



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:59 PM UTC

PDB ID : 5C8W / pdb_00005c8w
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 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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

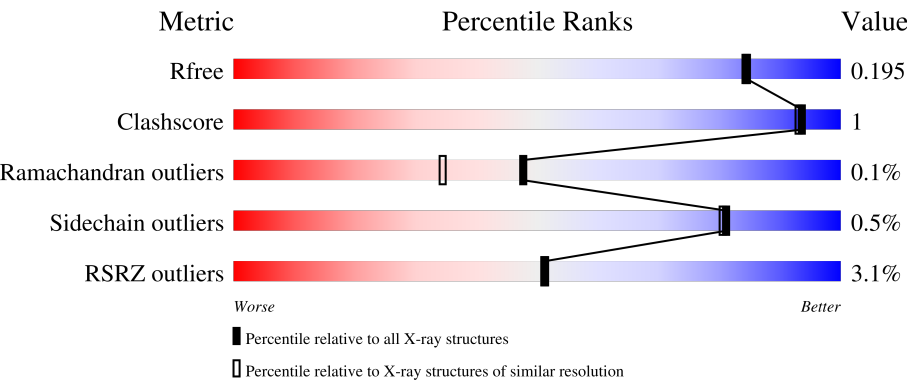
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (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 of 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 $\leq 5\%$. 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	143	% 81%16%
1	B	143	2% 81%15%
1	C	143	2% 82%15%
1	D	143	% 81%17%

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Mol	Chain	Length	Quality of chain
1	E	143	% 82% 17%
1	F	143	7% 78% 17%

2 Entry composition

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.

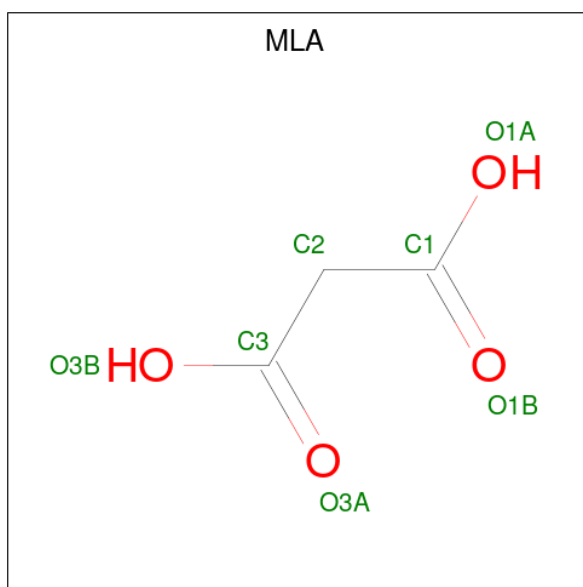
- Molecule 1 is a protein called cGMP-dependent protein kinase 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	120	Total	C	H	N	O	S	0	0	0
			1936	613	971	168	178	6			
1	B	121	Total	C	H	N	O	S	0	0	0
			1897	609	943	161	178	6			
1	C	121	Total	C	H	N	O	S	0	0	0
			1914	611	953	165	179	6			
1	D	119	Total	C	H	N	O	S	0	0	0
			1896	603	951	162	174	6			
1	E	119	Total	C	H	N	O	S	0	0	0
			1908	606	954	166	176	6			
1	F	118	Total	C	H	N	O	S	0	0	0
			1742	576	848	148	164	6			

There are 12 discrepancies between the modelled and reference sequences:

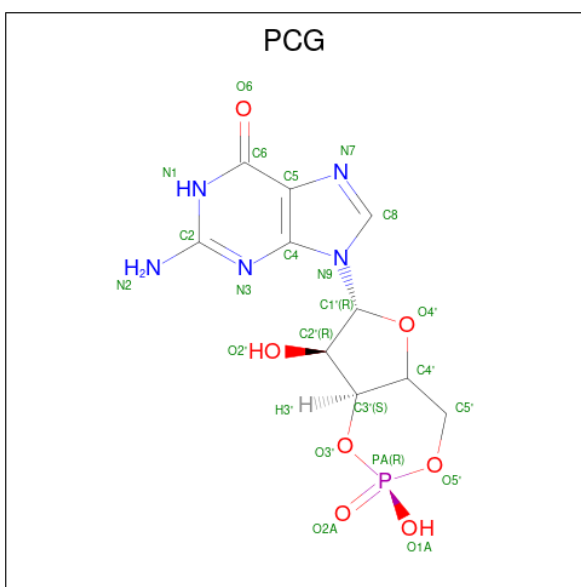
Chain	Residue	Modelled	Actual	Comment	Reference
A	135	GLY	-	expression tag	UNP Q13237
A	136	SER	-	expression tag	UNP Q13237
B	135	GLY	-	expression tag	UNP Q13237
B	136	SER	-	expression tag	UNP Q13237
C	135	GLY	-	expression tag	UNP Q13237
C	136	SER	-	expression tag	UNP Q13237
D	135	GLY	-	expression tag	UNP Q13237
D	136	SER	-	expression tag	UNP Q13237
E	135	GLY	-	expression tag	UNP Q13237
E	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 (CCD ID: MLA) (formula: C₃H₄O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			9	3	2	4		
2	B	1	Total	C	H	O	0	0
			9	3	2	4		
2	B	1	Total	C	H	O	0	0
			9	3	2	4		
2	C	1	Total	C	H	O	0	0
			9	3	2	4		
2	D	1	Total	C	H	O	0	0
			9	3	2	4		
2	E	1	Total	C	H	O	0	0
			9	3	2	4		
2	F	1	Total	C	H	O	0	0
			9	3	2	4		

- Molecule 3 is CYCLIC GUANOSINE MONOPHOSPHATE (CCD ID: PCG) (formula: C₁₀H₁₂N₅O₇P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	B	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	C	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	D	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	E	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	F	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Na	0	0
			1	1		
4	C	1	Total	Na	0	0
			1	1		
4	F	1	Total	Na	0	0
			1	1		

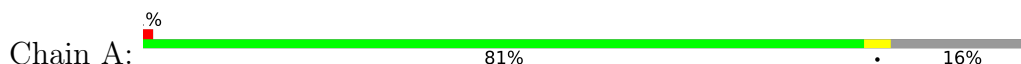
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	162	Total 162	O 162	0	0
5	B	155	Total 155	O 155	0	0
5	C	139	Total 139	O 139	0	0
5	D	98	Total 98	O 98	0	0
5	E	91	Total 91	O 91	0	0
5	F	67	Total 67	O 67	0	0

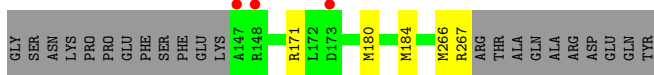
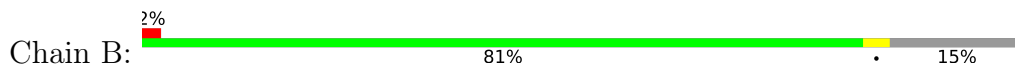
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

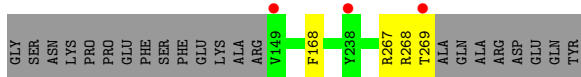
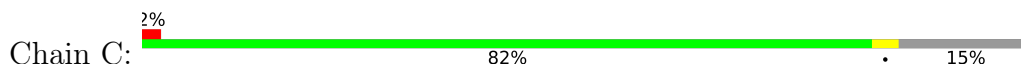
- Molecule 1: cGMP-dependent protein kinase 2



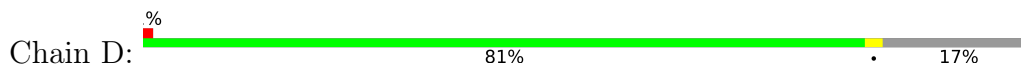
- Molecule 1: cGMP-dependent protein kinase 2



