Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2024 – 06:23 PM EST

PDB ID	:	8T4V
Title	:	Crystal structure of compound 1 bound to K-Ras(G12D)
Authors	:	Zhang, Z.; Zheng, Q.; Guiley, K.Z.; Shokat, K.M.
Deposited on	:	2023-06-10
Resolution	:	1.47 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:

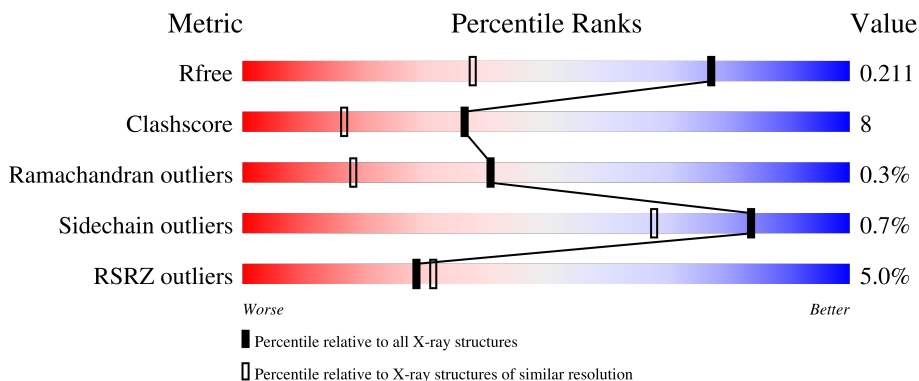|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.47 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		0.211
Clashscore		8
Ramachandran outliers		0.3%
Sidechain outliers		0.7%
RSRZ outliers		5.0%

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	4690 (1.50-1.46)
Clashscore	141614	4955 (1.50-1.46)
Ramachandran outliers	138981	4846 (1.50-1.46)
Sidechain outliers	138945	4844 (1.50-1.46)
RSRZ outliers	127900	4614 (1.50-1.46)

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	187	7% / 76% 14% · 9%
1	B	187	2% / 83% 8% 9%

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 3211 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	170	Total	C	N	O	S	0	0	0
			1360	852	233	271	4			
1	B	170	Total	C	N	O	S	0	0	0
			1360	852	233	271	4			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-17	MET	-	initiating methionine	UNP P01116
A	-16	HIS	-	expression tag	UNP P01116
A	-15	HIS	-	expression tag	UNP P01116
A	-14	HIS	-	expression tag	UNP P01116
A	-13	HIS	-	expression tag	UNP P01116
A	-12	HIS	-	expression tag	UNP P01116
A	-11	HIS	-	expression tag	UNP P01116
A	-10	SER	-	expression tag	UNP P01116
A	-9	SER	-	expression tag	UNP P01116
A	-8	GLY	-	expression tag	UNP P01116
A	-7	ARG	-	expression tag	UNP P01116
A	-6	GLU	-	expression tag	UNP P01116
A	-5	ASN	-	expression tag	UNP P01116
A	-4	LEU	-	expression tag	UNP P01116
A	-3	TYR	-	expression tag	UNP P01116
A	-2	PHE	-	expression tag	UNP P01116
A	-1	GLN	-	expression tag	UNP P01116
A	0	GLY	-	expression tag	UNP P01116
A	12	ASP	GLY	variant	UNP P01116
A	51	SER	CYS	conflict	UNP P01116
A	80	LEU	CYS	conflict	UNP P01116
A	118	SER	CYS	conflict	UNP P01116
B	-17	MET	-	initiating methionine	UNP P01116
B	-16	HIS	-	expression tag	UNP P01116
B	-15	HIS	-	expression tag	UNP P01116

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	expression tag	UNP P01116
B	-13	HIS	-	expression tag	UNP P01116
B	-12	HIS	-	expression tag	UNP P01116
B	-11	HIS	-	expression tag	UNP P01116
B	-10	SER	-	expression tag	UNP P01116
B	-9	SER	-	expression tag	UNP P01116
B	-8	GLY	-	expression tag	UNP P01116
B	-7	ARG	-	expression tag	UNP P01116
B	-6	GLU	-	expression tag	UNP P01116
B	-5	ASN	-	expression tag	UNP P01116
B	-4	LEU	-	expression tag	UNP P01116
B	-3	TYR	-	expression tag	UNP P01116
B	-2	PHE	-	expression tag	UNP P01116
B	-1	GLN	-	expression tag	UNP P01116
B	0	GLY	-	expression tag	UNP P01116
B	12	ASP	GLY	variant	UNP P01116
B	51	SER	CYS	conflict	UNP P01116
B	80	LEU	CYS	conflict	UNP P01116
B	118	SER	CYS	conflict	UNP P01116

- Molecule 2 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).
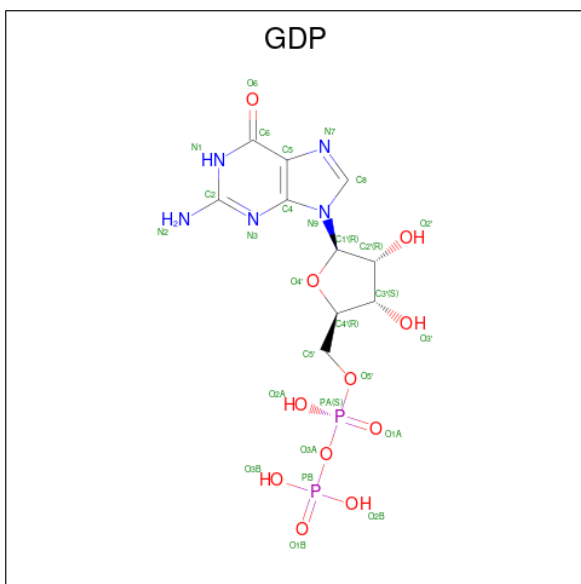
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	28	10	5	11	2	0	0

