



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:38 PM UTC

PDB ID : 4UCI / pdb_00004uci
Title : X-ray structure and activities of an essential Mononegavirales L- protein domain
Authors : Paesen, G.C.; Collet, A.; Sallamand, C.; Debart, F.; Vasseur, J.J.; Canard, B.; Decroly, E.; Grimes, J.M.
Deposited on : 2014-12-03
Resolution : 2.21 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)
Xtrriage (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

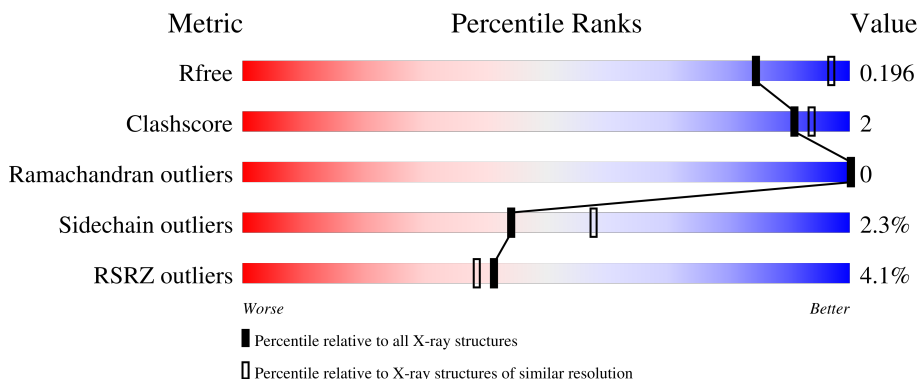
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.21 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	7682 (2.24-2.20)
Clashscore	190562	8402 (2.24-2.20)
Ramachandran outliers	187476	8303 (2.24-2.20)
Sidechain outliers	187428	8304 (2.24-2.20)
RSRZ outliers	180081	7683 (2.24-2.20)

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	415	 4% 81% 6% 13%
1	B	415	 3% 83% 6% 11%

2 Entry composition i

There are 7 unique types of molecules in this entry. The entry contains 6551 atoms, of which 26 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 RNA-DIRECTED RNA POLYMERASE L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	361	2937	1889	503	525	20	0	0	0
1	B	370	3006	1934	514	538	20	0	0	0

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1599	MET	-	expression tag	UNP Q6WB93
A	2006	SER	-	expression tag	UNP Q6WB93
A	2007	GLY	-	expression tag	UNP Q6WB93
A	2008	HIS	-	expression tag	UNP Q6WB93
A	2009	HIS	-	expression tag	UNP Q6WB93
A	2010	HIS	-	expression tag	UNP Q6WB93
A	2011	HIS	-	expression tag	UNP Q6WB93
A	2012	HIS	-	expression tag	UNP Q6WB93
A	2013	HIS	-	expression tag	UNP Q6WB93
A	1606	PRO	SER	conflict	UNP Q6WB93
A	1620	GLU	THR	conflict	UNP Q6WB93
A	1860	ASN	SER	conflict	UNP Q6WB93
A	1912	ASN	ASP	conflict	UNP Q6WB93
A	1935	VAL	ILE	conflict	UNP Q6WB93
A	1946	ASN	SER	conflict	UNP Q6WB93
B	1599	MET	-	expression tag	UNP Q6WB93
B	2006	SER	-	expression tag	UNP Q6WB93
B	2007	GLY	-	expression tag	UNP Q6WB93
B	2008	HIS	-	expression tag	UNP Q6WB93
B	2009	HIS	-	expression tag	UNP Q6WB93
B	2010	HIS	-	expression tag	UNP Q6WB93
B	2011	HIS	-	expression tag	UNP Q6WB93
B	2012	HIS	-	expression tag	UNP Q6WB93
B	2013	HIS	-	expression tag	UNP Q6WB93
B	1606	PRO	SER	conflict	UNP Q6WB93

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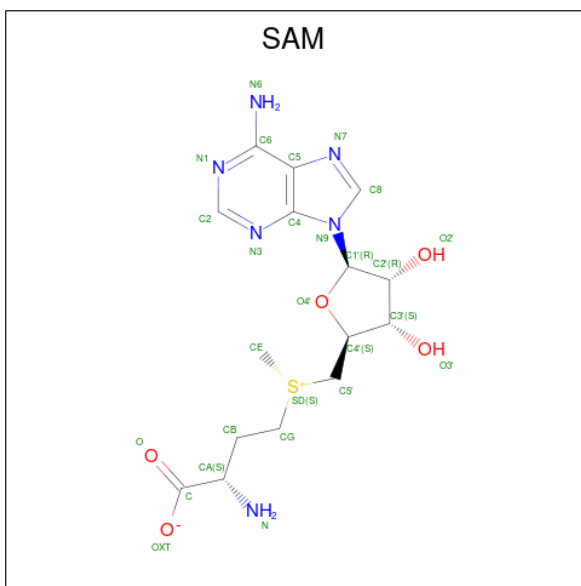
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Chain	Residue	Modelled	Actual	Comment	Reference
B	1620	GLU	THR	conflict	UNP Q6WB93
B	1860	ASN	SER	conflict	UNP Q6WB93
B	1912	ASN	ASP	conflict	UNP Q6WB93
B	1935	VAL	ILE	conflict	UNP Q6WB93
B	1946	ASN	SER	conflict	UNP Q6WB93