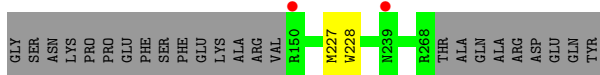
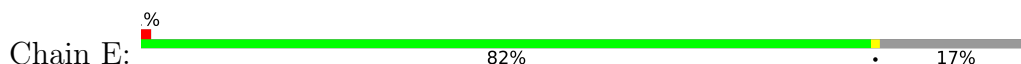
- Molecule 1: cGMP-dependent protein kinase 2



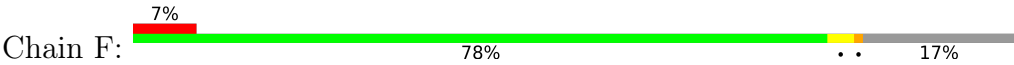
- Molecule 1: cGMP-dependent protein kinase 2



- Molecule 1: cGMP-dependent protein kinase 2



- Molecule 1: cGMP-dependent protein kinase 2



GLY	SER	ASN	LYS	PRO	GLU	PHE	SER	PHE	GLU	LYS	ALA	ARG	VAL	ARG	K151	D152	S153	S154	E155	L158	L172	G202	I205	E219	W228	N239	W266	R267	R268	THR	ALA	GLN	ALA	ARG	ASP	GLU	GLN	TYR
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	46.71Å 103.45Å 176.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	51.73 – 1.80 51.73 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.6 (51.73-1.80) 99.6 (51.73-1.80)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.29 (at 1.79Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.162 , 0.196 0.164 , 0.195	Depositor 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)	0.39 , 51.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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: NA, PCG, MLA

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	0.67	0/981	0.83	2/1320 (0.2%)
1	B	0.66	0/970	0.79	0/1308
1	C	0.67	0/977	0.80	0/1317
1	D	0.65	0/961	0.78	0/1295
1	E	0.50	0/970	0.78	0/1306
1	F	0.54	0/910	0.77	0/1235
All	All	0.62	0/5769	0.79	2/7781 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	201	PRO	CA-C-N	-5.42	116.31	121.57
1	A	201	PRO	C-N-CA	-5.42	116.31	121.57

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	B	954	943	952	3	0
1	C	961	953	953	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	945	951	950	2	0
1	E	954	954	953	1	0
1	F	894	848	849	4	0
2	A	7	2	2	0	0
2	B	14	4	4	0	0
2	C	7	2	2	0	0
2	D	7	2	2	0	0
2	E	7	2	2	0	0
2	F	7	2	2	0	0
3	A	23	0	11	0	0
3	B	23	0	11	0	0
3	C	23	0	11	0	0
3	D	23	0	11	0	0
3	E	23	0	11	0	0
3	F	23	0	11	0	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	F	1	0	0	0	0
5	A	162	0	0	3	3
5	B	155	0	0	2	5
5	C	139	0	0	0	1
5	D	98	0	0	1	2
5	E	91	0	0	0	2
5	F	67	0	0	1	1
All	All	6575	5634	5708	16	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.

All (16) 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: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:F:172:LEU:HD21	1:F:266:MET:HE1	1.86	0.57
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:B:171:ARG:NH2	5:B:402:HOH:O	2.37	0.47
1:C:268:ARG:O	1:C:269:THR:OG1	2.26	0.46
1:D:205:ILE:HD11	1:D:262:PHE:CE2	2.50	0.45
1:C:267:ARG:C	1:C:269:THR:H	2.25	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:268:ARG:O	5:F:401:HOH:O	2.20	0.44
1:F:172:LEU:CD2	1:F:266:MET:HE1	2.48	0.43
1:F:158:LEU:HD13	1:F:228:TRP:CZ2	2.54	0.43
1:D:156:LYS:NZ	5:D:405:HOH:O	2.51	0.42
1:B:180:MET:O	1:B:184:MET:HG3	2.19	0.42
1:E:227:MET:HG3	1:E:228:TRP:CD1	2.56	0.40
1:C:168:PHE:CD1	1:C:168:PHE:C	3.00	0.40

All (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	Interatomic distance (Å)	Clash overlap (Å)
5:A:537:HOH:O	5:B:497:HOH:O[4_545]	2.12	0.08
5:B:461:HOH:O	5:E:476:HOH:O[2_555]	2.12	0.08
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:A:517:HOH:O	5:B:491:HOH:O[4_445]	2.18	0.02
5:E:481:HOH:O	5:F:437:HOH:O[3_654]	2.18	0.02
5:A:528:HOH:O	5:C:500:HOH:O[1_455]	2.19	0.01

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	118/143 (82%)	117 (99%)	1 (1%)	0	100	100
1	B	119/143 (83%)	117 (98%)	2 (2%)	0	100	100
1	C	119/143 (83%)	118 (99%)	1 (1%)	0	100	100
1	D	117/143 (82%)	116 (99%)	1 (1%)	0	100	100
1	E	117/143 (82%)	115 (98%)	2 (2%)	0	100	100
1	F	116/143 (81%)	113 (97%)	2 (2%)	1 (1%)	14	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	706/858 (82%)	696 (99%)	9 (1%)	1 (0%)	48 34

All (1) Ramachandran outliers are listed below:

Mol	Chain	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	B	102/126 (81%)	101 (99%)	1 (1%)	68 64
1	C	102/126 (81%)	102 (100%)	0	100 100
1	D	102/126 (81%)	102 (100%)	0	100 100
1	E	102/126 (81%)	102 (100%)	0	100 100
1	F	87/126 (69%)	85 (98%)	2 (2%)	44 33
All	All	599/756 (79%)	596 (100%)	3 (0%)	81 80

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

Mol	Chain	Res	Type
1	B	266	MET
1	F	153	SER
1	F	266	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	175	GLN
1	A	203	ASN
1	B	175	GLN

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Mol	Chain	Res	Type
1	B	188	ASN
1	B	203	ASN
1	D	167	GLN
1	E	175	GLN
1	F	264	ASN

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 oligosaccharides 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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	PCG	B	303	-	26,26,26	2.27	10 (38%)	39,41,41	2.35	15 (38%)
3	PCG	A	302	-	26,26,26	2.49	12 (46%)	39,41,41	2.07	12 (30%)
2	MLA	F	301	-	6,6,6	1.16	0	7,7,7	1.03	0
2	MLA	B	301	-	6,6,6	1.13	0	7,7,7	1.57	2 (28%)
3	PCG	F	302	-	26,26,26	2.03	10 (38%)	39,41,41	2.50	10 (25%)
2	MLA	B	302	-	6,6,6	1.43	0	7,7,7	1.70	3 (42%)
3	PCG	C	302	-	26,26,26	2.18	10 (38%)	39,41,41	2.22	13 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MLA	A	301	-	6,6,6	1.16	0	7,7,7	1.22	1 (14%)
3	PCG	D	302	-	26,26,26	2.50	11 (42%)	39,41,41	2.28	14 (35%)
2	MLA	C	301	-	6,6,6	1.06	0	7,7,7	1.61	1 (14%)
3	PCG	E	302	-	26,26,26	2.16	11 (42%)	39,41,41	2.50	12 (30%)
2	MLA	D	301	-	6,6,6	1.12	0	7,7,7	1.03	0
2	MLA	E	301	-	6,6,6	1.14	0	7,7,7	1.28	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	PCG	B	303	-	-	0/4/31/31	0/4/4/4
3	PCG	A	302	-	-	0/4/31/31	0/4/4/4
2	MLA	F	301	-	-	2/4/4/4	-
2	MLA	B	301	-	-	2/4/4/4	-
3	PCG	F	302	-	-	0/4/31/31	0/4/4/4
2	MLA	B	302	-	-	0/4/4/4	-
3	PCG	C	302	-	-	0/4/31/31	0/4/4/4
2	MLA	A	301	-	-	4/4/4/4	-
3	PCG	D	302	-	-	0/4/31/31	0/4/4/4
2	MLA	C	301	-	-	2/4/4/4	-
3	PCG	E	302	-	-	0/4/31/31	0/4/4/4
2	MLA	D	301	-	-	4/4/4/4	-
2	MLA	E	301	-	-	2/4/4/4	-