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

- Molecule 3 is MAGNESIUM ION (three-letter code: 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-{(1R,5S)-3-[(7P)-7-(8-ethynylnaphthalen-1-yl)-8-fluoro-2-{[(4s,7as)-tetrahydro-1H-pyrrolizin-7a(5H)-yl]methoxy}pyrido[4,3-d]pyrimidin-4-yl]-3,8-diazabicyclo[3.2.1]octan-8-yl}-4-oxobutanoic acid (three-letter code: Y63) (formula: $C_{37}H_{37}FN_6O_4$) (labeled as "Ligand of Interest" by depositor).
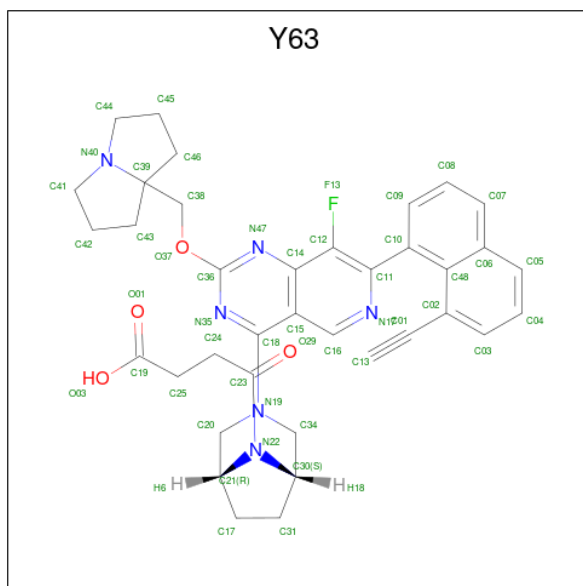
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	F	N	O	0	0
			48	37	1	6	4		
4	B	1	Total	C	F	N	O	0	0
			48	37	1	6	4		

- Molecule 5 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	167	Total 167	O 167	0	0
5	B	170	Total 170	O 170	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: GTPase KRas

Chain A:

• Molecule 1: GTPase KRas

Chain B:
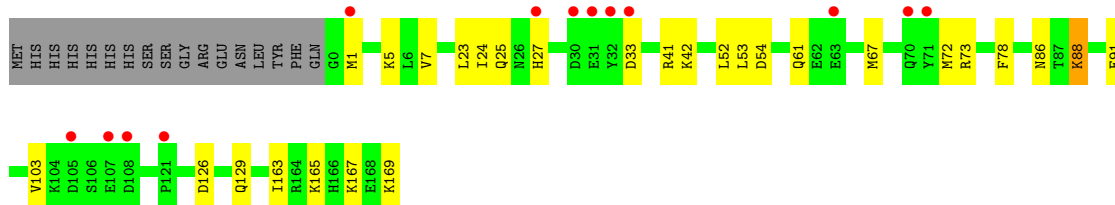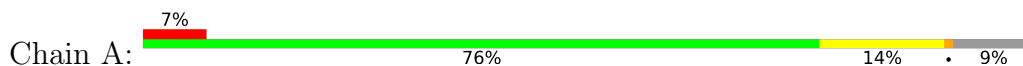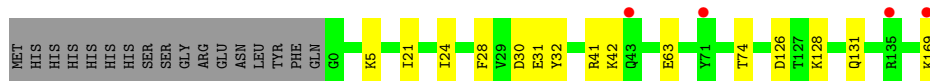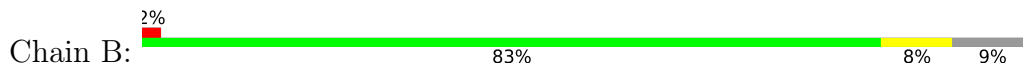
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	41.32Å　65.84Å　60.85Å 90.00°　101.75°　90.00°	Depositor
Resolution (Å)	59.57　–　1.47 59.57　–　1.47	Depositor EDS
% Data completeness (in resolution range)	99.1 (59.57-1.47) 99.1 (59.57-1.47)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.58 (at 1.46Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.190　,　0.211 0.188　,　0.211	Depositor DCC
R_{free} test set	2753 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	18.2	Xtriage
Anisotropy	0.443	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 41.4	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	3211	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.98% 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, GDP, Y63

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	0.41	0/1381	0.67	0/1862
1	B	0.41	0/1381	0.68	0/1862
All	All	0.41	0/2762	0.68	0/3724

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	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	41	ARG	Sidechain

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	1343	22	0
1	B	1360	0	1343	10	0
2	A	28	0	12	0	0
2	B	28	0	12	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	48	0	0	7	0
4	B	48	0	0	6	0
5	A	167	0	0	7	5
5	B	170	0	0	2	4
All	All	3211	0	2710	44	5

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 8.

