



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 06:54 PM UTC

PDB ID : 6S6W / pdb_00006s6w
Title : Crystal Structure of human ALDH1A3 in complex with 2,6-diphenylimidazo[1,2-a]pyridine (compound GA11) and NAD⁺
Authors : Gelardi, E.L.M.; Quattrini, L.; LaMotta, C.; Ferraris, D.M.; Garavaglia, S.
Deposited on : 2019-07-03
Resolution : 3.25 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

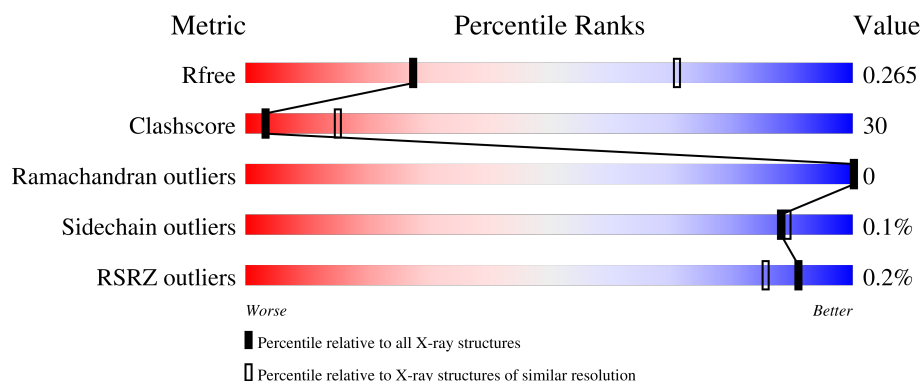
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 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	1605 (3.30-3.22)
Clashscore	190562	1660 (3.30-3.22)
Ramachandran outliers	187476	1630 (3.30-3.22)
Sidechain outliers	187428	1629 (3.30-3.22)
RSRZ outliers	180081	1605 (3.30-3.22)

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	489	 49% 48% . .
1	B	489	 50% 49% .

2 Entry composition [i](#)

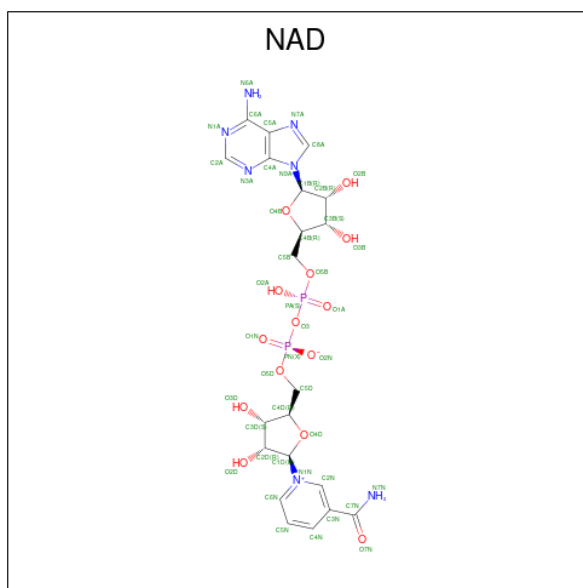
There are 5 unique types of molecules in this entry. The entry contains 7620 atoms, of which 30 are hydrogens and 0 are deuteriums.

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 Aldehyde dehydrogenase family 1 member A3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	476	Total	C	N	O	S	0	0	0
			3679	2344	628	687	20			
1	B	489	Total	C	N	O	S	0	0	0
			3779	2409	646	704	20			

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



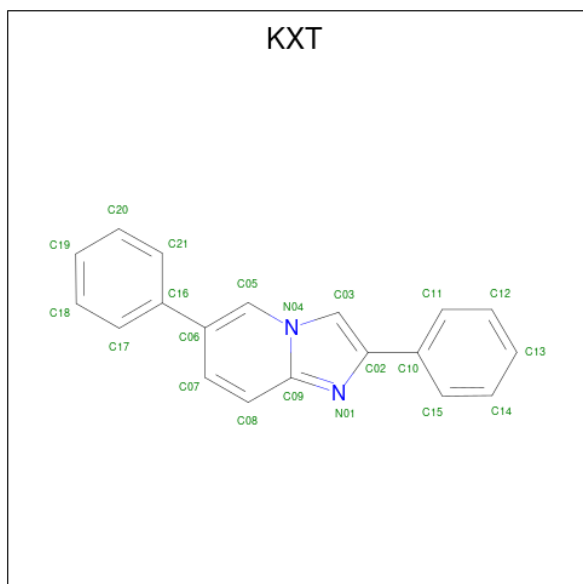
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			14	3	8	3		
3	A	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 4 is 2,6-diphenylimidazo[1,2-a]pyridine (CCD ID: KXT) (formula: $C_{19}H_{14}N_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	N	0	0
			35	19	14	2		

