



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 10:02 PM UTC

PDB ID : 5GY7 / pdb_00005gy7
Title : X-Ray structure of H243I mutant of UDP-Galactose 4-epimerase from E.coli:evidence for existence of open and closed active site during catalysis.
Authors : Singh, N.; Tiwari, P.; Phulera, S.; Dixit, A.; Choudhury, D.
Deposited on : 2016-09-21
Resolution : 1.43 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

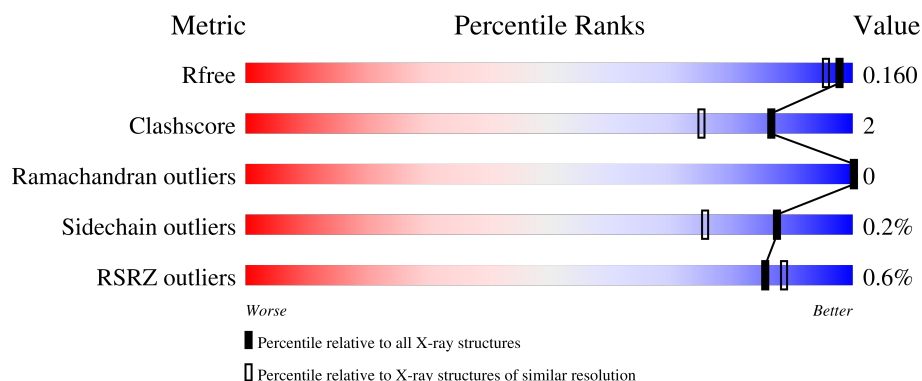
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.43 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	3234 (1.46-1.42)
Clashscore	190562	3289 (1.46-1.42)
Ramachandran outliers	187476	3248 (1.46-1.42)
Sidechain outliers	187428	3248 (1.46-1.42)
RSRZ outliers	180081	3234 (1.46-1.42)

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	344	% 88% 9% ..
1	B	344	% 88% 9% ..

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5934 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	338	Total	C	N	O	S	0	0	0
			2581	1632	452	486	11			
1	B	338	Total	C	N	O	S	0	0	0
			2561	1618	447	485	11			

There are 14 discrepancies between the modelled and reference sequences:

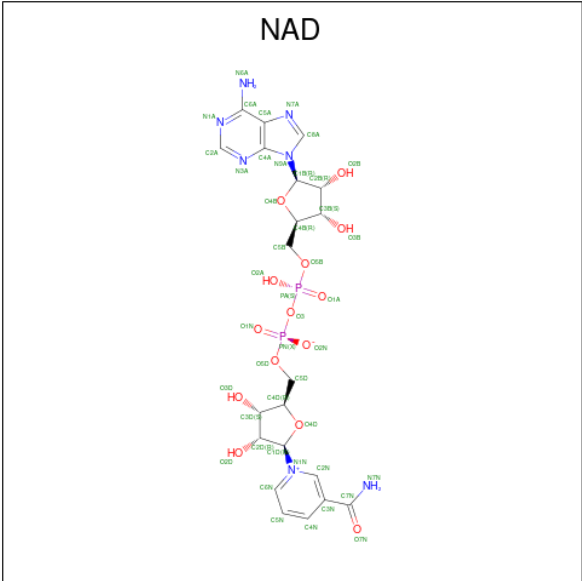
Chain	Residue	Modelled	Actual	Comment	Reference
A	243	ILE	HIS	engineered mutation	UNP P09147
A	339	HIS	-	expression tag	UNP P09147
A	340	HIS	-	expression tag	UNP P09147
A	341	HIS	-	expression tag	UNP P09147
A	342	HIS	-	expression tag	UNP P09147
A	343	HIS	-	expression tag	UNP P09147
A	344	HIS	-	expression tag	UNP P09147
B	243	ILE	HIS	engineered mutation	UNP P09147
B	339	HIS	-	expression tag	UNP P09147
B	340	HIS	-	expression tag	UNP P09147
B	341	HIS	-	expression tag	UNP P09147
B	342	HIS	-	expression tag	UNP P09147
B	343	HIS	-	expression tag	UNP P09147
B	344	HIS	-	expression tag	UNP P09147

- Molecule 2 is URIDINE-5'-DIPHOSPHATE (CCD ID: UDP) (formula: $C_9H_{14}N_2O_{12}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
2	B	1	Total	C	N	O	P	0	0
			25	9	2	12	2		

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



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

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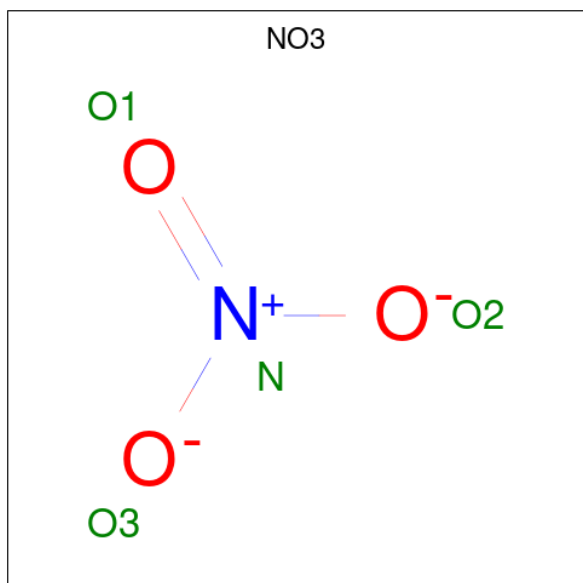
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is NITRATE ION (CCD ID: NO3) (formula: NO_3).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	N	O	0	0
			4	1	3		