All (64) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	302	PCG	PA-O5'	-6.35	1.50	1.57
3	C	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	B	303	PCG	O5'-C5'	-5.38	1.38	1.46
3	E	302	PCG	O5'-C5'	-5.02	1.39	1.46
3	F	302	PCG	O5'-C5'	-4.62	1.39	1.46
3	E	302	PCG	C5-N7	-4.06	1.30	1.39
3	F	302	PCG	C6-N1	-4.04	1.31	1.38
3	D	302	PCG	O5'-C5'	-3.97	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	303	PCG	PA-O1A	-3.88	1.37	1.55
3	D	302	PCG	C6-N1	-3.72	1.31	1.38
3	C	302	PCG	C5-N7	-3.70	1.31	1.39
3	D	302	PCG	O3'-C3'	-3.69	1.39	1.44
3	E	302	PCG	PA-O2A	-3.63	1.38	1.50
3	B	303	PCG	O3'-C3'	-3.57	1.39	1.44
3	C	302	PCG	O5'-C5'	-3.56	1.41	1.46
3	D	302	PCG	C5-N7	-3.52	1.32	1.39
3	A	302	PCG	C6-N1	-3.52	1.32	1.38
3	D	302	PCG	O4'-C4'	-3.52	1.37	1.45
3	B	303	PCG	O4'-C4'	-3.50	1.37	1.45
3	F	302	PCG	C5-N7	-3.47	1.32	1.39
3	A	302	PCG	C4-N9	-3.32	1.29	1.38
3	A	302	PCG	C5-N7	-3.28	1.32	1.39
3	B	303	PCG	C5-N7	-3.22	1.32	1.39
3	D	302	PCG	PA-O2A	-3.19	1.39	1.50
3	A	302	PCG	O4'-C4'	-3.13	1.38	1.45
3	A	302	PCG	PA-O2A	-3.10	1.40	1.50
3	E	302	PCG	O4'-C4'	-3.09	1.38	1.45
3	B	303	PCG	C4-N9	-3.06	1.30	1.38
3	D	302	PCG	PA-O1A	-3.06	1.41	1.55
3	C	302	PCG	PA-O1A	-2.97	1.41	1.55
3	E	302	PCG	C6-N1	-2.96	1.33	1.38
3	D	302	PCG	C4-N9	-2.87	1.30	1.38
3	C	302	PCG	O4'-C4'	-2.84	1.38	1.45
3	C	302	PCG	O3'-C3'	-2.83	1.40	1.44
3	E	302	PCG	C4-N9	-2.82	1.30	1.38
3	F	302	PCG	C4-N9	-2.77	1.31	1.38
3	B	303	PCG	C8-N9	-2.76	1.31	1.37
3	C	302	PCG	C4-N9	-2.70	1.31	1.38
3	E	302	PCG	O3'-C3'	-2.65	1.40	1.44
3	D	302	PCG	C8-N9	-2.63	1.31	1.37
3	A	302	PCG	PA-O1A	-2.59	1.43	1.55
3	F	302	PCG	C8-N9	-2.57	1.31	1.37
3	B	303	PCG	PA-O2A	-2.57	1.41	1.50
3	E	302	PCG	C8-N9	-2.57	1.31	1.37
3	C	302	PCG	C6-N1	-2.55	1.34	1.38
3	C	302	PCG	C8-N9	-2.54	1.31	1.37
3	A	302	PCG	C8-N9	-2.54	1.31	1.37
3	A	302	PCG	C5-C4	2.53	1.45	1.38
3	B	303	PCG	C6-N1	-2.53	1.34	1.38
3	F	302	PCG	PA-O1A	-2.52	1.43	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	302	PCG	O3'-C3'	-2.49	1.40	1.44
3	F	302	PCG	O4'-C4'	-2.43	1.39	1.45
3	E	302	PCG	C5-C4	2.42	1.45	1.38
3	B	303	PCG	C5-C4	2.36	1.45	1.38
3	F	302	PCG	C5-C4	2.36	1.45	1.38
3	C	302	PCG	C5-C4	2.19	1.44	1.38
3	E	302	PCG	PA-O3'	-2.15	1.54	1.57
3	F	302	PCG	O3'-C3'	-2.14	1.41	1.44
3	A	302	PCG	O6-C6	-2.09	1.19	1.23
3	D	302	PCG	C5-C4	2.08	1.44	1.38
3	F	302	PCG	PA-O5'	-2.05	1.55	1.57
3	E	302	PCG	C3'-C4'	-2.02	1.47	1.52