All (44) 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)
4:A:203:Y63:N19	4:A:203:Y63:C20	1.79	1.46
4:B:203:Y63:N19	4:B:203:Y63:C20	1.77	1.45
4:B:203:Y63:N19	4:B:203:Y63:C34	1.79	1.42
4:A:203:Y63:N19	4:A:203:Y63:C34	1.80	1.40
1:A:5:LYS:NZ	5:A:302:HOH:O	1.97	0.92
1:A:91:GLU:OE1	5:A:301:HOH:O	1.95	0.82
1:A:126:ASP:HB3	1:A:129:GLN:HG3	1.63	0.80
1:A:67:MET:HG2	5:A:424:HOH:O	1.90	0.69
4:B:203:Y63:C20	4:B:203:Y63:C18	2.71	0.66
4:A:203:Y63:C20	4:A:203:Y63:C18	2.74	0.63
4:A:203:Y63:C34	4:A:203:Y63:C18	2.74	0.61
1:B:31:GLU:OE1	5:B:301:HOH:O	2.16	0.61
1:A:88:LYS:HE2	1:A:88:LYS:H	1.68	0.59
4:B:203:Y63:C34	4:B:203:Y63:C18	2.77	0.59
4:B:203:Y63:C20	4:B:203:Y63:C34	2.80	0.59
4:A:203:Y63:C20	4:A:203:Y63:C34	2.79	0.59
1:A:41:ARG:NH2	5:A:308:HOH:O	2.37	0.57
1:B:169:LYS:HA	1:B:169:LYS:HE2	1.87	0.56
1:A:61:GLN:HG3	5:A:410:HOH:O	2.05	0.56
1:A:24:ILE:HD13	1:A:42:LYS:HB2	1.88	0.55
1:A:165:LYS:O	1:A:169:LYS:HD3	2.07	0.54
1:B:131:GLN:NE2	5:B:306:HOH:O	2.42	0.52
1:B:24:ILE:HD13	1:B:42:LYS:HB2	1.92	0.50
1:B:126:ASP:OD2	1:B:128:LYS:HG3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:GLU:CD	5:A:301:HOH:O	2.43	0.49
1:A:25:GLN:O	1:A:27:HIS:HD2	1.95	0.49
1:A:88:LYS:HD3	5:A:340:HOH:O	2.13	0.47
1:B:28:PHE:CE2	1:B:30:ASP:HB3	2.50	0.47
1:B:169:LYS:HE2	1:B:169:LYS:CA	2.44	0.47
1:A:5:LYS:HD2	1:A:54:ASP:O	2.16	0.46
1:A:86:ASN:OD1	1:A:88:LYS:HE2	2.16	0.45
4:B:203:Y63:C01	4:B:203:Y63:C11	2.95	0.45
1:A:163:ILE:HG22	1:A:167:LYS:HD2	1.99	0.44
1:A:73:ARG:NE	1:A:103:VAL:O	2.50	0.44
1:B:21:ILE:HD11	1:B:32:TYR:CD1	2.53	0.44
1:A:41:ARG:NH1	1:A:54:ASP:OD1	2.51	0.43
1:A:72:MET:HG3	4:A:203:Y63:C05	2.49	0.43
1:B:5:LYS:HE2	1:B:74:THR:O	2.17	0.43
1:B:21:ILE:HD11	1:B:32:TYR:CE1	2.53	0.42
1:A:23:LEU:HD11	1:A:53:LEU:HD12	2.02	0.42
4:A:203:Y63:C01	4:A:203:Y63:C11	2.98	0.42
1:A:88:LYS:HE2	1:A:88:LYS:HB2	1.77	0.41
1:A:7:VAL:HB	1:A:78:PHE:CD2	2.56	0.41
1:A:1:MET:SD	1:A:52:LEU:HB2	2.61	0.40

All (5) 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:446:HOH:O	5:B:414:HOH:O[2_556]	1.92	0.28
5:A:401:HOH:O	5:B:423:HOH:O[1_554]	1.95	0.25
5:A:406:HOH:O	5:A:433:HOH:O[2_546]	2.11	0.09
5:A:462:HOH:O	5:B:432:HOH:O[1_554]	2.11	0.09
5:A:429:HOH:O	5:B:447:HOH:O[2_657]	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	168/187 (90%)	163 (97%)	4 (2%)	1 (1%)	25	7
1	B	168/187 (90%)	167 (99%)	1 (1%)	0	100	100
All	All	336/374 (90%)	330 (98%)	5 (2%)	1 (0%)	41	18

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	33	ASP

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	150/166 (90%)	149 (99%)	1 (1%)	84	68
1	B	150/166 (90%)	149 (99%)	1 (1%)	84	68
All	All	300/332 (90%)	298 (99%)	2 (1%)	84	68

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	88	LYS
1	B	63	GLU

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	27	HIS
1	B	27	HIS
1	B	131	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 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	$\#|Z| > 2$
4	Y63	B	203	1	53,55,55	4.68	16 (30%)	63,82,82	1.83	14 (22%)
2	GDP	B	201	3	24,30,30	0.99	2 (8%)	30,47,47	1.05	3 (10%)
4	Y63	A	203	1	53,55,55	4.78	14 (26%)	63,82,82	2.03	16 (25%)
2	GDP	A	201	3	24,30,30	0.90	1 (4%)	30,47,47	1.09	3 (10%)

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
4	Y63	B	203	1	-	1/24/66/66	0/9/8/8
2	GDP	B	201	3	-	0/12/32/32	0/3/3/3
4	Y63	A	203	1	-	2/24/66/66	0/9/8/8
2	GDP	A	201	3	-	0/12/32/32	0/3/3/3

