Full wwPDB X-ray Structure Validation Report ⓘ

Oct 28, 2024 – 06:25 PM EDT

PDB ID	:	9BHP
Title	:	Crystal structure of KRAS G12C in a transition state mimetic complex with CYPA and RMC-7977
Authors	:	Pourfarjam, Y.; Goldgur, Y.; Cuevas-Navarro, A.; Lito, P.
Deposited on	:	2024-04-21
Resolution	:	2.10 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:

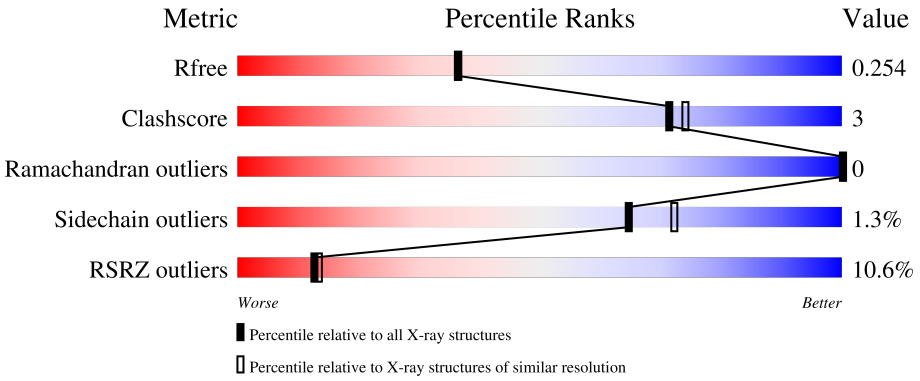
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 2.10 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	6234 (2.10-2.10)
Clashscore	180529	6893 (2.10-2.10)
Ramachandran outliers	177936	6839 (2.10-2.10)
Sidechain outliers	177891	6840 (2.10-2.10)
RSRZ outliers	164620	6234 (2.10-2.10)

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	B	166	93% 5%
1	D	166	89% 9%
2	A	170	91% 8%
2	C	170	38% 87% 11%

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	ZNI	B	201	X	-	-	-
3	ZNI	D	201	X	-	-	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 5513 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 Peptidyl-prolyl cis-trans isomerase A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	163	Total	C	N	O	S	0	0	0
			1248	792	216	232	8			
1	B	163	Total	C	N	O	S	0	0	0
			1248	792	216	232	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	0	GLY	-	expression tag	UNP P62937
B	0	GLY	-	expression tag	UNP P62937

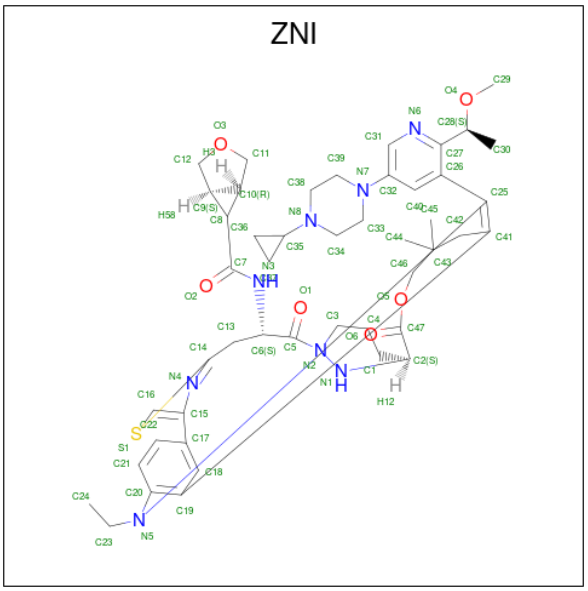
- Molecule 2 is a protein called Isoform 2B of GTPase KRas.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	168	Total	C	N	O	S	0	0	0
			1338	837	230	263	8			
2	C	167	Total	C	N	O	S	0	0	0
			1223	763	207	245	8			

There are 4 discrepancies between the modelled and reference sequences:

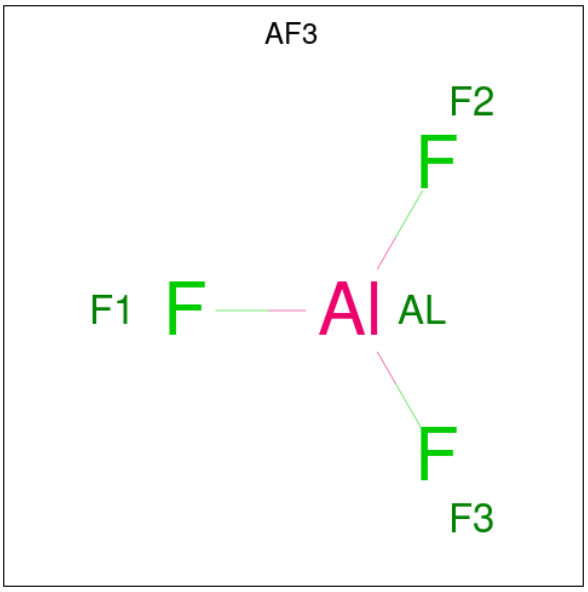
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP P01116
A	12	CYS	GLY	engineered mutation	UNP P01116
C	0	GLY	-	expression tag	UNP P01116
C	12	CYS	GLY	engineered mutation	UNP P01116

- Molecule 3 is (1R,5S,6r)-N-[(1P,7S,9S,13S,20M)-20-{5-(4-cyclopropylpiperazin-1-yl)-2-[(1S)-1-methoxyethyl]pyridin-3-yl}-21-ethyl-17,17-dimethyl-8,14-dioxo-15-oxa-4-thia-9,21,27,28-tetraazapentacyclo[17.5.2.1 2,5 .1 9,13 .0 22,26]octacosa-1(24),2,5(28),19,22,25-hexaen-7-yl]-3-oxabicyclo[3.1.0]hexane-6-carboxamide (three-letter code: ZNI) (formula: $C_{47}H_{60}N_8O_6S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	D	1	Total	C	N	O	S	0	0
			62	47	8	6	1		
3	B	1	Total	C	N	O	S	0	0
			62	47	8	6	1		

- Molecule 4 is ALUMINUM FLUORIDE (three-letter code: AF3) (formula: AlF_3) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Al	F	0	0
			4	1	3		

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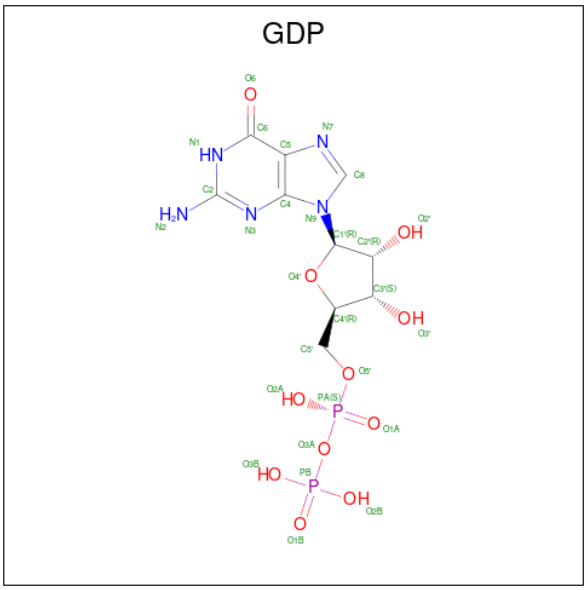
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total Al F 4 1 3	0	0

- Molecule 5 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



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

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	D	69	Total O 69 69	0	0

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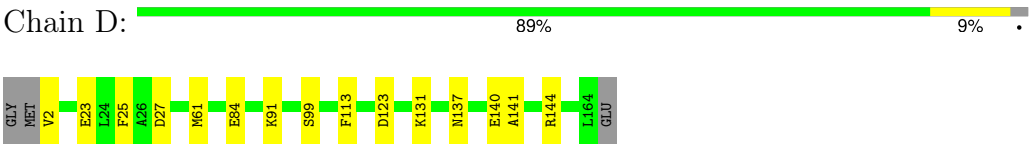
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	74	Total O 74 74	0	0
7	B	83	Total O 83 83	0	0
7	C	40	Total O 40 40	0	0

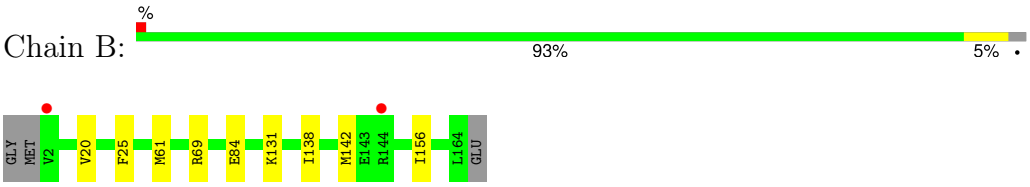
3 Residue-property plots (i)

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.

