wwPDB X-ray Structure Validation Summary Report (i)

Aug 4, 2026 – 07:24 AM EDT

PDB ID	:	5CJV / pdb_00005cjv
Title	:	Isobutyryl-CoA mutase fused with bound adenosylcobalamin, GDP, Mg (holo-IcmF/GDP), and substrate isovaleryl-coenzyme A
Authors	:	Jost, M.; Drennan, C.L.
Deposited on	:	2015-07-15
Resolution	:	3.45 Å(reported)

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

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

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

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

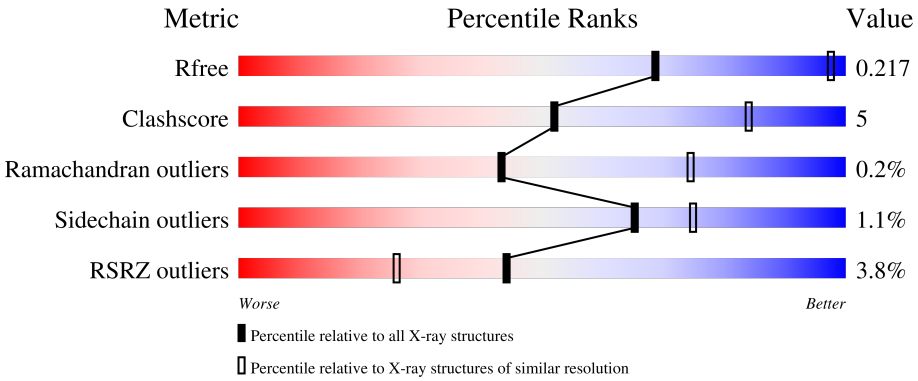
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 3.45 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	1070 (3.50-3.42)
Clashscore	190562	1128 (3.50-3.42)
Ramachandran outliers	187476	1101 (3.50-3.42)
Sidechain outliers	187428	1102 (3.50-3.42)
RSRZ outliers	180081	1070 (3.50-3.42)

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	1113	3% 82% 13% 5%
1	B	1113	4% 84% 12% 5%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 16519 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 Isobutyryl-CoA mutase fused.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1061	Total	C	N	O	S	0	0	0
			8093	5058	1449	1549	37			
1	B	1059	Total	C	N	O	S	0	0	0
			8067	5034	1453	1543	37			

There are 40 discrepancies between the modelled and reference sequences:

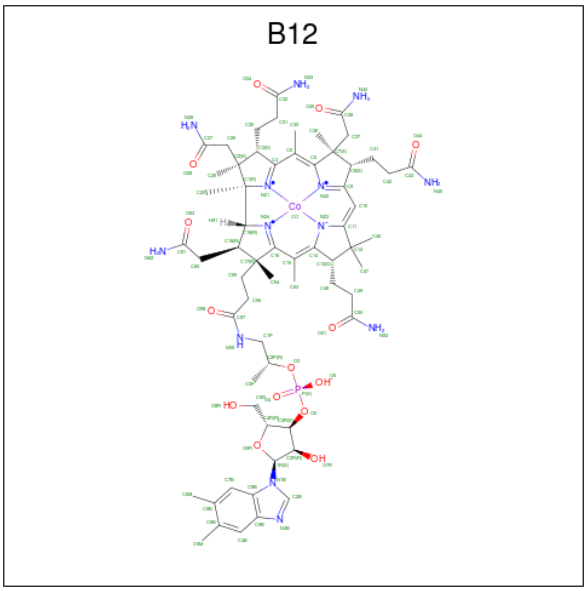
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP Q1LRY0
A	-18	GLY	-	expression tag	UNP Q1LRY0
A	-17	SER	-	expression tag	UNP Q1LRY0
A	-16	SER	-	expression tag	UNP Q1LRY0
A	-15	HIS	-	expression tag	UNP Q1LRY0
A	-14	HIS	-	expression tag	UNP Q1LRY0
A	-13	HIS	-	expression tag	UNP Q1LRY0
A	-12	HIS	-	expression tag	UNP Q1LRY0
A	-11	HIS	-	expression tag	UNP Q1LRY0
A	-10	HIS	-	expression tag	UNP Q1LRY0
A	-9	SER	-	expression tag	UNP Q1LRY0
A	-8	SER	-	expression tag	UNP Q1LRY0
A	-7	GLY	-	expression tag	UNP Q1LRY0
A	-6	LEU	-	expression tag	UNP Q1LRY0
A	-5	VAL	-	expression tag	UNP Q1LRY0
A	-4	PRO	-	expression tag	UNP Q1LRY0
A	-3	ARG	-	expression tag	UNP Q1LRY0
A	-2	GLY	-	expression tag	UNP Q1LRY0
A	-1	SER	-	expression tag	UNP Q1LRY0
A	0	HIS	-	expression tag	UNP Q1LRY0
B	-19	MET	-	initiating methionine	UNP Q1LRY0
B	-18	GLY	-	expression tag	UNP Q1LRY0
B	-17	SER	-	expression tag	UNP Q1LRY0
B	-16	SER	-	expression tag	UNP Q1LRY0
B	-15	HIS	-	expression tag	UNP Q1LRY0

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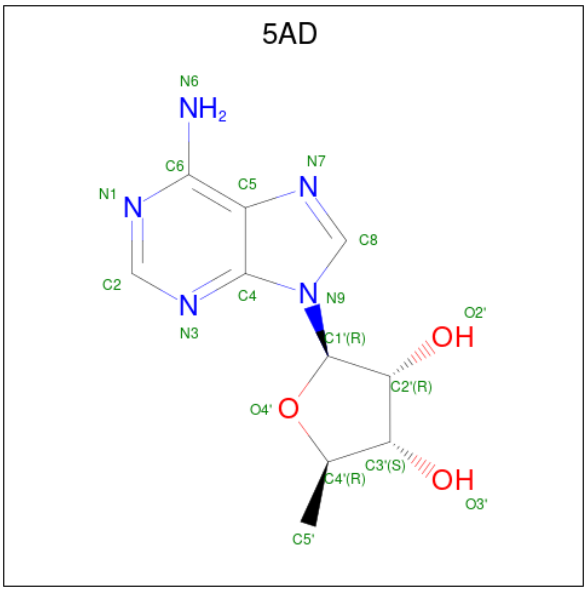
Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	expression tag	UNP Q1LRY0
B	-13	HIS	-	expression tag	UNP Q1LRY0
B	-12	HIS	-	expression tag	UNP Q1LRY0
B	-11	HIS	-	expression tag	UNP Q1LRY0
B	-10	HIS	-	expression tag	UNP Q1LRY0
B	-9	SER	-	expression tag	UNP Q1LRY0
B	-8	SER	-	expression tag	UNP Q1LRY0
B	-7	GLY	-	expression tag	UNP Q1LRY0
B	-6	LEU	-	expression tag	UNP Q1LRY0
B	-5	VAL	-	expression tag	UNP Q1LRY0
B	-4	PRO	-	expression tag	UNP Q1LRY0
B	-3	ARG	-	expression tag	UNP Q1LRY0
B	-2	GLY	-	expression tag	UNP Q1LRY0
B	-1	SER	-	expression tag	UNP Q1LRY0
B	0	HIS	-	expression tag	UNP Q1LRY0

- Molecule 2 is COBALAMIN (CCD ID: B12) (formula: $C_{62}H_{89}CoN_{13}O_{14}P$).



