



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 5, 2023 – 09:21 am GMT

PDB ID : 2C5A
Title : GDP-mannose-3', 5' -epimerase (Arabidopsis thaliana),Y174F, with 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 : 1.40 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

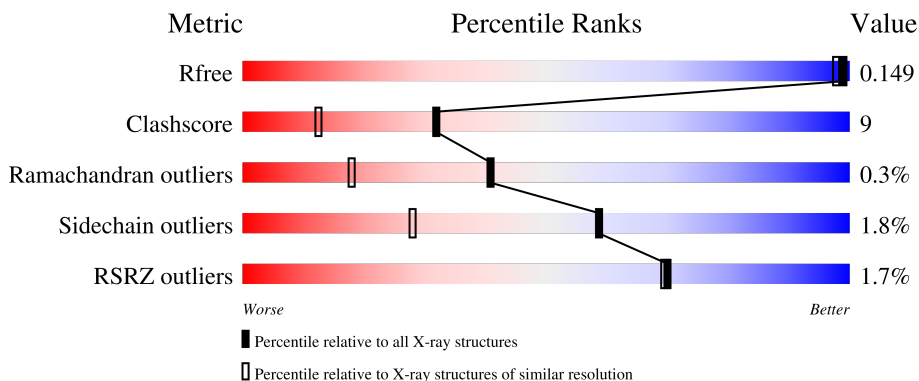
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.40 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	1714 (1.40-1.40)
Clashscore	141614	1812 (1.40-1.40)
Ramachandran outliers	138981	1763 (1.40-1.40)
Sidechain outliers	138945	1762 (1.40-1.40)
RSRZ outliers	127900	1674 (1.40-1.40)

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	379	
1	B	379	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	FMT	A	1388	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 7235 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.

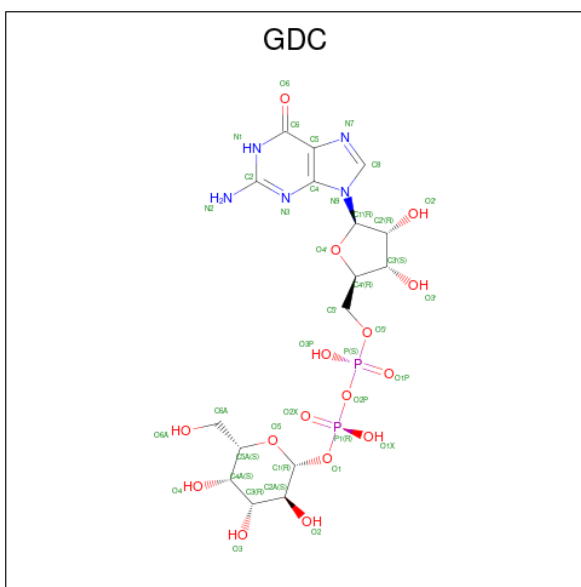
- Molecule 1 is a protein called GDP-MANNOSE-3', 5'-EPIMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	364	Total 2962	C 1880	N 510	O 548	S 24	0	12	1
1	B	361	Total 3024	C 1926	N 510	O 564	S 24	0	24	1

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	174	PHE	TYR	engineered mutation	UNP Q93VR3
B	174	PHE	TYR	engineered mutation	UNP Q93VR3

- Molecule 2 is GUANOSINE-5'-DIPHOSPHATE-BETA-L-GALACTOSE (three-letter code: GDC) (formula: $C_{16}H_{25}N_5O_{16}P_2$).



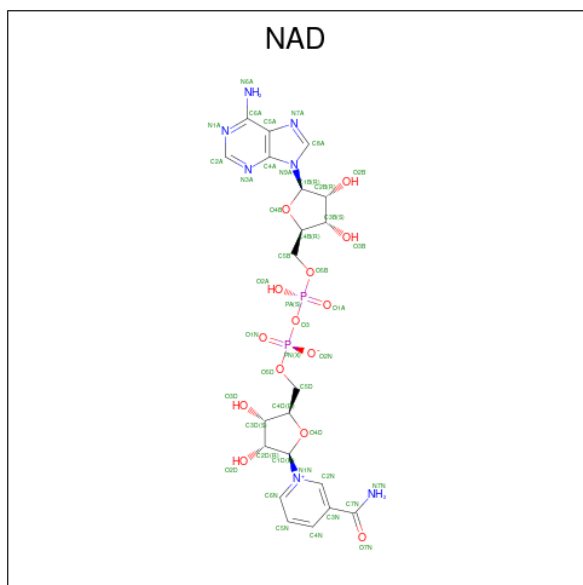
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	Total 39	C 16	N 5	O 16	P 2	0	0

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

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



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

- Molecule 4 is FORMIC ACID (three-letter code: FMT) (formula: CH₂O₂).



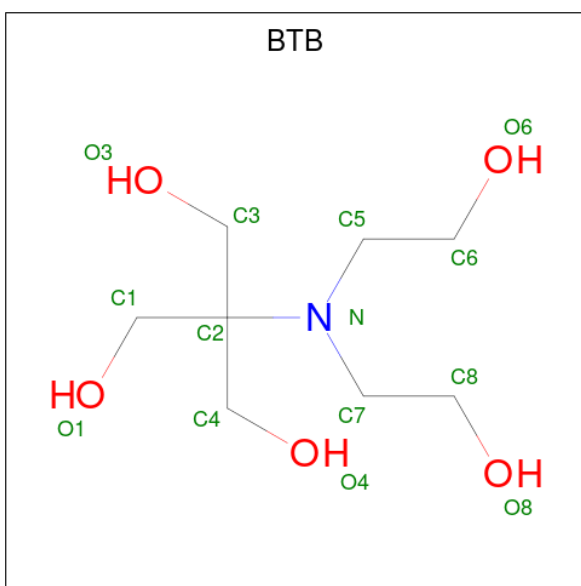
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 3 1 2	0	0
4	A	1	Total C O 3 1 2	0	0
4	A	1	Total C O 3 1 2	0	0
4	A	1	Total C O 3 1 2	0	0
4	A	1	Total C O 3 1 2	0	0
4	A	1	Total C O 3 1 2	0	0
4	A	1	Total C O 3 1 2	0	0
4	A	1	Total C O 3 1 2	0	0
4	A	1	Total C O 3 1 2	0	0
4	A	1	Total C O 3 1 2	0	0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

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

- Molecule 5 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPAN E-1,3-DIOL (three-letter code: BTB) (formula: C₈H₁₉NO₅).