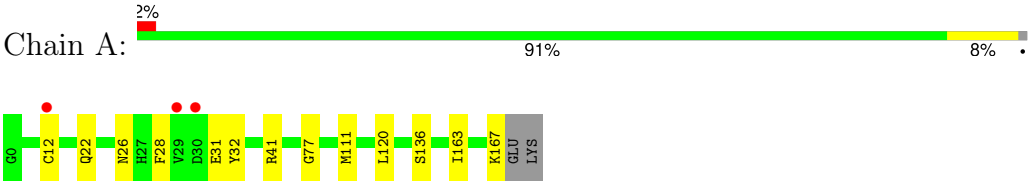
• Molecule 1: Peptidyl-prolyl cis-trans isomerase A



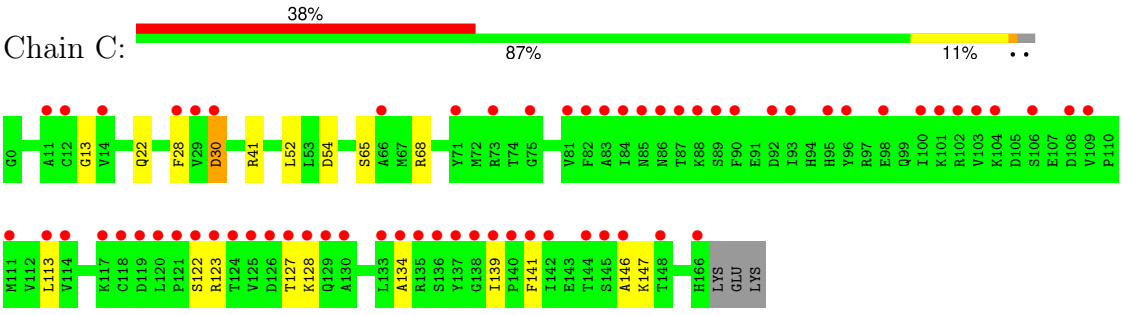
• Molecule 1: Peptidyl-prolyl cis-trans isomerase A



• Molecule 2: Isoform 2B of GTPase KRas



• Molecule 2: Isoform 2B of GTPase KRas



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	65.46Å 82.65Å 127.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.81 – 2.10 29.81 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.5 (29.81-2.10) 98.5 (29.81-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.14 (at 2.10Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.210 , 0.253 0.210 , 0.254	Depositor DCC
R_{free} test set	2084 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	30.7	Xtriage
Anisotropy	0.413	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 42.5	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	0.94	EDS
Total number of atoms	5513	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.62% 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: GDP, ZNI, MG, AF3

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	B	0.28	0/1276	0.52	0/1711
1	D	0.28	0/1276	0.52	0/1711
2	A	0.25	0/1359	0.52	0/1833
2	C	0.25	0/1240	0.49	0/1685
All	All	0.26	0/5151	0.51	0/6940

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	B	1248	0	1219	6	0
1	D	1248	0	1219	9	0
2	A	1338	0	1318	7	0
2	C	1223	0	1124	11	0
3	B	62	0	0	0	0
3	D	62	0	0	0	0
4	A	4	0	0	0	0
4	C	4	0	0	0	0
5	A	28	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	28	0	12	1	0
6	A	1	0	0	0	0
6	C	1	0	0	0	0
7	A	74	0	0	1	0
7	B	83	0	0	0	0
7	C	40	0	0	0	0
7	D	69	0	0	1	0
All	All	5513	0	4904	32	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 3.

All (32) 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)
2:C:41:ARG:HD2	2:C:52:LEU:HD11	1.70	0.72
2:A:41:ARG:NH2	7:A:301:HOH:O	2.23	0.71
1:D:2:VAL:N	7:D:301:HOH:O	2.33	0.61
1:D:25:PHE:HZ	1:D:131:LYS:HD3	1.65	0.61
1:B:25:PHE:CZ	1:B:131:LYS:HG2	2.38	0.59
1:B:25:PHE:HZ	1:B:131:LYS:HG2	1.66	0.59
2:A:12:CYS:SG	2:A:32:TYR:OH	2.61	0.58
1:D:84:GLU:H	1:D:84:GLU:CD	2.07	0.56
1:D:141:ALA:O	1:D:144:ARG:HG3	2.07	0.54
2:C:30:ASP:OD1	2:C:30:ASP:N	2.37	0.54
2:C:65:SER:O	2:C:68:ARG:HD2	2.10	0.52
2:A:31:GLU:HG2	1:B:69:ARG:NH1	2.24	0.52
2:C:13:GLY:HA2	5:C:202:GDP:H5'	1.91	0.52
2:C:22:GLN:NE2	2:C:146:ALA:O	2.43	0.51
2:C:134:ALA:HB1	2:C:139:ILE:O	2.12	0.50
1:D:23:GLU:OE1	1:D:131:LYS:NZ	2.46	0.49
2:C:41:ARG:NE	2:C:54:ASP:OD2	2.35	0.49
1:D:137:ASN:HA	1:D:140:GLU:OE2	2.15	0.47
2:C:122:SER:OG	2:C:123:ARG:N	2.50	0.45
1:B:84:GLU:H	1:B:84:GLU:CD	2.21	0.45
2:C:123:ARG:NH2	2:C:127:THR:OG1	2.50	0.44
1:D:91:LYS:HD2	1:D:123:ASP:HB3	2.00	0.43
2:A:120:LEU:HD23	2:A:120:LEU:HA	1.89	0.42
2:A:111:MET:HE3	2:A:111:MET:HB3	1.74	0.42
2:A:22:GLN:HE21	2:A:28:PHE:HB2	1.84	0.42
1:B:20:VAL:HG22	1:B:138:ILE:HB	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:99:SER:HB3	1:D:113:PHE:CZ	2.55	0.41
2:A:77:GLY:HA3	2:A:163:ILE:HD11	2.03	0.41
2:C:28:PHE:CD2	2:C:147:LYS:HD3	2.56	0.41
2:C:113:LEU:O	2:C:141:PHE:HA	2.21	0.40
1:B:142:MET:HG2	1:B:156:ILE:HG21	2.03	0.40
1:D:27:ASP:OD2	1:D:27:ASP:N	2.54	0.40

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	B	161/166 (97%)	158 (98%)	3 (2%)	0	100	100
1	D	161/166 (97%)	155 (96%)	6 (4%)	0	100	100
2	A	166/170 (98%)	164 (99%)	2 (1%)	0	100	100
2	C	165/170 (97%)	159 (96%)	6 (4%)	0	100	100
All	All	653/672 (97%)	636 (97%)	17 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	B	131/133 (98%)	130 (99%)	1 (1%)	79	84
1	D	131/133 (98%)	130 (99%)	1 (1%)	79	84
2	A	148/150 (99%)	145 (98%)	3 (2%)	50	57
2	C	121/150 (81%)	119 (98%)	2 (2%)	56	63
All	All	531/566 (94%)	524 (99%)	7 (1%)	65	72

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	61	MET
2	A	26	ASN
2	A	136	SER
2	A	167	LYS
1	B	61	MET
2	C	30	ASP
2	C	128	LYS

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

Mol	Chain	Res	Type
2	A	25	GLN
2	A	70	GLN
2	A	95	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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	ZNI	D	201	-	63,71,71	3.41	22 (34%)	73,107,107	3.00	32 (43%)
4	AF3	A	201	-	0,3,3	-	-	-		
4	AF3	C	201	-	0,3,3	-	-	-		
5	GDP	A	202	6	25,30,30	3.80	12 (48%)	30,47,47	1.28	4 (13%)
5	GDP	C	202	6	25,30,30	3.87	15 (60%)	30,47,47	1.54	4 (13%)
3	ZNI	B	201	-	63,71,71	2.83	22 (34%)	73,107,107	2.96	33 (45%)

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	ZNI	D	201	-	1/1/14/16	9/55/96/96	0/8/10/10
5	GDP	C	202	6	-	0/12/32/32	0/3/3/3
3	ZNI	B	201	-	1/1/14/16	12/55/96/96	0/8/10/10
5	GDP	A	202	6	-	3/12/32/32	0/3/3/3

