



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:16 AM UTC

PDB ID : 1MV8 / pdb_00001mv8
Title : 1.55 Å crystal structure of a ternary complex of GDP-mannose dehydrogenase from *Pseudomonas aeruginosa*
Authors : Snook, C.F.; Tipton, P.A.; Beamer, L.J.
Deposited on : 2002-09-24
Resolution : 1.55 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
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	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

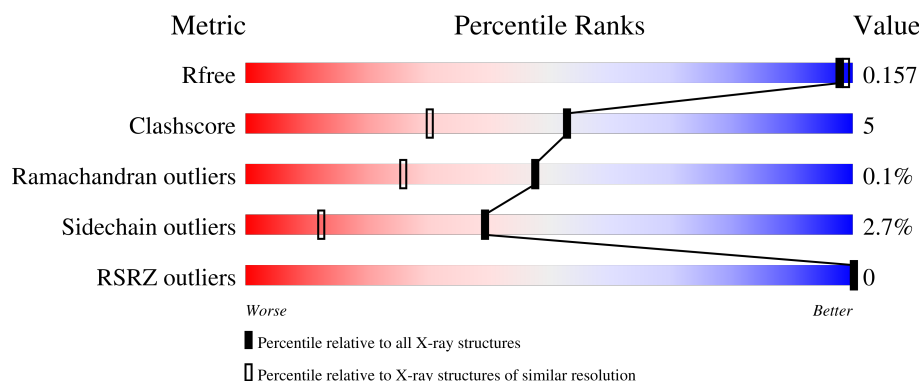
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

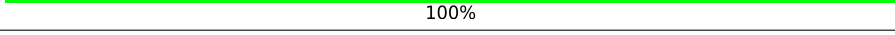
The reported resolution of this entry is 1.55 Å.

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	2145 (1.56-1.56)
Clashscore	190562	2189 (1.56-1.56)
Ramachandran outliers	187476	2153 (1.56-1.56)
Sidechain outliers	187428	2150 (1.56-1.56)
RSRZ outliers	180081	2146 (1.56-1.56)

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	436	 87% 11% .
1	B	436	 91% 8% .
1	C	436	 91% 9% .
1	D	436	 89% 10% .
2	E	2	 100%

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Mol	Chain	Length	Quality of chain
2	F	2	

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
5	ACY	C	2010	-	-	X	-

2 Entry composition

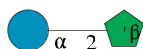
There are 7 unique types of molecules in this entry. The entry contains 14879 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 6-dehydrogenase.

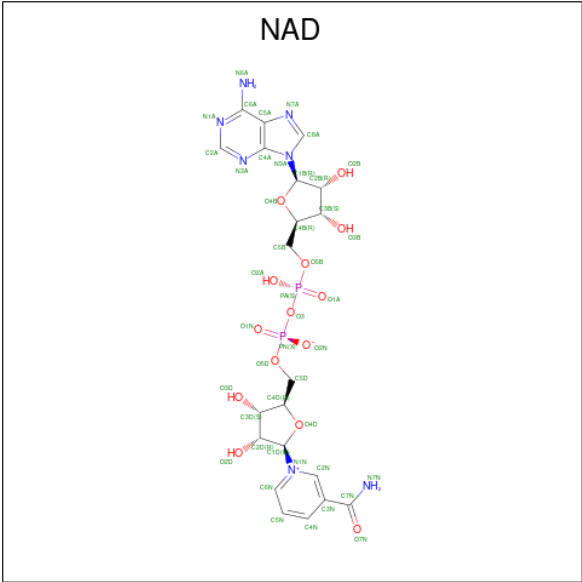
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	436	Total	C	N	O	S	0	0	0
			3280	2065	562	635	18			
1	B	436	Total	C	N	O	S	0	0	0
			3273	2066	562	627	18			
1	C	436	Total	C	N	O	S	0	0	0
			3297	2077	566	636	18			
1	D	436	Total	C	N	O	S	0	0	0
			3291	2075	565	633	18			

- Molecule 2 is an oligosaccharide called beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose.



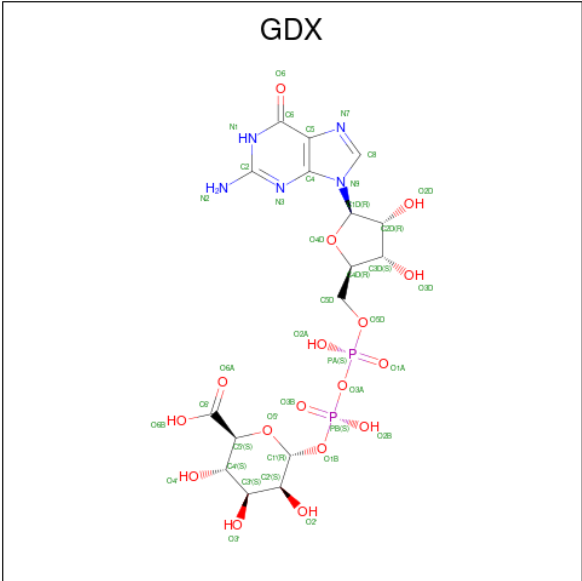
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	E	2	Total	C	O	0	0	0
			23	12	11			
2	F	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



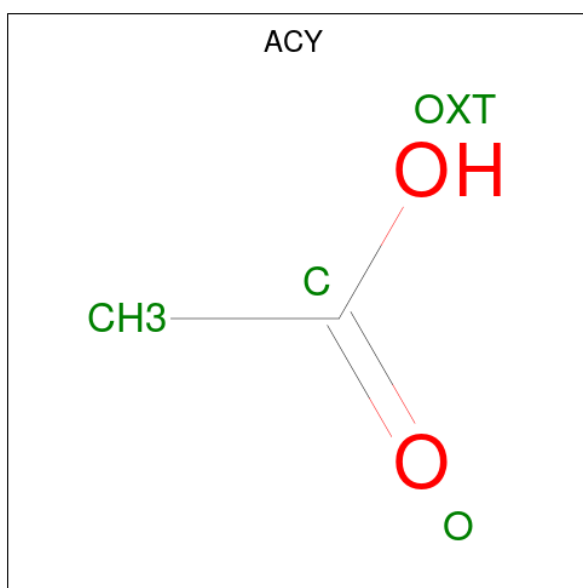
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			35	15	5	13	2		
3	B	1	Total	C	N	O	P	0	0
			35	15	5	13	2		
3	C	1	Total	C	N	O	P	0	0
			35	15	5	13	2		
3	D	1	Total	C	N	O	P	0	0
			35	15	5	13	2		

- Molecule 4 is GUANOSINE 5'-(TRIHYDROGEN DIPHOSPHATE), P'-D-MANNOPYRANOSYL ESTER (CCD ID: GDX) (formula: C₁₆H₂₃N₅O₁₇P₂).



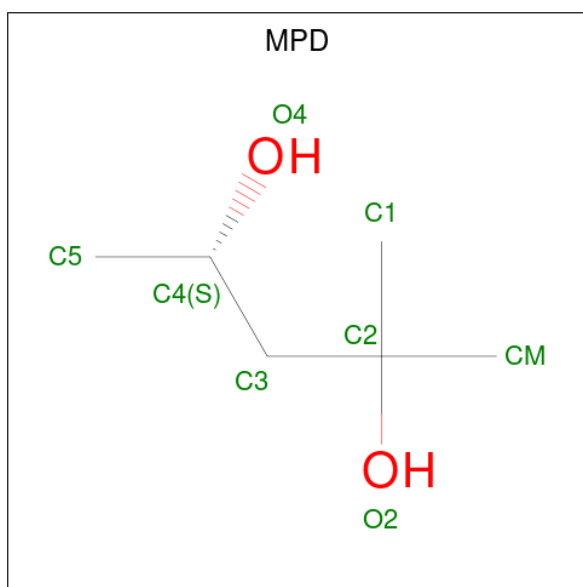
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			40	16	5	17	2		
4	A	1	Total	C	N	O	P	0	0
			40	16	5	17	2		
4	D	1	Total	C	N	O	P	0	0
			40	16	5	17	2		
4	D	1	Total	C	N	O	P	0	0
			40	16	5	17	2		

- Molecule 5 is ACETIC ACID (CCD ID: ACY) (formula: C₂H₄O₂).



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

- Molecule 6 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	C	O	0	0
			8	6	2		

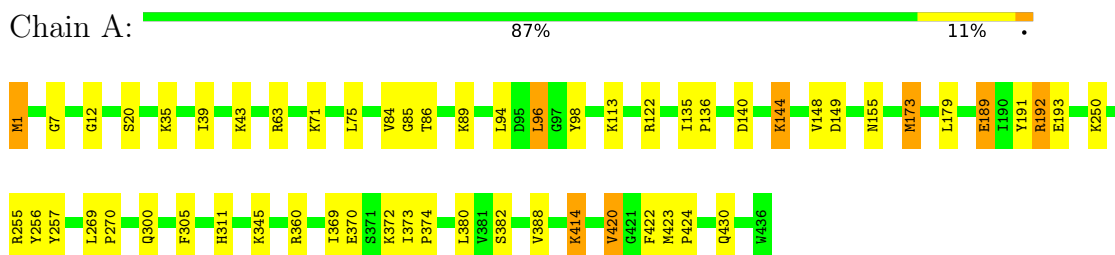
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	289	Total	O	0	0
			289	289		
7	B	301	Total	O	0	0
			301	301		
7	C	386	Total	O	0	0
			386	386		
7	D	400	Total	O	0	0
			400	400		

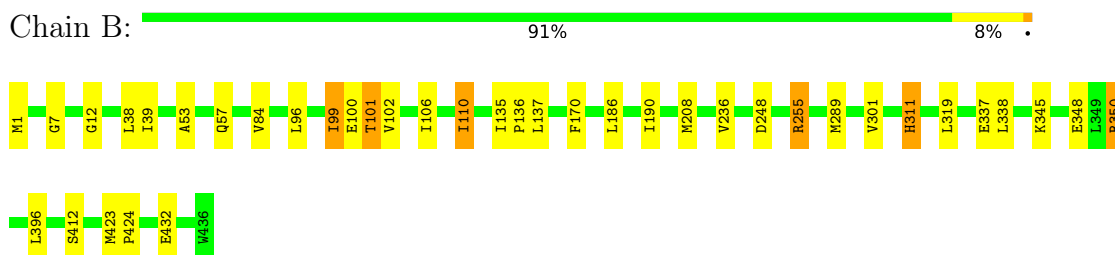
3 Residue-property plots

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.

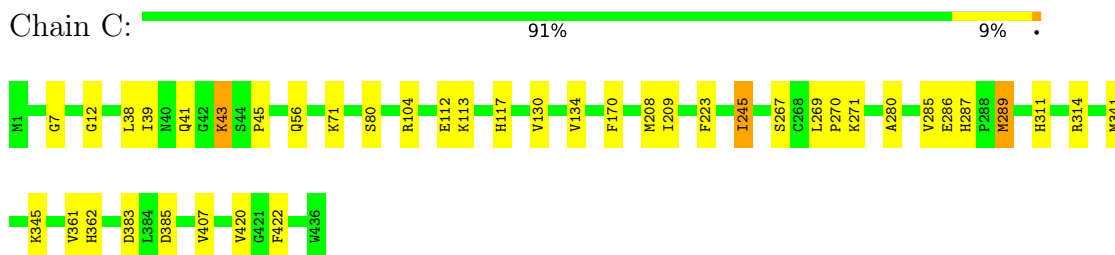
- Molecule 1: GDP-mannose 6-dehydrogenase



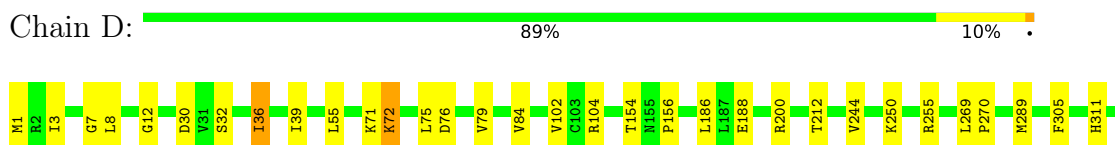
- Molecule 1: GDP-mannose 6-dehydrogenase



- Molecule 1: GDP-mannose 6-dehydrogenase



- Molecule 1: GDP-mannose 6-dehydrogenase





- Molecule 2: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain E:  100%



- Molecule 2: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain F:  50% 50%



4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	82.47Å 82.47Å 309.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.55 40.00 – 1.55	Depositor EDS
% Data completeness (in resolution range)	100.0 (40.00-1.55) 99.0 (40.00-1.55)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 1.55Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.174 , 0.194 0.150 , 0.157	Depositor DCC
R_{free} test set	14843 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	15.1	Xtriage
Anisotropy	0.019	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 27.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.176 for h,-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	14879	wwPDB-VP
Average B, all atoms (Å ²)	11.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.91% 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: GDX, ACY, MPD, GLC, FRU, 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	0.54	1/3333 (0.0%)	0.84	1/4520 (0.0%)
1	B	0.59	1/3327 (0.0%)	0.85	1/4511 (0.0%)
1	C	0.53	3/3351 (0.1%)	0.84	1/4543 (0.0%)
1	D	0.52	2/3345 (0.1%)	0.83	0/4533
All	All	0.55	7/13356 (0.1%)	0.84	3/18107 (0.0%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	289	MET	SD-CE	-16.98	1.37	1.79
1	A	173	MET	SD-CE	-11.38	1.51	1.79
1	C	289	MET	SD-CE	-6.53	1.63	1.79
1	D	289	MET	SD-CE	-6.03	1.64	1.79
1	C	341	MET	SD-CE	-5.75	1.65	1.79
1	D	341	MET	SD-CE	-5.23	1.66	1.79
1	C	208	MET	SD-CE	-5.17	1.66	1.79

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	311	HIS	N-CA-C	6.66	121.47	112.88
1	C	311	HIS	N-CA-C	6.40	121.14	112.88
1	B	311	HIS	N-CA-C	6.25	121.04	113.17

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	3280	0	3256	41	0
1	B	3273	0	3255	27	0
1	C	3297	0	3281	28	0
1	D	3291	0	3281	44	0
2	E	23	0	21	0	0
2	F	23	0	21	0	0
3	A	35	0	19	2	0
3	B	35	0	19	0	0
3	C	35	0	19	0	0
3	D	35	0	19	0	0
4	A	80	0	32	0	0
4	D	80	0	32	0	0
5	C	8	0	6	3	0
6	C	8	0	14	0	0
7	A	289	0	0	2	0
7	B	301	0	0	3	0
7	C	386	0	0	7	1
7	D	400	0	0	8	1
All	All	14879	0	13275	133	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 5.

