Full wwPDB X-ray Structure Validation Report ⓘ

Dec 4, 2023 – 07:43 pm GMT

PDB ID	:	2C59
Title	:	gdp-mannose-3', 5' -epimerase (arabidopsis thaliana), with gdp-alpha-d-mannose and gdp-beta-l-galactose bound in the active site.
Authors	:	Major, L.L.; Wolucka, B.A.; Naismith, J.H.
Deposited on	:	2005-10-26
Resolution	:	2.00 Å(reported)

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

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

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

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

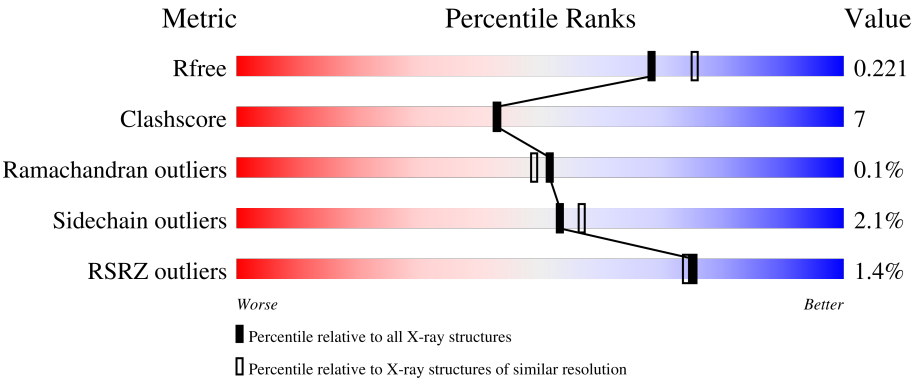
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	379	2% 82% 13% .
1	B	379	% 83% 12% . .

2 Entry composition (i)

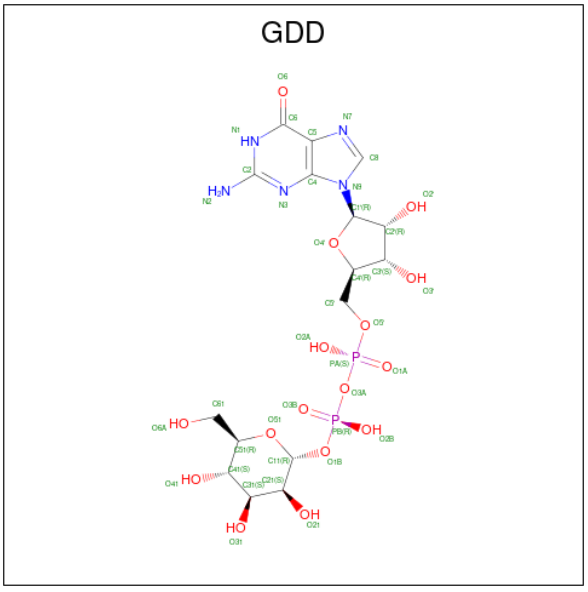
There are 7 unique types of molecules in this entry. The entry contains 7048 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 GDP-MANNOSE-3', 5'-EPIMERASE.

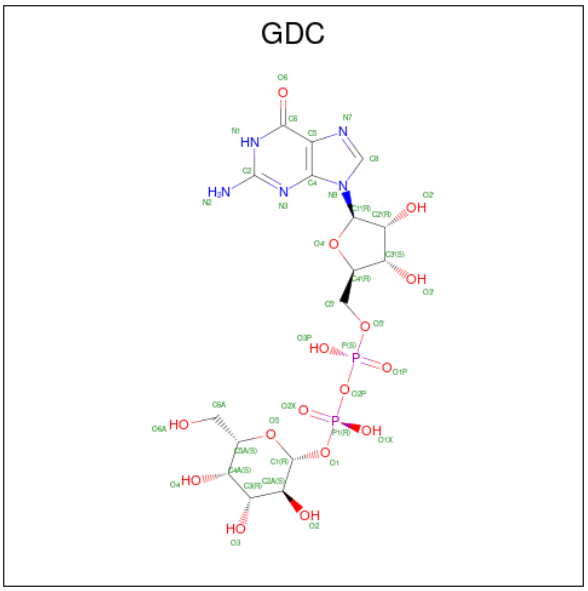
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	364	Total	C	N	O	S	0	7	0
			2944	1864	504	554	22			
1	B	362	Total	C	N	O	S	0	16	0
			2975	1888	511	553	23			

- Molecule 2 is GUANOSINE-5'-DIPHOSPHATE-ALPHA-D-MANNOSE (three-letter code: GDD) (formula: $C_{16}H_{25}N_5O_{16}P_2$).



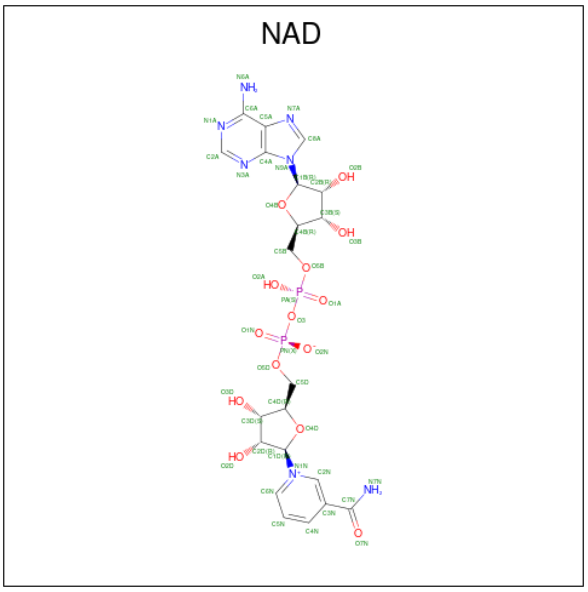
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	1
			39	16	5	16	2		
2	B	1	Total	C	N	O	P	0	1
			39	16	5	16	2		

- Molecule 3 is GUANOSINE-5'-DIPHOSPHATE-BETA-L-GALACTOSE (three-letter code: GDC) (formula: $C_{16}H_{25}N_5O_{16}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	1
			39	16	5	16	2		
3	B	1	Total	C	N	O	P	0	1
			39	16	5	16	2		

- Molecule 4 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

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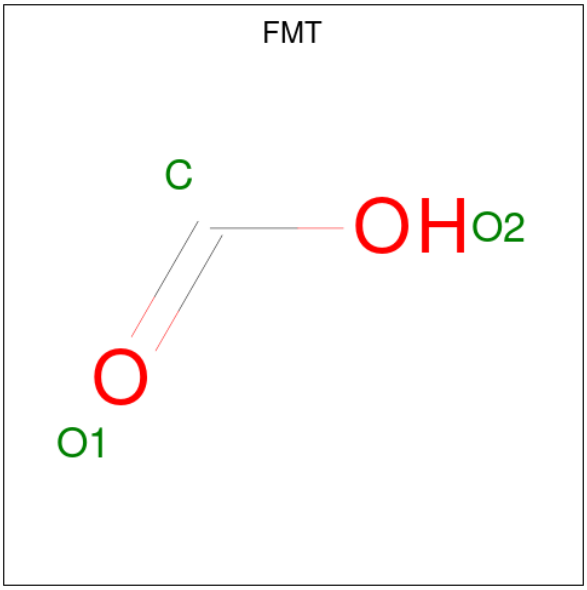
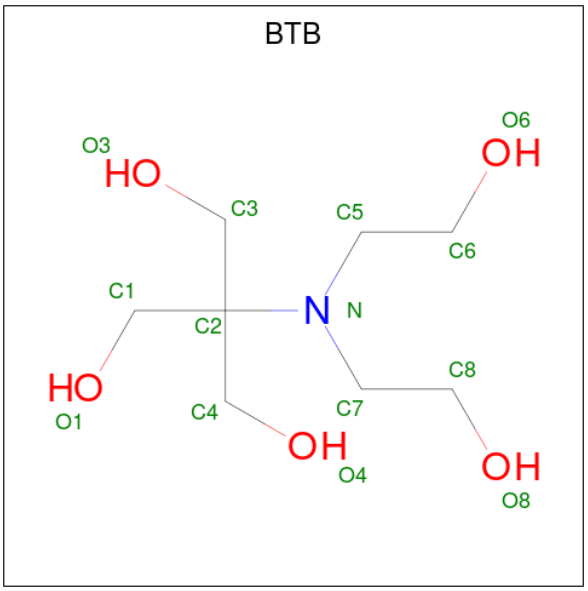
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 5 is FORMIC ACID (three-letter code: FMT) (formula: CH_2O_2).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O		0	0
			3	1	2			
5	A	1	Total	C	O		0	0
			3	1	2			
5	A	1	Total	C	O		0	0
			3	1	2			
5	B	1	Total	C	O		0	0
			3	1	2			
5	B	1	Total	C	O		0	0
			3	1	2			
5	B	1	Total	C	O		0	0
			3	1	2			
5	B	1	Total	C	O		0	0
			3	1	2			
5	B	1	Total	C	O		0	0
			3	1	2			

- Molecule 6 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: BTB) (formula: $C_8H_{19}NO_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C N O 14 8 1 5	0	0

- Molecule 7 is water.