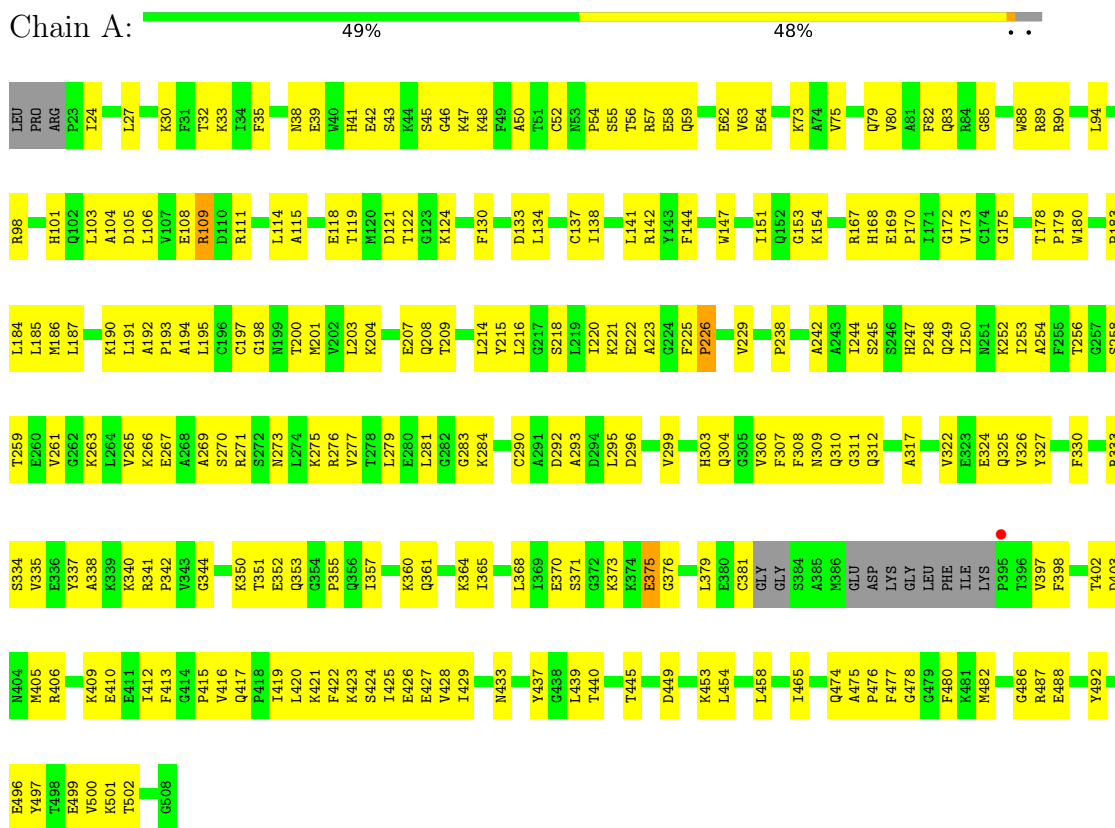
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	5	Total 5	O 5	0	0
5	B	6	Total 6	O 6	0	0

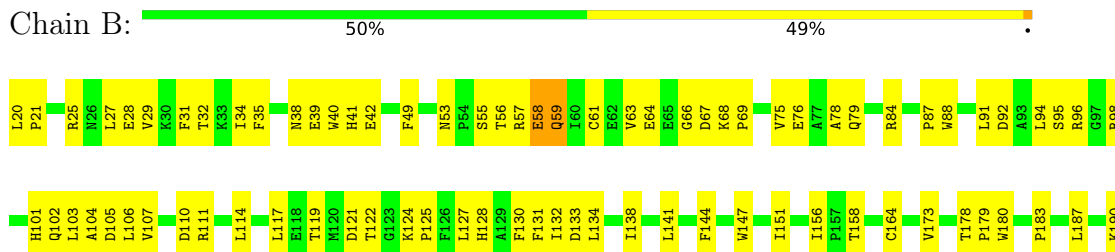
3 Residue-property plots

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: Aldehyde dehydrogenase family 1 member A3



