Full wwPDB X-ray Structure Validation Report (i)

Apr 28, 2025 – 06:14 PM EDT

PDB ID	:	9BL0 / pdb_00009bl0
Title	:	KRAS G12D Mutant KRAS 1-169 at 298 K bound to MRTX-1133
Authors	:	Xu, M.; Deck, S.L.; Milano, S.K.; Aplin, C.; Cerione, R.A.
Deposited on	:	2024-04-29
Resolution	:	1.66 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

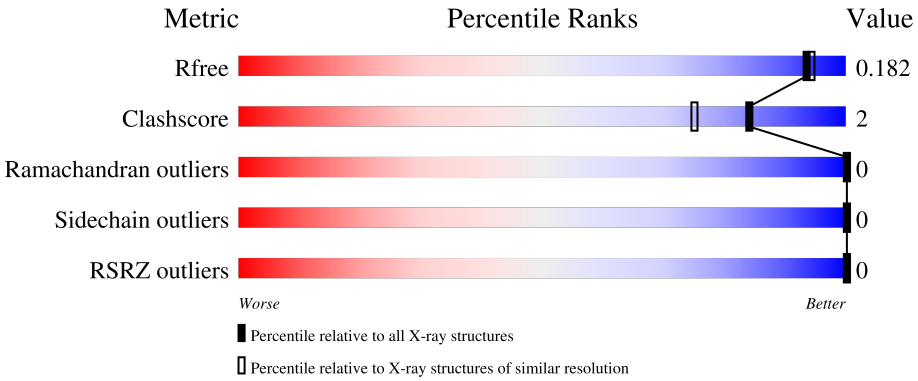
MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

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 1.66 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}	164625	2328 (1.66-1.66)
Clashscore	180529	2515 (1.66-1.66)
Ramachandran outliers	177936	2475 (1.66-1.66)
Sidechain outliers	177891	2475 (1.66-1.66)
RSRZ outliers	164620	2328 (1.66-1.66)

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	169	96% .
1	B	169	93% 7%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 3007 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.

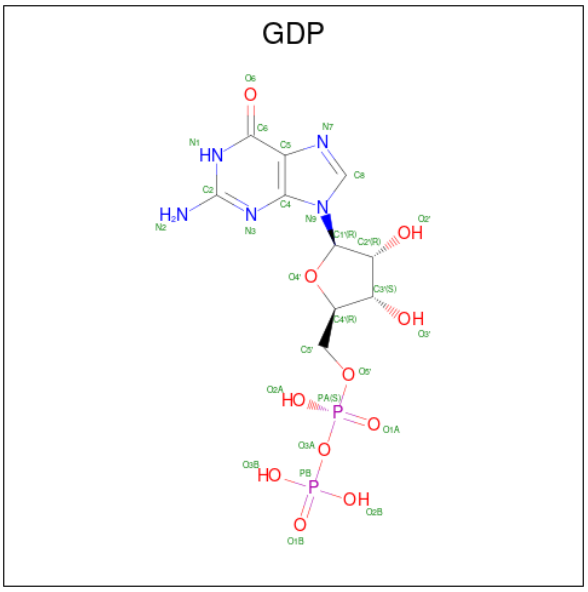
- Molecule 1 is a protein called Isoform 2B of GTPase KRas.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	169	Total	C	N	O	S	0	1	0
			1360	852	232	272	4			
1	B	169	Total	C	N	O	S	0	1	0
			1359	852	232	271	4			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	12	ASP	GLY	engineered mutation	UNP P01116
A	51	SER	CYS	engineered mutation	UNP P01116
A	80	LEU	CYS	engineered mutation	UNP P01116
A	118	SER	CYS	engineered mutation	UNP P01116
B	12	ASP	GLY	engineered mutation	UNP P01116
B	51	SER	CYS	engineered mutation	UNP P01116
B	80	LEU	CYS	engineered mutation	UNP P01116
B	118	SER	CYS	engineered mutation	UNP P01116

- Molecule 2 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).

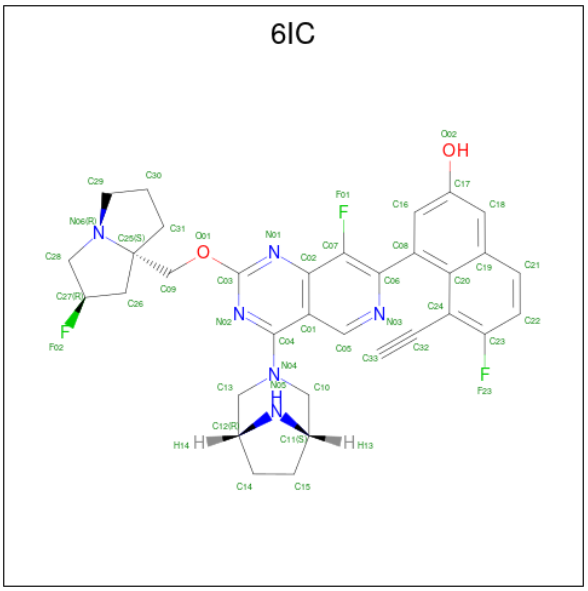


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
2	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 4 is 4-(4-[(1R,5S)-3,8-diazabicyclo[3.2.1]octan-3-yl]-8-fluoro-2-{[(2R,4R,7aS)-2-fluorotetrahydro-1H-pyrrolizin-7a(5H)-yl]methoxy}pyrido[4,3-d]pyrimidin-7-yl)-5-ethynyl-6-fluoronaphthalen-2-ol (CCD ID: 6IC) (formula: $C_{33}H_{31}F_3N_6O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C F N O 44 33 3 6 2	0	0
4	B	1	Total C F N O 44 33 3 6 2	0	0

- Molecule 5 is water.

