



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:25 PM UTC

PDB ID : 7U8H / pdb_00007u8h
Title : Discovery of a KRAS G12V Inhibitor in vivo Tool Compound starting from an HSQC-NMR based Fragment Hit
Authors : Phan, J.; Fesik, S.W.
Deposited on : 2022-03-08
Resolution : 1.70 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

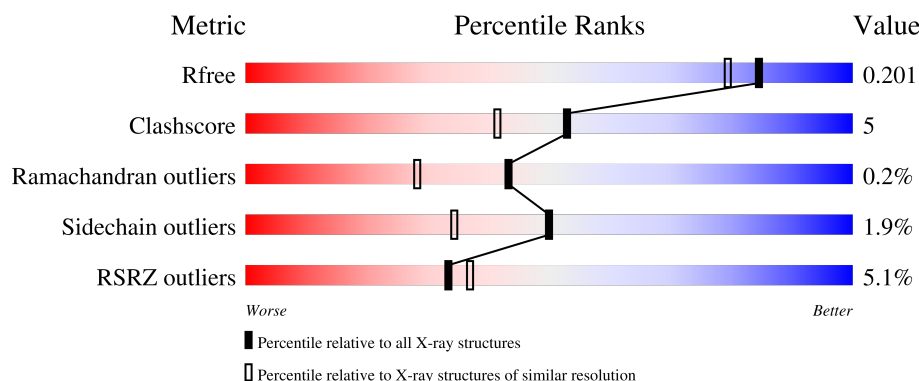
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	170	2% 89% 10% .
1	B	170	4% 90% 9% .
1	C	170	12% 82% 11% . 6%
1	D	170	2% 86% 12% ..

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
5	LX6	A	204	-	X	-	-
5	LX6	B	204	-	X	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6340 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.

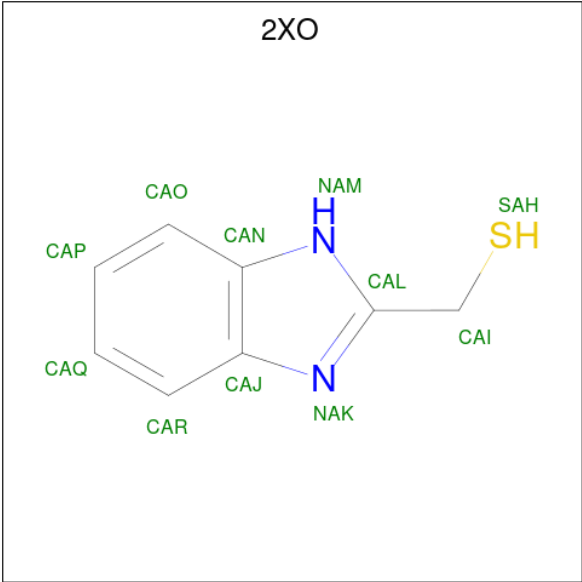
- Molecule 1 is a protein called GTPase KRas.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	169	Total	C	N	O	S	0	9	0
			1411	884	242	276	9			
1	B	168	Total	C	N	O	S	0	5	0
			1379	864	238	269	8			
1	C	160	Total	C	N	O	S	0	5	0
			1302	815	225	255	7			
1	D	168	Total	C	N	O	S	0	10	0
			1432	893	254	275	10			

There are 16 discrepancies between the modelled and reference sequences:

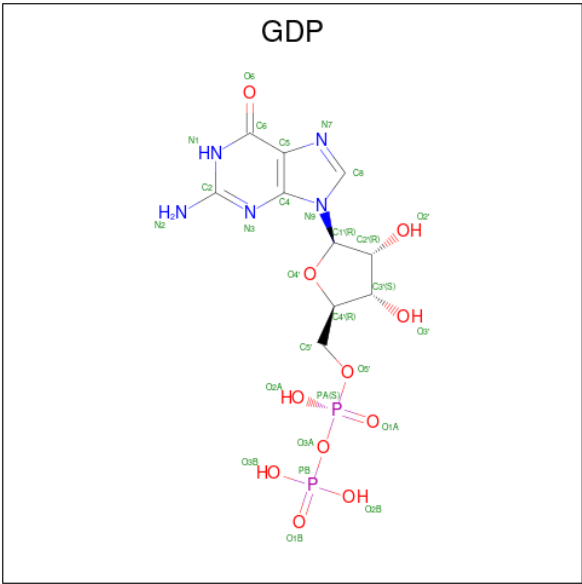
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP P01116
A	12	VAL	GLY	engineered mutation	UNP P01116
A	39	CYS	SER	conflict	UNP P01116
A	118	SER	CYS	conflict	UNP P01116
B	0	GLY	-	expression tag	UNP P01116
B	12	VAL	GLY	engineered mutation	UNP P01116
B	39	CYS	SER	conflict	UNP P01116
B	118	SER	CYS	conflict	UNP P01116
C	0	GLY	-	expression tag	UNP P01116
C	12	VAL	GLY	engineered mutation	UNP P01116
C	39	CYS	SER	conflict	UNP P01116
C	118	SER	CYS	conflict	UNP P01116
D	0	GLY	-	expression tag	UNP P01116
D	12	VAL	GLY	engineered mutation	UNP P01116
D	39	CYS	SER	conflict	UNP P01116
D	118	SER	CYS	conflict	UNP P01116

- Molecule 2 is 1H-benzimidazol-2-ylmethanethiol (CCD ID: 2XO) (formula: C₈H₈N₂S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	S	0	0
			11	8	2	1		
2	B	1	Total	C	N	S	0	0
			11	8	2	1		
2	C	1	Total	C	N	S	0	0
			11	8	2	1		
2	D	1	Total	C	N	S	0	0
			11	8	2	1		

- Molecule 3 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).

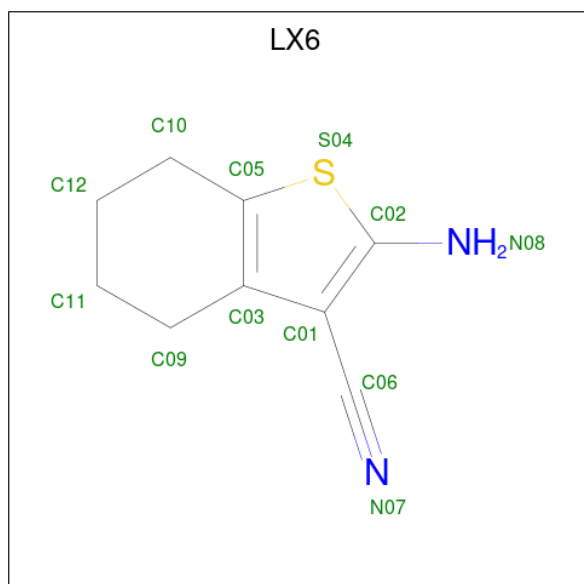


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
3	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
3	C	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
3	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 5 is 2-amino-4,5,6,7-tetrahydro-1-benzothiophene-3-carbonitrile (CCD ID: LX6) (formula: C₉H₁₀N₂S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	S	0	0
			12	9	2	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	S	0	0
			12	9	2	1		

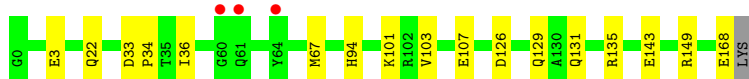
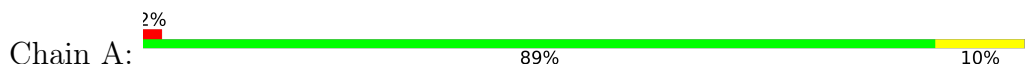
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	175	Total	O	0	0
			175	175		
6	B	169	Total	O	0	0
			169	169		
6	C	105	Total	O	0	0
			105	105		
6	D	183	Total	O	0	0
			183	183		

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.