All (71) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	201	ZNI	C42-C43	12.96	1.60	1.55
3	B	201	ZNI	C42-C43	12.04	1.60	1.55
3	D	201	ZNI	C26-C25	11.01	1.62	1.48
5	C	202	GDP	C2'-C3'	-10.76	1.24	1.53
5	A	202	GDP	C2'-C3'	-10.63	1.24	1.53
3	D	201	ZNI	C13-C14	8.76	1.55	1.49
3	D	201	ZNI	C17-C15	7.87	1.61	1.49
5	C	202	GDP	O4'-C1'	-7.61	1.30	1.40
3	B	201	ZNI	C13-C14	7.47	1.54	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	202	GDP	O6-C6	7.40	1.40	1.23
5	A	202	GDP	O4'-C1'	-7.32	1.31	1.40
5	C	202	GDP	O6-C6	7.13	1.40	1.23
3	B	201	ZNI	C26-C25	6.79	1.57	1.48
3	D	201	ZNI	C41-C19	6.73	1.51	1.41
3	D	201	ZNI	C5-N2	6.44	1.44	1.35
3	B	201	ZNI	C41-C19	6.40	1.51	1.41
5	C	202	GDP	PA-O3A	5.46	1.65	1.59
3	B	201	ZNI	C5-N2	5.33	1.42	1.35
3	D	201	ZNI	C2-N1	5.30	1.52	1.47
5	A	202	GDP	PA-O3A	5.12	1.65	1.59
5	C	202	GDP	C2-N2	4.83	1.45	1.34
3	D	201	ZNI	C32-N7	4.83	1.52	1.38
5	A	202	GDP	C2-N2	4.81	1.45	1.34
3	B	201	ZNI	C17-C15	4.34	1.55	1.49
3	D	201	ZNI	C7-N3	4.13	1.42	1.34
5	C	202	GDP	C5'-C4'	-4.06	1.39	1.51
3	B	201	ZNI	C32-N7	3.91	1.49	1.38
5	A	202	GDP	C5'-C4'	-3.85	1.40	1.51
3	B	201	ZNI	N1-N2	-3.67	1.39	1.43
3	B	201	ZNI	C7-N3	3.49	1.41	1.34
3	D	201	ZNI	C15-N4	3.46	1.48	1.37
3	B	201	ZNI	C42-C41	3.45	1.56	1.52
3	D	201	ZNI	C40-C32	3.41	1.45	1.39
5	C	202	GDP	C3'-C4'	3.25	1.61	1.53
5	A	202	GDP	O3'-C3'	3.25	1.51	1.43
5	A	202	GDP	C3'-C4'	3.19	1.61	1.53
5	C	202	GDP	C5-C6	-3.19	1.41	1.47
5	C	202	GDP	O3'-C3'	3.18	1.50	1.43
5	A	202	GDP	C5-C6	-3.15	1.41	1.47
5	A	202	GDP	C6-N1	-3.12	1.33	1.37
5	C	202	GDP	C6-N1	-3.11	1.33	1.37
5	C	202	GDP	C1'-N9	-3.10	1.41	1.50
3	B	201	ZNI	C15-N4	3.09	1.47	1.37
3	D	201	ZNI	C42-C41	3.08	1.55	1.52
3	D	201	ZNI	C16-S1	3.05	1.75	1.70
3	B	201	ZNI	C2-N1	3.02	1.50	1.47
3	B	201	ZNI	C16-S1	2.89	1.75	1.70
3	D	201	ZNI	C33-N7	2.85	1.51	1.46
5	A	202	GDP	O4'-C4'	2.85	1.51	1.45
3	D	201	ZNI	C8-C10	2.82	1.56	1.51
3	B	201	ZNI	C40-C32	2.80	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	202	GDP	C1'-N9	-2.79	1.42	1.50
3	D	201	ZNI	C21-C20	2.78	1.46	1.41
5	C	202	GDP	O4'-C4'	2.74	1.51	1.45
3	D	201	ZNI	C22-C17	2.54	1.44	1.39
3	B	201	ZNI	C21-C20	2.50	1.45	1.41
3	D	201	ZNI	C39-N7	2.47	1.51	1.46
3	D	201	ZNI	C31-N6	2.46	1.39	1.34
3	D	201	ZNI	C26-C27	2.43	1.45	1.41
3	B	201	ZNI	C22-C17	2.41	1.44	1.39
3	B	201	ZNI	C8-C10	2.41	1.56	1.51
3	D	201	ZNI	C18-C19	2.36	1.46	1.42
3	B	201	ZNI	C26-C27	2.35	1.45	1.41
3	B	201	ZNI	C39-N7	2.28	1.50	1.46
3	B	201	ZNI	C31-N6	2.17	1.38	1.34
5	C	202	GDP	O2'-C2'	2.12	1.48	1.43
5	C	202	GDP	C2-N1	-2.10	1.32	1.37
3	D	201	ZNI	C40-C26	2.06	1.43	1.39
3	B	201	ZNI	C35-N8	-2.03	1.43	1.48
3	B	201	ZNI	C18-C19	2.02	1.46	1.42
5	C	202	GDP	C5-C4	-2.01	1.38	1.43

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	201	ZNI	C36-C35-N8	11.99	131.06	117.84
3	B	201	ZNI	C36-C35-N8	11.83	130.88	117.84
3	D	201	ZNI	C40-C32-C31	-10.57	110.39	119.67
3	B	201	ZNI	C40-C32-C31	-9.99	110.90	119.67
3	B	201	ZNI	C10-C8-C7	6.74	132.78	117.18
3	B	201	ZNI	C37-C35-N8	-6.62	110.54	117.84
3	D	201	ZNI	C37-C35-N8	-5.28	112.02	117.84
3	D	201	ZNI	C26-C40-C32	5.28	128.90	119.30
3	D	201	ZNI	C10-C8-C7	5.25	129.33	117.18
5	C	202	GDP	C4'-O4'-C1'	-5.14	105.21	109.92
3	B	201	ZNI	C31-C32-N7	5.06	129.49	121.80
3	D	201	ZNI	C9-C8-C7	4.96	128.67	117.18
3	B	201	ZNI	C26-C40-C32	4.95	128.30	119.30
3	D	201	ZNI	C31-C32-N7	4.89	129.22	121.80
3	D	201	ZNI	O5-C46-C43	4.65	117.23	109.25
3	D	201	ZNI	C13-C6-C5	-4.38	100.76	109.94
3	B	201	ZNI	C9-C8-C7	4.01	126.47	117.18
3	B	201	ZNI	O5-C46-C43	3.77	115.73	109.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	201	ZNI	C13-C6-C5	-3.75	102.09	109.94
5	A	202	GDP	C8-N7-C5	3.66	108.78	102.55
5	C	202	GDP	C8-N7-C5	3.62	108.72	102.55
3	D	201	ZNI	C8-C7-N3	3.61	123.00	114.82
3	D	201	ZNI	C31-N6-C27	3.61	124.72	118.88
3	D	201	ZNI	C13-C6-N3	3.59	118.28	110.83
3	D	201	ZNI	C21-C20-C19	-3.52	116.15	120.94
3	D	201	ZNI	C4-C1-C2	3.48	115.56	110.97
3	D	201	ZNI	O5-C47-C2	3.40	119.58	111.58
3	B	201	ZNI	C31-N6-C27	3.32	124.25	118.88
3	B	201	ZNI	O3-C11-C10	-3.25	101.79	106.27
5	A	202	GDP	C4'-O4'-C1'	-3.22	106.98	109.92
3	B	201	ZNI	O5-C47-C2	3.19	119.08	111.58
3	D	201	ZNI	C22-C17-C18	-3.14	112.82	118.03
3	B	201	ZNI	C4-C1-C2	3.08	115.03	110.97
3	B	201	ZNI	C14-C13-C6	-3.07	106.80	113.86
3	D	201	ZNI	O5-C47-O6	-3.06	118.54	124.14
3	B	201	ZNI	O5-C47-O6	-3.06	118.54	124.14
3	B	201	ZNI	C13-C6-N3	3.01	117.06	110.83
3	B	201	ZNI	C33-C34-N8	2.99	115.86	110.61
3	B	201	ZNI	C44-C43-C42	2.98	113.41	109.27
3	B	201	ZNI	C21-C20-C19	-2.92	116.97	120.94
3	D	201	ZNI	C17-C18-C19	2.71	128.01	122.18
5	C	202	GDP	C5-C6-N1	2.69	119.20	114.07
3	D	201	ZNI	O3-C11-C10	-2.68	102.56	106.27
3	D	201	ZNI	C22-C21-C20	2.63	123.62	119.82
3	D	201	ZNI	C44-C43-C42	2.63	112.92	109.27
3	D	201	ZNI	O2-C7-N3	-2.60	118.30	122.96
3	B	201	ZNI	C39-C38-N8	2.60	115.19	110.61
5	A	202	GDP	C5-C6-N1	2.55	118.93	114.07
3	B	201	ZNI	C34-N8-C35	-2.55	106.31	112.79
3	D	201	ZNI	C39-C38-N8	2.54	115.07	110.61
3	D	201	ZNI	C34-N8-C35	-2.53	106.35	112.79
3	B	201	ZNI	C39-N7-C33	-2.52	105.89	111.57
3	B	201	ZNI	C22-C17-C15	2.47	125.19	121.28
3	D	201	ZNI	C39-N7-C33	-2.47	106.02	111.57
3	B	201	ZNI	C22-C21-C20	2.45	123.36	119.82
3	B	201	ZNI	C22-C17-C18	-2.42	114.01	118.03
3	B	201	ZNI	C17-C18-C19	2.42	127.38	122.18
5	C	202	GDP	C2-N1-C6	-2.42	120.68	125.11
3	D	201	ZNI	C25-C26-C27	2.41	124.04	119.86
3	D	201	ZNI	C22-C17-C15	2.34	124.99	121.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	201	ZNI	C1-C4-C3	2.33	113.82	110.75
3	D	201	ZNI	C24-C23-N5	2.32	115.11	111.72
3	D	201	ZNI	C46-O5-C47	2.30	121.43	117.17
3	D	201	ZNI	C14-C13-C6	-2.29	108.60	113.86
3	B	201	ZNI	C40-C26-C25	2.25	121.83	118.75
3	D	201	ZNI	C40-C26-C25	2.24	121.81	118.75
3	B	201	ZNI	C6-N3-C7	2.24	126.45	121.65
3	B	201	ZNI	C8-C7-N3	2.23	119.87	114.82
5	A	202	GDP	C2-N1-C6	-2.22	121.04	125.11
3	B	201	ZNI	C18-C19-C20	-2.18	117.03	119.65
3	B	201	ZNI	O2-C7-N3	-2.09	119.21	122.96
3	D	201	ZNI	C38-N8-C35	2.09	118.10	112.79
3	B	201	ZNI	C25-C26-C27	2.08	123.46	119.86