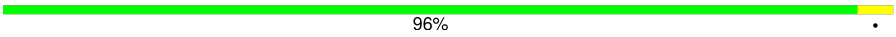
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	67	Total O 67 67	0	0
5	B	75	Total O 75 75	0	0

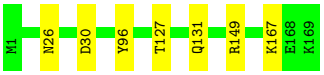
3 Residue-property plots (i)

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: Isoform 2B of GTPase KRas

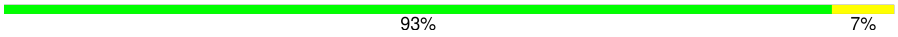
Chain A:





- Molecule 1: Isoform 2B of GTPase KRas

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	75.36Å 75.36Å 203.86Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.17 – 1.66 40.17 – 1.66	Depositor EDS
% Data completeness (in resolution range)	95.7 (40.17-1.66) 95.8 (40.17-1.66)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.09 (at 1.65Å)	Xtriage
Refinement program	PHENIX (1.21.1_5286: ???)	Depositor
R, R_{free}	0.179 , 0.195 0.178 , 0.182	Depositor DCC
R_{free} test set	46917 reflections (4.07%)	wwPDB-VP
Wilson B-factor (Å^2)	23.4	Xtriage
Anisotropy	0.006	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 23.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.489 for -h-k,k,-l	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	3007	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.09% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: 6IC, MG, GDP

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	0.37	0/1384	0.57	0/1865
1	B	0.39	0/1383	0.59	0/1865
All	All	0.38	0/2767	0.58	0/3730

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

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	1360	0	1345	6	0
1	B	1359	0	1345	6	0
2	A	28	0	12	1	0
2	B	28	0	12	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	44	0	0	1	0
4	B	44	0	0	0	0
5	A	67	0	0	1	0
5	B	75	0	0	0	0
All	All	3007	0	2714	12	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 2.

All (12) 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:B:123:ARG:NH2	1:B:143:GLU:OE2	2.22	0.70
1:B:3:GLU:OE2	1:B:5:LYS:NZ	2.27	0.68
1:A:167:LYS:NZ	5:A:301:HOH:O	2.30	0.64
1:B:149:ARG:HH12	1:B:153:ASP:CG	2.17	0.53
1:A:149:ARG:HG2	1:A:149:ARG:O	2.14	0.48
1:B:1:MET:HE1	1:B:43:GLN:NE2	2.30	0.47
1:B:126:ASP:OD1	1:B:129:GLN:HB2	2.15	0.47
1:A:127:THR:HG22	1:A:131:GLN:OE1	2.15	0.46
1:A:30:ASP:O	2:A:201:GDP:O2'	2.20	0.45
1:B:41:ARG:NH1	1:B:52:LEU:HD21	2.31	0.45
1:A:26:ASN:HA	1:A:149:ARG:HH12	1.83	0.43
1:A:96:TYR:CE1	4:A:203:6IC:C33	3.03	0.42

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	168/169 (99%)	160 (95%)	8 (5%)	0	100	100
1	B	168/169 (99%)	162 (96%)	6 (4%)	0	100	100
All	All	336/338 (99%)	322 (96%)	14 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	151/150 (101%)	151 (100%)	0	100	100
1	B	151/150 (101%)	151 (100%)	0	100	100
All	All	302/300 (101%)	302 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	GLN
1	B	43	GLN
1	B	129	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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
2	GDP	A	201	3	25,30,30	0.96	1 (4%)	30,47,47	1.11	2 (6%)
4	6IC	A	203	-	49,51,51	4.26	22 (44%)	57,78,78	4.52	25 (43%)
4	6IC	B	203	-	49,51,51	4.25	23 (46%)	57,78,78	4.47	25 (43%)
2	GDP	B	201	3	25,30,30	1.08	3 (12%)	30,47,47	0.69	1 (3%)

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	GDP	A	201	3	-	0/12/32/32	0/3/3/3
4	6IC	A	203	-	-	0/14/55/55	0/8/8/8
4	6IC	B	203	-	-	0/14/55/55	0/8/8/8
2	GDP	B	201	3	-	0/12/32/32	0/3/3/3