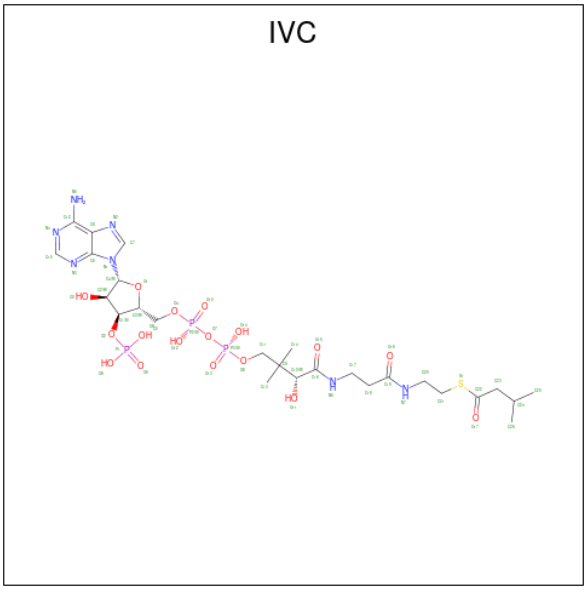
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		
2	B	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		

- Molecule 3 is 5'-DEOXYADENOSINE (CCD ID: 5AD) (formula: $C_{10}H_{13}N_5O_3$).



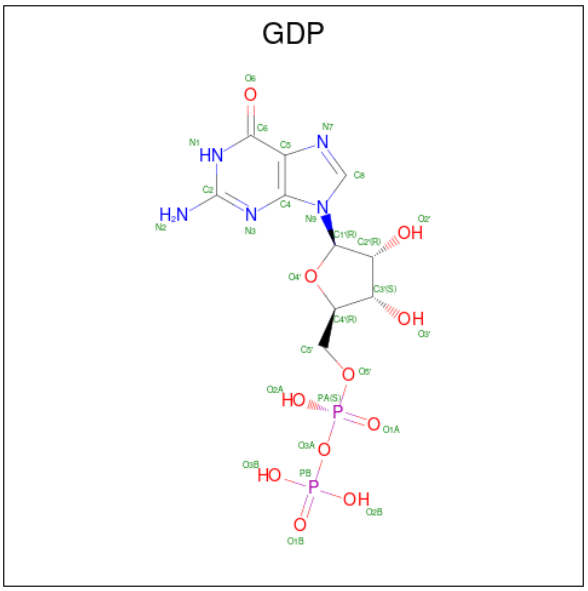
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 36 20 10 6	0	1

- Molecule 4 is Isovaleryl-coenzyme A (CCD ID: IVC) (formula: $C_{26}H_{44}N_7O_{17}P_3S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O P S 54 26 7 17 3 1	0	0
4	B	1	Total C N O P 27 10 5 10 2	0	0

- Molecule 5 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: 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	0	0
			28	10	5	11	2		
5	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total	Mg	0	0
			2	2		
6	B	2	Total	Mg	0	0
			2	2		

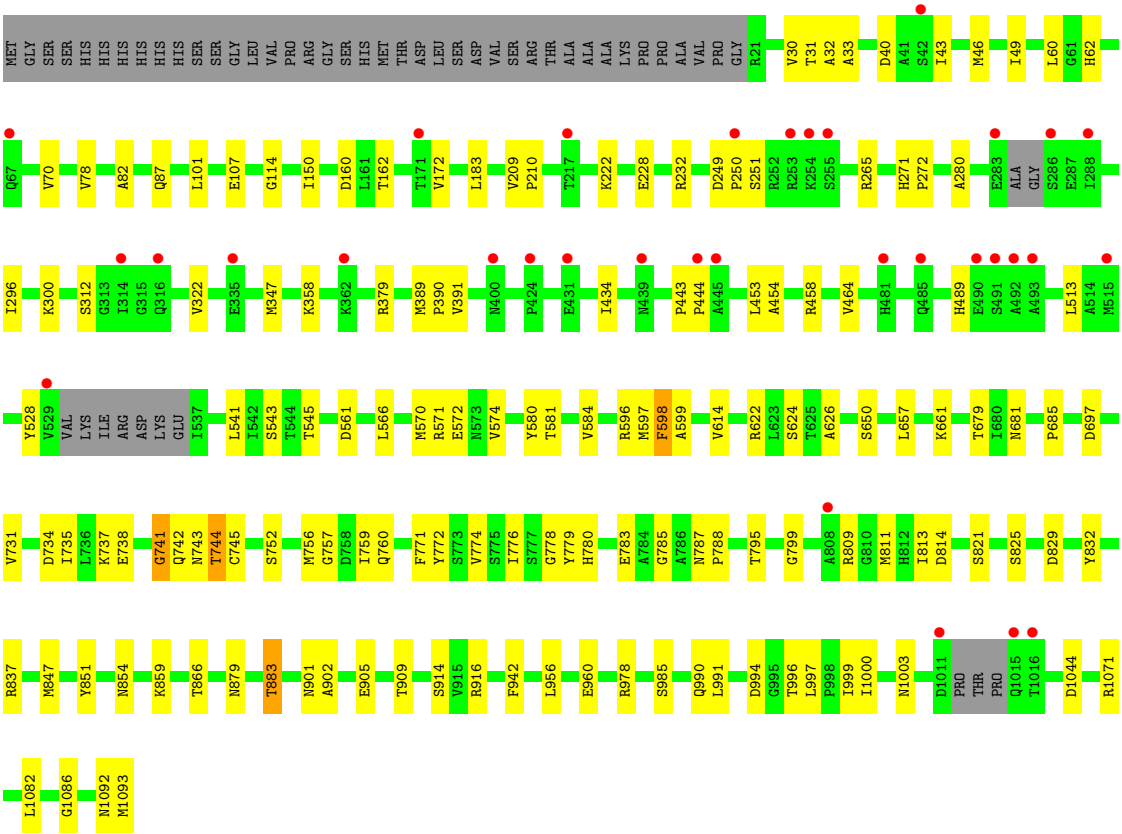
3 Residue-property plots (i)

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: Isobutyryl-CoA mutase fused

Chain A:

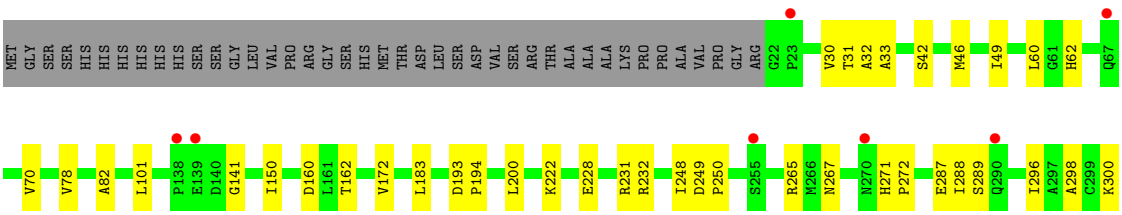


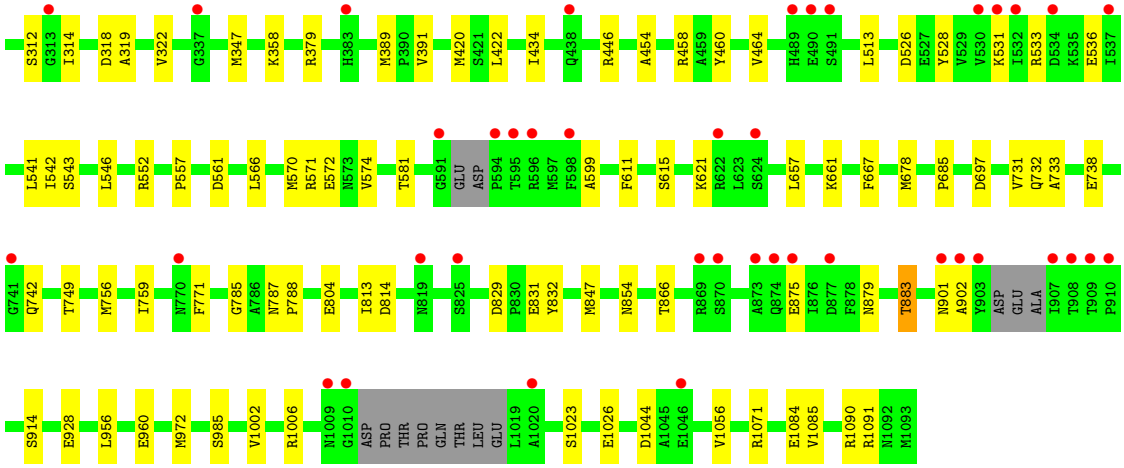


• Molecule 1: Isobutyryl-CoA mutase fused

Chain B:






S312 G313 I314 D318 A319 V322 G337 M347 K358 R379 H383 M389 P390 V391 M420 S421 L422 I434 Q438 R446 A454 R458 A459 Y460 V464 H489 E490 S491 L513 D526 E527 Y528 V529 V530 K531 I532 R533 D534 K535 E536 I537
L541 I542 S543 L546 R552 P557 D561 L566 M570 R571 E572 N573 V574 T581 G591 GLU ASP P594 T595 R596 M597 F598 A599 F611 S615 K621 R622 L623 S624 L657 K661 F667 M678 P685 D697 V731 Q732 A733 E738
G741 Q742 T749 M756 I759 N770 F771 G785 A786 N787 P788 E804 I813 D814 N819 S825 D829 P830 E831 Y832 M847 N854 T866 R869 S870 A873 Q874 E875 I876 D877 F878 N879 T883 N901 A902 Y903 ASP GLU ALA I907 T908 T909 P910
S914 E928 L956 E960 M972 S985 V1002 R1006 N1009 G1010 ASP PRO THR PRO GLN THR LEU GLU L1019 A1020 S1023 E1026 D1044 A1045 E1046 V1056 R1071 E1084 V1085 R1090 R1091 N1092 M1093

4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	317.56Å 317.56Å 343.52Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	34.91 – 3.45 34.91 – 3.45	Depositor EDS
% Data completeness (in resolution range)	99.0 (34.91-3.45) 99.0 (34.91-3.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$< I/\sigma(I) >$ [1]	1.72 (at 3.47Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.193 , 0.214 0.198 , 0.217	Depositor DCC
R_{free} test set	4357 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	89.2	Xtriage
Anisotropy	0.274	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 65.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	16519	wwPDB-VP
Average B, all atoms (Å^2)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.08% 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: MG, B12, 5AD, GDP, IVC

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	0.28	0/8234	0.70	0/11154
1	B	0.29	0/8205	0.71	3/11107 (0.0%)
All	All	0.28	0/16439	0.71	3/22261 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	552	ARG	NE-CZ-NH2	6.54	125.08	119.20
1	B	552	ARG	NE-CZ-NH1	-5.98	115.52	121.50
1	B	533	ARG	CB-CA-C	-5.06	110.35	117.23

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8093	0	7834	92	0
1	B	8067	0	7806	69	0
2	A	91	0	88	10	0
2	B	91	0	88	6	0
3	A	36	0	26	3	0
4	A	54	0	42	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	27	0	13	0	0
5	A	28	0	12	3	0
5	B	28	0	12	3	0
6	A	2	0	0	0	0
6	B	2	0	0	0	0
All	All	16519	0	15921	164	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 5.

The worst 5 of 164 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:GLN:HE22	2:A:1101:B12:H421	1.44	0.82
1:A:783:GLU:HB3	2:A:1101:B12:H532	1.64	0.78
1:B:615:SER:O	1:B:621:LYS:NZ	2.25	0.69
1:A:779:TYR:OH	3:A:1102[B]:5AD:O3'	2.13	0.66
1:A:821:SER:HG	4:A:1103:IVC:H25	1.39	0.66

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	1053/1113 (95%)	1009 (96%)	42 (4%)	2 (0%)	43 74
1	B	1051/1113 (94%)	1014 (96%)	34 (3%)	3 (0%)	36 67
All	All	2104/2226 (94%)	2023 (96%)	76 (4%)	5 (0%)	43 74

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	732	GLN
1	B	1091	ARG
1	A	489	HIS
1	B	319	ALA
1	A	741	GLY

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	823/906 (91%)	812 (99%)	11 (1%)	61	73
1	B	817/906 (90%)	810 (99%)	7 (1%)	70	76
All	All	1640/1812 (90%)	1622 (99%)	18 (1%)	65	75

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	574	VAL
1	B	1044	ASP
1	B	883	THR
1	A	909	THR
1	B	543	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	872	HIS
1	B	899	HIS
1	B	901	ASN
1	A	732	GLN
1	A	707	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 (i)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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	$\#\|Z\| >$
3	5AD	A	1102[B]	-	20,20,20	0.09	0	28,30,30	0.19	0
4	IVC	A	1103	-	54,56,56	0.42	0	77,83,83	0.52	0
2	B12	B	1101	1	94,101,101	0.75	4 (4%)	149,166,166	1.02	12 (8%)
5	GDP	A	1104	6	29,30,30	2.52	11 (37%)	45,47,47	1.66	9 (20%)
3	5AD	A	1102[A]	-	20,20,20	0.10	0	28,30,30	0.30	0
5	GDP	B	1103	6	29,30,30	2.53	11 (37%)	45,47,47	1.66	9 (20%)
4	IVC	B	1102	-	29,29,56	0.40	0	44,45,83	0.53	1 (2%)
2	B12	A	1101	1	94,101,101	0.77	4 (4%)	149,166,166	1.08	13 (8%)