- Molecule 1: Aldehyde dehydrogenase family 1 member A3



L191	A192	P193	L195	C196	C197	T200	M201	V202	L203	K204	E207	Q208	T209	P210	L211	L214	Y215	L216	G217	S218	L219	I220	E221	E222	F225	P226	P227	G228	V229	V233	V240	I244	S245	S246	H247	F248	Q249	I250	H251	K252	I253	A254	F255	T256	G257	S258	T259	E260	V261	V265		
K266	E267	A268	A269	S270	R271	K275	L279	E280	L281	G282	G283	K284	M285	A293	D294	L295	D296	L297	A298	V299	E300	C301	A302	H303	Q304	G305	V306	F307	F308	N309	Q310	G311	Q312	G313	C314	T315	A316	A317	S318	R319	V322	E323	E324	Q325	V326	Y327	F330	V331	V335	E336	K339	
V343	G344	D345	P346	F347	D348	V349	K350	T351	Q352	Q353	G354	P355	Q356	I357	D358	Q359	K360	Q361	F362	D363	I365	L366	E367	L368	S371	K374	E375	L379	E380	C381	G382	G383	S384	A385	M386	K394	P395	T396	S399	E400	V401	T402	D403	M404	M405	R406	I407	A408	K409	I412	F413	G414
P415	V416	Q417	P418	I419	L420	K421	F422	K423	S424	I425	I429	K430	R431	A432	T435	D436	Y437	G438	L439	A442	Y443	F444	K450	L454	A457	L458	E459	Y468	P476	F477	G478	G479	F480	K481	R487	E491	Y492	A493	L494	A495	E496	E499	T502	I505	G508							

4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	81.56Å 89.36Å 159.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.00 – 3.25 48.00 – 3.25	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.00-3.25) 99.5 (48.00-3.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 3.25Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.177 , 0.256 0.202 , 0.265	Depositor DCC
R_{free} test set	912 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	82.2	Xtriage
Anisotropy	0.432	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 65.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7620	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.10% 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: KXT, NAD, GOL

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	0.30	1/3753 (0.0%)	0.60	10/5076 (0.2%)
1	B	0.21	0/3857	0.52	5/5219 (0.1%)
All	All	0.26	1/7610 (0.0%)	0.56	15/10295 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	226	PRO	C-N	12.13	1.49	1.33

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	226	PRO	CA-C-N	12.34	132.48	119.89
1	A	226	PRO	C-N-CA	12.34	132.48	119.89
1	B	375	GLU	N-CA-C	11.53	127.45	113.16
1	A	109	ARG	N-CA-C	8.75	120.59	111.14
1	A	109	ARG	CB-CA-C	-8.73	97.10	110.90

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	3679	0	3702	238	0
1	B	3779	0	3811	239	0
2	A	44	0	23	5	0
2	B	44	0	24	2	0
3	A	12	16	16	2	0
4	A	21	14	0	0	0
5	A	5	0	0	1	0
5	B	6	0	0	0	0
All	All	7590	30	7576	462	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 30.

The worst 5 of 462 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:GLY:O	1:A:405:MET:HE1	1.56	1.05
1:A:371:SER:HB2	1:A:406:ARG:HD3	1.42	1.00
1:B:306:VAL:HG22	1:B:317:ALA:HB3	1.40	0.99
1:B:283:GLY:HA3	1:B:437:TYR:HB3	1.43	0.98
1:A:290:CYS:HB2	1:A:445:THR:HG22	1.42	0.97

There are no symmetry-related clashes.

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	470/489 (96%)	427 (91%)	43 (9%)	0	100	100
1	B	487/489 (100%)	441 (91%)	46 (9%)	0	100	100
All	All	957/978 (98%)	868 (91%)	89 (9%)	0	100	100

There are no Ramachandran outliers to report.