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	302	PCG	O3'-C3'-C4'	-6.93	105.48	110.71
3	D	302	PCG	C5-C4-N3	-6.47	118.10	128.39
3	E	302	PCG	C5-C4-N3	-6.28	118.40	128.39
3	F	302	PCG	C5-C4-N3	-6.26	118.43	128.39
3	E	302	PCG	O3'-C3'-C4'	-6.05	106.14	110.71
3	B	303	PCG	C5-C4-N3	-5.92	118.97	128.39
3	E	302	PCG	C2-N3-C4	5.66	122.04	112.30
3	E	302	PCG	N9-C4-N3	5.65	137.25	125.95
3	B	303	PCG	C2-N3-C4	5.53	121.82	112.30
3	C	302	PCG	C5-C4-N3	-5.48	119.67	128.39
3	B	303	PCG	N9-C4-N3	5.44	136.82	125.95
3	F	302	PCG	C2-N3-C4	5.43	121.64	112.30
3	D	302	PCG	C2-N3-C4	5.36	121.53	112.30
3	F	302	PCG	N9-C4-N3	5.20	136.34	125.95
3	D	302	PCG	N9-C4-N3	5.18	136.32	125.95
3	C	302	PCG	N9-C4-N3	4.96	135.86	125.95
3	C	302	PCG	O3'-C3'-C4'	-4.55	107.28	110.71
3	A	302	PCG	C5-C4-N3	-4.53	121.17	128.39
3	C	302	PCG	C2-N3-C4	4.44	119.95	112.30
3	D	302	PCG	O3'-C3'-C4'	-4.21	107.53	110.71
3	A	302	PCG	N9-C4-N3	4.17	134.29	125.95
3	A	302	PCG	O3'-C3'-C2'	4.16	119.69	115.61
3	A	302	PCG	C2-N3-C4	4.03	119.23	112.30
3	F	302	PCG	O1A-PA-O2A	3.86	120.42	108.56
3	B	303	PCG	O3'-C3'-C2'	3.65	119.19	115.61
3	C	302	PCG	O3'-C3'-C2'	3.60	119.13	115.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	302	PCG	O3'-C3'-C4'	-3.55	108.03	110.71
3	B	303	PCG	O3'-C3'-C4'	-3.52	108.05	110.71
3	F	302	PCG	O3'-C3'-C2'	3.44	118.97	115.61
3	F	302	PCG	C6-C5-N7	3.41	136.50	130.29
3	E	302	PCG	O1A-PA-O2A	3.41	119.03	108.56
3	D	302	PCG	C6-C5-N7	3.32	136.33	130.29
3	A	302	PCG	C6-C5-N7	3.31	136.31	130.29
3	E	302	PCG	O6-C6-C5	-3.25	117.95	126.53
3	B	303	PCG	C6-C5-N7	3.23	136.18	130.29
3	E	302	PCG	O5'-PA-O3'	-3.14	101.49	105.70
3	B	303	PCG	O1A-PA-O2A	3.09	118.07	108.56
3	B	303	PCG	O5'-PA-O3'	-3.08	101.58	105.70
3	F	302	PCG	O5'-PA-O3'	-3.03	101.65	105.70
3	C	302	PCG	O5'-PA-O2A	-3.02	103.46	110.44
3	C	302	PCG	O6-C6-C5	-3.01	118.58	126.53
3	C	302	PCG	O1A-PA-O2A	3.01	117.81	108.56
3	A	302	PCG	O6-C6-C5	-3.00	118.60	126.53
3	E	302	PCG	C2'-C3'-C4'	-3.00	97.98	103.24
2	B	301	MLA	O3B-C3-C2	2.90	123.49	114.51
2	C	301	MLA	O1A-C1-C2	2.84	123.30	114.51
3	D	302	PCG	O1A-PA-O2A	2.77	117.07	108.56
3	A	302	PCG	O4'-C4'-C5'	2.71	120.58	112.38
3	E	302	PCG	O3'-C3'-C2'	2.68	118.24	115.61
3	D	302	PCG	C4-C5-N7	-2.66	106.45	110.67
3	A	302	PCG	O5'-PA-O3'	-2.66	102.14	105.70
3	B	303	PCG	C8-N9-C4	2.65	111.00	106.03
3	B	303	PCG	C4-C5-N7	-2.60	106.55	110.67
3	C	302	PCG	O6-C6-N1	2.57	124.95	120.11
3	D	302	PCG	O6-C6-C5	-2.57	119.74	126.53
2	B	302	MLA	O1A-C1-O1B	-2.56	116.75	123.33
3	C	302	PCG	O5'-PA-O3'	-2.52	102.33	105.70
3	E	302	PCG	C6-C5-N7	2.48	134.80	130.29
3	C	302	PCG	C4'-O4'-C1'	-2.46	104.04	109.47
3	F	302	PCG	C4-C5-N7	-2.44	106.80	110.67
3	B	303	PCG	O6-C6-C5	-2.44	120.10	126.53
3	D	302	PCG	O3'-C3'-C2'	2.43	117.99	115.61
2	B	302	MLA	O3B-C3-O3A	-2.42	117.11	123.33
2	A	301	MLA	O3B-C3-C2	2.38	121.87	114.51
3	C	302	PCG	C6-C5-N7	2.36	134.58	130.29
3	D	302	PCG	C2-N1-C6	-2.35	120.84	125.11
3	A	302	PCG	O1A-PA-O2A	2.31	115.66	108.56
3	E	302	PCG	O3'-PA-O2A	-2.29	105.48	110.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	303	PCG	O3'-PA-O2A	-2.29	105.48	110.39
3	B	303	PCG	C8-N7-C5	2.25	108.27	104.26
3	A	302	PCG	C5'-C4'-C3'	-2.24	108.35	112.56
3	D	302	PCG	C5-C6-N1	2.24	118.94	113.25
3	B	303	PCG	C2'-C3'-C4'	-2.18	99.42	103.24
2	B	301	MLA	O3A-C3-C2	-2.16	115.97	122.11
3	D	302	PCG	O4'-C4'-C5'	2.14	118.86	112.38
2	B	302	MLA	O3B-C3-C2	2.12	121.09	114.51
3	C	302	PCG	C4-C5-N7	-2.10	107.33	110.67
3	F	302	PCG	C8-N9-C4	2.10	109.96	106.03
3	E	302	PCG	C5-C6-N1	2.10	118.59	113.25
3	D	302	PCG	C2'-C3'-C4'	-2.08	99.59	103.24
3	D	302	PCG	C8-N7-C5	2.06	107.94	104.26
3	B	303	PCG	O1A-PA-O3'	2.04	111.78	107.04
3	A	302	PCG	O6-C6-N1	2.03	123.93	120.11

There are no chirality outliers.

All (16) torsion outliers are listed below:

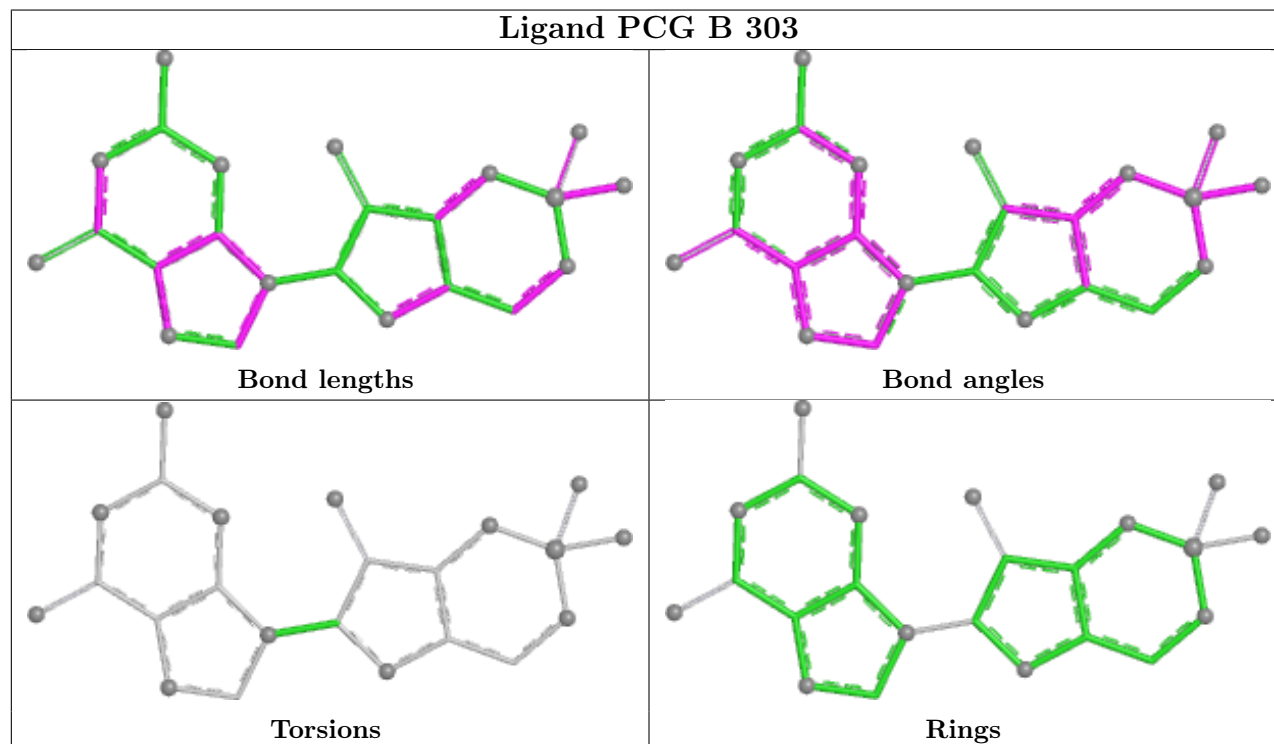
Mol	Chain	Res	Type	Atoms
2	B	301	MLA	O1A-C1-C2-C3
2	E	301	MLA	O1B-C1-C2-C3
2	A	301	MLA	C1-C2-C3-O3A
2	B	301	MLA	O1B-C1-C2-C3
2	C	301	MLA	C1-C2-C3-O3B
2	A	301	MLA	C1-C2-C3-O3B
2	C	301	MLA	C1-C2-C3-O3A
2	D	301	MLA	C1-C2-C3-O3A
2	D	301	MLA	C1-C2-C3-O3B
2	E	301	MLA	O1A-C1-C2-C3
2	A	301	MLA	O1A-C1-C2-C3
2	F	301	MLA	O1A-C1-C2-C3
2	A	301	MLA	O1B-C1-C2-C3
2	F	301	MLA	O1B-C1-C2-C3
2	D	301	MLA	O1A-C1-C2-C3
2	D	301	MLA	O1B-C1-C2-C3