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	5AD	A	1102[B]	-	-	0/4/20/20	0/3/3/3
4	IVC	A	1103	-	-	13/55/71/71	0/3/3/3
2	B12	B	1101	1	-	15/56/223/223	0/3/11/11
5	GDP	A	1104	6	-	0/16/32/32	0/3/3/3
3	5AD	A	1102[A]	-	-	0/4/20/20	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GDP	B	1103	6	-	0/16/32/32	0/3/3/3
4	IVC	B	1102	-	-	3/15/31/71	0/3/3/3
2	B12	A	1101	1	-	16/56/223/223	0/3/11/11

The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1103	GDP	O6-C6	7.13	1.37	1.23
5	A	1104	GDP	O6-C6	7.08	1.37	1.23
5	B	1103	GDP	C2-N2	6.04	1.48	1.34
5	A	1104	GDP	C2-N2	6.03	1.48	1.34
2	B	1101	B12	C14-N23	4.19	1.40	1.35

The worst 5 of 44 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1104	GDP	C5-C4-N3	-5.29	119.97	128.39
5	B	1103	GDP	C5-C4-N3	-5.28	119.98	128.39
5	A	1104	GDP	C2-N3-C4	4.58	120.19	112.30
5	B	1103	GDP	C2-N3-C4	4.56	120.15	112.30
5	B	1103	GDP	N9-C4-N3	3.62	133.19	125.95

There are no chirality outliers.

5 of 47 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1101	B12	C1P-C2P-O3-P
2	A	1101	B12	C3P-C2P-O3-P
4	A	1103	IVC	C5-O4-P2-O12
4	A	1103	IVC	C5-O4-P2-O10
4	A	1103	IVC	C5-O4-P2-O7

There are no ring outliers.

7 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1102[B]	5AD	2	0
4	A	1103	IVC	7	0
2	B	1101	B12	6	0
5	A	1104	GDP	3	0

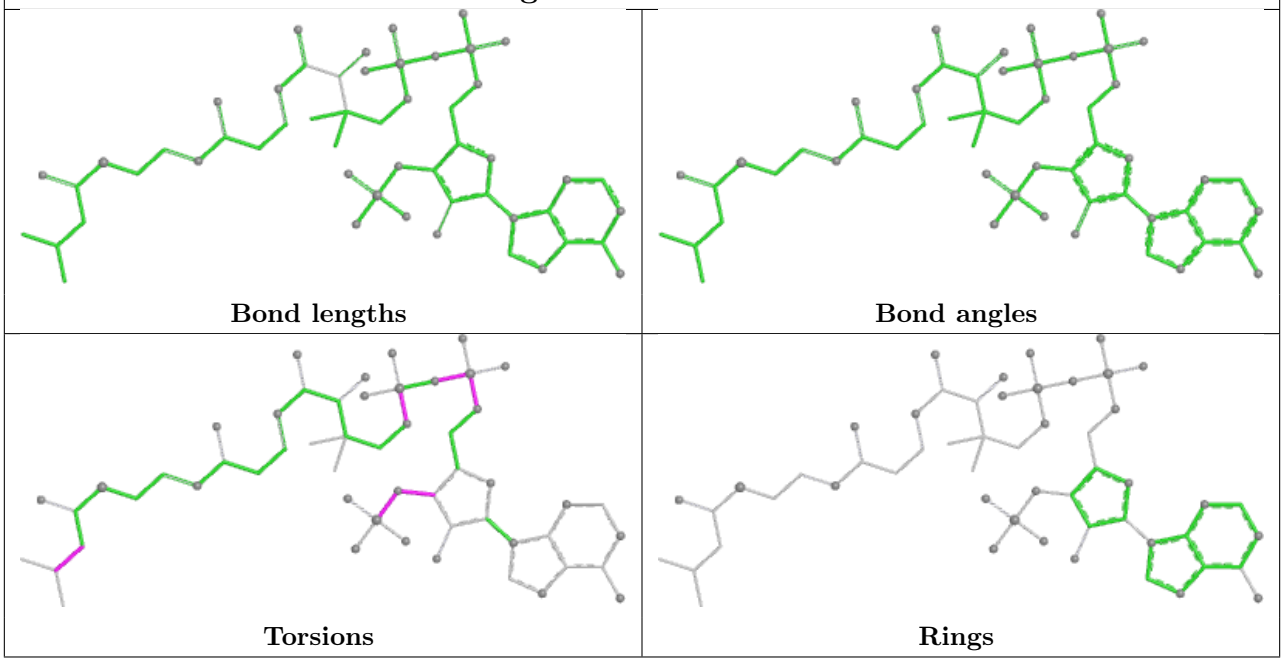
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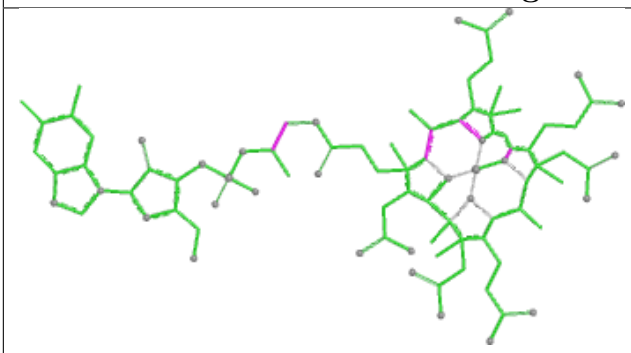
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1102[A]	5AD	1	0
5	B	1103	GDP	3	0
2	A	1101	B12	10	0

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.