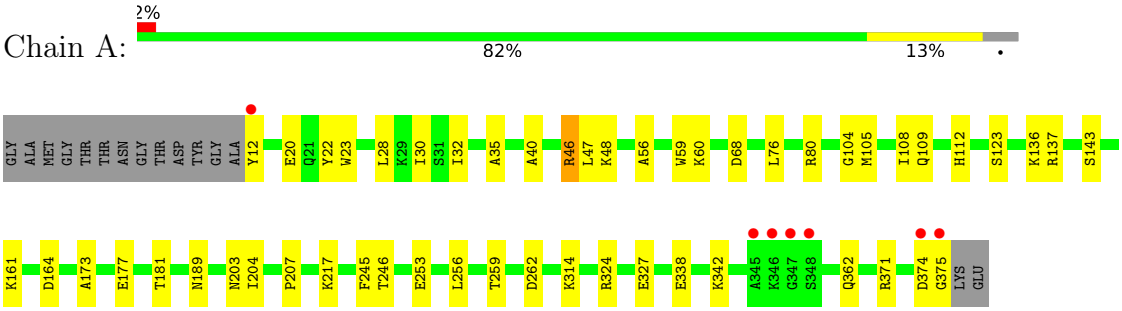
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	391	Total O 391 391	0	0
7	B	456	Total O 456 456	0	0

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.

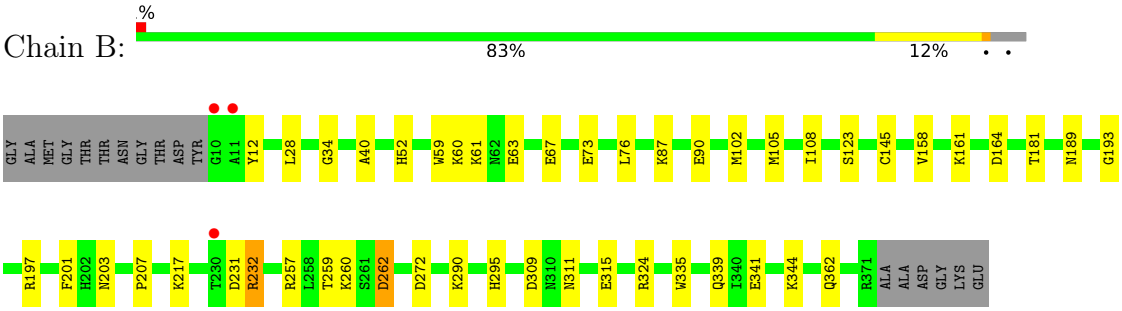
• Molecule 1: GDP-MANNOSE-3', 5'-EPIMERASE

Chain A:



• Molecule 1: GDP-MANNOSE-3', 5'-EPIMERASE

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	62.81Å 83.81Å 66.29Å 90.00° 98.91° 90.00°	Depositor
Resolution (Å)	29.88 – 2.00 29.64 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.6 (29.88-2.00) 99.6 (29.64-2.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.10 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.147 , 0.223 0.145 , 0.221	Depositor DCC
R_{free} test set	2324 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	23.9	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 68.5	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	0.97	EDS
Total number of atoms	7048	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.02% 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: FMT, GDC, GDD, BTB, NAD

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	0.94	2/3037 (0.1%)	0.82	1/4086 (0.0%)
1	B	0.93	1/3102 (0.0%)	0.82	2/4169 (0.0%)
All	All	0.93	3/6139 (0.0%)	0.82	3/8255 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	201	PHE	CE1-CZ	5.66	1.48	1.37
1	A	253	GLU	CB-CG	5.23	1.62	1.52
1	A	245	PHE	CE1-CZ	5.17	1.47	1.37

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	272	ASP	CB-CG-OD1	5.95	123.65	118.30
1	B	309	ASP	CB-CG-OD1	5.56	123.30	118.30
1	A	80	ARG	NE-CZ-NH2	-5.29	117.65	120.30

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	2944	0	2864	41	0
1	B	2975	0	2917	37	0
2	A	39	0	23	1	0
2	B	39	0	23	3	0
3	A	39	0	23	1	0
3	B	39	0	23	0	0
4	A	44	0	26	0	0
4	B	44	0	26	1	0
5	A	9	0	3	0	0
5	B	15	0	5	1	0
6	B	14	0	19	4	0
7	A	391	0	0	10	1
7	B	456	0	0	15	1
All	All	7048	0	5952	83	1

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 7.