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	D	201	ZNI	N2
3	B	201	ZNI	N2

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	201	ZNI	C14-C13-C6-N3
3	D	201	ZNI	C26-C27-C28-C30
3	D	201	ZNI	C26-C27-C28-O4
3	B	201	ZNI	C14-C13-C6-N3
3	B	201	ZNI	C26-C27-C28-C30
3	B	201	ZNI	C26-C27-C28-O4
3	D	201	ZNI	C14-C13-C6-C5
3	B	201	ZNI	C14-C13-C6-C5
3	D	201	ZNI	O6-C47-O5-C46
3	D	201	ZNI	C2-C47-O5-C46
3	B	201	ZNI	O6-C47-O5-C46
3	B	201	ZNI	C2-C47-O5-C46
3	D	201	ZNI	C27-C28-O4-C29
3	B	201	ZNI	C27-C28-O4-C29
5	A	202	GDP	PA-O3A-PB-O1B
3	B	201	ZNI	O2-C7-C8-C9
3	B	201	ZNI	N3-C7-C8-C9
3	B	201	ZNI	C30-C28-O4-C29
3	D	201	ZNI	C44-C43-C46-O5

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Mol	Chain	Res	Type	Atoms
5	A	202	GDP	PA-O3A-PB-O2B
5	A	202	GDP	PA-O3A-PB-O3B
3	B	201	ZNI	C31-C32-N7-C33
3	D	201	ZNI	C30-C28-O4-C29
3	B	201	ZNI	N6-C27-C28-O4

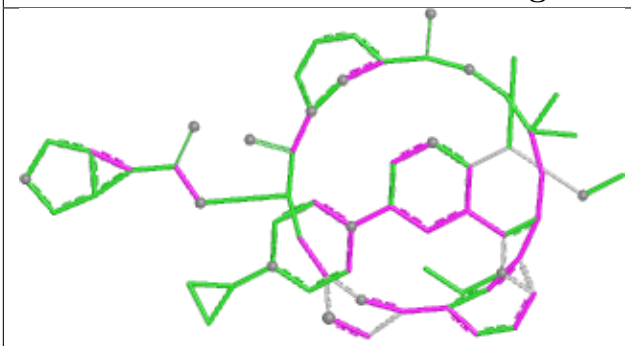
There are no ring outliers.

1 monomer is involved in 1 short contact:

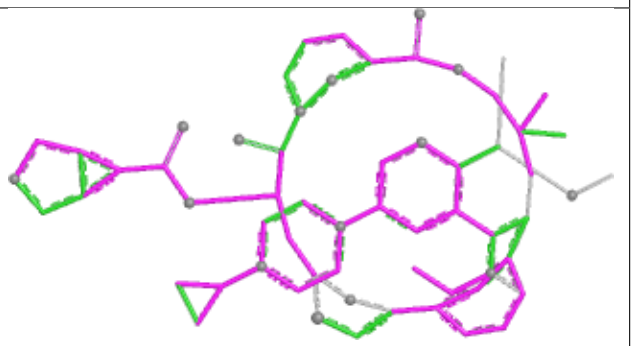
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	202	GDP	1	0

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.