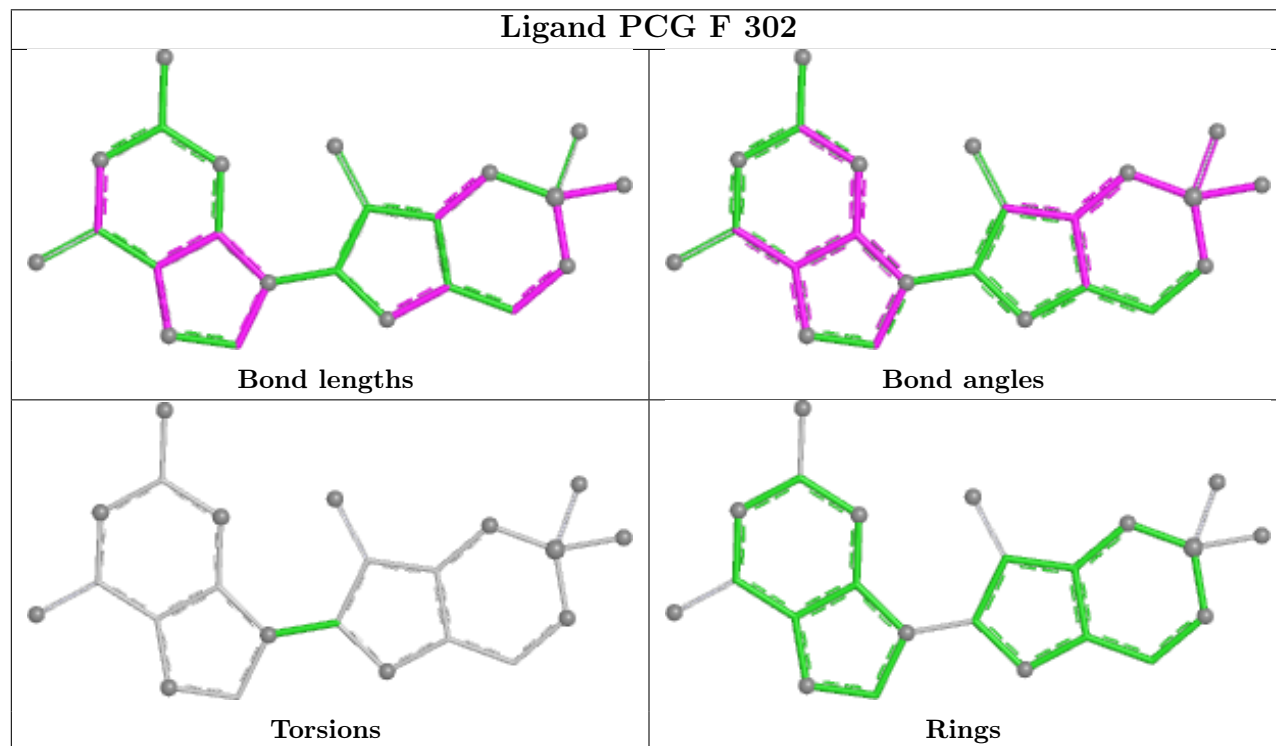
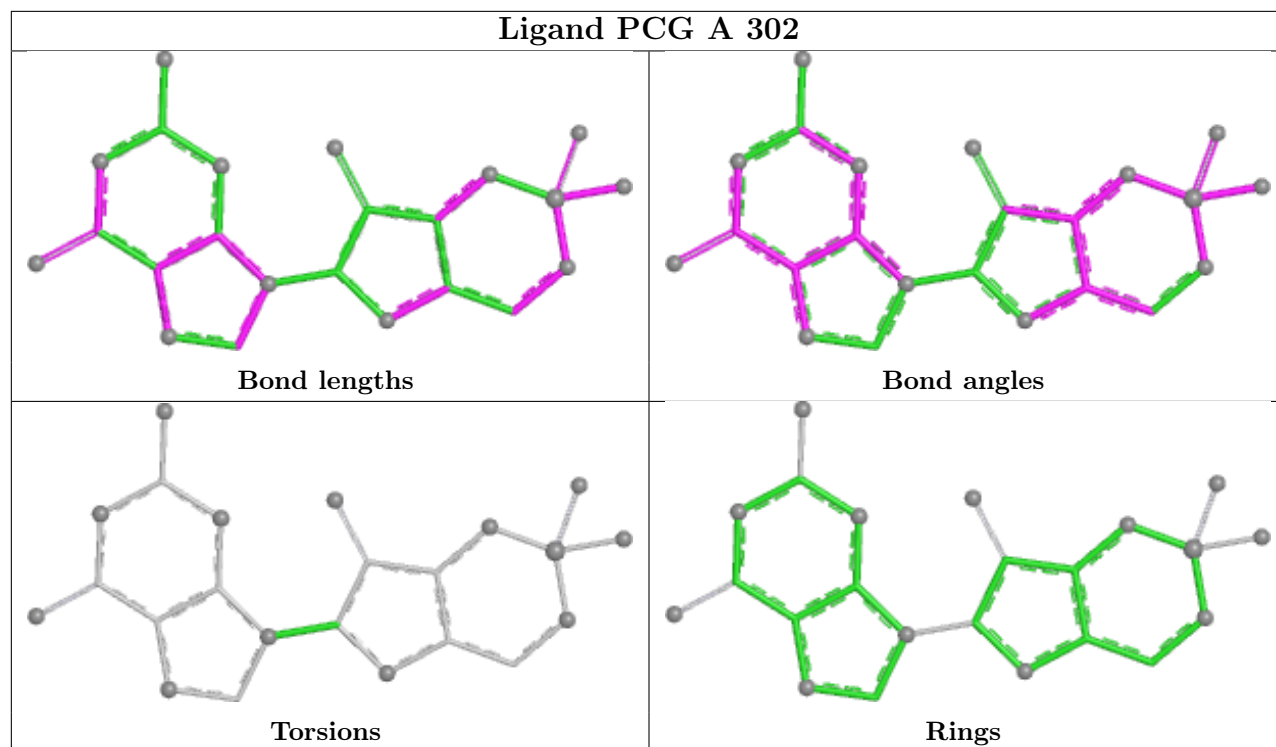
There are no ring outliers.