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	395/405 (98%)	395 (100%)	0	100	100
1	B	405/405 (100%)	404 (100%)	1 (0%)	87	87
All	All	800/810 (99%)	799 (100%)	1 (0%)	88	89

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

Mol	Chain	Res	Type
1	B	76	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	HIS
1	A	251	ASN
1	B	251	ASN
1	B	310	GLN
1	B	353	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

5 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	GOL	A	602	-	5,5,5	1.19	0	5,5,5	1.52	1 (20%)
3	GOL	A	604	-	5,5,5	0.93	0	5,5,5	1.13	1 (20%)
2	NAD	A	601	1	46,48,48	4.06	20 (43%)	64,73,73	1.82	13 (20%)
2	NAD	B	601	-	46,48,48	4.06	20 (43%)	64,73,73	2.02	12 (18%)
4	KXT	A	603	-	24,24,24	2.04	4 (16%)	32,33,33	1.79	5 (15%)

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	GOL	A	602	-	-	0/4/4/4	-
3	GOL	A	604	-	-	0/4/4/4	-
2	NAD	A	601	1	-	3/30/62/62	0/5/5/5
2	NAD	B	601	-	-	7/30/62/62	0/5/5/5
4	KXT	A	603	-	-	8/8/8/8	0/4/4/4

The worst 5 of 44 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	NAD	O4D-C1D	16.61	1.62	1.40
2	B	601	NAD	O4D-C1D	16.19	1.62	1.40
2	B	601	NAD	O4B-C1B	8.53	1.61	1.42
2	A	601	NAD	O4B-C1B	8.52	1.61	1.42
2	B	601	NAD	C2B-C1B	-7.69	1.29	1.53

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	NAD	C4D-O4D-C1D	-8.99	101.69	109.92
4	A	603	KXT	C02-N01-C09	5.53	108.20	105.64
2	A	601	NAD	N3A-C2A-N1A	-5.40	120.41	128.58
2	B	601	NAD	N3A-C2A-N1A	-5.39	120.42	128.58
2	B	601	NAD	C5A-C4A-N3A	-4.86	120.02	126.72

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

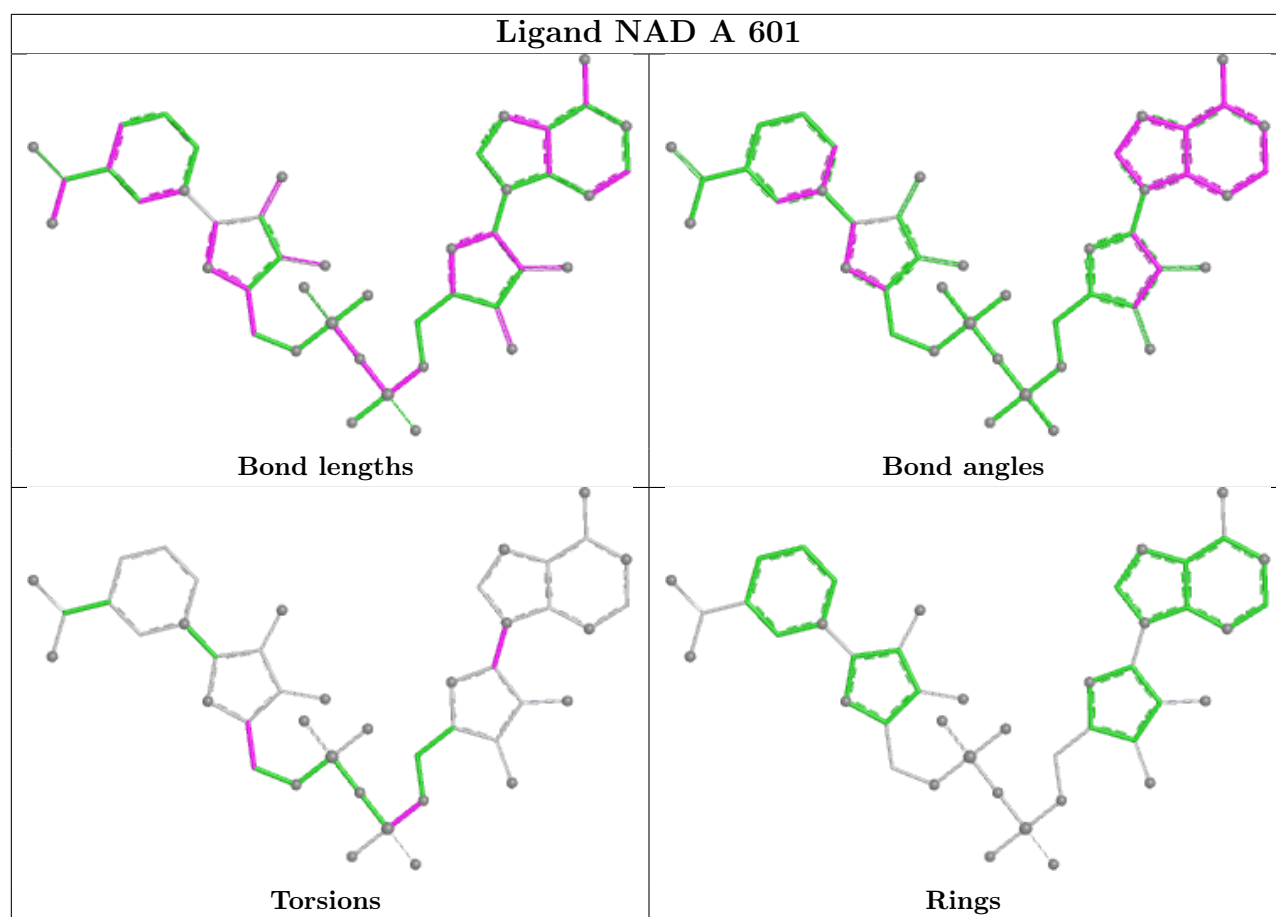
Mol	Chain	Res	Type	Atoms
2	B	601	NAD	PA-O3-PN-O5D
2	B	601	NAD	O4D-C1D-N1N-C6N
4	A	603	KXT	C03-C02-C10-C11
4	A	603	KXT	C03-C02-C10-C15
4	A	603	KXT	N01-C02-C10-C11