All (133) 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:D:305:PHE:HZ	1:D:345:LYS:CD	1.47	1.26
1:B:348:GLU:OE2	1:B:350:ARG:NH2	1.82	1.11
1:D:305:PHE:CZ	1:D:345:LYS:CD	2.35	1.08
1:D:305:PHE:HZ	1:D:345:LYS:HD3	1.15	1.05
1:D:305:PHE:CZ	1:D:345:LYS:HD3	1.94	1.02
1:A:382:SER:OG	7:A:2295:HOH:O	1.78	1.00
1:B:350:ARG:HG3	1:B:350:ARG:HH11	1.33	0.94
1:D:188:GLU:OE2	1:D:200:ARG:HD2	1.69	0.93
1:A:360:ARG:HD2	1:A:370:GLU:OE2	1.69	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:305:PHE:CZ	1:D:345:LYS:HD2	2.05	0.89
1:C:383:ASP:OD2	1:C:385:ASP:HB2	1.75	0.86
1:A:122:ARG:NH1	1:A:191:TYR:OH	2.10	0.85
1:B:106:ILE:O	1:B:110:ILE:HG23	1.74	0.85
1:D:360:ARG:HD2	7:D:2401:HOH:O	1.76	0.84
1:A:122:ARG:NH1	1:A:155:ASN:OD1	2.12	0.83
1:D:30:ASP:HB3	1:D:36:ILE:HD11	1.63	0.80
1:A:122:ARG:NH1	1:A:191:TYR:HH	1.82	0.77
1:D:188:GLU:OE2	1:D:200:ARG:CD	2.32	0.77
1:B:255:ARG:NH1	7:B:2126:HOH:O	2.19	0.76
5:C:2009:ACY:C	5:C:2010:ACY:O	2.34	0.75
1:B:345:LYS:HE3	1:D:340:GLU:OE1	1.86	0.74
1:C:286:GLU:OE2	7:C:2063:HOH:O	2.07	0.71
1:A:84:VAL:HG11	1:A:98:TYR:HB3	1.72	0.70
1:A:71:LYS:O	1:A:75:LEU:HD23	1.93	0.68
1:B:350:ARG:HG3	1:B:350:ARG:NH1	2.06	0.67
1:D:255:ARG:NH1	7:D:2413:HOH:O	2.28	0.66
1:B:345:LYS:HE3	1:D:340:GLU:CD	2.20	0.66
1:B:84:VAL:HG11	1:B:102:VAL:HG21	1.77	0.65
1:D:361:VAL:HG22	1:D:362:HIS:CD2	2.32	0.64
1:C:280:ALA:HB2	7:C:2376:HOH:O	1.97	0.64
1:B:345:LYS:CE	1:D:340:GLU:OE1	2.46	0.63
1:A:84:VAL:HG12	1:A:85:GLY:N	2.14	0.63
1:C:285:VAL:O	1:C:287:HIS:HD2	1.83	0.61
1:A:173:MET:HE3	1:B:248:ASP:HB2	1.81	0.61
1:C:267:SER:O	1:C:271:LYS:NZ	2.26	0.60
1:C:45:PRO:HG2	7:C:2330:HOH:O	2.00	0.60
1:D:30:ASP:CB	1:D:36:ILE:HD11	2.30	0.59
1:A:372:LYS:C	1:A:374:PRO:HD2	2.27	0.59
1:D:30:ASP:HB3	1:D:36:ILE:CD1	2.32	0.59
1:C:80:SER:OG	1:C:117:HIS:HE1	1.85	0.59
1:A:122:ARG:HD2	1:A:155:ASN:O	2.02	0.59
1:D:32:SER:O	1:D:36:ILE:HD13	2.04	0.57
1:D:8:LEU:HD13	1:D:39:ILE:HD13	1.87	0.57
1:B:101:THR:HG21	7:B:2072:HOH:O	2.05	0.56
1:B:311:HIS:HE1	1:B:432:GLU:OE2	1.88	0.56
1:B:99:ILE:HG13	1:B:100:GLU:N	2.21	0.56
1:A:420:VAL:HG11	1:A:422:PHE:CE2	2.40	0.56
1:D:84:VAL:HG11	1:D:102:VAL:HG21	1.88	0.55
1:D:305:PHE:HZ	1:D:345:LYS:CE	2.18	0.55
1:C:314:ARG:CZ	7:C:2076:HOH:O	2.53	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:VAL:HG13	3:A:2001:NAD:C8A	2.37	0.55
1:C:113:LYS:HZ3	1:C:117:HIS:HD2	1.55	0.54
1:B:348:GLU:CD	1:B:350:ARG:HH22	2.08	0.54
1:A:84:VAL:CG1	1:A:98:TYR:HB3	2.38	0.54
1:C:113:LYS:NZ	1:C:117:HIS:HD2	2.05	0.54
1:A:373:ILE:N	1:A:374:PRO:CD	2.71	0.53
1:C:287:HIS:HE1	7:C:2081:HOH:O	1.91	0.53
1:B:350:ARG:NH1	1:B:350:ARG:CG	2.71	0.53
1:D:71:LYS:O	1:D:75:LEU:HD13	2.09	0.53
1:B:53:ALA:O	1:B:57:GLN:HG3	2.09	0.52
1:D:305:PHE:CZ	1:D:345:LYS:NZ	2.73	0.52
1:D:311:HIS:HE1	7:D:2240:HOH:O	1.92	0.51
1:D:424:PRO:HB2	1:D:425:HIS:CD2	2.45	0.51
1:C:420:VAL:O	5:C:2010:ACY:H1	2.11	0.51
1:A:84:VAL:CG1	3:A:2001:NAD:C8A	2.89	0.50
1:A:84:VAL:HG12	1:A:85:GLY:H	1.77	0.50
1:C:41:GLN:HB2	1:C:43:LYS:HG3	1.93	0.50
1:D:104:ARG:CZ	7:D:2360:HOH:O	2.59	0.50
1:A:20:SER:O	1:A:63:ARG:NH1	2.45	0.49
1:C:223:PHE:HB2	1:C:289:MET:HE1	1.93	0.49
1:A:86:THR:HB	1:A:94:LEU:HD11	1.96	0.48
1:A:250:LYS:NZ	1:B:170:PHE:O	2.43	0.48
1:B:1:MET:HE1	1:B:190:ILE:HG13	1.97	0.47
1:B:186:LEU:HD23	1:B:186:LEU:C	2.40	0.47
1:A:135:ILE:HB	1:A:136:PRO:HD3	1.96	0.47
1:A:189:GLU:OE1	1:A:192:ARG:NE	2.36	0.47
1:C:383:ASP:OD2	1:C:385:ASP:CB	2.56	0.47
1:B:7:GLY:O	1:B:12:GLY:HA3	2.16	0.46
1:D:72:LYS:HD3	1:D:76:ASP:OD2	2.15	0.46
1:D:410:THR:HG21	7:D:2337:HOH:O	2.15	0.46
1:A:420:VAL:HG11	1:A:422:PHE:HE2	1.80	0.46
1:D:3:ILE:HG12	1:D:79:VAL:CG1	2.45	0.46
1:D:7:GLY:O	1:D:12:GLY:HA3	2.16	0.46
1:D:255:ARG:NH2	7:D:2413:HOH:O	2.48	0.46
1:C:170:PHE:O	1:D:250:LYS:NZ	2.40	0.45
1:B:311:HIS:CE1	1:B:432:GLU:OE2	2.67	0.45
1:C:209:ILE:HD13	1:D:244:VAL:HG11	1.98	0.45
1:D:36:ILE:CD1	1:D:36:ILE:N	2.79	0.45
1:A:7:GLY:O	1:A:12:GLY:HA3	2.17	0.45
1:C:420:VAL:HG13	5:C:2010:ACY:H2	1.99	0.45
1:D:305:PHE:CE2	1:D:345:LYS:NZ	2.78	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:ILE:HB	1:B:136:PRO:HD3	1.99	0.44
1:B:423:MET:HA	1:B:424:PRO:HD2	1.90	0.44
1:D:396:LEU:HD22	1:D:396:LEU:N	2.32	0.44
1:B:301:VAL:HG11	1:B:337:GLU:OE1	2.18	0.44
1:A:360:ARG:HG2	1:A:369:ILE:HG21	2.00	0.43
1:A:75:LEU:HD13	1:A:113:LYS:HG3	2.00	0.43
1:A:89:LYS:HE3	7:A:2237:HOH:O	2.16	0.43
1:A:373:ILE:N	1:A:374:PRO:HD2	2.32	0.43
1:A:269:LEU:HB2	1:A:270:PRO:HD3	2.01	0.43
1:C:7:GLY:O	1:C:12:GLY:HA3	2.18	0.43
1:A:84:VAL:CG1	1:A:85:GLY:N	2.79	0.43
1:D:394:LEU:HD13	1:D:406:LEU:HD11	1.99	0.43
1:A:144:LYS:HG2	1:A:149:ASP:HB3	2.01	0.43
1:A:360:ARG:CD	1:A:370:GLU:OE2	2.55	0.42
1:A:256:TYR:HD2	1:A:257:TYR:CE2	2.37	0.42
1:D:423:MET:HA	1:D:424:PRO:HD3	1.94	0.42
1:B:319:LEU:HD12	1:B:396:LEU:HD23	2.01	0.42
1:C:104:ARG:NH2	7:C:2308:HOH:O	2.51	0.42
1:C:71:LYS:NZ	1:C:112:GLU:OE2	2.49	0.42
1:A:300:GLN:HE21	1:A:300:GLN:HA	1.84	0.42
1:A:388:VAL:O	1:A:414:LYS:HE3	2.19	0.42
1:C:245:ILE:HD11	1:D:212:THR:HB	2.02	0.42
1:C:269:LEU:HB2	1:C:270:PRO:HD3	2.01	0.42
1:B:255:ARG:HG2	7:B:2027:HOH:O	2.20	0.41
1:A:1:MET:HE2	1:A:1:MET:HB2	1.75	0.41
1:C:407:VAL:HG21	1:C:422:PHE:HB3	2.03	0.41
1:D:269:LEU:HB2	1:D:270:PRO:HD3	2.02	0.41
1:C:104:ARG:NE	7:C:2308:HOH:O	2.53	0.41
1:D:255:ARG:CZ	7:D:2413:HOH:O	2.64	0.41
1:D:371:SER:C	1:D:374:PRO:HD3	2.45	0.41
1:A:35:LYS:O	1:A:39:ILE:HG12	2.20	0.41
1:A:94:LEU:HG	1:A:96:LEU:HD13	2.03	0.41
1:A:305:PHE:HZ	1:A:345:LYS:HG3	1.86	0.41
1:C:130:VAL:HA	1:C:134:VAL:HB	2.02	0.41
1:D:1:MET:HE1	1:D:186:LEU:HD11	2.03	0.41
1:D:311:HIS:CE1	7:D:2240:HOH:O	2.70	0.41
1:C:361:VAL:HG23	1:C:362:HIS:CD2	2.55	0.41
1:A:423:MET:HA	1:A:424:PRO:HD3	1.97	0.40
1:C:113:LYS:NZ	1:C:117:HIS:CD2	2.88	0.40
1:A:84:VAL:CG1	1:A:85:GLY:H	2.34	0.40
1:B:100:GLU:HG2	1:B:137:LEU:HD11	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:154:THR:HG22	1:D:156:PRO:HD3	2.02	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:C:2358:HOH:O	7:D:2112:HOH:O[4_545]	1.98	0.22

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	434/436 (100%)	421 (97%)	12 (3%)	1 (0%)	43	24
1	B	434/436 (100%)	420 (97%)	14 (3%)	0	100	100
1	C	434/436 (100%)	421 (97%)	13 (3%)	0	100	100
1	D	434/436 (100%)	422 (97%)	12 (3%)	0	100	100
All	All	1736/1744 (100%)	1684 (97%)	51 (3%)	1 (0%)	48	26

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	192	ARG

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	356/370 (96%)	342 (96%)	14 (4%)	28	5
1	B	353/370 (95%)	341 (97%)	12 (3%)	32	7
1	C	359/370 (97%)	353 (98%)	6 (2%)	53	25
1	D	358/370 (97%)	352 (98%)	6 (2%)	53	25
All	All	1426/1480 (96%)	1388 (97%)	38 (3%)	39	12

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	43	LYS
1	A	96	LEU
1	A	140	ASP
1	A	144	LYS
1	A	148	VAL
1	A	179	LEU
1	A	189	GLU
1	A	193	GLU
1	A	255	ARG
1	A	380	LEU
1	A	414	LYS
1	A	420	VAL
1	A	430	GLN
1	B	38	LEU
1	B	39	ILE
1	B	96	LEU
1	B	99	ILE
1	B	101	THR
1	B	110	ILE
1	B	208	MET
1	B	236	VAL
1	B	255	ARG
1	B	338	LEU
1	B	350	ARG
1	B	412	SER
1	C	38	LEU
1	C	39	ILE
1	C	43	LYS
1	C	56	GLN
1	C	245	ILE

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Mol	Chain	Res	Type
1	C	345	LYS
1	D	36	ILE
1	D	55	LEU
1	D	72	LYS
1	D	361	VAL
1	D	379	LEU
1	D	406	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	299	ASN
1	A	300	GLN
1	B	155	ASN
1	B	229	ASN
1	B	311	HIS
1	B	355	ASN
1	B	362	HIS
1	B	365	ASN
1	B	425	HIS
1	C	117	HIS
1	C	155	ASN
1	C	229	ASN
1	C	287	HIS
1	D	155	ASN
1	D	300	GLN
1	D	311	HIS
1	D	425	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

4 monosaccharides 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$
2	GLC	E	1	2	11,11,12	0.57	0	15,15,17	0.58	0
2	FRU	E	2	2	11,12,12	0.53	0	10,18,18	0.63	0
2	GLC	F	1	2	11,11,12	0.52	0	15,15,17	0.98	1 (6%)
2	FRU	F	2	2	11,12,12	0.54	0	10,18,18	0.41	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
2	GLC	E	1	2	-	0/2/19/22	0/1/1/1
2	FRU	E	2	2	-	5/5/24/24	0/1/1/1
2	GLC	F	1	2	-	0/2/19/22	0/1/1/1
2	FRU	F	2	2	-	2/5/24/24	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1	GLC	C1-O5-C5	3.04	116.26	112.19

There are no chirality outliers.

