W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 3, 2024 – 07:24 PM EST

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

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

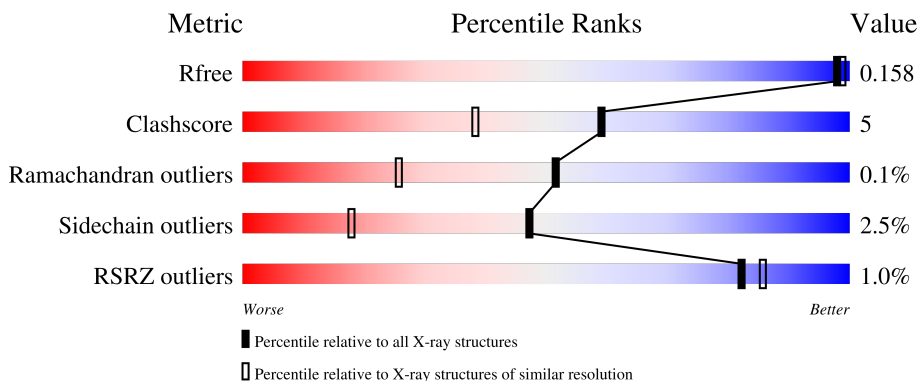|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 1.55 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	Percentile Ranks	Value
Rfree		0.158
Clashscore		5
Ramachandran outliers		0.1%
Sidechain outliers		2.5%
RSRZ outliers		1.0%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	1483 (1.56-1.56)
Clashscore	141614	1529 (1.56-1.56)
Ramachandran outliers	138981	1498 (1.56-1.56)
Sidechain outliers	138945	1495 (1.56-1.56)
RSRZ outliers	127900	1465 (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 <=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	% 86% 12% ·
1	B	436	% 91% 8% ·
1	C	436	91% 8%
1	D	436	% 89% 10% ·
2	E	2	100%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	2	50% 50%

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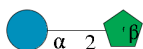
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	E	2	Total	C	O	0	0	0
			23	12	11			
2	F	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).

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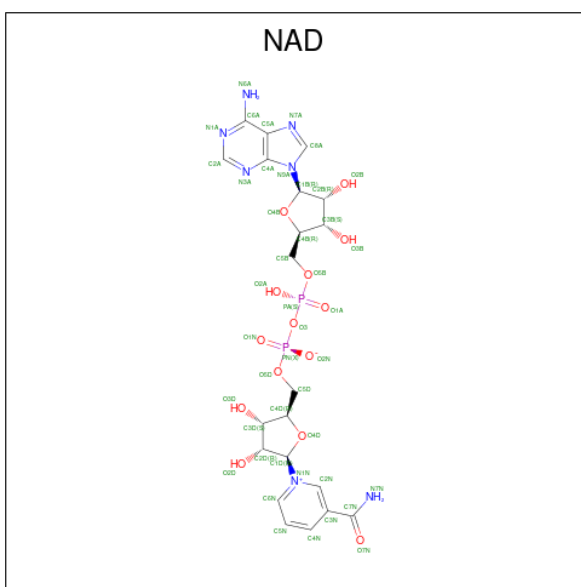
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			35	15	5	13	2		
3	B	1	Total	C	N	O	P	0	0
			35	15	5	13	2		
3	C	1	Total	C	N	O	P	0	0
			35	15	5	13	2		
3	D	1	Total	C	N	O	P	0	0
			35	15	5	13	2		

- Molecule 4 is GUANOSINE 5'-(TRIHYDROGEN DIPHOSPHATE), P'-D-MANNOPYRANOSYL ESTER (three-letter code: GDX) (formula: $C_{16}H_{23}N_5O_{17}P_2$).
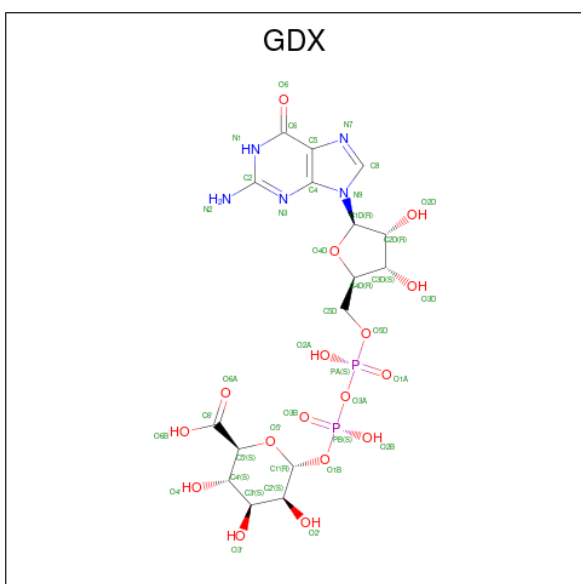
GDX

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 (three-letter code: ACY) (formula: $C_2H_4O_2$).
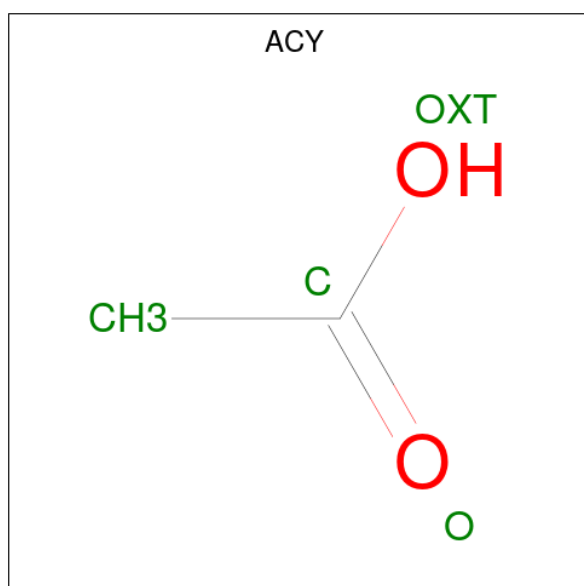
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).

MPD

O4

OH

C1

C5

C4(S)

C2

CM

C3

OH

O2

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

- Molecule 7 is water.

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

WORLDWIDE
PDB
PROTEIN DATA BANK

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.
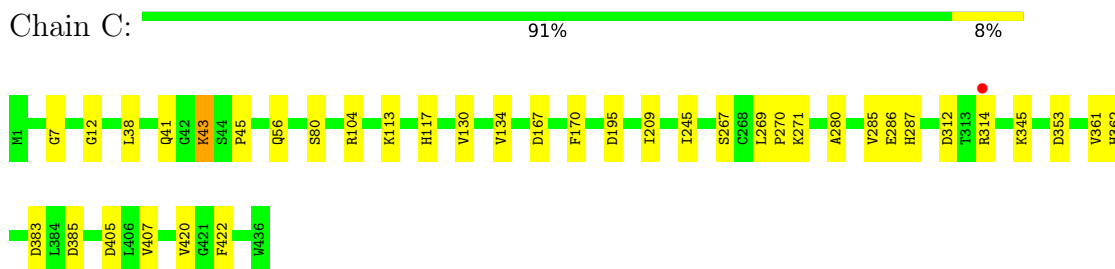
• Molecule 1: GDP-mannose 6-dehydrogenase
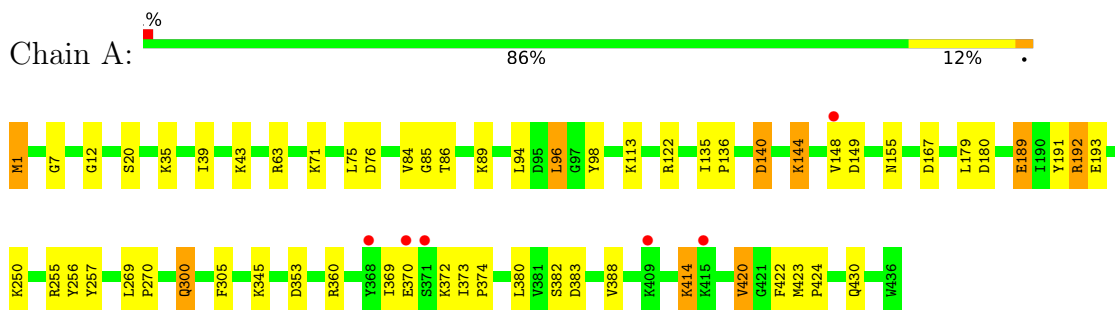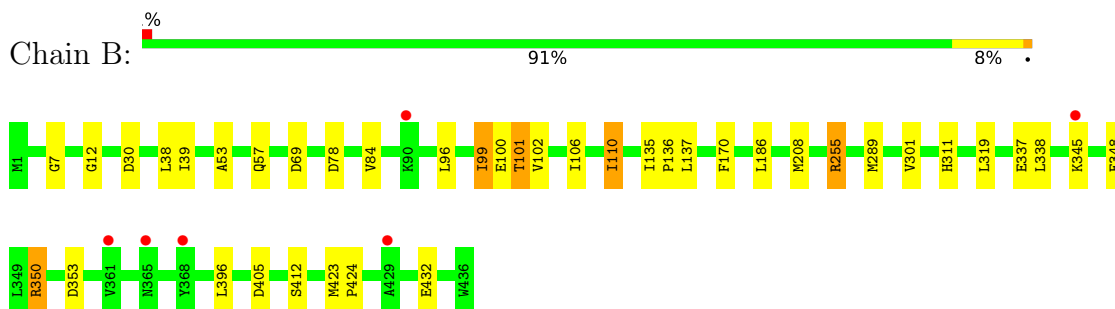
• Molecule 1: GDP-mannose 6-dehydrogenase