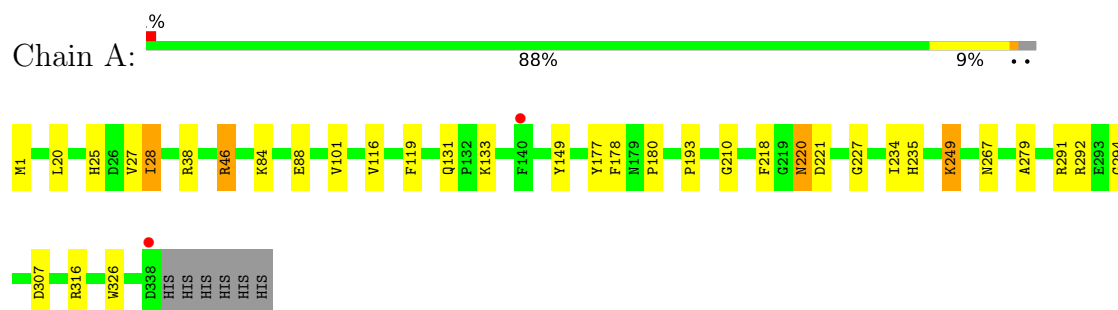
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	332	Total	O	0	0
			332	332		
6	B	312	Total	O	0	0
			312	312		

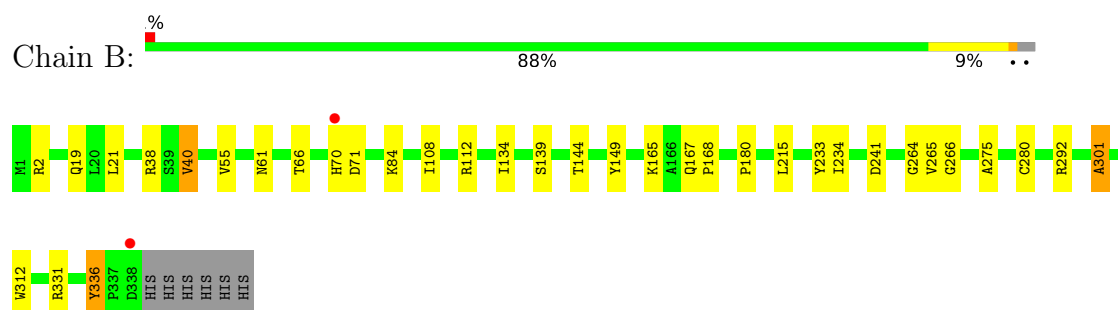
3 Residue-property plots [i](#)

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 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	47.11Å 91.16Å 80.26Å 90.00° 99.87° 90.00°	Depositor
Resolution (Å)	79.07 – 1.43 79.07 – 1.43	Depositor EDS
% Data completeness (in resolution range)	98.7 (79.07-1.43) 98.7 (79.07-1.43)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.73 (at 1.43Å)	Xtriage
Refinement program	REFMAC 5.8.0151	Depositor
R, R_{free}	0.134 , 0.160 0.134 , 0.160	Depositor DCC
R_{free} test set	6040 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	9.3	Xtriage
Anisotropy	0.421	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 36.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	5934	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 5.05% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NO3, UDP, GOL, 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	1.70	23/2646 (0.9%)	1.44	7/3611 (0.2%)
1	B	1.70	19/2624 (0.7%)	1.46	15/3584 (0.4%)
All	All	1.70	42/5270 (0.8%)	1.45	22/7195 (0.3%)

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	B	0	1

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	210	GLY	CA-C	-8.34	1.40	1.51
1	B	266	GLY	CA-C	-7.45	1.46	1.52
1	B	167	GLN	CA-CB	-7.03	1.44	1.53
1	B	112	ARG	C-O	6.92	1.32	1.24
1	B	38	ARG	CA-CB	6.65	1.64	1.53
1	A	133	LYS	N-CA	-6.45	1.38	1.46
1	A	220	ASN	CA-CB	6.31	1.64	1.53
1	B	71	ASP	N-CA	6.22	1.54	1.46
1	A	46	ARG	CA-C	-6.10	1.45	1.52
1	B	139	SER	CB-OG	-6.09	1.29	1.42
1	A	88	GLU	N-CA	-5.92	1.39	1.46
1	B	21	LEU	N-CA	5.90	1.53	1.46
1	A	279	ALA	CA-C	-5.78	1.45	1.52
1	A	1	MET	SD-CE	-5.77	1.65	1.79
1	B	265	VAL	CA-CB	-5.77	1.45	1.55
1	B	134	ILE	CA-C	-5.72	1.48	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	307	ASP	CA-C	5.68	1.60	1.52
1	A	291	ARG	C-O	-5.61	1.17	1.23
1	A	119	PHE	N-CA	5.61	1.53	1.46
1	A	116	VAL	CA-CB	5.59	1.60	1.54
1	B	55	VAL	CA-C	-5.57	1.45	1.52
1	A	249	LYS	CA-C	-5.52	1.45	1.52
1	A	227	GLY	N-CA	-5.51	1.36	1.45
1	A	20	LEU	CA-C	-5.50	1.45	1.52
1	A	220	ASN	CA-C	5.49	1.59	1.52
1	B	233	TYR	CA-C	-5.45	1.46	1.52
1	A	101	VAL	C-O	5.44	1.29	1.24
1	A	27	VAL	N-CA	5.38	1.52	1.46
1	B	215	LEU	CA-C	-5.28	1.46	1.52
1	A	25	HIS	CA-C	-5.28	1.46	1.52
1	A	267	ASN	CA-C	-5.19	1.46	1.52
1	B	165	LYS	C-O	5.17	1.30	1.24
1	B	312	TRP	CA-C	-5.14	1.46	1.52
1	B	108	ILE	CB-CG1	-5.14	1.43	1.53
1	B	40	VAL	CA-CB	5.12	1.61	1.54
1	B	331	ARG	CA-C	-5.09	1.45	1.52
1	B	61	ASN	CA-CB	-5.07	1.46	1.52
1	A	221	ASP	N-CA	5.07	1.52	1.46
1	B	280	CYS	C-N	-5.07	1.26	1.33
1	A	131	GLN	C-N	5.06	1.39	1.34
1	A	193	PRO	CA-C	-5.05	1.46	1.52
1	A	177	TYR	CA-C	-5.03	1.46	1.52