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

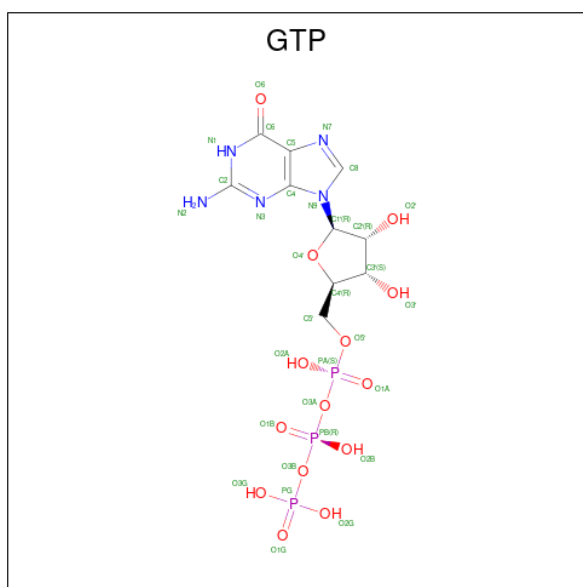
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0
2	B	1	Total Zn 1 1	0	0

- Molecule 3 is S-ADENOSYLMETHIONINE (CCD ID: SAM) (formula: C₁₅H₂₂N₆O₅S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O S 27 15 6 5 1	0	0
3	B	1	Total C N O S 27 15 6 5 1	0	0

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf		
			Total	C	N	O			P	
4	A	1	Total	32	10	5	14	3	0	0
4	B	1	Total	32	10	5	14	3	0	0

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



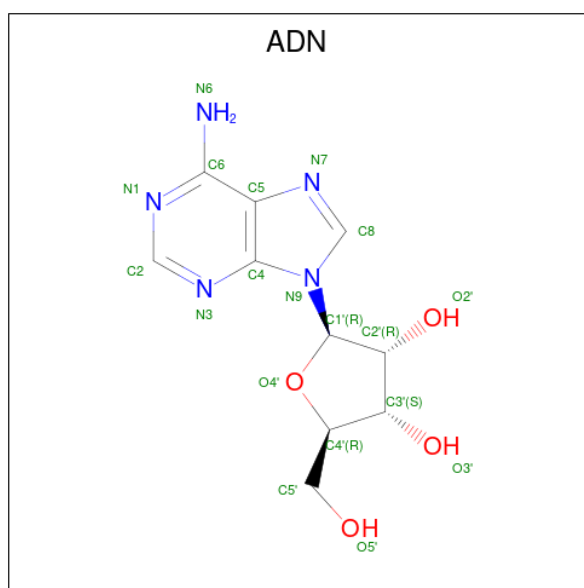
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
			Total	C	O			
5	A	1	Total	6	3	3	0	0
5	A	1	Total	6	3	3	0	0

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

- Molecule 6 is ADENOSINE (CCD ID: ADN) (formula: $C_{10}H_{13}N_5O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C H N O 32 10 13 5 4	0	0
6	B	1	Total C H N O 32 10 13 5 4	0	0

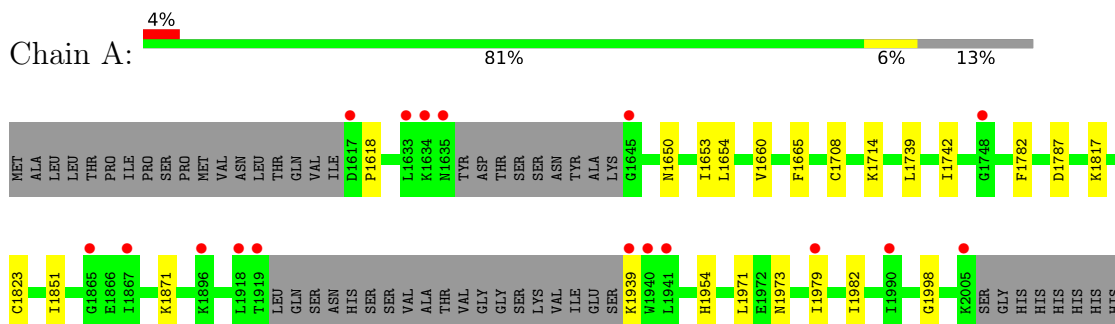
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	177	Total O 177 177	0	0
7	B	205	Total O 205 205	0	0