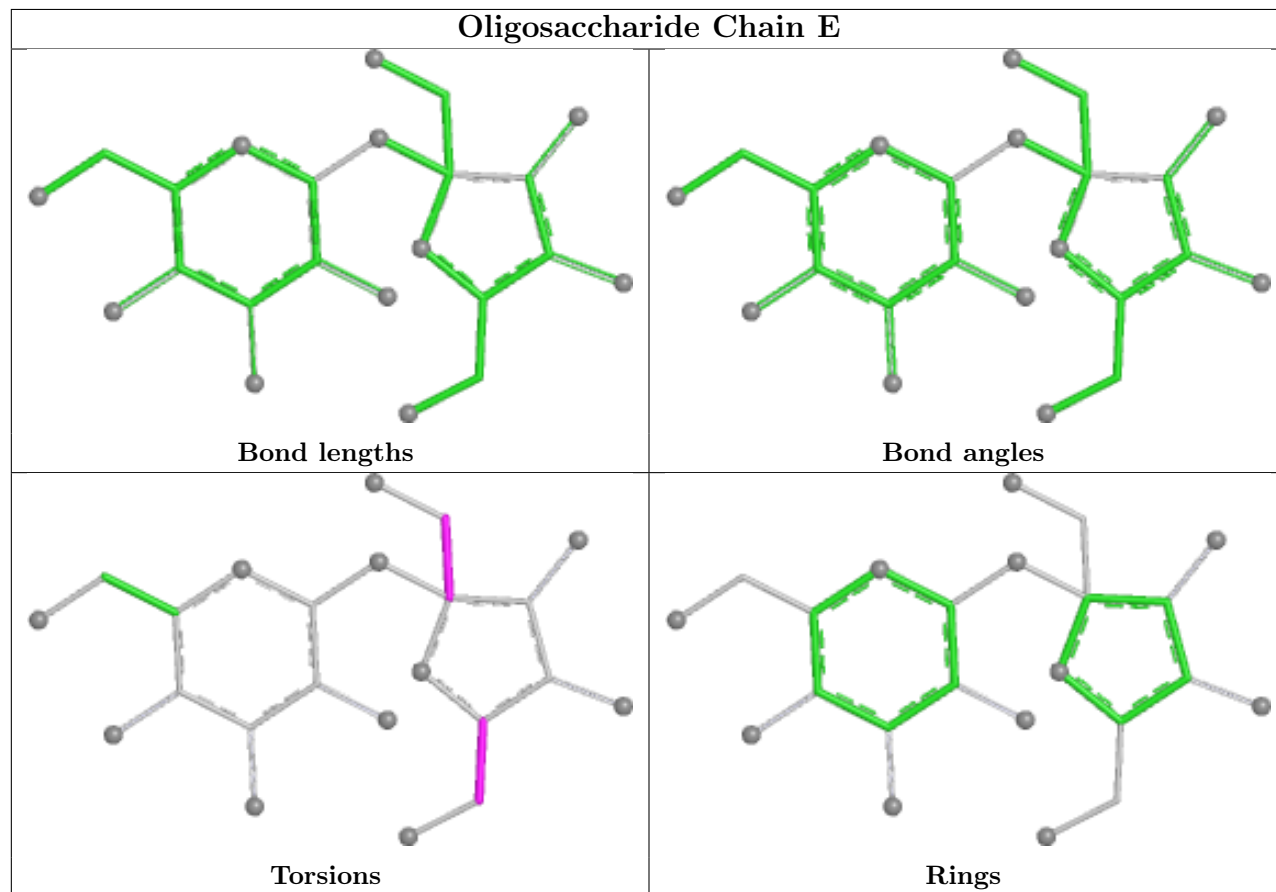
All (7) torsion outliers are listed below:

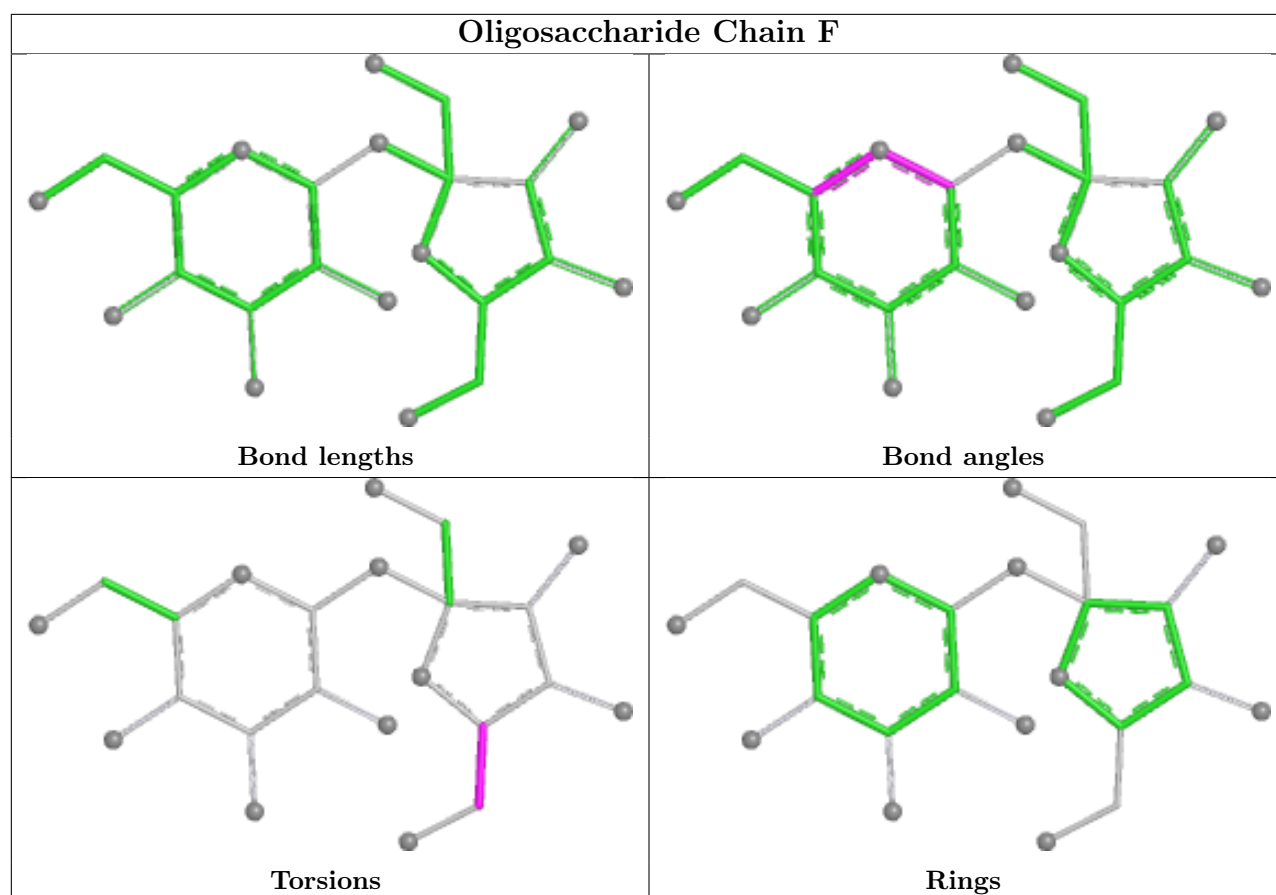
Mol	Chain	Res	Type	Atoms
2	E	2	FRU	O1-C1-C2-O2
2	E	2	FRU	C4-C5-C6-O6
2	E	2	FRU	O5-C5-C6-O6
2	F	2	FRU	C4-C5-C6-O6
2	F	2	FRU	O5-C5-C6-O6
2	E	2	FRU	O1-C1-C2-O5
2	E	2	FRU	O1-C1-C2-C3

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.





5.6 Ligand geometry [i](#)

11 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	$\# Z > 2$
3	NAD	A	2001	-	38,38,48	1.01	2 (5%)	53,58,73	1.65	10 (18%)
3	NAD	D	2004	-	38,38,48	1.06	3 (7%)	53,58,73	1.68	10 (18%)
5	ACY	C	2010	-	3,3,3	0.83	0	3,3,3	0.65	0
3	NAD	C	2003	-	38,38,48	1.18	3 (7%)	53,58,73	1.59	8 (15%)
4	GDX	D	2008	-	42,43,43	3.69	17 (40%)	63,67,67	1.91	17 (26%)
4	GDX	A	2006	-	42,43,43	3.71	18 (42%)	63,67,67	2.01	17 (26%)
3	NAD	B	2002	-	38,38,48	1.12	5 (13%)	53,58,73	1.76	13 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GDX	D	2007	-	42,43,43	3.65	17 (40%)	63,67,67	1.95	17 (26%)
5	ACY	C	2009	-	3,3,3	0.74	0	3,3,3	1.12	0
4	GDX	A	2005	-	42,43,43	3.74	18 (42%)	63,67,67	1.97	18 (28%)
6	MPD	C	2011	-	7,7,7	0.29	0	9,10,10	0.30	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	NAD	A	2001	-	-	0/22/51/62	0/4/4/5
3	NAD	D	2004	-	-	1/22/51/62	0/4/4/5
3	NAD	C	2003	-	-	0/22/51/62	0/4/4/5
4	GDX	D	2008	-	-	1/25/61/61	0/4/4/4
4	GDX	A	2006	-	-	0/25/61/61	0/4/4/4
3	NAD	B	2002	-	-	1/22/51/62	0/4/4/5
4	GDX	D	2007	-	-	0/25/61/61	0/4/4/4
4	GDX	A	2005	-	-	1/25/61/61	0/4/4/4
6	MPD	C	2011	-	-	2/5/5/5	-