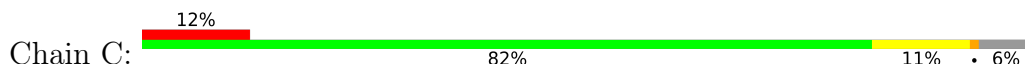
- Molecule 1: GTPase KRas



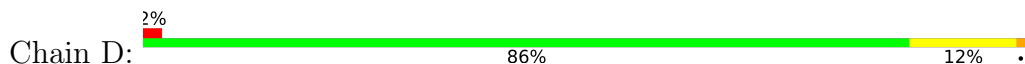
- Molecule 1: GTPase KRas



- Molecule 1: GTPase KRas



- Molecule 1: GTPase KRas



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	94.83Å 98.48Å 149.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.82 – 1.70 29.82 – 1.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.82-1.70) 99.9 (29.82-1.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.50 (at 1.70Å)	Xtriage
Refinement program	PHENIX 1.8.1_1168	Depositor
R, R_{free}	0.172 , 0.199 0.173 , 0.201	Depositor DCC
R_{free} test set	3861 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	17.3	Xtriage
Anisotropy	0.633	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 46.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.025 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6340	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 4.06% 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: 2XO, LX6, GDP, MG

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	0.36	0/1442	0.66	0/1945
1	B	0.35	0/1400	0.64	0/1888
1	C	0.33	0/1321	0.68	0/1783
1	D	0.36	0/1457	0.67	0/1962
All	All	0.35	0/5620	0.66	0/7578

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	1411	0	1394	14	0
1	B	1379	0	1364	8	0
1	C	1302	0	1282	19	0
1	D	1432	0	1414	15	0
2	A	11	0	7	0	0
2	B	11	0	7	0	0
2	C	11	0	7	0	0
2	D	11	0	7	0	0
3	A	28	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	28	0	12	0	0
3	C	28	0	12	6	0
3	D	28	0	12	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	12	0	0	1	0
5	B	12	0	0	0	0
6	A	175	0	0	7	3
6	B	169	0	0	1	2
6	C	105	0	0	9	1
6	D	183	0	0	3	2
All	All	6340	0	5530	56	4

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.

All (56) 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:126:ASP:OD1	6:A:301:HOH:O	1.92	0.88
1:C:31:GLU:O	6:C:302:HOH:O	1.97	0.81
3:C:202:GDP:O2A	6:C:301:HOH:O	1.97	0.81
1:C:82:PHE:HE2	1:C:125[B]:VAL:HG21	1.49	0.78
1:D:164:ARG:NH1	6:D:303:HOH:O	2.16	0.77
1:D:43:GLN:OE1	6:D:301:HOH:O	2.03	0.76
1:C:24:ILE:O	6:C:303:HOH:O	2.05	0.73
1:C:22:GLN:O	1:C:149:ARG:NH1	2.25	0.70
1:C:16:LYS:NZ	3:C:202:GDP:O1B	2.22	0.68
1:C:13:GLY:HA2	3:C:202:GDP:H5'	1.76	0.67
1:A:94[B]:HIS:ND1	6:A:303:HOH:O	2.29	0.65
1:D:94:HIS:O	1:D:98:GLU:HG2	1.96	0.65
1:C:33:ASP:N	6:C:302:HOH:O	2.30	0.64
1:B:97[A]:ARG:HG3	1:B:111[A]:MET:HE1	1.79	0.64
1:A:126:ASP:HB3	1:A:129:GLN:HG3	1.79	0.63
1:A:94[B]:HIS:CE1	6:A:303:HOH:O	2.53	0.61
1:C:143:GLU:OE2	6:C:304:HOH:O	2.16	0.60
1:D:78:PHE:HB2	1:D:111[A]:MET:HG2	1.83	0.59
1:B:1:MET:HE3	1:B:52:LEU:HB2	1.84	0.59
1:C:29:VAL:N	6:C:305:HOH:O	2.17	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94[B]:HIS:CG	6:A:303:HOH:O	2.58	0.56
1:C:82:PHE:CE2	1:C:125[B]:VAL:HG21	2.37	0.55
1:D:37:GLU:OE2	1:D:68[B]:ARG:NH1	2.30	0.54
1:C:29:VAL:HG12	1:C:31:GLU:HG2	1.88	0.54
1:B:3:GLU:HG2	1:B:52:LEU:HB3	1.90	0.52
1:D:101:LYS:HZ2	1:D:109:VAL:H	1.57	0.51
1:C:34:PRO:O	6:C:306:HOH:O	2.19	0.50
1:B:118[B]:SER:OG	1:B:143:GLU:HG2	2.11	0.50
1:C:117:LYS:HG2	3:C:202:GDP:C6	2.48	0.49
1:A:103:VAL:HG21	5:A:204:LX6:S04	2.54	0.47
1:B:39:CYS:HB3	6:B:303:HOH:O	2.14	0.47
1:D:65:SER:OG	1:D:68[A]:ARG:HG2	2.14	0.47
1:D:68[B]:ARG:HD2	6:D:339:HOH:O	2.14	0.47
1:A:131:GLN:HG2	6:A:456:HOH:O	2.15	0.46
1:C:117:LYS:HB3	1:C:120:LEU:HD22	1.97	0.46
1:D:46:ILE:O	1:D:164:ARG:NH2	2.48	0.46
1:D:101:LYS:HD2	1:D:106:SER:O	2.16	0.46
1:B:135:ARG:NH2	1:C:3:GLU:OE2	2.41	0.46
1:C:88:LYS:HB2	6:C:355:HOH:O	2.14	0.46
1:C:117:LYS:HG2	3:C:202:GDP:C5	2.51	0.46
1:C:72:MET:HB2	1:C:103:VAL:HG11	1.98	0.45
1:D:97[B]:ARG:HG3	1:D:111[B]:MET:HE1	1.99	0.44
1:D:65:SER:CB	1:D:68[A]:ARG:HG2	2.48	0.43
1:A:135:ARG:HA	6:A:398:HOH:O	2.19	0.43
1:B:22:GLN:HG3	1:B:149:ARG:HG3	2.01	0.43
1:A:33:ASP:HB3	1:A:36:ILE:HG12	2.01	0.43
1:A:22:GLN:CD	1:A:149:ARG:HG2	2.45	0.42
1:B:33:ASP:HA	1:B:34:PRO:HD3	1.90	0.42
1:A:3:GLU:OE2	1:D:135[B]:ARG:NH2	2.44	0.42
1:D:65:SER:HB3	1:D:68[A]:ARG:HG2	2.01	0.42
1:C:118[A]:SER:OG	1:C:150:GLN:OE1	2.36	0.41
1:A:101:LYS:NZ	1:A:107:GLU:OE1	2.39	0.41
1:A:143:GLU:CD	6:A:306:HOH:O	2.62	0.41
3:C:202:GDP:H5''	6:C:301:HOH:O	2.20	0.41
1:A:33:ASP:HA	1:A:34:PRO:HD3	1.88	0.41
1:D:33:ASP:HA	1:D:34:PRO:HD3	1.92	0.40

All (4) 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)
6:C:334:HOH:O	6:D:344:HOH:O[7_545]	1.99	0.21
6:A:387:HOH:O	6:B:429:HOH:O[5_455]	2.03	0.17
6:A:456:HOH:O	6:B:429:HOH:O[5_455]	2.11	0.09
6:A:432:HOH:O	6:D:370:HOH:O[7_555]	2.14	0.06