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	203	Y63	C34-N19	17.04	1.80	1.46
4	B	203	Y63	C34-N19	16.35	1.79	1.46
4	A	203	Y63	C20-N19	16.28	1.79	1.46
4	B	203	Y63	C20-N19	15.45	1.77	1.46
4	A	203	Y63	C30-N22	-14.40	1.29	1.47
4	B	203	Y63	C30-N22	-14.30	1.29	1.47
4	B	203	Y63	C21-N22	-14.17	1.29	1.47
4	A	203	Y63	C21-N22	-12.97	1.31	1.47
4	A	203	Y63	C02-C01	8.59	1.53	1.44
4	B	203	Y63	C02-C01	6.70	1.51	1.44
4	B	203	Y63	C23-N22	6.68	1.44	1.36
4	A	203	Y63	O37-C36	6.65	1.41	1.34
4	B	203	Y63	O37-C36	6.11	1.41	1.34
4	A	203	Y63	C23-N22	6.11	1.44	1.36
4	A	203	Y63	C39-N40	-4.80	1.43	1.49
4	B	203	Y63	C39-N40	-4.45	1.44	1.49
4	A	203	Y63	C31-C17	-3.98	1.43	1.54
4	B	203	Y63	C31-C17	-3.69	1.43	1.54
4	B	203	Y63	C02-C48	-3.47	1.39	1.44
4	A	203	Y63	C18-N19	3.19	1.46	1.37
4	A	203	Y63	C12-C14	-3.14	1.33	1.41
4	B	203	Y63	C18-N19	3.04	1.46	1.37
4	A	203	Y63	C15-C14	-2.94	1.35	1.42
4	B	203	Y63	C16-N17	2.89	1.38	1.32
4	A	203	Y63	C16-N17	2.72	1.38	1.32
4	B	203	Y63	C12-C14	-2.60	1.35	1.41
4	B	203	Y63	C15-C14	-2.56	1.36	1.42
4	A	203	Y63	C02-C48	-2.50	1.40	1.44
2	B	201	GDP	C6-N1	-2.42	1.34	1.37
4	B	203	Y63	C10-C48	-2.24	1.40	1.43
2	B	201	GDP	O4'-C1'	2.08	1.44	1.41
4	B	203	Y63	C17-C21	2.08	1.58	1.53
2	A	201	GDP	C6-N1	-2.04	1.34	1.37

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	203	Y63	C44-N40-C41	-6.10	106.67	115.25
4	B	203	Y63	C44-N40-C41	-5.39	107.68	115.25
4	A	203	Y63	C10-C11-N17	4.70	124.75	115.52
4	B	203	Y63	C10-C11-N17	4.34	124.04	115.52
4	A	203	Y63	C10-C11-C12	-4.24	113.17	123.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	203	Y63	C34-N19-C20	-4.09	102.08	113.42
4	A	203	Y63	C07-C06-C05	-3.98	113.87	123.19
4	B	203	Y63	C10-C11-C12	-3.98	113.79	123.26
4	B	203	Y63	C03-C02-C01	-3.93	116.17	119.95
4	A	203	Y63	C21-C20-N19	3.83	114.56	109.57
4	B	203	Y63	C18-C15-C14	3.70	120.88	116.20
4	A	203	Y63	C17-C21-C20	-3.59	108.34	111.63
4	B	203	Y63	C34-N19-C20	-3.46	103.84	113.42
4	B	203	Y63	C46-C39-N40	3.37	109.62	102.49
4	A	203	Y63	C46-C39-N40	3.33	109.54	102.49
4	B	203	Y63	C07-C06-C05	-3.15	115.83	123.19
4	A	203	Y63	C24-C25-C19	-3.13	106.88	113.60
4	A	203	Y63	C43-C39-N40	3.02	108.89	102.49
4	A	203	Y63	C18-C15-C14	3.00	119.99	116.20
4	A	203	Y63	C30-C34-N19	2.77	113.18	109.57
2	A	201	GDP	C8-N7-C5	2.77	108.27	102.99
4	A	203	Y63	C43-C39-C46	-2.61	109.09	113.55
4	B	203	Y63	C43-C39-N40	2.60	108.00	102.49
4	B	203	Y63	C21-C20-N19	2.57	112.91	109.57
4	A	203	Y63	C05-C06-C48	2.54	123.37	118.27
4	A	203	Y63	C34-C30-N22	2.52	112.01	108.77
4	B	203	Y63	C24-C25-C19	-2.35	108.55	113.60
2	A	201	GDP	PA-O3A-PB	-2.35	124.77	132.83
2	B	201	GDP	C5-C6-N1	2.30	118.01	113.95
4	B	203	Y63	C20-C21-N22	2.26	111.67	108.77
2	B	201	GDP	C8-N7-C5	2.24	107.25	102.99
4	A	203	Y63	C07-C06-C48	2.24	122.75	118.27
2	B	201	GDP	O3'-C3'-C4'	-2.21	104.66	111.05
4	B	203	Y63	C17-C21-C20	-2.10	109.70	111.63
4	B	203	Y63	O29-C23-N22	-2.06	120.12	122.29
2	A	201	GDP	C5-C6-N1	2.02	117.51	113.95