All (83) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	2007	GDX	C4'-C5'	-10.19	1.36	1.53
4	D	2008	GDX	C4'-C5'	-10.16	1.36	1.53
4	A	2005	GDX	C4'-C5'	-10.05	1.36	1.53
4	A	2006	GDX	C4'-C5'	-10.03	1.36	1.53
4	A	2005	GDX	C5'-C6'	-8.06	1.36	1.53
4	A	2006	GDX	C5'-C6'	-7.85	1.36	1.53
4	D	2007	GDX	C5'-C6'	-7.58	1.37	1.53
4	D	2008	GDX	C5'-C6'	-7.42	1.37	1.53
4	A	2006	GDX	O2'-C2'	-6.82	1.26	1.43
4	A	2006	GDX	O3'-C3'	-6.64	1.26	1.43
4	D	2008	GDX	C3D-C4D	-6.56	1.36	1.53
4	A	2005	GDX	C3D-C4D	-6.54	1.36	1.53
4	D	2008	GDX	O4'-C4'	-6.52	1.26	1.43
4	A	2005	GDX	O3'-C3'	-6.48	1.26	1.43
4	A	2005	GDX	O2'-C2'	-6.47	1.26	1.43
4	D	2008	GDX	O2'-C2'	-6.44	1.27	1.43
4	D	2008	GDX	O3'-C3'	-6.38	1.27	1.43
4	D	2007	GDX	O4'-C4'	-6.33	1.27	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	2007	GDX	O3'-C3'	-6.33	1.27	1.43
4	D	2007	GDX	C3D-C4D	-6.33	1.36	1.53
4	A	2006	GDX	O4'-C4'	-6.32	1.27	1.43
4	A	2006	GDX	C3D-C4D	-6.27	1.37	1.53
4	A	2006	GDX	C3D-C2D	-6.25	1.36	1.53
4	D	2007	GDX	O2'-C2'	-6.22	1.27	1.43
4	A	2005	GDX	O2D-C2D	-6.21	1.27	1.43
4	D	2008	GDX	C3D-C2D	-6.11	1.36	1.53
4	A	2005	GDX	O4'-C4'	-6.10	1.27	1.43
4	D	2007	GDX	C3D-C2D	-6.10	1.36	1.53
4	A	2005	GDX	C3D-C2D	-6.04	1.37	1.53
4	D	2007	GDX	O2D-C2D	-5.94	1.28	1.43
4	D	2008	GDX	O2D-C2D	-5.89	1.28	1.43
4	A	2006	GDX	C3'-C2'	-5.76	1.37	1.52
4	A	2005	GDX	C4'-C3'	-5.65	1.37	1.52
4	A	2006	GDX	C4'-C3'	-5.64	1.37	1.52
4	A	2006	GDX	O2D-C2D	-5.61	1.29	1.43
4	A	2005	GDX	C3'-C2'	-5.58	1.37	1.52
4	D	2008	GDX	C4'-C3'	-5.37	1.38	1.52
4	D	2007	GDX	C3'-C2'	-5.34	1.38	1.52
4	A	2005	GDX	C2D-C1D	-5.29	1.36	1.53
4	D	2008	GDX	C3'-C2'	-5.24	1.38	1.52
4	D	2007	GDX	C1'-C2'	-5.23	1.37	1.52
4	D	2007	GDX	C4'-C3'	-5.21	1.38	1.52
4	D	2008	GDX	C1'-C2'	-5.13	1.37	1.52
4	A	2006	GDX	C1'-C2'	-5.11	1.37	1.52
4	D	2007	GDX	C2D-C1D	-5.06	1.37	1.53
4	A	2006	GDX	C2D-C1D	-5.04	1.37	1.53
4	A	2005	GDX	C1'-C2'	-4.94	1.38	1.52
4	D	2008	GDX	C2D-C1D	-4.91	1.38	1.53
4	A	2005	GDX	C1D-N9	-3.42	1.37	1.47
3	C	2003	NAD	PA-O3	3.38	1.63	1.59
4	A	2005	GDX	C5-C4	3.33	1.47	1.38
4	D	2008	GDX	C5-C4	3.24	1.47	1.38
4	A	2006	GDX	C5-C4	3.22	1.47	1.38
4	D	2007	GDX	C5-C4	3.13	1.47	1.38
4	A	2006	GDX	C1D-N9	-3.13	1.38	1.47
4	D	2008	GDX	C1D-N9	-3.12	1.38	1.47
3	A	2001	NAD	PA-O3	3.04	1.62	1.59
4	D	2007	GDX	C1D-N9	-2.90	1.39	1.47
3	C	2003	NAD	C2A-N3A	2.89	1.39	1.33
3	D	2004	NAD	C2A-N3A	2.79	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2002	NAD	C2A-N3A	2.68	1.38	1.33
3	B	2002	NAD	PA-O3	2.65	1.62	1.59
3	B	2002	NAD	C8A-N7A	2.58	1.36	1.31
3	C	2003	NAD	C8A-N7A	2.47	1.36	1.31
3	D	2004	NAD	C2A-N1A	2.40	1.38	1.33
3	B	2002	NAD	C2A-N1A	2.36	1.38	1.33
4	A	2006	GDX	C4-N9	-2.31	1.32	1.38
4	A	2006	GDX	C5-N7	-2.27	1.34	1.39
3	A	2001	NAD	C2A-N3A	2.25	1.37	1.33
4	A	2005	GDX	C6-N1	-2.23	1.34	1.38
4	A	2005	GDX	O6B-C6'	-2.20	1.23	1.30
4	A	2005	GDX	C4-N9	-2.18	1.32	1.38
4	D	2008	GDX	C6-N1	-2.17	1.34	1.38
4	D	2007	GDX	O6B-C6'	-2.17	1.23	1.30
4	D	2007	GDX	C4-N9	-2.12	1.32	1.38
4	A	2005	GDX	C5-N7	-2.11	1.34	1.39
4	A	2006	GDX	O6B-C6'	-2.11	1.23	1.30
4	D	2008	GDX	O5'-C1'	2.10	1.47	1.41
4	A	2006	GDX	C6-N1	-2.10	1.34	1.38
4	D	2008	GDX	O5'-C5'	2.09	1.47	1.43
3	B	2002	NAD	PN-O2N	-2.07	1.45	1.55
4	D	2007	GDX	C5-N7	-2.07	1.34	1.39
3	D	2004	NAD	C8A-N7A	2.04	1.35	1.31

All (110) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2002	NAD	N3A-C2A-N1A	-5.98	119.53	128.58
4	A	2005	GDX	N9-C4-N3	5.73	137.40	125.95
4	A	2006	GDX	N9-C4-N3	5.62	137.18	125.95
3	A	2001	NAD	N3A-C2A-N1A	-5.32	120.53	128.58
4	D	2007	GDX	N9-C4-N3	5.28	136.52	125.95
4	D	2008	GDX	N9-C4-N3	5.22	136.39	125.95
3	C	2003	NAD	N3A-C2A-N1A	-5.11	120.84	128.58
3	D	2004	NAD	N3A-C2A-N1A	-5.04	120.96	128.58
4	A	2005	GDX	C5-C4-N3	-5.03	120.38	128.39
4	A	2006	GDX	C5-C4-N3	-5.00	120.43	128.39
4	D	2008	GDX	C5-C4-N3	-4.90	120.59	128.39
4	D	2007	GDX	C5-C4-N3	-4.89	120.61	128.39
4	A	2006	GDX	C2-N3-C4	4.35	119.79	112.30
4	D	2008	GDX	C2-N3-C4	4.34	119.78	112.30
3	B	2002	NAD	N9A-C8A-N7A	-4.26	107.89	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2006	GDX	O6B-C6'-O6A	-4.22	114.50	124.08
3	D	2004	NAD	N9A-C8A-N7A	-4.17	108.02	113.94
4	A	2005	GDX	C8-N9-C4	4.15	113.81	106.03
4	D	2007	GDX	O6B-C6'-O6A	-4.09	114.81	124.08
4	D	2007	GDX	C2-N3-C4	4.03	119.25	112.30
4	A	2006	GDX	C8-N9-C4	4.00	113.53	106.03
4	A	2005	GDX	C2-N3-C4	3.96	119.12	112.30
4	A	2006	GDX	O5'-C1'-O1B	-3.96	106.19	111.36
4	D	2007	GDX	C8-N9-C4	3.94	113.41	106.03
4	D	2008	GDX	C2D-C1D-N9	3.92	124.15	113.25
3	C	2003	NAD	N9A-C8A-N7A	-3.90	108.41	113.94
4	D	2007	GDX	C3D-C2D-C1D	3.75	108.56	101.46
3	A	2001	NAD	C5A-C4A-N3A	-3.74	121.56	126.72
4	A	2005	GDX	O6B-C6'-O6A	-3.73	115.62	124.08
3	A	2001	NAD	N9A-C8A-N7A	-3.68	108.72	113.94
4	A	2006	GDX	C2D-C1D-N9	3.60	123.28	113.25
4	A	2006	GDX	C2D-C3D-C4D	3.55	109.46	102.61
4	D	2008	GDX	C8-N9-C4	3.54	112.66	106.03
4	D	2007	GDX	C2D-C1D-N9	3.53	123.09	113.25
3	D	2004	NAD	C5A-C4A-N3A	-3.53	121.86	126.72
3	C	2003	NAD	C5A-C4A-N3A	-3.49	121.91	126.72
4	D	2008	GDX	C3D-C2D-C1D	3.47	108.02	101.46
4	D	2008	GDX	O6B-C6'-O6A	-3.41	116.34	124.08
3	D	2004	NAD	C5A-N7A-C8A	3.38	108.76	103.45
4	A	2005	GDX	C2D-C1D-N9	3.34	122.54	113.25
3	A	2001	NAD	C5A-N7A-C8A	3.32	108.67	103.45
4	A	2005	GDX	O4D-C1D-N9	3.31	115.87	108.36
4	A	2005	GDX	N9-C8-N7	-3.27	107.33	113.40
3	C	2003	NAD	C5A-N7A-C8A	3.27	108.59	103.45
3	B	2002	NAD	C5A-C4A-N3A	-3.26	122.22	126.72
4	A	2005	GDX	C2D-C3D-C4D	3.25	108.89	102.61
3	B	2002	NAD	C2A-N3A-C4A	3.24	119.74	111.83
4	D	2007	GDX	O4D-C1D-N9	3.23	115.67	108.36
3	B	2002	NAD	C5A-N7A-C8A	3.16	108.42	103.45
3	D	2004	NAD	O4B-C1B-N9A	3.16	114.15	108.09
4	A	2005	GDX	C3D-C2D-C1D	3.13	107.39	101.46
4	D	2007	GDX	N9-C8-N7	-3.12	107.61	113.40
3	C	2003	NAD	O4D-C4D-C3D	3.03	107.43	104.63
4	A	2006	GDX	N9-C8-N7	-3.02	107.81	113.40
3	B	2002	NAD	O2A-PA-O3	2.99	115.36	107.27
4	D	2007	GDX	C2D-C3D-C4D	2.99	108.38	102.61
3	A	2001	NAD	C2A-N3A-C4A	2.94	119.00	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	2008	GDX	C6-C5-N7	2.93	135.62	130.29
3	C	2003	NAD	C2A-N3A-C4A	2.84	118.77	111.83
4	D	2008	GDX	N9-C8-N7	-2.82	108.18	113.40
4	A	2006	GDX	C3D-C2D-C1D	2.79	106.74	101.46
3	A	2001	NAD	O4B-C1B-N9A	2.76	113.39	108.09
3	D	2004	NAD	O4D-C4D-C3D	2.76	107.18	104.63
4	D	2008	GDX	C2D-C3D-C4D	2.75	107.92	102.61
3	A	2001	NAD	C4A-C5A-N7A	-2.70	107.50	110.58
4	A	2006	GDX	O6B-C6'-C5'	2.70	123.38	113.64
3	D	2004	NAD	C2A-N3A-C4A	2.68	118.37	111.83
3	B	2002	NAD	O2N-PN-O3	2.65	114.45	107.27
4	A	2006	GDX	O4D-C1D-N9	2.60	114.26	108.36
3	D	2004	NAD	C4A-N9A-C8A	2.60	108.47	105.74
4	A	2005	GDX	C4'-C3'-C2'	2.56	115.32	110.83
3	D	2004	NAD	C4A-C5A-N7A	-2.54	107.67	110.58
4	D	2008	GDX	O5'-C1'-O1B	-2.52	108.07	111.36
4	A	2005	GDX	C6-C5-N7	2.49	134.82	130.29
3	C	2003	NAD	C4A-C5A-N7A	-2.46	107.77	110.58
3	B	2002	NAD	C4A-N9A-C8A	2.45	108.31	105.74
3	A	2001	NAD	O2A-PA-O3	2.45	113.91	107.27
4	A	2006	GDX	C6-C5-N7	2.40	134.66	130.29
4	D	2007	GDX	O6B-C6'-C5'	2.40	122.28	113.64
3	C	2003	NAD	O4B-C1B-N9A	2.39	112.69	108.09
4	A	2005	GDX	C8-N7-C5	2.39	108.52	104.26
4	A	2005	GDX	O3D-C3D-C4D	-2.39	104.23	111.08
4	A	2005	GDX	O6B-C6'-C5'	2.38	122.23	113.64
4	D	2008	GDX	C8-N7-C5	2.38	108.50	104.26
4	D	2008	GDX	O4D-C1D-N9	2.37	113.73	108.36
4	D	2007	GDX	C6-C5-N7	2.37	134.61	130.29
4	D	2007	GDX	C4'-C3'-C2'	2.37	114.99	110.83
4	D	2008	GDX	O3D-C3D-C4D	-2.36	104.30	111.08
3	B	2002	NAD	C4A-C5A-N7A	-2.32	107.92	110.58
3	B	2002	NAD	C4A-N9A-C1B	-2.32	121.22	126.63
3	B	2002	NAD	O4D-C4D-C3D	2.30	106.76	104.63
3	D	2004	NAD	N3A-C4A-N9A	2.30	131.07	127.17
4	D	2008	GDX	O6B-C6'-C5'	2.29	121.91	113.64
4	A	2006	GDX	C1'-C2'-C3'	2.29	114.82	110.01
4	D	2008	GDX	C4'-C3'-C2'	2.25	114.79	110.83
4	D	2007	GDX	O6-C6-C5	-2.23	120.64	126.53
4	D	2007	GDX	O4'-C4'-C3'	2.18	115.52	110.38
4	A	2005	GDX	C1'-C2'-C3'	2.15	114.52	110.01
3	A	2001	NAD	O3-PA-O1A	-2.12	104.31	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2006	GDX	C4'-C3'-C2'	2.12	114.56	110.83
3	B	2002	NAD	O3-PA-O1A	-2.12	104.33	110.70
4	D	2007	GDX	C8-N7-C5	2.11	108.02	104.26
4	D	2008	GDX	C1'-C2'-C3'	2.06	114.34	110.01
4	D	2007	GDX	O5'-C1'-O1B	-2.05	108.69	111.36
4	A	2005	GDX	O6-C6-C5	-2.04	121.16	126.53
4	A	2006	GDX	O6-C6-C5	-2.04	121.16	126.53
3	B	2002	NAD	O4B-C1B-N9A	2.02	111.97	108.09
3	A	2001	NAD	C5A-C4A-N9A	2.01	108.01	105.81
4	A	2006	GDX	O4'-C4'-C3'	2.01	115.12	110.38
4	A	2005	GDX	O4'-C4'-C3'	2.00	115.10	110.38

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	2005	GDX	C1'-O1B-PB-O3A
4	D	2008	GDX	C1'-O1B-PB-O3A
3	D	2004	NAD	O4B-C4B-C5B-O5B
3	B	2002	NAD	O4B-C4B-C5B-O5B
6	C	2011	MPD	C1-C2-C3-C4
6	C	2011	MPD	CM-C2-C3-C4