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	176/170 (104%)	170 (97%)	6 (3%)	0	100	100
1	B	171/170 (101%)	167 (98%)	4 (2%)	0	100	100
1	C	161/170 (95%)	156 (97%)	4 (2%)	1 (1%)	21	9
1	D	176/170 (104%)	171 (97%)	5 (3%)	0	100	100
All	All	684/680 (101%)	664 (97%)	19 (3%)	1 (0%)	43	31

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	31	GLU

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	158/150 (105%)	156 (99%)	2 (1%)	61	48
1	B	153/150 (102%)	151 (99%)	2 (1%)	61	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	145/150 (97%)	143 (99%)	2 (1%)	59	46
1	D	159/150 (106%)	154 (97%)	5 (3%)	35	18
All	All	615/600 (102%)	604 (98%)	11 (2%)	50	36

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	MET
1	A	168	GLU
1	B	79	LEU
1	B	105	ASP
1	C	120	LEU
1	C	128	LYS
1	D	1	MET
1	D	49	GLU
1	D	52	LEU
1	D	164	ARG
1	D	168	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	GLN
1	B	166	HIS
1	C	25	GLN
1	C	26	ASN
1	D	43	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 4 are monoatomic - leaving 10 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$
5	LX6	A	204	-	13,13,13	6.90	9 (69%)	18,18,18	7.16	12 (66%)
3	GDP	B	202	4	29,30,30	1.16	4 (13%)	45,47,47	1.71	6 (13%)
3	GDP	A	202	4	29,30,30	1.15	3 (10%)	45,47,47	1.72	6 (13%)
3	GDP	D	202	4	29,30,30	1.09	2 (6%)	45,47,47	1.64	6 (13%)
2	2XO	A	201	-	11,12,12	2.90	2 (18%)	13,16,16	1.87	4 (30%)
2	2XO	B	201	-	11,12,12	2.94	2 (18%)	13,16,16	1.86	4 (30%)
3	GDP	C	202	4	29,30,30	1.12	2 (6%)	45,47,47	1.77	7 (15%)
5	LX6	B	204	-	13,13,13	6.87	9 (69%)	18,18,18	7.08	13 (72%)
2	2XO	D	201	-	11,12,12	2.73	2 (18%)	13,16,16	1.89	4 (30%)
2	2XO	C	201	-	11,12,12	2.92	2 (18%)	13,16,16	1.93	4 (30%)

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
5	LX6	A	204	-	-	0/0/9/9	0/2/2/2
3	GDP	B	202	4	-	2/16/32/32	0/3/3/3
3	GDP	A	202	4	-	0/16/32/32	0/3/3/3
3	GDP	D	202	4	-	2/16/32/32	0/3/3/3
2	2XO	A	201	-	-	0/0/10/10	0/2/2/2
2	2XO	B	201	-	-	0/0/10/10	0/2/2/2
3	GDP	C	202	4	-	1/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	LX6	B	204	-	-	0/0/9/9	0/2/2/2
2	2XO	D	201	-	-	0/0/10/10	0/2/2/2
2	2XO	C	201	-	-	0/0/10/10	0/2/2/2

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	204	LX6	C05-C03	17.36	1.57	1.36
5	A	204	LX6	C05-C03	17.24	1.57	1.36
5	B	204	LX6	C01-C02	9.94	1.52	1.39
5	A	204	LX6	C01-C02	9.86	1.52	1.39
5	A	204	LX6	C05-S04	-9.74	1.54	1.74
5	B	204	LX6	C05-S04	-9.38	1.55	1.74
2	C	201	2XO	CAI-SAH	-8.81	1.66	1.82
2	B	201	2XO	CAI-SAH	-8.79	1.66	1.82
2	A	201	2XO	CAI-SAH	-8.72	1.67	1.82
2	D	201	2XO	CAI-SAH	-8.18	1.67	1.82
5	A	204	LX6	C02-S04	-6.99	1.61	1.73
5	B	204	LX6	C02-S04	-6.80	1.62	1.73
5	A	204	LX6	C01-C03	4.91	1.58	1.44
5	B	204	LX6	C01-C03	4.73	1.58	1.44
5	B	204	LX6	C02-N08	4.65	1.43	1.35
5	A	204	LX6	C02-N08	4.65	1.43	1.35
2	B	201	2XO	CAL-NAK	3.56	1.38	1.32
2	A	201	2XO	CAL-NAK	3.32	1.37	1.32
5	A	204	LX6	C11-C09	-3.19	1.41	1.52
3	C	202	GDP	C5-C4	3.17	1.47	1.38
2	C	201	2XO	CAL-NAK	3.15	1.37	1.32
5	A	204	LX6	C12-C10	-3.11	1.42	1.52
5	B	204	LX6	C11-C09	-3.09	1.42	1.52
3	A	202	GDP	C5-C4	3.08	1.47	1.38
3	B	202	GDP	C5-C4	3.07	1.47	1.38
5	B	204	LX6	C12-C10	-3.07	1.42	1.52
2	D	201	2XO	CAL-NAK	3.03	1.37	1.32
3	D	202	GDP	C5-C4	2.92	1.46	1.38
5	A	204	LX6	C06-C01	2.86	1.49	1.43
5	B	204	LX6	C06-C01	2.80	1.49	1.43
3	C	202	GDP	C6-N1	-2.33	1.34	1.38
3	B	202	GDP	C4-N9	-2.25	1.32	1.38
3	B	202	GDP	C6-N1	-2.14	1.34	1.38
3	B	202	GDP	PA-O3A	2.11	1.61	1.59
3	A	202	GDP	C6-N1	-2.07	1.35	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	202	GDP	C4-N9	-2.05	1.32	1.38
3	D	202	GDP	C6-N1	-2.04	1.35	1.38