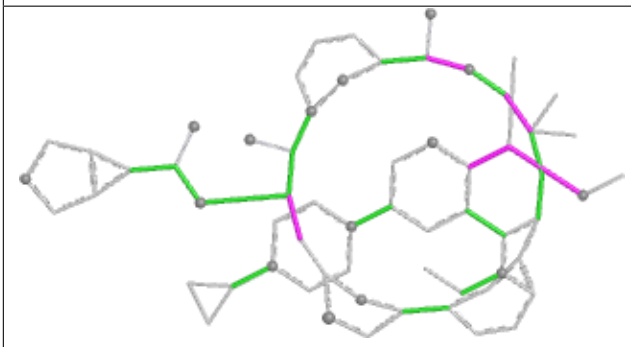
Ligand ZNI D 201



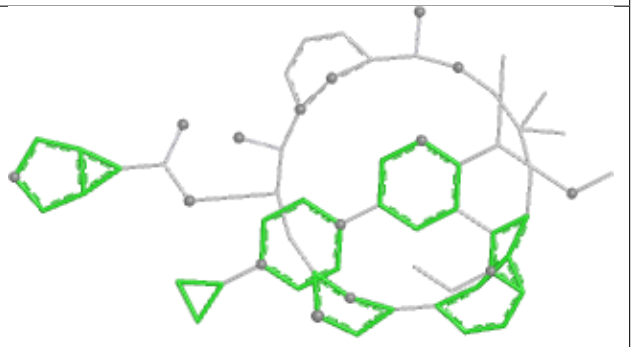
Bond lengths



Bond angles

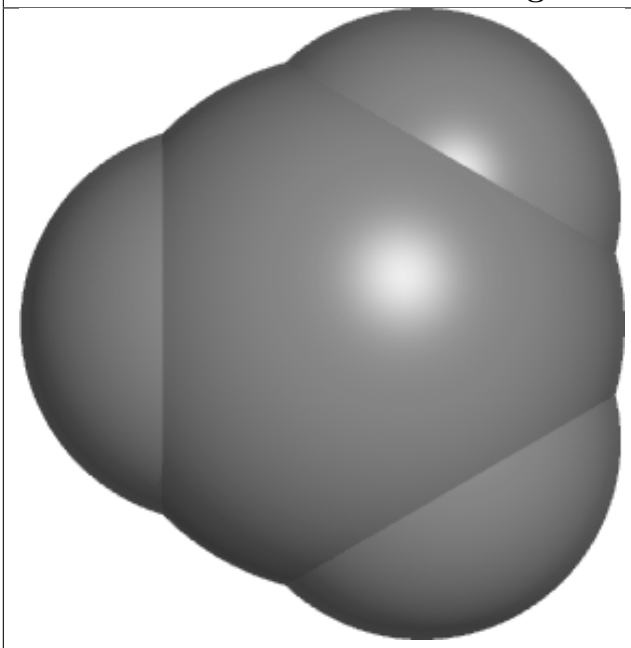


Torsions

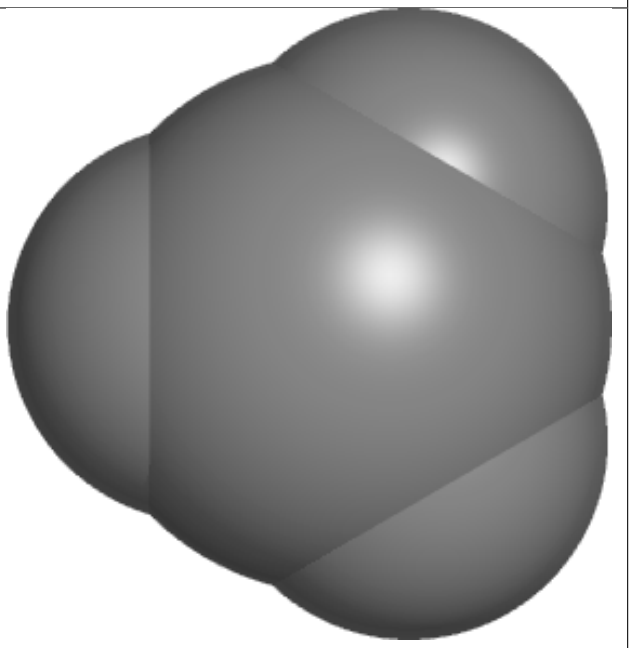


Rings

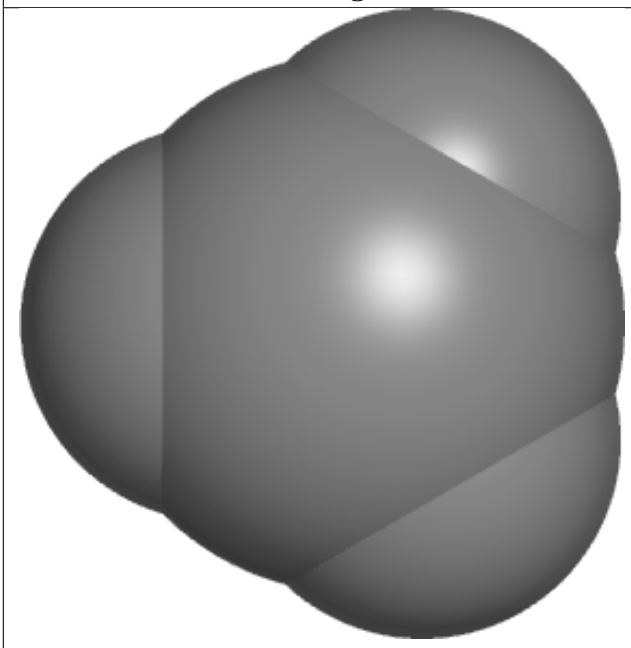
Ligand AF3 A 201



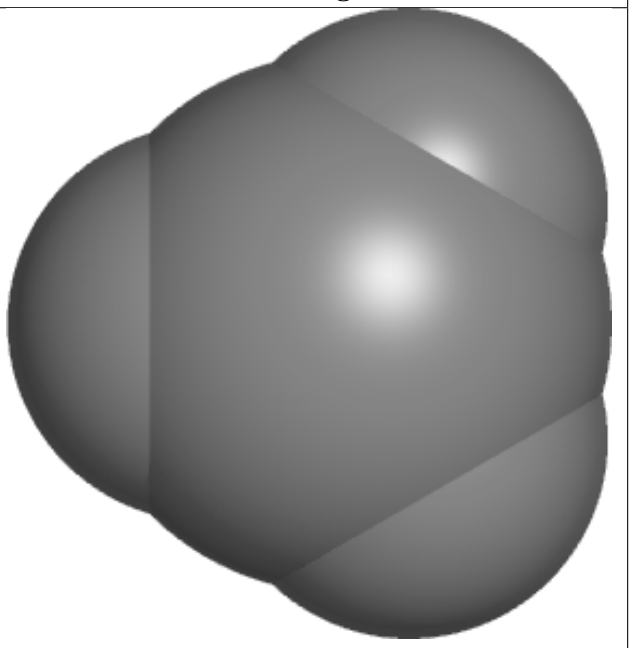
Bond lengths



Bond angles

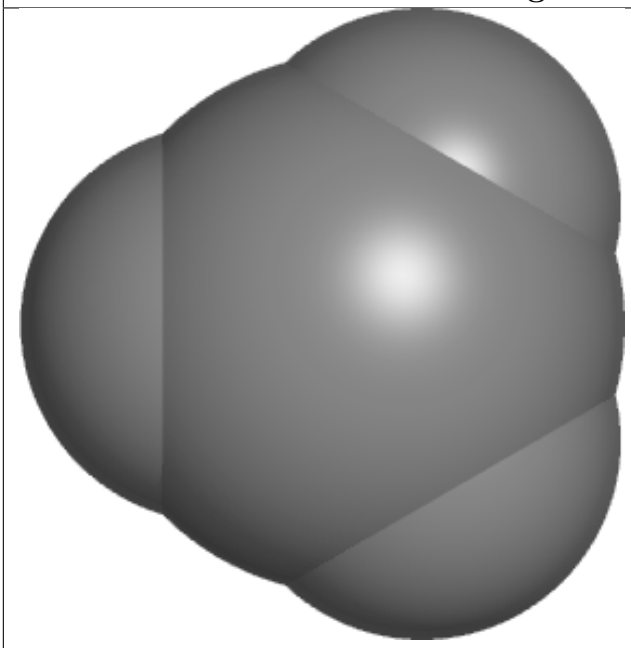


Torsions

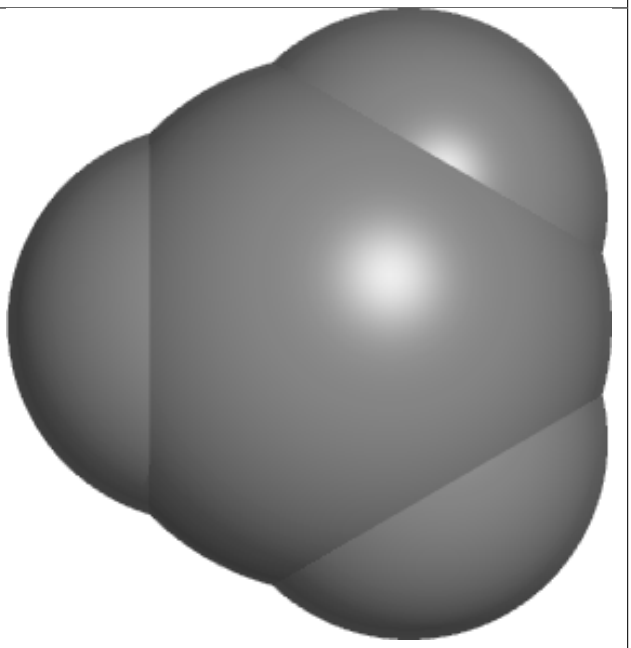


Rings

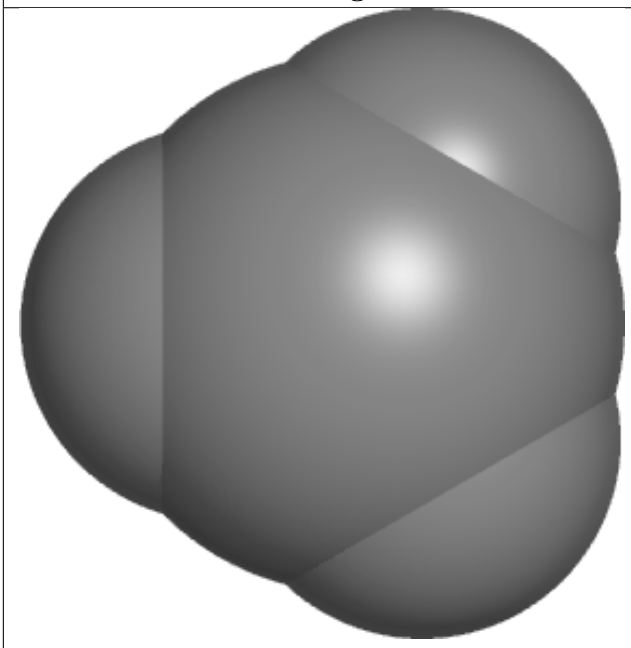
Ligand AF3 C 201



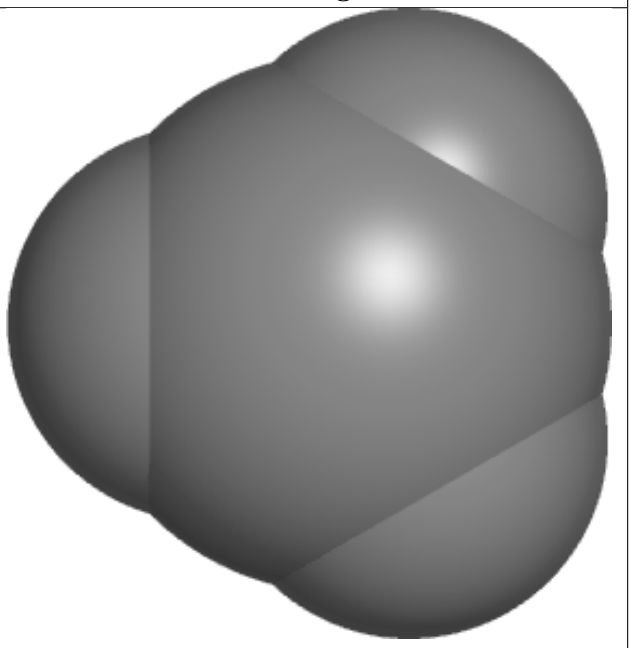
Bond lengths



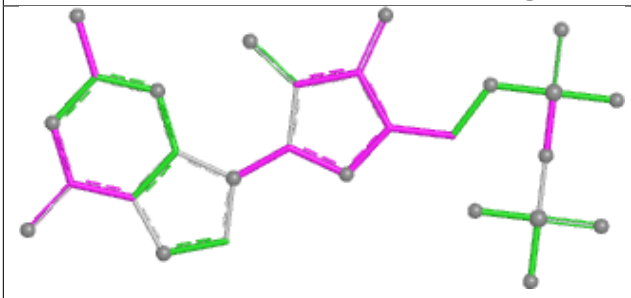
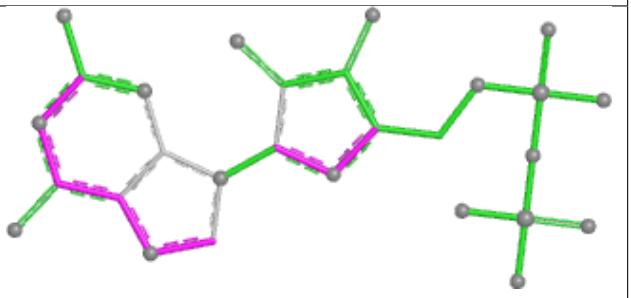
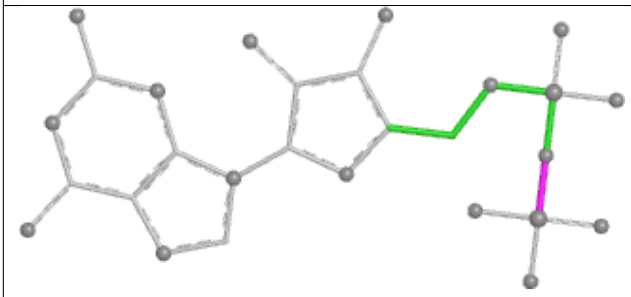
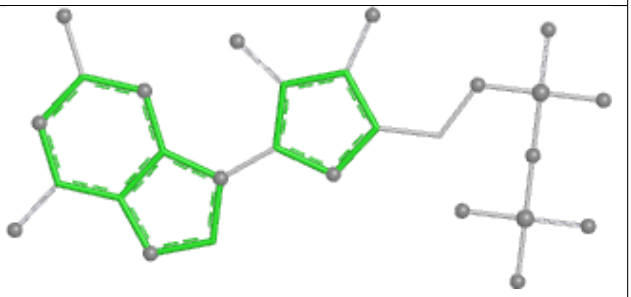
Bond angles

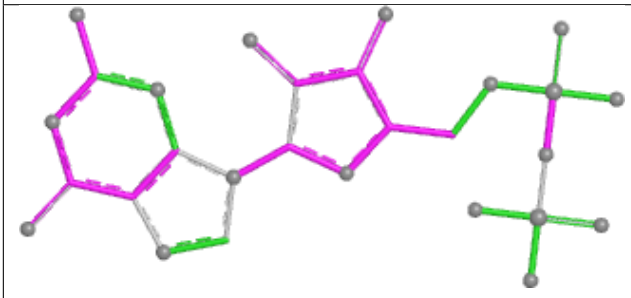
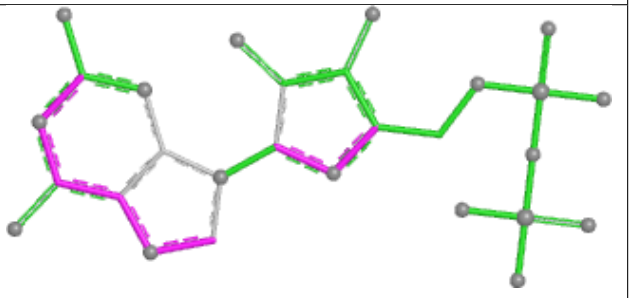
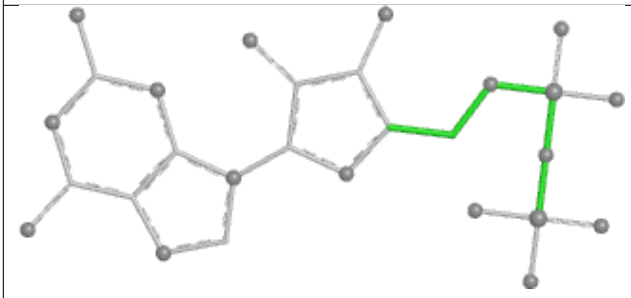
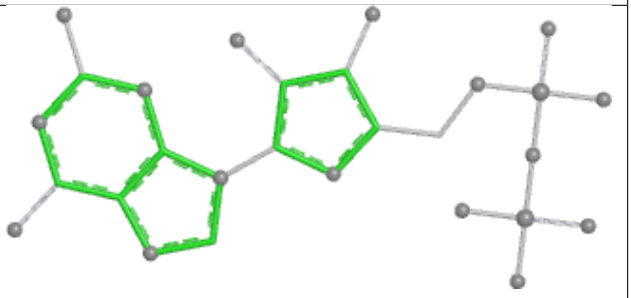