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

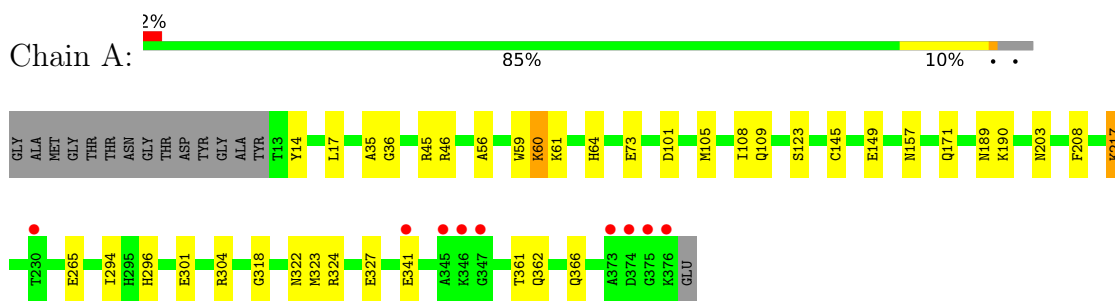
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	465	Total	O	0	0
			465	465		
6	B	553	Total	O	0	0
			553	553		

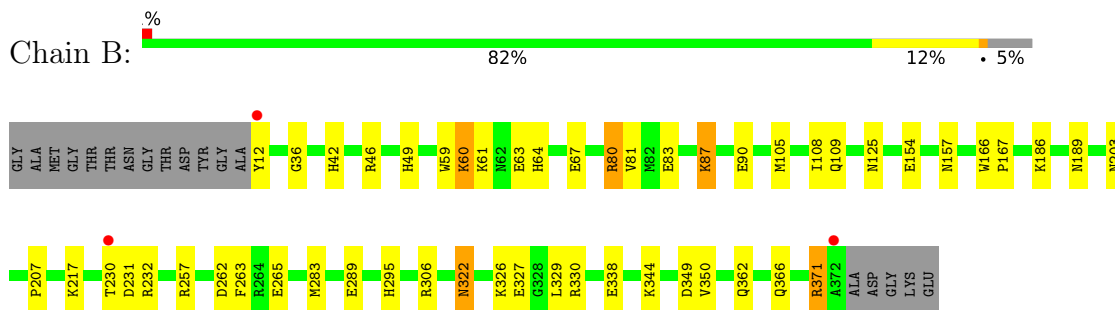
3 Residue-property plots [i](#)

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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	62.50Å 83.27Å 66.12Å 90.00° 98.89° 90.00°	Depositor
Resolution (Å)	21.61 – 1.40 21.15 – 1.40	Depositor EDS
% Data completeness (in resolution range)	96.5 (21.61-1.40) 96.5 (21.15-1.40)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.98 (at 1.40Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.103 , 0.140 0.115 , 0.149	Depositor DCC
R_{free} test set	6337 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	9.6	Xtrriage
Anisotropy	0.113	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 52.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	7235	wwPDB-VP
Average B, all atoms (Å ²)	13.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.67% 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: NAD, GDC, FMT, BTB

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	0.92	4/3061 (0.1%)	0.94	5/4116 (0.1%)
1	B	0.91	3/3161 (0.1%)	0.94	7/4249 (0.2%)
All	All	0.92	7/6222 (0.1%)	0.94	12/8365 (0.1%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	67	GLU	CD-OE2	6.78	1.33	1.25
1	A	123	SER	CA-CB	5.95	1.61	1.52
1	A	265	GLU	CG-CD	-5.83	1.43	1.51
1	B	154	GLU	CG-CD	-5.74	1.43	1.51
1	A	73	GLU	CB-CG	-5.20	1.42	1.52
1	A	301	GLU	CD-OE1	5.18	1.31	1.25
1	B	366	GLN	CB-CG	-5.17	1.38	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	371	ARG	NE-CZ-NH1	12.35	126.48	120.30
1	B	371	ARG	NE-CZ-NH2	-10.83	114.88	120.30
1	B	46	ARG	NE-CZ-NH1	9.67	125.14	120.30
1	A	46	ARG	NE-CZ-NH1	8.41	124.50	120.30
1	B	46	ARG	NE-CZ-NH2	-7.80	116.40	120.30
1	A	46	ARG	NE-CZ-NH2	-7.35	116.63	120.30
1	A	304	ARG	NE-CZ-NH2	-6.21	117.19	120.30
1	B	306	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	B	257	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	A	45	ARG	NE-CZ-NH2	-5.53	117.53	120.30
1	B	80	ARG	NE-CZ-NH2	-5.09	117.76	120.30
1	A	208	PHE	CB-CG-CD2	-5.01	117.30	120.80

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	2962	0	2929	39	0
1	B	3024	0	3005	66	0
2	A	39	0	23	10	0
2	B	39	0	23	5	0
3	A	44	0	26	0	0
3	B	44	0	26	1	0
4	A	36	0	12	7	0
4	B	15	0	5	0	0
5	B	14	0	19	2	0
6	A	465	0	0	15	0
6	B	553	0	0	17	1
All	All	7235	0	6068	109	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 9.