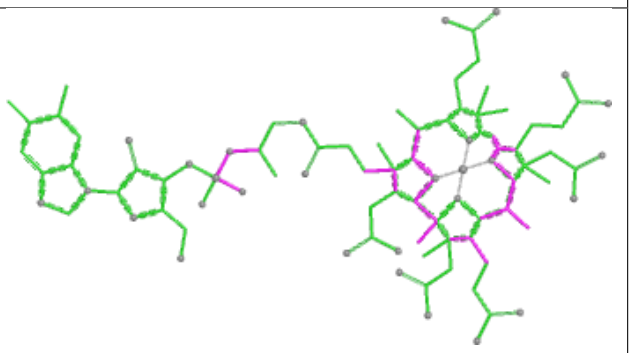
Ligand IVC A 1103



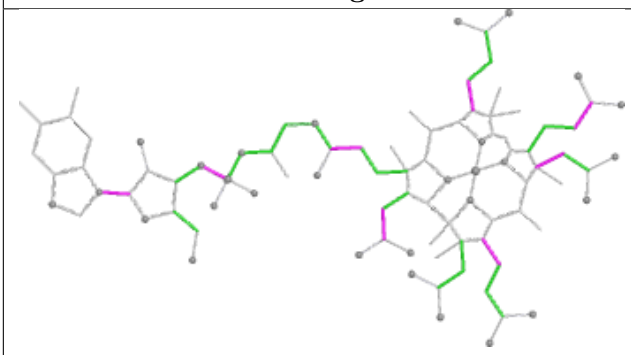
Ligand B12 B 1101



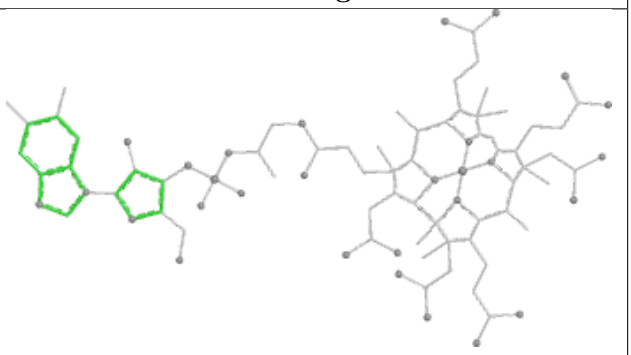
Bond lengths



Bond angles

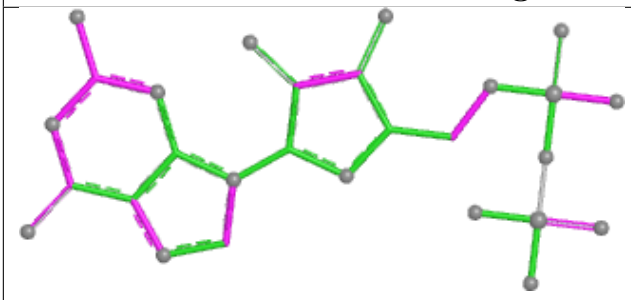


Torsions

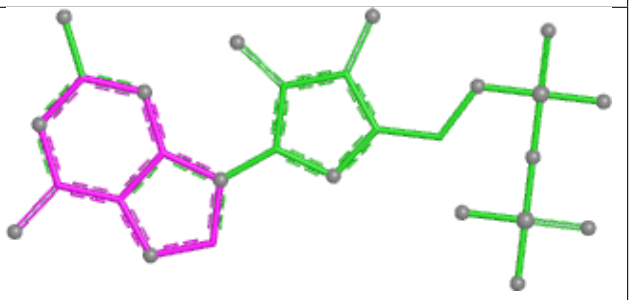


Rings

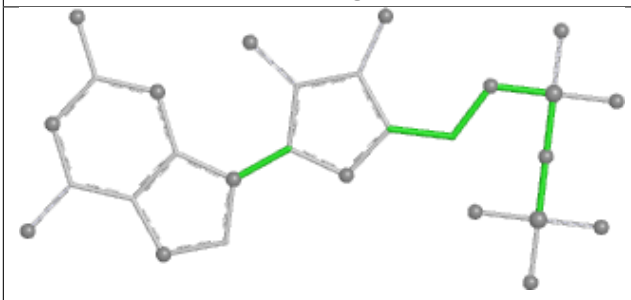
Ligand GDP A 1104



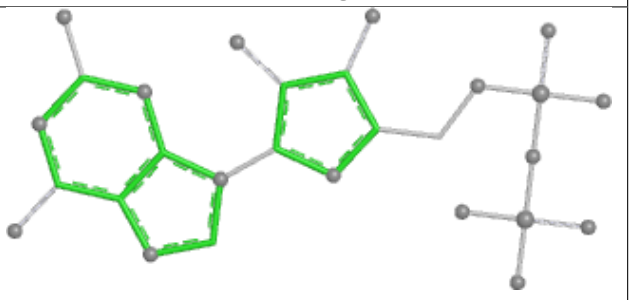
Bond lengths



Bond angles

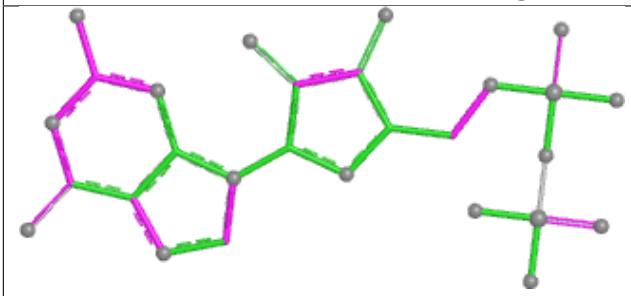


Torsions

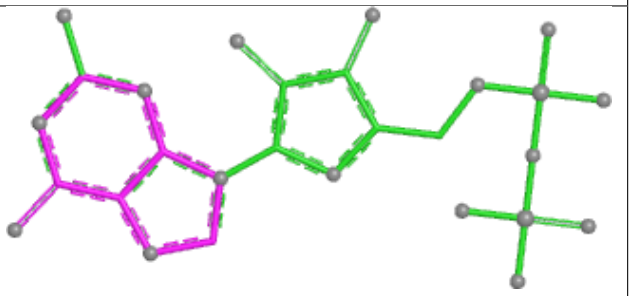


Rings

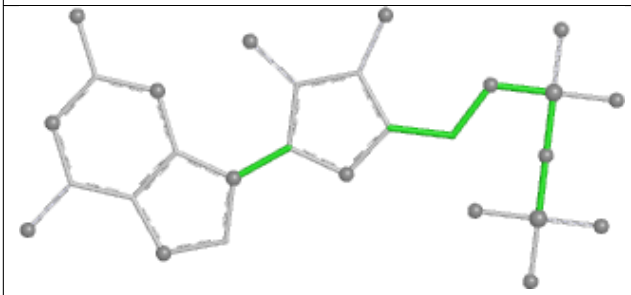
Ligand GDP B 1103



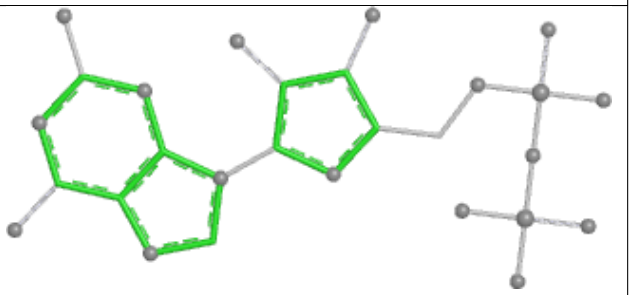
Bond lengths



Bond angles