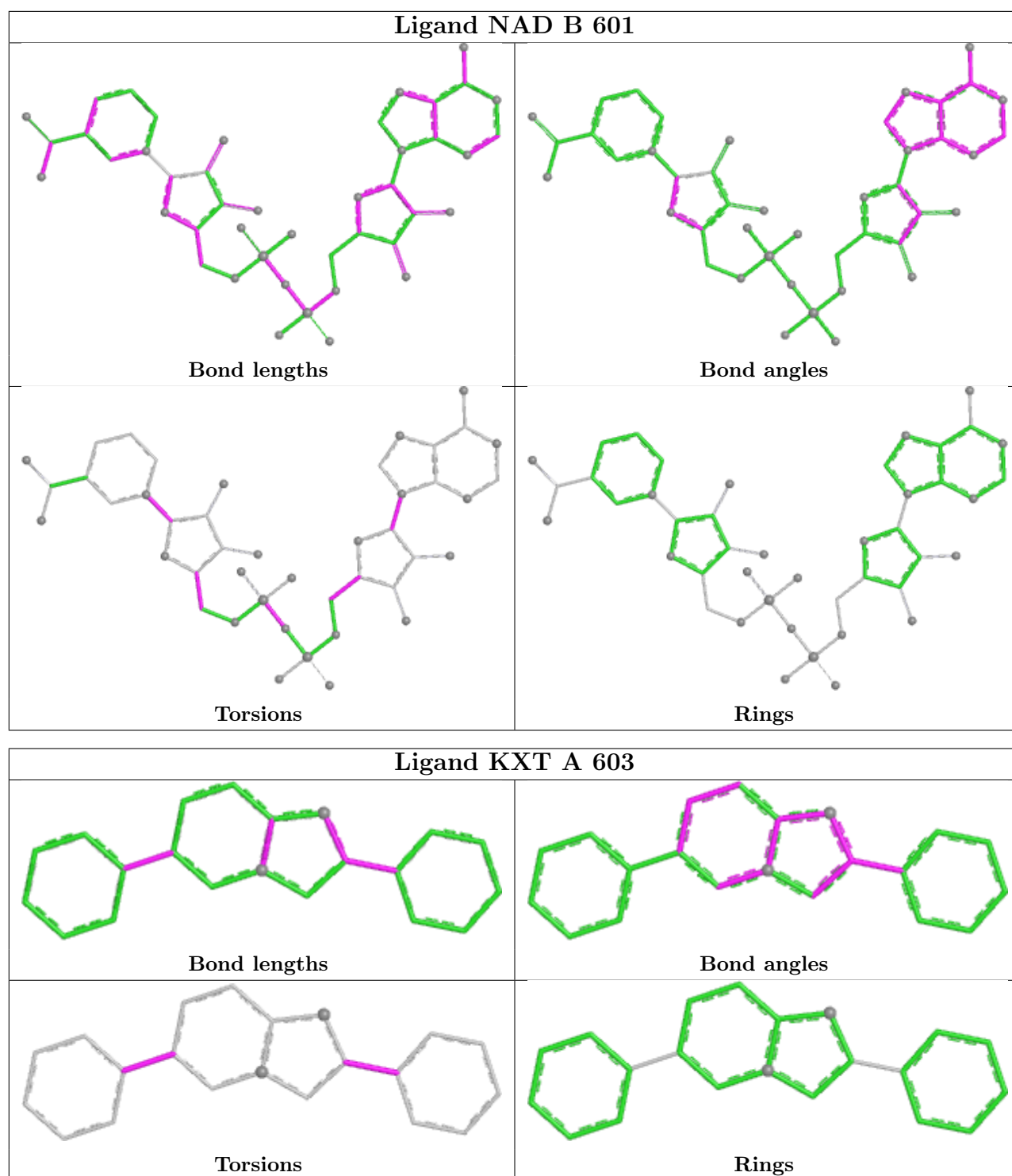
There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	604	GOL	2	0
2	A	601	NAD	5	0
2	B	601	NAD	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.