All (109) 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:217[B]:LYS:NZ	2:A:1376:GDC:H3	1.13	1.40
1:A:36:GLY:O	1:A:60:LYS:NZ	1.70	1.24
1:A:217[B]:LYS:NZ	2:A:1376:GDC:C3	2.09	1.14
1:B:217[A]:LYS:HZ1	2:B:1372:GDC:H5A	1.13	1.13
1:B:60[A]:LYS:NZ	1:B:63:GLU:HG3	1.77	1.00
1:A:14:TYR:CD2	1:A:323[B]:MET:SD	2.55	0.99
1:A:217[B]:LYS:HZ3	2:A:1376:GDC:C3	1.70	0.98
1:B:289:GLU:OE2	6:B:2416:HOH:O	1.84	0.93
1:B:217[A]:LYS:NZ	2:B:1372:GDC:H5A	1.85	0.90
1:B:90[A]:GLU:OE1	6:B:2171:HOH:O	1.91	0.87
1:A:217[B]:LYS:HZ1	2:A:1376:GDC:H3	1.07	0.87
1:A:366[B]:GLN:NE2	6:A:2427:HOH:O	2.08	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60[A]:LYS:HZ1	1:B:63:GLU:HG3	1.44	0.83
1:A:217[B]:LYS:HZ1	2:A:1376:GDC:C3	1.80	0.82
1:A:318:GLY:O	4:A:1387:FMT:H	1.79	0.82
1:B:283[B]:MET:HE2	1:B:329:LEU:HD12	1.62	0.81
1:B:60[A]:LYS:NZ	1:B:61:LYS:O	2.12	0.80
1:A:14:TYR:CE2	1:A:323[B]:MET:CG	2.65	0.80
1:B:60[B]:LYS:NZ	1:B:371:ARG:HD3	1.98	0.79
1:A:14:TYR:CE2	1:A:323[B]:MET:SD	2.77	0.78
1:B:60[B]:LYS:HZ3	1:B:371:ARG:HD3	1.49	0.77
1:B:283[B]:MET:CE	1:B:326:LYS:HA	2.16	0.75
1:A:341:GLU:HG3	6:A:2386:HOH:O	1.87	0.72
1:B:283[B]:MET:CE	1:B:329:LEU:HD12	2.19	0.72
1:B:217[A]:LYS:HZ2	2:B:1372:GDC:H3	1.55	0.71
1:A:322:ASN:OD1	6:A:2378:HOH:O	2.09	0.70
1:A:217[B]:LYS:HZ3	2:A:1376:GDC:H3	0.89	0.70
1:B:81:VAL:HG12	1:B:83[B]:GLU:HG2	1.74	0.70
1:B:60[A]:LYS:HZ3	1:B:63:GLU:HG3	1.58	0.69
1:B:262[B]:ASP:OD1	6:B:2383:HOH:O	2.10	0.68
1:A:14:TYR:CE2	1:A:323[B]:MET:HG3	2.29	0.68
1:B:125:ASN:ND2	6:B:2156:HOH:O	2.27	0.65
1:B:125:ASN:CB	6:B:2156:HOH:O	2.45	0.65
1:B:60[B]:LYS:HE2	1:B:371:ARG:HD2	1.78	0.64
1:A:217[B]:LYS:HZ1	2:A:1376:GDC:C2A	2.12	0.63
1:B:60[B]:LYS:NZ	6:B:2098:HOH:O	1.95	0.62
1:B:105[B]:MET:CE	1:B:109:GLN:HG3	2.30	0.62
1:A:149:GLU:CD	1:A:171:GLN:HE21	2.03	0.62
1:B:283[B]:MET:HE1	1:B:326:LYS:HA	1.81	0.61
1:B:49[A]:HIS:CE1	6:B:2078:HOH:O	2.52	0.61
1:B:125:ASN:HB2	6:B:2156:HOH:O	2.00	0.61
1:B:105[B]:MET:HE3	1:B:109:GLN:HG3	1.84	0.60
4:A:1385:FMT:O1	6:A:2460:HOH:O	2.17	0.60
1:A:327:GLU:HG2	6:A:2152:HOH:O	2.03	0.59
4:A:1388:FMT:O1	6:A:2465:HOH:O	2.17	0.57
1:A:157:ASN:ND2	6:A:2194:HOH:O	2.37	0.57
1:B:60[B]:LYS:HE2	3:B:1374:NAD:O2B	2.05	0.56
1:B:64:HIS:HD2	6:B:2478:HOH:O	1.89	0.55
1:B:186:LYS:NZ	5:B:1380:BTB:O4	2.34	0.55
1:B:232:ARG:HD3	1:B:295:HIS:CE1	2.41	0.55
1:A:190:LYS:NZ	6:A:2228:HOH:O	2.22	0.55
1:B:283[B]:MET:HE3	1:B:326:LYS:HA	1.90	0.53
1:B:80:ARG:C	6:B:2156:HOH:O	2.46	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:217[A]:LYS:NZ	2:B:1372:GDC:H3	2.23	0.52
