



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:48 PM UTC

PDB ID : 9HJN / pdb\_00009hjn  
Title : Structure of UDP-Galactose-4-epimerase (GalE) bound to fragment from Diamond XChem experiment.  
Authors : Browne, W.  
Deposited on : 2024-11-29  
Resolution : 1.65 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](mailto: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>.

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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

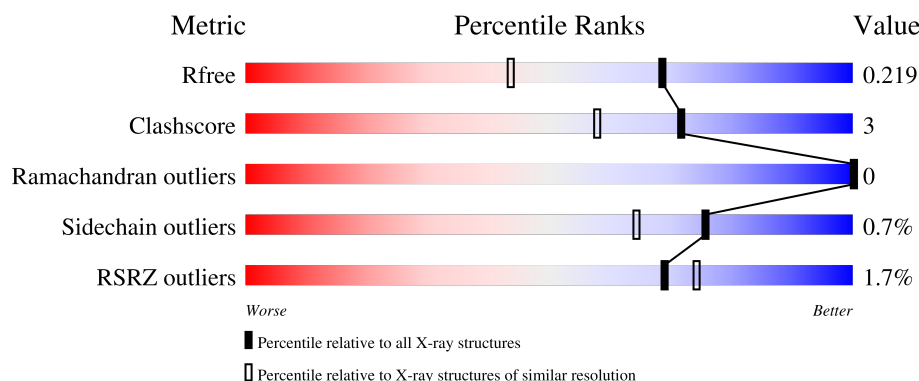
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.65 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	2563 (1.66-1.66)
Clashscore	190562	2662 (1.66-1.66)
Ramachandran outliers	187476	2621 (1.66-1.66)
Sidechain outliers	187428	2621 (1.66-1.66)
RSRZ outliers	180081	2564 (1.66-1.66)

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  $\geq 3$ , 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	348	<div> <div>%</div> <div> <div></div> <div>90%</div> <div>8%</div> <div>.</div> </div> </div>
1	B	348	<div> <div>3%</div> <div> <div></div> <div>90%</div> <div>8%</div> <div>.</div> </div> </div>

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	MLI	A	403	-	-	X	-
4	MLI	B	404	-	-	X	-

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 5830 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 UDP-glucose 4-epimerase.

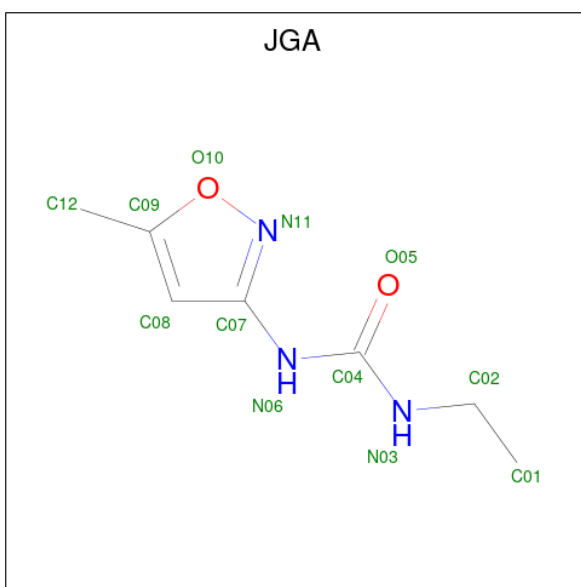
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	343	Total	C	N	O	S	0	1	0
			2647	1679	458	495	15			
1	B	343	Total	C	N	O	S	0	0	0
			2634	1671	458	490	15			

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula:  $C_{21}H_{27}N_7O_{14}P_2$ ).



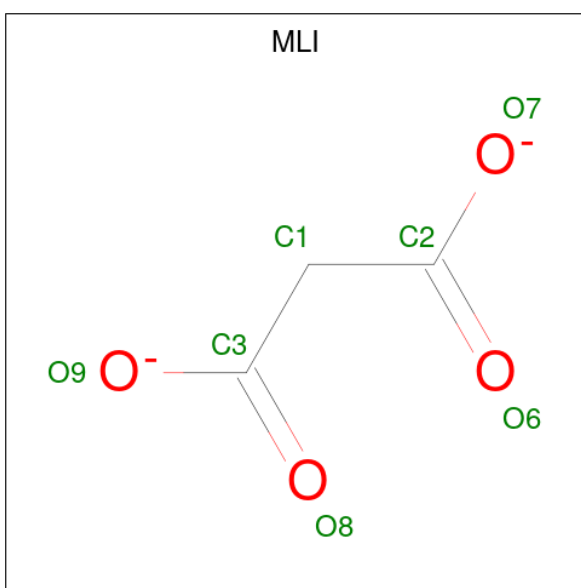
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is N-ethyl-N'-(5-methyl-1,2-oxazol-3-yl)urea (CCD ID: JGA) (formula:  $C_7H_{11}N_3O_2$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			12	7	3	2		
3	B	1	Total	C	N	O	0	0
			12	7	3	2		

- Molecule 4 is MALONATE ION (CCD ID: MLI) (formula:  $C_3H_2O_4$ ).