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	203	6IC	C26-C25	-17.85	1.33	1.54
4	B	203	6IC	C26-C25	-17.25	1.34	1.54
4	B	203	6IC	C29-N06	10.89	1.62	1.47
4	A	203	6IC	C29-N06	10.87	1.62	1.47
4	B	203	6IC	C10-N04	9.73	1.64	1.46
4	A	203	6IC	C10-N04	9.49	1.64	1.46
4	B	203	6IC	C13-N04	8.98	1.63	1.46
4	A	203	6IC	C13-N04	8.95	1.63	1.46
4	B	203	6IC	O01-C03	6.45	1.41	1.34
4	B	203	6IC	C28-N06	-6.41	1.35	1.47
4	A	203	6IC	C28-N06	-6.30	1.36	1.47
4	A	203	6IC	O01-C03	6.18	1.41	1.34
4	B	203	6IC	C31-C30	4.57	1.67	1.52
4	A	203	6IC	C31-C30	4.55	1.67	1.52
4	A	203	6IC	C24-C20	-4.35	1.37	1.43
4	B	203	6IC	C24-C20	-4.32	1.37	1.43
4	B	203	6IC	C31-C25	4.12	1.58	1.54
4	B	203	6IC	C12-N05	-4.04	1.31	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	203	6IC	C12-N05	-4.04	1.31	1.49
4	A	203	6IC	C31-C25	3.95	1.58	1.54
4	B	203	6IC	C15-C14	-3.68	1.44	1.54
4	A	203	6IC	C15-C14	-3.66	1.44	1.54
4	A	203	6IC	C24-C32	3.64	1.50	1.43
4	B	203	6IC	C24-C32	3.51	1.50	1.43
4	B	203	6IC	C01-C02	-3.38	1.33	1.42
4	A	203	6IC	C01-C02	-3.30	1.33	1.42
4	A	203	6IC	C11-N05	-3.19	1.34	1.49
4	B	203	6IC	C11-N05	-3.16	1.35	1.49
4	A	203	6IC	C03-N01	3.08	1.39	1.33
4	B	203	6IC	C03-N01	2.92	1.38	1.33
4	B	203	6IC	C04-C01	-2.92	1.38	1.43
4	B	203	6IC	C06-C07	2.83	1.43	1.38
2	B	201	GDP	C5-C6	-2.75	1.42	1.47
4	A	203	6IC	C06-C07	2.66	1.43	1.38
4	B	203	6IC	C20-C19	-2.59	1.36	1.42
4	A	203	6IC	C14-C12	2.55	1.59	1.52
4	B	203	6IC	C04-N04	2.55	1.47	1.39
4	A	203	6IC	C20-C19	-2.54	1.37	1.42
4	A	203	6IC	C04-N04	2.49	1.47	1.39
4	B	203	6IC	C14-C12	2.44	1.59	1.52
4	A	203	6IC	C04-C01	-2.44	1.39	1.43
2	B	201	GDP	C8-N7	-2.27	1.31	1.34
4	B	203	6IC	F01-C07	2.23	1.39	1.35
4	B	203	6IC	C08-C20	-2.14	1.40	1.43
4	B	203	6IC	C02-N01	2.10	1.41	1.37
4	A	203	6IC	F01-C07	2.05	1.38	1.35
2	B	201	GDP	C5-C4	-2.01	1.38	1.43
2	A	201	GDP	O4'-C1'	2.01	1.43	1.40
4	A	203	6IC	C09-C25	2.00	1.56	1.52

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	203	6IC	N02-C04-N04	-14.77	106.61	117.17
4	B	203	6IC	C29-N06-C28	13.87	140.55	114.48
4	A	203	6IC	C29-N06-C28	13.66	140.15	114.48
4	B	203	6IC	N02-C04-N04	-13.40	107.59	117.17
4	A	203	6IC	C08-C06-N03	10.54	135.38	115.27
4	B	203	6IC	C08-C06-N03	10.22	134.79	115.27
4	A	203	6IC	C16-C08-C06	-9.39	104.98	119.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	203	6IC	C16-C08-C06	-9.24	105.21	119.16
4	A	203	6IC	C09-O01-C03	-8.94	103.12	116.89
4	B	203	6IC	C09-O01-C03	-8.52	103.77	116.89
4	B	203	6IC	O01-C03-N02	8.03	141.62	116.17
4	A	203	6IC	O01-C03-N02	7.84	141.00	116.17
4	B	203	6IC	C14-C12-C13	-7.31	104.81	111.70
4	A	203	6IC	C04-C01-C02	7.10	122.29	115.66
4	B	203	6IC	C04-C01-C02	6.87	122.07	115.66
4	A	203	6IC	C15-C11-C10	-6.75	105.35	111.70
4	B	203	6IC	C15-C11-C10	-6.65	105.44	111.70
4	A	203	6IC	C01-C04-N04	6.48	132.28	121.18
4	A	203	6IC	C14-C12-C13	-5.99	106.06	111.70
4	B	203	6IC	C01-C04-N04	5.71	130.96	121.18
4	B	203	6IC	O01-C03-N01	-5.69	98.13	116.17
4	A	203	6IC	O01-C03-N01	-5.62	98.35	116.17
4	B	203	6IC	F01-C07-C02	-5.58	106.76	118.17
4	B	203	6IC	O01-C09-C25	5.48	114.56	106.59
4	A	203	6IC	O01-C09-C25	5.33	114.34	106.59
4	A	203	6IC	F01-C07-C02	-5.09	107.78	118.17
4	B	203	6IC	C01-C05-N03	-4.79	120.90	124.70
4	B	203	6IC	C30-C29-N06	4.40	110.25	103.94
4	A	203	6IC	C01-C05-N03	-4.36	121.24	124.70
4	A	203	6IC	C30-C29-N06	4.18	109.93	103.94
4	B	203	6IC	N01-C03-N02	-4.09	120.23	127.66
4	B	203	6IC	C07-C02-N01	4.07	127.61	119.29
4	A	203	6IC	C07-C02-N01	3.97	127.42	119.29
4	B	203	6IC	C08-C20-C24	-3.89	118.33	124.36
4	A	203	6IC	N01-C03-N02	-3.88	120.62	127.66
4	A	203	6IC	C08-C20-C24	-3.66	118.68	124.36
4	B	203	6IC	C08-C20-C19	3.57	123.39	118.03
4	A	203	6IC	C08-C20-C19	3.38	123.11	118.03
4	B	203	6IC	C20-C24-C32	3.17	129.47	123.78
4	A	203	6IC	C11-C10-N04	3.15	112.67	110.19
4	A	203	6IC	C01-C02-N01	-3.10	116.34	122.66
4	B	203	6IC	C11-C10-N04	3.08	112.61	110.19
4	B	203	6IC	C01-C02-N01	-3.06	116.41	122.66
4	A	203	6IC	C26-C25-C31	-3.01	108.56	113.58
4	B	203	6IC	C26-C25-C31	-2.89	108.75	113.58
2	A	201	GDP	C4'-O4'-C1'	2.83	112.52	109.92
4	A	203	6IC	C20-C24-C32	2.80	128.80	123.78
4	B	203	6IC	C03-N01-C02	2.76	119.87	116.22
4	A	203	6IC	C03-N01-C02	2.72	119.82	116.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	201	GDP	C8-N7-C5	2.60	106.98	102.55
4	B	203	6IC	C10-N04-C04	-2.51	110.30	118.91
4	A	203	6IC	C10-N04-C04	-2.46	110.50	118.91
2	B	201	GDP	O6-C6-C5	2.00	128.29	124.32