1:B:60[A]:LYS:NZ	1:B:63:GLU:CG	2.62	0.52
1:A:145:CYS:SG	2:A:1376:GDC:O4	2.64	0.52
1:A:296:HIS:HE1	6:A:2337:HOH:O	1.93	0.51
1:B:60[B]:LYS:CE	1:B:371:ARG:CD	2.89	0.51
1:B:81:VAL:CG1	1:B:83[B]:GLU:HG2	2.38	0.51
1:A:217[B]:LYS:HZ3	2:A:1376:GDC:C4A	2.24	0.51
1:B:87[B]:LYS:HE2	6:B:2165:HOH:O	2.09	0.50
1:A:101:ASP:OD2	4:A:1388:FMT:C	2.59	0.50
1:B:60[B]:LYS:CE	1:B:371:ARG:HD2	2.40	0.50
1:B:157:ASN:O	6:B:2267:HOH:O	2.19	0.50
1:B:36:GLY:O	1:B:60[A]:LYS:HE3	2.11	0.50
1:A:366[B]:GLN:CG	6:A:2427:HOH:O	2.61	0.49
1:A:61:LYS:NZ	6:A:2075:HOH:O	2.42	0.48
1:A:14:TYR:CZ	1:A:323[B]:MET:HG2	2.48	0.48
1:B:230[A]:THR:HG23	1:B:231:ASP:OD2	2.13	0.48
1:B:60[A]:LYS:HZ1	1:B:63:GLU:CG	2.20	0.48
1:B:283[B]:MET:CE	1:B:326:LYS:CA	2.89	0.48
1:B:108[B]:ILE:HD12	6:B:2297:HOH:O	2.12	0.48
1:B:283[B]:MET:HE3	1:B:326:LYS:CB	2.44	0.48
1:B:87[B]:LYS:HE3	1:B:87[B]:LYS:HB3	1.67	0.48
1:A:362[B]:GLN:NE2	4:A:1388:FMT:O2	2.46	0.47
1:A:64:HIS:HE1	6:A:2241:HOH:O	1.96	0.47
1:A:361:THR:H	4:A:1381:FMT:C	2.28	0.47
1:A:14:TYR:CZ	1:A:323[B]:MET:CG	3.00	0.45
1:B:166:TRP:HA	1:B:167:PRO:C	2.36	0.45
1:B:42:HIS:HE1	1:B:207:PRO:O	2.00	0.45
1:B:217[A]:LYS:HZ2	2:B:1372:GDC:C3	2.28	0.45
1:A:64:HIS:HD2	6:A:2392:HOH:O	2.00	0.44
1:B:283[B]:MET:HE1	1:B:326:LYS:CA	2.46	0.44
1:B:344:LYS:HE2	1:B:350:VAL:HG21	1.98	0.44
1:B:60[A]:LYS:HZ3	1:B:63:GLU:CG	2.29	0.44
1:B:105[B]:MET:HE1	1:B:109:GLN:HG3	1.99	0.44
1:B:64:HIS:HE1	6:B:2327:HOH:O	2.01	0.44
1:B:263:PHE:CE2	1:B:265[A]:GLU:HB2	2.53	0.43
1:B:87[A]:LYS:HE2	6:B:2059:HOH:O	2.18	0.43
1:A:105:MET:HE3	1:A:109:GLN:HG3	1.99	0.43
1:A:217[B]:LYS:HE2	2:A:1376:GDC:H5A	2.01	0.43
1:B:322:ASN:C	1:B:322:ASN:HD22	2.22	0.43
1:B:327[B]:GLU:CD	1:B:330:ARG:HH12	2.22	0.42
5:B:1380:BTB:H31	5:B:1380:BTB:H71	1.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:GLU:OE2	1:A:171:GLN:NE2	2.41	0.42
1:A:14:TYR:CD2	1:A:17:LEU:HB2	2.55	0.42
1:B:60[B]:LYS:HZ3	1:B:371:ARG:CD	2.25	0.42
4:A:1388:FMT:O1	6:A:2464:HOH:O	2.22	0.41
1:B:12:TYR:HB3	1:B:207:PRO:HG2	2.01	0.41
1:A:108[B]:ILE:HD12	6:A:2212:HOH:O	2.20	0.41
1:B:283[B]:MET:HE3	1:B:326:LYS:CA	2.50	0.41
1:B:338[B]:GLU:CD	6:B:2474:HOH:O	2.59	0.41
1:B:60[B]:LYS:NZ	1:B:371:ARG:CD	2.77	0.41
1:B:60[B]:LYS:HD3	1:B:371:ARG:CG	2.51	0.41
1:B:362[A]:GLN:NE2	6:B:2512:HOH:O	2.54	0.41
1:A:294:ILE:N	1:A:294:ILE:HD13	2.35	0.41
1:A:35:ALA:HB3	1:A:56:ALA:HB1	2.03	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)
6:B:2093:HOH:O	6:B:2200:HOH:O[1_455]	2.14	0.06