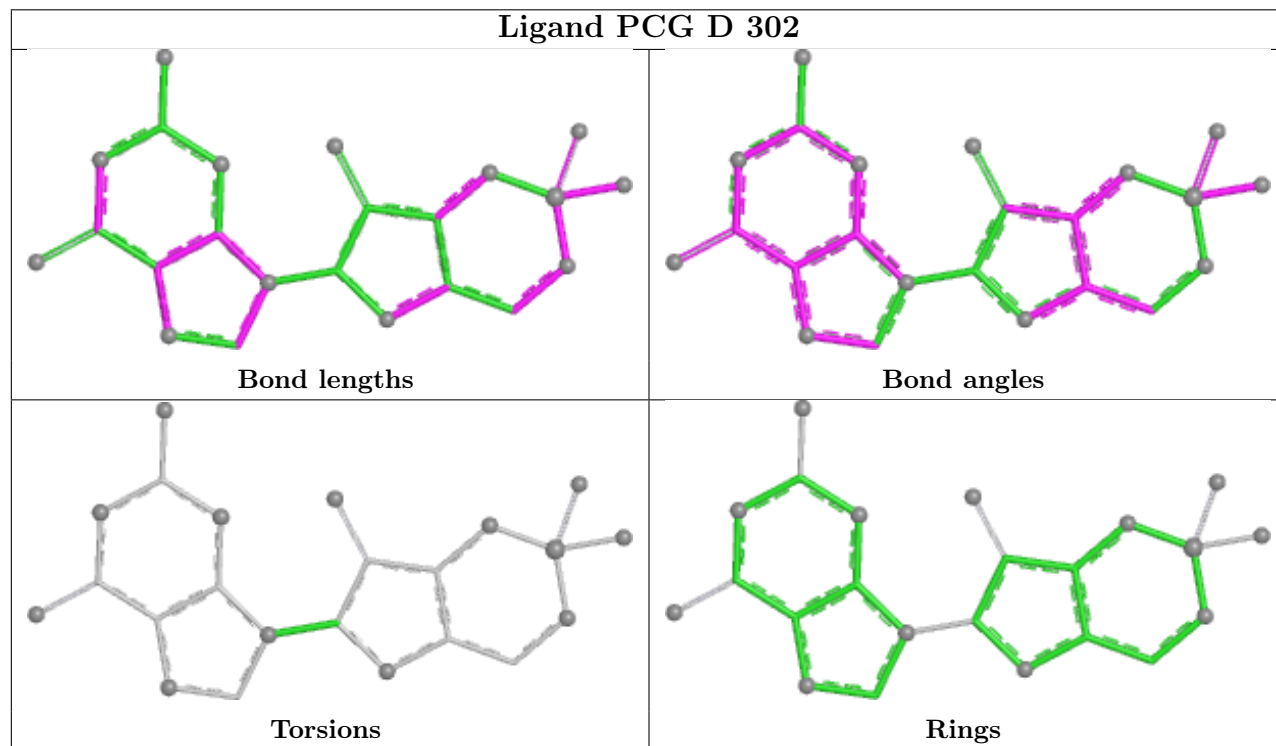
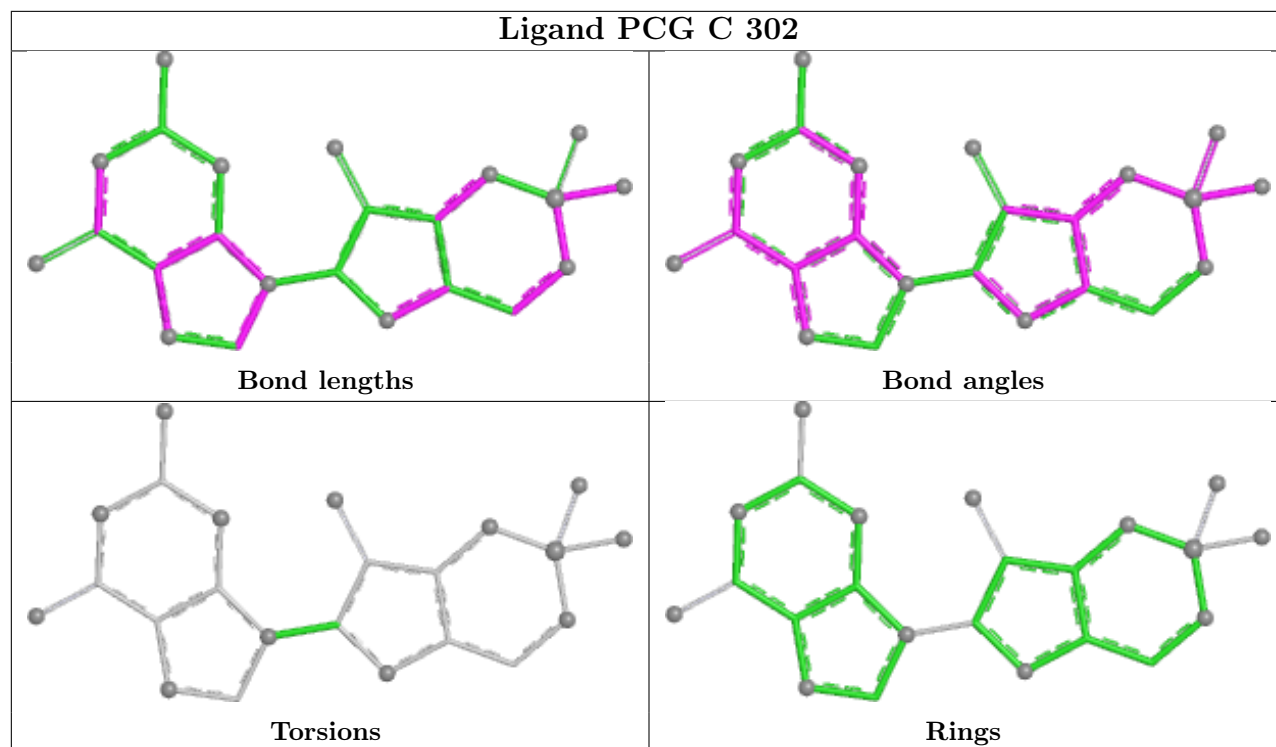
No monomer is involved in short contacts.

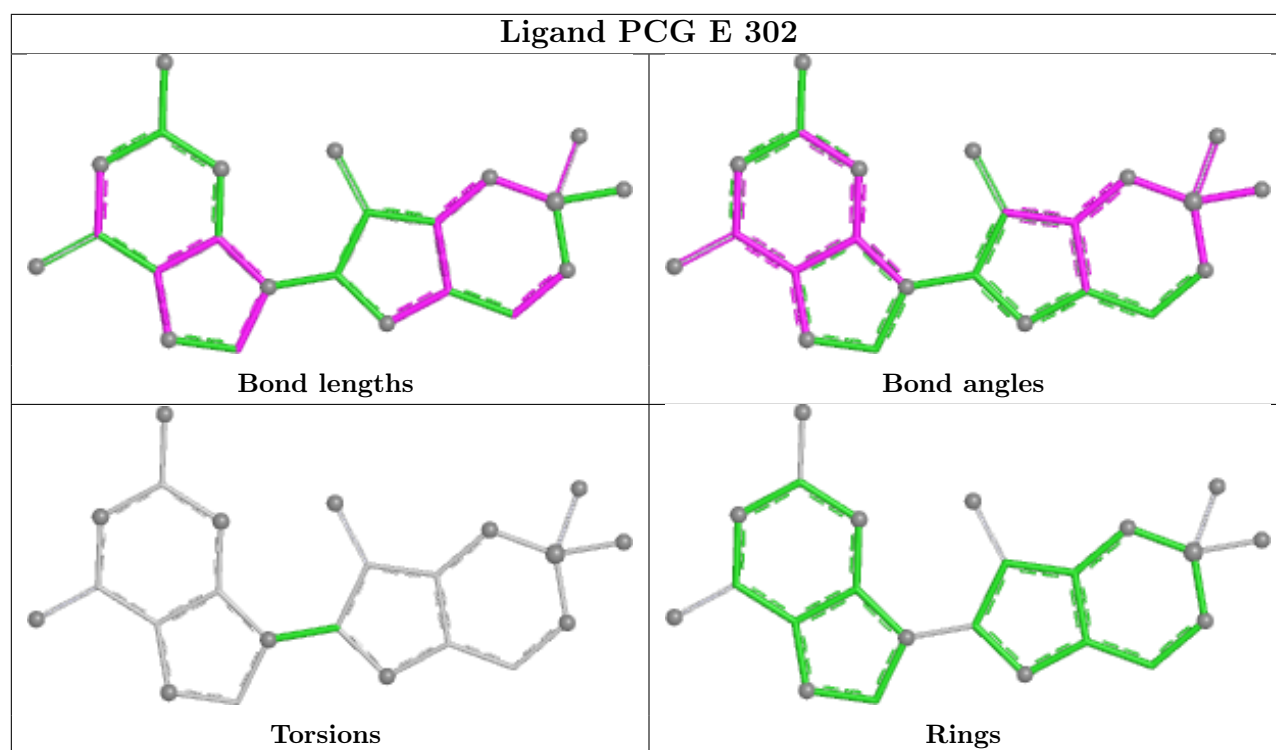
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 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 ⓘ