There are no chirality outliers.

There are no torsion outliers.

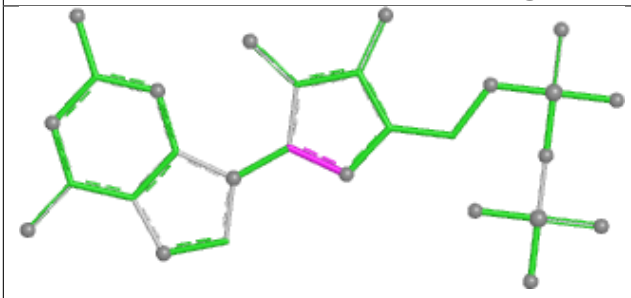
There are no ring outliers.

2 monomers are involved in 2 short contacts:

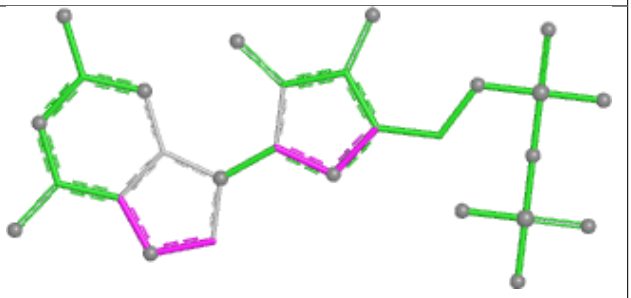
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	201	GDP	1	0
4	A	203	6IC	1	0