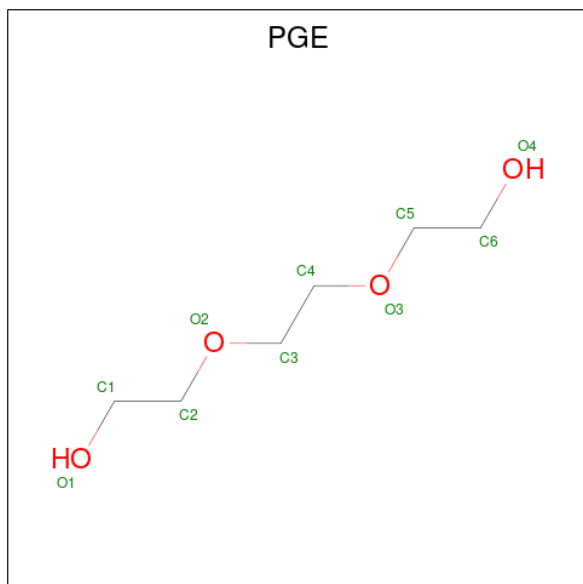
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	3	4		
4	B	1	Total	C	O	0	0
			7	3	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			7	3	4		

- Molecule 5 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula:  $C_6H_{14}O_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			10	6	4		
5	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula:  $C_2H_6O_2$ ).



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

- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Cl	0	0
			1	1		

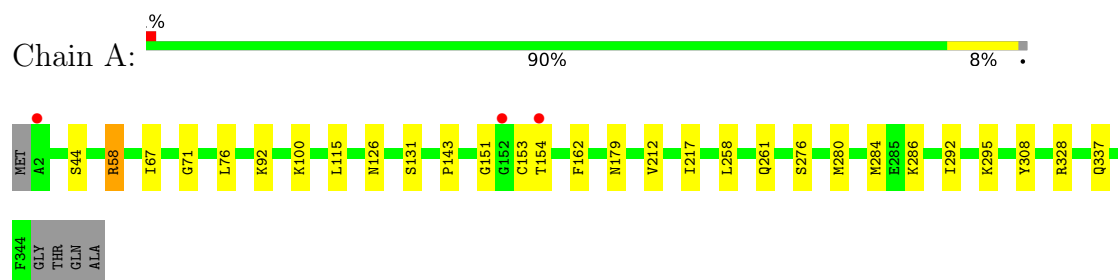
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	206	Total	O	0	0
			206	206		
8	B	176	Total	O	0	0
			176	176		

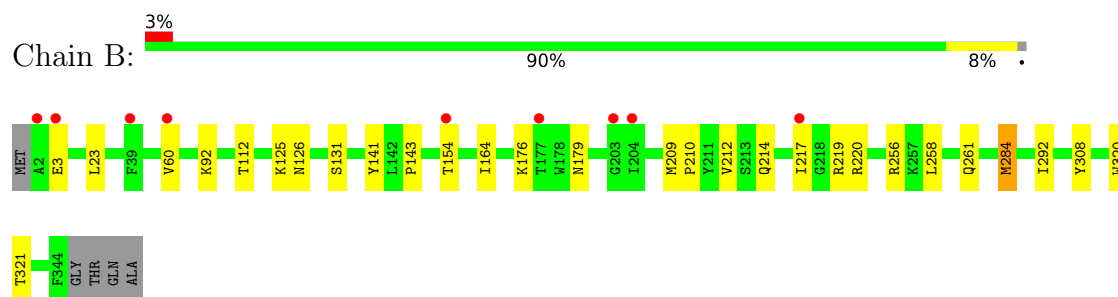
### 3 Residue-property plots [i](#)

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: UDP-glucose 4-epimerase



- Molecule 1: UDP-glucose 4-epimerase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	46.14Å 108.33Å 137.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.72 – 1.65 43.72 – 1.65	Depositor EDS
% Data completeness (in resolution range)	99.6 (43.72-1.65) 99.6 (43.72-1.65)	Depositor EDS
$R_{merge}$	0.44	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.41 (at 1.65Å)	Xtriage
Refinement program	REFMAC 5.8.0430 (refmacat 0.4.88)	Depositor
R, $R_{free}$	0.190 , 0.219 0.190 , 0.219	Depositor DCC
$R_{free}$ test set	4221 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	19.3	Xtriage
Anisotropy	0.411	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 29.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5830	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 20.11 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.3366e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: JGA, NAD, PGE, CL, MLI, EDO

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	0.58	0/2704	1.04	4/3663 (0.1%)
1	B	0.57	0/2691	1.03	3/3644 (0.1%)
All	All	0.57	0/5395	1.03	7/7307 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
All	All	0	3

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	284	MET	CG-SD-CE	-7.46	84.48	100.90
1	B	321	THR	OG1-CB-CG2	-6.61	96.08	109.30
1	A	295	LYS	CB-CG-CD	6.02	125.15	111.30
1	A	328	ARG	CG-CD-NE	-5.91	98.99	112.00
1	A	100	LYS	CB-CA-C	-5.62	103.84	111.21
1	A	286	LYS	CG-CD-CE	5.12	123.07	111.30
1	B	3	GLU	CB-CG-CD	-5.07	103.99	112.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	58[A]	ARG	Sidechain
1	B	219	ARG	Sidechain
1	B	220	ARG	Sidechain