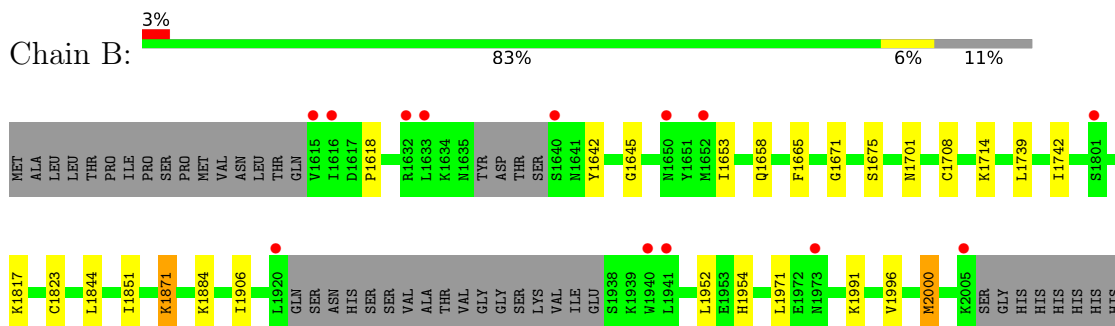
3 Residue-property plots [i](#)

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: RNA-DIRECTED RNA POLYMERASE L



- Molecule 1: RNA-DIRECTED RNA POLYMERASE L



4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	80.22Å 83.61Å 182.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.20 – 2.21 44.20 – 2.21	Depositor EDS
% Data completeness (in resolution range)	99.9 (44.20-2.21) 99.9 (44.20-2.21)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 2.20Å)	Xtrriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.190 , 0.201 0.190 , 0.196	Depositor DCC
R_{free} test set	3154 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	58.3	Xtrriage
Anisotropy	0.395	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 53.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.021 for k,h,-l	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6551	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.29% 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: GTP, SAM, ADN, ZN, GOL

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	0.72	0/3000	1.25	1/4043 (0.0%)
1	B	0.75	1/3070 (0.0%)	1.25	1/4138 (0.0%)
All	All	0.73	1/6070 (0.0%)	1.25	2/8181 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	2000	MET	SD-CE	-8.94	1.57	1.79

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1665	PHE	CA-CB-CG	-5.37	108.43	113.80
1	A	1665	PHE	CA-CB-CG	-5.21	108.59	113.80

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	2937	0	2980	9	0
1	B	3006	0	3054	14	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
3	A	27	0	22	0	0
3	B	27	0	22	0	0
4	A	32	0	12	0	0
4	B	32	0	12	2	0
5	A	18	0	24	0	0
5	B	24	0	32	0	0
6	A	19	13	13	0	0
6	B	19	13	13	0	0
7	A	177	0	0	0	0
7	B	205	0	0	0	0
All	All	6525	26	6184	21	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (21) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1844:LEU:O	1:B:1871:LYS:HE2	1.82	0.79
1:B:1952:LEU:HD22	1:B:2000:MET:HE1	1.67	0.77
1:B:1671:GLY:H	1:B:1701:ASN:HD22	1.36	0.74
1:B:1658:GLN:HG3	4:B:2410:GTP:O2A	1.98	0.64
1:B:1906:ILE:HD13	1:B:2000:MET:HE2	1.81	0.62
1:B:1739:LEU:HG	1:B:1742:ILE:HD12	1.85	0.59
1:A:1739:LEU:HG	1:A:1742:ILE:HD12	1.84	0.58
1:B:1996:VAL:HG12	1:B:2000:MET:HE3	1.87	0.56
1:B:1952:LEU:HD22	1:B:2000:MET:CE	2.36	0.54
1:A:1979:ILE:HD12	1:A:1982:ILE:HD11	1.91	0.51
1:A:1650:ASN:O	1:B:1645:GLY:HA3	2.15	0.46
1:A:1973:ASN:HB3	1:B:1642:TYR:HB2	1.98	0.46
1:A:1654:LEU:HD13	1:A:1982:ILE:HD13	1.97	0.46
1:A:1660:VAL:O	1:A:1998:GLY:HA3	2.17	0.45
1:A:1618:PRO:HB2	1:A:1708:CYS:HA	1.97	0.45
1:B:1671:GLY:N	1:B:1701:ASN:HD22	2.09	0.45
1:A:1954:HIS:HE1	1:A:1971:LEU:O	2.00	0.44
1:B:1618:PRO:HB2	1:B:1708:CYS:HA	1.98	0.44
1:B:1991:LYS:HE3	4:B:2410:GTP:C5	2.52	0.44
1:B:1954:HIS:HE1	1:B:1971:LEU:O	2.03	0.41
1:A:1782:PHE:HB3	1:A:1787:ASP:HB2	2.03	0.41

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	355/415 (86%)	348 (98%)	7 (2%)	0	100	100
1	B	364/415 (88%)	357 (98%)	7 (2%)	0	100	100
All	All	719/830 (87%)	705 (98%)	14 (2%)	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	A	326/374 (87%)	319 (98%)	7 (2%)	47	61
1	B	334/374 (89%)	326 (98%)	8 (2%)	43	56
All	All	660/748 (88%)	645 (98%)	15 (2%)	44	58

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1653	ILE
1	A	1714	LYS
1	A	1817	LYS
1	A	1823	CYS
1	A	1851	ILE

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Mol	Chain	Res	Type
1	A	1871	LYS
1	A	1939	LYS
1	B	1653	ILE
1	B	1675	SER
1	B	1714	LYS
1	B	1817	LYS
1	B	1823	CYS
1	B	1851	ILE
1	B	1871	LYS
1	B	1884	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1635	ASN
1	A	1659	HIS
1	A	1868	GLN
1	A	1914	GLN
1	A	1943	ASN
1	A	1946	ASN
1	A	1954	HIS
1	A	1973	ASN
1	B	1635	ASN
1	B	1701	ASN
1	B	1864	HIS
1	B	1954	HIS
1	B	1973	ASN