• Molecule 1: GDP-mannose 6-dehydrogenase

• Molecule 1: GDP-mannose 6-dehydrogenase

M1 R2 I3 G7 L8 G12 D30 V31 S32 I36 D37 L38 I39 L55 K71 K72 L75 D76 S77 D78 V79 V84 V102 C103 R104 T154 N155 P156 D180 E188 R200 T212 V244 K250 R255 L269 P270 F305 H311 D312

T313 R314 D328 E340 K345 D353 R360 V361 H362 Y368 S371 L379 L394 V395 L396 D400 D405 L406 T410 M423 P424 H425 W436
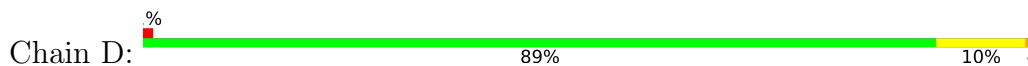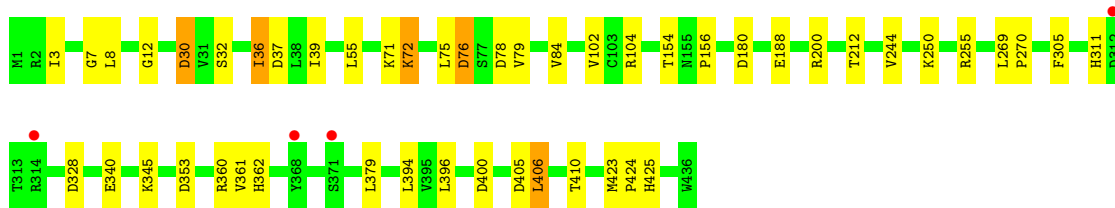
• Molecule 2: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain E: 100%

GLC1 FRU2

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

Chain F: 50%   50%

GLC1 FRU2

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 49.55 – 1.55	Depositor EDS
% Data completeness (in resolution range)	100.0 (40.00-1.55) 99.0 (49.55-1.55)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.68 (at 1.55Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.174 , 0.194 0.151 , 0.158	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)	0.35 , 31.8	EDS
L-test for twinning[2]	$< |L| > = 0.42, < L^2 > = 0.25$	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.*

---

[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: FRU, GLC, MPD, NAD, GDX, ACY

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	0.40	0/3333	0.73	6/4520 (0.1%)
1	B	0.41	1/3327 (0.0%)	0.75	5/4511 (0.1%)
1	C	0.40	0/3351	0.74	5/4543 (0.1%)
1	D	0.41	0/3345	0.75	9/4533 (0.2%)
All	All	0.41	1/13356 (0.0%)	0.74	25/18107 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	289	MET	SD-CE	-7.28	1.37	1.77

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	167	ASP	CB-CG-OD2	6.00	123.70	118.30
1	C	405	ASP	CB-CG-OD2	5.74	123.47	118.30
1	B	405	ASP	CB-CG-OD2	5.64	123.38	118.30
1	D	405	ASP	CB-CG-OD2	5.62	123.36	118.30
1	C	195	ASP	CB-CG-OD2	5.52	123.27	118.30

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.

W O R L D W I D E
wwPDB
PROTEIN DATA BANK

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3280	0	3256	40	0
1	B	3273	0	3255	25	0
1	C	3297	0	3281	26	0
1	D	3291	0	3281	42	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	127	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.

The worst 5 of 127 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

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 ⓘ

5.3.1 Protein backbone ⓘ

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%)	47	23
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%)	51	26

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	192	ARG

5.3.2 Protein sidechains ⓘ

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%)	341 (96%)	15 (4%)	30	5
1	B	353/370 (95%)	342 (97%)	11 (3%)	40	11
1	C	359/370 (97%)	355 (99%)	4 (1%)	73	53
1	D	358/370 (97%)	353 (99%)	5 (1%)	67	41
All	All	1426/1480 (96%)	1391 (98%)	35 (2%)	47	18

5 of 35 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	56	GLN
1	C	345	LYS
1	D	72	LYS
1	A	414	LYS
1	A	380	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	229	ASN
1	C	287	HIS
1	D	425	HIS
1	D	300	GLN
1	B	311	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	0.58	0	15,15,17	0.69	0
2	FRU	E	2	2	11,12,12	0.52	0	10,18,18	0.67	0
2	GLC	F	1	2	11,11,12	0.53	0	15,15,17	1.07	1 (6%)
2	FRU	F	2	2	11,12,12	0.53	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(^{o})	Ideal(^{o})
2	F	1	GLC	C1-O5-C5	3.01	116.26	112.19

There are no chirality outliers.

5 of 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

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.

Oligosaccharide Chain E

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain F

Bond lengths

Bond angles

Torsions

Rings
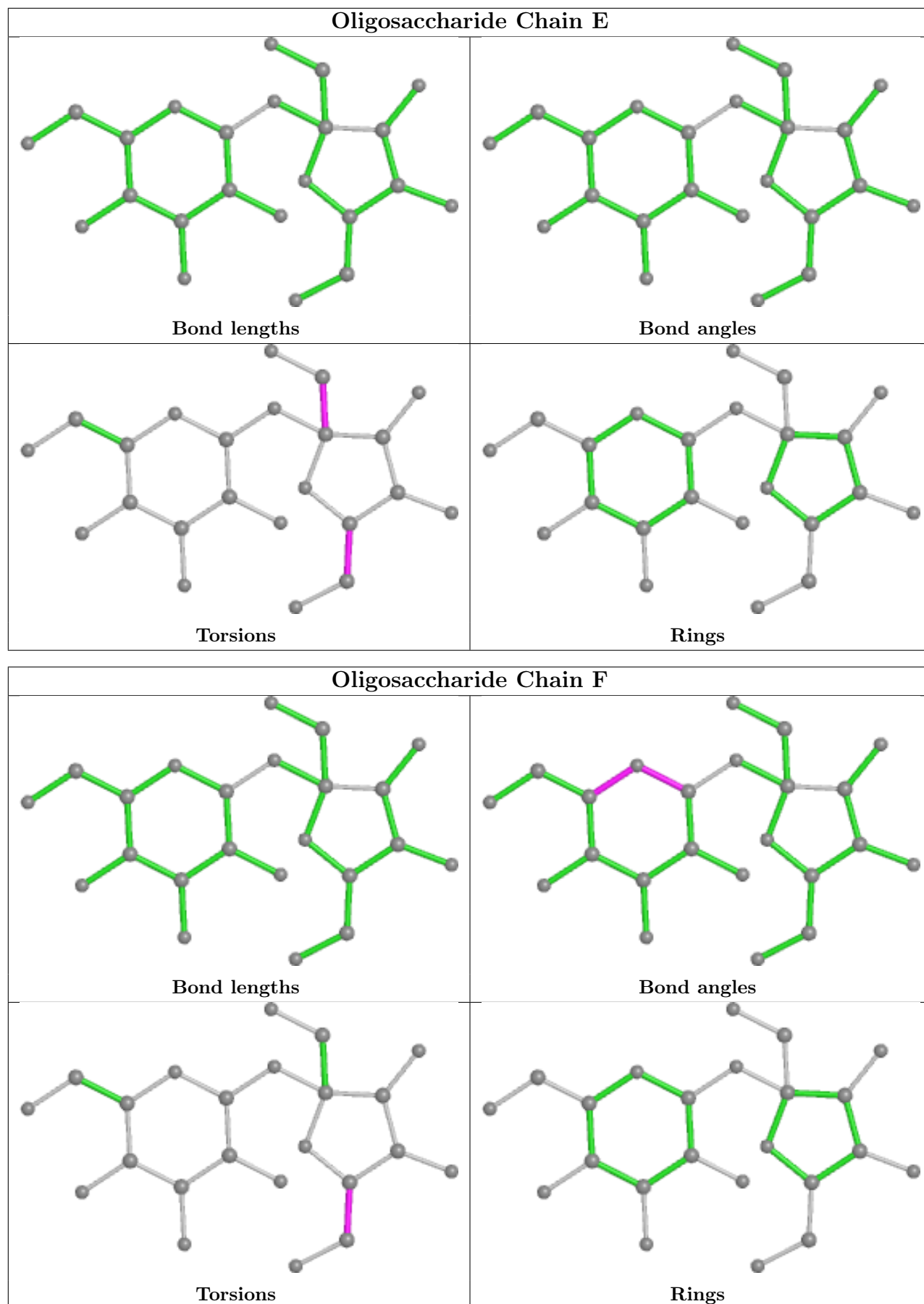
5.6 Ligand geometry (i)

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).