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	336	TYR	CA-C-N	-6.77	112.80	119.78
1	B	336	TYR	C-N-CA	-6.77	112.80	119.78
1	A	326	TRP	O-C-N	6.74	129.26	122.12
1	B	336	TYR	O-C-N	6.59	128.59	121.60
1	A	307	ASP	O-C-N	6.56	128.82	122.07
1	B	66	THR	O-C-N	6.34	129.38	122.15
1	B	144	THR	CB-CA-C	-5.88	104.35	110.17
1	B	70	HIS	CB-CA-C	-5.79	101.75	110.90
1	A	292	ARG	NH1-CZ-NH2	5.67	126.67	119.30
1	B	292	ARG	NE-CZ-NH1	-5.47	116.03	121.50
1	B	70	HIS	CA-C-O	-5.37	115.17	120.70
1	B	144	THR	CA-C-O	5.31	123.82	119.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	66	THR	CA-C-O	-5.25	114.86	120.42
1	A	218	PHE	CA-C-O	5.20	127.40	121.58
1	B	55	VAL	O-C-N	-5.13	117.76	123.20
1	B	275	ALA	CA-C-O	5.11	126.19	120.82
1	A	294	GLY	O-C-N	-5.10	116.89	122.65
1	B	292	ARG	NH1-CZ-NH2	5.07	125.89	119.30
1	B	168	PRO	CA-C-O	-5.05	112.33	118.99
1	A	178	PHE	CB-CA-C	5.03	120.43	110.42
1	B	2	ARG	CG-CD-NE	-5.03	100.94	112.00
1	A	38	ARG	NE-CZ-NH2	-5.02	114.68	119.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	301	ALA	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2581	0	2481	13	0
1	B	2561	0	2451	9	0
2	A	25	0	11	0	0
2	B	25	0	11	0	0
3	A	44	0	26	0	0
3	B	44	0	26	0	0
4	A	6	0	8	0	0
5	B	4	0	0	0	0
6	A	332	0	0	7	2
6	B	312	0	0	1	2
All	All	5934	0	5014	22	2

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 2.

All (22) 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:19:GLN:NE2	1:B:241:ASP:OD1	1.68	1.25
1:A:46:ARG:HD3	6:A:782:HOH:O	1.38	1.22
1:A:249:LYS:HE2	6:A:501:HOH:O	1.05	1.18
1:B:19:GLN:HG3	6:B:566:HOH:O	1.52	1.07
1:A:249:LYS:CE	6:A:501:HOH:O	1.66	0.94
1:A:46:ARG:CD	6:A:782:HOH:O	2.05	0.92
1:B:19:GLN:HE22	1:B:241:ASP:CG	1.98	0.70
1:A:249:LYS:NZ	6:A:501:HOH:O	1.90	0.66
1:A:46:ARG:CG	6:A:782:HOH:O	2.35	0.62
1:A:46:ARG:HG3	6:A:782:HOH:O	2.07	0.52
1:A:220:ASN:C	1:A:220:ASN:OD1	2.52	0.50
1:A:84:LYS:HA	1:A:149:TYR:CE1	2.49	0.47
1:B:19:GLN:CD	1:B:241:ASP:OD1	2.51	0.47
1:B:84:LYS:HA	1:B:149:TYR:CE1	2.49	0.47
1:A:235:HIS:CD2	1:A:316:ARG:HD3	2.50	0.46
1:B:180:PRO:HA	1:B:234:ILE:O	2.15	0.46
1:A:180:PRO:HA	1:A:234:ILE:O	2.15	0.45
1:B:40:VAL:HG23	1:B:336:TYR:CZ	2.52	0.44
1:A:235:HIS:CG	1:A:316:ARG:HD3	2.54	0.42
1:A:28:ILE:HD12	1:A:28:ILE:N	2.35	0.41
1:B:19:GLN:HE22	1:B:241:ASP:HA	1.86	0.41
1:B:264:GLY:HA2	1:B:301:ALA:O	2.20	0.41

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:504:HOH:O	6:B:591:HOH:O[1_454]	1.92	0.28
6:A:782:HOH:O	6:B:642:HOH:O[1_554]	2.10	0.10

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	336/344 (98%)	333 (99%)	3 (1%)	0	100	100
1	B	336/344 (98%)	332 (99%)	4 (1%)	0	100	100
All	All	672/688 (98%)	665 (99%)	7 (1%)	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	271/288 (94%)	270 (100%)	1 (0%)	84	69
1	B	267/288 (93%)	267 (100%)	0	100	100
All	All	538/576 (93%)	537 (100%)	1 (0%)	87	76

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	GLN
1	A	158	GLN
1	A	267	ASN
1	B	19	GLN

5.3.3 RNA ⓘ

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](#)

6 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	402	-	46,48,48	1.56	11 (23%)	64,73,73	1.46	11 (17%)
2	UDP	A	401	-	25,26,26	1.08	2 (8%)	38,40,40	1.32	4 (10%)
5	NO3	B	403	-	1,3,3	0.96	0	0,3,3	-	-
4	GOL	A	403	-	5,5,5	1.89	1 (20%)	5,5,5	2.17	1 (20%)
3	NAD	B	402	-	46,48,48	1.72	8 (17%)	64,73,73	1.33	9 (14%)
2	UDP	B	401	-	25,26,26	1.08	2 (8%)	38,40,40	1.21	5 (13%)