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

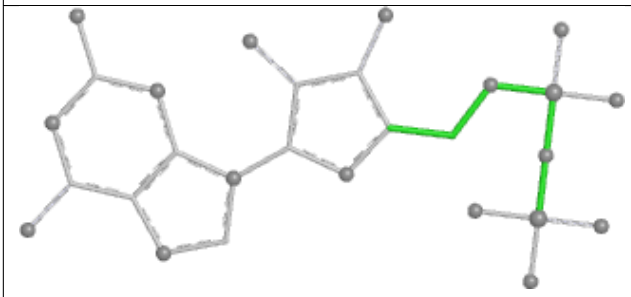
Ligand GDP A 201



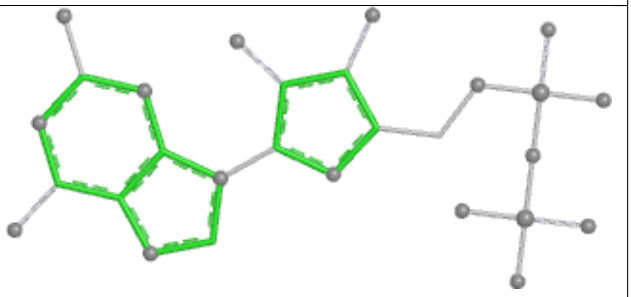
Bond lengths



Bond angles

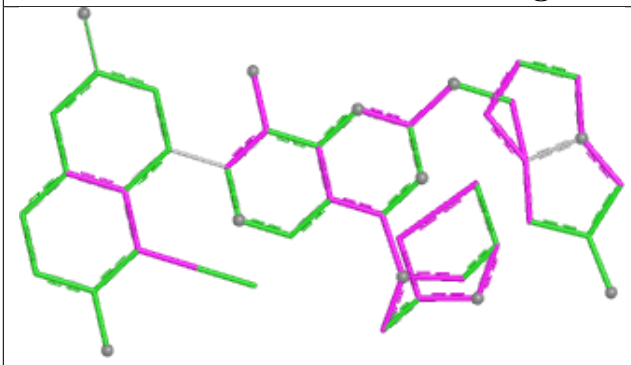


Torsions

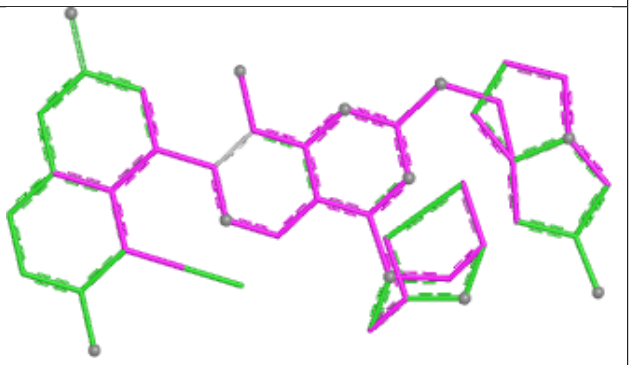


Rings

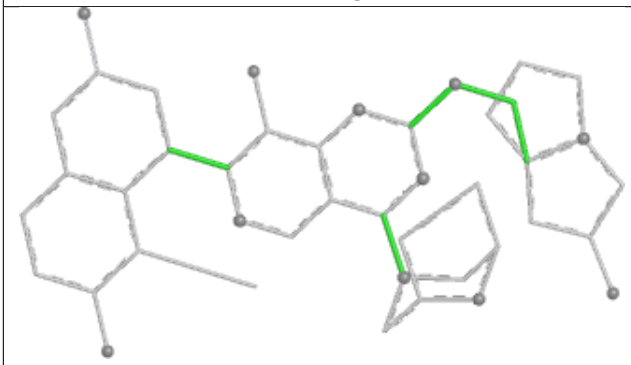
Ligand 6IC A 203



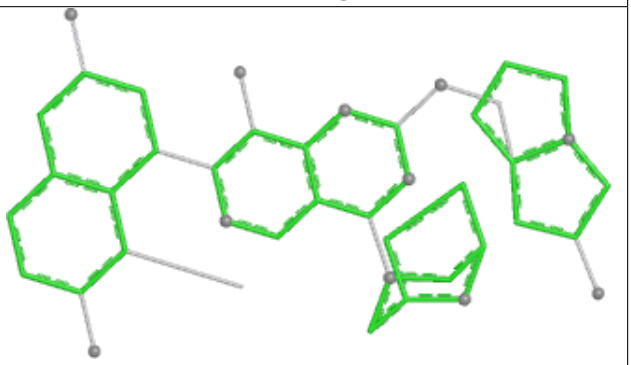
Bond lengths



Bond angles

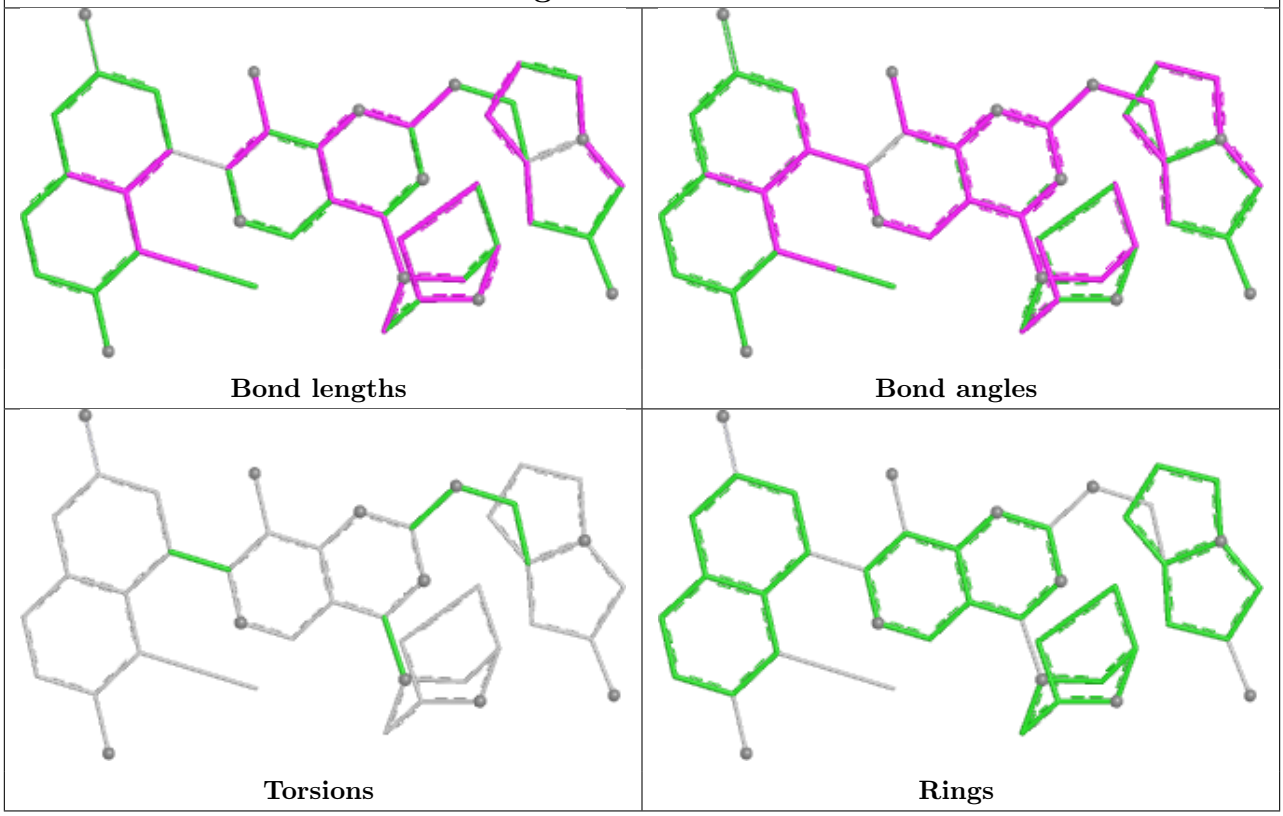


Torsions

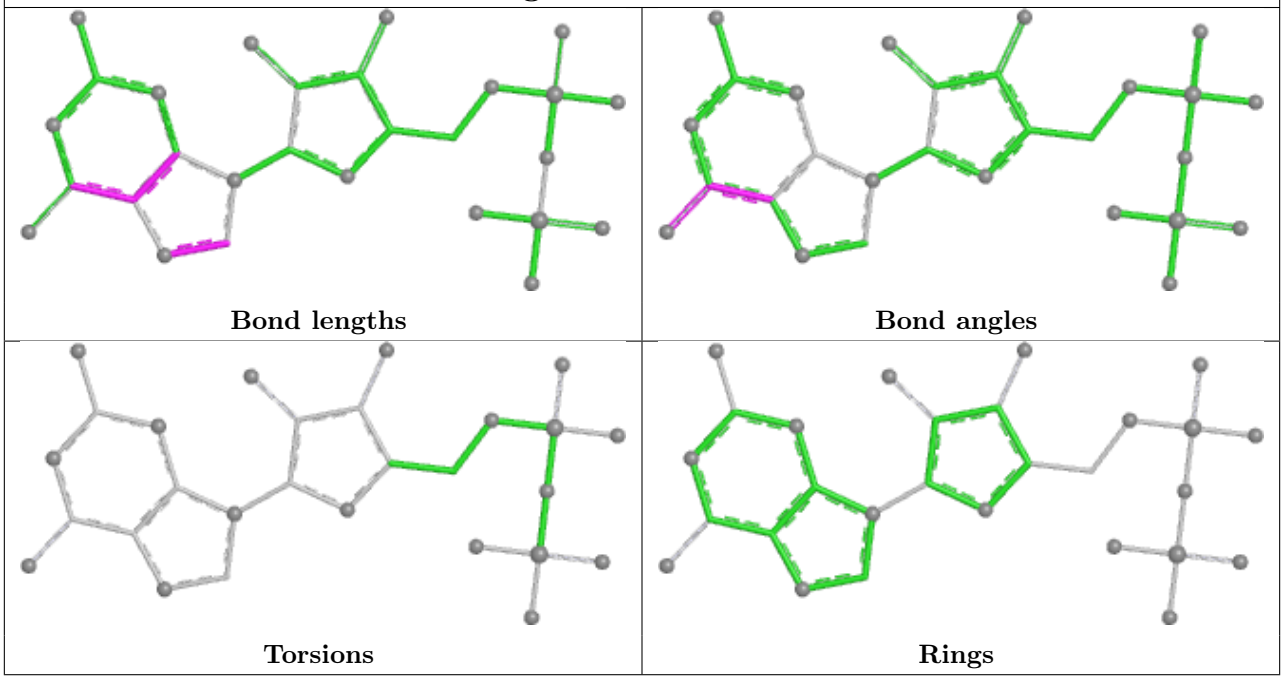