There are no chirality outliers.
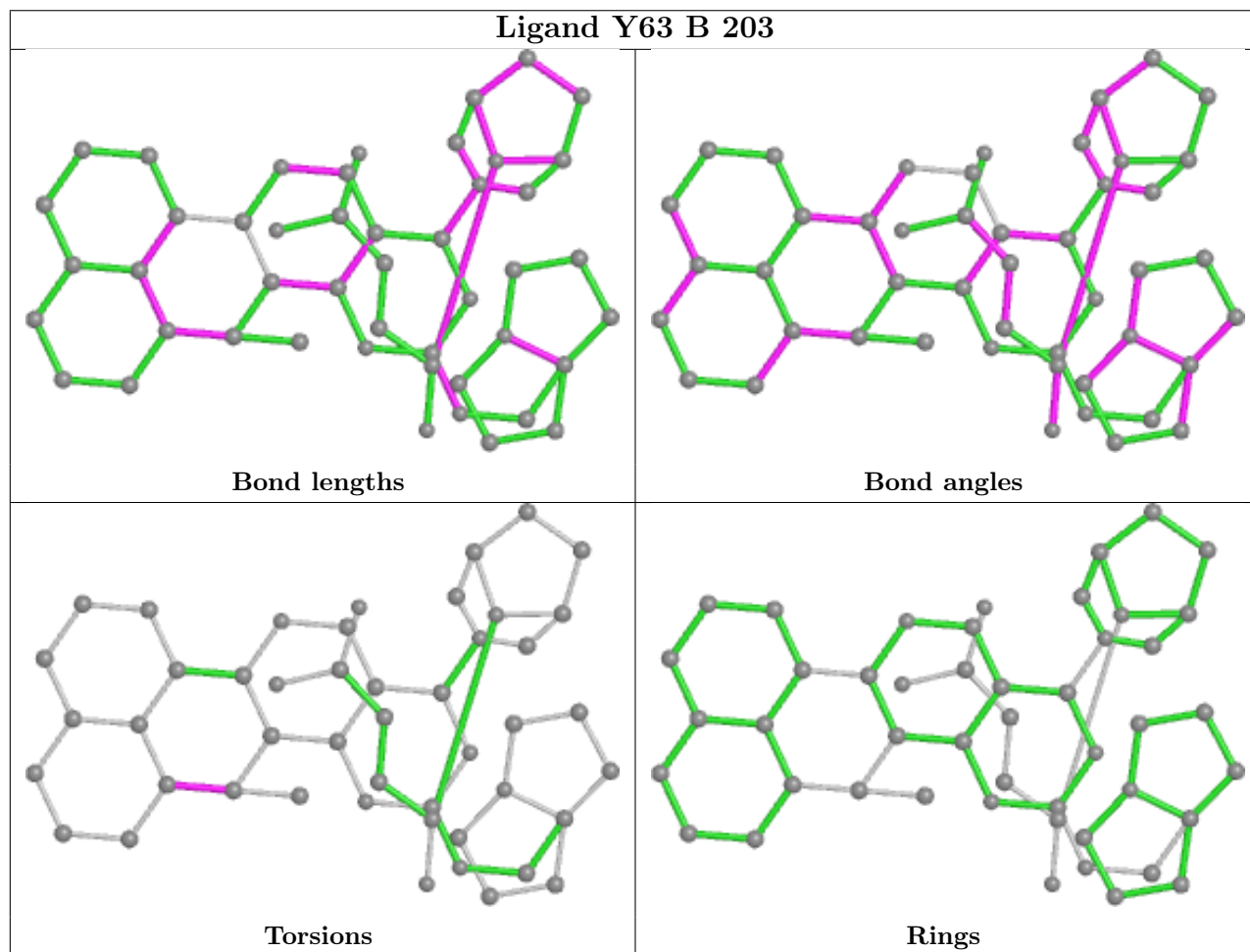
All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	203	Y63	O03-C19-C25-C24
4	A	203	Y63	O01-C19-C25-C24
4	B	203	Y63	C13-C01-C02-C03

