WORLDWIDE PDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 26, 2023 – 02:32 PM EDT

PDB ID	:	3GCM
Title	:	Crystal Structure of E. coli polynucleotide phosphorylase bound to RNA and RNase E
Authors	:	Nurmohamed, S.; Luisi, B.L.
Deposited on	:	2009-02-22
Resolution	:	2.50 Å(reported)

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

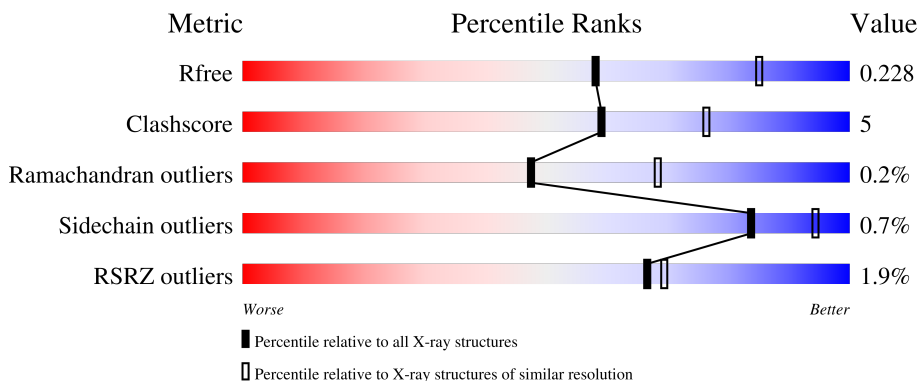|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1　Overall quality at a glance ⓘ

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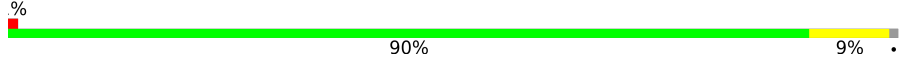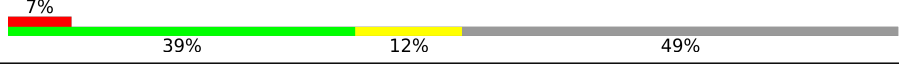*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.
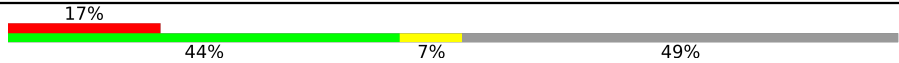
Metric	Percentile Ranks	Value
Rfree		0.228
Clashscore		5
Ramachandran outliers		0.2%
Sidechain outliers		0.7%
RSRZ outliers		1.9%

Worse　　　　　　　　　　　　　　　　　　*Better*

▌Percentile relative to all X-ray structures
▯Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 <=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	549	2% 91% 7% ••
1	B	549	% 92% 7% •
1	C	549	% 90% 9% •
2	D	41	7% 39% 12% 49%
2	E	41	7% 46% • 51%

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Mol	Chain	Length	Quality of chain
2	F	41	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	FLC	B	552	-	-	X	-
5	5GP	B	550	-	-	-	X
5	5GP	C	550	-	-	-	X

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 13916 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 Polyribonucleotide nucleotidyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	544	Total	C	N	O	S	8	4	0
			4151	2604	724	802	21			
1	B	544	Total	C	N	O	S	0	5	0
			4170	2614	732	803	21			
1	C	544	Total	C	N	O	S	0	2	0
			4142	2598	721	802	21			

- Molecule 2 is a protein called Ribonuclease E.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	21	Total	C	N	O	0	0	0
			134	80	30	24			
2	E	20	Total	C	N	O	0	0	0
			130	78	29	23			
2	F	21	Total	C	N	O	0	0	0
			138	82	31	25			

- Molecule 3 is CITRATE ANION (three-letter code: FLC) (formula: $C_6H_5O_7$).

FLC

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 13	C 6	O 7	0	0
3	A	1	Total 13	C 6	O 7	0	0
3	B	1	Total 13	C 6	O 7	0	0
3	B	1	Total 13	C 6	O 7	0	0
3	B	1	Total 13	C 6	O 7	0	0
3	B	1	Total 13	C 6	O 7	0	0
3	C	1	Total 13	C 6	O 7	0	0
3	C	1	Total 13	C 6	O 7	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	Mg 1	0	0
4	B	1	Total 1	Mg 1	0	0
4	C	1	Total 1	Mg 1	0	0

- Molecule 5 is GUANOSINE-5'-MONOPHOSPHATE (three-letter code: 5GP) (formula:

$C_{10}H_{14}N_5O_8P$).
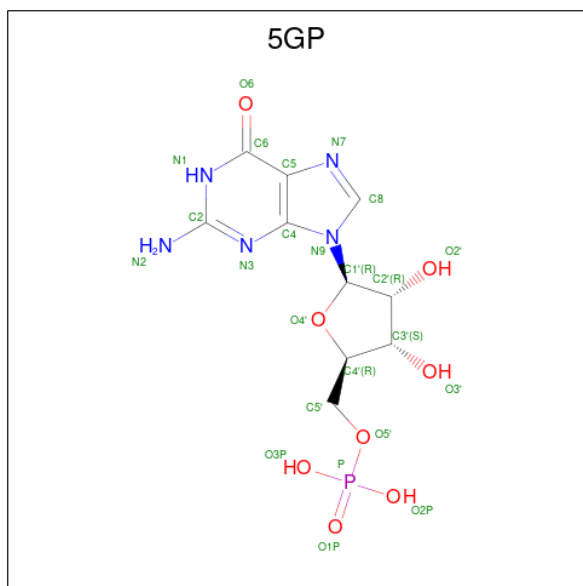
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total 20	C 10	N 5	O 5	0	0
5	B	1	Total 20	C 10	N 5	O 5	0	0
5	C	1	Total 20	C 10	N 5	O 5	0	0

- Molecule 6 is water.

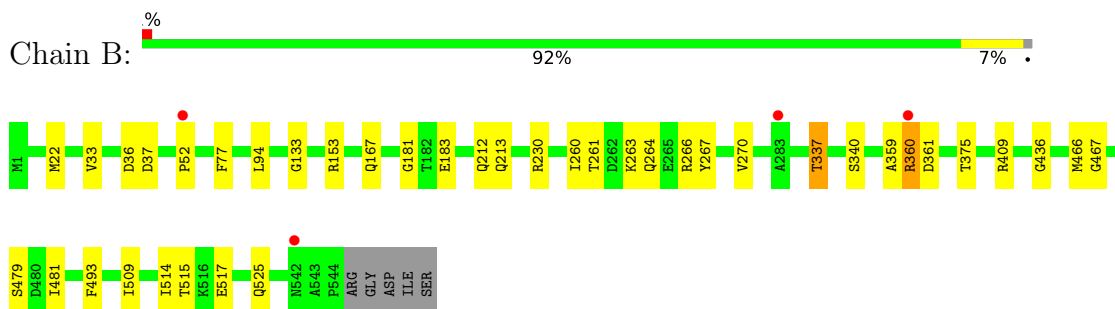| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	334	Total 334	O 334	0	0
6	D	8	Total 8	O 8	0	0
6	B	280	Total 280	O 280	0	0
6	E	9	Total 9	O 9	0	0
6	C	247	Total 247	O 247	0	0
6	F	6	Total 6	O 6	0	0

3 Residue-property plots ⓘ

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.
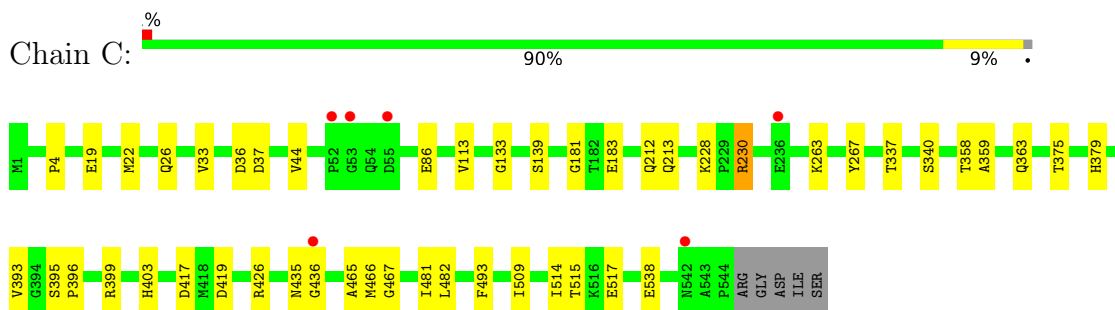
• Molecule 1: Polyribonucleotide nucleotidyltransferase
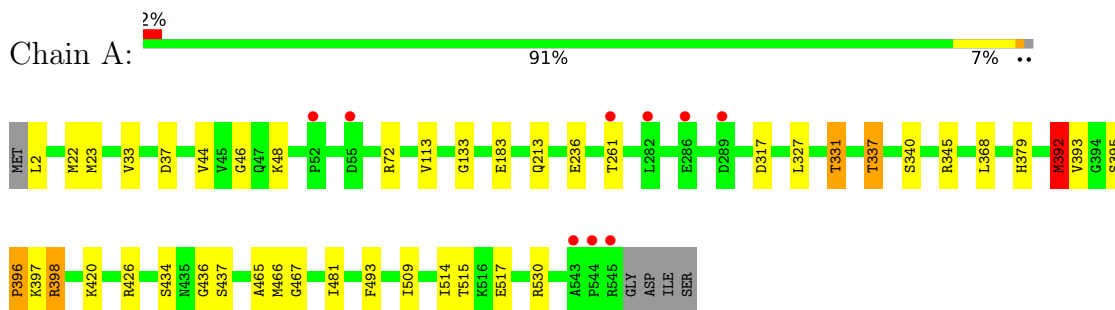
Chain A:

• Molecule 1: Polyribonucleotide nucleotidyltransferase

Chain B:

• Molecule 1: Polyribonucleotide nucleotidyltransferase

Chain C:

• Molecule 2: Ribonuclease E

Chain D:

GLU ALA PRO ARG HIS SER ASP TRP GLN ARG PRO THR PHE ALA PHE GLU GLY LYS G1039 G1043 H1044 T1045 A1046 T1047 H1048 H1049 P1059 VAL GLU

• Molecule 2: Ribonuclease E

7%

Chain E:

46%   •   51%

GLU ALA PRO ARG HIS SER ASP TRP GLN ARG PRO THR PHE ALA PHE GLU GLY LYS GLY A1040 G1043 H1044 T1045 Q1058 P1059 VAL GLU

• Molecule 2: Ribonuclease E

17%

Chain F:

44%   7%   49%

GLU ALA PRO ARG HIS SER ASP TRP GLN ARG PRO THR PHE ALA PHE GLU GLY LYS G1039 A1040 G1043 H1044 T1045 A1046 P1059 VAL GLU
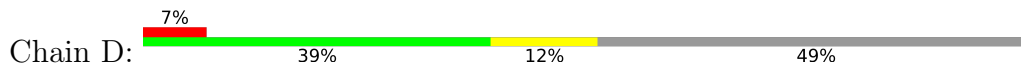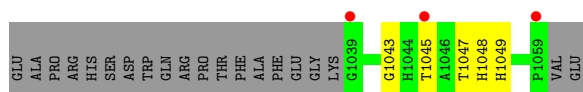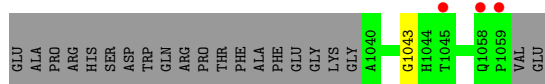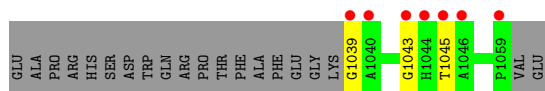
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	176.34Å 176.34Å 189.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50 43.46 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.4 (20.00-2.50) 99.3 (43.46-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.71 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.166 , 0.221 0.200 , 0.228	Depositor DCC
R_{free} test set	5134 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å²)	28.9	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent k_{sol}(e/Å³), B_{sol}(Å²)	0.34 , 37.6	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	13916	wwPDB-VP
Average B, all atoms (Å²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.42% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 5GP, FLC

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	#$\mid Z \mid$ >5	RMSZ	#$\mid Z \mid$ >5
1	A	0.51	4/4226 (0.1%)	0.52	2/5728 (0.0%)
1	B	0.35	0/4245	0.47	0/5751
1	C	0.36	0/4211	0.47	0/5708
2	D	0.34	0/139	0.49	0/191
2	E	0.29	0/135	0.46	0/186
2	F	0.33	0/143	0.43	0/196
All	All	0.41	4/13099 (0.0%)	0.49	2/17760 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	1
1	C	0	1
All	All	0	5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	392[A]	MET	CA-C	-10.84	1.24	1.52
1	A	392[B]	MET	CA-C	-10.84	1.24	1.52
1	A	398[A]	ARG	N-CA	-9.54	1.27	1.46
1	A	398[B]	ARG	N-CA	-9.54	1.27	1.46

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	398[A]	ARG	NE-CZ-NH1	5.97	123.28	120.30
1	A	398[B]	ARG	NE-CZ-NH1	5.97	123.28	120.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	392[A]	MET	Mainchain
1	A	392[B]	MET	Mainchain
1	A	436	GLY	Peptide
1	B	436	GLY	Peptide
1	C	436	GLY	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4151	0	4170	35	0
1	B	4170	0	4203	33	0
1	C	4142	0	4160	47	0
2	D	134	0	119	4	0
2	E	130	0	116	3	0
2	F	138	0	125	6	0
3	A	26	0	10	0	0
3	B	52	0	20	6	0
3	C	26	0	10	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
5	B	40	0	24	4	0
5	C	20	0	12	0	0
6	A	334	0	0	12	0
6	B	280	0	0	10	0
6	C	247	0	0	11	0
6	D	8	0	0	1	0
6	E	9	0	0	0	0
6	F	6	0	0	0	0
All	All	13916	0	12969	123	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 5.

The worst 5 of 123 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)
5:B:550:5GP:C5'	5:B:551:5GP:H8	1.75	1.18
5:B:550:5GP:H5'1	5:B:551:5GP:C8	1.78	1.10
1:B:264:GLN:NE2	1:C:26:GLN:HA	1.74	1.02
5:B:550:5GP:H5'1	5:B:551:5GP:H8	0.94	0.93
1:B:77:PHE:HB2	5:B:550:5GP:H2'	1.50	0.92