## 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	2647	0	2588	19	0
1	B	2634	0	2576	17	0
2	A	44	0	26	1	0
2	B	44	0	26	1	0
3	A	12	0	0	0	0
3	B	12	0	0	0	0
4	A	7	0	2	2	0
4	B	14	0	4	3	0
5	A	10	0	14	3	0
5	B	7	0	9	1	0
6	A	8	0	12	1	0
6	B	8	0	12	0	0
7	B	1	0	0	0	0
8	A	206	0	0	2	0
8	B	176	0	0	2	0
All	All	5830	0	5269	35	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (35) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:256:ARG:HD3	4:B:404:MLI:O7	1.72	0.89
1:A:154:THR:O	8:A:501:HOH:O	1.98	0.81
1:B:176:LYS:HD2	5:B:406:PGE:H2	1.70	0.72
1:B:125:LYS:HE3	8:B:590:HOH:O	1.91	0.69
1:B:154:THR:CB	8:B:505:HOH:O	2.46	0.63
1:A:76:LEU:HD12	4:A:403:MLI:O7	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:GLY:HA3	5:A:404:PGE:H3	1.80	0.63
1:B:214:GLN:HA	1:B:217:ILE:HG22	1.80	0.63
1:A:162:PHE:CE2	5:A:404:PGE:H2	2.35	0.60
1:A:212:VAL:HG12	1:A:284:MET:HG2	1.87	0.57
1:A:58[A]:ARG:HH21	1:B:320:TRP:HA	1.71	0.55
1:A:217:ILE:HD12	1:A:337:GLN:HG3	1.89	0.54
1:A:143:PRO:HB3	1:A:308:TYR:CE2	2.44	0.53
1:B:212:VAL:HG12	1:B:284:MET:HG2	1.91	0.52
1:B:141:TYR:HA	4:B:403:MLI:H12	1.92	0.51
1:A:58[B]:ARG:HD3	8:A:654:HOH:O	2.11	0.50
1:B:212:VAL:HG13	1:B:292:ILE:HD13	1.93	0.49
1:A:276:SER:O	1:A:280:MET:HG2	2.13	0.49
1:B:143:PRO:HB3	1:B:308:TYR:CE2	2.48	0.48
1:A:67:ILE:HD11	1:A:115:LEU:HB2	1.94	0.48
1:A:126:ASN:HB3	1:A:258:LEU:HD13	1.96	0.48
1:B:256:ARG:HD3	4:B:404:MLI:C2	2.40	0.48
1:B:209:MET:N	1:B:210:PRO:HD2	2.29	0.47
1:A:212:VAL:HG13	1:A:292:ILE:HD13	1.97	0.47
1:B:23:LEU:HD11	1:B:60:VAL:HG22	1.99	0.45
1:A:131:SER:O	2:A:401:NAD:H6N	2.17	0.44
1:A:71:GLY:HA3	6:A:405:EDO:H12	1.99	0.43
1:B:179:ASN:HD21	1:B:261:GLN:NE2	2.15	0.43
1:B:131:SER:O	2:B:401:NAD:H6N	2.19	0.43
1:A:162:PHE:HE2	5:A:404:PGE:H2	1.78	0.42
1:A:76:LEU:HA	4:A:403:MLI:O7	2.19	0.41
1:A:179:ASN:HD21	1:A:261:GLN:NE2	2.17	0.41
1:A:212:VAL:CG1	1:A:292:ILE:HD13	2.50	0.41
1:B:112:THR:HG21	1:B:164:ILE:HG23	2.03	0.41
1:B:126:ASN:HB3	1:B:258:LEU:HD13	2.03	0.40

There are no symmetry-related clashes.

## 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	342/348 (98%)	336 (98%)	6 (2%)	0	100	100
1	B	341/348 (98%)	333 (98%)	8 (2%)	0	100	100
All	All	683/696 (98%)	669 (98%)	14 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	273/281 (97%)	270 (99%)	3 (1%)	65	48
1	B	271/281 (96%)	270 (100%)	1 (0%)	84	77
All	All	544/562 (97%)	540 (99%)	4 (1%)	76	64

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	SER
1	A	92	LYS
1	A	153	CYS
1	B	92	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	138	ASN
1	A	173	GLN
1	A	214	GLN
1	A	224	ASN
1	A	261	GLN
1	A	282	GLN
1	B	74	GLN
1	B	122	HIS
1	B	138	ASN