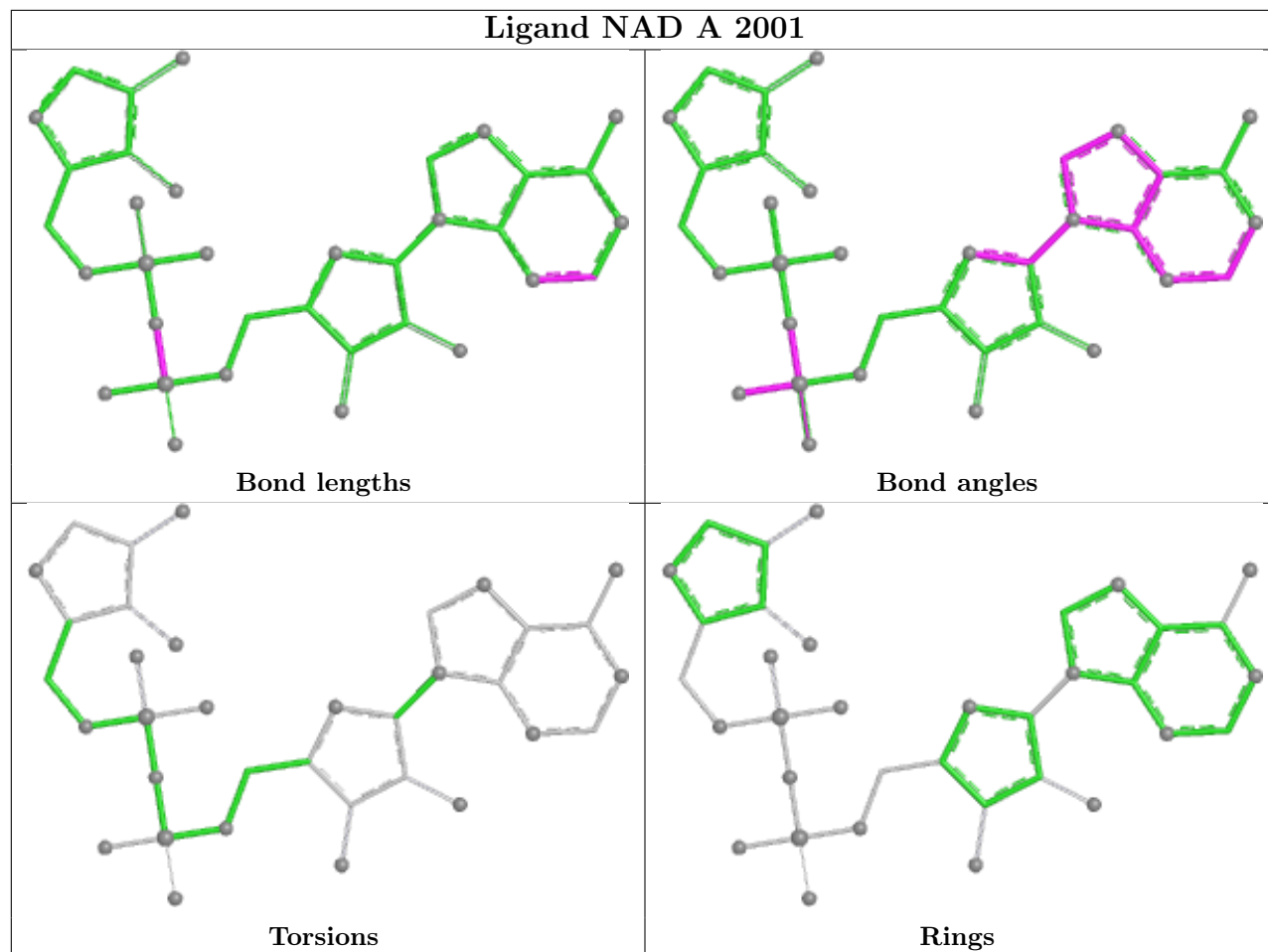
There are no ring outliers.

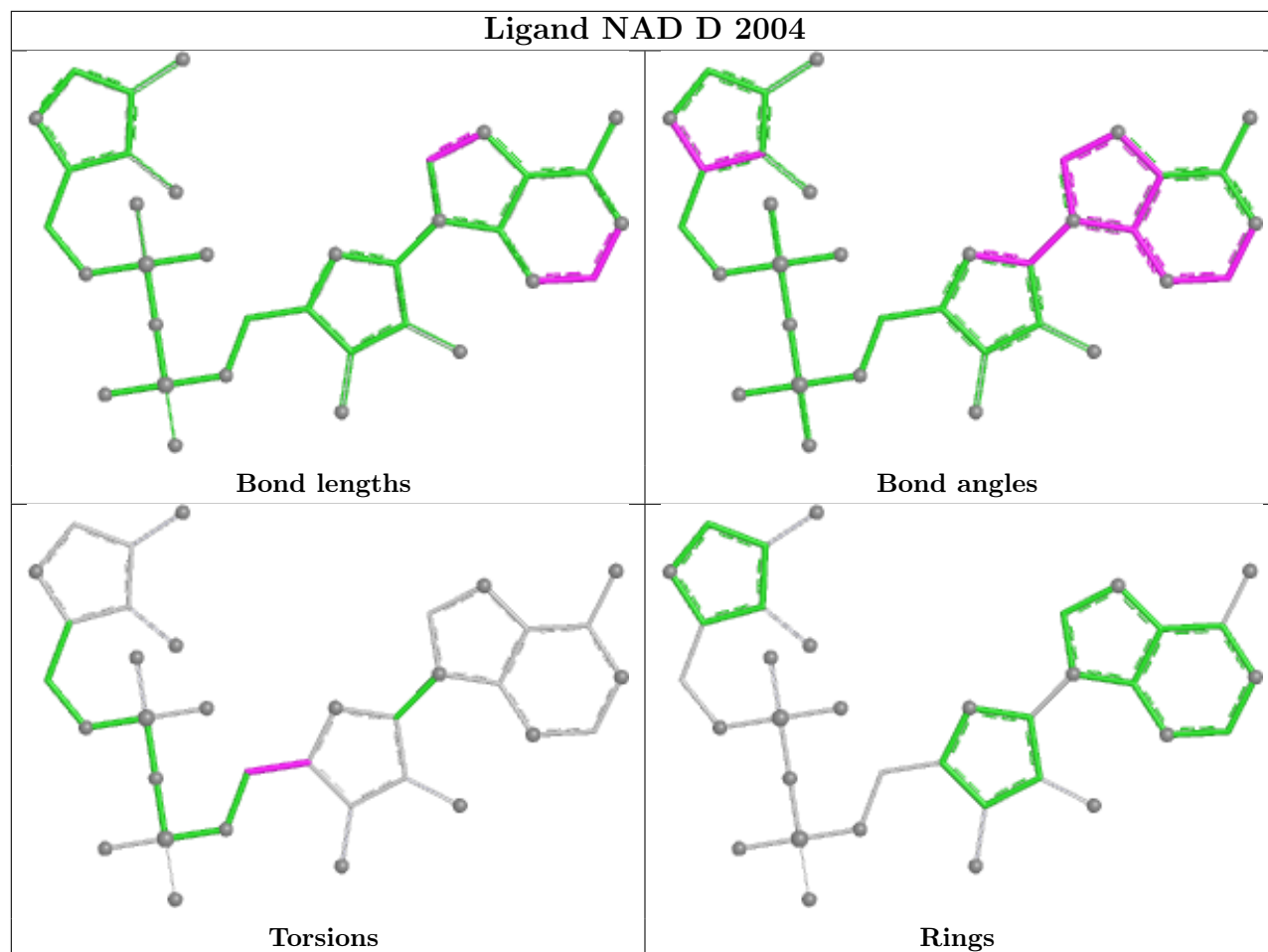
3 monomers are involved in 5 short contacts:

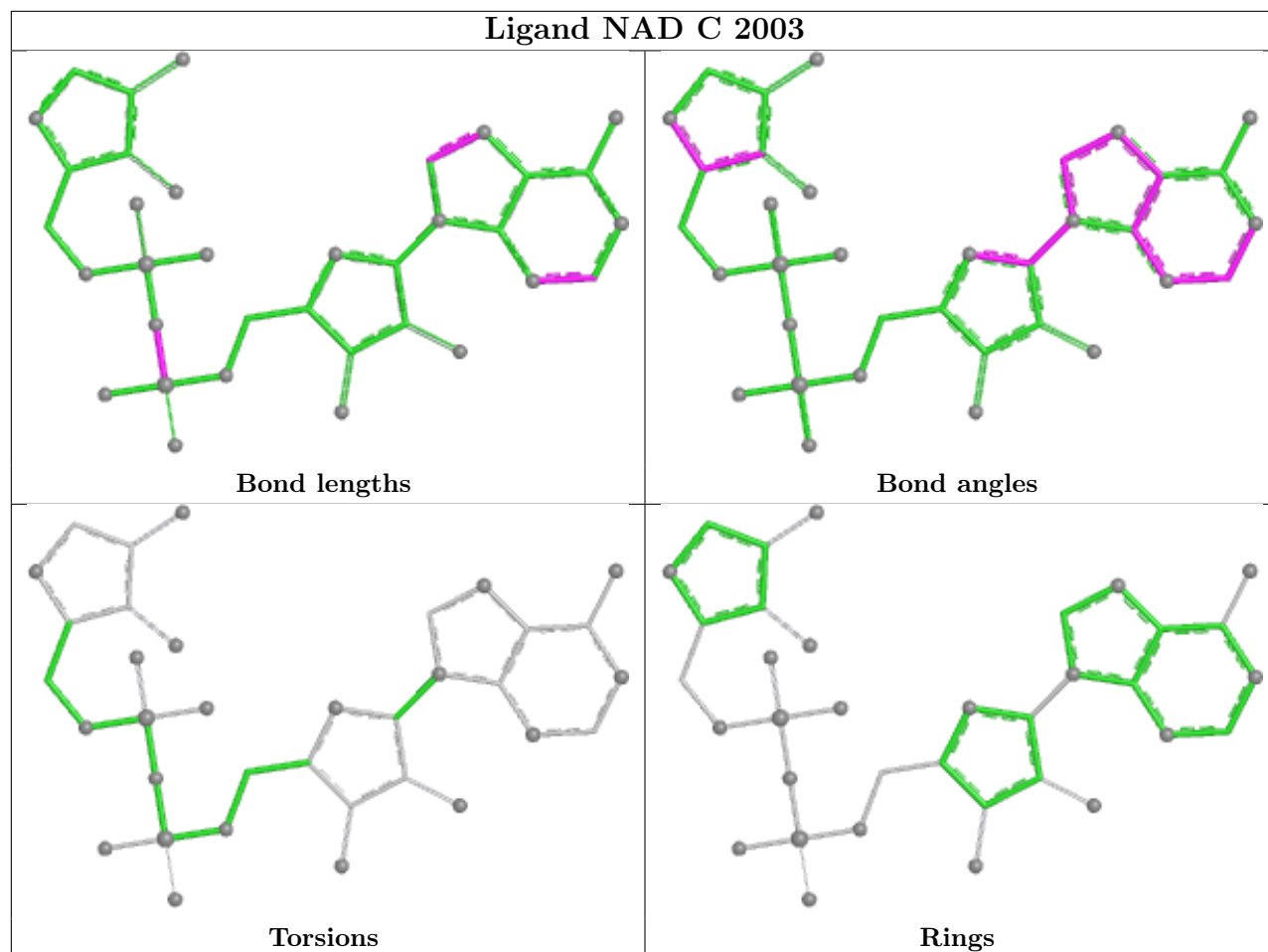
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2001	NAD	2	0
5	C	2010	ACY	3	0
5	C	2009	ACY	1	0

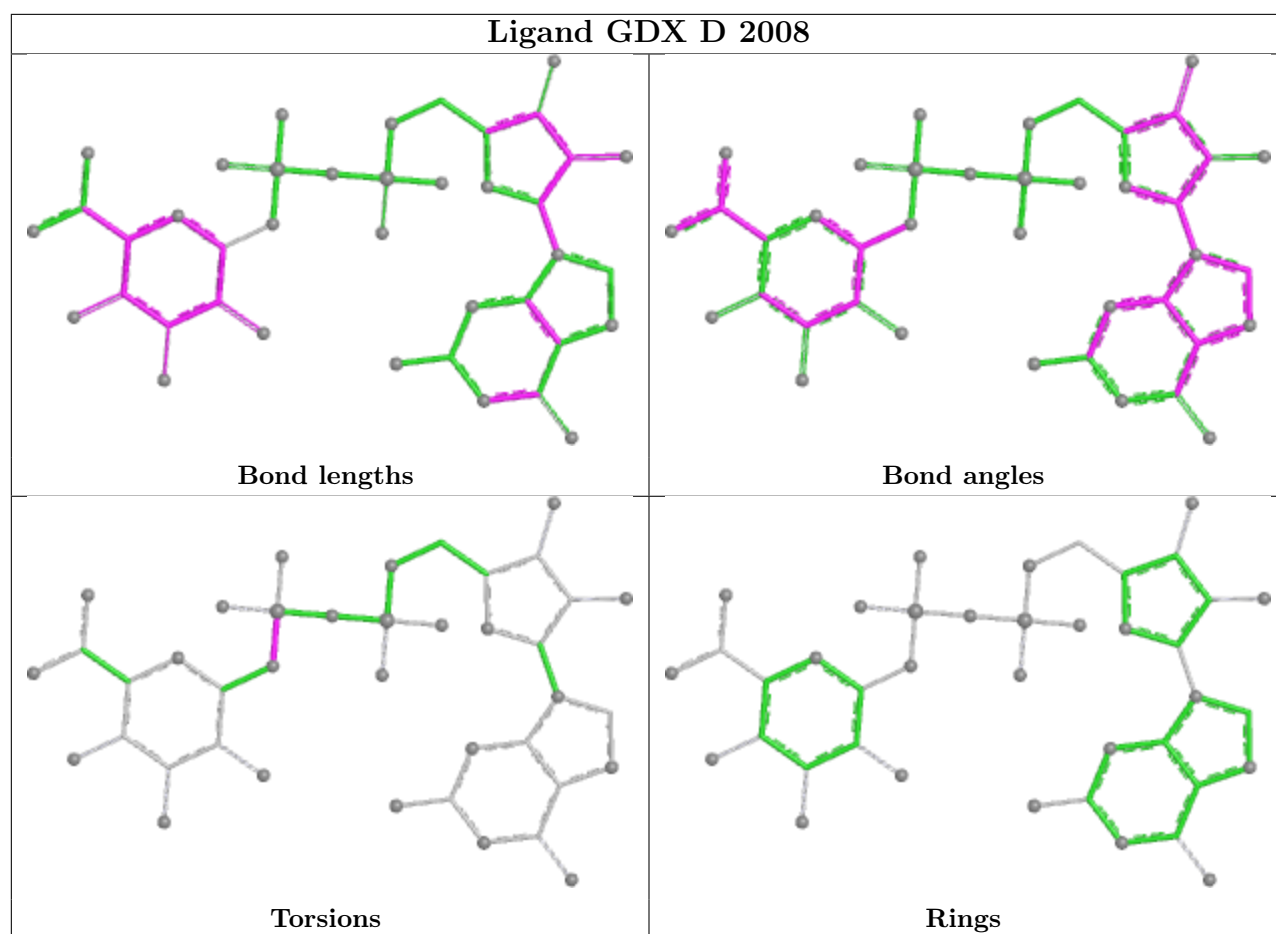
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient