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	546/549 (100%)	532 (97%)	11 (2%)	3 (0%)	29	48
1	B	547/549 (100%)	530 (97%)	15 (3%)	2 (0%)	34	54
1	C	544/549 (99%)	532 (98%)	12 (2%)	0	100	100
2	D	19/41 (46%)	18 (95%)	1 (5%)	0	100	100
2	E	18/41 (44%)	18 (100%)	0	0	100	100
2	F	19/41 (46%)	19 (100%)	0	0	100	100
All	All	1693/1770 (96%)	1649 (97%)	39 (2%)	5 (0%)	47	61

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	360	ARG
1	A	392[A]	MET
1	A	392[B]	MET

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Mol	Chain	Res	Type
1	A	396	PRO
1	B	52	PRO

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	441/446 (99%)	435 (99%)	6 (1%)	67	86
1	B	444/446 (100%)	442 (100%)	2 (0%)	88	96
1	C	440/446 (99%)	438 (100%)	2 (0%)	88	96
2	D	10/28 (36%)	9 (90%)	1 (10%)	7	15
2	E	10/28 (36%)	10 (100%)	0	100	100
2	F	11/28 (39%)	11 (100%)	0	100	100
All	All	1356/1422 (95%)	1345 (99%)	11 (1%)	84	93

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	230	ARG
1	B	337	THR
1	C	230	ARG
1	C	86	GLU
1	A	398[B]	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	3	ASN
1	C	167	GLN
1	C	62	ASN
1	C	212	GLN
1	B	47	GLN

5.3.3 RNA ⓘ

There are no RNA molecules 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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 14 ligands modelled in this entry, 3 are monoatomic - leaving 11 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	FLC	C	552	-	12,12,12	1.03	0	17,17,17	1.35	2 (11%)
3	FLC	B	554	-	12,12,12	1.03	0	17,17,17	1.32	2 (11%)
3	FLC	A	550	-	12,12,12	1.02	0	17,17,17	1.26	2 (11%)
3	FLC	A	551	-	12,12,12	1.01	0	17,17,17	1.33	2 (11%)
3	FLC	B	555	-	12,12,12	1.00	0	17,17,17	1.36	2 (11%)
3	FLC	B	552	-	12,12,12	1.04	0	17,17,17	1.43	2 (11%)
3	FLC	B	553	-	12,12,12	0.99	0	17,17,17	1.31	2 (11%)
3	FLC	C	551	-	12,12,12	1.02	0	17,17,17	1.32	2 (11%)
5	5GP	B	551	-	18,22,26	1.03	2 (11%)	19,33,40	0.78	1 (5%)
5	5GP	B	550	-	18,22,26	1.01	2 (11%)	19,33,40	0.78	0
5	5GP	C	550	-	18,22,26	1.06	2 (11%)	19,33,40	0.56	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	FLC	C	552	-	-	0/16/16/16	-
3	FLC	B	554	-	-	5/16/16/16	-
3	FLC	A	550	-	-	0/16/16/16	-
3	FLC	A	551	-	-	4/16/16/16	-
3	FLC	B	555	-	-	2/16/16/16	-
3	FLC	B	552	-	-	2/16/16/16	-
3	FLC	B	553	-	-	2/16/16/16	-
3	FLC	C	551	-	-	0/16/16/16	-
5	5GP	B	551	-	-	1/2/22/26	0/3/3/3
5	5GP	B	550	-	-	0/2/22/26	0/3/3/3
5	5GP	C	550	-	-	0/2/22/26	0/3/3/3

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	550	5GP	C5-C6	-2.63	1.42	1.47
5	C	550	5GP	C8-N7	-2.55	1.30	1.35
5	B	551	5GP	C8-N7	-2.51	1.30	1.35
5	B	551	5GP	C5-C6	-2.46	1.42	1.47
5	B	550	5GP	C5-C6	-2.42	1.42	1.47

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	554	FLC	OB2-CBC-CB	3.59	119.28	113.05
3	C	551	FLC	OB2-CBC-CB	3.56	119.23	113.05
3	B	553	FLC	OB2-CBC-CB	3.55	119.22	113.05
3	B	555	FLC	OB2-CBC-CB	3.55	119.21	113.05
3	B	552	FLC	OB2-CBC-CB	3.53	119.17	113.05