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Mol	Chain	Res	Type
1	B	206	ASN
1	B	224	ASN
1	B	261	GLN
1	B	282	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 1 is monoatomic - leaving 13 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
6	EDO	A	405	-	3,3,3	0.57	0	2,2,2	0.12	0
4	MLI	B	403	-	6,6,6	1.57	1 (16%)	7,7,7	1.01	0
5	PGE	B	406	-	6,6,9	0.30	0	5,5,8	0.14	0
3	JGA	A	402	-	12,12,12	0.55	0	15,15,15	0.64	0
2	NAD	A	401	-	46,48,48	0.90	3 (6%)	64,73,73	1.01	3 (4%)
6	EDO	A	406	-	3,3,3	0.11	0	2,2,2	0.33	0
6	EDO	B	407	-	3,3,3	0.42	0	2,2,2	0.29	0
3	JGA	B	402	-	12,12,12	0.50	0	15,15,15	1.01	1 (6%)
5	PGE	A	404	-	9,9,9	0.24	0	8,8,8	0.25	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAD	B	401	-	46,48,48	0.88	2 (4%)	64,73,73	0.98	3 (4%)
4	MLI	A	403	-	6,6,6	1.27	1 (16%)	7,7,7	1.38	1 (14%)
6	EDO	B	405	-	3,3,3	0.07	0	2,2,2	0.14	0
4	MLI	B	404	-	6,6,6	1.67	1 (16%)	7,7,7	0.83	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
6	EDO	A	405	-	-	1/1/1/1	-
4	MLI	B	403	-	-	4/4/4/4	-
5	PGE	B	406	-	-	3/4/4/7	-
3	JGA	A	402	-	-	0/7/7/7	0/1/1/1
2	NAD	A	401	-	-	5/30/62/62	0/5/5/5
6	EDO	A	406	-	-	1/1/1/1	-
6	EDO	B	407	-	-	0/1/1/1	-
3	JGA	B	402	-	-	2/7/7/7	0/1/1/1
5	PGE	A	404	-	-	7/7/7/7	-
2	NAD	B	401	-	-	4/30/62/62	0/5/5/5
4	MLI	A	403	-	-	2/4/4/4	-
6	EDO	B	405	-	-	1/1/1/1	-
4	MLI	B	404	-	-	2/4/4/4	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	NAD	C2N-N1N	3.88	1.39	1.35
2	B	401	NAD	C2N-N1N	3.75	1.39	1.35
4	B	404	MLI	O7-C2	-2.88	1.21	1.30
2	B	401	NAD	O4D-C1D	2.62	1.44	1.40
2	A	401	NAD	PN-O3	2.49	1.62	1.59
4	B	403	MLI	O7-C2	-2.41	1.22	1.30
2	A	401	NAD	O4D-C1D	2.05	1.43	1.40
4	A	403	MLI	O9-C3	-2.01	1.24	1.30

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	NAD	C2N-C3N-C4N	3.15	121.92	118.26
4	A	403	MLI	C3-C1-C2	-2.61	103.74	112.95
2	A	401	NAD	C4D-O4D-C1D	-2.49	107.64	109.92
2	B	401	NAD	O3-PN-O1N	-2.45	103.34	110.70
2	A	401	NAD	C5D-C4D-C3D	-2.29	106.99	115.21
3	B	402	JGA	C01-C02-N03	2.24	118.96	111.53
2	B	401	NAD	C2N-C3N-C4N	2.01	120.60	118.26
2	B	401	NAD	O2N-PN-O3	2.01	112.70	107.27

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	404	PGE	C6-C5-O3-C4
5	A	404	PGE	O2-C3-C4-O3
5	A	404	PGE	O3-C5-C6-O4
5	A	404	PGE	O1-C1-C2-O2
6	B	405	EDO	O1-C1-C2-O2
2	A	401	NAD	PN-O3-PA-O5B
2	B	401	NAD	PN-O3-PA-O5B
4	A	403	MLI	C2-C1-C3-O8
3	B	402	JGA	O05-C04-N03-C02
5	A	404	PGE	C3-C4-O3-C5
4	A	403	MLI	C2-C1-C3-O9
2	B	401	NAD	PA-O3-PN-O1N
4	B	404	MLI	C3-C1-C2-O7
6	A	406	EDO	O1-C1-C2-O2
2	A	401	NAD	C5D-O5D-PN-O1N
2	B	401	NAD	C5D-O5D-PN-O1N
4	B	404	MLI	C3-C1-C2-O6
2	A	401	NAD	PA-O3-PN-O1N
3	B	402	JGA	N06-C04-N03-C02
5	B	406	PGE	C1-C2-O2-C3
2	A	401	NAD	PA-O3-PN-O2N
5	B	406	PGE	O2-C3-C4-O3
6	A	405	EDO	O1-C1-C2-O2
4	B	403	MLI	C2-C1-C3-O8
5	A	404	PGE	C1-C2-O2-C3
2	B	401	NAD	PA-O3-PN-O2N
2	A	401	NAD	O4B-C4B-C5B-O5B
4	B	403	MLI	C3-C1-C2-O6
5	A	404	PGE	C4-C3-O2-C2
5	B	406	PGE	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	B	403	MLI	C3-C1-C2-O7
4	B	403	MLI	C2-C1-C3-O9