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	120/143 (83%)	-0.59	2 (1%) 69 69	13, 22, 51, 77	0
1	B	121/143 (84%)	-0.54	3 (2%) 58 58	14, 22, 53, 84	0
1	C	121/143 (84%)	-0.38	3 (2%) 58 58	16, 25, 54, 79	0
1	D	119/143 (83%)	-0.22	2 (1%) 69 69	16, 30, 58, 69	0
1	E	119/143 (83%)	0.06	2 (1%) 69 69	22, 36, 65, 88	0
1	F	118/143 (82%)	0.46	10 (8%) 16 14	26, 38, 64, 99	0
All	All	718/858 (83%)	-0.21	22 (3%) 51 51	13, 30, 61, 99	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	149	VAL	6.8
1	B	147	ALA	5.2
1	A	150	ARG	4.5
1	F	152	ASP	4.2
1	E	150	ARG	4.1
1	F	155	GLU	3.9
1	F	239	ASN	3.8
1	F	154	SER	3.7
1	C	269	THR	3.5
1	F	153	SER	3.3
1	F	219	GLU	3.1
1	D	219	GLU	2.9
1	F	151	LYS	2.7
1	A	239	ASN	2.7
1	F	202	GLY	2.7
1	C	238	TYR	2.5
1	F	205	ILE	2.5
1	F	268	ARG	2.3
1	B	148	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	239	ASN	2.3
1	D	149	VAL	2.2
1	B	173	ASP	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

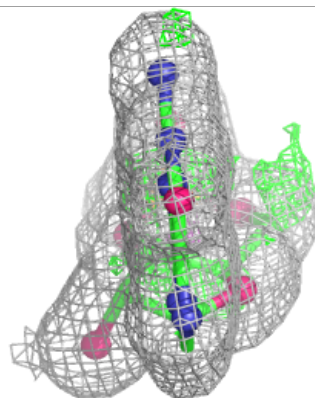
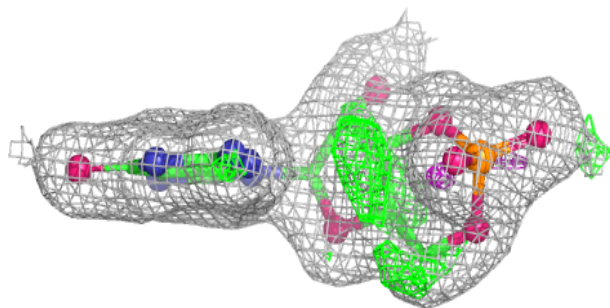
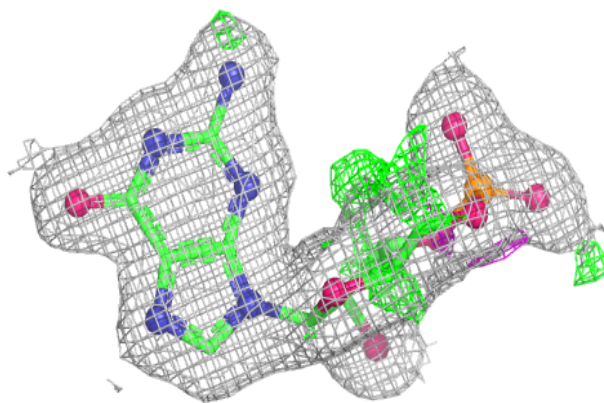
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MLA	B	302	7/7	0.82	0.16	36,50,59,61	0
2	MLA	E	301	7/7	0.90	0.11	33,42,51,51	0
2	MLA	F	301	7/7	0.94	0.09	27,47,56,57	0
2	MLA	C	301	7/7	0.95	0.07	23,25,32,43	0
3	PCG	F	302	23/23	0.96	0.08	17,23,36,45	0
4	NA	F	303	1/1	0.96	0.10	37,37,37,37	0
3	PCG	D	302	23/23	0.97	0.06	16,22,29,38	0
3	PCG	E	302	23/23	0.97	0.07	12,19,23,28	0
2	MLA	B	301	7/7	0.97	0.07	20,26,39,40	0
4	NA	A	303	1/1	0.97	0.09	20,20,20,20	0
4	NA	C	303	1/1	0.97	0.09	28,28,28,28	0
2	MLA	D	301	7/7	0.97	0.07	28,38,46,49	0
2	MLA	A	301	7/7	0.98	0.06	19,21,34,36	0
3	PCG	B	303	23/23	0.98	0.05	9,14,17,25	0
3	PCG	C	302	23/23	0.98	0.06	13,18,22,35	0
3	PCG	A	302	23/23	0.99	0.04	9,13,17,19	0

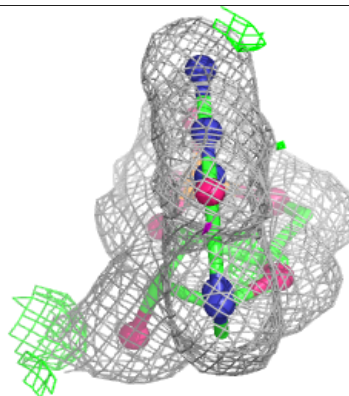
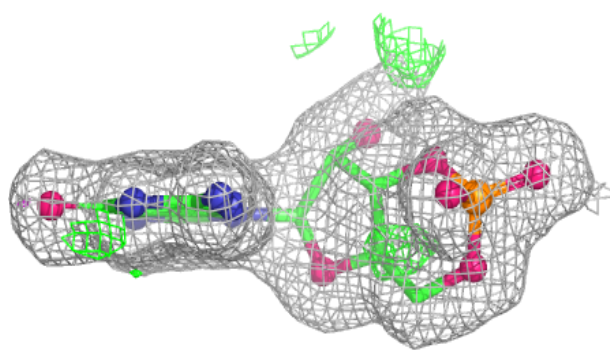
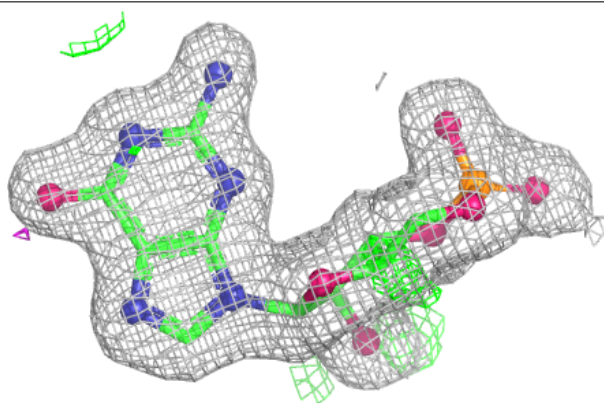
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