There are no chirality outliers.
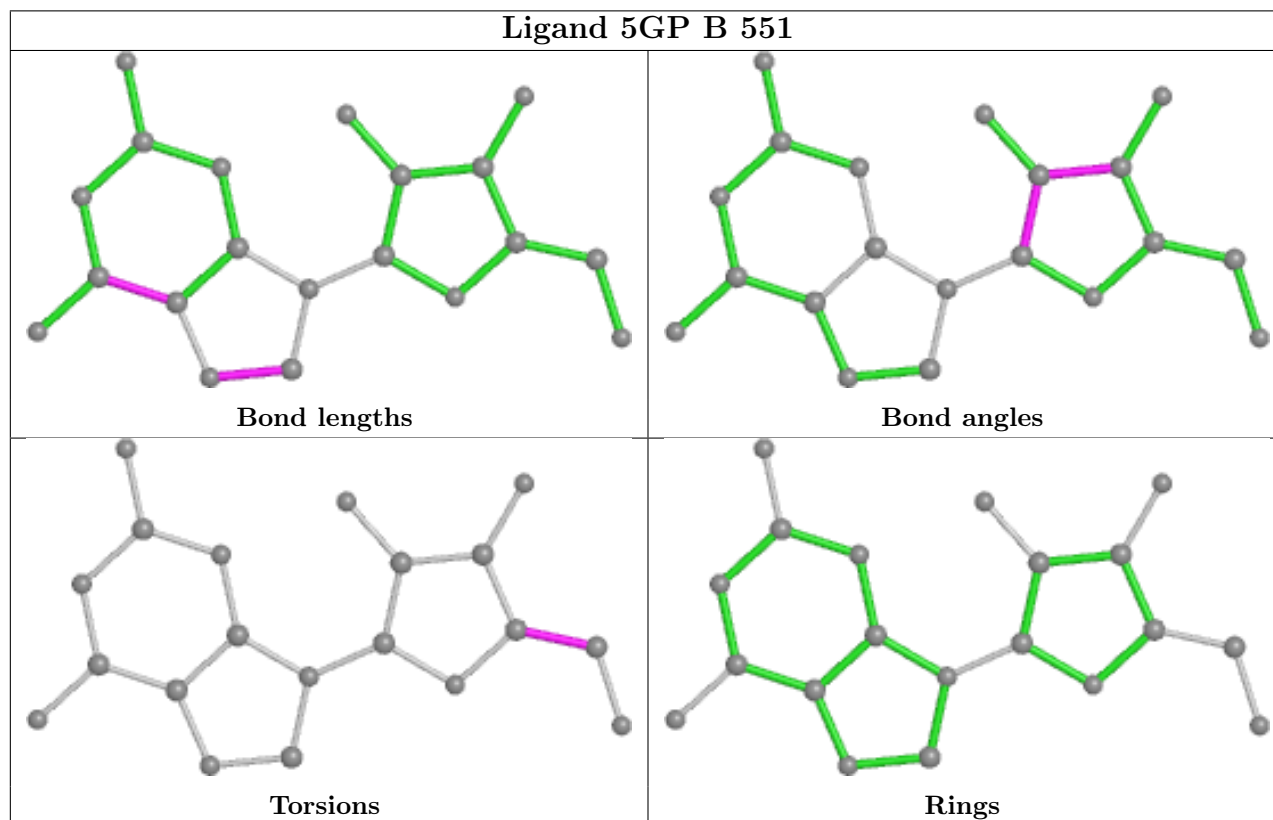
5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	554	FLC	CAC-CA-CB-OHB
3	B	554	FLC	CAC-CA-CB-CBC
3	B	554	FLC	CAC-CA-CB-CG
3	B	552	FLC	CA-CB-CG-CGC
3	B	553	FLC	CBC-CB-CG-CGC

There are no ring outliers.

3 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	552	FLC	6	0
5	B	551	5GP	3	0
5	B	550	5GP	4	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.