Torsions

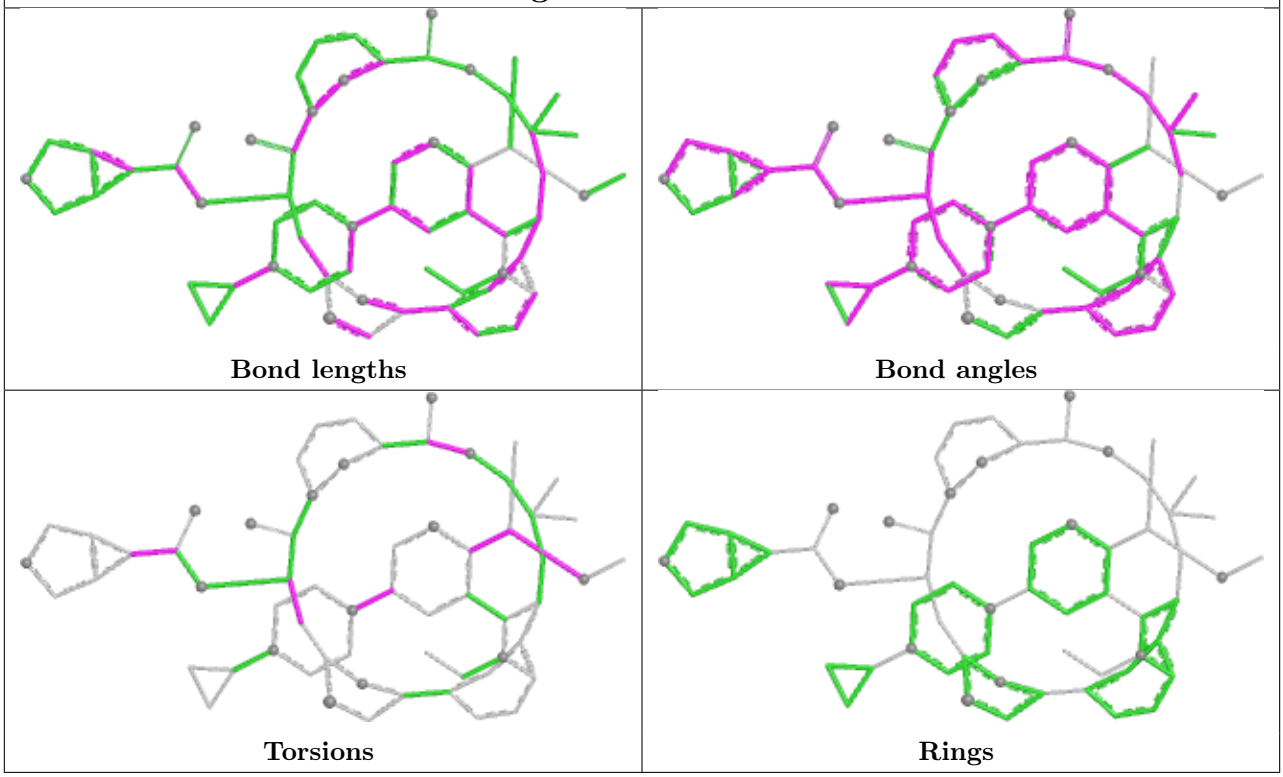


Rings

Ligand GDP A 202	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GDP C 202	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ZNI 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	B	163/166 (98%)	-0.28	2 (1%) 76 77	19, 29, 40, 58	0
1	D	163/166 (98%)	-0.15	0 100 100	25, 33, 44, 64	0
2	A	168/170 (98%)	0.17	3 (1%) 67 69	23, 37, 56, 68	0
2	C	167/170 (98%)	1.78	65 (38%) 1 1	34, 68, 103, 113	0
All	All	661/672 (98%)	0.39	70 (10%) 13 13	19, 35, 89, 113	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	84	ILE	5.8
2	C	118	CYS	5.3
2	C	125	VAL	5.2
2	C	100	ILE	5.2
2	C	82	PHE	4.9
2	C	127	THR	4.7
2	C	120	LEU	4.7
2	C	133	LEU	4.7
2	C	126	ASP	4.6
2	C	108	ASP	4.4
2	C	130	ALA	4.1
2	C	124	THR	4.0
2	C	128	LYS	3.8
2	C	121	PRO	3.8
2	C	139	ILE	3.7
2	C	134	ALA	3.7
2	C	93	ILE	3.7
2	C	89	SER	3.6
2	C	119	ASP	3.6
2	C	103	VAL	3.6
2	C	90	PHE	3.5