There are no ring outliers.
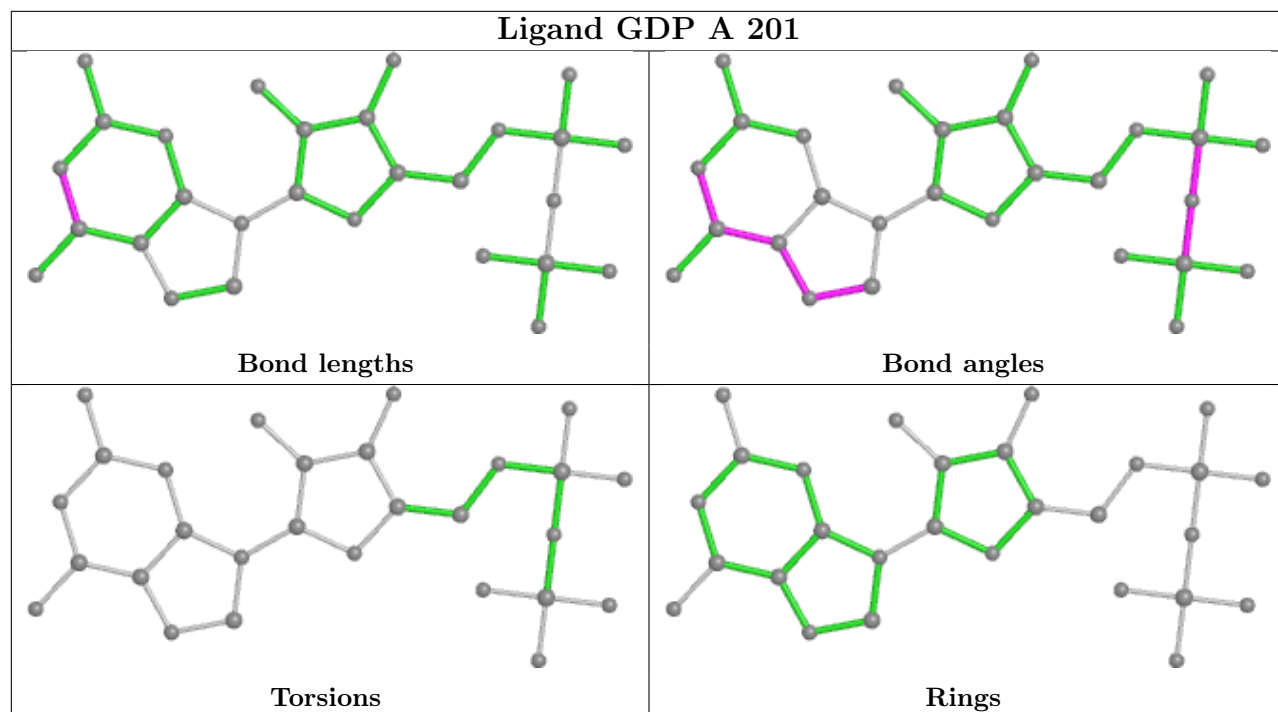
2 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	203	Y63	6	0
4	A	203	Y63	7	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 Y63 B 203

Bond lengths

Bond angles

Torsions

Rings

Ligand GDP B 201

Bond lengths

Bond angles

Torsions

Rings

Ligand Y63 A 203

Bond lengths

Bond angles

Torsions

Rings

Ligand GDP A 201
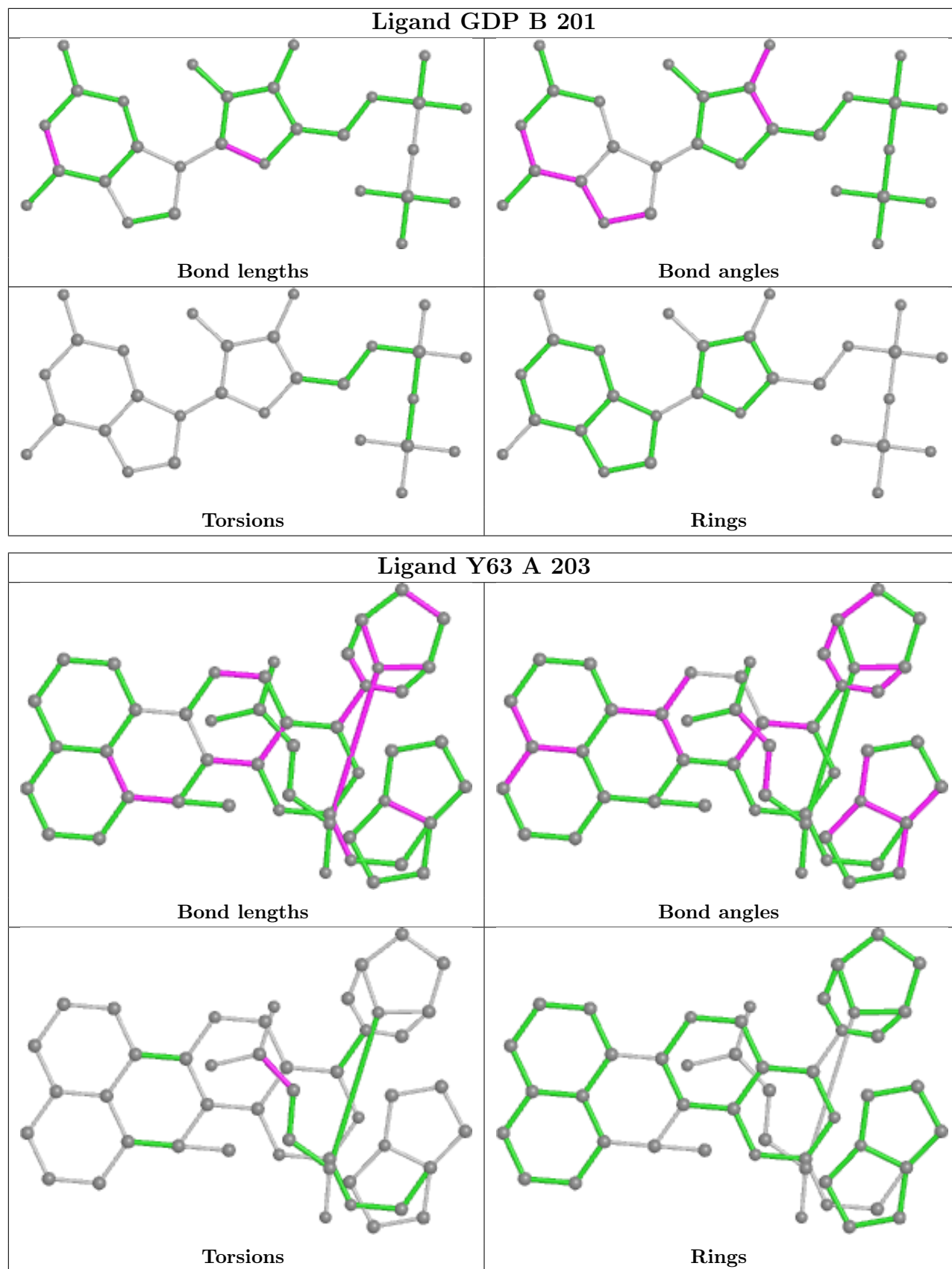
5.7 Other polymers (i)