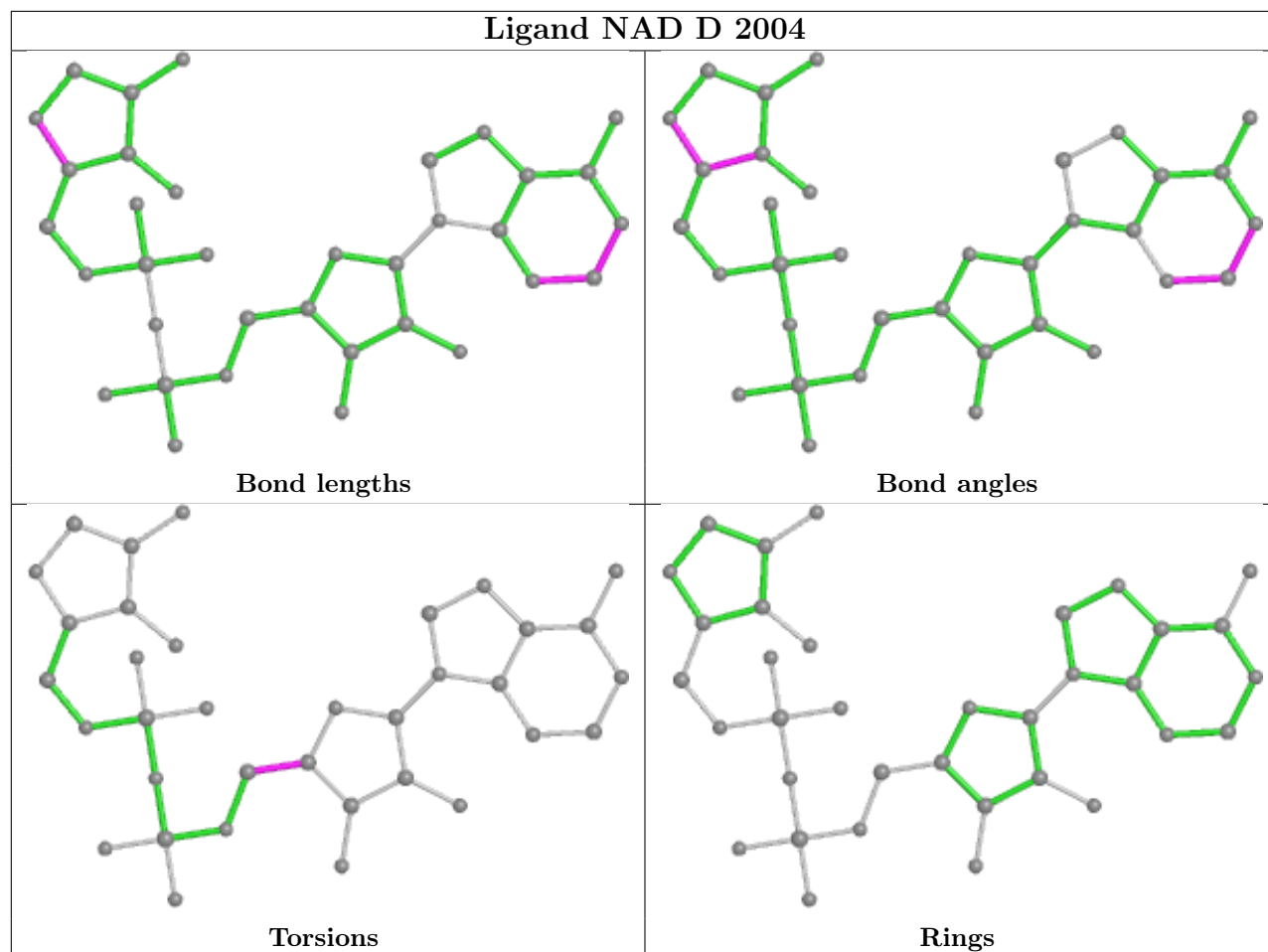| Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
3	NAD	C	2003	-	33,38,48	1.13	1 (3%)	37,58,73	1.38	4 (10%)
6	MPD	C	2011	-	7,7,7	0.26	0	9,10,10	0.32	0
4	GDX	D	2008	-	36,43,43	4.22	16 (44%)	47,67,67	1.56	10 (21%)
3	NAD	B	2002	-	33,38,48	1.14	3 (9%)	37,58,73	1.46	4 (10%)
5	ACY	C	2009	-	3,3,3	0.69	0	3,3,3	1.12	0
3	NAD	D	2004	-	33,38,48	1.15	3 (9%)	37,58,73	1.34	2 (5%)
3	NAD	A	2001	-	33,38,48	1.01	1 (3%)	37,58,73	1.33	3 (8%)
4	GDX	A	2006	-	36,43,43	4.25	14 (38%)	47,67,67	1.67	10 (21%)
4	GDX	D	2007	-	36,43,43	4.20	15 (41%)	47,67,67	1.69	12 (25%)
4	GDX	A	2005	-	36,43,43	4.29	16 (44%)	47,67,67	1.58	9 (19%)
5	ACY	C	2010	-	3,3,3	0.78	0	3,3,3	0.64	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	C	2003	-	-	1/18/51/62	0/4/4/5
6	MPD	C	2011	-	-	0/5/5/5	-
4	GDX	D	2008	-	-	1/21/61/61	0/4/4/4
3	NAD	B	2002	-	-	1/18/51/62	0/4/4/5
3	NAD	D	2004	-	-	1/18/51/62	0/4/4/5
3	NAD	A	2001	-	-	1/18/51/62	0/4/4/5
4	GDX	A	2006	-	-	2/21/61/61	0/4/4/4
4	GDX	D	2007	-	-	2/21/61/61	0/4/4/4
4	GDX	A	2005	-	-	1/21/61/61	0/4/4/4

The worst 5 of 69 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2005	GDX	C2D-C1D	-11.14	1.36	1.53
4	D	2007	GDX	C2D-C1D	-10.66	1.37	1.53
4	A	2006	GDX	C2D-C1D	-10.61	1.37	1.53
4	D	2008	GDX	C2D-C1D	-10.36	1.38	1.53
4	D	2007	GDX	C4'-C5'	-9.93	1.36	1.53

The worst 5 of 54 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	2002	NAD	N3A-C2A-N1A	-5.86	119.53	128.68
3	A	2001	NAD	N3A-C2A-N1A	-5.21	120.53	128.68
4	D	2007	GDX	C3D-C2D-C1D	5.03	108.56	100.98
3	C	2003	NAD	N3A-C2A-N1A	-5.01	120.84	128.68
3	D	2004	NAD	N3A-C2A-N1A	-4.94	120.96	128.68

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	2005	GDX	C1'-O1B-PB-O3A
4	A	2006	GDX	C1'-O1B-PB-O3A
4	D	2007	GDX	C1'-O1B-PB-O3A
4	D	2008	GDX	C1'-O1B-PB-O3A
4	D	2007	GDX	C5D-O5D-PA-O3A