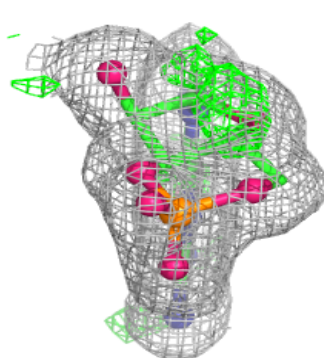
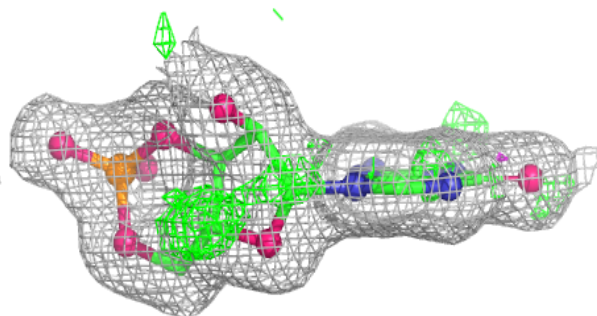
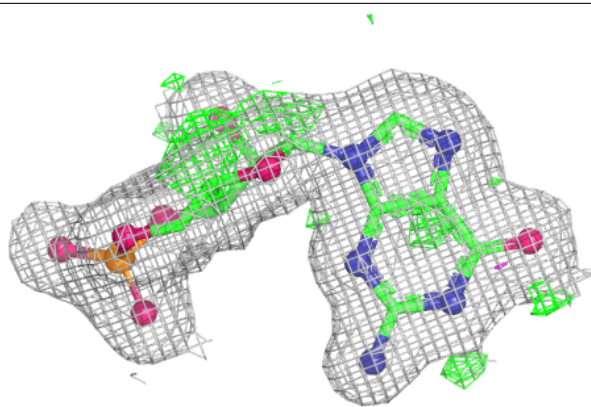
**Electron density around PCG D 302:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

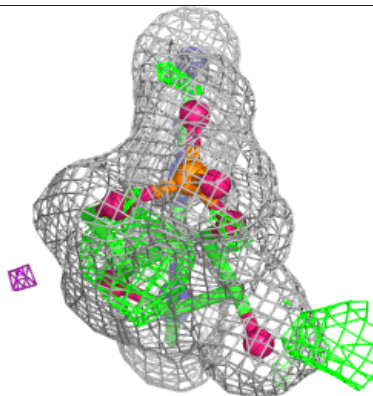
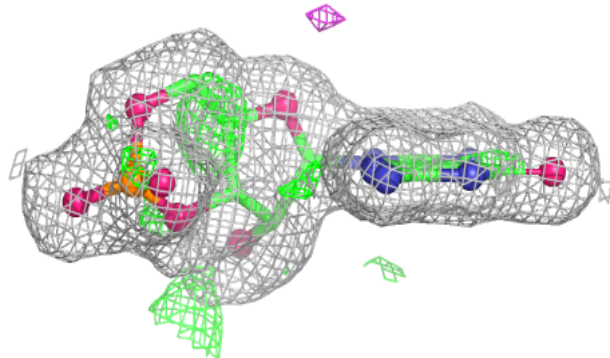
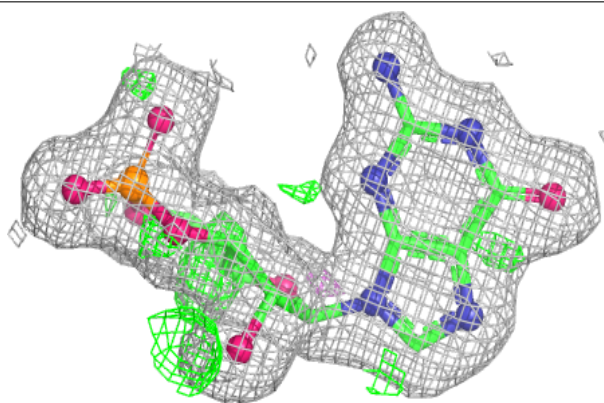


Electron density around PCG E 302:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

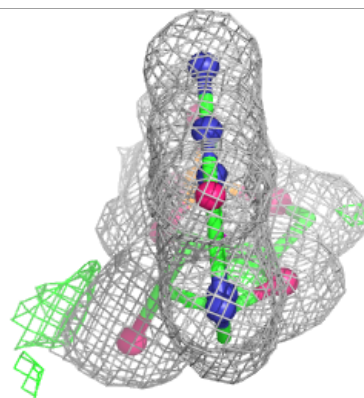
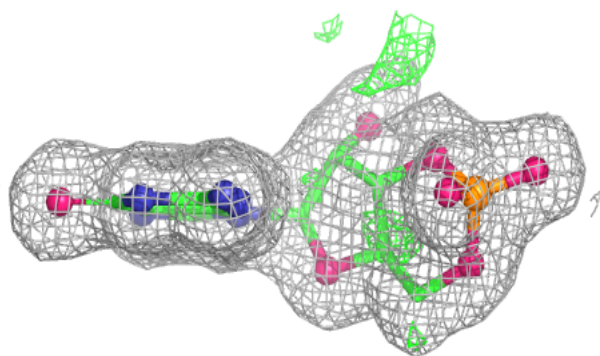
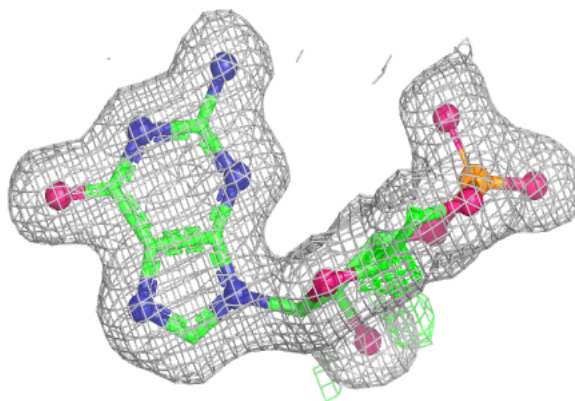
**Electron density around PCG B 303:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

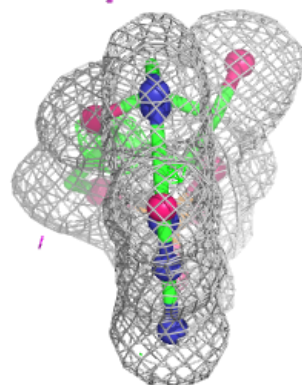
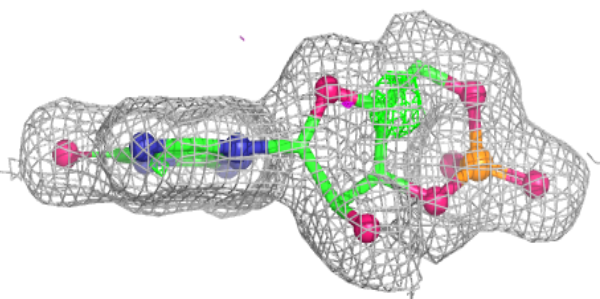
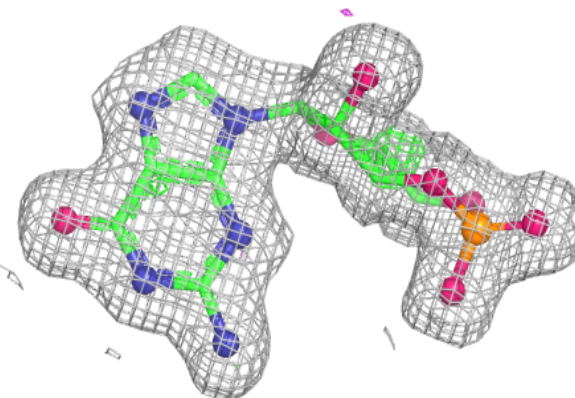


Electron density around PCG C 302:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around PCG A 302:**

$2mF_o-DF_c$ (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.