All (83) 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:262[B]:ASP:OD2	7:B:2312:HOH:O	1.62	1.15
1:B:87:LYS:HD2	7:B:2140:HOH:O	1.50	1.11
1:A:374:ASP:HB2	1:A:375:GLY:HA3	1.28	1.08
1:B:262[A]:ASP:OD2	7:B:2313:HOH:O	1.73	1.07
1:A:177[A]:GLU:OE2	7:A:2181:HOH:O	1.76	1.02
1:A:262[B]:ASP:OD1	7:A:2241:HOH:O	1.80	0.97
1:A:105:MET:CE	1:A:108[B]:ILE:HD11	1.96	0.96
1:B:28:LEU:H	1:B:52:HIS:HD2	1.11	0.90
1:B:231:ASP:HB3	1:B:232:ARG:HH21	1.34	0.89
1:A:105:MET:HE3	1:A:108[B]:ILE:HD11	1.58	0.86
1:A:327[B]:GLU:OE2	7:A:2330:HOH:O	1.93	0.84
1:B:262[A]:ASP:OD1	7:B:2311:HOH:O	1.94	0.84
1:B:145:CYS:SG	2:B:1377[A]:GDD:O41	2.20	0.80
1:B:73:GLU:OE1	6:B:1376:BTB:H71	1.83	0.78
1:A:177[A]:GLU:OE2	7:A:2183:HOH:O	2.06	0.74
1:A:108[B]:ILE:HD13	1:A:109:GLN:N	2.02	0.73
1:A:105:MET:HA	1:A:108[B]:ILE:HD12	1.71	0.71
1:A:324:ARG:HB2	1:A:327[B]:GLU:HG3	1.72	0.70
1:A:136:LYS:NZ	7:A:2134:HOH:O	2.25	0.69
1:B:28:LEU:H	1:B:52:HIS:CD2	2.03	0.68
1:B:60[A]:LYS:HE2	1:B:63:GLU:OE2	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:362:GLN:HG2	7:B:2194:HOH:O	1.93	0.67
1:A:108[B]:ILE:HD13	1:A:109:GLN:H	1.58	0.67
1:A:374:ASP:HB2	1:A:375:GLY:CA	2.16	0.63
1:B:257:ARG:HA	1:B:260:LYS:HE2	1.82	0.61
1:A:374:ASP:CB	1:A:375:GLY:HA3	2.15	0.60
6:B:1376:BTB:H81	7:B:2141:HOH:O	2.00	0.60
1:B:231:ASP:HB3	1:B:232:ARG:NH2	2.14	0.59
1:B:145:CYS:HG	2:B:1377[A]:GDD:C41	2.13	0.58
1:A:60:LYS:HG2	1:A:371:ARG:HB2	1.86	0.58
1:A:12:TYR:OH	1:A:338:GLU:OE1	2.22	0.57
1:A:177[A]:GLU:HG2	7:A:2181:HOH:O	2.05	0.57
1:A:22:TYR:HB2	1:A:256:LEU:HD13	1.87	0.56
6:B:1376:BTB:H31	7:B:2448:HOH:O	2.06	0.56
1:A:48:LYS:HE2	1:A:68:ASP:O	2.05	0.56
1:B:232:ARG:HD3	1:B:295:HIS:CE1	2.41	0.55
1:A:342:LYS:NZ	7:A:2336:HOH:O	2.40	0.55
1:A:105:MET:HA	1:A:108[B]:ILE:CD1	2.36	0.54
1:B:311[B]:ASN:ND2	7:B:2365:HOH:O	2.40	0.54
1:B:108:ILE:HD13	2:B:1377[A]:GDD:O31	2.07	0.54
1:A:23:TRP:CD1	1:A:28:LEU:HD11	2.43	0.53
6:B:1376:BTB:H41	6:B:1376:BTB:C8	2.39	0.52
1:A:105:MET:HE1	1:A:108[B]:ILE:HD11	1.87	0.51
1:A:177[A]:GLU:CG	7:A:2181:HOH:O	2.58	0.51
1:A:204:ILE:HD13	1:A:246:THR:HB	1.92	0.50
1:B:60[A]:LYS:HE2	7:B:2092:HOH:O	2.11	0.50
1:B:61[A]:LYS:NZ	1:B:67:GLU:OE2	2.36	0.50
1:A:137:ARG:HD3	1:A:259:THR:O	2.13	0.49
1:B:28:LEU:N	1:B:52:HIS:HD2	1.94	0.49
1:A:20:GLU:O	1:A:46:ARG:NH2	2.45	0.49
1:A:143:SER:OG	2:A:1377[A]:GDD:O41	2.31	0.48
1:A:327[B]:GLU:CD	7:A:2329:HOH:O	2.51	0.48
1:B:123:SER:HB3	1:B:181:THR:HG21	1.95	0.48
1:A:161:LYS:O	1:A:164:ASP:HB2	2.14	0.47
1:B:102[B]:MET:HG2	4:B:1380:NAD:O3	2.13	0.47
1:A:203:ASN:N	3:A:1378[B]:GDC:O6A	2.40	0.47
1:B:52:HIS:HE1	7:B:2077:HOH:O	1.97	0.47
1:A:112:HIS:HD2	1:A:173:ALA:H	1.63	0.46
1:B:231:ASP:CB	1:B:232:ARG:HH21	2.17	0.46
1:B:197:ARG:HG3	1:B:259:THR:HA	1.98	0.46
1:B:12:TYR:HB3	1:B:207:PRO:HG2	1.98	0.46
1:B:90[A]:GLU:HG3	7:B:2143:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:ALA:HB3	1:A:56:ALA:HB1	1.97	0.45
1:B:108:ILE:HD12	7:B:2244:HOH:O	2.16	0.45
1:A:104:GLY:O	1:A:108[B]:ILE:HG23	2.17	0.45
1:A:12:TYR:HB3	1:A:207:PRO:HG2	2.00	0.43
1:B:335:TRP:O	1:B:339:GLN:HG2	2.18	0.43
1:B:105[A]:MET:HE1	1:B:108:ILE:HD11	1.99	0.43
1:B:61[A]:LYS:HE2	1:B:76:LEU:HD22	2.00	0.42
1:B:324[B]:ARG:NH1	7:B:2381:HOH:O	2.52	0.42
1:A:204:ILE:HA	1:A:246:THR:O	2.20	0.42
1:B:161:LYS:O	1:B:164:ASP:HB2	2.20	0.42
1:A:362:GLN:HE21	1:A:362:GLN:HB2	1.67	0.42
1:B:193:GLY:HA2	7:B:2270:HOH:O	2.18	0.42
1:A:123:SER:HB3	1:A:181:THR:HG21	2.01	0.41
1:A:30:ILE:HD13	1:A:47:LEU:HD13	2.03	0.41
1:B:290:LYS:O	7:B:2345:HOH:O	2.22	0.41
1:A:32:ILE:HG22	1:A:40:ALA:HB1	2.03	0.41
1:B:34:GLY:O	1:B:40:ALA:HB3	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:2288:HOH:O	7:B:2088:HOH:O[2_656]	2.05	0.15

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	369/379 (97%)	357 (97%)	12 (3%)	0	100	100
1	B	376/379 (99%)	368 (98%)	7 (2%)	1 (0%)	41	37
All	All	745/758 (98%)	725 (97%)	19 (3%)	1 (0%)	51	49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	203	ASN

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	317/319 (99%)	312 (98%)	5 (2%)	62	67
1	B	325/319 (102%)	315 (97%)	10 (3%)	40	40
All	All	642/638 (101%)	627 (98%)	15 (2%)	53	53

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

Mol	Chain	Res	Type
1	A	46	ARG
1	A	59	TRP
1	A	76	LEU
1	A	189	ASN
1	A	217	LYS
1	B	59	TRP
1	B	158	VAL
1	B	189	ASN
1	B	217	LYS
1	B	232	ARG
1	B	262[A]	ASP
1	B	262[B]	ASP
1	B	341	GLU
1	B	344[A]	LYS
1	B	344[B]	LYS

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

Mol	Chain	Res	Type
1	A	42	HIS

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Mol	Chain	Res	Type
1	A	112	HIS
1	A	362	GLN
1	B	52	HIS
1	B	362	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

15 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	FMT	B	1372	-	2,2,2	0.76	0	1,1,1	0.24	0
3	GDC	B	1378[B]	-	35,42,42	0.89	0	46,65,65	1.53	6 (13%)
6	BTB	B	1376	-	13,13,13	1.27	2 (15%)	7,16,16	1.45	2 (28%)
5	FMT	A	1381	-	2,2,2	0.60	0	1,1,1	0.12	0
4	NAD	A	1379	-	42,48,48	1.68	3 (7%)	50,73,73	1.74	8 (16%)
2	GDD	B	1377[A]	-	35,42,42	0.75	0	46,65,65	1.44	8 (17%)
5	FMT	B	1374	-	2,2,2	0.91	0	1,1,1	0.42	0
5	FMT	B	1375	-	2,2,2	0.69	0	1,1,1	0.10	0
5	FMT	A	1382	-	2,2,2	0.65	0	1,1,1	0.15	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	GDD	A	1377[A]	-	35,42,42	0.91	1 (2%)	46,65,65	1.35	7 (15%)
5	FMT	B	1371	-	2,2,2	0.71	0	1,1,1	0.23	0
5	FMT	A	1380	-	2,2,2	0.76	0	1,1,1	0.17	0
3	GDC	A	1378[B]	-	35,42,42	0.99	1 (2%)	46,65,65	1.93	9 (19%)
4	NAD	B	1380	-	42,48,48	1.61	4 (9%)	50,73,73	1.56	5 (10%)
5	FMT	B	1373	-	2,2,2	0.65	0	1,1,1	0.22	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
3	GDC	B	1378[B]	-	-	1/19/59/59	0/4/4/4
6	BTB	B	1376	-	-	10/21/21/21	-
4	NAD	A	1379	-	-	5/26/62/62	0/5/5/5
2	GDD	B	1377[A]	-	-	2/19/59/59	0/4/4/4
2	GDD	A	1377[A]	-	-	1/19/59/59	0/4/4/4
3	GDC	A	1378[B]	-	-	5/19/59/59	0/4/4/4
4	NAD	B	1380	-	-	4/26/62/62	0/5/5/5

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1379	NAD	O7N-C7N	7.62	1.38	1.24
4	B	1380	NAD	O7N-C7N	7.57	1.38	1.24
4	A	1379	NAD	C2A-N3A	4.41	1.39	1.32
4	B	1380	NAD	C2A-N3A	3.37	1.37	1.32
4	A	1379	NAD	C2A-N1A	3.20	1.39	1.33
6	B	1376	BTB	C5-N	3.17	1.52	1.48
4	B	1380	NAD	C2N-N1N	3.06	1.38	1.35
2	A	1377[A]	GDD	O4'-C1'	2.33	1.44	1.41
3	A	1378[B]	GDC	O4'-C1'	2.33	1.44	1.41
4	B	1380	NAD	O4B-C4B	-2.18	1.40	1.45
6	B	1376	BTB	C7-N	2.06	1.51	1.48