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

Of 15 ligands modelled in this entry, 2 are monoatomic - leaving 13 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	GTP	B	2410	-	33,34,34	0.72	1 (3%)	50,54,54	1.05	4 (8%)
4	GTP	A	2410	-	33,34,34	0.47	0	50,54,54	0.82	3 (6%)
5	GOL	B	2412	-	5,5,5	0.05	0	5,5,5	0.26	0
6	ADN	A	2414	-	21,21,21	0.18	0	31,31,31	0.40	0
5	GOL	B	2413	-	5,5,5	0.06	0	5,5,5	0.32	0
5	GOL	B	2411	-	5,5,5	0.05	0	5,5,5	0.09	0
6	ADN	B	2415	-	21,21,21	0.15	0	31,31,31	0.37	0
3	SAM	A	2409	-	27,29,29	0.52	0	34,42,42	0.57	0
5	GOL	A	2412	-	5,5,5	0.05	0	5,5,5	0.16	0
5	GOL	A	2411	-	5,5,5	0.08	0	5,5,5	0.19	0
5	GOL	A	2413	-	5,5,5	0.06	0	5,5,5	0.12	0
5	GOL	B	2414	-	5,5,5	0.08	0	5,5,5	0.14	0
3	SAM	B	2409	-	27,29,29	0.54	0	34,42,42	0.55	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GTP	B	2410	-	-	8/22/38/38	0/3/3/3
4	GTP	A	2410	-	-	3/22/38/38	0/3/3/3
5	GOL	B	2412	-	-	0/4/4/4	-
6	ADN	A	2414	-	-	0/6/22/22	0/3/3/3
5	GOL	B	2413	-	-	0/4/4/4	-
5	GOL	B	2411	-	-	0/4/4/4	-
6	ADN	B	2415	-	-	0/6/22/22	0/3/3/3
3	SAM	A	2409	-	-	1/17/33/33	0/3/3/3
5	GOL	A	2412	-	-	0/4/4/4	-
5	GOL	A	2411	-	-	0/4/4/4	-
5	GOL	A	2413	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	B	2414	-	-	0/4/4/4	-
3	SAM	B	2409	-	-	1/17/33/33	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	2410	GTP	PB-O3B	-3.13	1.56	1.59

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	2410	GTP	O2B-PB-O3B	-3.86	96.85	107.27
4	B	2410	GTP	O2A-PA-O5'	-3.03	93.85	107.57
4	A	2410	GTP	O2B-PB-O3A	-2.75	99.85	107.27
4	A	2410	GTP	O2B-PB-O3B	-2.69	100.00	107.27
4	B	2410	GTP	O3B-PB-O1B	2.39	117.89	110.70
4	B	2410	GTP	O2B-PB-O3A	-2.05	101.73	107.27
4	A	2410	GTP	O2A-PA-O5'	-2.05	98.27	107.57

There are no chirality outliers.

All (13) torsion outliers are listed below:

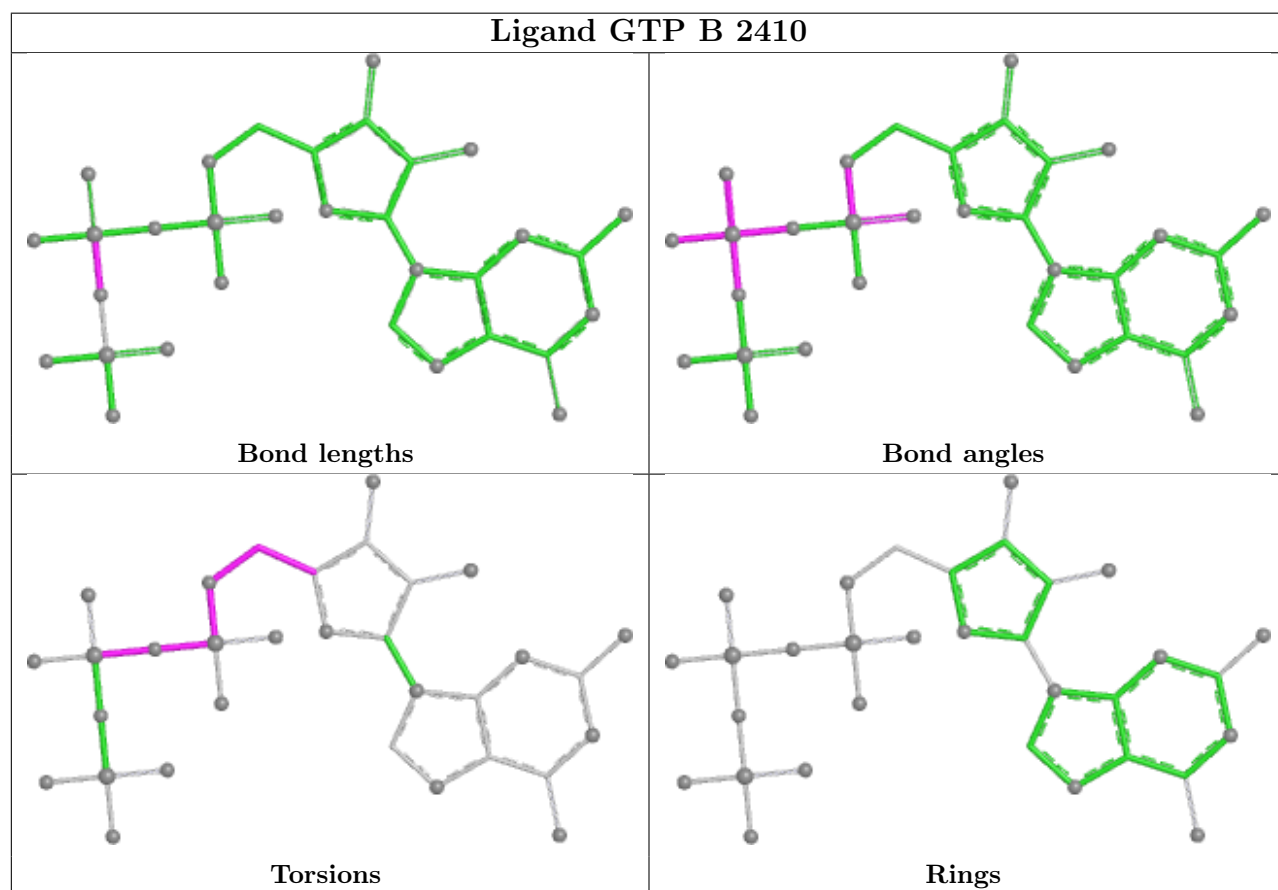
Mol	Chain	Res	Type	Atoms
4	B	2410	GTP	C5'-O5'-PA-O2A
4	B	2410	GTP	C3'-C4'-C5'-O5'
4	A	2410	GTP	O4'-C4'-C5'-O5'
4	B	2410	GTP	O4'-C4'-C5'-O5'
4	A	2410	GTP	C3'-C4'-C5'-O5'
4	B	2410	GTP	PB-O3A-PA-O5'
4	A	2410	GTP	C4'-C5'-O5'-PA
4	B	2410	GTP	C4'-C5'-O5'-PA
3	B	2409	SAM	C2'-C1'-N9-C8
3	A	2409	SAM	C2'-C1'-N9-C8
4	B	2410	GTP	PB-O3A-PA-O1A
4	B	2410	GTP	PA-O3A-PB-O2B
4	B	2410	GTP	PB-O3A-PA-O2A

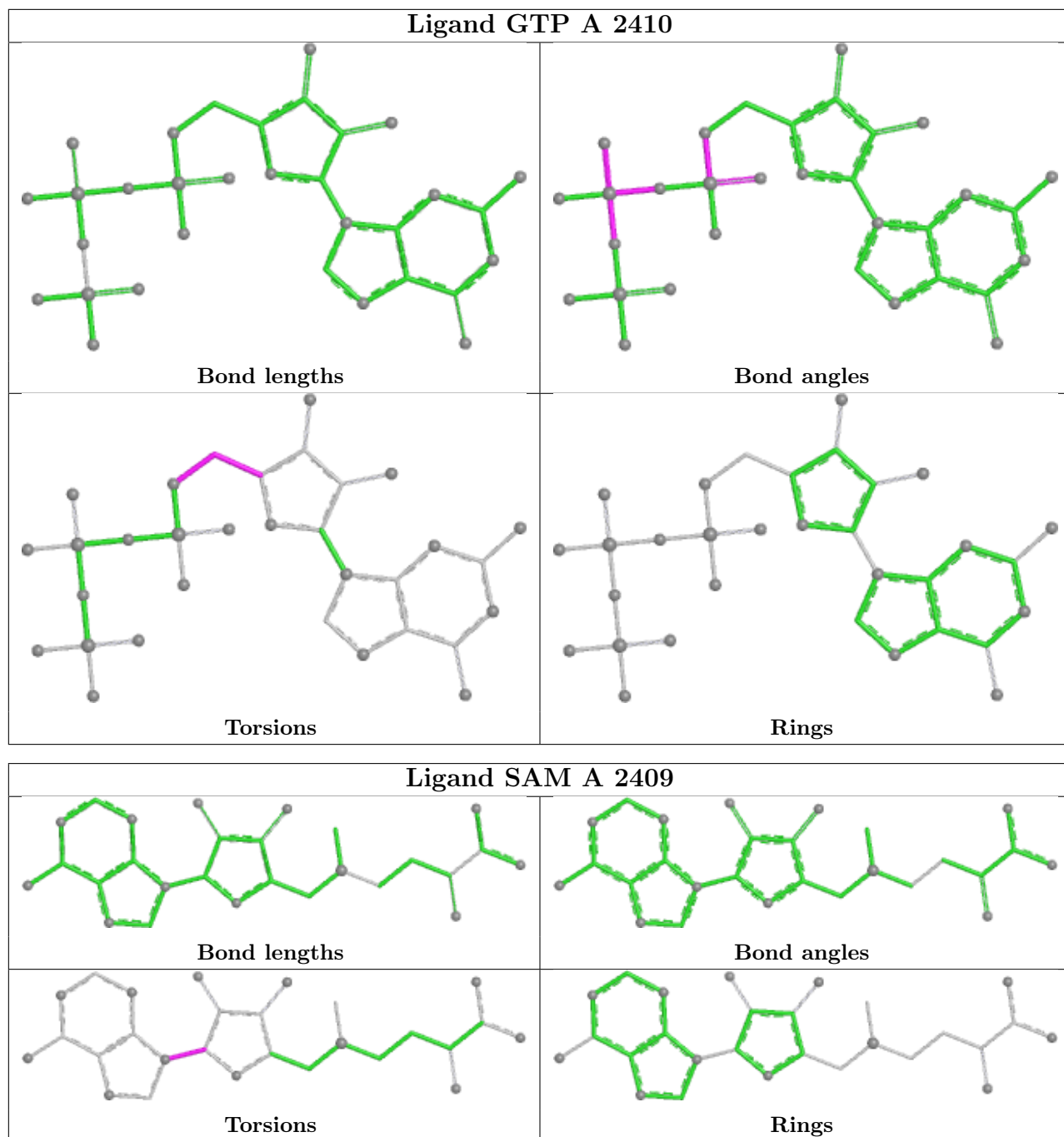
There are no ring outliers.