Rings

Ligand 6IC B 203



Ligand GDP B 201



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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	169/169 (100%)	-1.36	0	100	100	15, 25, 46, 68	1 (0%)
1	B	169/169 (100%)	-1.33	0	100	100	15, 25, 49, 71	1 (0%)
All	All	338/338 (100%)	-1.34	0	100	100	15, 25, 48, 71	2 (0%)

There are no RSRZ outliers to report.

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

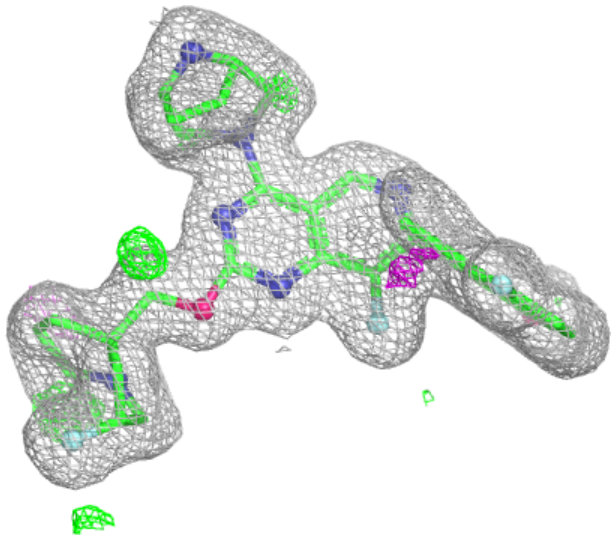
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