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1378[B]	GDC	O1-C1-C2A	8.07	123.16	108.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1379	NAD	C3N-C7N-N7N	5.61	124.48	117.75
4	A	1379	NAD	N3A-C2A-N1A	-5.59	119.94	128.68
4	B	1380	NAD	N3A-C2A-N1A	-5.39	120.25	128.68
4	A	1379	NAD	O7N-C7N-C3N	-5.31	113.28	119.63
4	B	1380	NAD	C3N-C7N-N7N	4.96	123.71	117.75
3	B	1378[B]	GDC	O1-C1-C2A	4.84	117.25	108.38
3	A	1378[B]	GDC	C1-O5-C5A	3.96	121.47	113.69
4	B	1380	NAD	O4D-C1D-C2D	-3.66	101.57	106.93
2	B	1377[A]	GDD	O6-C6-C5	-3.62	117.29	124.37
3	B	1378[B]	GDC	O6-C6-C5	-3.62	117.29	124.37
2	B	1377[A]	GDD	O51-C11-O1B	-3.58	106.69	111.36
2	A	1377[A]	GDD	O6-C6-C5	-3.49	117.56	124.37
3	A	1378[B]	GDC	O6-C6-C5	-3.49	117.56	124.37
2	A	1377[A]	GDD	O1B-C11-C21	3.20	114.25	108.38
4	B	1380	NAD	O7N-C7N-C3N	-3.08	115.95	119.63
2	B	1377[A]	GDD	O6-C6-N1	3.02	124.22	120.65
3	B	1378[B]	GDC	O6-C6-N1	3.02	124.22	120.65
3	A	1378[B]	GDC	O2P-P1-O1	2.94	108.42	102.48
2	A	1377[A]	GDD	C5-C6-N1	2.85	118.98	113.95
3	A	1378[B]	GDC	C5-C6-N1	2.85	118.98	113.95
4	A	1379	NAD	C4A-C5A-N7A	-2.80	106.48	109.40
3	A	1378[B]	GDC	O5-C1-C2A	-2.72	104.60	110.35
2	B	1377[A]	GDD	C5-C6-N1	2.56	118.48	113.95
3	B	1378[B]	GDC	C5-C6-N1	2.56	118.48	113.95
6	B	1376	BTB	O8-C8-C7	2.56	121.81	111.19
3	A	1378[B]	GDC	O4-C4A-C3	2.55	116.23	110.35
2	A	1377[A]	GDD	PB-O1B-C11	-2.54	109.91	119.74
4	A	1379	NAD	C6N-N1N-C2N	-2.54	119.66	121.97
2	B	1377[A]	GDD	O21-C21-C31	-2.51	104.54	110.35
4	A	1379	NAD	O4D-C1D-C2D	-2.40	103.42	106.93
2	A	1377[A]	GDD	C8-N7-C5	2.38	107.52	102.99
3	A	1378[B]	GDC	C8-N7-C5	2.38	107.52	102.99
2	A	1377[A]	GDD	O6-C6-N1	2.36	123.43	120.65
3	A	1378[B]	GDC	O6-C6-N1	2.36	123.43	120.65
4	A	1379	NAD	C2A-N1A-C6A	2.33	122.74	118.75
2	B	1377[A]	GDD	O41-C41-C31	-2.24	105.16	110.35
2	A	1377[A]	GDD	O51-C11-O1B	-2.20	108.49	111.36
2	B	1377[A]	GDD	O4'-C1'-C2'	-2.17	103.75	106.93
3	B	1378[B]	GDC	O4'-C1'-C2'	-2.17	103.75	106.93
6	B	1376	BTB	C6-C5-N	2.12	119.87	111.59
4	B	1380	NAD	O4B-C1B-C2B	-2.07	103.91	106.93
4	A	1379	NAD	C5A-C6A-N6A	2.04	123.46	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1377[A]	GDD	N2-C2-N1	2.01	120.99	116.71
3	B	1378[B]	GDC	N2-C2-N1	2.01	120.99	116.71

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1377[A]	GDD	PB-O3A-PA-O5'
4	A	1379	NAD	C5D-O5D-PN-O1N
4	B	1380	NAD	C5D-O5D-PN-O1N
6	B	1376	BTB	C4-C2-C3-O3
6	B	1376	BTB	C1-C2-N-C7
6	B	1376	BTB	C3-C2-N-C7
6	B	1376	BTB	C4-C2-N-C7
6	B	1376	BTB	N-C7-C8-O8
3	A	1378[B]	GDC	C4A-C5A-C6A-O6A
2	B	1377[A]	GDD	O51-C51-C61-O6A
3	A	1378[B]	GDC	O5-C5A-C6A-O6A
2	B	1377[A]	GDD	C41-C51-C61-O6A
3	A	1378[B]	GDC	P1-O2P-P-O5'
3	B	1378[B]	GDC	P1-O2P-P-O5'
4	A	1379	NAD	C5D-O5D-PN-O3
4	B	1380	NAD	C5D-O5D-PN-O3
4	A	1379	NAD	C5D-O5D-PN-O2N
6	B	1376	BTB	C1-C2-C3-O3
6	B	1376	BTB	N-C2-C4-O4
6	B	1376	BTB	C1-C2-N-C5
6	B	1376	BTB	C3-C2-N-C5
3	A	1378[B]	GDC	C1-O1-P1-O2P
3	A	1378[B]	GDC	P1-O2P-P-O1P
4	B	1380	NAD	O4B-C4B-C5B-O5B
4	A	1379	NAD	O4B-C4B-C5B-O5B
4	A	1379	NAD	C4B-C5B-O5B-PA
4	B	1380	NAD	C5D-O5D-PN-O2N
6	B	1376	BTB	C1-C2-C4-O4

There are no ring outliers.

6 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	1376	BTB	4	0

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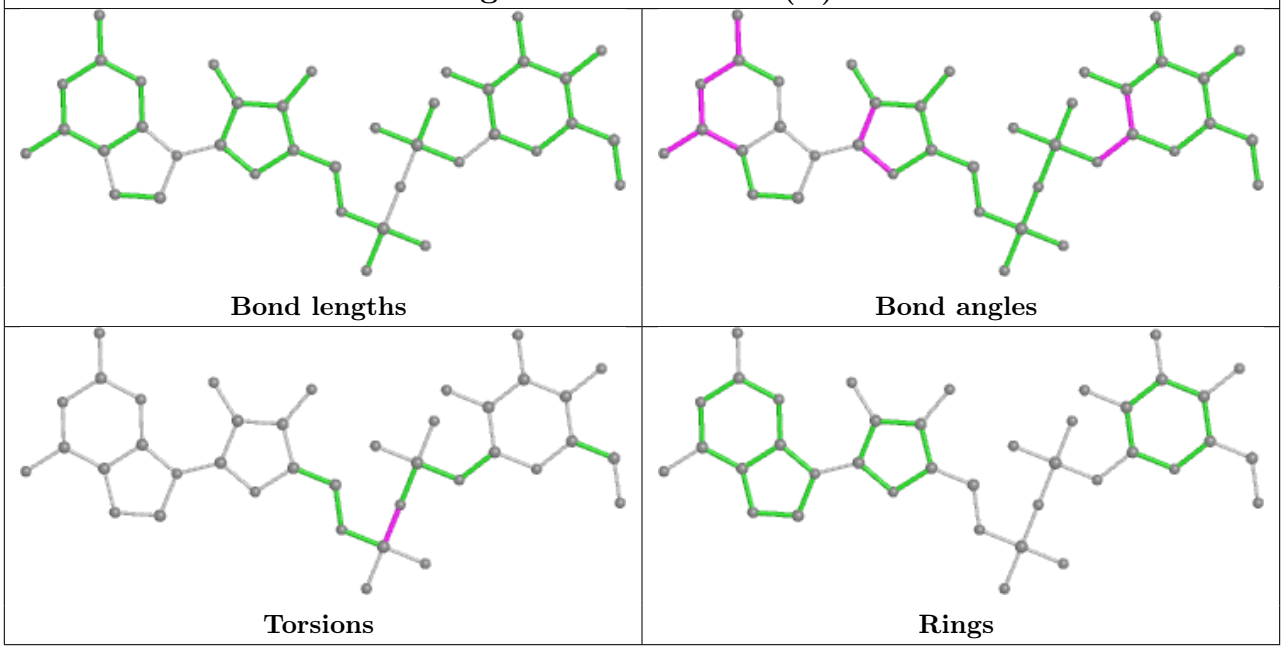
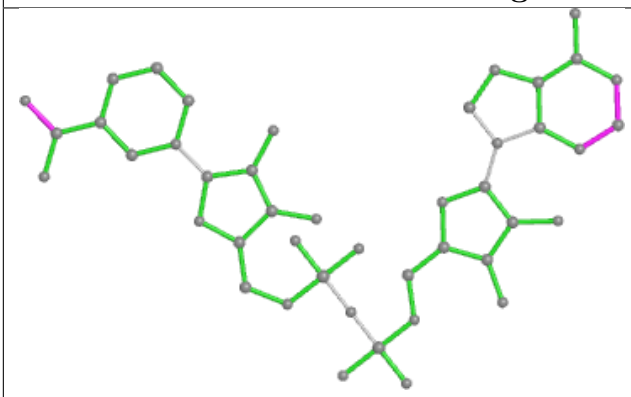
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1377[A]	GDD	3	0
2	A	1377[A]	GDD	1	0
3	A	1378[B]	GDC	1	0
4	B	1380	NAD	1	0
5	B	1373	FMT	1	0

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.