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	204	LX6	C05-S04-C02	24.12	107.53	91.55
5	B	204	LX6	C05-S04-C02	22.87	106.71	91.55
5	B	204	LX6	C10-C05-C03	-12.38	116.23	125.85
5	A	204	LX6	C10-C05-C03	-11.01	117.30	125.85
5	B	204	LX6	C05-C03-C01	-8.66	107.83	111.77
5	A	204	LX6	C05-C03-C01	-7.93	108.16	111.77
5	B	204	LX6	C10-C05-S04	7.39	135.24	121.01
5	A	204	LX6	C10-C05-S04	7.13	134.74	121.01
3	C	202	GDP	C5-C4-N3	-5.79	119.17	128.39
3	A	202	GDP	C5-C4-N3	-5.52	119.60	128.39
3	B	202	GDP	C5-C4-N3	-5.33	119.91	128.39
3	D	202	GDP	C5-C4-N3	-5.03	120.39	128.39
3	C	202	GDP	C2-N3-C4	4.84	120.64	112.30
3	A	202	GDP	C2-N3-C4	4.81	120.59	112.30
5	A	204	LX6	C03-C05-S04	-4.74	107.96	112.43
3	B	202	GDP	C2-N3-C4	4.66	120.33	112.30
3	D	202	GDP	C2-N3-C4	4.46	119.99	112.30
5	A	204	LX6	C09-C03-C01	4.41	134.26	125.68
2	B	201	2XO	NAM-CAL-NAK	-4.19	107.61	112.72
3	C	202	GDP	N9-C4-N3	4.17	134.29	125.95
5	B	204	LX6	C03-C05-S04	-4.14	108.52	112.43
5	B	204	LX6	C09-C03-C01	4.08	133.62	125.68
3	A	202	GDP	C6-C5-N7	4.04	137.64	130.29
3	B	202	GDP	C6-C5-N7	3.95	137.48	130.29
2	C	201	2XO	NAM-CAL-NAK	-3.92	107.94	112.72
2	A	201	2XO	NAM-CAL-NAK	-3.92	107.95	112.72
5	A	204	LX6	C02-C01-C03	-3.91	108.14	113.32
3	B	202	GDP	N9-C4-N3	3.89	133.73	125.95
3	D	202	GDP	C6-C5-N7	3.81	137.23	130.29
3	A	202	GDP	N9-C4-N3	3.79	133.53	125.95
3	D	202	GDP	N9-C4-N3	3.75	133.45	125.95
5	B	204	LX6	C02-C01-C03	-3.66	108.47	113.32
5	A	204	LX6	C09-C03-C05	-3.65	117.58	121.39
2	D	201	2XO	NAM-CAL-NAK	-3.58	108.35	112.72
3	C	202	GDP	C6-C5-N7	3.51	136.68	130.29
5	B	204	LX6	C01-C02-N08	-3.15	125.32	128.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	201	2XO	CAJ-NAK-CAL	3.14	109.32	105.25
2	A	201	2XO	CAJ-NAK-CAL	3.12	109.30	105.25
2	D	201	2XO	CAJ-NAK-CAL	3.11	109.29	105.25
3	A	202	GDP	C4-C5-N7	-3.11	105.73	110.67
5	A	204	LX6	C12-C10-C05	3.08	116.12	110.38
3	B	202	GDP	C4-C5-N7	-3.04	105.85	110.67
2	B	201	2XO	CAJ-NAK-CAL	2.92	109.04	105.25
5	B	204	LX6	S04-C02-N08	2.91	126.20	120.07
5	B	204	LX6	C06-C01-C02	2.73	126.82	121.62
3	C	202	GDP	C4-C5-N7	-2.72	106.36	110.67
5	B	204	LX6	C09-C03-C05	-2.71	118.56	121.39
3	D	202	GDP	C4-C5-N7	-2.70	106.39	110.67
5	B	204	LX6	C12-C10-C05	2.68	115.38	110.38
5	A	204	LX6	C06-C01-C02	2.67	126.71	121.62
5	A	204	LX6	S04-C02-N08	2.57	125.48	120.07
2	B	201	2XO	CAN-NAM-CAL	2.51	110.14	107.23
3	C	202	GDP	O2A-PA-O3A	2.47	113.94	107.27
3	C	202	GDP	O3B-PB-O3A	2.41	112.73	104.64
2	D	201	2XO	CAR-CAJ-CAN	2.38	122.88	120.26
2	C	201	2XO	CAN-CAJ-NAK	-2.33	106.23	109.42
3	B	202	GDP	C8-N7-C5	2.28	108.31	104.26
3	D	202	GDP	O6-C6-C5	-2.25	120.59	126.53
2	D	201	2XO	CAN-CAJ-NAK	-2.22	106.37	109.42
2	A	201	2XO	CAN-CAJ-NAK	-2.20	106.40	109.42
5	B	204	LX6	C11-C09-C03	2.17	116.52	111.85
3	A	202	GDP	C8-N7-C5	2.16	108.11	104.26
5	A	204	LX6	C01-C02-N08	-2.07	126.32	128.22
2	C	201	2XO	CAN-NAM-CAL	2.05	109.60	107.23
2	B	201	2XO	CAN-CAJ-NAK	-2.02	106.65	109.42
2	A	201	2XO	CAR-CAJ-CAN	2.01	122.47	120.26

There are no chirality outliers.

All (5) torsion outliers are listed below:

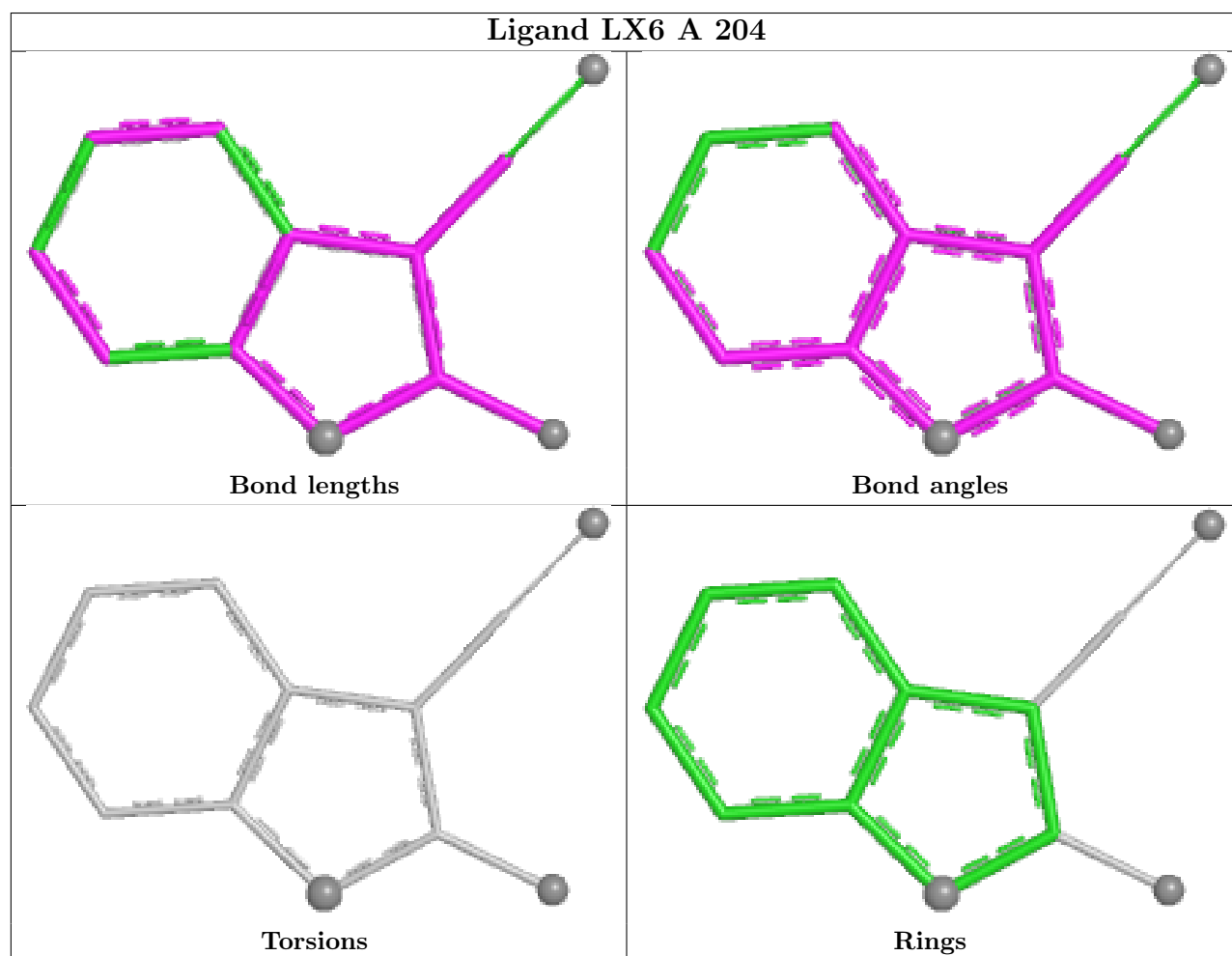
Mol	Chain	Res	Type	Atoms
3	B	202	GDP	PA-O3A-PB-O3B
3	D	202	GDP	PA-O3A-PB-O2B
3	B	202	GDP	PA-O3A-PB-O1B
3	D	202	GDP	PA-O3A-PB-O1B
3	C	202	GDP	PB-O3A-PA-O2A

