA	В	301	7/7	0.97	0.10	20,26,39,40	0
3	PCG	С	302	23/23	0.97	0.09	13,18,22,35	0
3	PCG	E	302	23/23	0.97	0.09	12,19,23,28	0
2	MLA	С	301	7/7	0.97	0.08	23,25,32,43	0
2	MLA	D	301	7/7	0.98	0.08	28,38,46,49	0
2	MLA	A	301	7/7	0.98	0.10	19,21,34,36	0
3	PCG	В	303	23/23	0.98	0.12	9,14,17,25	0
3	PCG	D	302	23/23	0.98	0.07	16,22,29,38	0
4	NA	F	303	1/1	0.98	0.13	37,37,37,37	0
3	PCG	A	302	23/23	0.98	0.10	9,13,17,19	0
4	NA	A	303	1/1	0.99	0.19	20,20,20,20	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 PCG F 302: 2mF_o-DF_c (at 0.7 rmsd) in gray mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around PCG E 302: $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray mF_o -DF_c (at 3 rmsd) in purple (negative) and green (positive) Electron density around PCG B 303: $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray mF_o -DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around PCG D 302: $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray mF_o -DF_c (at 3 rmsd) in purple (negative) and green (positive) Electron density around PCG A 302: $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray mF_o -DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.