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	374/379 (99%)	363 (97%)	10 (3%)	1 (0%)	41	18
1	B	384/379 (101%)	377 (98%)	6 (2%)	1 (0%)	41	18
All	All	758/758 (100%)	740 (98%)	16 (2%)	2 (0%)	41	18

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	203	ASN
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	321/319 (101%)	315 (98%)	6 (2%)	57	25
1	B	334/319 (105%)	326 (98%)	8 (2%)	49	16
All	All	655/638 (103%)	641 (98%)	14 (2%)	59	21

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	TRP
1	A	60	LYS
1	A	189	ASN
1	A	217[A]	LYS
1	A	217[B]	LYS
1	A	324	ARG
1	B	59	TRP
1	B	60[A]	LYS
1	B	60[B]	LYS
1	B	87[A]	LYS
1	B	87[B]	LYS
1	B	189	ASN
1	B	322	ASN
1	B	349	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	ASN
1	A	64	HIS
1	A	157	ASN

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Mol	Chain	Res	Type
1	A	171	GLN
1	A	296	HIS
1	B	42	HIS
1	B	64	HIS
1	B	322	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

22 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	BTB	B	1380	-	13,13,13	1.85	3 (23%)	7,16,16	1.86	3 (42%)
4	FMT	A	1381	-	2,2,2	0.59	0	1,1,1	0.44	0
4	FMT	B	1378	-	2,2,2	0.57	0	1,1,1	0.76	0
2	GDC	B	1372	-	35,42,42	1.02	3 (8%)	46,65,65	1.35	4 (8%)
4	FMT	B	1377	-	2,2,2	0.76	0	1,1,1	0.63	0
4	FMT	A	1387	-	2,2,2	0.65	0	1,1,1	0.11	0
4	FMT	A	1389	-	2,2,2	0.67	0	1,1,1	0.33	0
4	FMT	A	1385	-	2,2,2	0.82	0	1,1,1	0.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	FMT	B	1379	-	2,2,2	0.69	0	1,1,1	0.52	0
4	FMT	A	1388	-	2,2,2	1.26	0	1,1,1	0.73	0
4	FMT	B	1375	-	2,2,2	0.69	0	1,1,1	0.39	0
4	FMT	A	1382	-	2,2,2	0.84	0	1,1,1	0.54	0
3	NAD	B	1374	-	42,48,48	1.34	6 (14%)	50,73,73	1.84	7 (14%)
4	FMT	A	1383	-	2,2,2	1.02	0	1,1,1	0.45	0
4	FMT	A	1386	-	2,2,2	1.01	0	1,1,1	0.11	0
4	FMT	A	1380	-	2,2,2	1.05	0	1,1,1	0.34	0
4	FMT	A	1379	-	2,2,2	0.84	0	1,1,1	0.32	0
4	FMT	A	1390	-	2,2,2	0.83	0	1,1,1	0.21	0
4	FMT	B	1376	-	2,2,2	0.86	0	1,1,1	0.85	0
4	FMT	A	1384	-	2,2,2	0.72	0	1,1,1	0.65	0
3	NAD	A	1378	-	42,48,48	1.49	5 (11%)	50,73,73	1.44	4 (8%)
2	GDC	A	1376	-	35,42,42	0.92	0	46,65,65	1.20	4 (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
5	BTB	B	1380	-	-	4/21/21/21	-
3	NAD	A	1378	-	-	5/26/62/62	0/5/5/5
2	GDC	A	1376	-	-	1/19/59/59	0/4/4/4
2	GDC	B	1372	-	-	1/19/59/59	0/4/4/4
3	NAD	B	1374	-	-	4/26/62/62	0/5/5/5

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1374	NAD	O7N-C7N	4.61	1.33	1.24
3	A	1378	NAD	O7N-C7N	4.51	1.32	1.24
5	B	1380	BTB	C5-N	4.24	1.54	1.48
3	A	1378	NAD	C2B-C1B	3.02	1.58	1.53
5	B	1380	BTB	C2-N	3.01	1.54	1.48
3	A	1378	NAD	C2N-N1N	2.93	1.38	1.35
5	B	1380	BTB	C3-C2	-2.81	1.49	1.53
3	A	1378	NAD	C4N-C3N	2.71	1.43	1.39
3	B	1374	NAD	C2A-N3A	2.70	1.36	1.32
3	B	1374	NAD	C4N-C3N	2.67	1.43	1.39
3	A	1378	NAD	C3N-C7N	-2.53	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1372	GDC	O5-C5A	-2.43	1.38	1.44
2	B	1372	GDC	C6-N1	-2.29	1.34	1.37
3	B	1374	NAD	C2N-N1N	2.20	1.37	1.35
3	B	1374	NAD	C3N-C7N	-2.10	1.47	1.50
2	B	1372	GDC	C5-C6	-2.07	1.43	1.47
3	B	1374	NAD	C2D-C1D	-2.06	1.50	1.53

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1374	NAD	C5N-C4N-C3N	-5.89	113.38	120.34
3	B	1374	NAD	C2N-C3N-C4N	5.84	124.87	118.26
2	B	1372	GDC	O5-C1-O1	-5.41	104.29	111.36
3	A	1378	NAD	C3N-C7N-N7N	5.35	124.18	117.75
3	A	1378	NAD	O7N-C7N-C3N	-5.09	113.54	119.63
3	B	1374	NAD	C3N-C7N-N7N	4.46	123.10	117.75
3	B	1374	NAD	C3N-C2N-N1N	-4.01	116.51	120.43
3	B	1374	NAD	N3A-C2A-N1A	-3.72	122.87	128.68
2	A	1376	GDC	O5-C1-O1	-3.56	106.72	111.36
5	B	1380	BTB	O3-C3-C2	-3.15	102.82	111.44
3	A	1378	NAD	C5A-C6A-N6A	3.06	125.00	120.35
2	B	1372	GDC	O3-C3-C2A	-2.79	103.89	110.35
3	B	1374	NAD	C6N-C5N-C4N	2.57	123.18	119.44
5	B	1380	BTB	C8-C7-N	2.55	121.56	111.59
3	B	1374	NAD	O7N-C7N-C3N	-2.46	116.69	119.63
2	B	1372	GDC	C1-O5-C5A	-2.42	108.94	113.69
3	A	1378	NAD	N3A-C2A-N1A	-2.29	125.11	128.68
2	B	1372	GDC	O5-C5A-C4A	2.27	113.83	109.69
2	A	1376	GDC	O4-C4A-C3	2.15	115.31	110.35
2	A	1376	GDC	O4'-C4'-C3'	2.07	109.20	105.11
2	A	1376	GDC	O1-P1-O2X	-2.06	101.73	109.47
5	B	1380	BTB	C6-C5-N	2.04	119.53	111.59

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1378	NAD	C5D-O5D-PN-O1N
3	B	1374	NAD	C5D-O5D-PN-O1N
5	B	1380	BTB	C1-C2-N-C7
5	B	1380	BTB	C3-C2-N-C7
5	B	1380	BTB	C4-C2-N-C7