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 [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	476/489 (97%)	-0.12	1 (0%) 91 85	43, 69, 131, 153	0
1	B	489/489 (100%)	-0.22	1 (0%) 91 85	39, 70, 116, 144	0
All	All	965/978 (98%)	-0.17	2 (0%) 91 85	39, 70, 125, 153	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	395	PRO	2.4
1	B	211	LEU	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 [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.

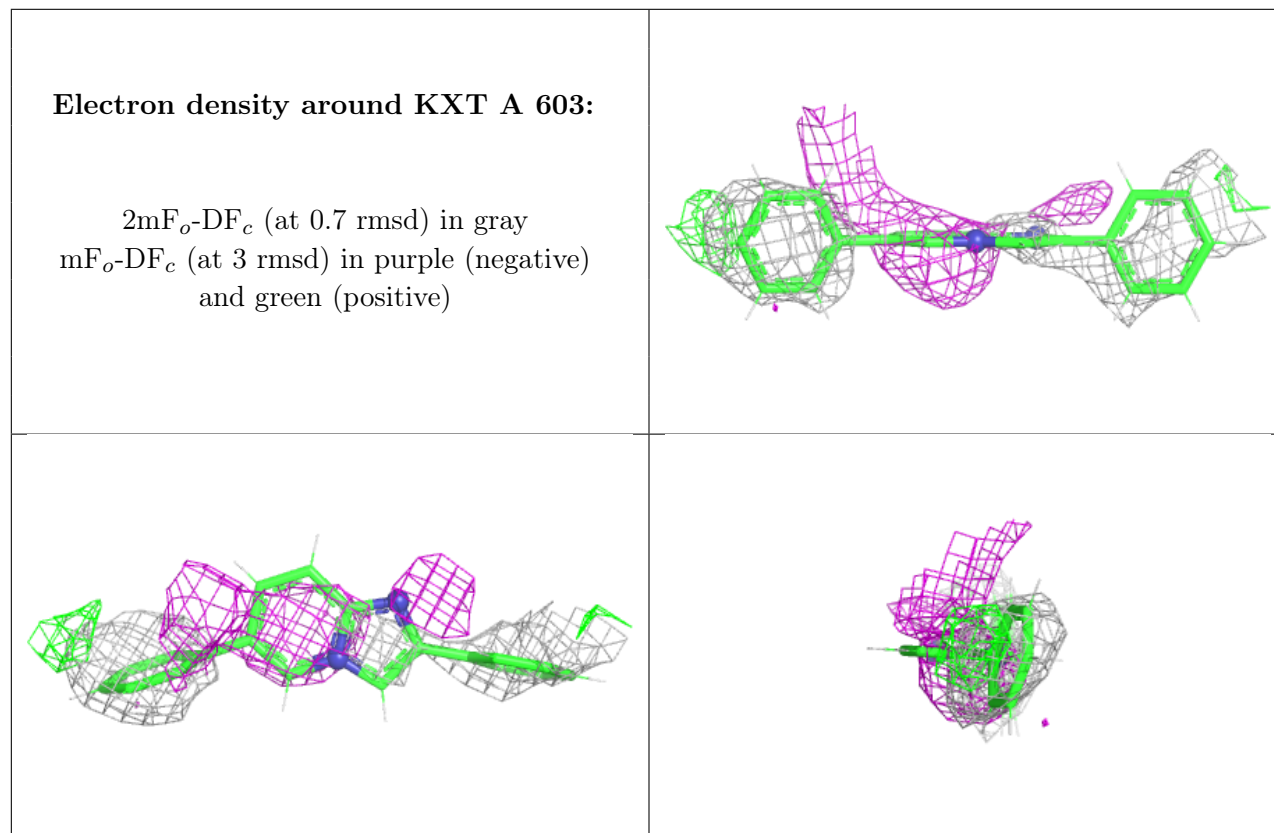
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	KXT	A	603	21/21	0.61	0.19	79,122,154,160	0
3	GOL	A	604	6/6	0.84	0.12	61,80,97,97	0
2	NAD	A	601	44/44	0.88	0.11	50,76,133,136	0