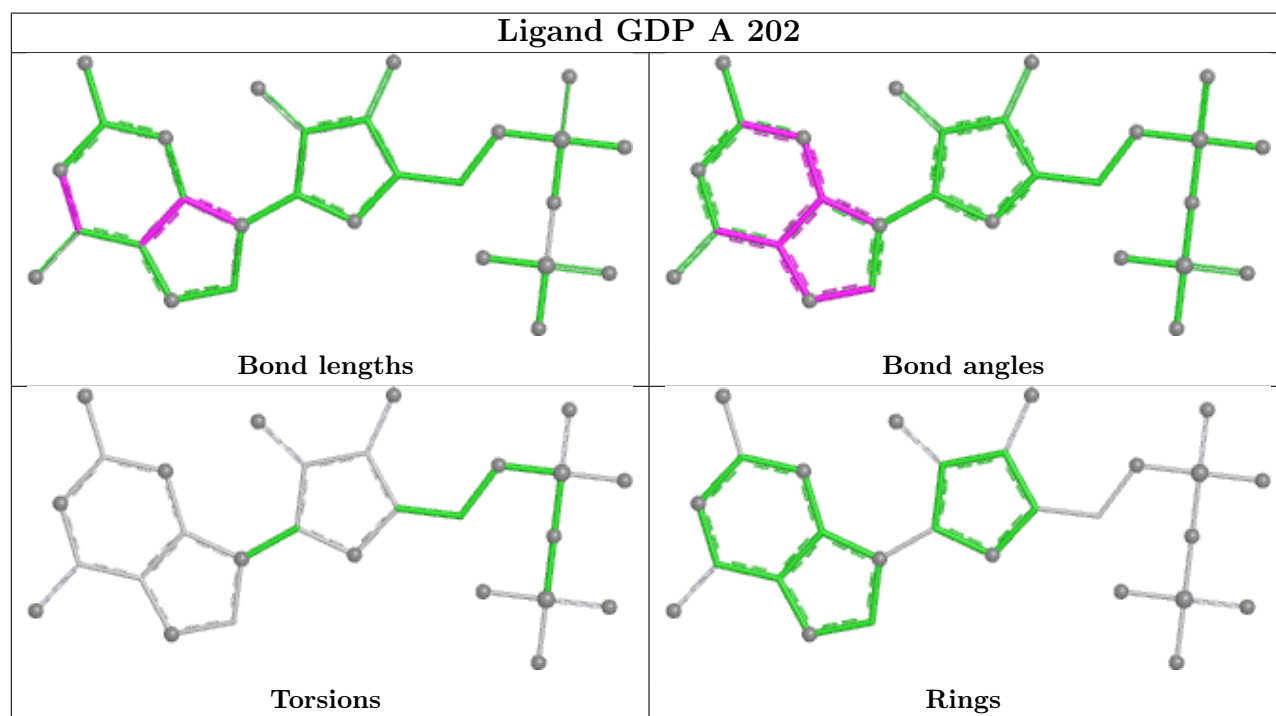
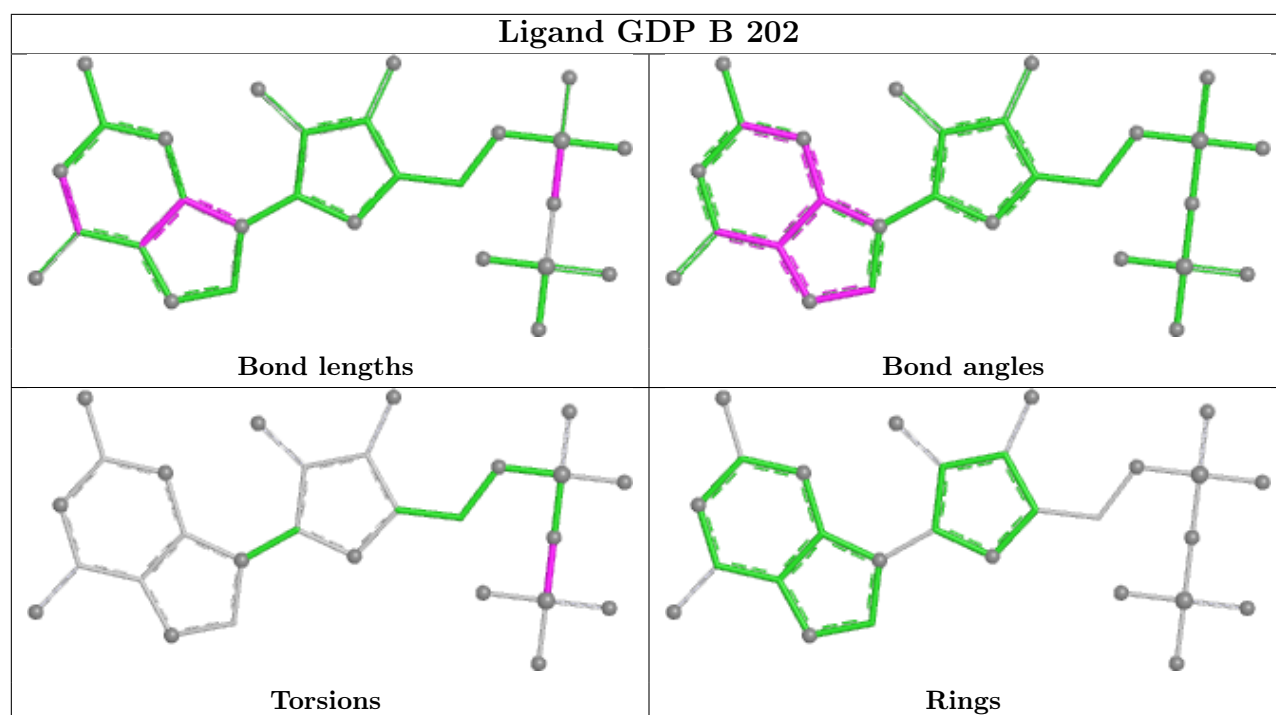
There are no ring outliers.