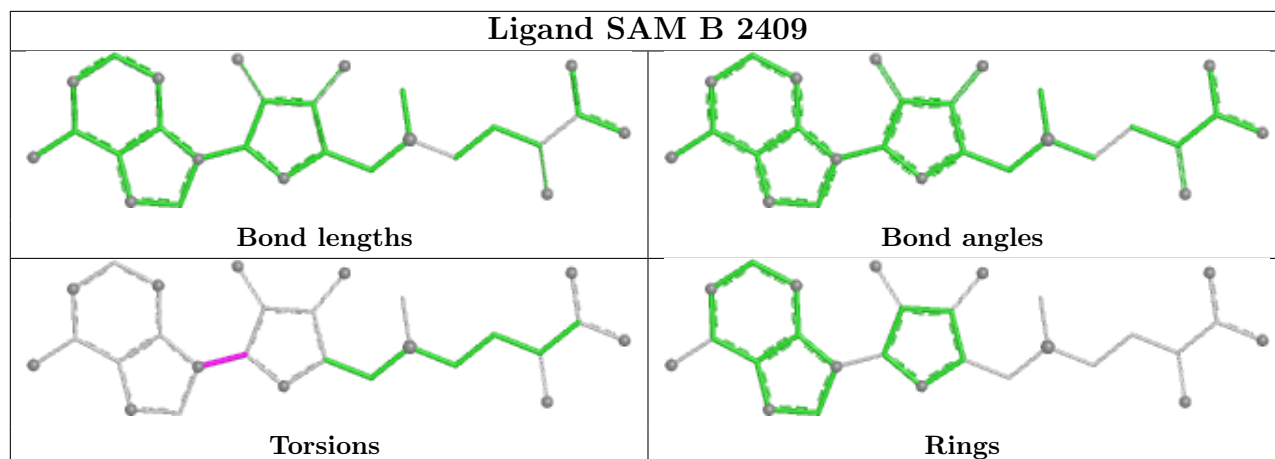
1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	2410	GTP	2	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	361/415 (86%)	0.27	17 (4%) 36 33	51, 65, 98, 134	0
1	B	370/415 (89%)	0.24	13 (3%) 47 44	48, 62, 98, 148	0
All	All	731/830 (88%)	0.25	30 (4%) 41 38	48, 64, 98, 148	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1615	VAL	4.0
1	A	1919	THR	3.8
1	B	1920	LEU	3.7
1	B	2005	LYS	3.6
1	B	1940	TRP	3.4
1	A	1635	ASN	3.3
1	B	1650	ASN	3.1
1	A	1634	LYS	3.1
1	A	1940	TRP	3.0
1	A	1748	GLY	2.9
1	A	1865	GLY	2.8
1	B	1616	ILE	2.8
1	A	1633	LEU	2.8
1	A	1939	LYS	2.7
1	B	1652	MET	2.6
1	A	1941	LEU	2.6
1	A	1979	ILE	2.5
1	A	2005	LYS	2.4
1	B	1941	LEU	2.4
1	B	1973	ASN	2.4
1	B	1633	LEU	2.4
1	A	1645	GLY	2.4
1	B	1640	SER	2.3
1	B	1801	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	1867	ILE	2.1
1	A	1617	ASP	2.1
1	A	1918	LEU	2.1
1	B	1632	ARG	2.1
1	A	1896	LYS	2.1
1	A	1990	ILE	2.1

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.