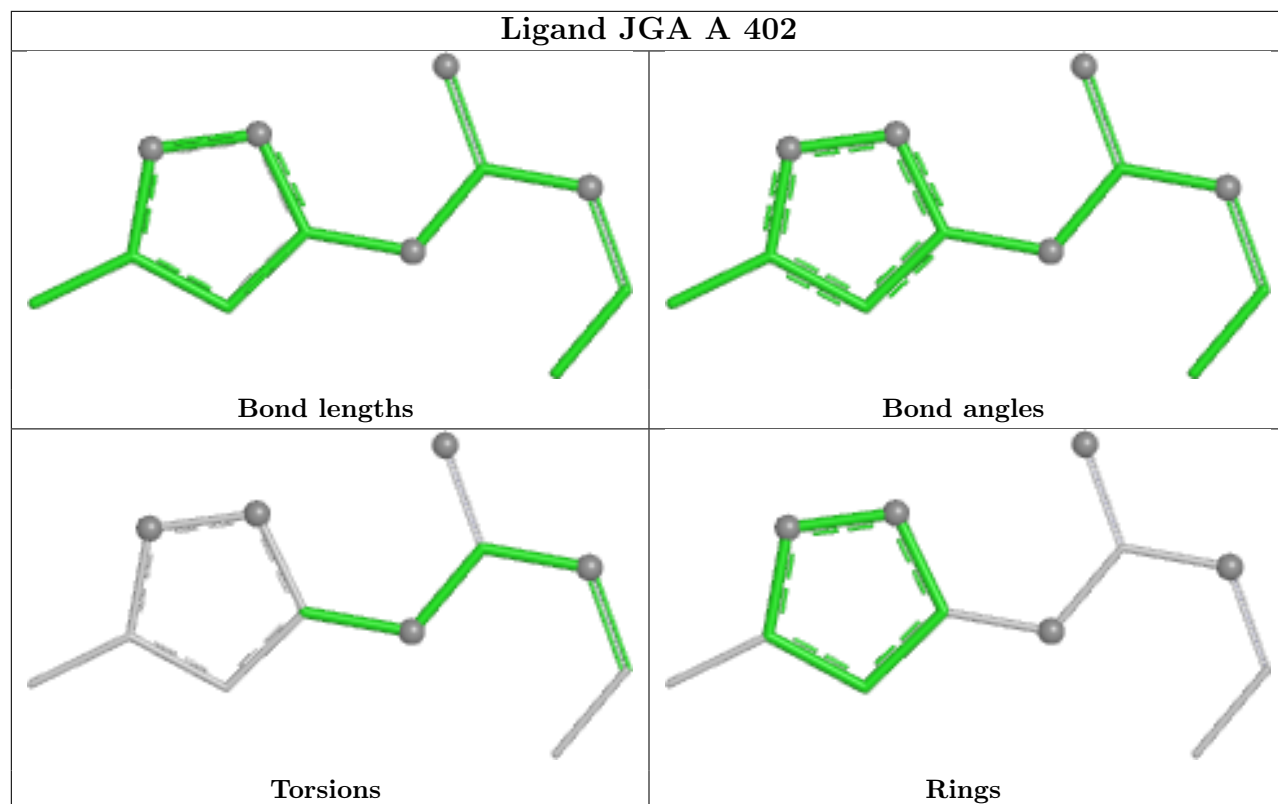
There are no ring outliers.

8 monomers are involved in 12 short contacts:

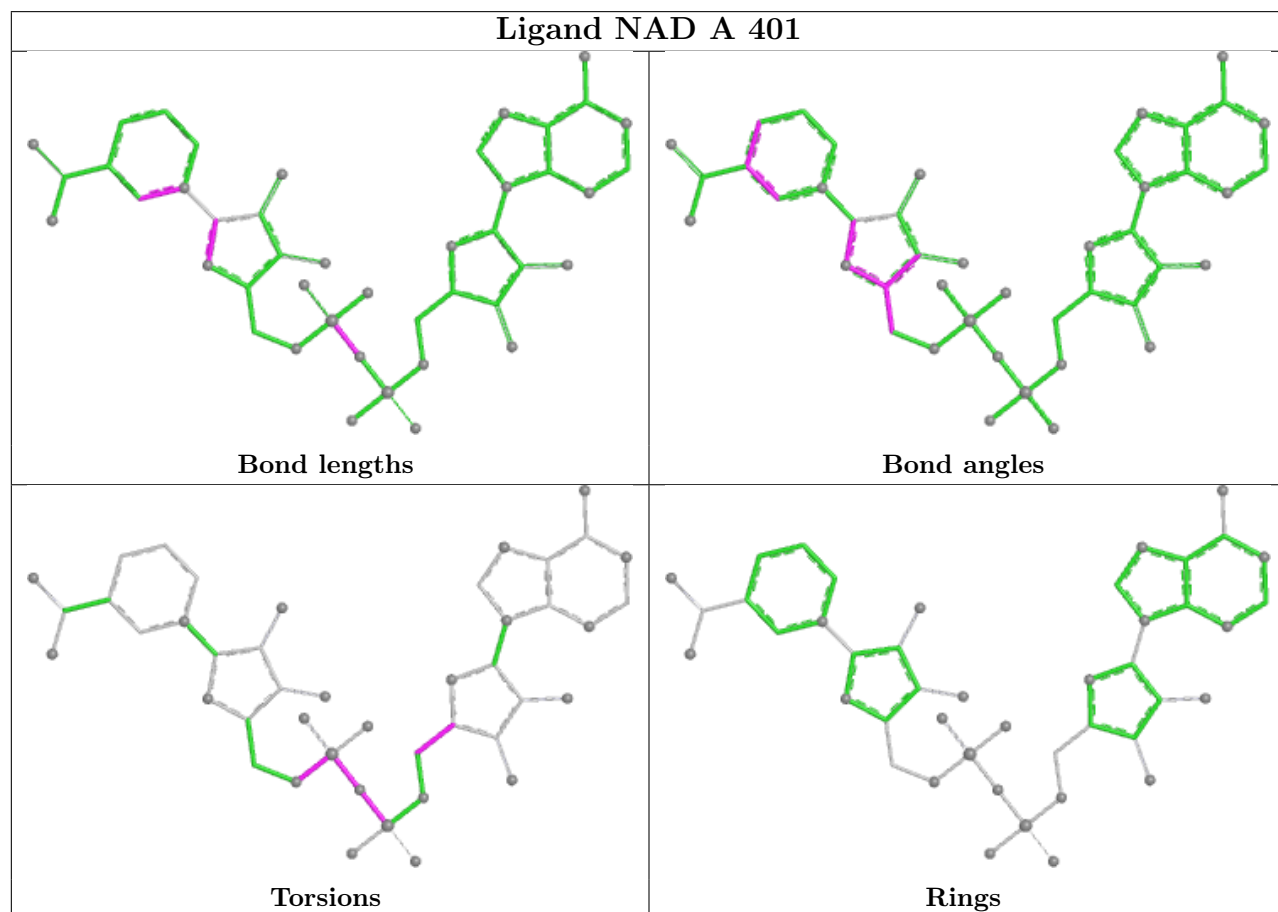
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	405	EDO	1	0
4	B	403	MLI	1	0
5	B	406	PGE	1	0
2	A	401	NAD	1	0
5	A	404	PGE	3	0
2	B	401	NAD	1	0
4	A	403	MLI	2	0
4	B	404	MLI	2	0