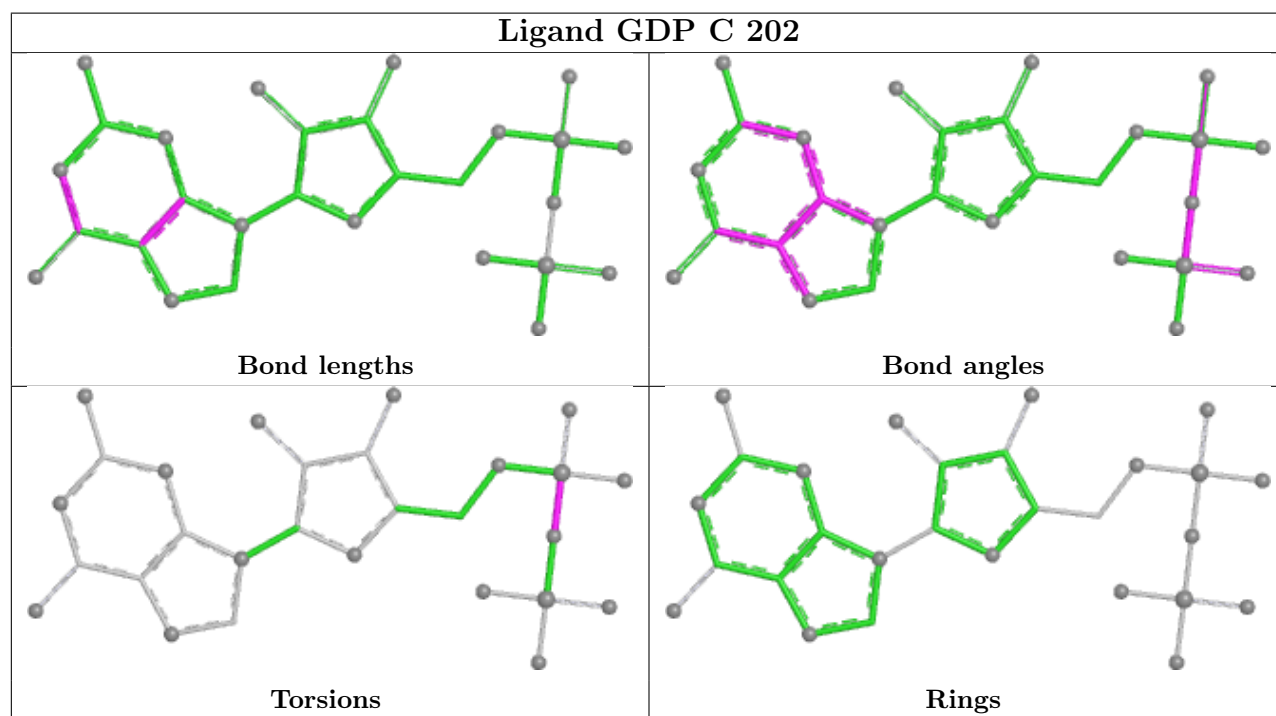
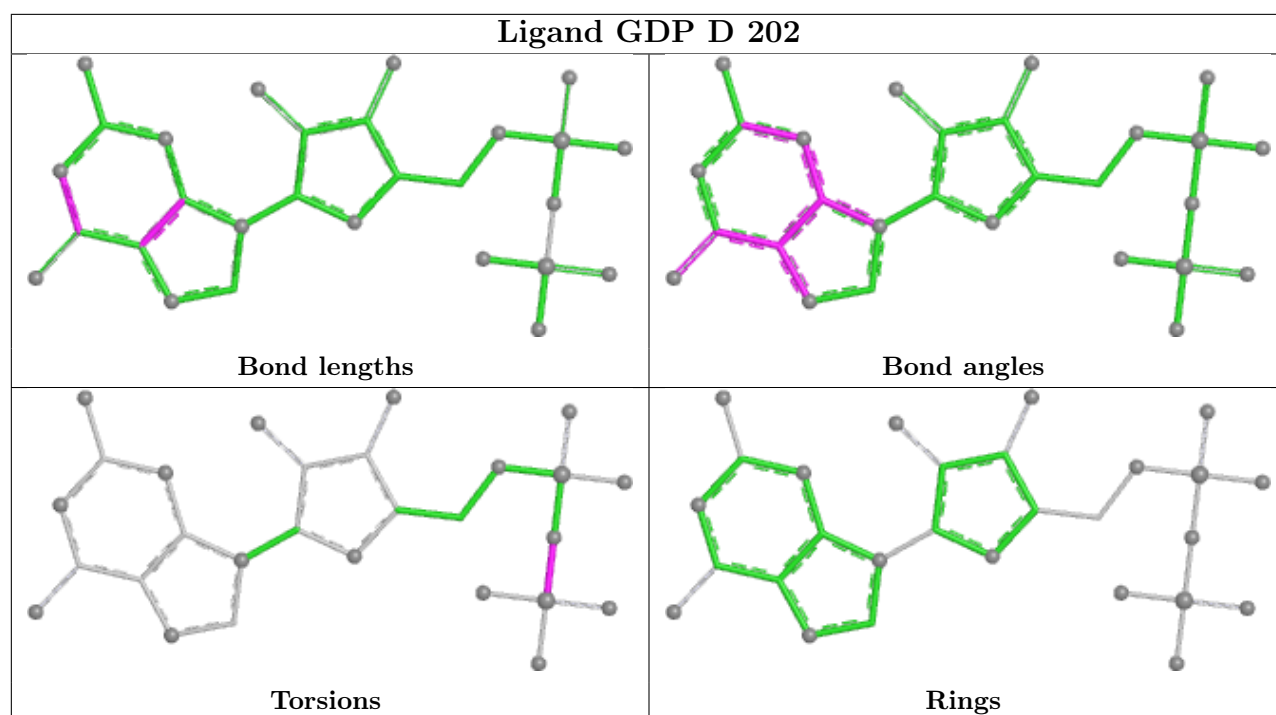
2 monomers are involved in 7 short contacts:

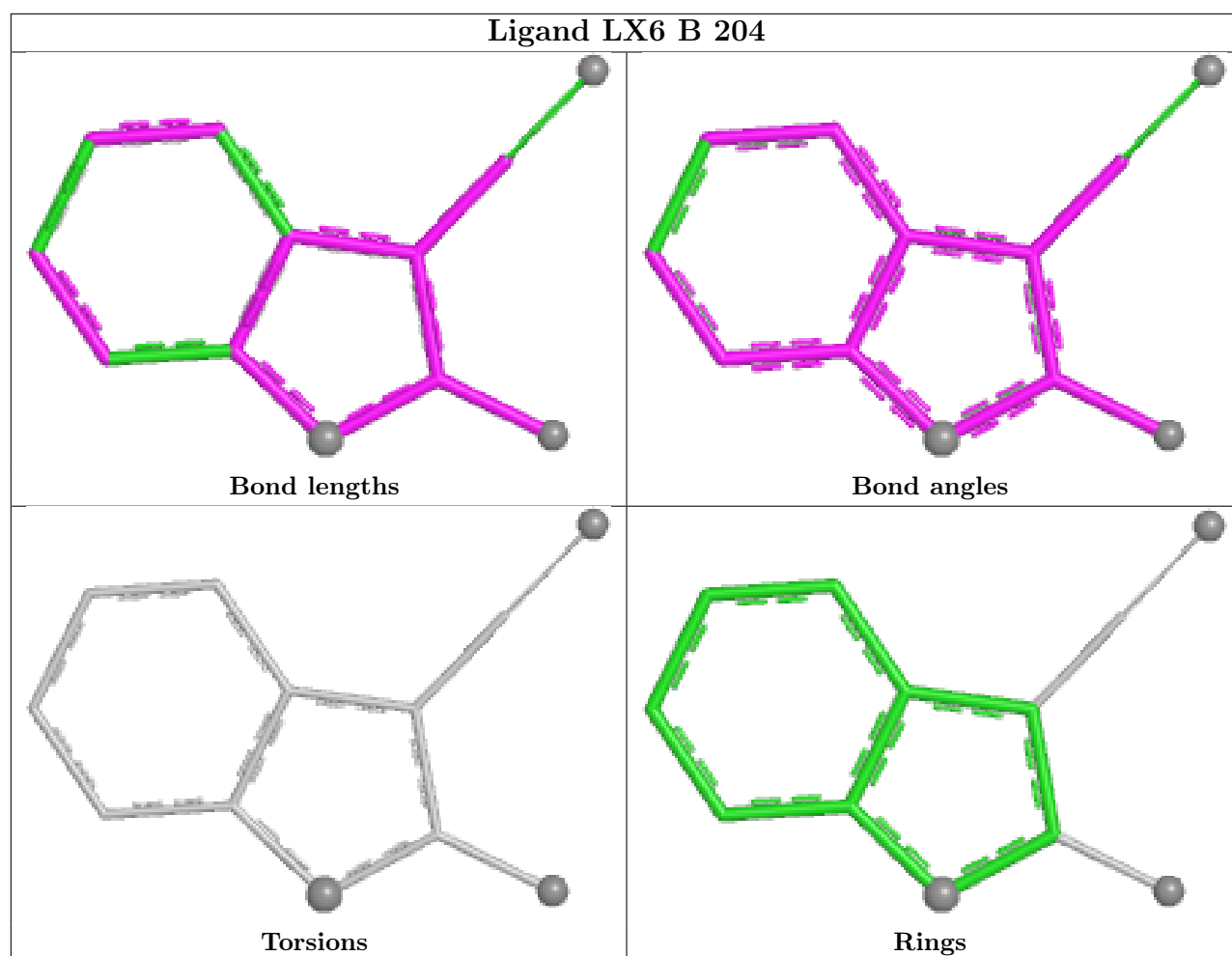
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	204	LX6	1	0
3	C	202	GDP	6	0