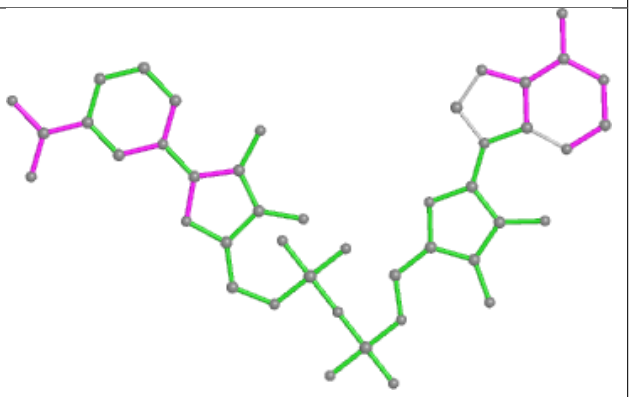
Ligand GDC B 1378 (B)



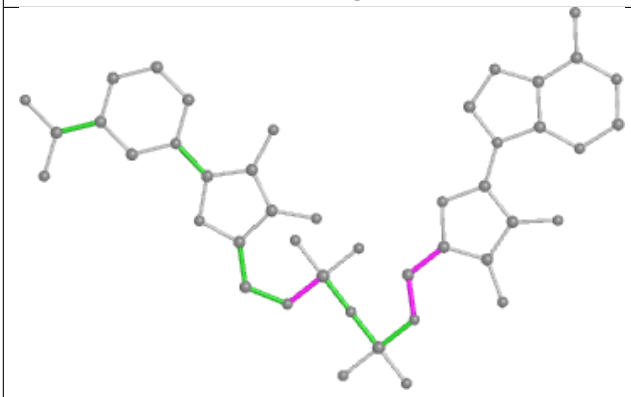
Ligand NAD A 1379



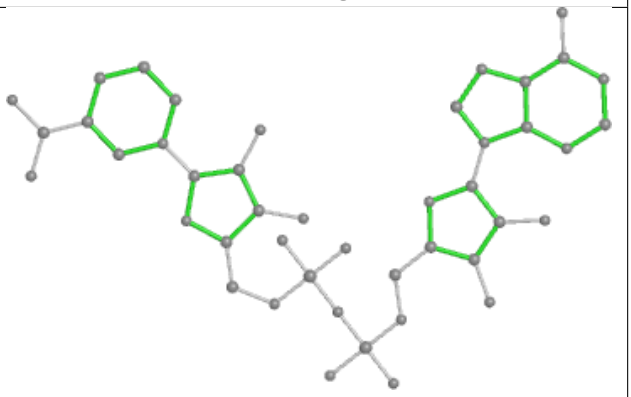
Bond lengths



Bond angles

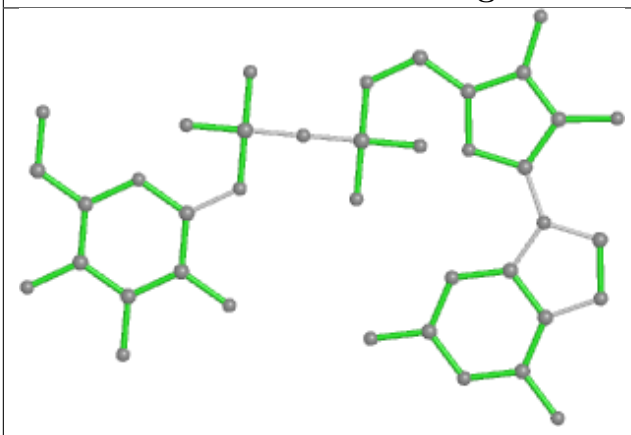


Torsions

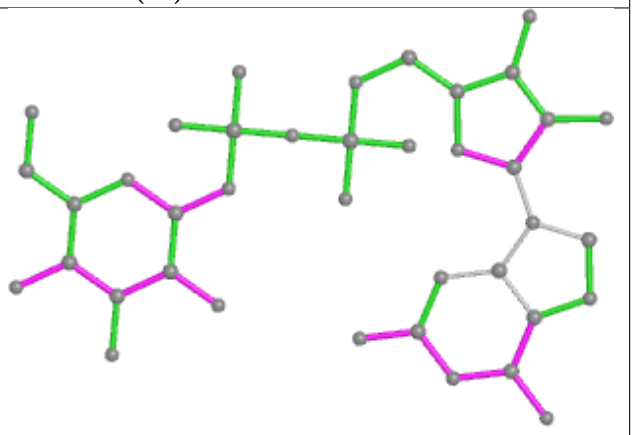


Rings

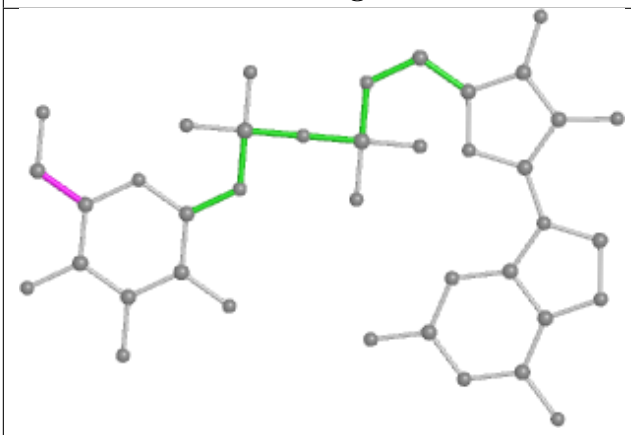
Ligand GDD B 1377 (A)