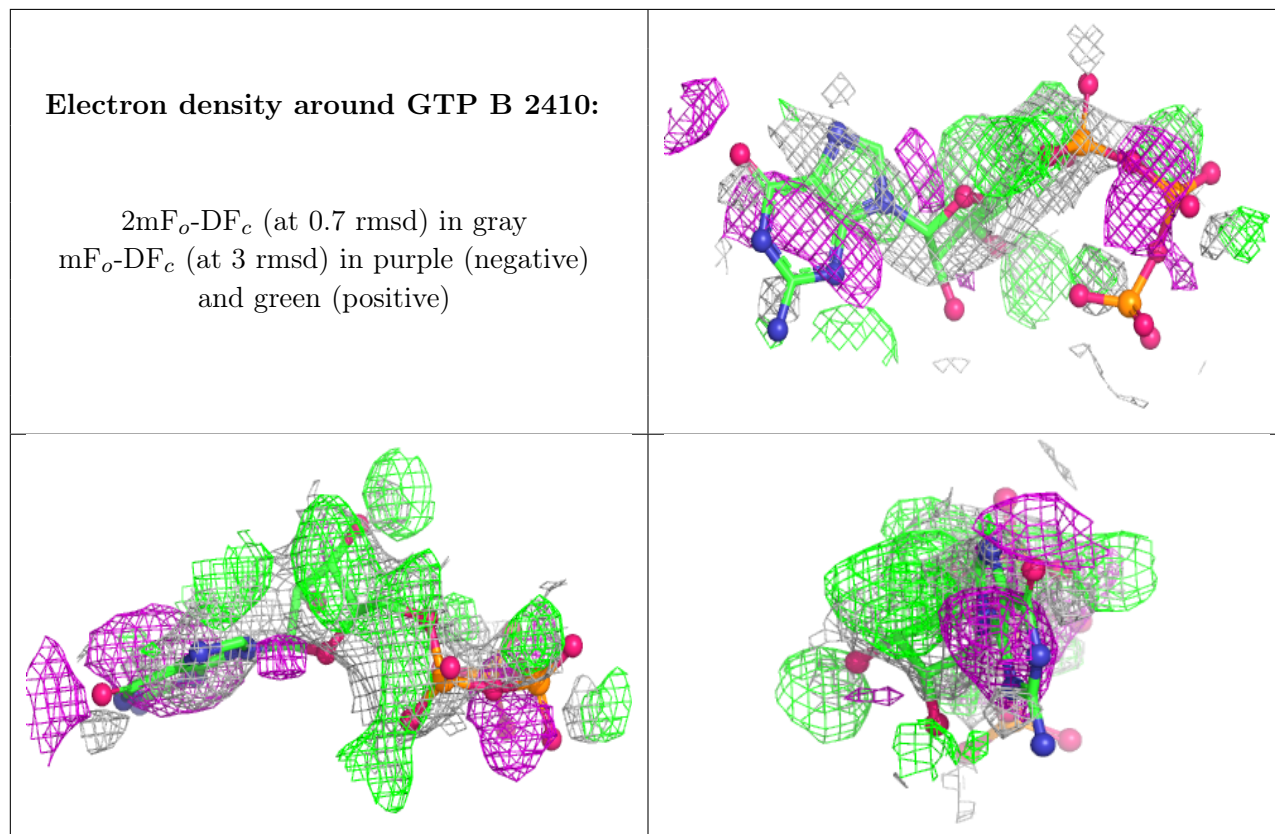
6.4 Ligands [i](#)

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
5	GOL	A	2413	6/6	0.49	0.19	132,133,133,134	0
4	GTP	B	2410	32/32	0.65	0.34	145,150,155,155	12
4	GTP	A	2410	32/32	0.65	0.31	149,154,157,157	12
5	GOL	A	2412	6/6	0.70	0.20	101,104,104,105	0
5	GOL	B	2411	6/6	0.78	0.27	119,120,121,121	0
5	GOL	B	2414	6/6	0.78	0.20	96,100,102,103	0
6	ADN	A	2414	19/19	0.78	0.14	62,90,98,98	0
5	GOL	B	2413	6/6	0.81	0.14	99,102,103,104	0
5	GOL	A	2411	6/6	0.84	0.18	94,99,100,101	0
6	ADN	B	2415	19/19	0.84	0.13	60,83,96,96	0
5	GOL	B	2412	6/6	0.88	0.20	94,96,97,98	0
3	SAM	B	2409	27/27	0.97	0.07	45,54,59,62	0
3	SAM	A	2409	27/27	0.97	0.06	51,57,61,64	0
2	ZN	A	2408	1/1	0.99	0.04	60,60,60,60	0
2	ZN	B	2408	1/1	1.00	0.02	56,56,56,56	0