Ligand 5GP B 551

Bond lengths

Bond angles

Torsions

Rings

Ligand 5GP B 550

Bond lengths

Bond angles

Torsions

Rings

Ligand 5GP C 550

Bond lengths

Bond angles

Torsions

Rings
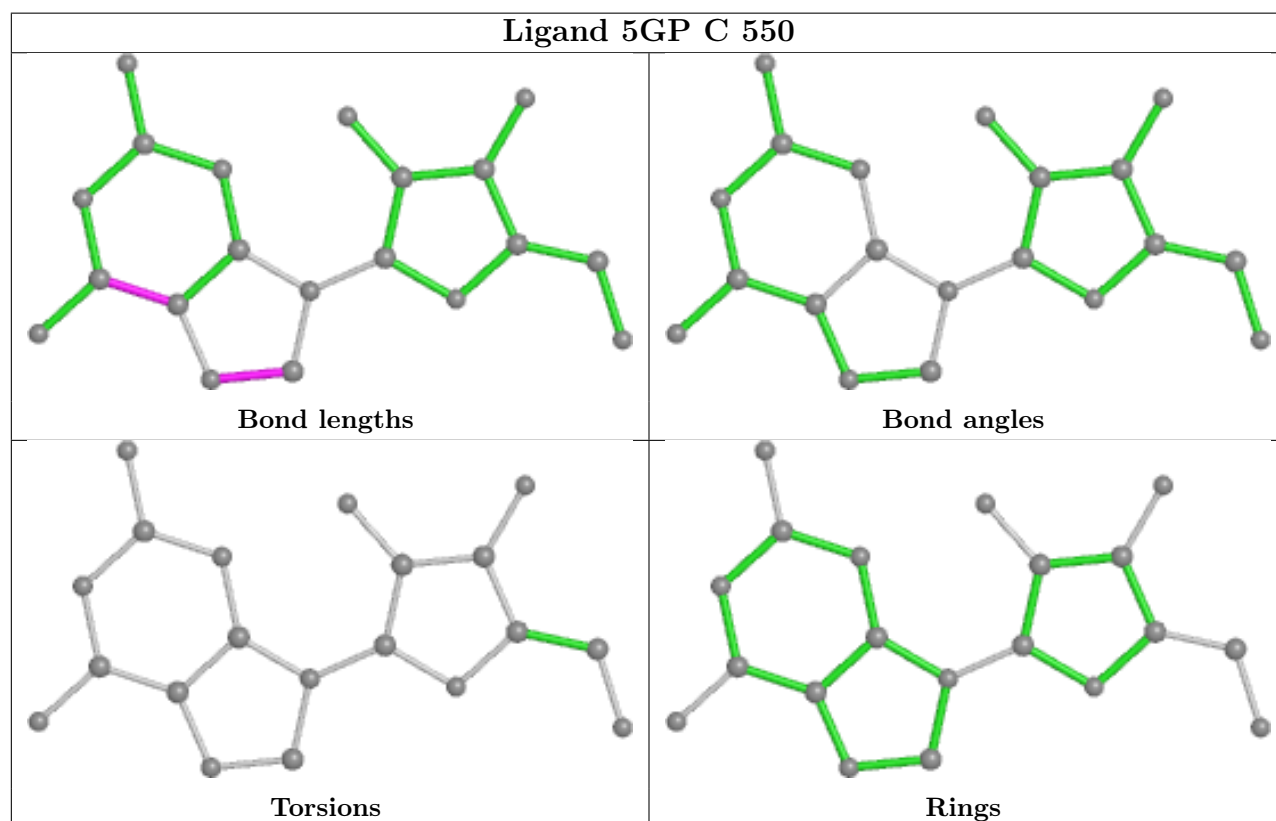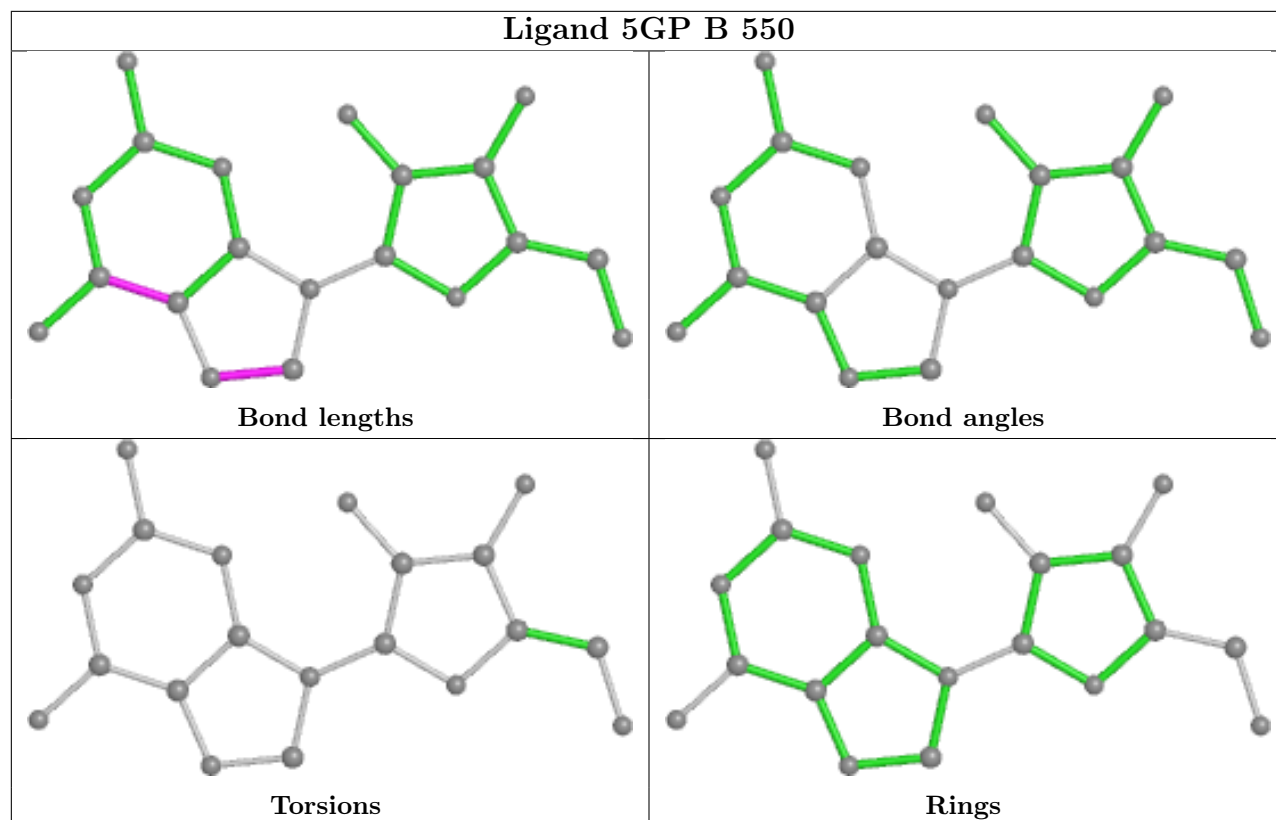
5.7 Other polymers ⓘ