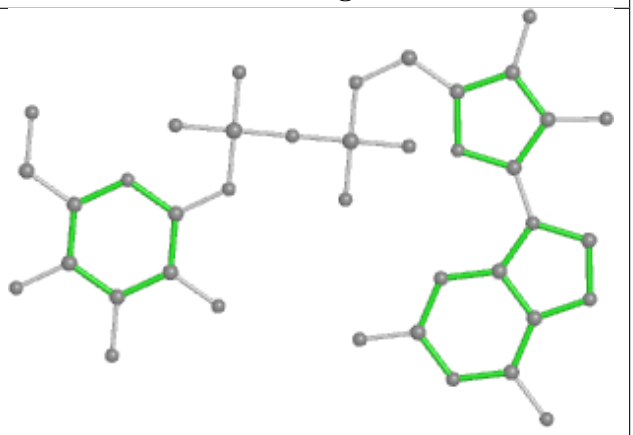
Bond lengths



Bond angles

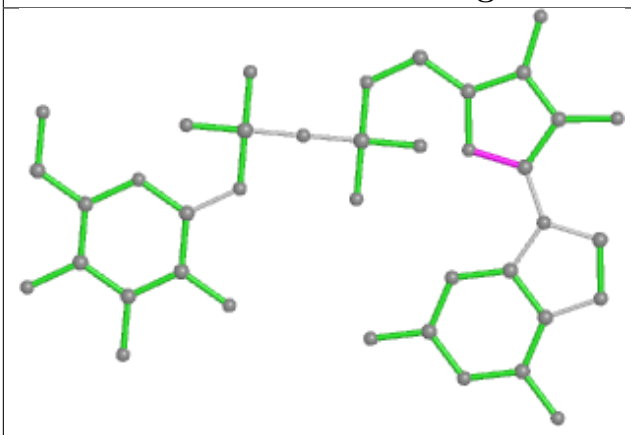


Torsions

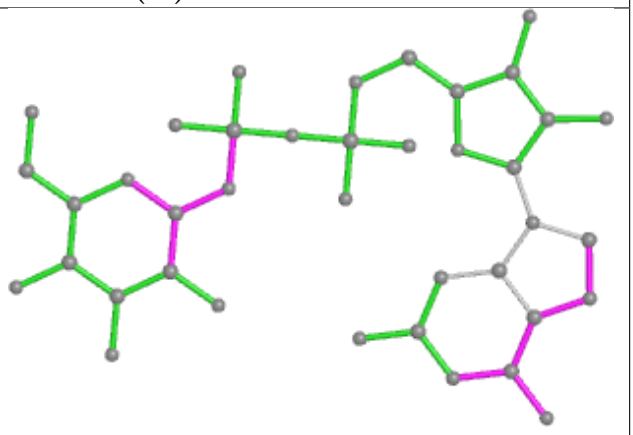


Rings

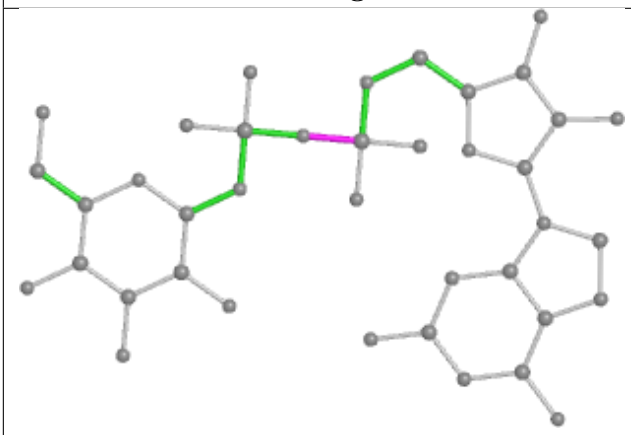
Ligand GDD A 1377 (A)



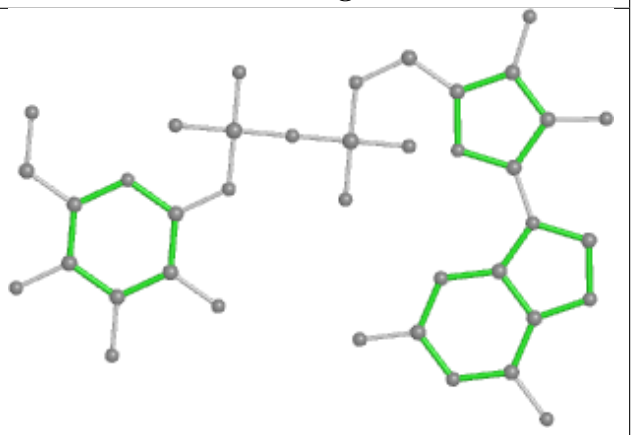
Bond lengths



Bond angles

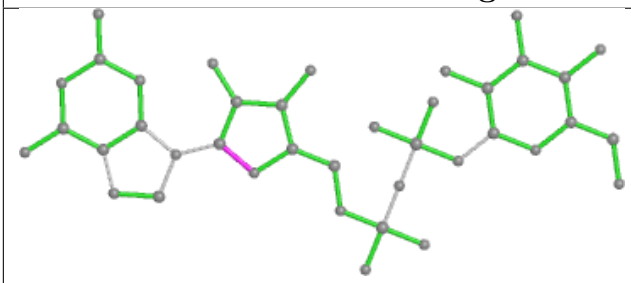


Torsions

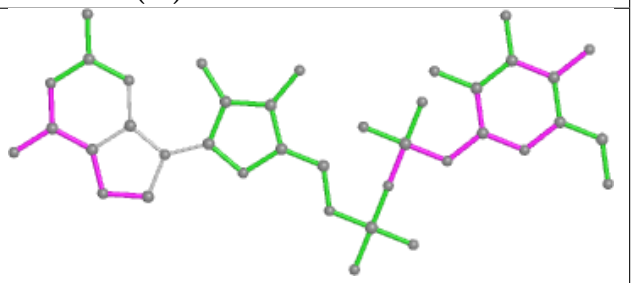


Rings

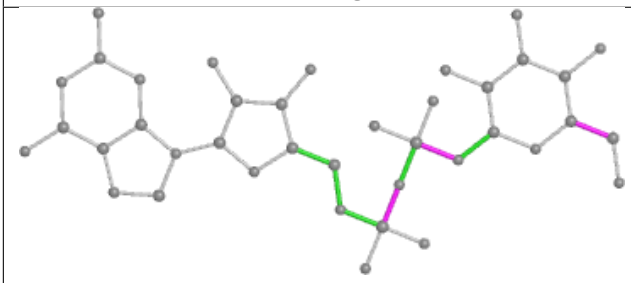
Ligand GDC A 1378 (B)



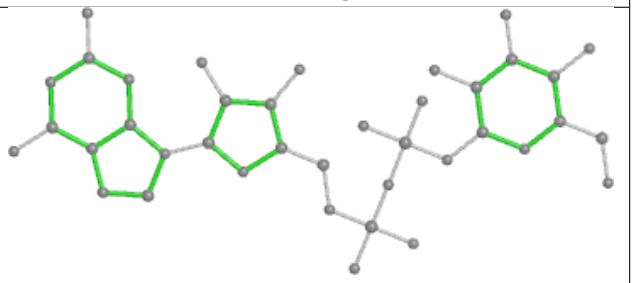
Bond lengths



Bond angles

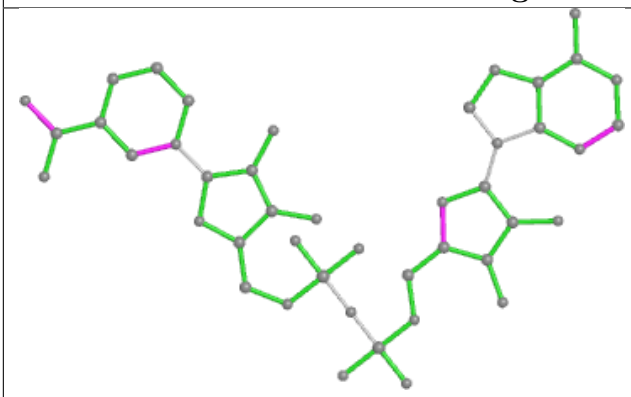


Torsions

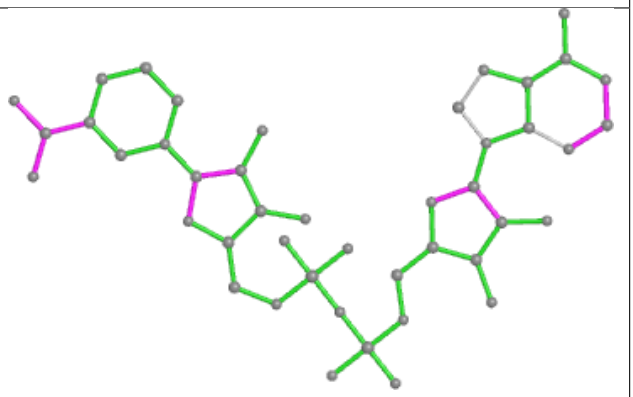


Rings

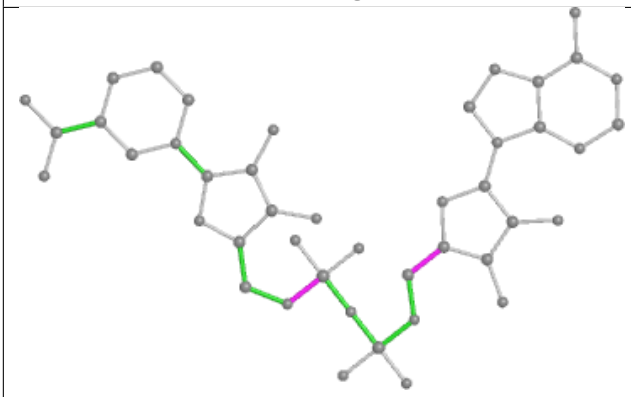
Ligand NAD B 1380



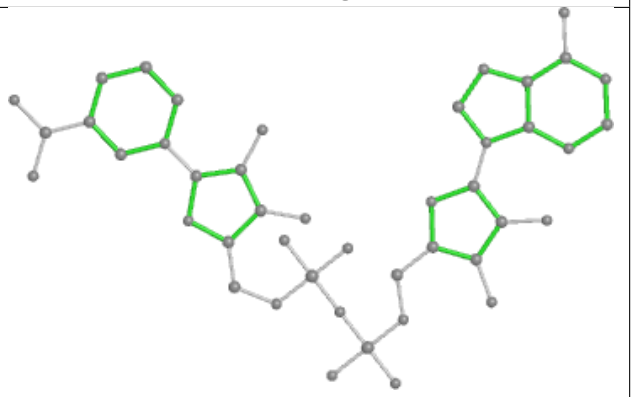
Bond lengths



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	364/379 (96%)	-0.38	7 (1%)	66	65	14, 20, 40, 51	6 (1%)
1	B	362/379 (95%)	-0.46	3 (0%)	86	85	13, 19, 32, 46	6 (1%)
All	All	726/758 (95%)	-0.42	10 (1%)	75	74	13, 19, 36, 51	12 (1%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	347	GLY	5.0
1	A	374	ASP	3.8
1	A	345	ALA	3.2
1	A	375	GLY	3.1
1	B	10	GLY	3.0
1	A	12	TYR	3.0
1	A	346	LYS	2.9
1	B	11	ALA	2.8
1	B	230[A]	THR	2.4
1	A	348	SER	2.0

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 monosaccharides in this entry.