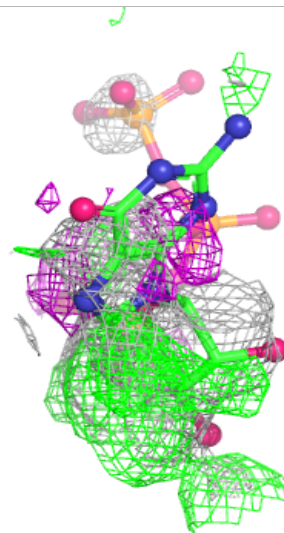
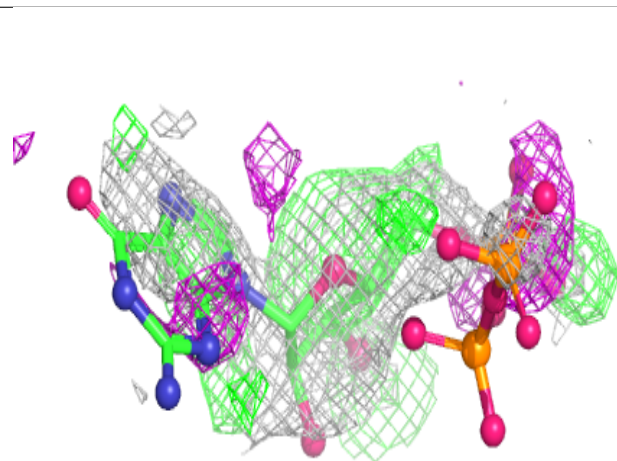
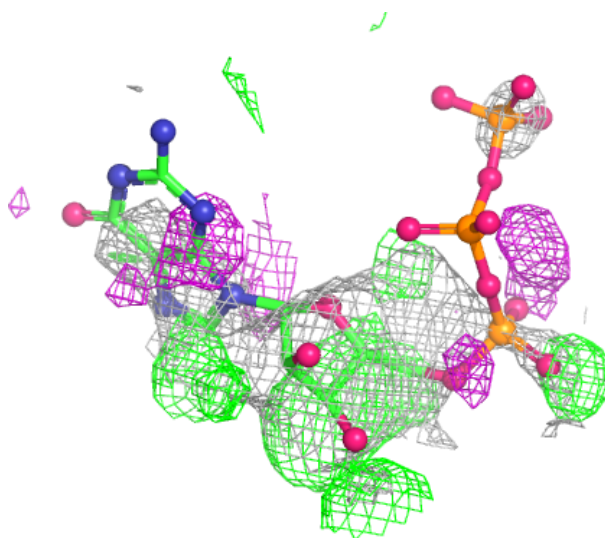
The following is a graphical depiction of the model fit to experimental electron density of all

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.



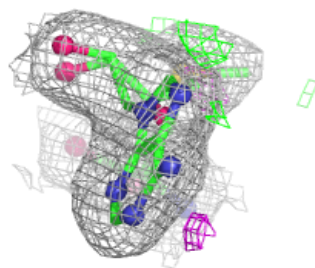
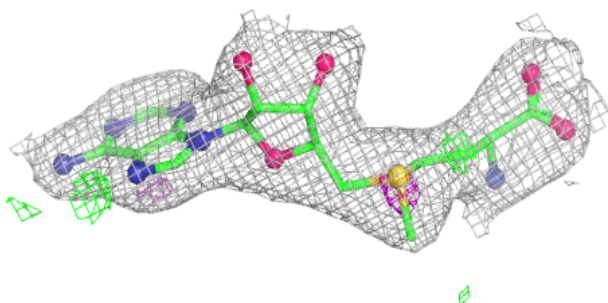
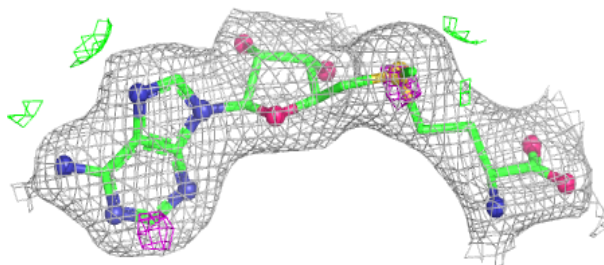
Electron density around GTP A 2410:

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

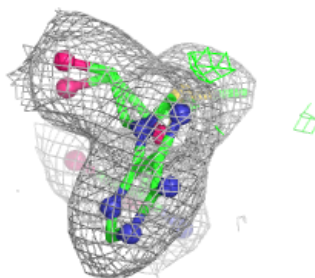
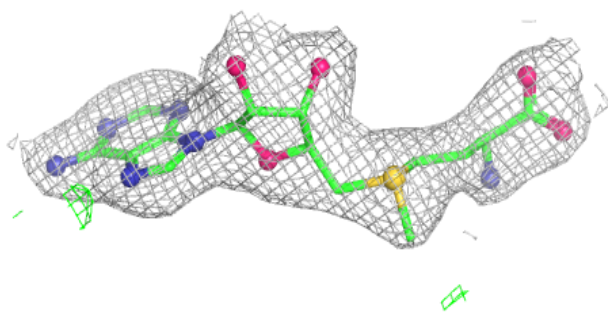
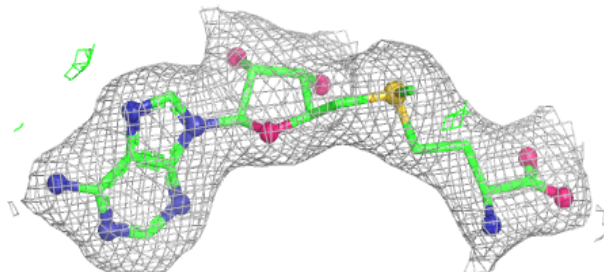


Electron density around SAM B 2409:

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

**Electron density around SAM A 2409:**

$2mF_o-DF_c$ (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.