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, 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	170/187 (90%)	0.65	13 (7%)	13	15	13, 21, 36, 48	0
1	B	170/187 (90%)	0.47	4 (2%)	59	63	11, 21, 32, 35	0
All	All	340/374 (90%)	0.56	17 (5%)	28	31	11, 21, 34, 48	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	33	ASP	5.4
1	A	31	GLU	5.3
1	A	105	ASP	4.5
1	A	71	TYR	3.9
1	B	169	LYS	2.9
1	B	71	TYR	2.8
1	A	107	GLU	2.8
1	A	27	HIS	2.6
1	B	43	GLN	2.5
1	A	63	GLU	2.4
1	B	135	ARG	2.3
1	A	32	TYR	2.3
1	A	121	PRO	2.1
1	A	1	MET	2.0
1	A	70	GLN	2.0
1	A	108	ASP	2.0
1	A	30	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

W O R L D W I D E
wwPDB
PROTEIN DATA BANK

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
4	Y63	A	203	48/48	0.87	0.12	17,21,30,47	0
4	Y63	B	203	48/48	0.91	0.11	14,17,27,39	0
2	GDP	A	201	28/28	0.97	0.09	14,18,24,28	0
2	GDP	B	201	28/28	0.97	0.09	11,14,19,22	0
3	MG	A	202	1/1	0.98	0.07	16,16,16,16	0
3	MG	B	202	1/1	1.00	0.08	12,12,12,12	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.
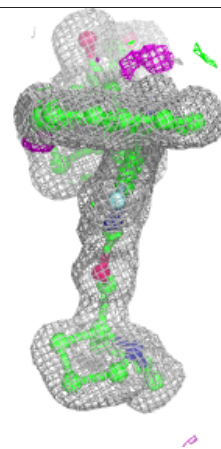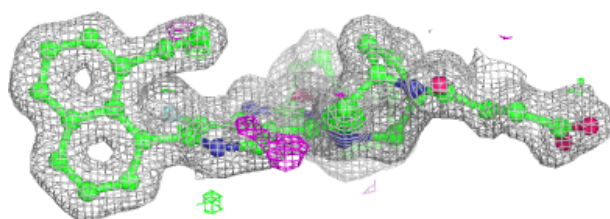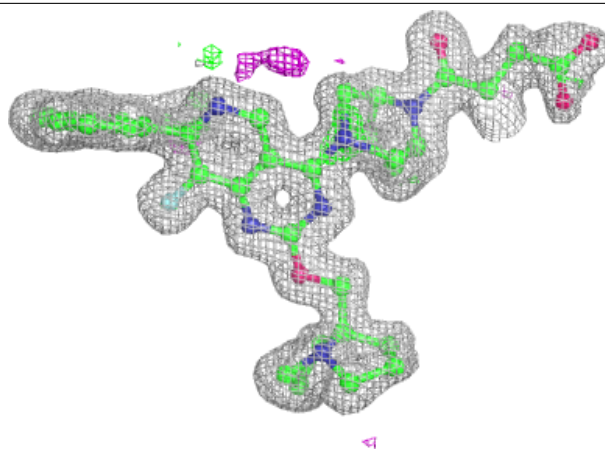
Electron density around Y63 A 203:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
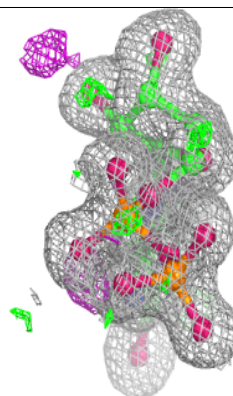mF_o-DF_c (at 3 rmsd) in purple (negative)
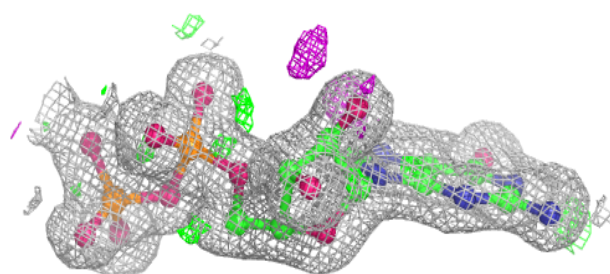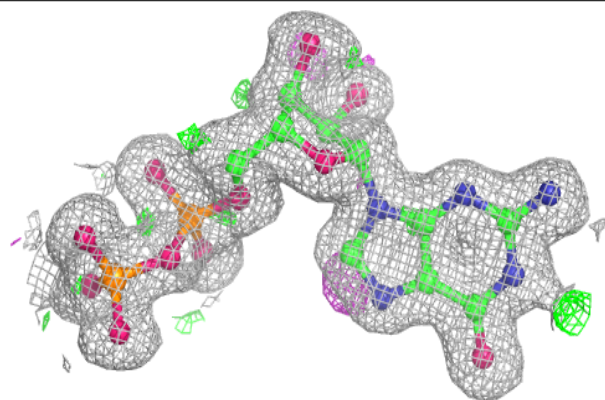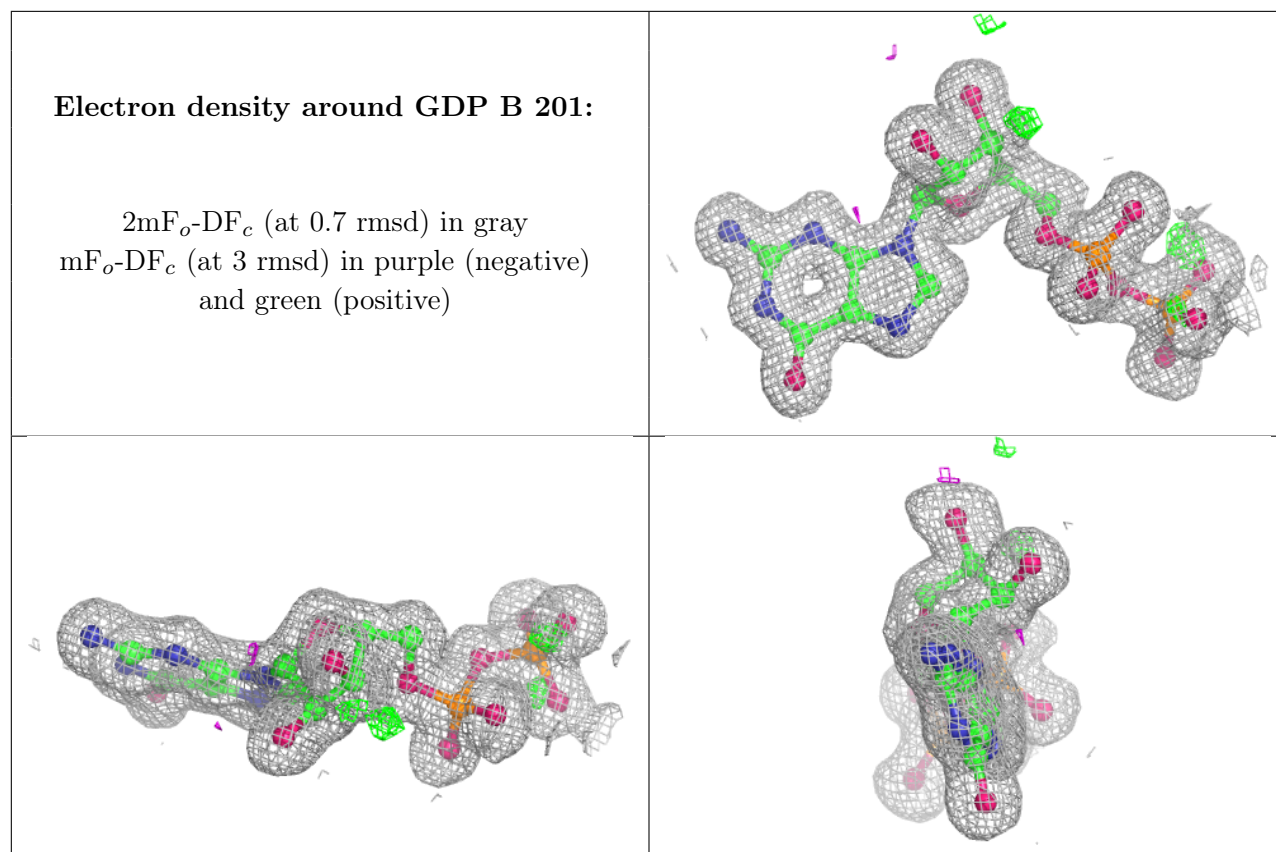and green (positive)
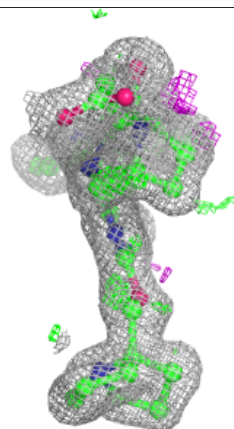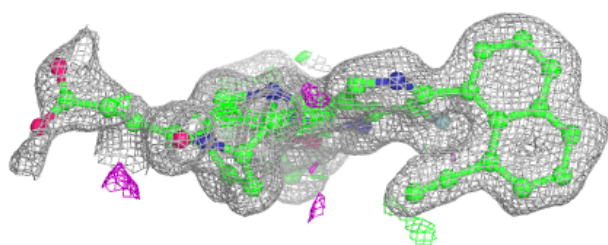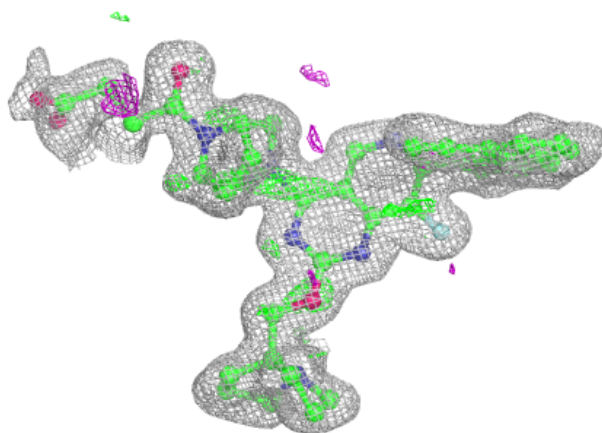
Electron density around Y63 B 203:

$2mF_o$-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 ⓘ

There are no such residues in this entry.