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	402	-	-	4/30/62/62	0/5/5/5
2	UDP	A	401	-	-	1/16/32/32	0/2/2/2
4	GOL	A	403	-	-	1/4/4/4	-
3	NAD	B	402	-	-	5/30/62/62	0/5/5/5
2	UDP	B	401	-	-	1/16/32/32	0/2/2/2

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	402	NAD	C4N-C3N	5.11	1.47	1.39
3	A	402	NAD	C5N-C4N	4.53	1.46	1.38
3	B	402	NAD	C3N-C7N	-4.14	1.44	1.50
3	B	402	NAD	C5N-C4N	4.00	1.45	1.38
3	B	402	NAD	O4D-C1D	3.73	1.45	1.40
4	A	403	GOL	O2-C2	3.60	1.53	1.43
3	A	402	NAD	C4N-C3N	3.49	1.44	1.39
2	A	401	UDP	C2-N3	-3.23	1.32	1.38
3	B	402	NAD	C2N-C3N	-2.74	1.34	1.39
3	A	402	NAD	C2N-C3N	-2.59	1.34	1.39
3	A	402	NAD	C6N-N1N	2.59	1.41	1.35
3	A	402	NAD	C8A-N7A	2.55	1.36	1.31
3	B	402	NAD	C8A-N7A	2.53	1.36	1.31
3	B	402	NAD	C6N-C5N	-2.53	1.33	1.38
3	A	402	NAD	PN-O3	2.44	1.62	1.59
3	A	402	NAD	O4D-C1D	2.40	1.44	1.40
2	B	401	UDP	C4-N3	-2.39	1.34	1.38
3	A	402	NAD	C5A-C4A	2.38	1.43	1.39
3	A	402	NAD	C2B-C3B	-2.25	1.47	1.53
2	B	401	UDP	PA-O3A	-2.25	1.57	1.59
3	A	402	NAD	C6N-C5N	-2.22	1.34	1.38
3	B	402	NAD	PN-O3	2.19	1.61	1.59
3	A	402	NAD	O4B-C1B	2.04	1.46	1.42
2	A	401	UDP	PA-O2A	-2.00	1.46	1.55

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	402	NAD	C5N-C4N-C3N	-4.84	115.61	120.36
4	A	403	GOL	O2-C2-C1	4.17	126.44	109.18
2	A	401	UDP	N3-C2-N1	3.73	119.75	114.89
3	A	402	NAD	C4A-N9A-C8A	3.52	109.43	105.74
3	B	402	NAD	C2N-C3N-C7N	3.47	129.46	119.46
3	A	402	NAD	C5N-C4N-C3N	-3.41	117.01	120.36
3	A	402	NAD	N9A-C8A-N7A	-3.03	109.64	113.94
3	B	402	NAD	C4N-C3N-C7N	-2.81	113.39	121.06
2	B	401	UDP	C5-C4-N3	2.66	118.53	114.80
3	B	402	NAD	N3A-C2A-N1A	-2.59	124.66	128.58
2	A	401	UDP	C4-N3-C2	-2.55	123.44	126.61
3	A	402	NAD	C4D-O4D-C1D	-2.55	107.59	109.92
2	A	401	UDP	O2A-PA-O3A	2.54	114.13	107.27
3	A	402	NAD	O4B-C1B-C2B	-2.52	101.22	106.62
3	A	402	NAD	C3B-C2B-C1B	2.49	106.17	101.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	402	NAD	O7N-C7N-C3N	2.46	122.61	119.60
2	B	401	UDP	O2-C2-N1	-2.42	119.65	122.80
3	B	402	NAD	C2A-N1A-C6A	2.39	122.65	118.73
3	B	402	NAD	C6N-N1N-C2N	-2.33	119.89	121.88
2	B	401	UDP	N3-C2-N1	2.30	117.88	114.89
3	A	402	NAD	C5A-N7A-C8A	2.30	107.06	103.45
3	A	402	NAD	C4A-N9A-C1B	-2.26	121.35	126.63
3	A	402	NAD	C6N-N1N-C2N	-2.24	119.97	121.88
2	A	401	UDP	O3B-PB-O3A	-2.20	97.26	104.64
2	B	401	UDP	C1'-N1-C2	2.16	121.47	117.59
3	A	402	NAD	O4D-C4D-C3D	2.13	109.39	105.15
2	B	401	UDP	C6-N1-C2	-2.13	118.41	121.00
3	B	402	NAD	O7N-C7N-N7N	-2.12	119.55	122.62
3	A	402	NAD	C6A-C5A-N7A	2.08	136.10	132.09
3	B	402	NAD	C6N-C5N-C4N	2.04	122.38	119.45

There are no chirality outliers.

All (12) torsion outliers are listed below:

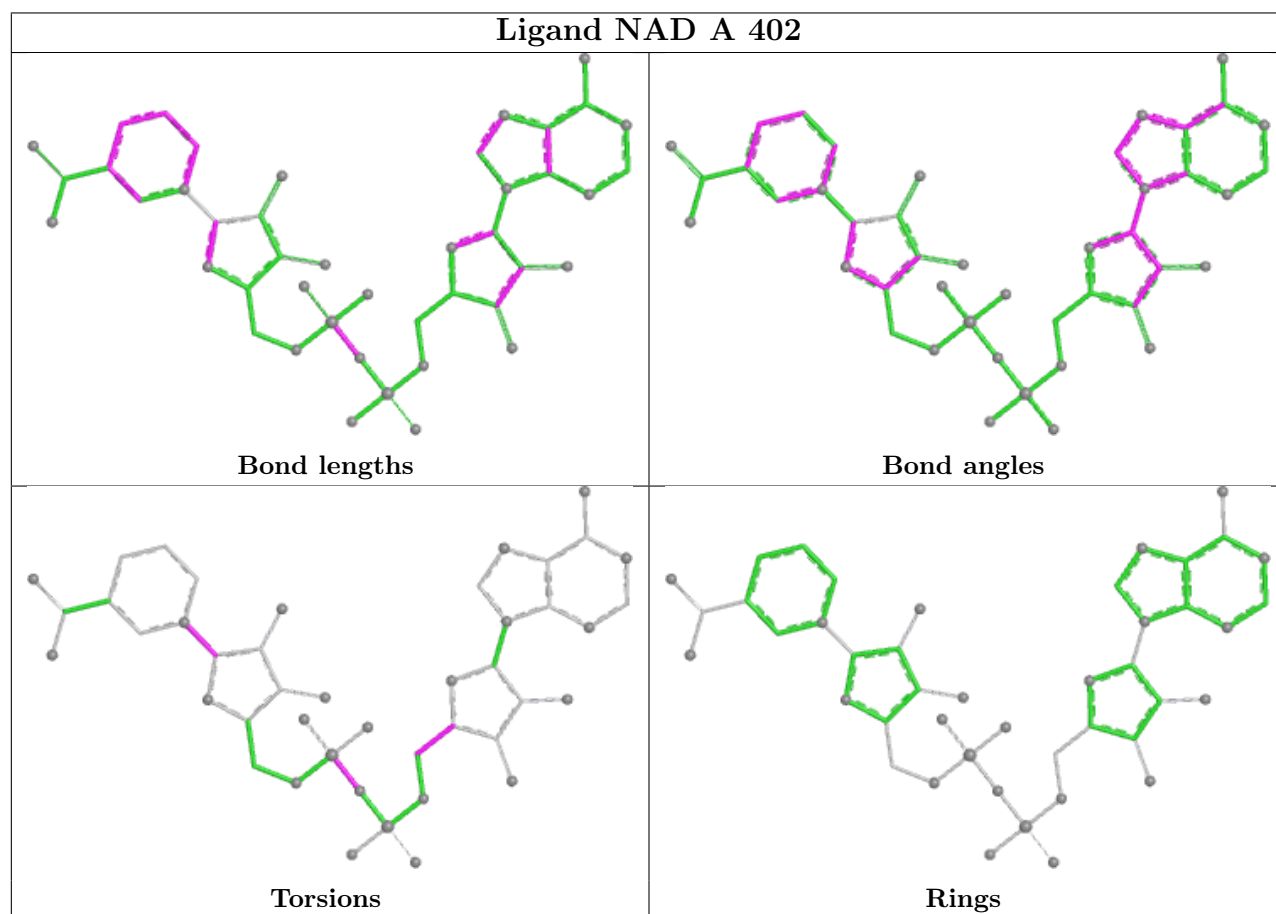
Mol	Chain	Res	Type	Atoms
2	A	401	UDP	PB-O3A-PA-O5'
2	B	401	UDP	PB-O3A-PA-O5'
3	A	402	NAD	O4D-C1D-N1N-C2N
3	B	402	NAD	C5D-O5D-PN-O1N
3	B	402	NAD	O4D-C1D-N1N-C2N
4	A	403	GOL	C1-C2-C3-O3
3	B	402	NAD	C5D-O5D-PN-O3
3	A	402	NAD	O4D-C1D-N1N-C6N
3	B	402	NAD	O4D-C1D-N1N-C6N
3	B	402	NAD	PA-O3-PN-O2N
3	A	402	NAD	PA-O3-PN-O2N
3	A	402	NAD	O4B-C4B-C5B-O5B