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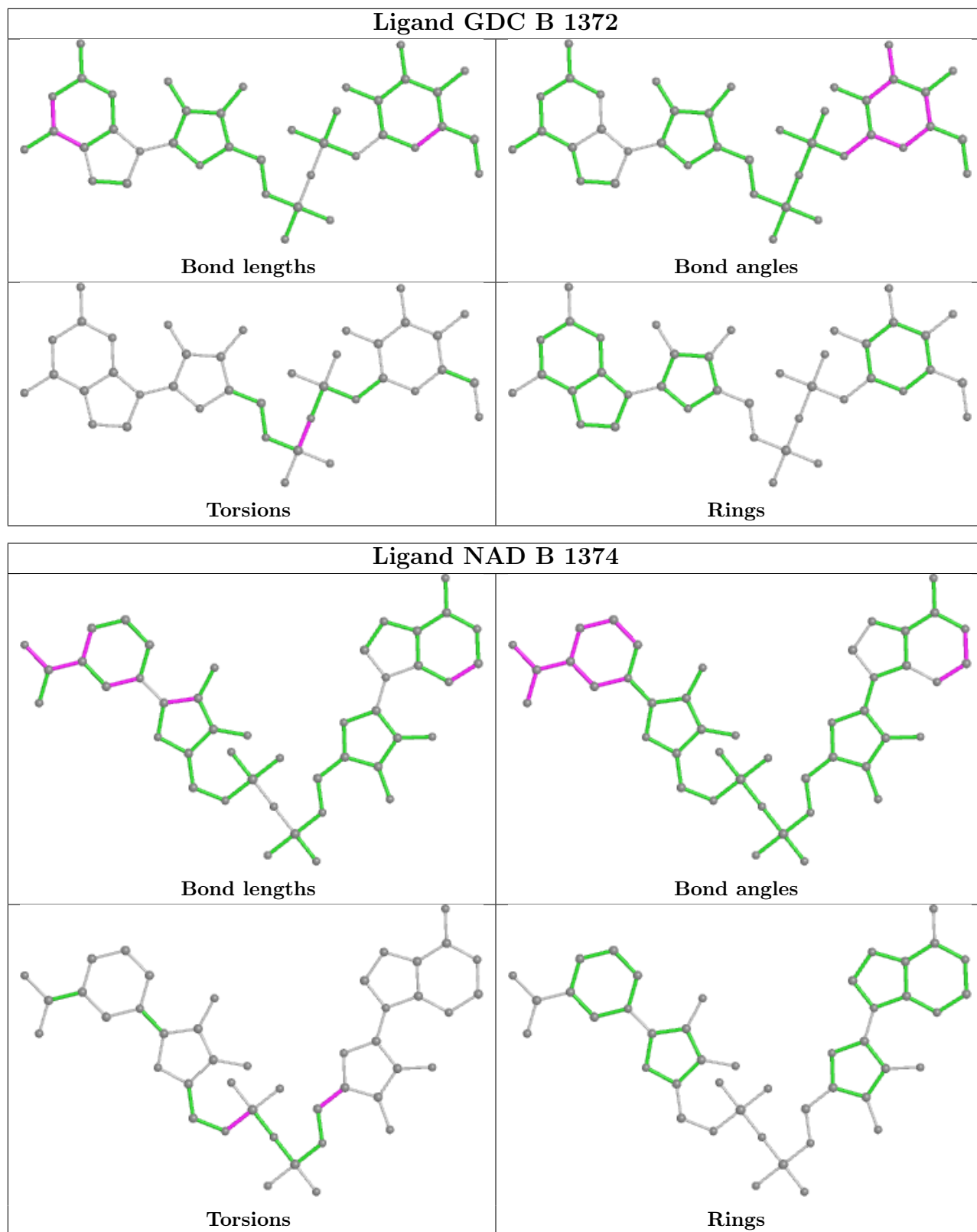
Mol	Chain	Res	Type	Atoms
5	B	1380	BTB	C6-C5-N-C7
2	A	1376	GDC	P1-O2P-P-O5'
2	B	1372	GDC	P1-O2P-P-O5'
3	A	1378	NAD	C5D-O5D-PN-O3
3	B	1374	NAD	C5D-O5D-PN-O3
3	A	1378	NAD	C5D-O5D-PN-O2N
3	B	1374	NAD	C5D-O5D-PN-O2N
3	B	1374	NAD	O4B-C4B-C5B-O5B
3	A	1378	NAD	O4B-C4B-C5B-O5B
3	A	1378	NAD	PA-O3-PN-O2N

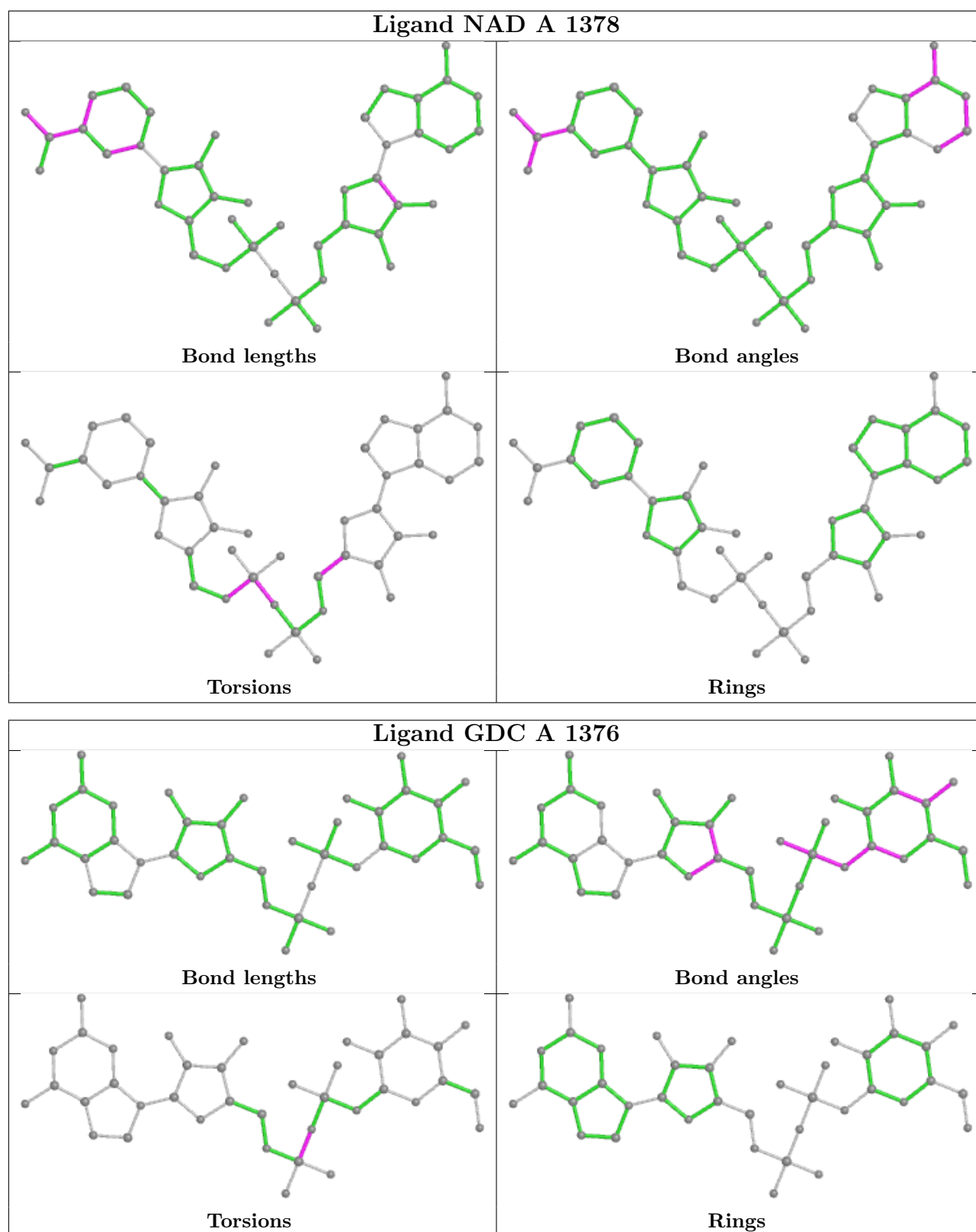
There are no ring outliers.