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	2009	ACY	1	0
3	A	2001	NAD	2	0
5	C	2010	ACY	3	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.
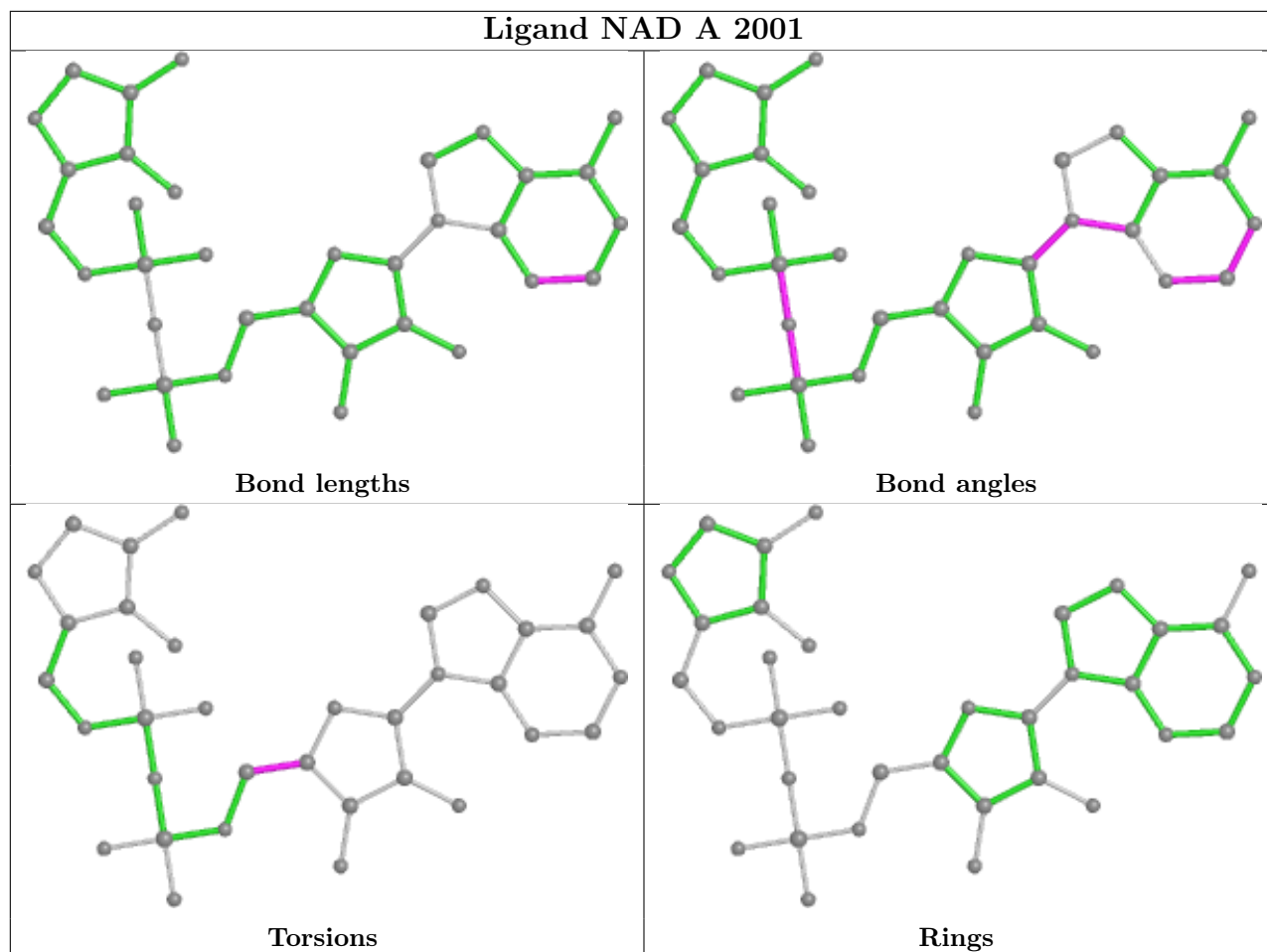
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.
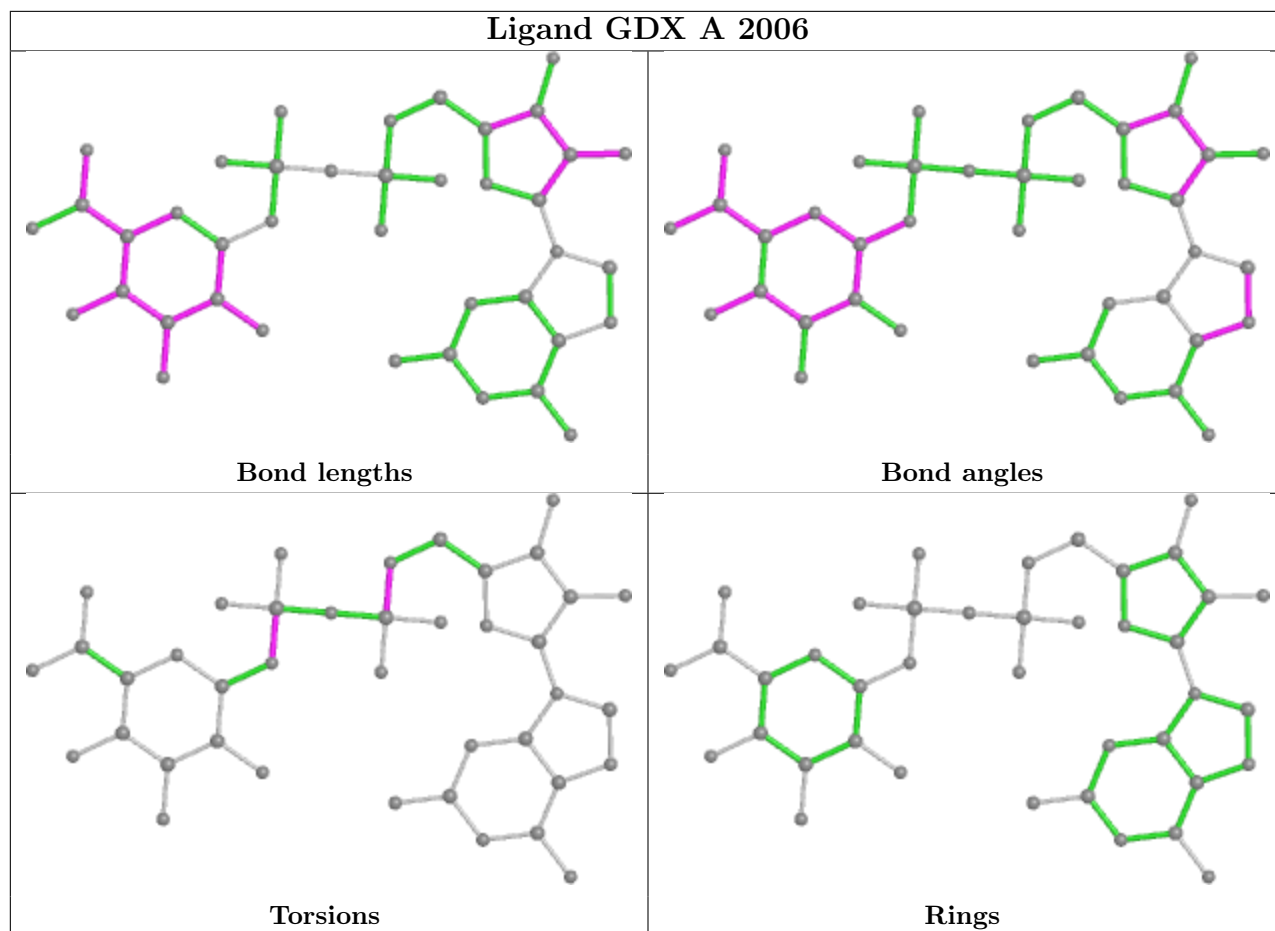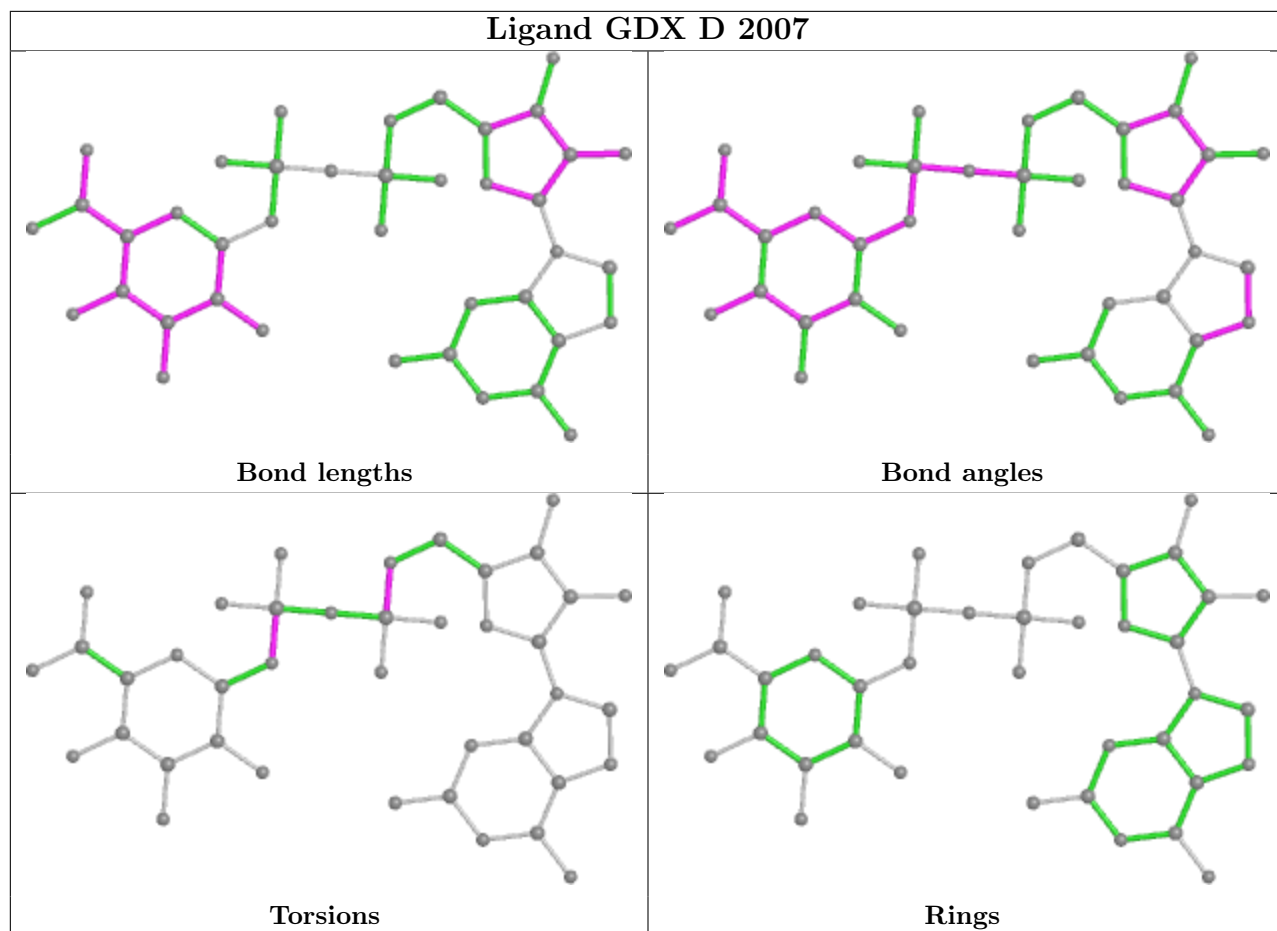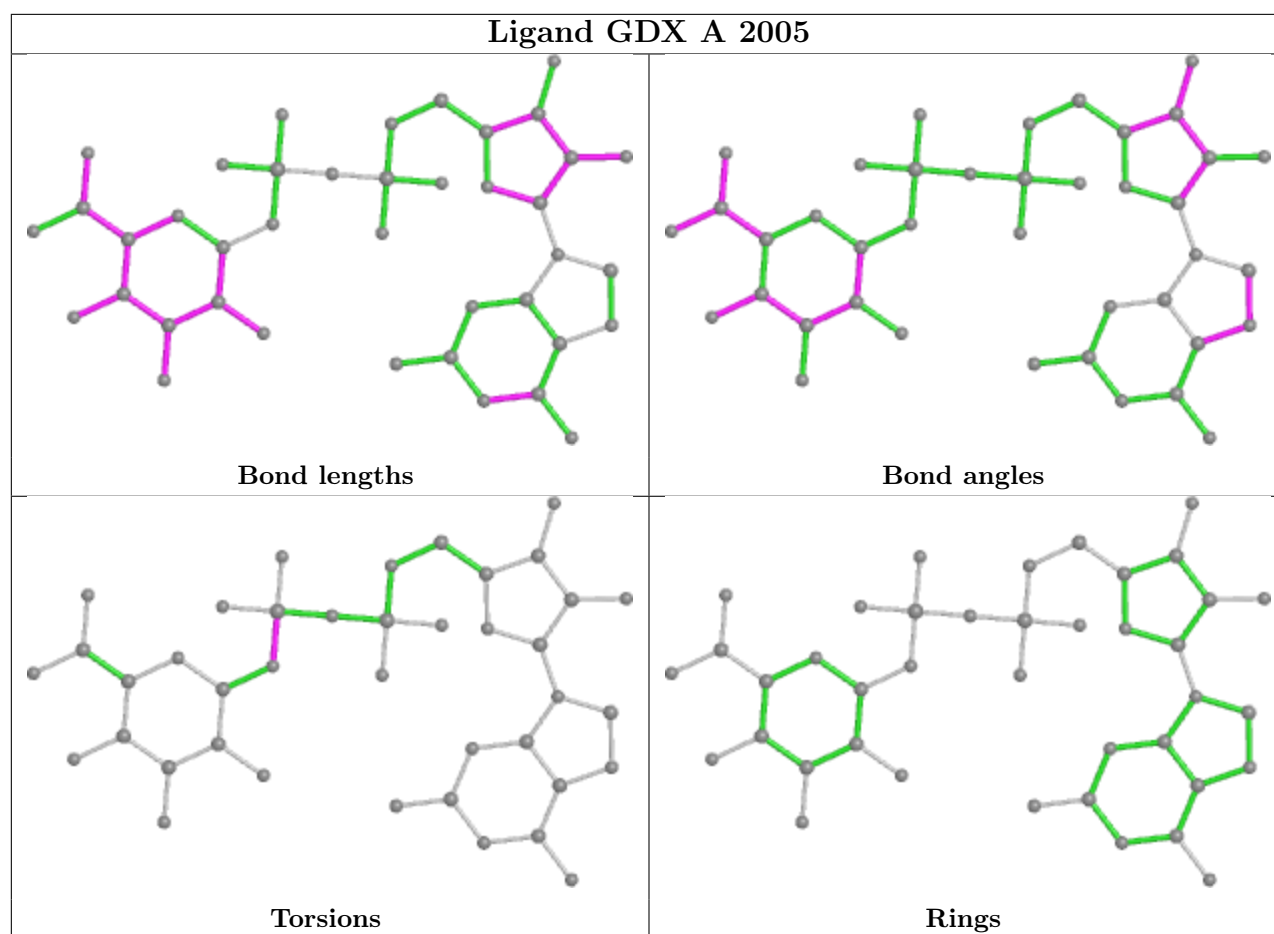