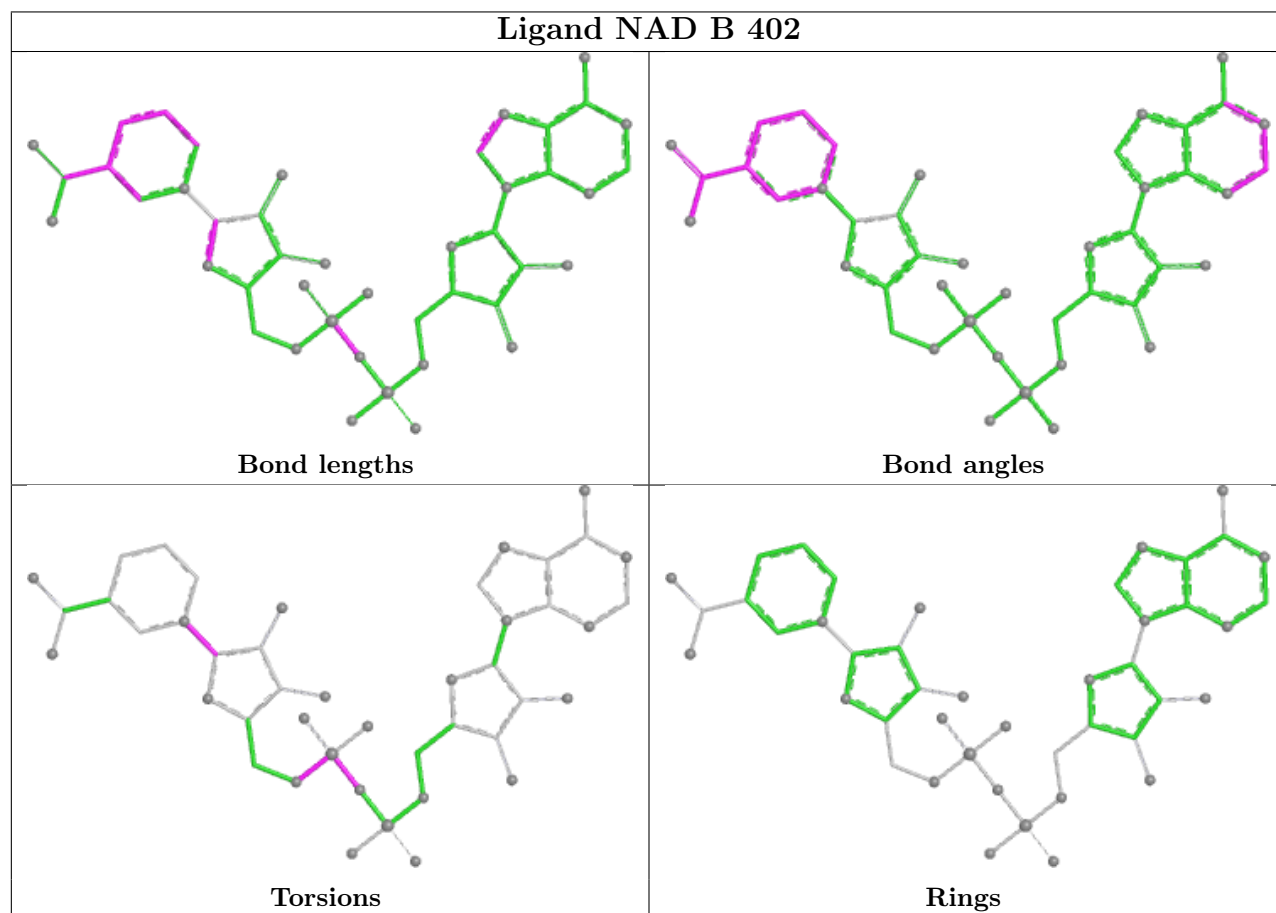
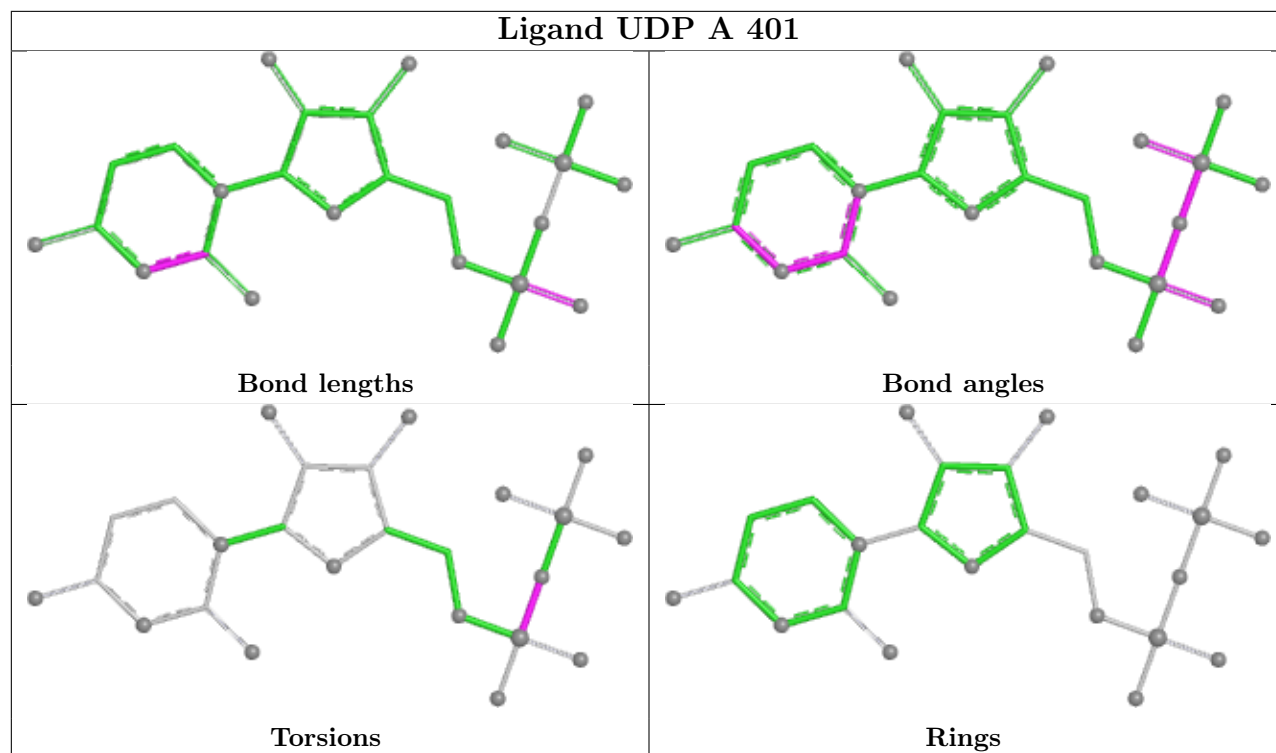
There are no ring outliers.