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Mol	Chain	Res	Type	RSRZ
2	C	122	SER	3.5
2	C	129	GLN	3.4
2	C	12	CYS	3.3
2	C	113	LEU	3.3
2	A	29	VAL	3.2
2	C	144	THR	3.0
2	C	166	HIS	3.0
2	C	85	ASN	3.0
2	C	11	ALA	3.0
2	C	83	ALA	3.0
2	C	123	ARG	3.0
2	C	136	SER	3.0
2	C	109	VAL	3.0
2	C	96	TYR	2.9
2	C	148	THR	2.9
2	C	141	PHE	2.9
2	C	71	TYR	2.8
2	C	29	VAL	2.8
2	C	117	LYS	2.8
2	C	75	GLY	2.7
2	C	138	GLY	2.7
2	A	12	CYS	2.6
2	C	102	ARG	2.6
2	C	92	ASP	2.6
2	C	114	VAL	2.5
2	C	30	ASP	2.5
2	C	95	HIS	2.5
2	C	73	ARG	2.5
2	C	14	VAL	2.5
2	C	86	ASN	2.5
2	C	106	SER	2.4
2	C	28	PHE	2.4
2	A	30	ASP	2.3
2	C	66	ALA	2.3
2	C	111	MET	2.3
2	C	87	THR	2.3
2	C	135	ARG	2.2
2	C	146	ALA	2.2
2	C	81	VAL	2.2
2	C	104	LYS	2.2
2	C	101	LYS	2.2
1	B	144	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
2	C	137	TYR	2.1
2	C	88	LYS	2.1
2	C	142	ILE	2.1
2	C	140	PRO	2.0
1	B	2	VAL	2.0
2	C	145	SER	2.0
2	C	98	GLU	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 monosaccharides in this entry.

6.4 Ligands (i)

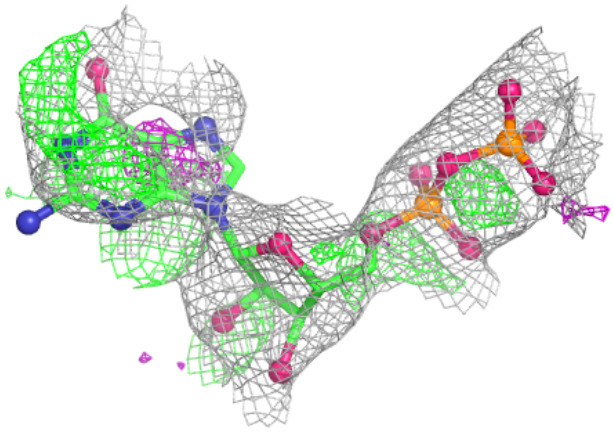
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

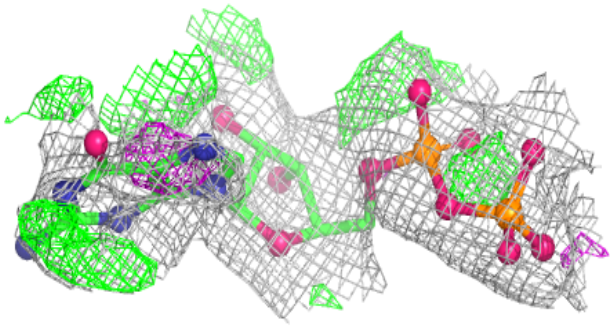
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	GDP	C	202	28/28	0.88	0.15	51,69,77,81	0
3	ZNI	D	201	62/62	0.89	0.13	28,35,45,48	0
4	AF3	C	201	4/4	0.91	0.11	49,56,56,57	0
3	ZNI	B	201	62/62	0.91	0.10	19,24,32,37	0
4	AF3	A	201	4/4	0.94	0.09	26,26,28,28	0
5	GDP	A	202	28/28	0.97	0.07	21,27,30,33	0
6	MG	A	203	1/1	0.98	0.03	22,22,22,22	0
6	MG	C	203	1/1	0.99	0.04	47,47,47,47	0

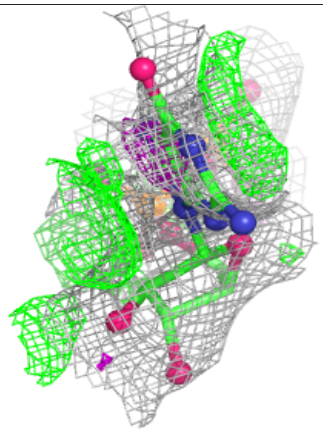
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

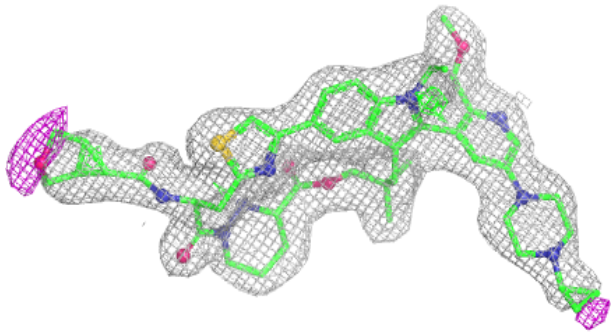


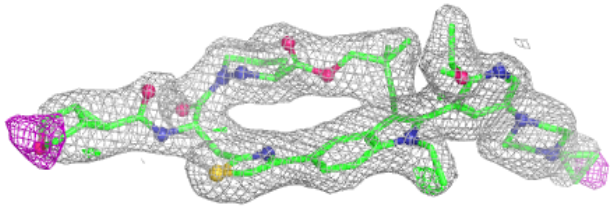


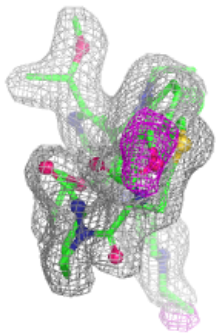


Electron density around ZNI D 201:

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

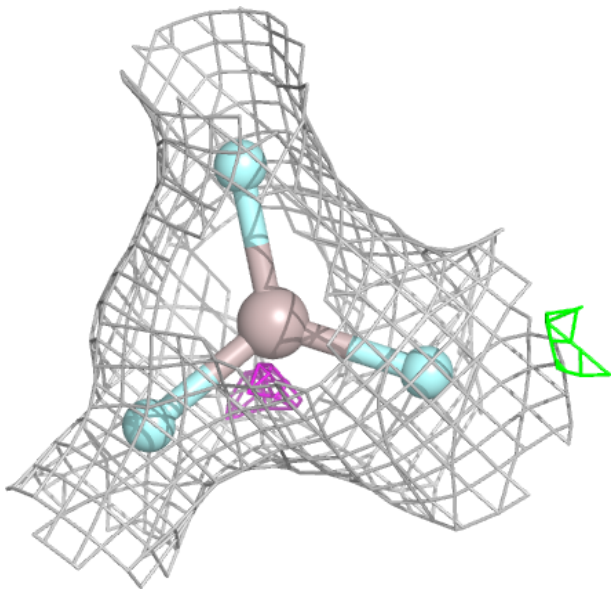


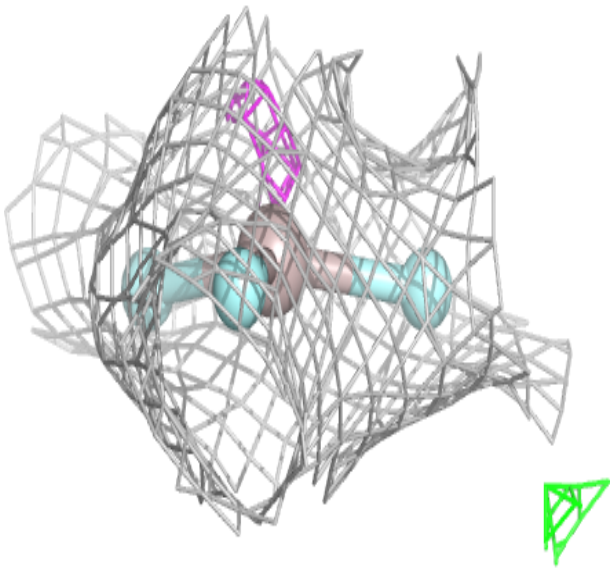


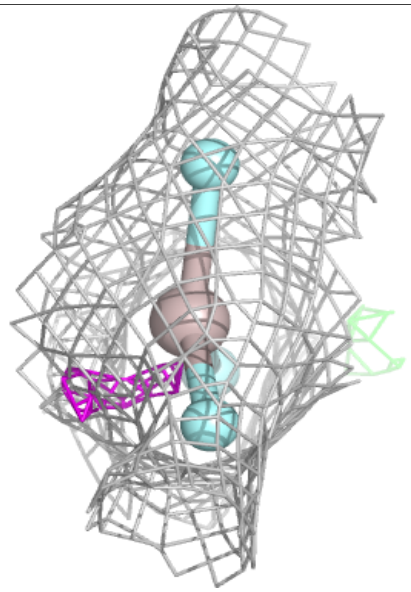


Electron density around AF3 C 201:

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

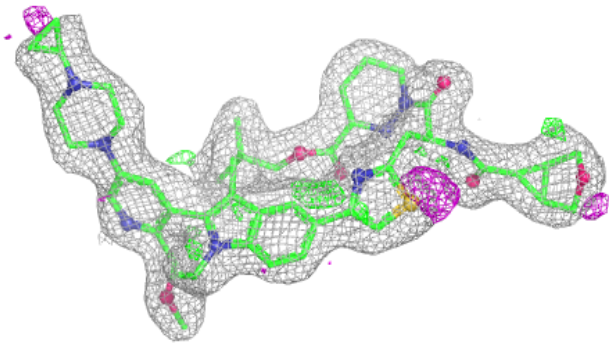


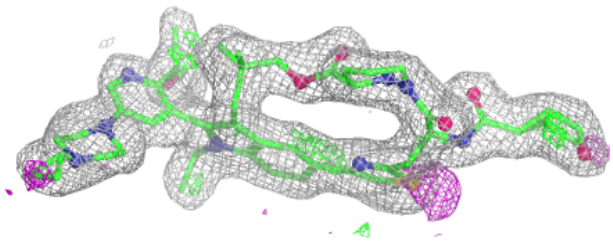


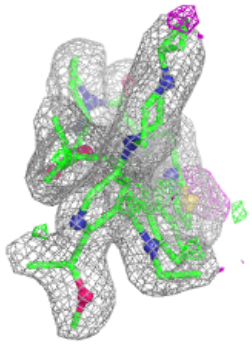


Electron density around ZNI B 201:

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

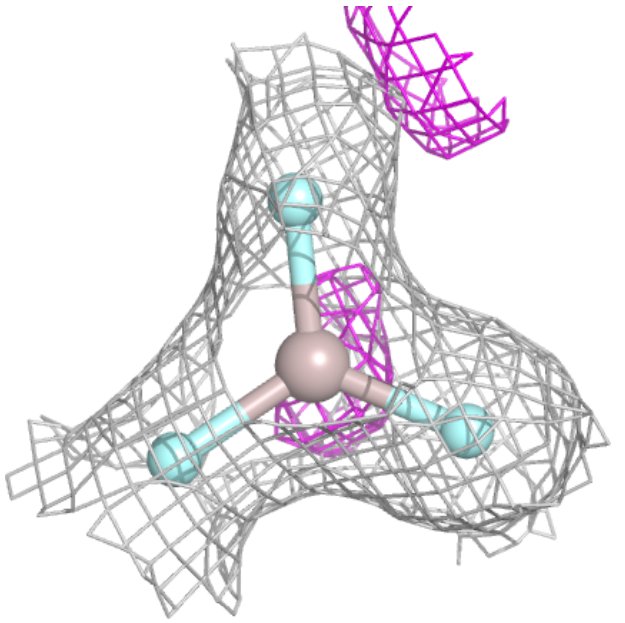


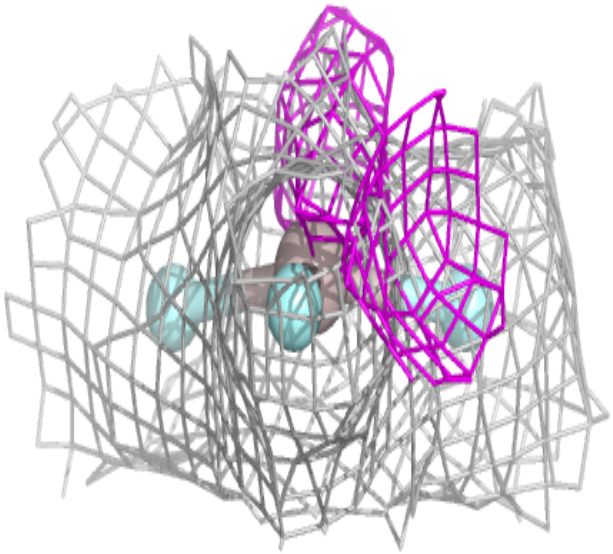


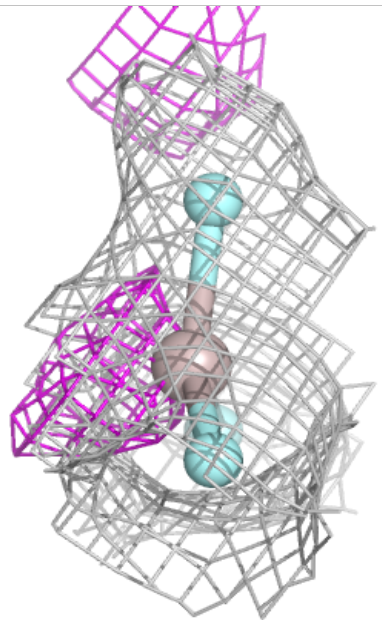


Electron density around AF3 A 201:

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

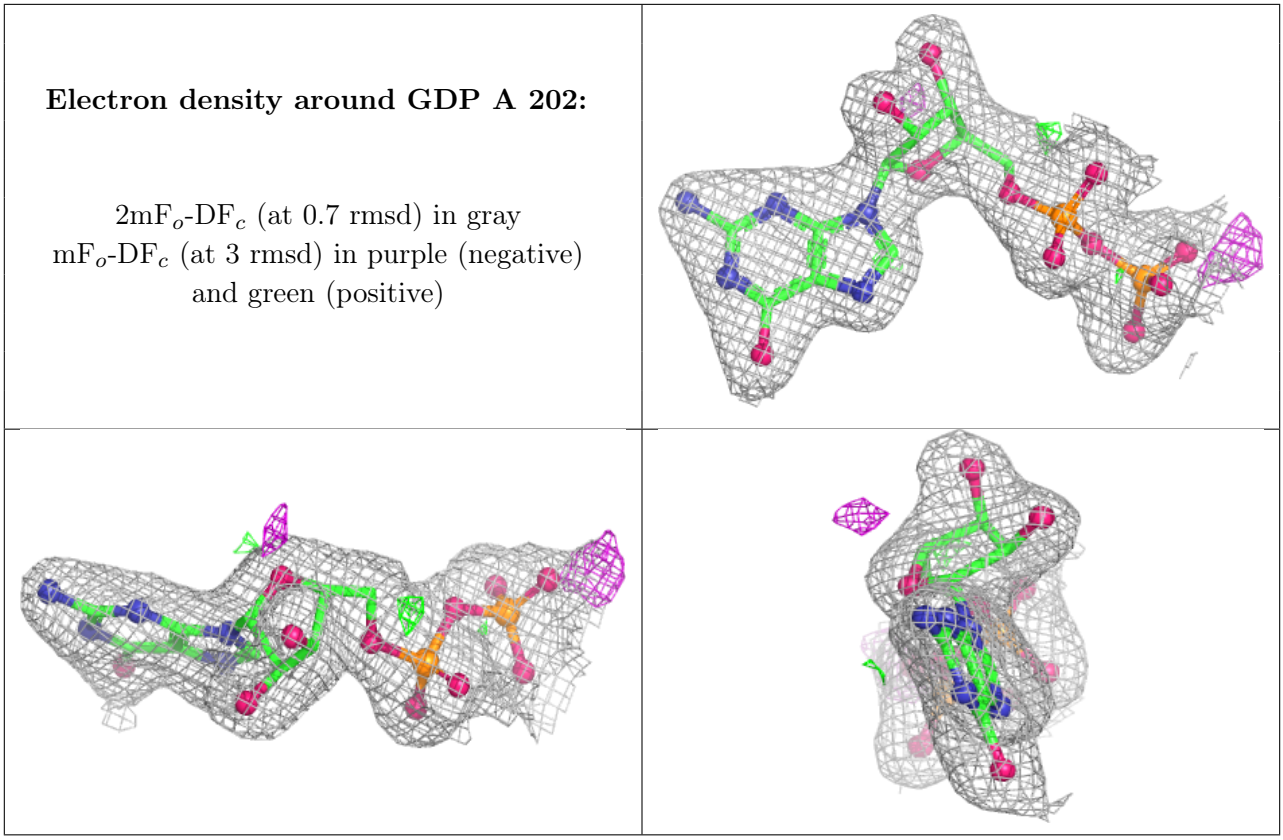






Electron density around GDP A 202:

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



6.5 Other polymers (i)

There are no such residues in this entry.