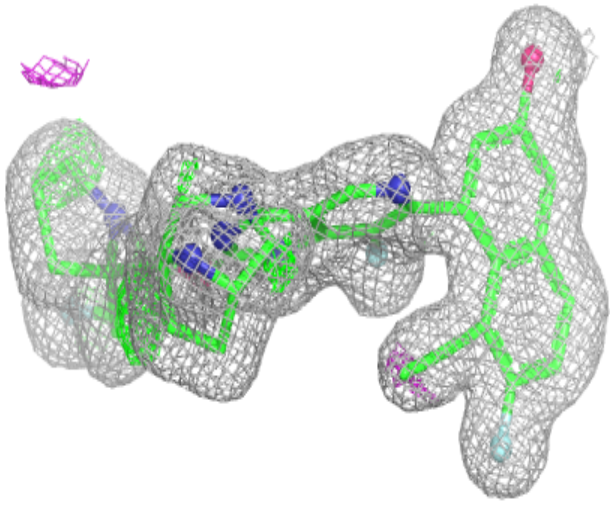
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	6IC	A	203	44/44	0.99	0.03	24,24,24,28	0
4	6IC	B	203	44/44	0.99	0.03	24,24,25,27	0
3	MG	A	202	1/1	1.00	0.01	16,16,16,16	0
3	MG	B	202	1/1	1.00	0.01	17,17,17,17	0
2	GDP	A	201	28/28	1.00	0.02	15,21,27,31	0
2	GDP	B	201	28/28	1.00	0.02	15,24,30,33	0

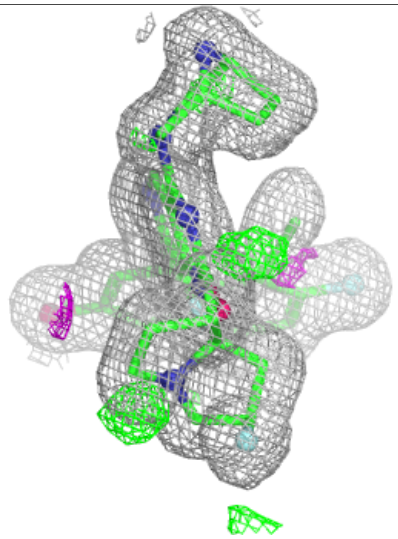
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 6IC A 203:

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

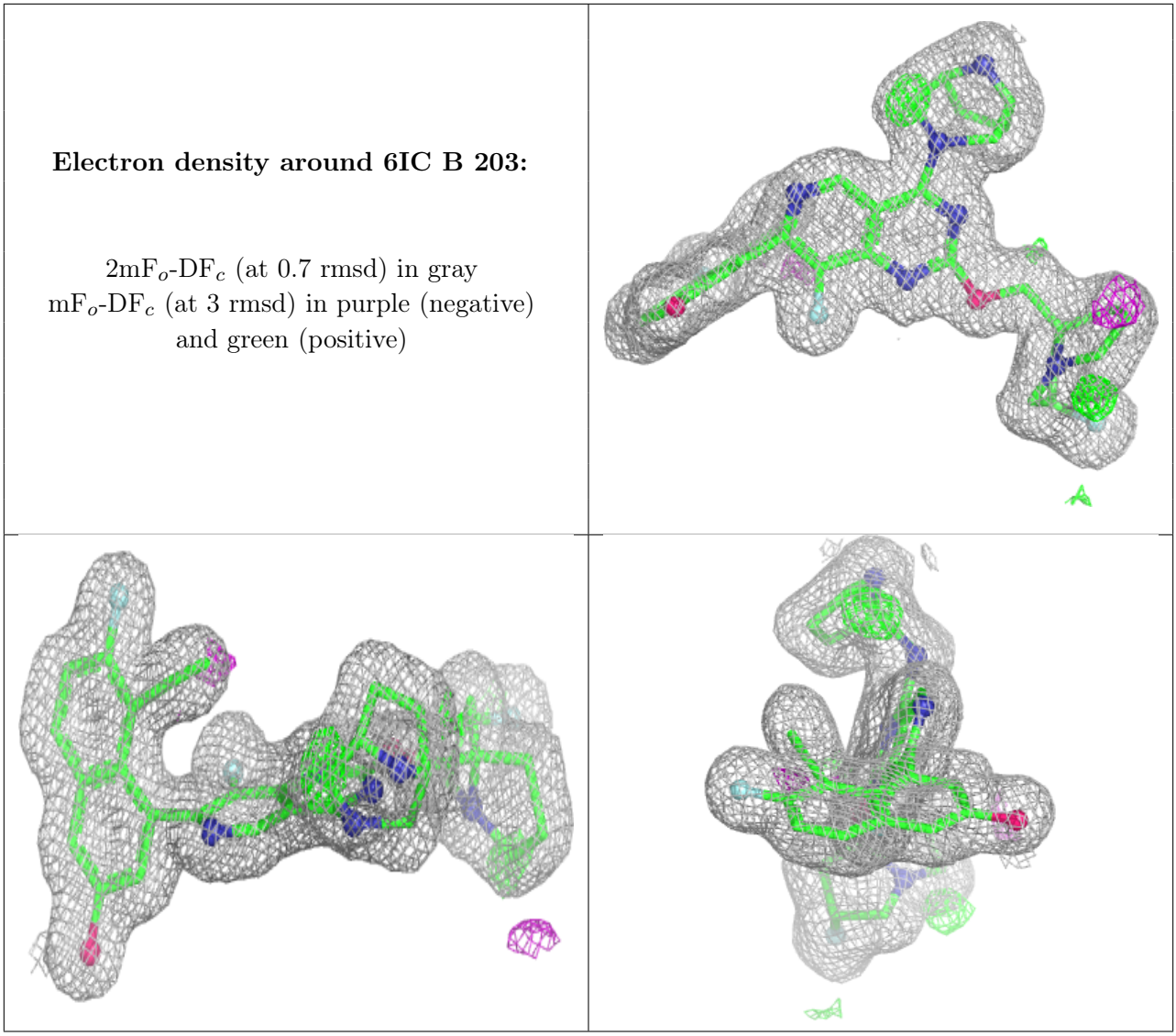






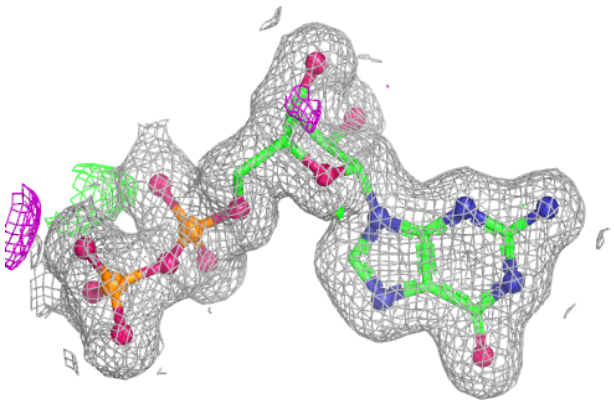
Electron density around 6IC B 203:

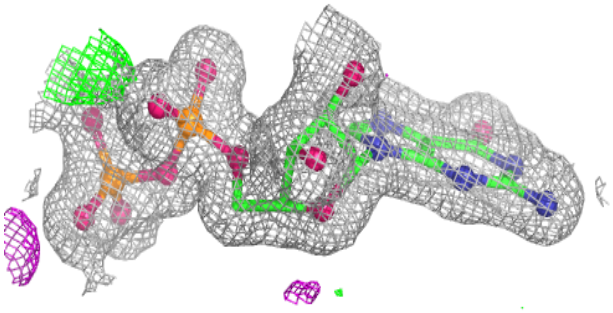
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

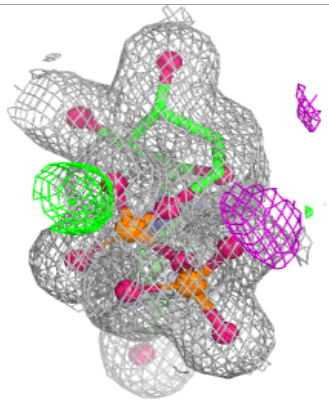


Electron density around GDP A 201:

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

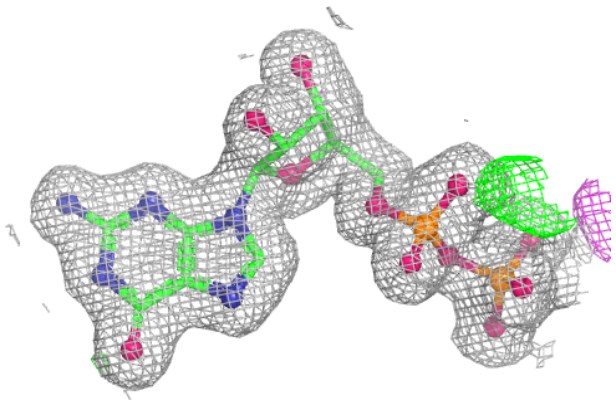


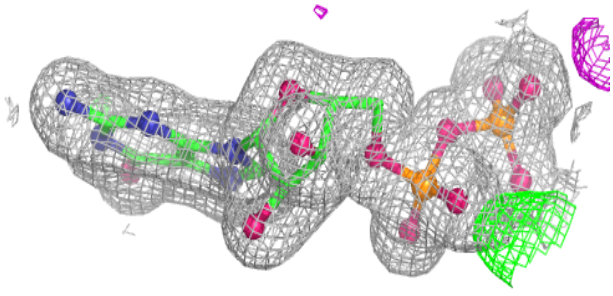


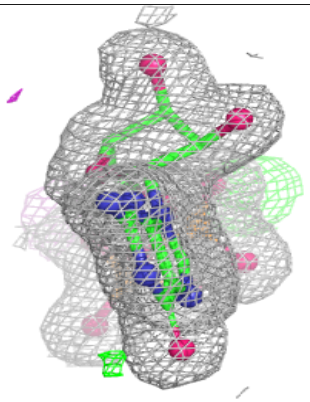


Electron density around GDP B 201:

$2mF_o$-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.