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	544/549 (99%)	-0.34	9 (1%)	70	72	10, 21, 44, 62	1 (0%)
1	B	544/549 (99%)	-0.32	4 (0%)	87	89	11, 23, 46, 68	1 (0%)
1	C	544/549 (99%)	-0.23	6 (1%)	80	82	12, 25, 47, 64	1 (0%)
2	D	21/41 (51%)	0.57	3 (14%)	2	2	17, 37, 47, 52	0
2	E	20/41 (48%)	0.84	3 (15%)	2	2	33, 50, 62, 65	0
2	F	21/41 (51%)	1.45	7 (33%)	0	0	24, 48, 61, 61	0
All	All	1694/1770 (95%)	-0.25	32 (1%)	66	69	10, 24, 49, 68	3 (0%)

The worst 5 of 32 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	1045	THR	4.7
2	F	1059	PRO	4.4
2	F	1039	GLY	4.4
2	F	1046	ALA	4.3
2	E	1045	THR	4.2

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 monosaccharides 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. 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.

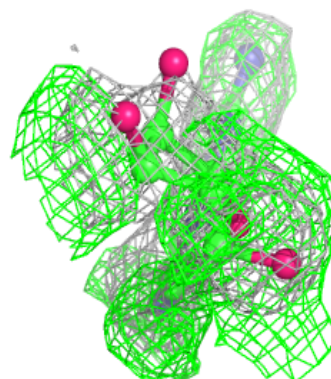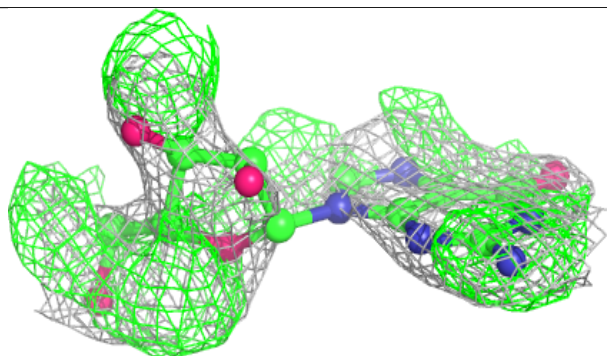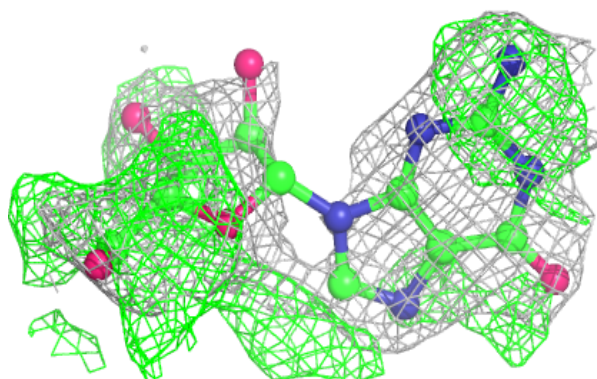| Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	5GP	C	550	20/24	0.69	0.49	23,24,29,31	20
5	5GP	B	550	20/24	0.72	0.48	18,20,23,25	20