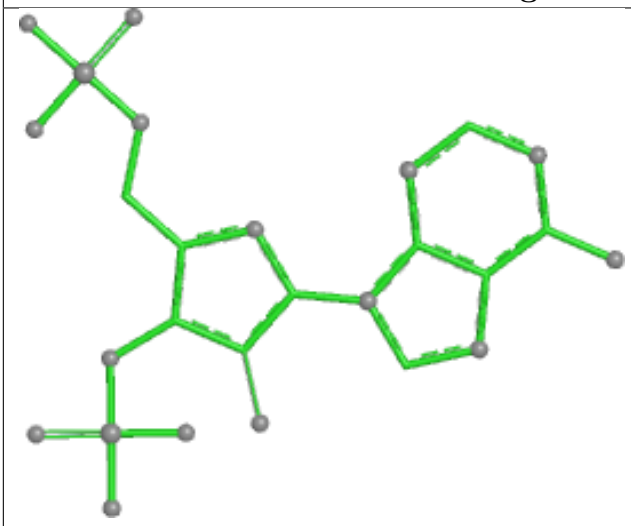


Torsions

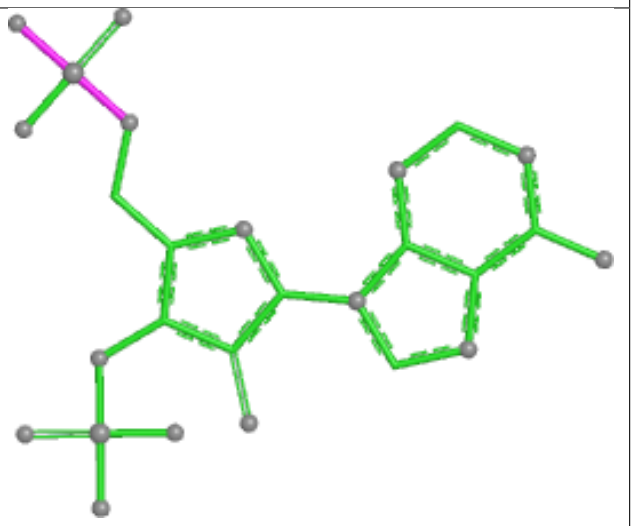


Rings

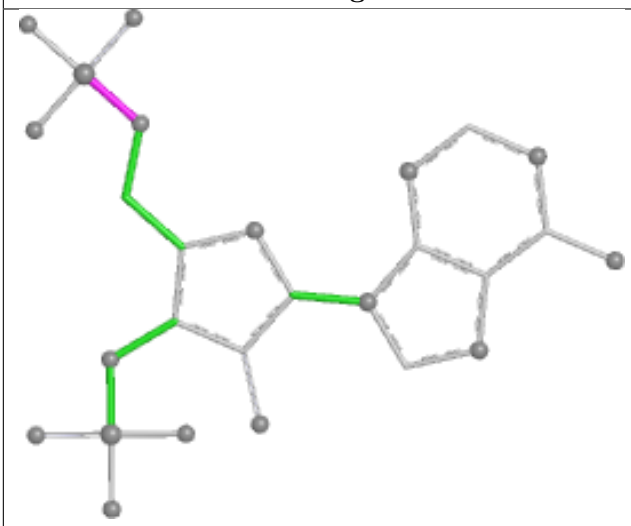
Ligand IVC B 1102



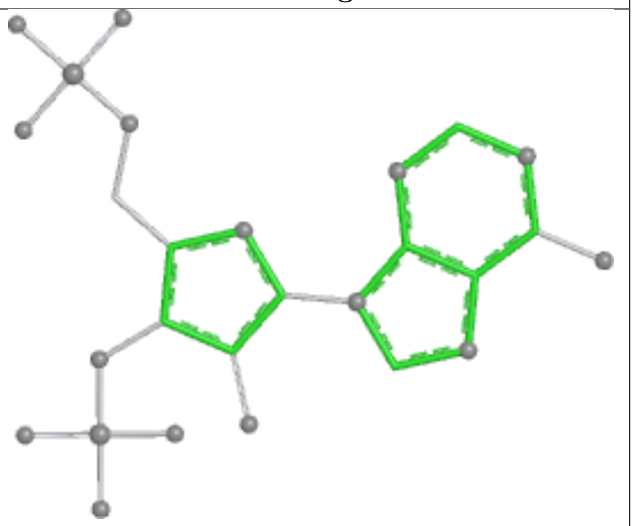
Bond lengths



Bond angles

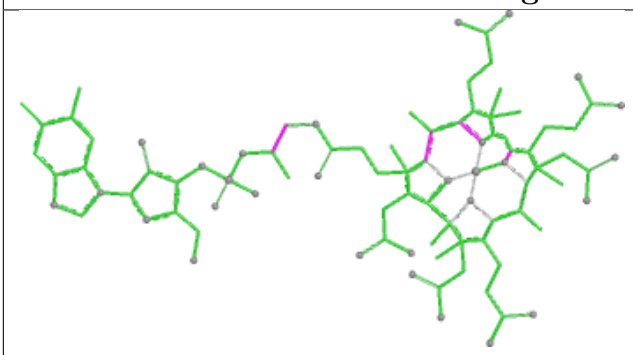


Torsions

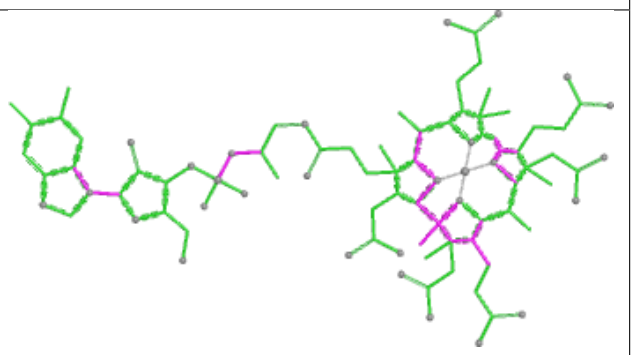


Rings

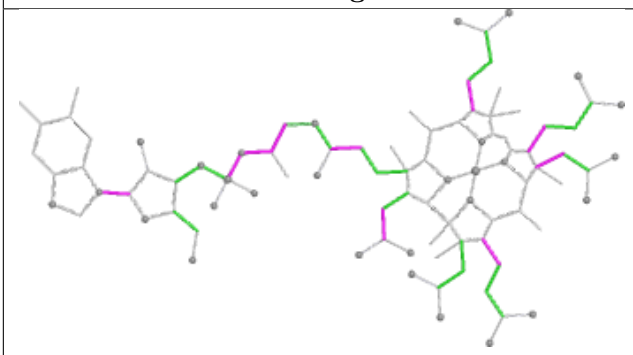
Ligand B12 A 1101



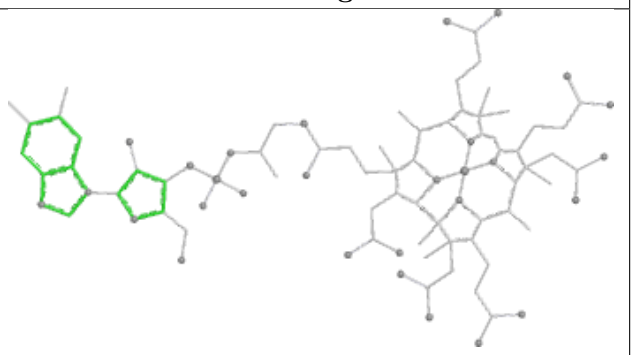
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	1061/1113 (95%)	0.16	33 (3%)	51	31	58, 88, 139, 180	0
1	B	1059/1113 (95%)	0.12	47 (4%)	39	23	55, 82, 137, 212	0
All	All	2120/2226 (95%)	0.14	80 (3%)	44	26	55, 85, 139, 212	0