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.

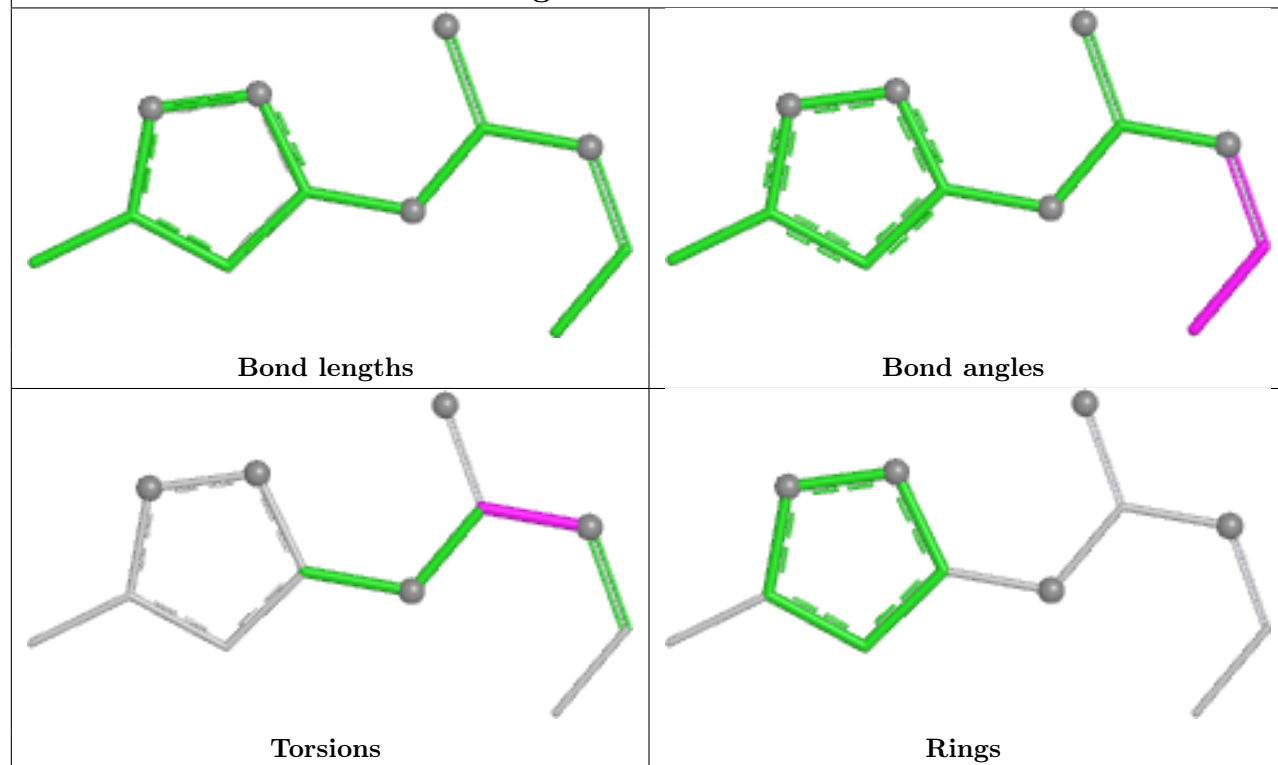
## Ligand JGA A 402



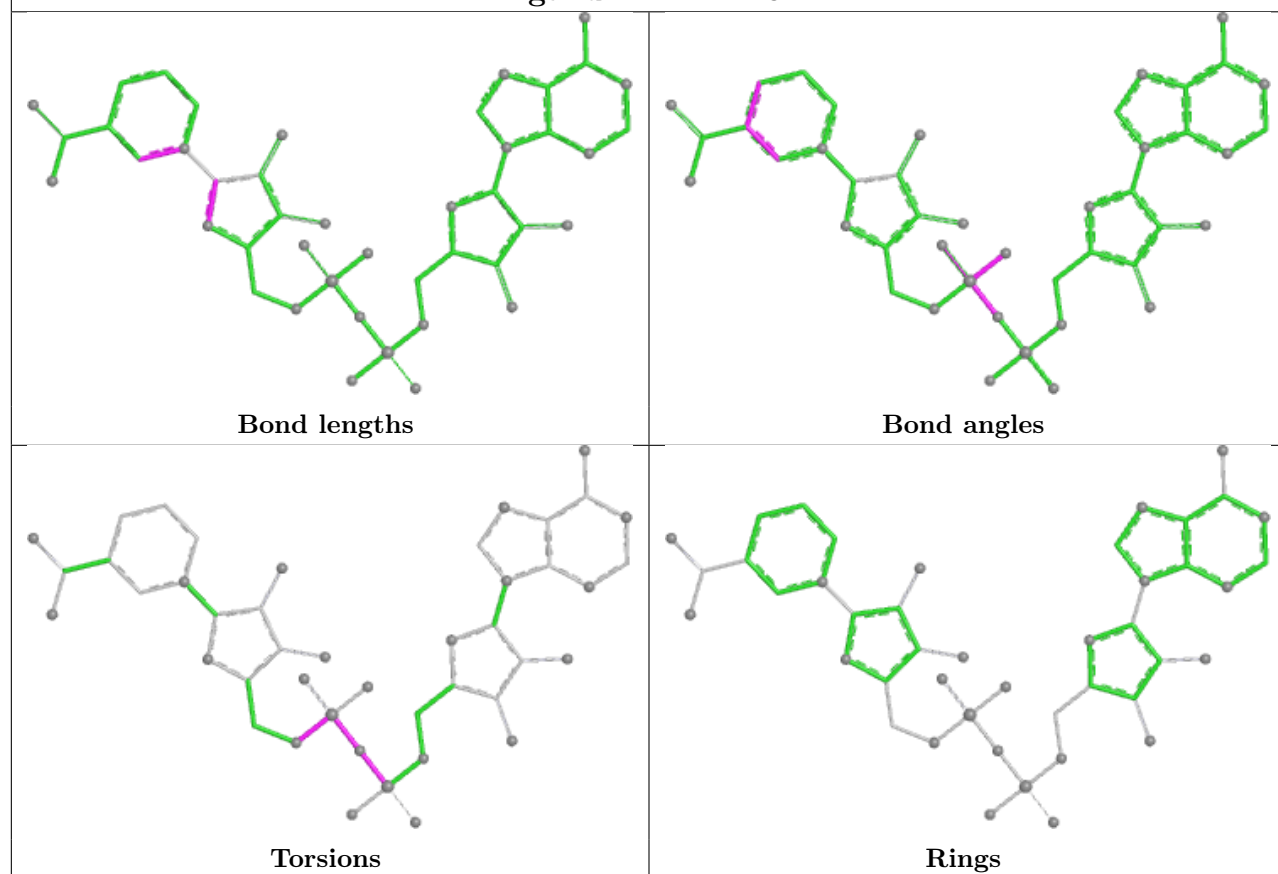
## Ligand NAD A 401



## Ligand JGA B 402



## Ligand NAD B 401



## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	343/348 (98%)	-0.24	3 (0%) 81 86	13, 19, 34, 50	1 (0%)
1	B	343/348 (98%)	-0.04	9 (2%) 57 62	15, 22, 39, 55	0
All	All	686/696 (98%)	-0.14	12 (1%) 69 74	13, 21, 37, 55	1 (0%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2	ALA	4.9
1	A	154	THR	3.2
1	B	204	ILE	3.1
1	A	2	ALA	3.0
1	B	39	PHE	2.7
1	A	152	GLY	2.6
1	B	60	VAL	2.6
1	B	154	THR	2.5
1	B	203	GLY	2.2
1	B	177	THR	2.2
1	B	217	ILE	2.1
1	B	3	GLU	2.1

### 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 oligosaccharides in this entry.

## 6.4 Ligands

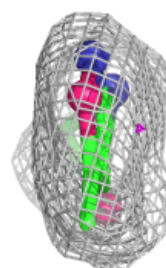