3	FLC	B	554	13/13	0.74	0.26	77,80,81,81	0
5	5GP	B	551	20/24	0.80	0.37	15,16,18,21	20
3	FLC	B	552	13/13	0.80	0.37	60,62,64,64	0
4	MG	C	553	1/1	0.82	0.20	40,40,40,40	0
3	FLC	B	553	13/13	0.87	0.20	41,48,52,54	0
3	FLC	A	550	13/13	0.88	0.18	46,49,50,50	0
4	MG	A	552	1/1	0.88	0.16	33,33,33,33	0
3	FLC	C	551	13/13	0.89	0.18	45,48,51,53	0
3	FLC	A	551	13/13	0.89	0.19	30,42,51,54	0
3	FLC	B	555	13/13	0.90	0.19	40,47,54,57	0
3	FLC	C	552	13/13	0.93	0.15	30,43,51,55	0
4	MG	B	556	1/1	0.94	0.16	36,36,36,36	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.
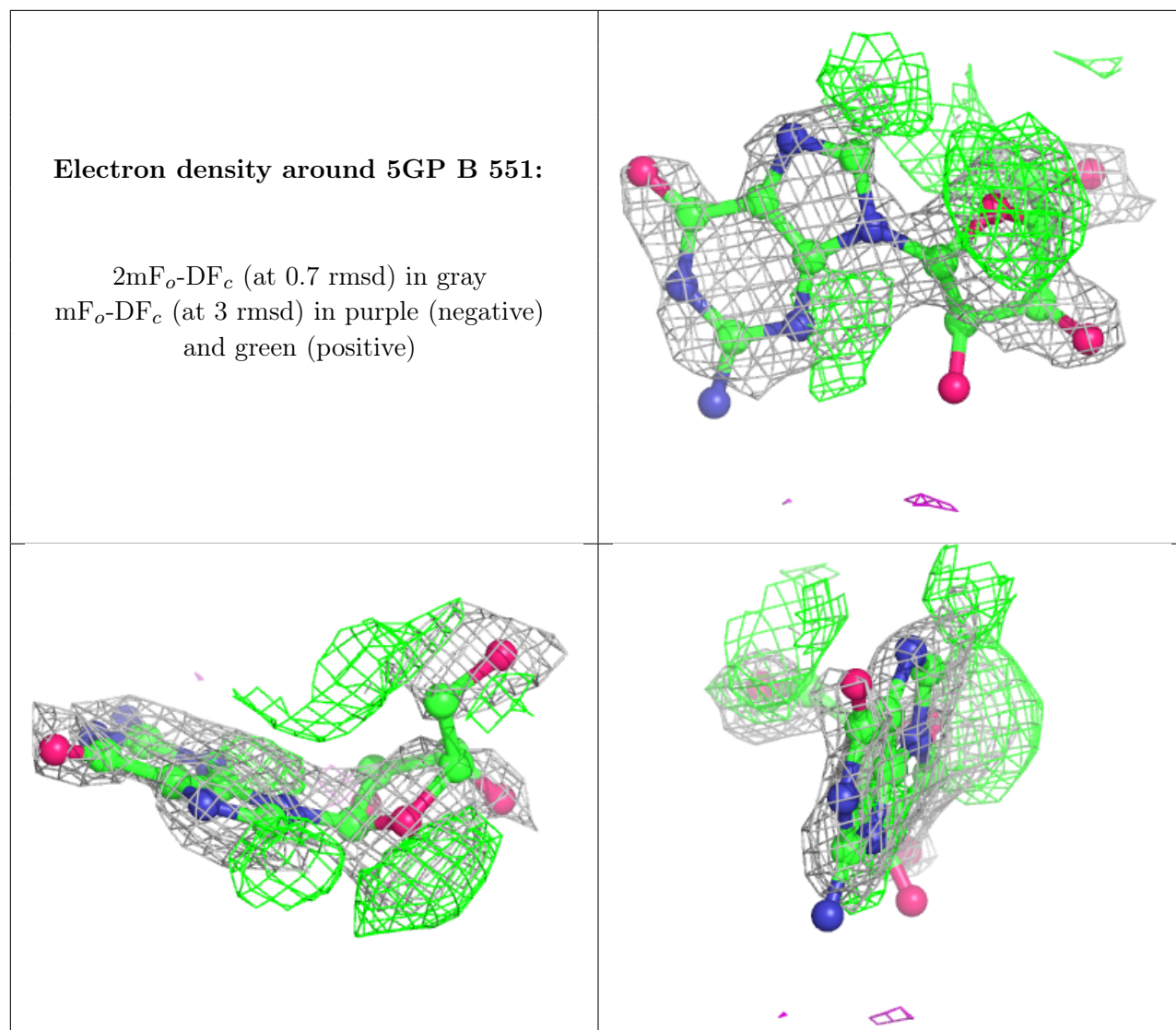
Electron density around 5GP C 550:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
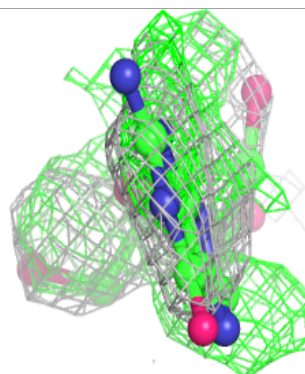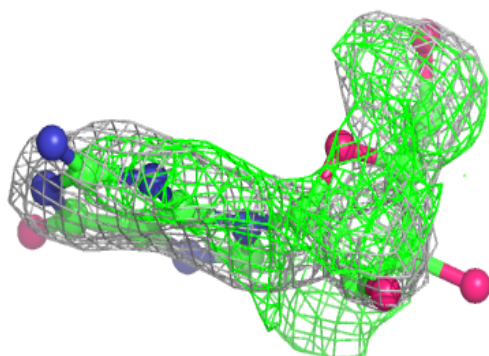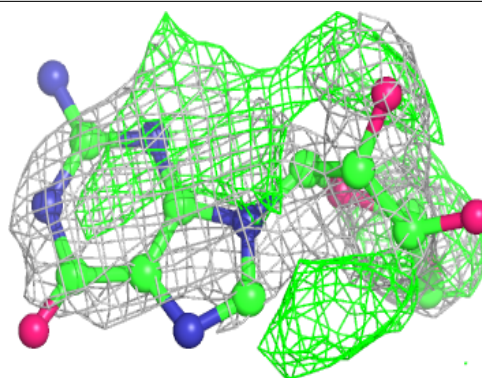
Electron density around 5GP B 550:

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

Electron density around 5GP B 551:

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 ⓘ

There are no such residues in this entry.