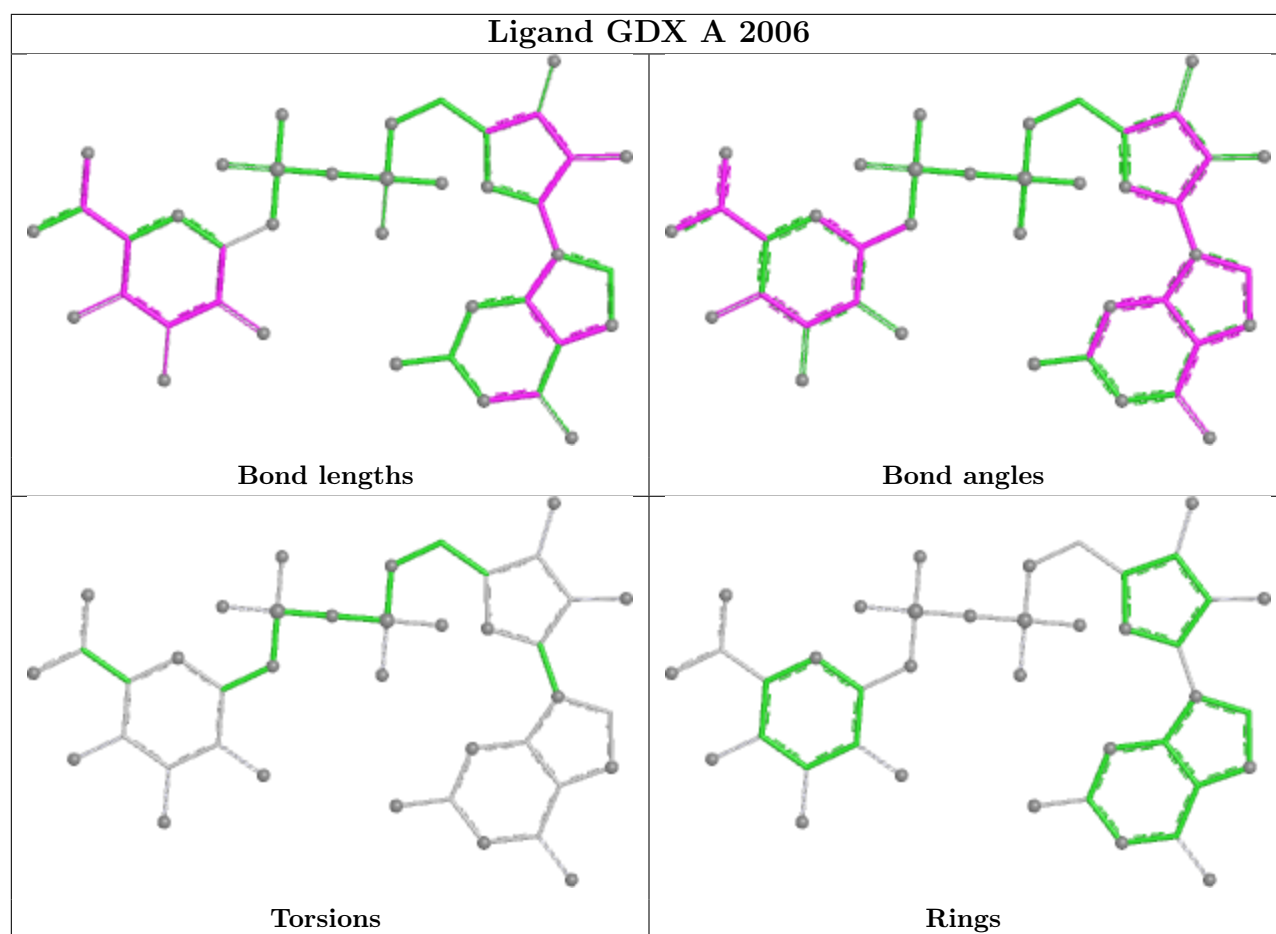
equivalents in the CSD to analyse the geometry.