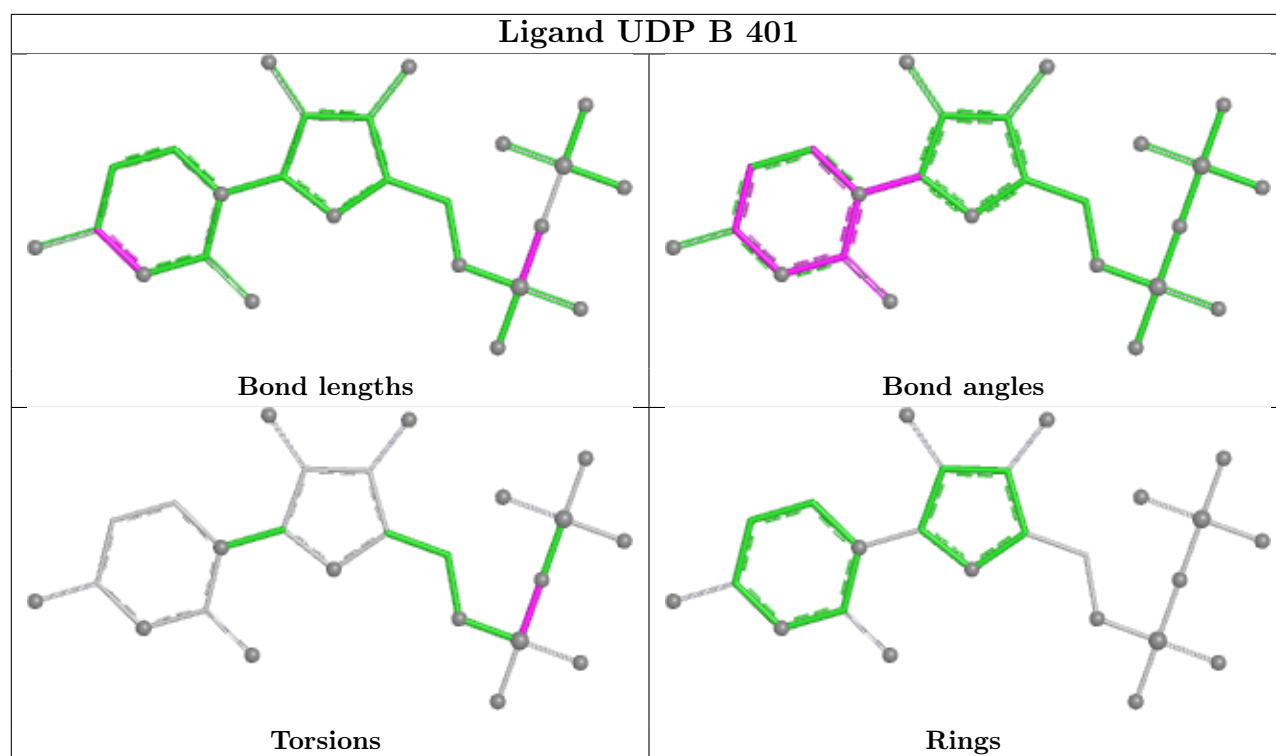
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for 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	338/344 (98%)	-0.47	2 (0%) 85 89	6, 10, 17, 28	0
1	B	338/344 (98%)	-0.50	2 (0%) 85 89	5, 9, 16, 30	0
All	All	676/688 (98%)	-0.48	4 (0%) 85 89	5, 9, 17, 30	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	338	ASP	3.5
1	B	338	ASP	3.1
1	B	70	HIS	2.5
1	A	140	PHE	2.2

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 [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
4	GOL	A	403	6/6	0.93	0.10	12,18,22,27	0

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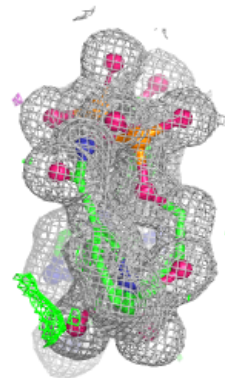
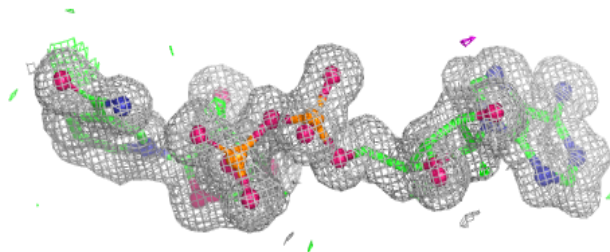
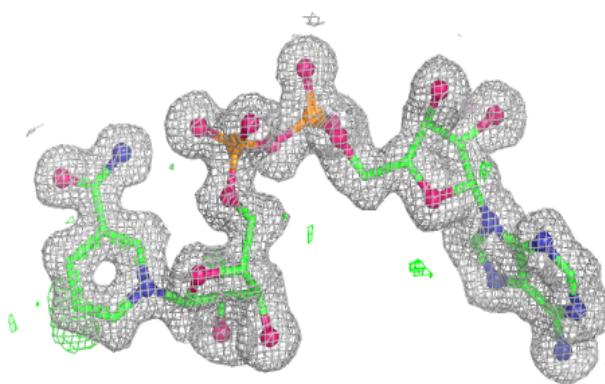
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	NO3	B	403	4/4	0.94	0.16	21,21,22,26	0
3	NAD	A	402	44/44	0.99	0.03	5,6,9,11	0
3	NAD	B	402	44/44	0.99	0.04	5,6,9,11	0
2	UDP	A	401	25/25	0.99	0.03	7,7,10,15	0
2	UDP	B	401	25/25	0.99	0.03	5,6,9,13	0

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

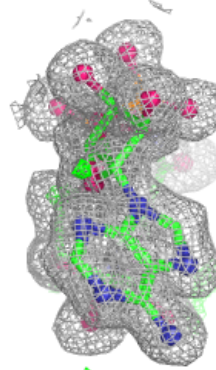
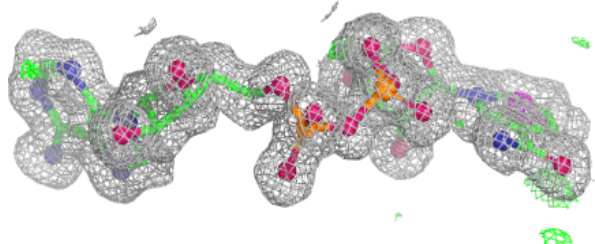
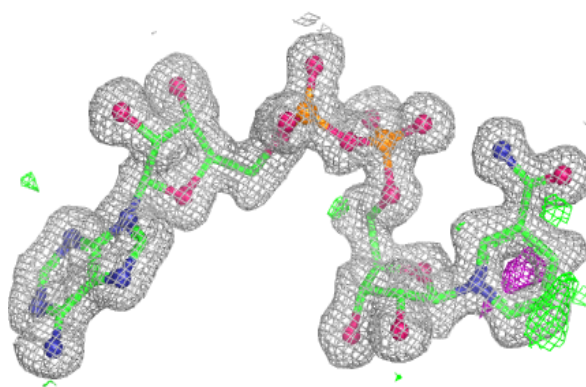
Electron density around NAD A 402:

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

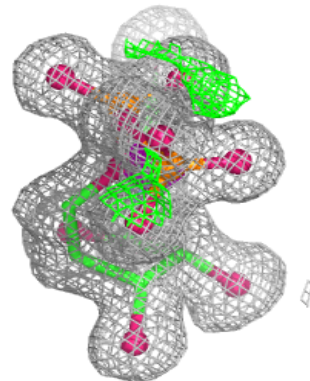
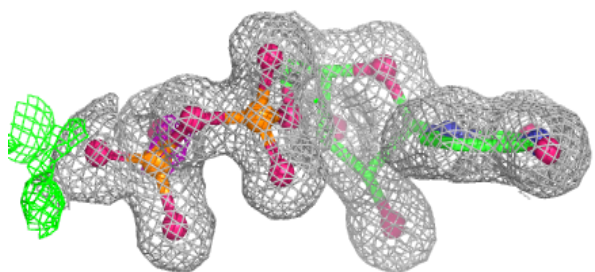
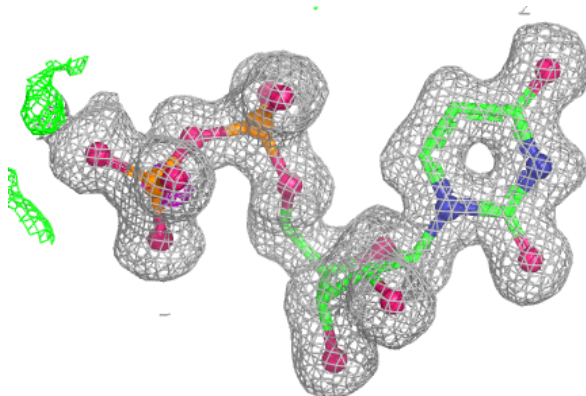


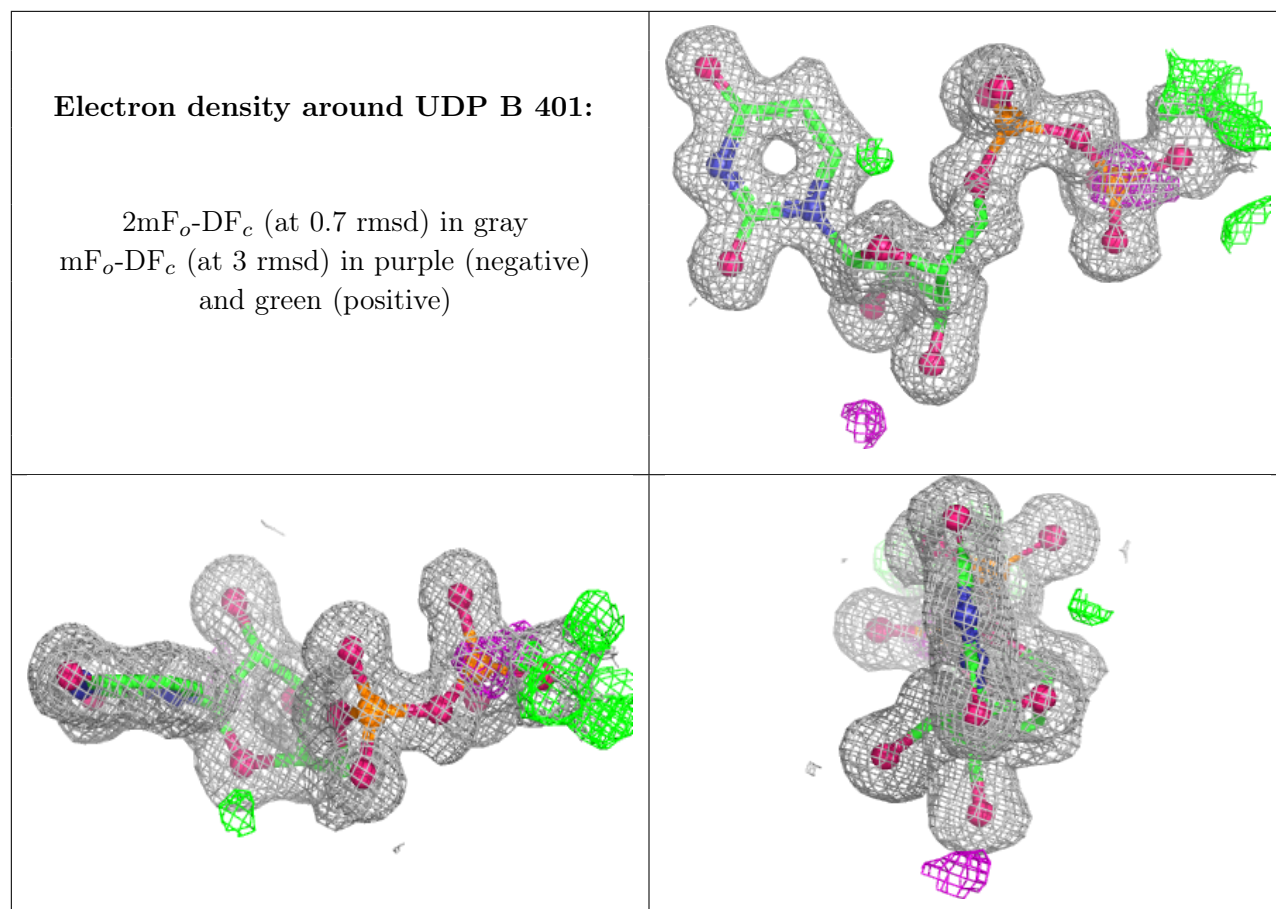
Electron density around NAD B 402:

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

**Electron density around UDP 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)





6.5 Other polymers ⓘ

There are no such residues in this entry.