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 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	169/170 (99%)	-0.07	3 (1%) 67 72	6, 17, 45, 62	9 (5%)
1	B	168/170 (98%)	-0.05	6 (3%) 46 50	9, 22, 45, 64	5 (2%)
1	C	160/170 (94%)	0.90	21 (13%) 7 7	9, 36, 62, 71	5 (3%)
1	D	168/170 (98%)	-0.14	4 (2%) 59 64	7, 17, 47, 82	10 (5%)
All	All	665/680 (97%)	0.15	34 (5%) 33 37	6, 23, 57, 82	29 (4%)

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	32	TYR	5.9
1	C	60	GLY	4.5
1	C	29	VAL	4.5
1	C	71	TYR	4.4
1	C	28	PHE	4.2
1	A	60	GLY	3.8
1	A	64	TYR	3.4
1	C	30	ASP	3.4
1	D	60	GLY	3.4
1	C	95	HIS	3.2
1	A	61	GLN	3.0
1	C	27	HIS	2.9
1	D	64	TYR	2.8
1	C	68	ARG	2.8
1	C	0	GLY	2.7
1	D	59	ALA	2.7
1	D	68[A]	ARG	2.6
1	B	29	VAL	2.6
1	B	64	TYR	2.6
1	C	108	ASP	2.5
1	C	26	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	120	LEU	2.5
1	C	31	GLU	2.5
1	B	30	ASP	2.4
1	B	105	ASP	2.4
1	C	125[A]	VAL	2.4
1	C	146	ALA	2.4
1	B	122	SER	2.3
1	C	149	ARG	2.3
1	C	148	THR	2.2
1	B	106	SER	2.1
1	C	103	VAL	2.0
1	C	121	PRO	2.0
1	C	130	ALA	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
4	MG	C	203	1/1	0.82	0.11	26,26,26,26	0
2	2XO	D	201	11/11	0.85	0.11	14,16,31,37	0
3	GDP	C	202	28/28	0.89	0.12	18,34,38,39	0
2	2XO	C	201	11/11	0.90	0.08	16,21,30,43	0
2	2XO	B	201	11/11	0.91	0.10	17,25,36,110	0
5	LX6	B	204	12/12	0.91	0.12	27,33,38,42	0
5	LX6	A	204	12/12	0.92	0.10	29,33,41,42	0
2	2XO	A	201	11/11	0.93	0.07	13,18,32,49	0
4	MG	B	203	1/1	0.98	0.03	15,15,15,15	0
3	GDP	B	202	28/28	0.98	0.06	12,18,26,29	0

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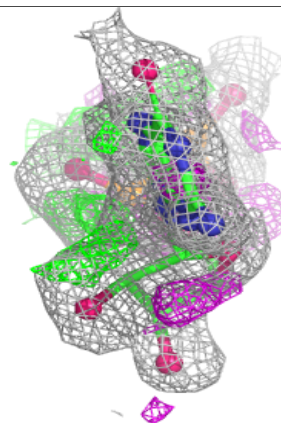
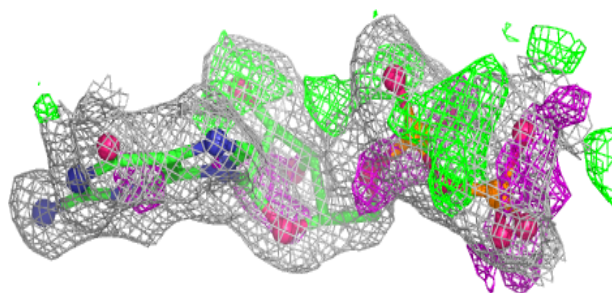
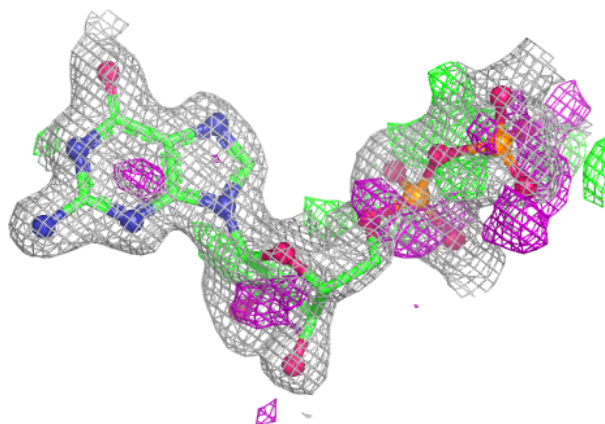
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GDP	A	202	28/28	0.98	0.06	10,14,25,31	0
4	MG	A	203	1/1	0.98	0.03	13,13,13,13	0
3	GDP	D	202	28/28	0.99	0.04	7,9,14,17	0
4	MG	D	203	1/1	0.99	0.02	9,9,9,9	0

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.

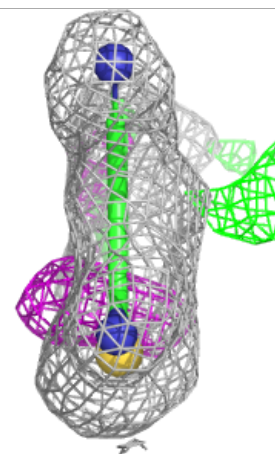
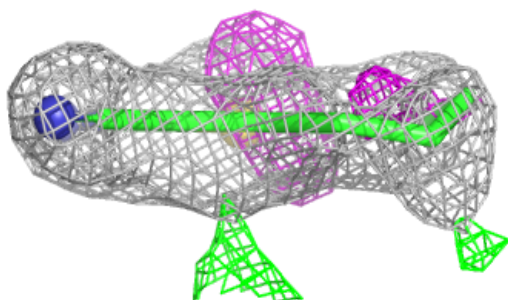
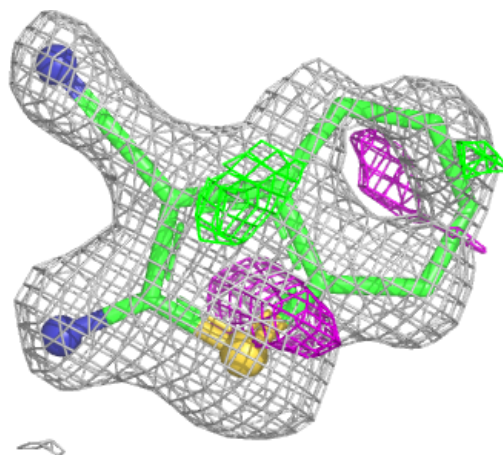
Electron density around GDP C 202:

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



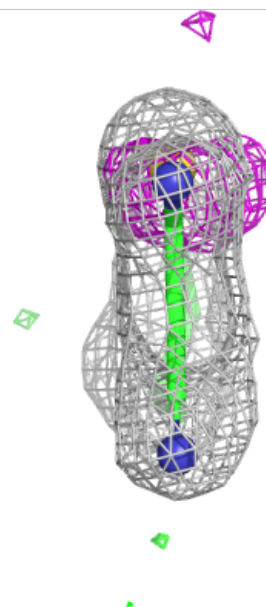
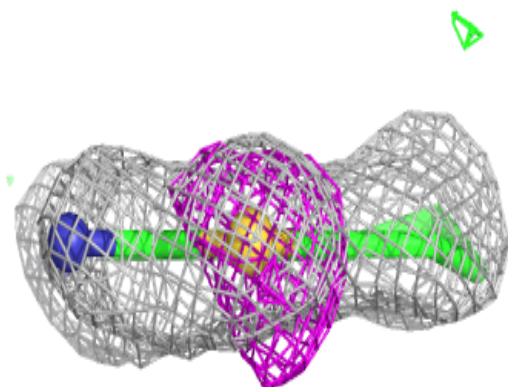
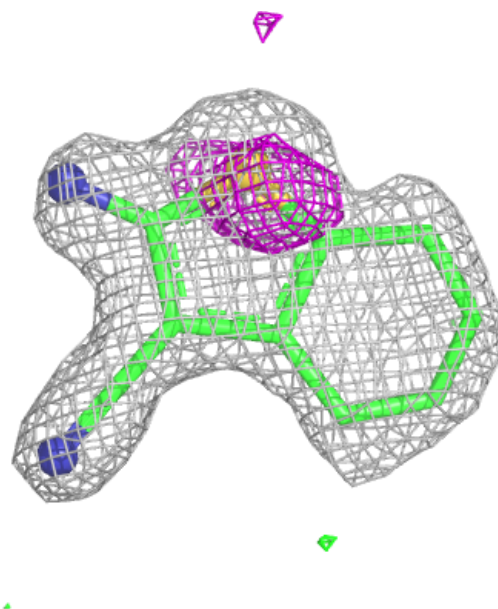
Electron density around LX6 B 204:

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



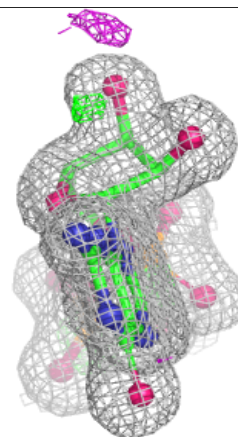
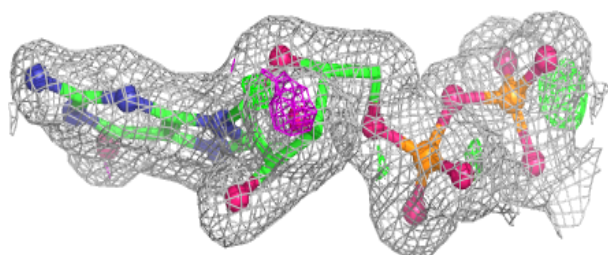
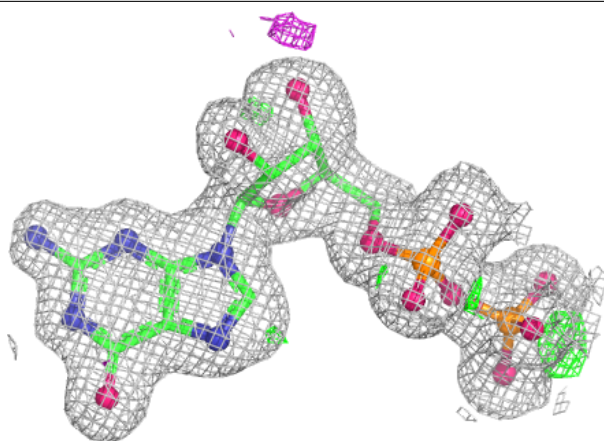
Electron density around LX6 A 204:

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

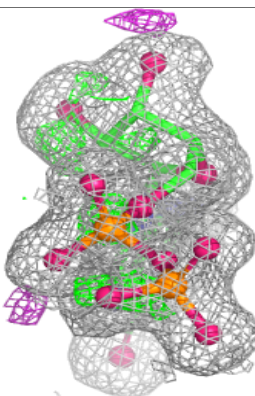
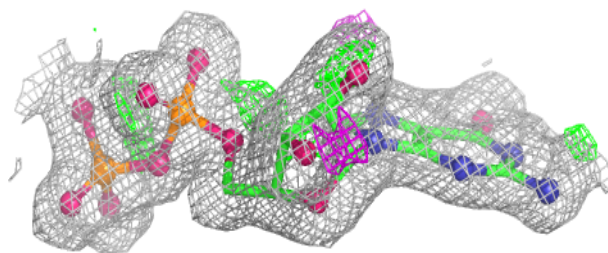
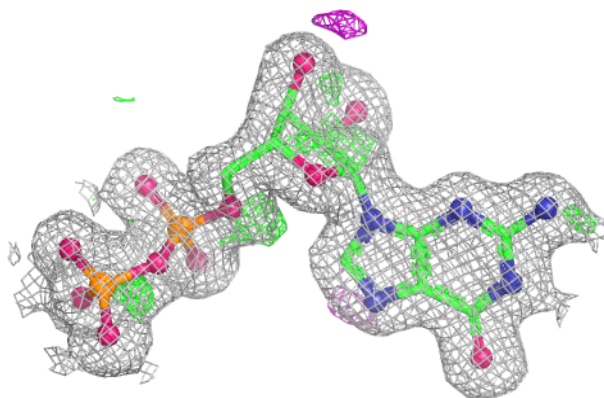


Electron density around GDP B 202:

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

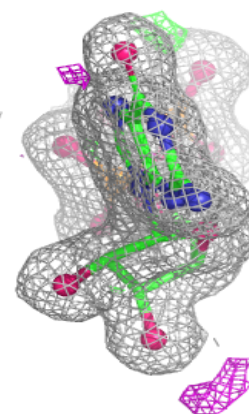
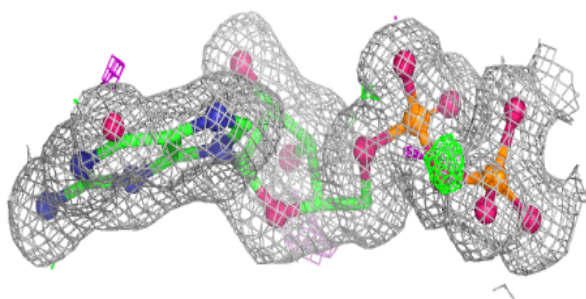
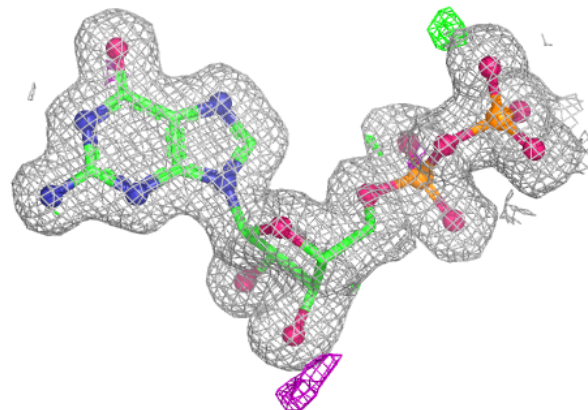
**Electron density around GDP A 202:**

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



Electron density around GDP D 202:

$2mF_o - DF_c$ (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.