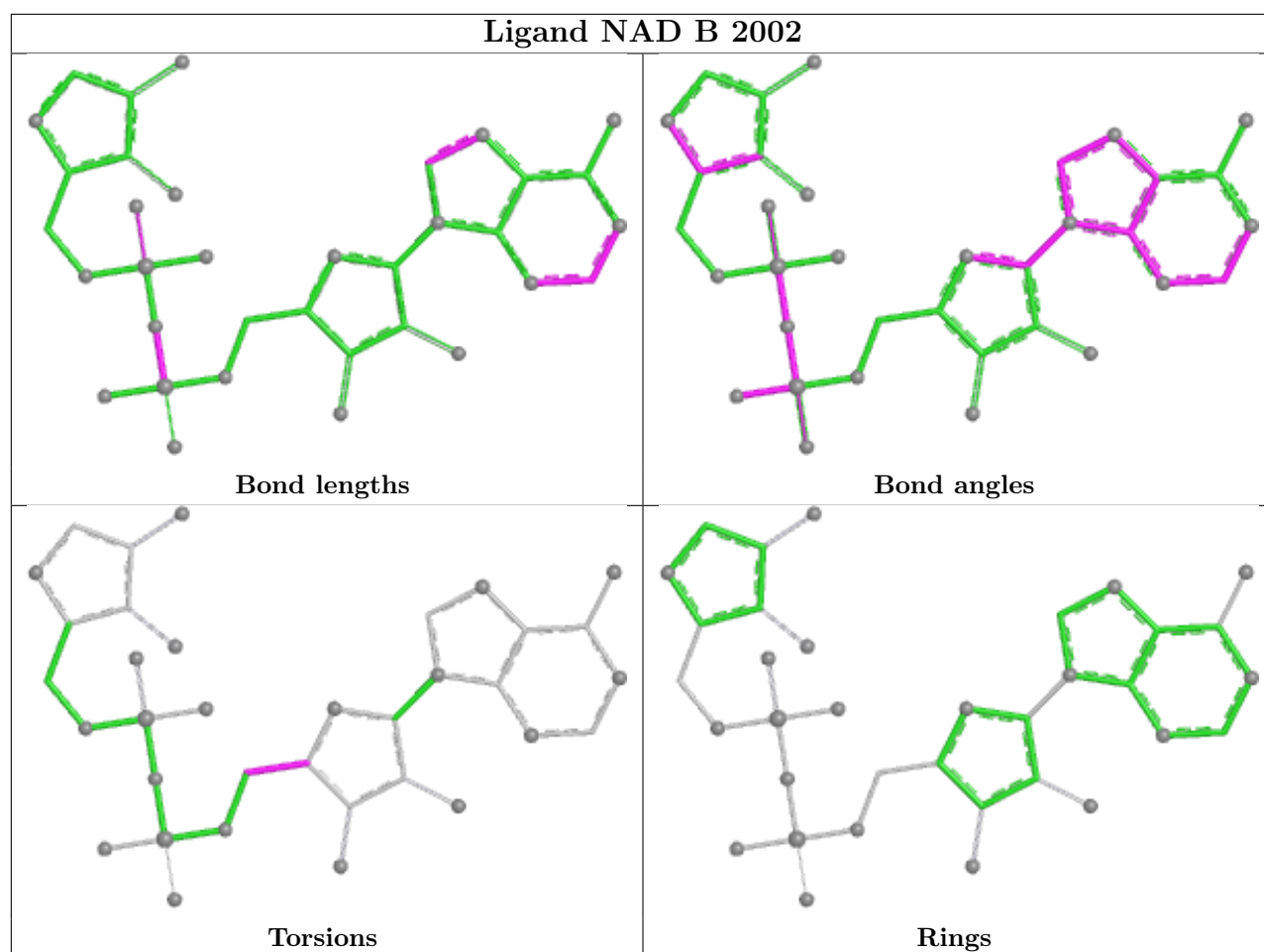


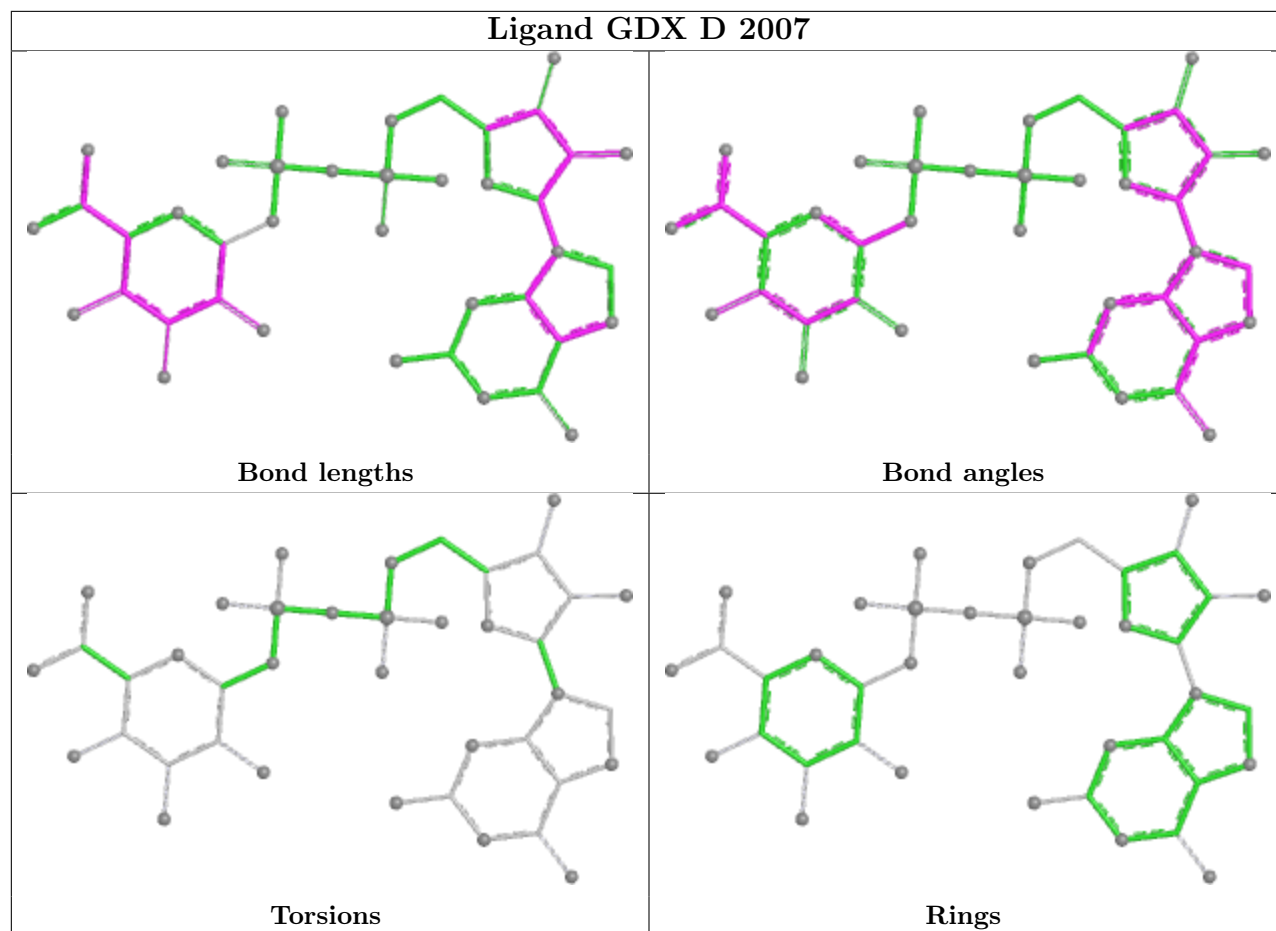


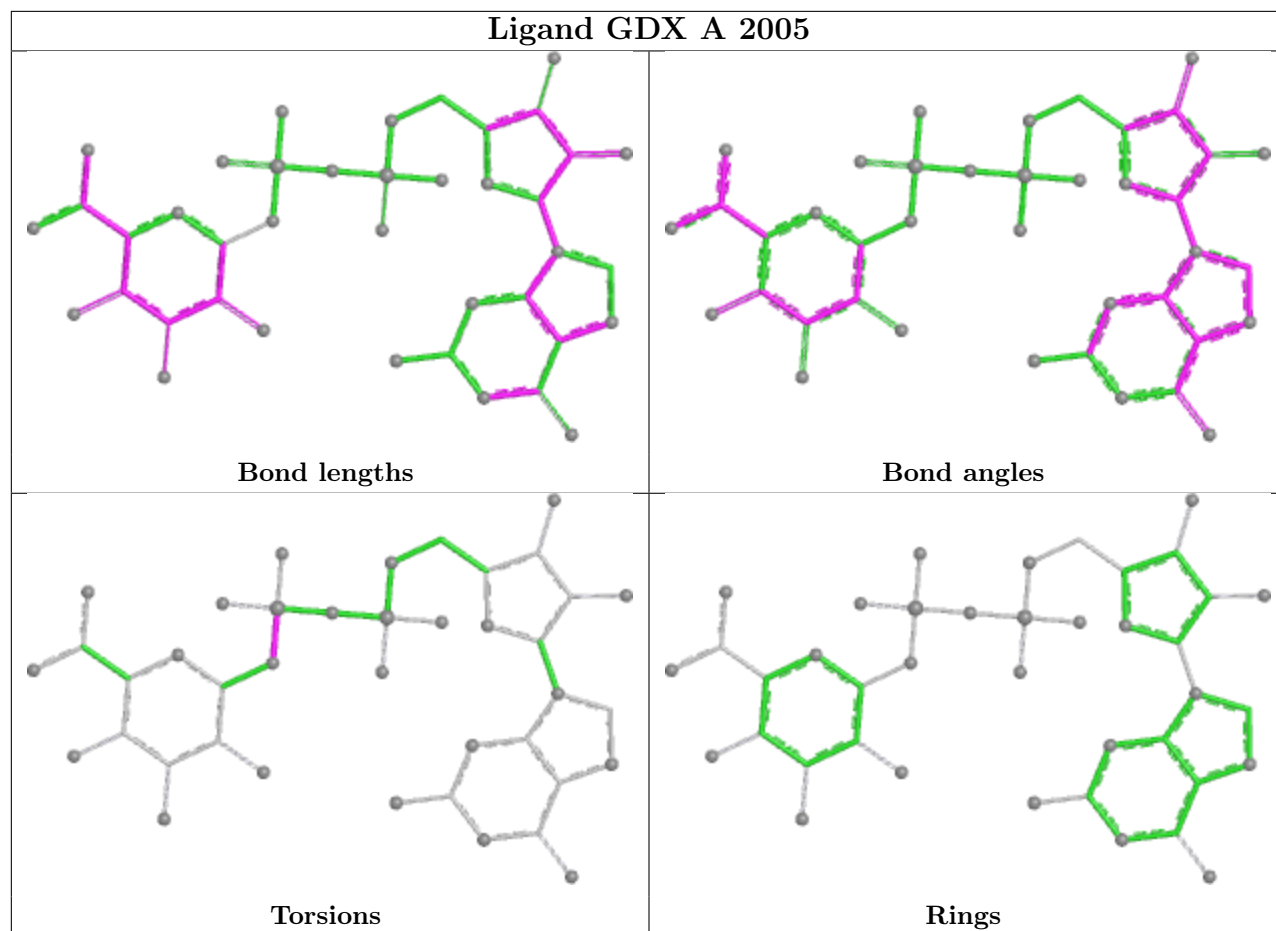












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	436/436 (100%)	-1.10	0 100 100	4, 9, 18, 25	1 (0%)
1	B	436/436 (100%)	-1.14	0 100 100	3, 9, 17, 23	2 (0%)
1	C	436/436 (100%)	-1.24	0 100 100	3, 8, 16, 21	0
1	D	436/436 (100%)	-1.23	0 100 100	3, 7, 16, 25	0
All	All	1744/1744 (100%)	-1.18	0 100 100	3, 8, 17, 25	3 (0%)

There are no RSRZ outliers to report.

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](#)

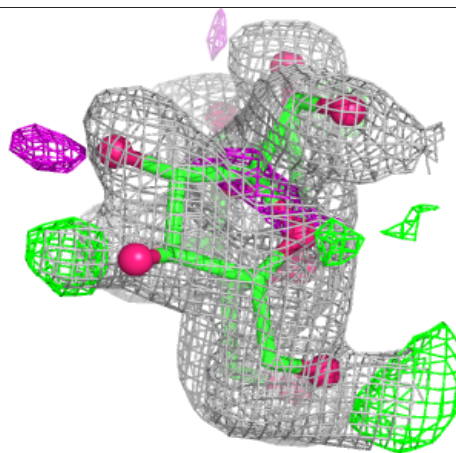
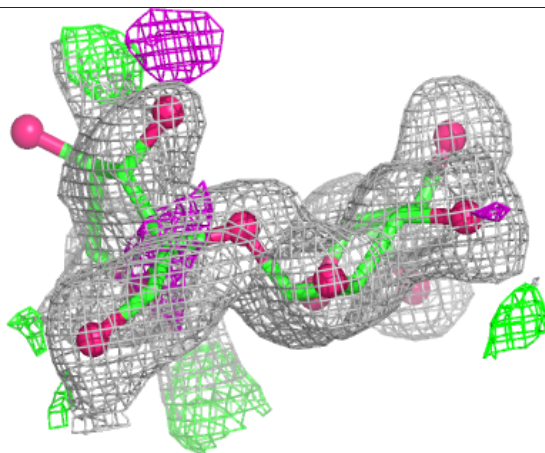
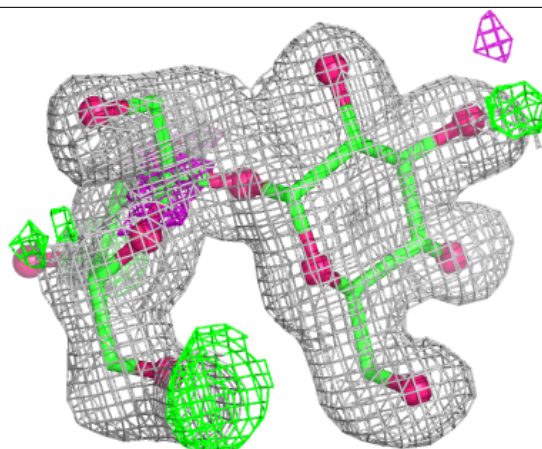
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

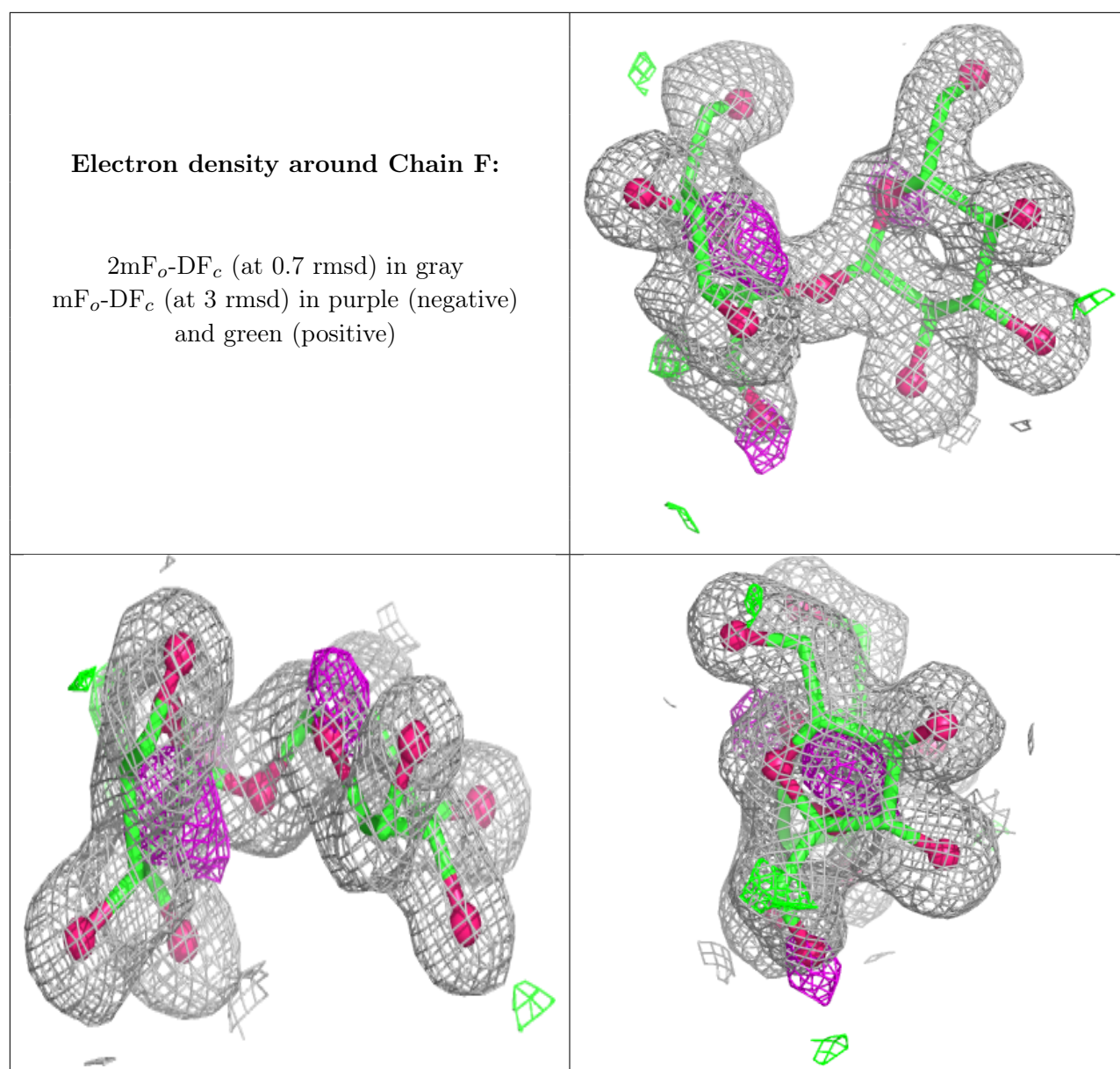
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	FRU	E	2	12/12	0.91	0.09	35,38,41,41	0
2	FRU	F	2	12/12	0.96	0.07	28,29,31,32	0
2	GLC	E	1	11/12	0.98	0.06	31,32,34,34	0
2	GLC	F	1	11/12	0.99	0.05	25,25,26,27	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain E:

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





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
6	MPD	C	2011	8/8	0.90	0.12	38,39,39,40	0
3	NAD	B	2002	35/44	0.99	0.03	15,17,19,19	0
5	ACY	C	2009	4/4	0.99	0.04	26,26,27,27	0
5	ACY	C	2010	4/4	0.99	0.05	26,26,26,27	0
3	NAD	A	2001	35/44	0.99	0.03	14,17,21,23	0

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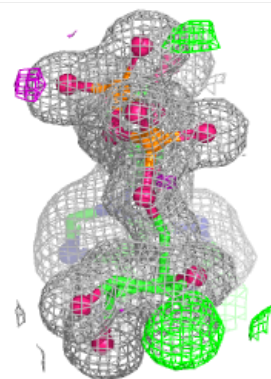
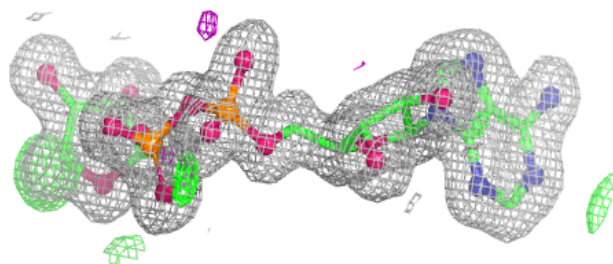
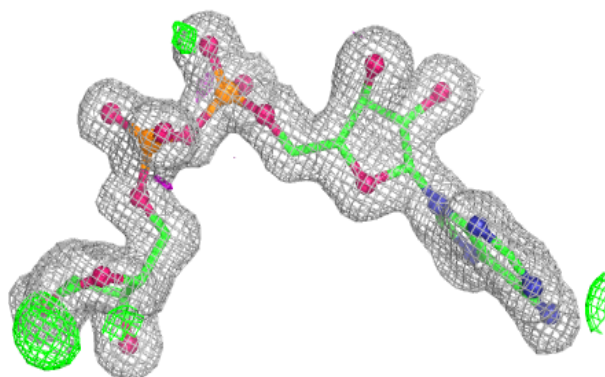
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	GDX	A	2006	40/40	1.00	0.02	12,14,16,18	0
4	GDX	D	2007	40/40	1.00	0.02	11,13,14,16	0
4	GDX	D	2008	40/40	1.00	0.02	11,13,15,16	0
3	NAD	C	2003	35/44	1.00	0.02	12,16,18,19	0
3	NAD	D	2004	35/44	1.00	0.02	12,15,16,18	0
4	GDX	A	2005	40/40	1.00	0.03	13,15,16,17	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.