Ligand NAD C 2003

Bond lengths

Bond angles

Torsions

Rings

Ligand GDX D 2008

Bond lengths

Bond angles

Torsions

Rings

Ligand NAD B 2002

Bond lengths

Bond angles

Torsions

Rings

Ligand NAD D 2004

Bond lengths

Bond angles

Torsions

Rings

Ligand NAD A 2001

Bond lengths

Bond angles

Torsions

Rings

Ligand GDX A 2006

Bond lengths

Bond angles

Torsions

Rings

Ligand GDX D 2007

Bond lengths

Bond angles

Torsions

Rings

Ligand GDX A 2005

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	436/436 (100%)	-0.32	6 (1%)	75	80	4, 9, 18, 25	1 (0%)
1	B	436/436 (100%)	-0.37	6 (1%)	75	80	4, 9, 17, 23	2 (0%)
1	C	436/436 (100%)	-0.43	1 (0%)	95	95	3, 8, 16, 21	0
1	D	436/436 (100%)	-0.42	4 (0%)	84	87	3, 7, 16, 25	0
All	All	1744/1744 (100%)	-0.39	17 (0%)	82	86	3, 8, 17, 25	3 (0%)

The worst 5 of 17 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	368	TYR	4.7
1	B	345	LYS	3.6
1	D	368	TYR	3.6
1	A	371	SER	3.0
1	A	148	VAL	2.8