The worst 5 of 80 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1011	ASP	10.7
1	B	903	TYR	7.3
1	B	908	THR	6.0
1	B	877	ASP	5.9
1	B	909	THR	5.3

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

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

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

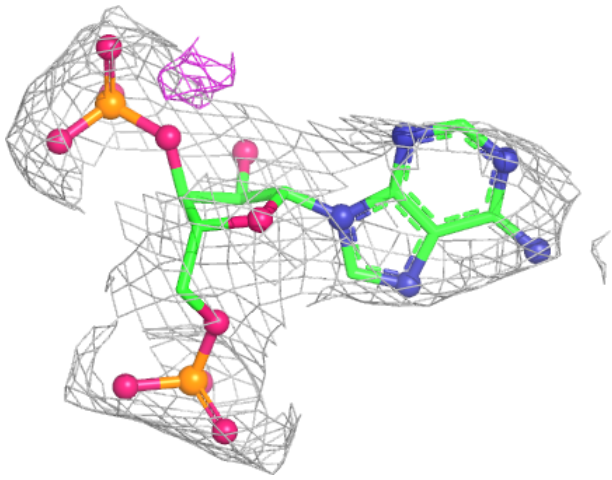
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

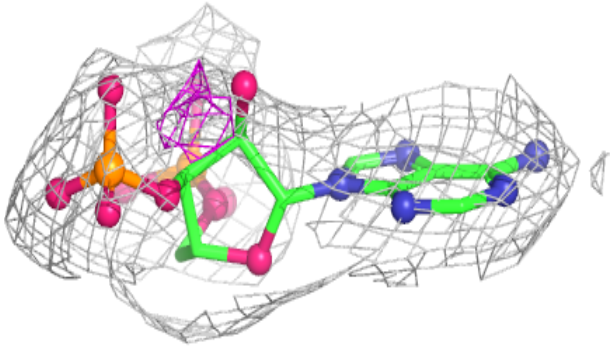
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	IVC	B	1102	27/54	0.78	0.12	130,147,183,185	0
3	5AD	A	1102[B]	18/18	0.86	0.25	108,113,115,115	18
3	5AD	A	1102[A]	18/18	0.86	0.25	107,112,115,115	18
4	IVC	A	1103	54/54	0.92	0.14	76,114,161,164	0
2	B12	B	1101	91/91	0.94	0.13	91,113,136,139	0
6	MG	A	1106	1/1	0.96	0.07	78,78,78,78	0
5	GDP	B	1103	28/28	0.97	0.07	55,65,72,123	0
2	B12	A	1101	91/91	0.97	0.09	51,65,80,83	0
5	GDP	A	1104	28/28	0.98	0.06	70,89,96,98	0
6	MG	A	1105	1/1	0.99	0.04	64,64,64,64	0
6	MG	B	1104	1/1	0.99	0.05	42,42,42,42	0
6	MG	B	1105	1/1	0.99	0.07	43,43,43,43	0

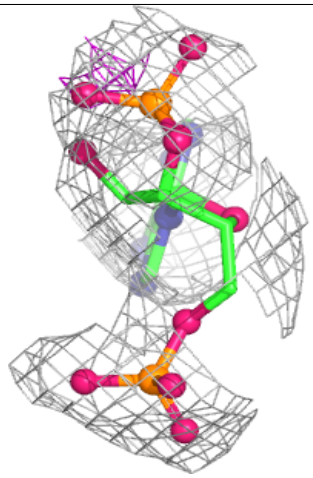
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around IVC B 1102:

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

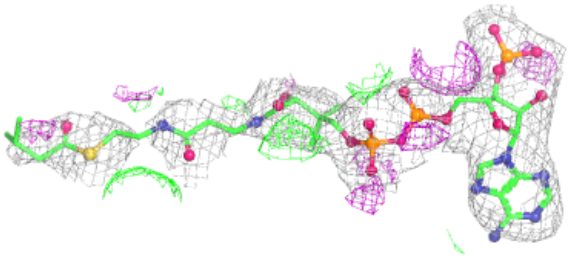




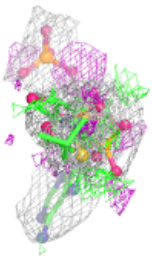


Electron density around IVC A 1103:

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

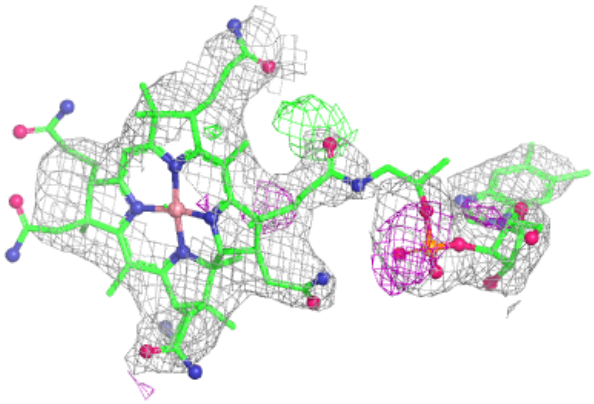


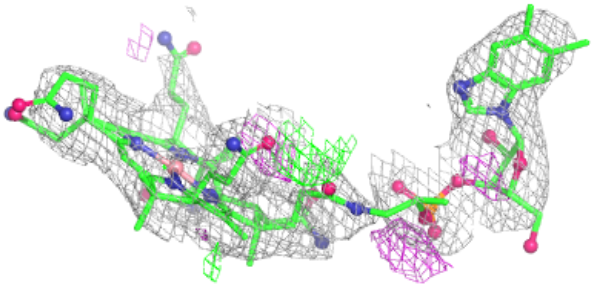


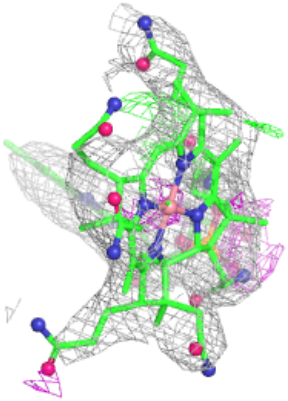


Electron density around B12 B 1101:

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

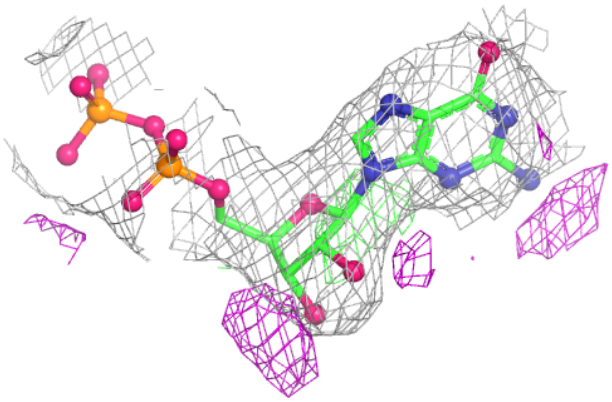


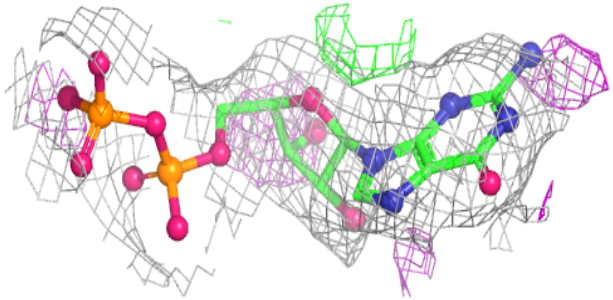


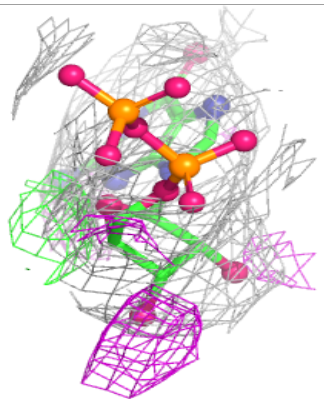


Electron density around GDP B 1103:

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

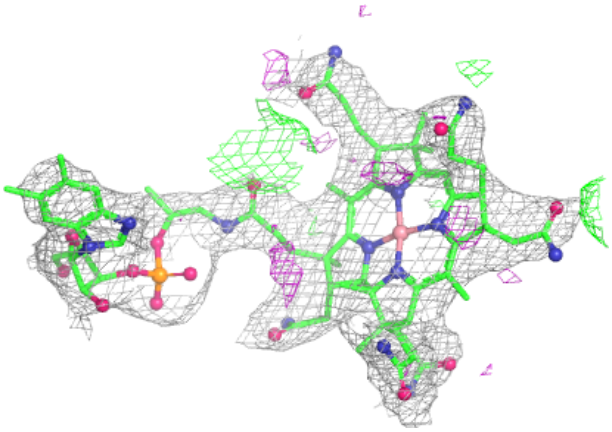


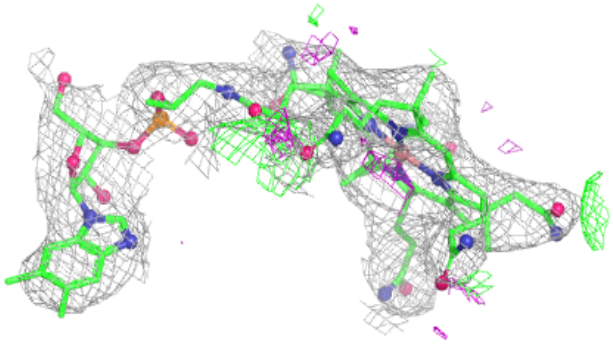


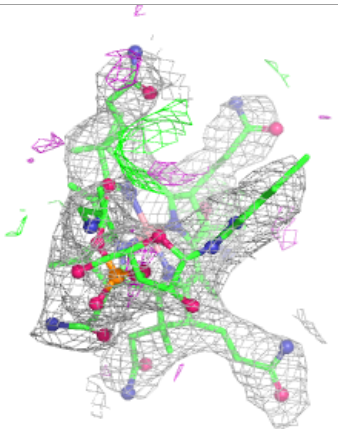


Electron density around B12 A 1101:

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

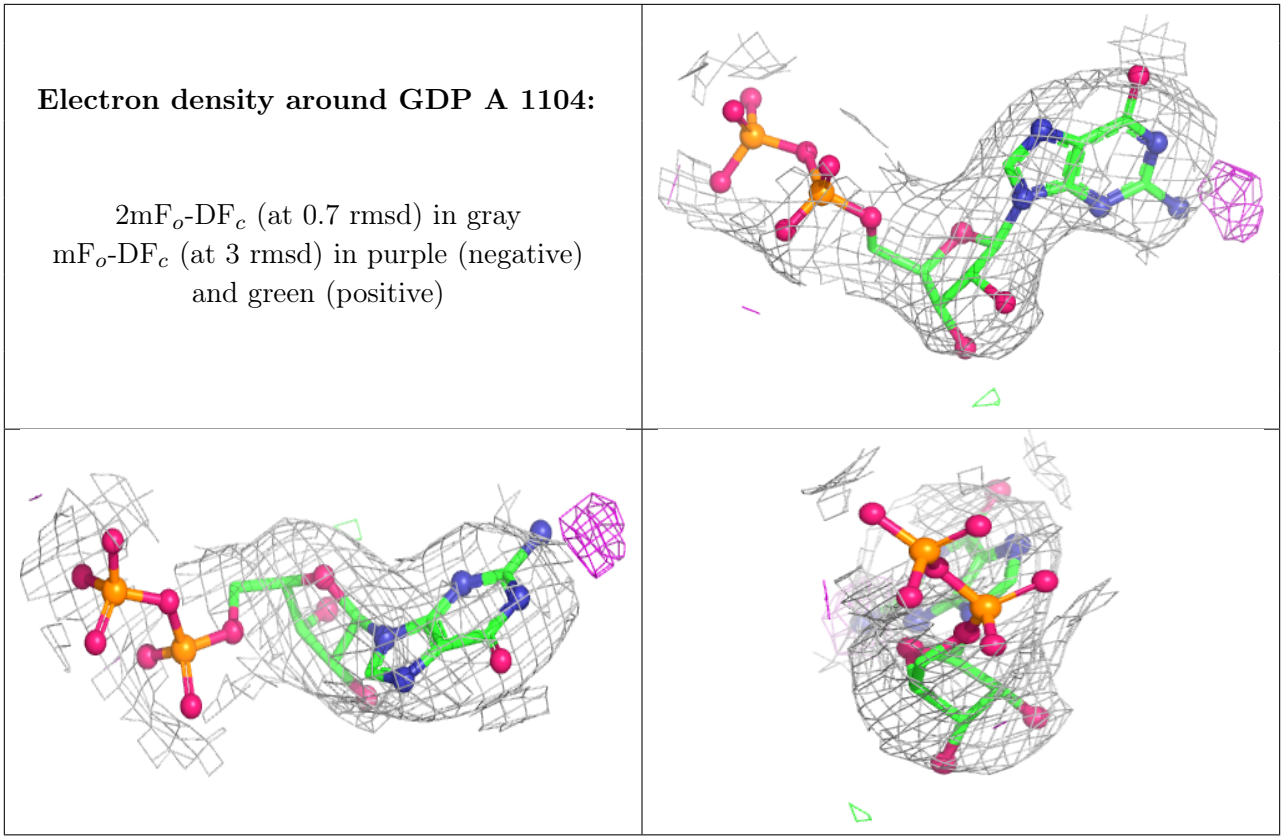






Electron density around GDP A 1104:

$2mF_o$-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.