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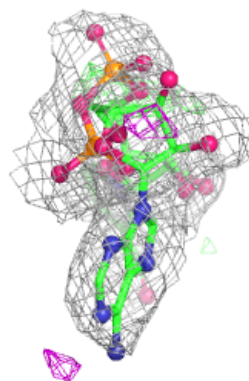
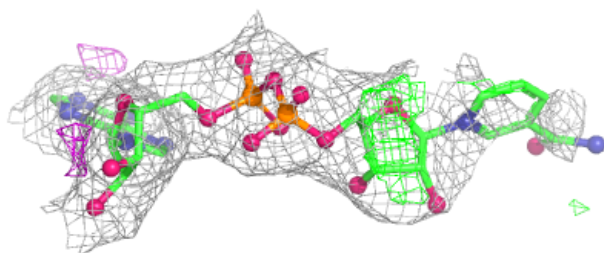
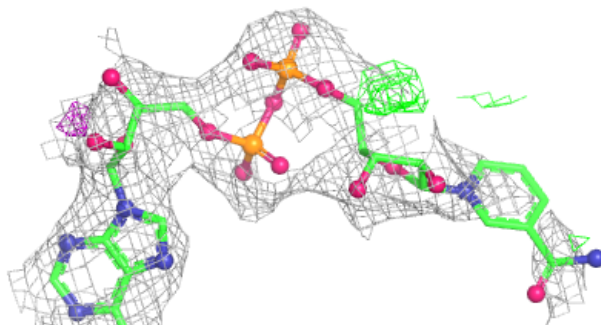
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAD	B	601	44/44	0.88	0.10	64,83,142,143	0
3	GOL	A	602	6/6	0.89	0.14	62,81,100,100	0

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.

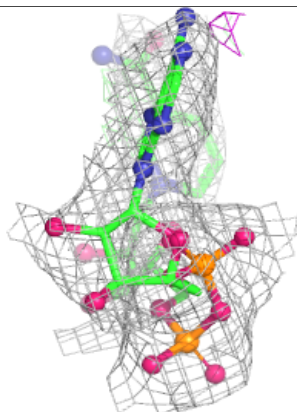
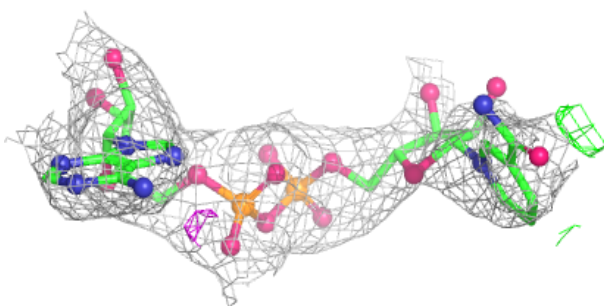
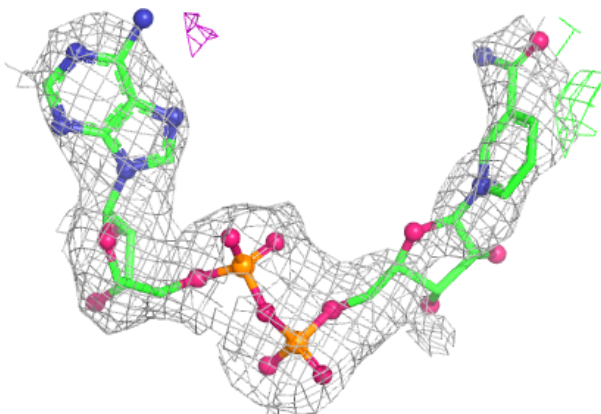


Electron density around NAD A 601:

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

**Electron density around NAD B 601:**

$2mF_o-DF_c$ (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.