6.4 Ligands (i)

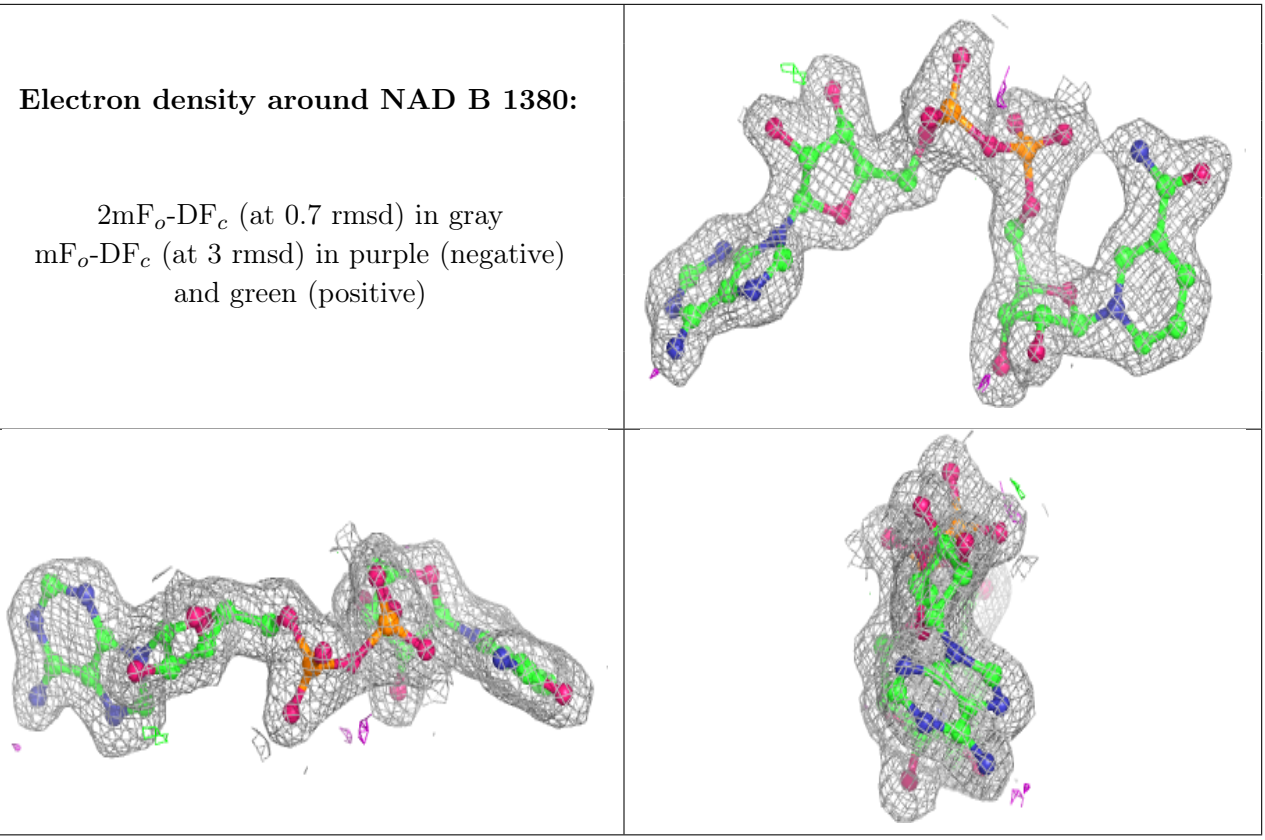
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
6	BTB	B	1376	14/14	0.77	0.21	23,28,31,34	14
5	FMT	A	1381	3/3	0.78	0.30	58,58,58,59	0
5	FMT	A	1382	3/3	0.81	0.25	38,38,40,40	0
5	FMT	B	1371	3/3	0.86	0.35	71,71,71,71	0
5	FMT	B	1375	3/3	0.89	0.41	42,42,42,43	0
5	FMT	B	1373	3/3	0.93	0.21	46,46,46,47	0
5	FMT	B	1372	3/3	0.96	0.17	35,35,36,36	0
4	NAD	B	1380	44/44	0.97	0.10	14,18,21,24	0
5	FMT	A	1380	3/3	0.97	0.07	34,34,36,36	0
4	NAD	A	1379	44/44	0.97	0.08	12,19,23,25	0
3	GDC	A	1378[B]	39/39	0.98	0.11	2,15,19,20	39
3	GDC	B	1378[B]	39/39	0.98	0.13	3,14,18,19	39
2	GDD	A	1377[A]	39/39	0.98	0.11	14,18,26,29	39
2	GDD	B	1377[A]	39/39	0.98	0.12	10,16,18,19	39
5	FMT	B	1374	3/3	0.99	0.05	20,20,22,24	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.

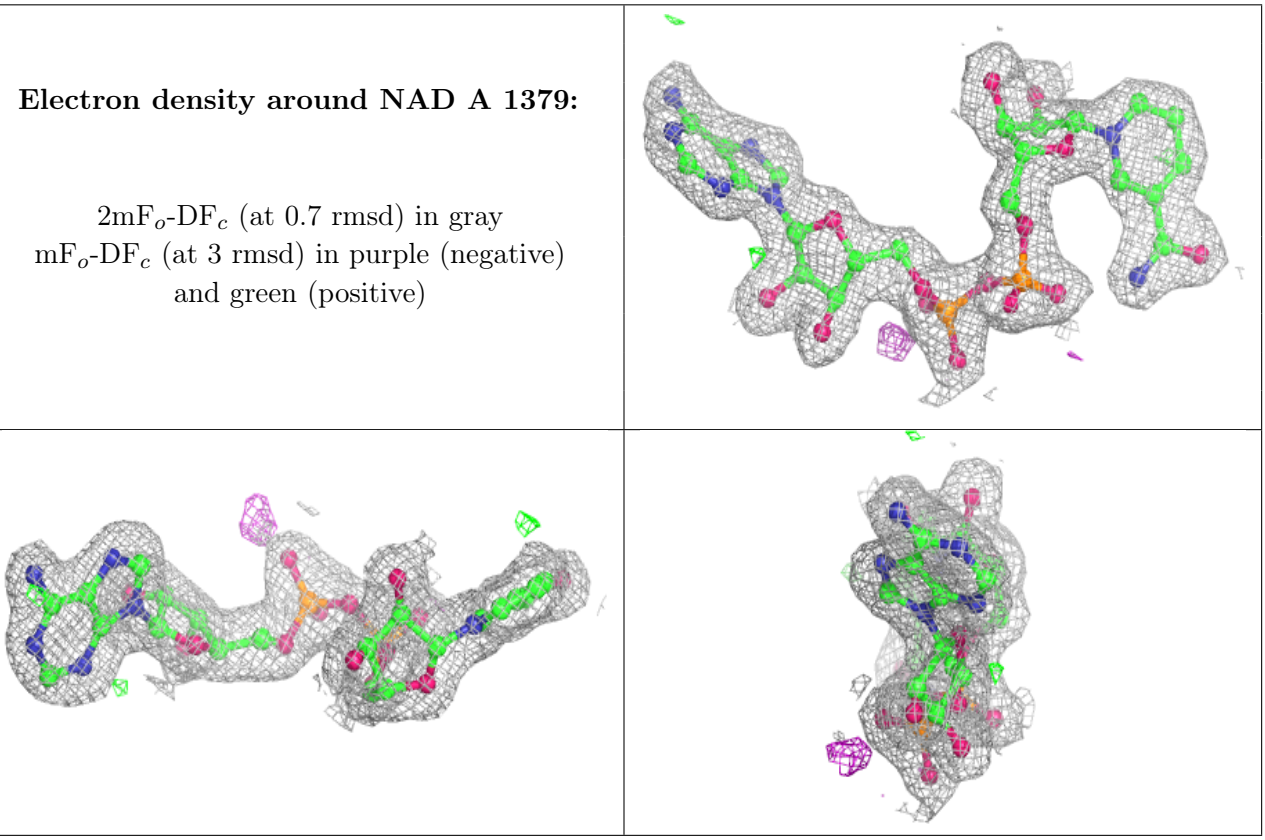
Electron density around NAD B 1380:

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



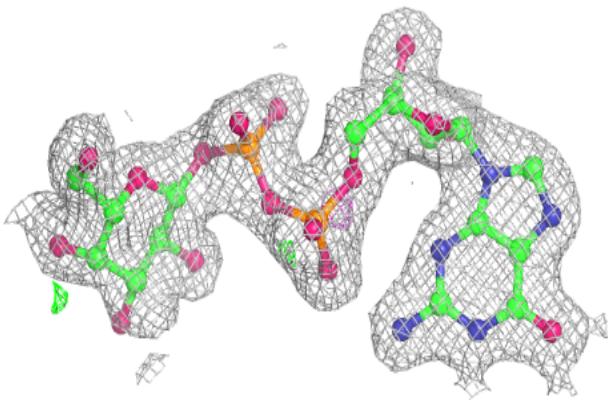
Electron density around NAD A 1379:

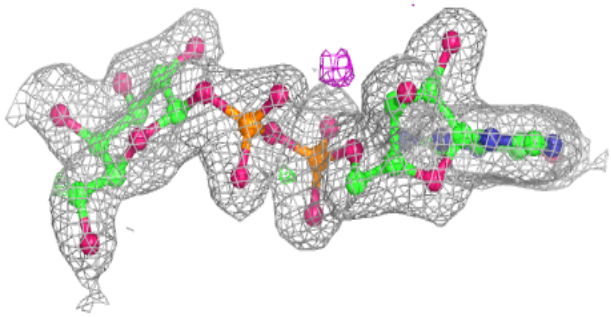
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

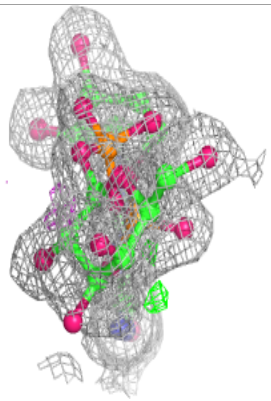


Electron density around GDC A 1378 (B):

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

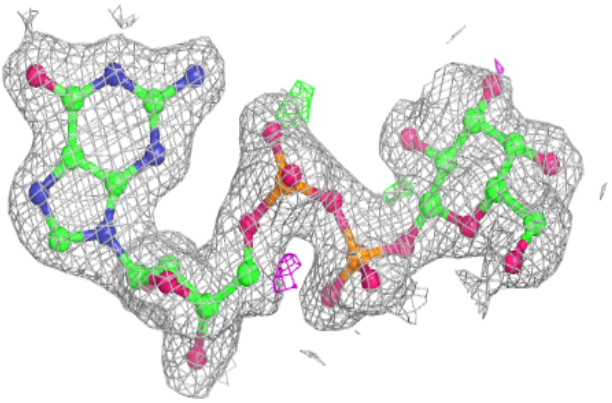


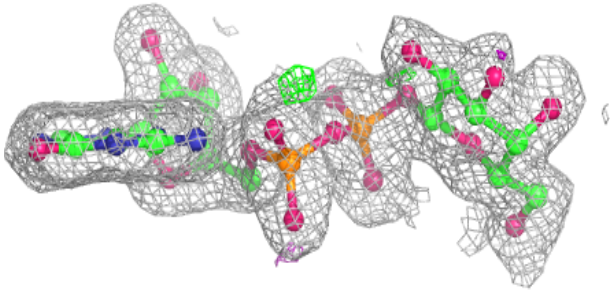


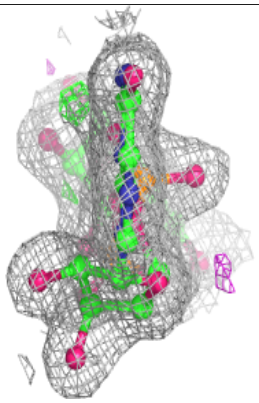


Electron density around GDC B 1378 (B):

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

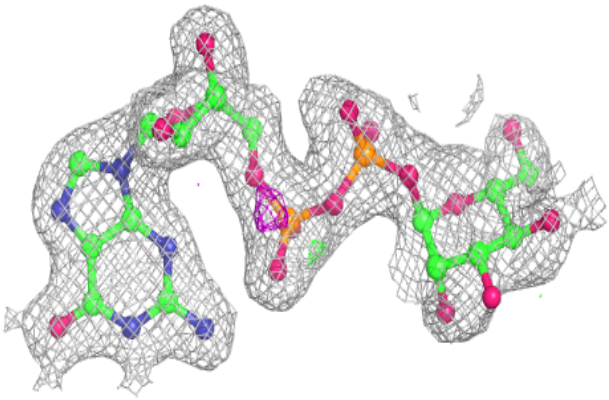


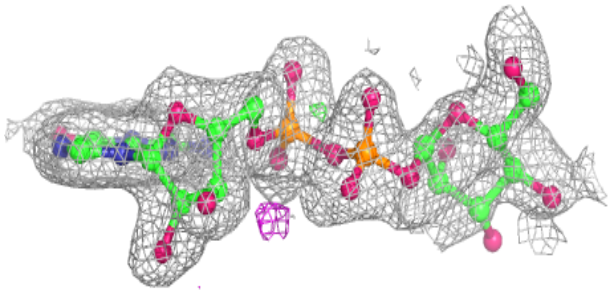


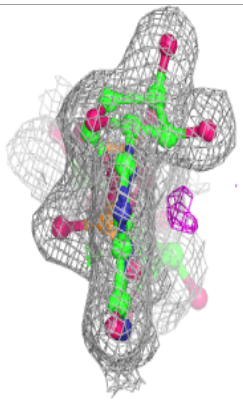


Electron density around GDD A 1377 (A):

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

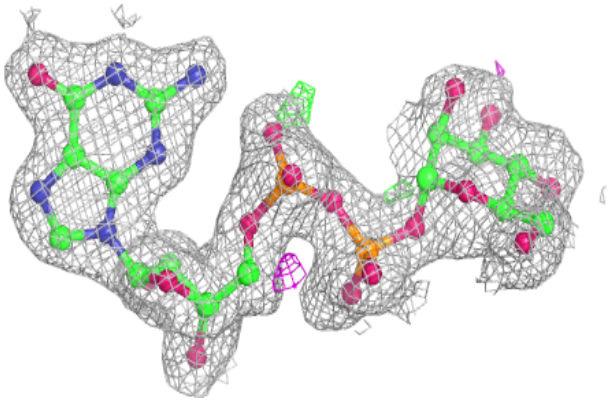


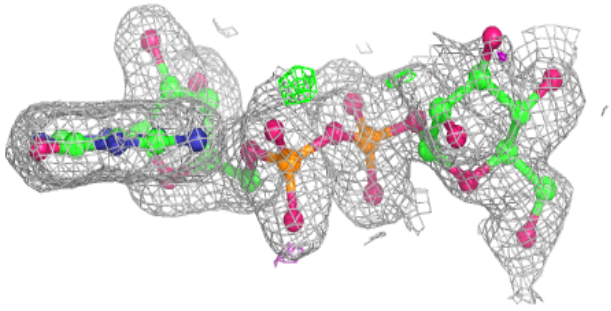


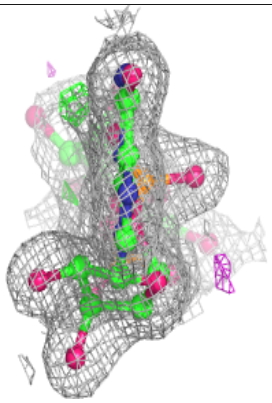


Electron density around GDD B 1377 (A):

$2mF_o$-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.