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 ⓘ

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.
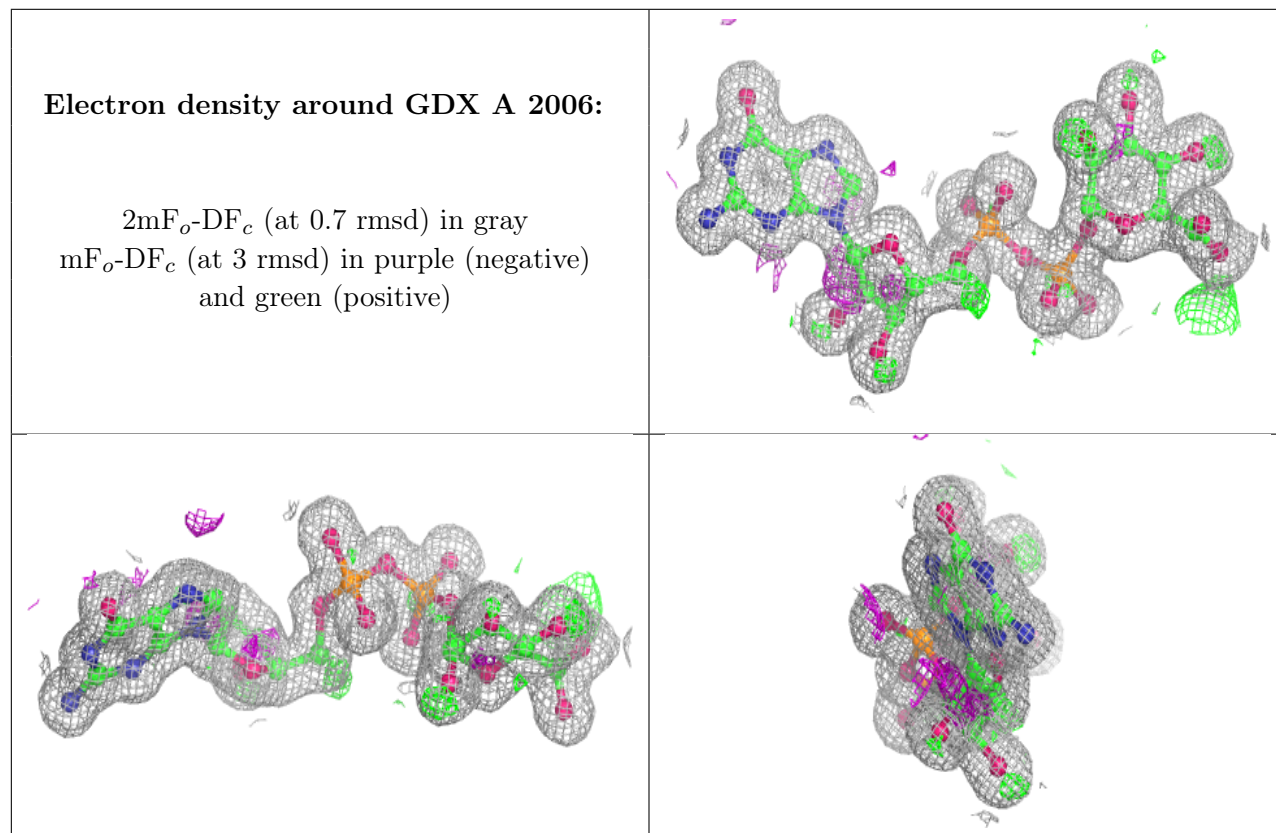
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FRU	E	2	12/12	0.69	0.30	35,38,41,41	0
2	FRU	F	2	12/12	0.83	0.13	28,29,31,32	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GLC	E	1	11/12	0.89	0.14	31,32,34,34	0
2	GLC	F	1	11/12	0.93	0.13	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.
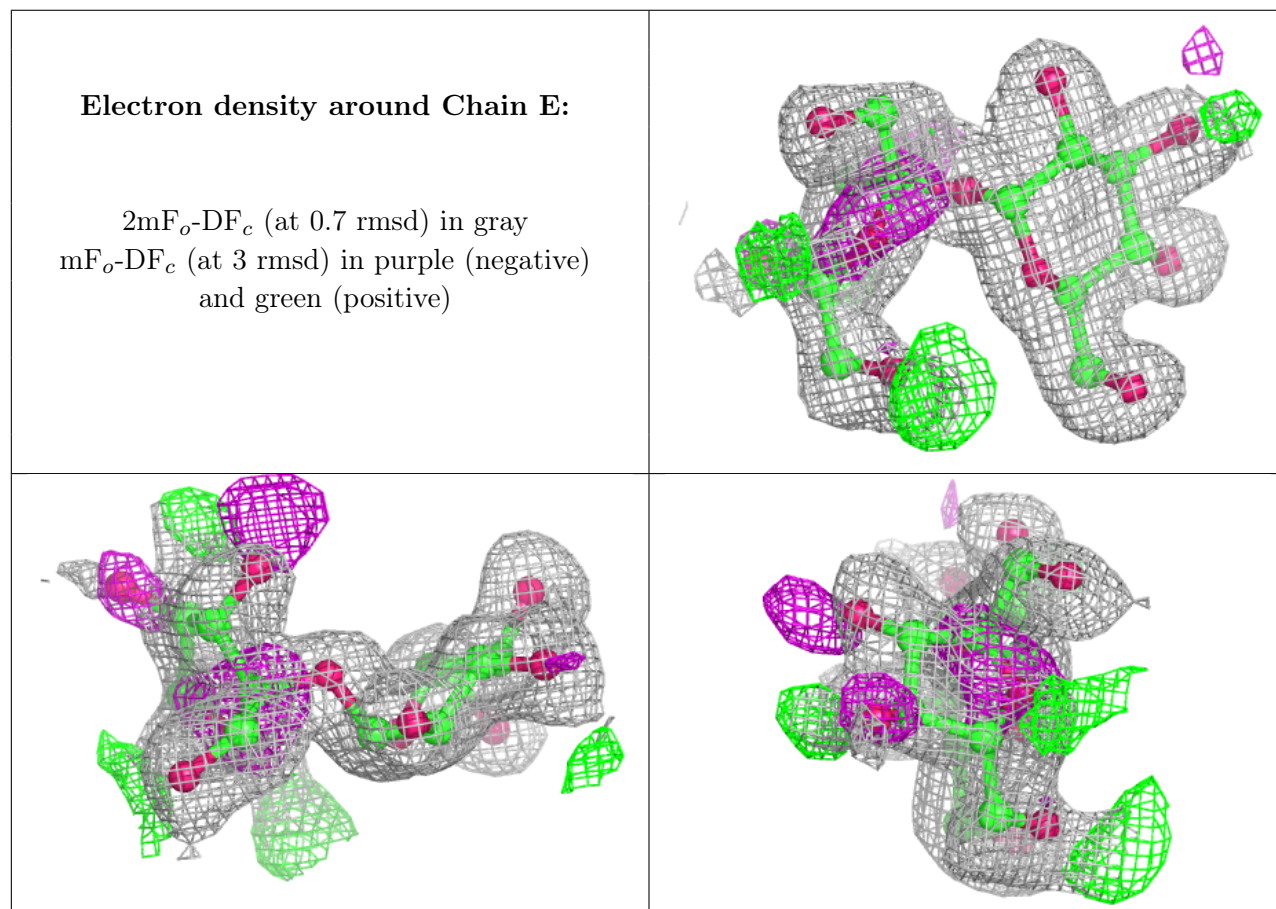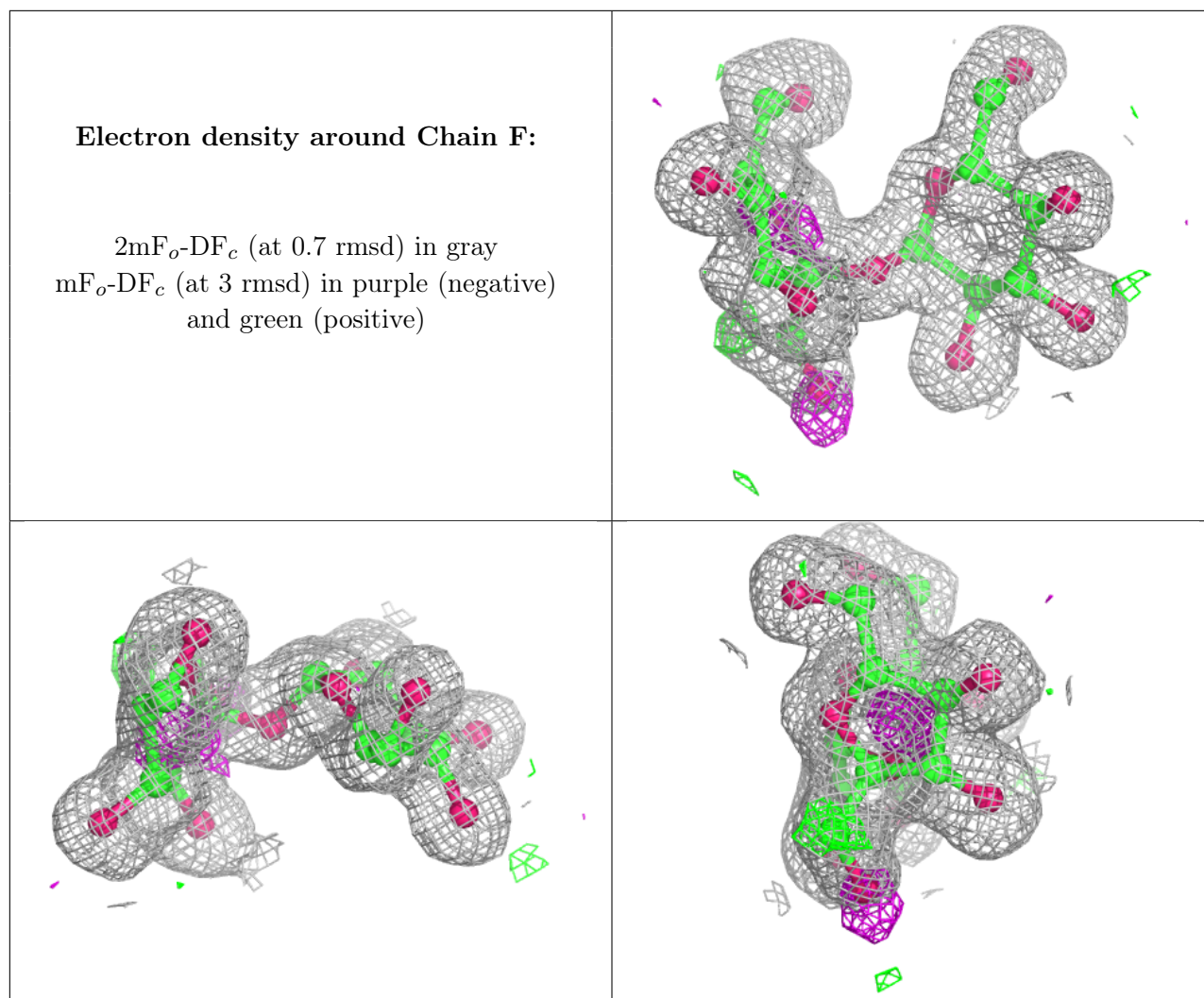
Electron density around Chain E:

$2\text{mF}_o\text{-DF}_c$ (at 0.7 rmsd) in gray
$\text{mF}_o\text{-DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

Electron density around Chain F:

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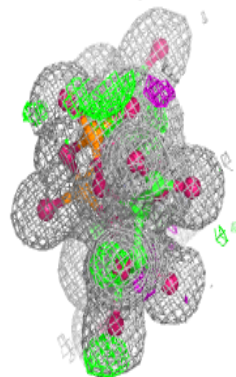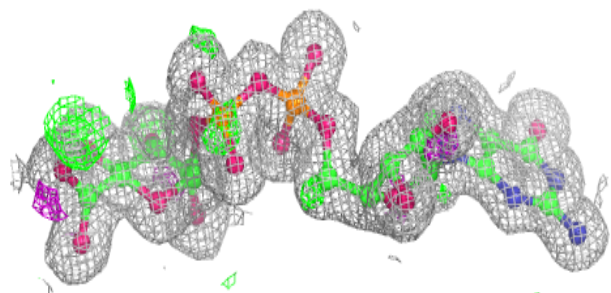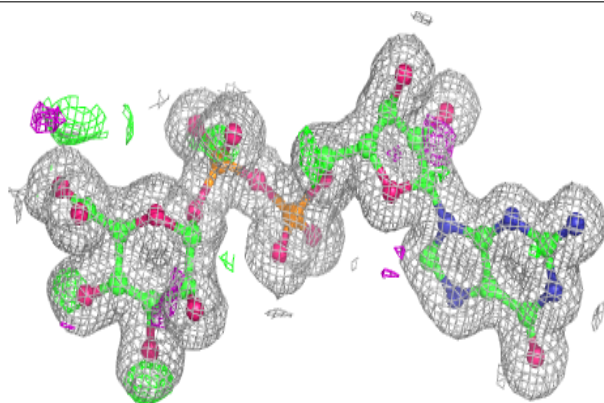and green (positive)

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	0.53	0.38	38,39,39,40	0
5	ACY	C	2010	4/4	0.93	0.10	26,26,26,27	0
5	ACY	C	2009	4/4	0.94	0.06	26,26,27,27	0
4	GDX	A	2006	40/40	0.97	0.08	12,14,16,18	0
4	GDX	A	2005	40/40	0.97	0.08	13,15,16,17	0
3	NAD	B	2002	35/44	0.98	0.06	15,17,19,19	0
4	GDX	D	2007	40/40	0.98	0.07	11,13,14,16	0
4	GDX	D	2008	40/40	0.98	0.07	11,13,15,16	0
3	NAD	C	2003	35/44	0.98	0.07	12,16,18,19	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
3	NAD	D	2004	35/44	0.98	0.06	12,15,16,18	0
3	NAD	A	2001	35/44	0.98	0.06	14,17,21,23	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 GDX A 2006:

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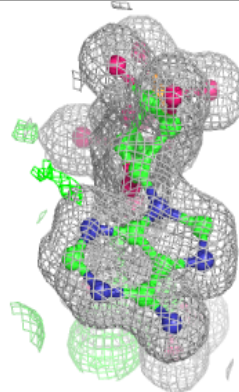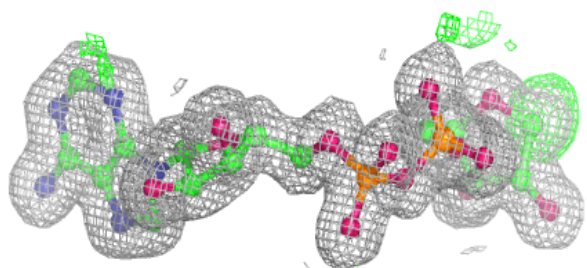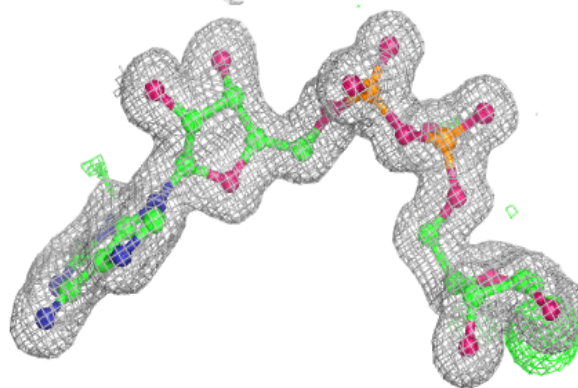and green (positive)