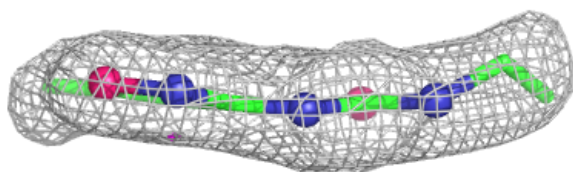
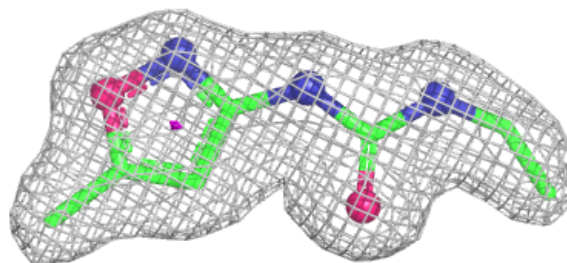
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	MLI	B	404	7/7	0.63	0.23	57,65,70,73	0
6	EDO	B	405	4/4	0.63	0.24	49,54,57,57	0
4	MLI	A	403	7/7	0.76	0.20	39,41,54,61	0
5	PGE	B	406	7/10	0.78	0.18	32,46,56,57	0
5	PGE	A	404	10/10	0.79	0.16	39,43,48,49	0
4	MLI	B	403	7/7	0.84	0.16	48,53,64,70	0
6	EDO	A	406	4/4	0.86	0.12	33,38,41,41	0
6	EDO	A	405	4/4	0.88	0.13	33,40,43,43	0
7	CL	B	408	1/1	0.91	0.16	51,51,51,51	0
6	EDO	B	407	4/4	0.93	0.09	33,33,33,35	0
3	JGA	B	402	12/12	0.94	0.09	25,28,35,36	0
3	JGA	A	402	12/12	0.96	0.06	22,24,28,28	0
2	NAD	A	401	44/44	0.98	0.04	12,14,16,22	0
2	NAD	B	401	44/44	0.98	0.05	15,17,24,25	0