8 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1380	BTB	2	0
4	A	1381	FMT	1	0
2	B	1372	GDC	5	0
4	A	1387	FMT	1	0
4	A	1385	FMT	1	0
4	A	1388	FMT	4	0
3	B	1374	NAD	1	0
2	A	1376	GDC	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 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

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	364/379 (96%)	-0.36	9 (2%) 57 57	6, 11, 26, 39	0
1	B	361/379 (95%)	-0.51	3 (0%) 86 84	5, 9, 20, 30	0
All	All	725/758 (95%)	-0.44	12 (1%) 70 69	5, 10, 23, 39	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	376	LYS	8.1
1	A	375	GLY	6.2
1	B	372	ALA	4.4
1	A	346	LYS	3.6
1	A	230	THR	3.4
1	A	345	ALA	3.3
1	A	347	GLY	3.0
1	B	12	TYR	3.0
1	A	374	ASP	2.7
1	B	230[A]	THR	2.5
1	A	341	GLU	2.1
1	A	373	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands

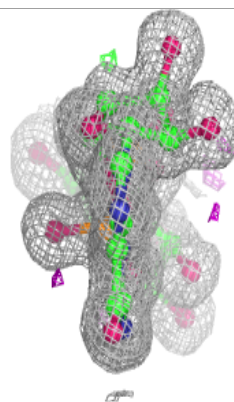
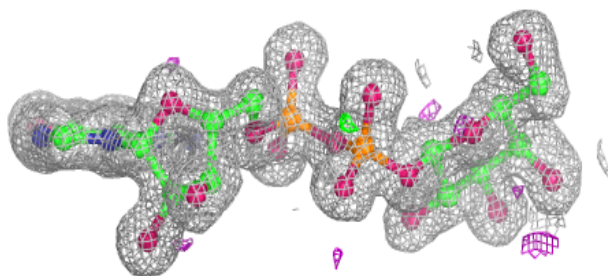
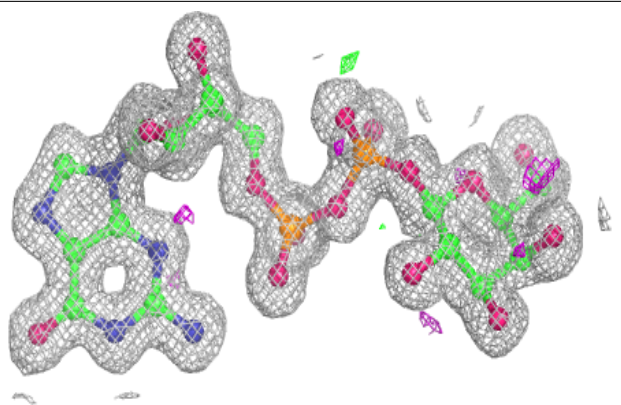
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	FMT	A	1389	3/3	0.74	0.21	43,43,45,46	0
4	FMT	A	1385	3/3	0.85	0.24	35,35,35,35	0
4	FMT	B	1376	3/3	0.85	0.26	26,26,28,29	0
4	FMT	A	1382	3/3	0.88	0.11	26,26,27,28	0
5	BTB	B	1380	14/14	0.89	0.14	18,21,24,29	0
4	FMT	A	1387	3/3	0.92	0.21	26,26,29,31	0
4	FMT	B	1377	3/3	0.93	0.16	15,15,18,23	0
4	FMT	A	1381	3/3	0.93	0.35	33,33,34,34	0
4	FMT	A	1379	3/3	0.94	0.19	23,23,25,27	0
4	FMT	B	1375	3/3	0.95	0.28	29,29,31,33	0
4	FMT	B	1379	3/3	0.95	0.07	18,18,21,24	0
4	FMT	A	1383	3/3	0.95	0.13	18,18,24,28	0
4	FMT	A	1390	3/3	0.96	0.06	19,19,22,23	0
4	FMT	A	1384	3/3	0.97	0.14	24,24,26,26	0
4	FMT	B	1378	3/3	0.97	0.11	19,19,20,21	0
4	FMT	A	1388	3/3	0.97	0.28	25,25,28,28	0
4	FMT	A	1386	3/3	0.97	0.21	26,26,26,27	0
2	GDC	A	1376	39/39	0.98	0.06	7,9,15,17	0
3	NAD	A	1378	44/44	0.99	0.04	5,7,8,10	0
3	NAD	B	1374	44/44	0.99	0.04	5,6,7,9	0
2	GDC	B	1372	39/39	0.99	0.05	5,6,14,16	0
4	FMT	A	1380	3/3	0.99	0.05	10,10,10,13	0