Electron density around GDX A 2005:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
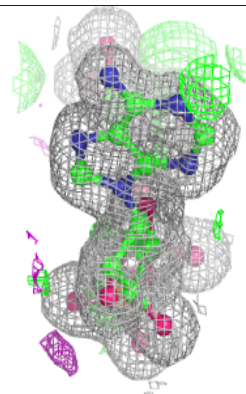mF_o-DF_c (at 3 rmsd) in purple (negative)
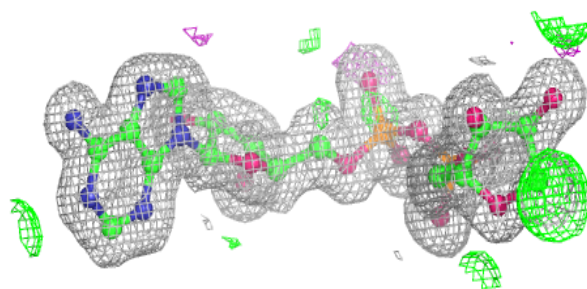and green (positive)
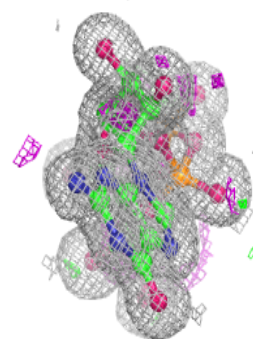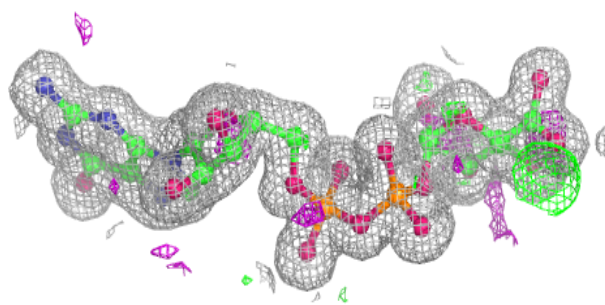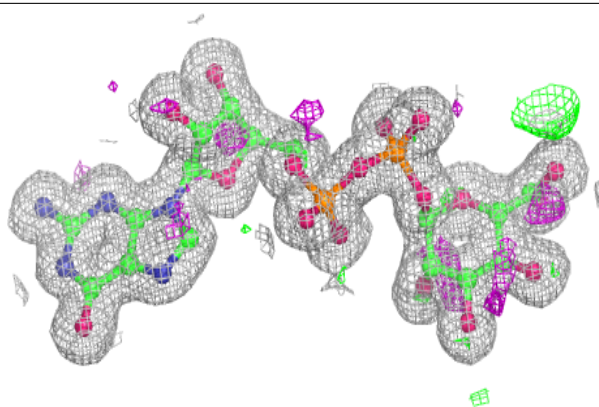
Electron density around NAD B 2002:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
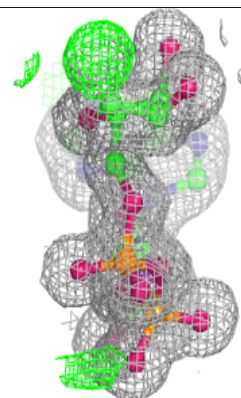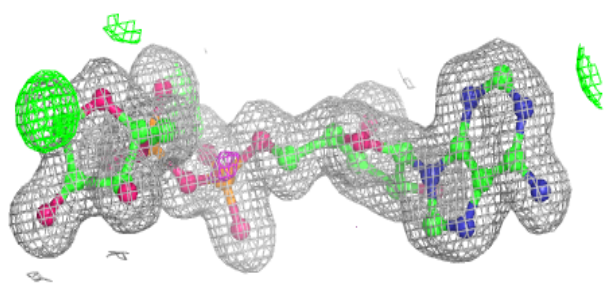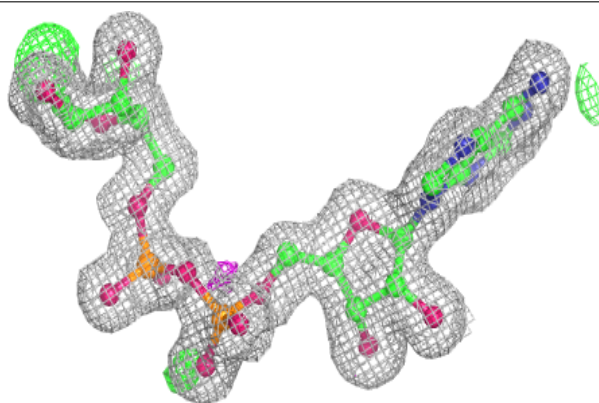
Electron density around GDX D 2007:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
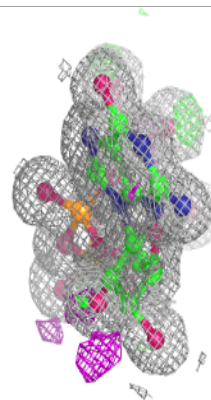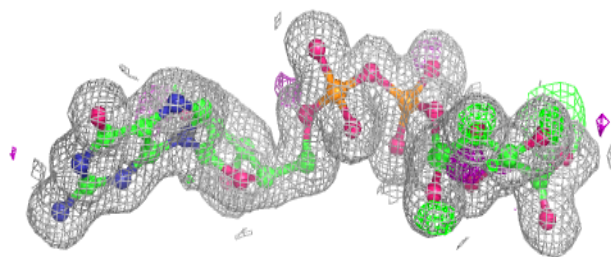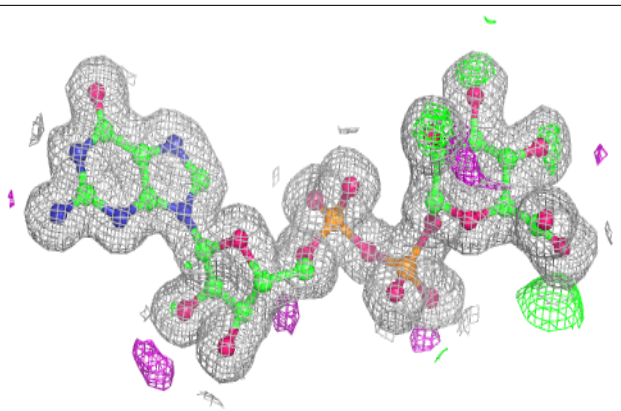
Electron density around GDX D 2008:

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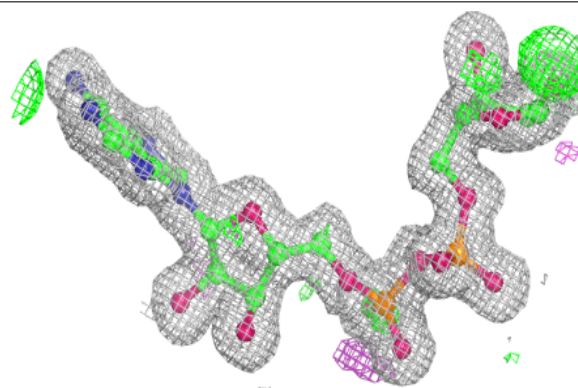and green (positive)

Electron density around NAD C 2003:

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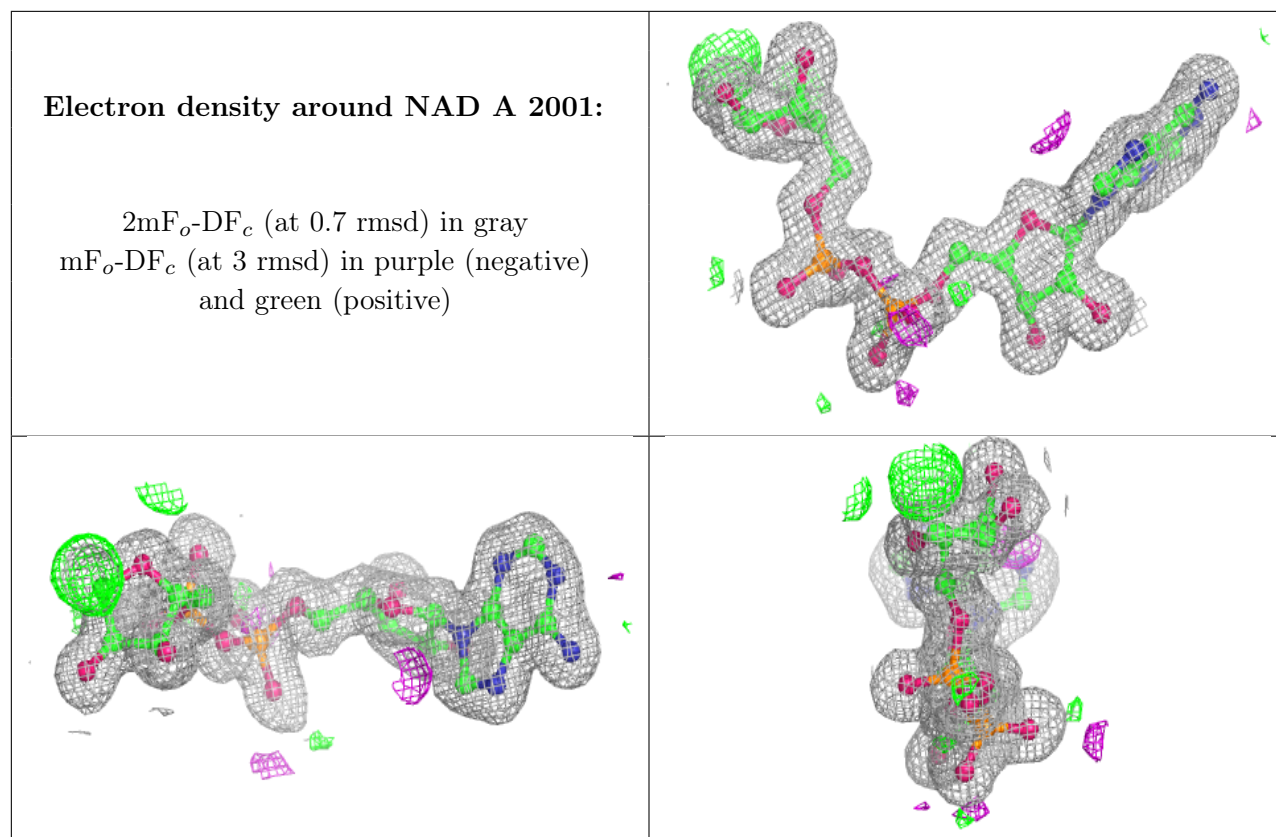mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

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 NAD A 2001:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.