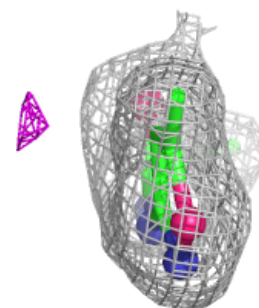
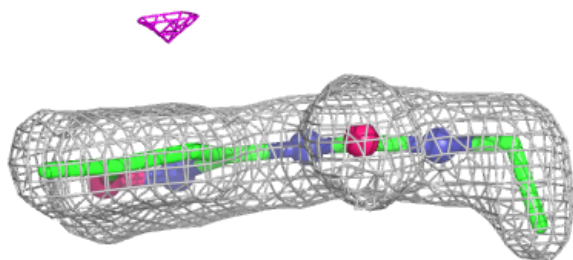
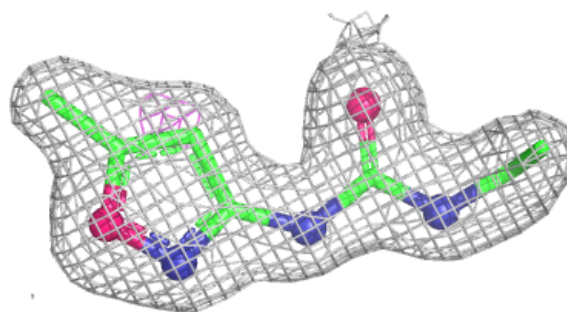
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around JGA B 402:**

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

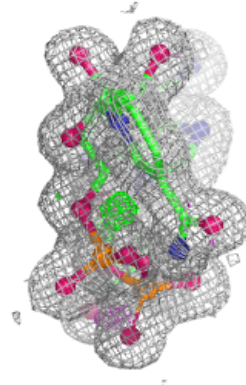
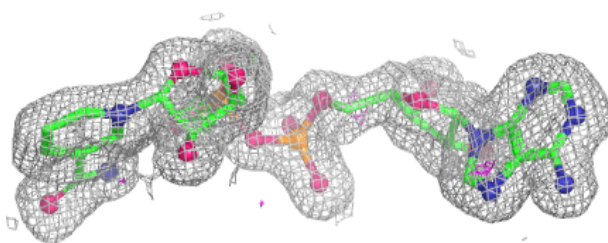
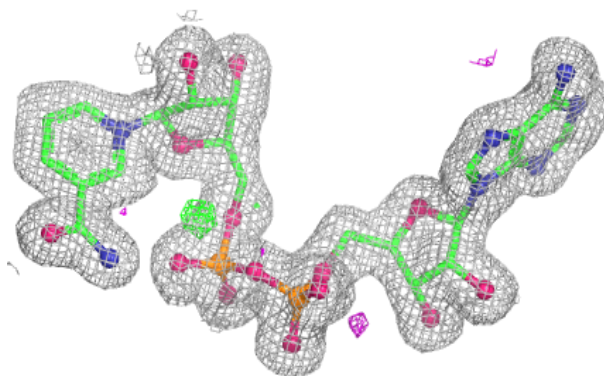
**Electron density around JGA A 402:**

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

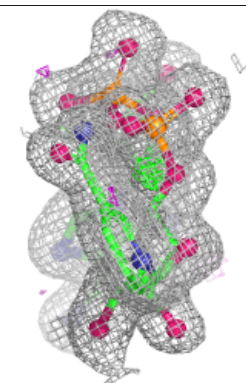
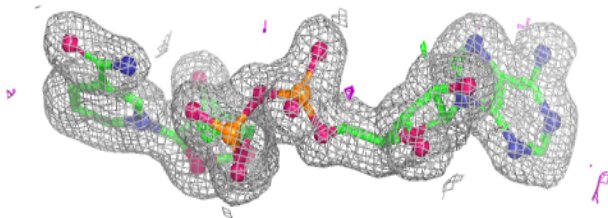
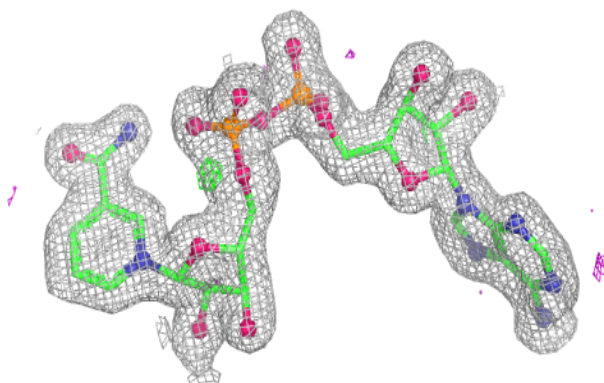


**Electron density around NAD A 401:**

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

**Electron density around NAD B 401:**

$2mF_o-DF_c$  (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.