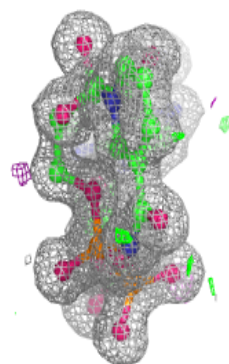
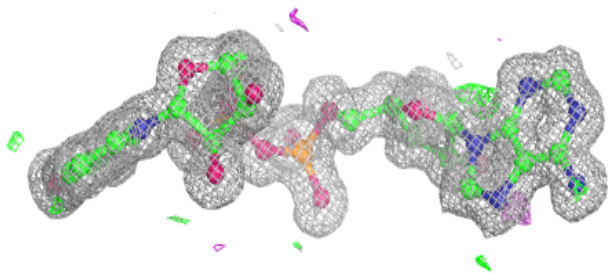
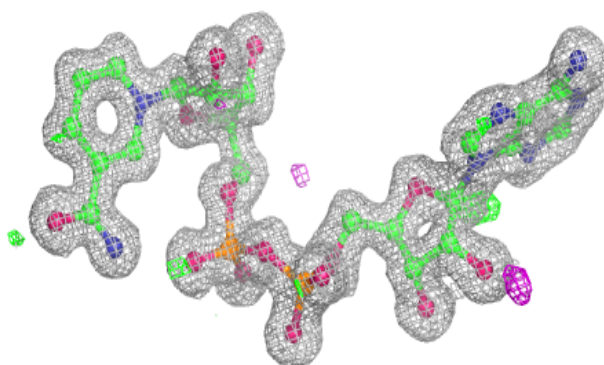
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GDC A 1376:

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

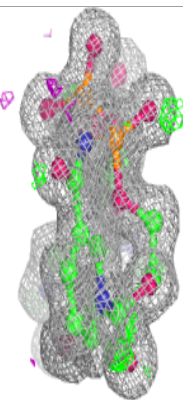
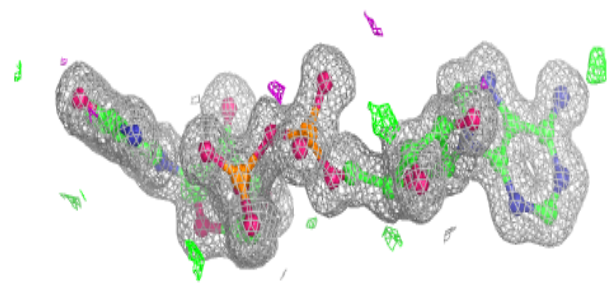
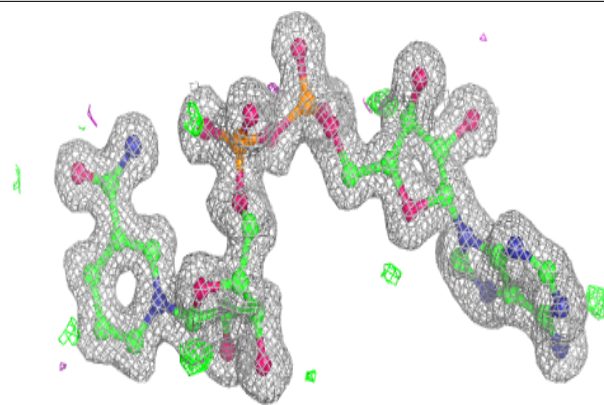
**Electron density around NAD A 1378:**

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

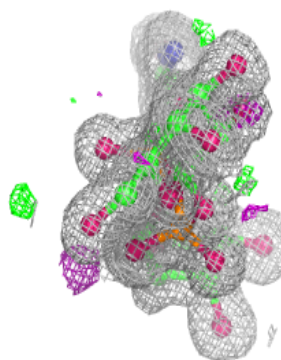
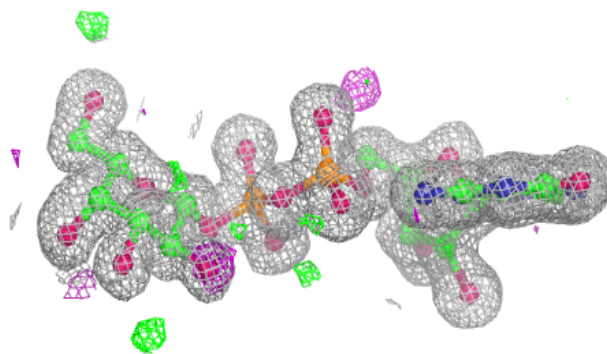
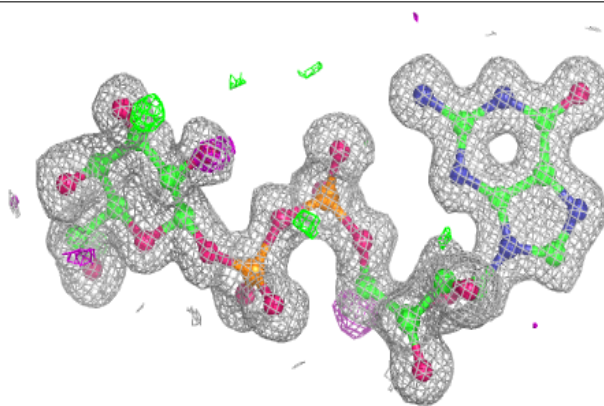


Electron density around NAD B 1374:

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

**Electron density around GDC B 1372:**

$2mF_o-DF_c$ (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.