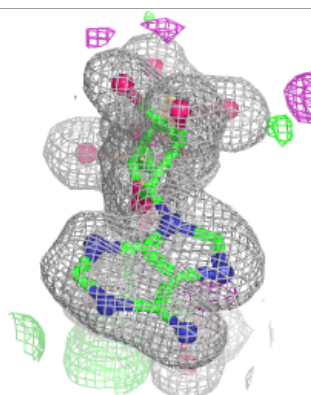
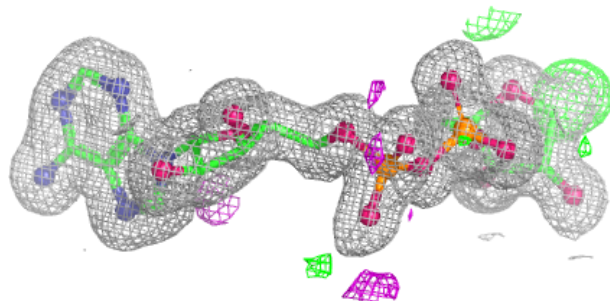
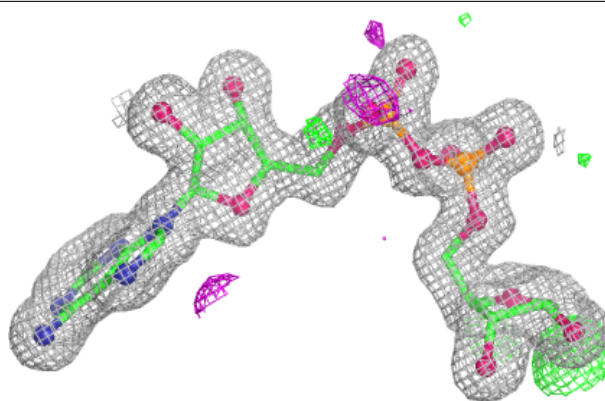
Electron density around NAD B 2002:

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mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

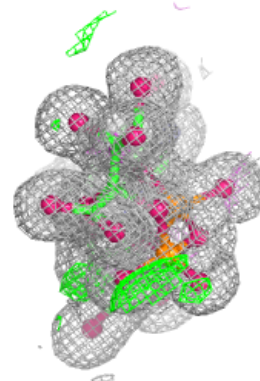
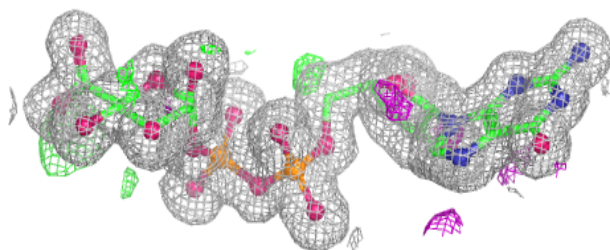
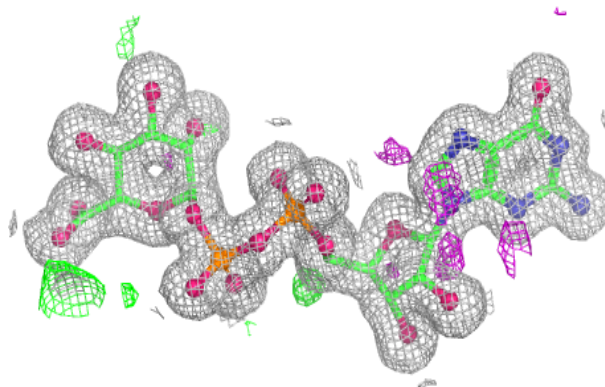


Electron density around NAD A 2001:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

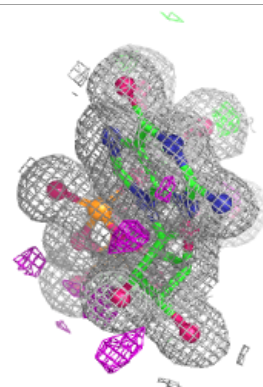
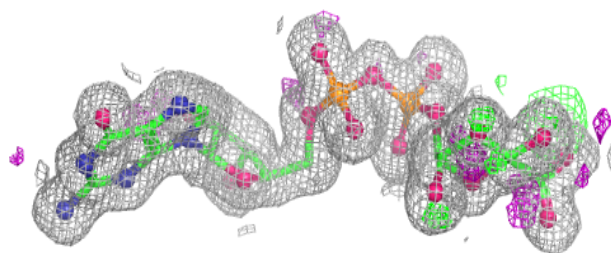
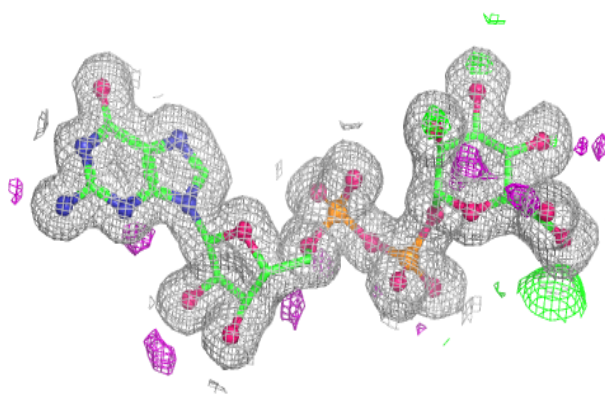
**Electron density around GDX A 2006:**

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

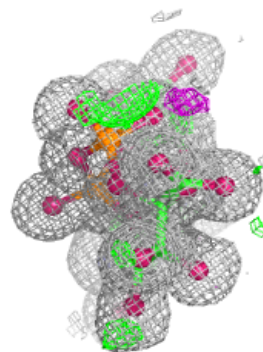
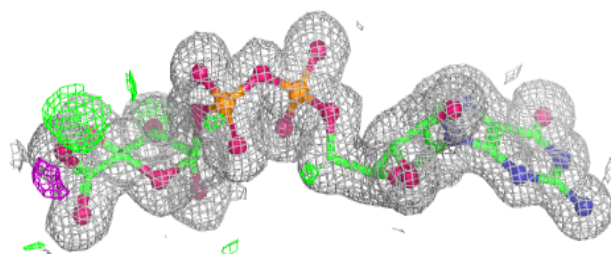
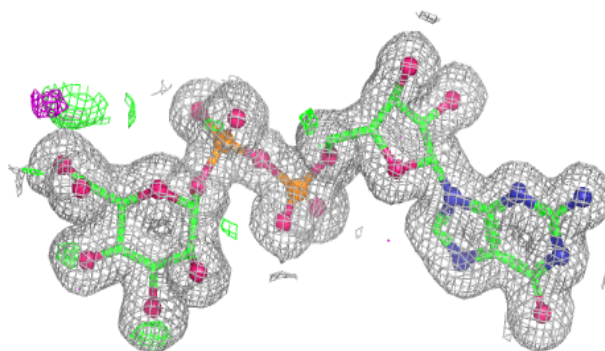


Electron density around GDX D 2007:

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

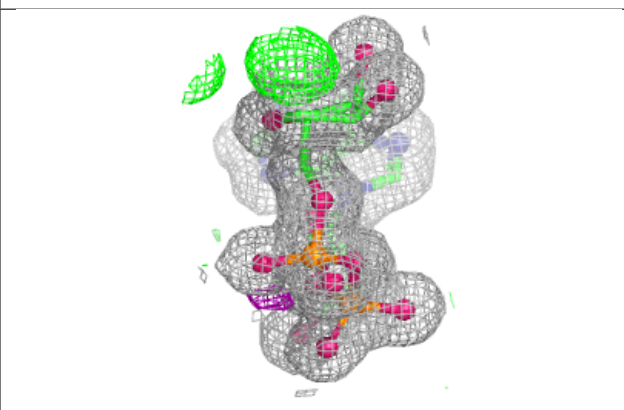
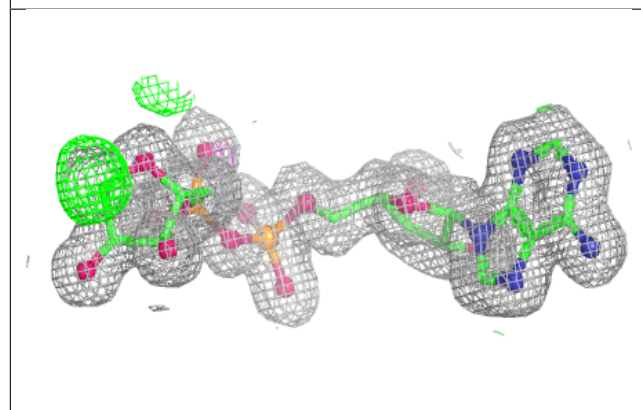
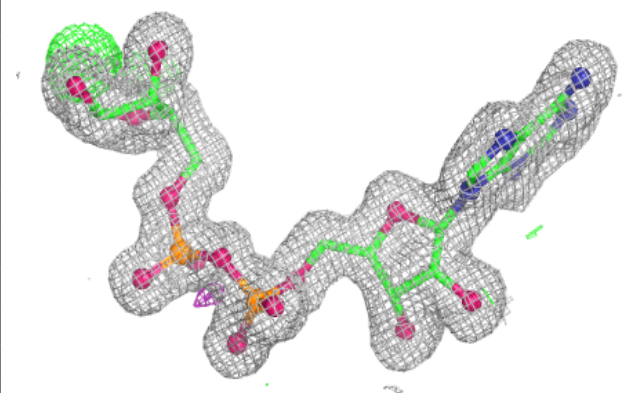
**Electron density around GDX D 2008:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

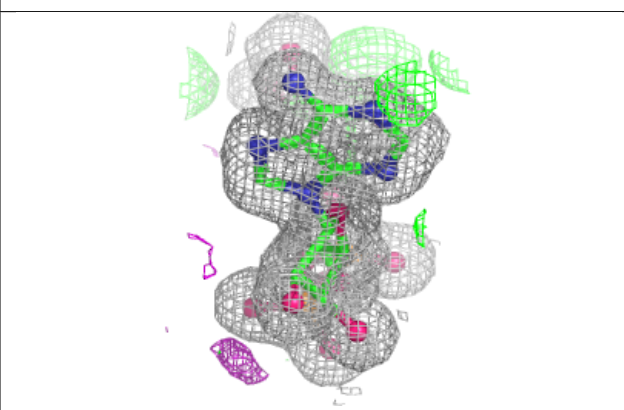
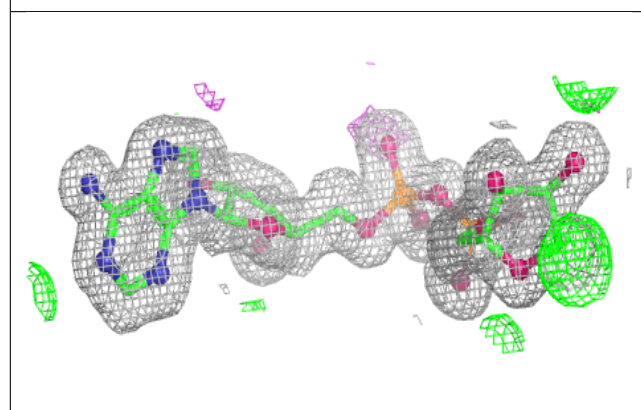
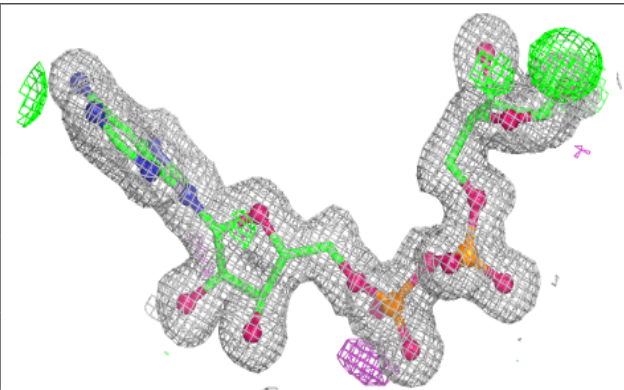


Electron density around NAD C 2003:

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

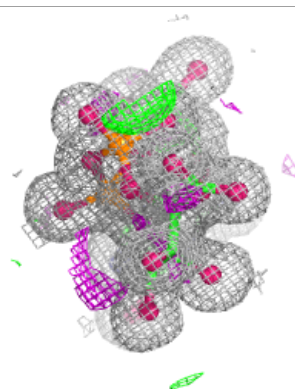
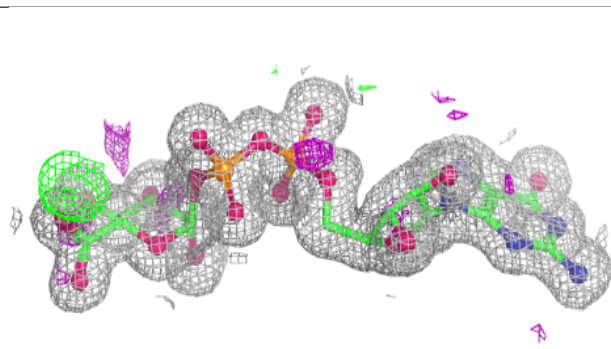
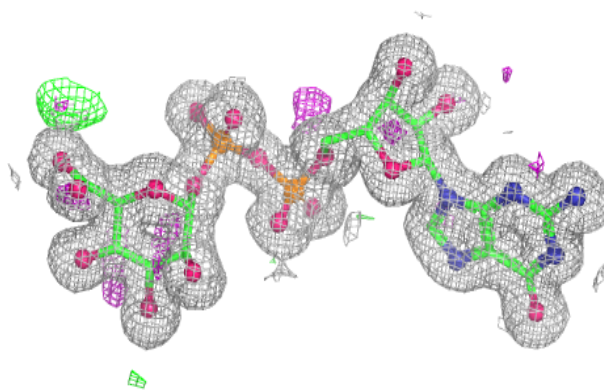
**Electron density around NAD D 2004:**

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



Electron density around GDX A 2005:

$2mF_o-DF_c$ (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.