



Full wwPDB X-ray Structure Validation Report ⓘ

May 31, 2022 – 04:35 PM EDT

PDB ID : 7MJD
Title : Crystal Structure Analysis of ALDH1B1
Authors : Fernandez, D.; Chen, J.K.
Deposited on : 2021-04-20
Resolution : 2.12 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 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 : 2.28.1
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) : 2.28.1

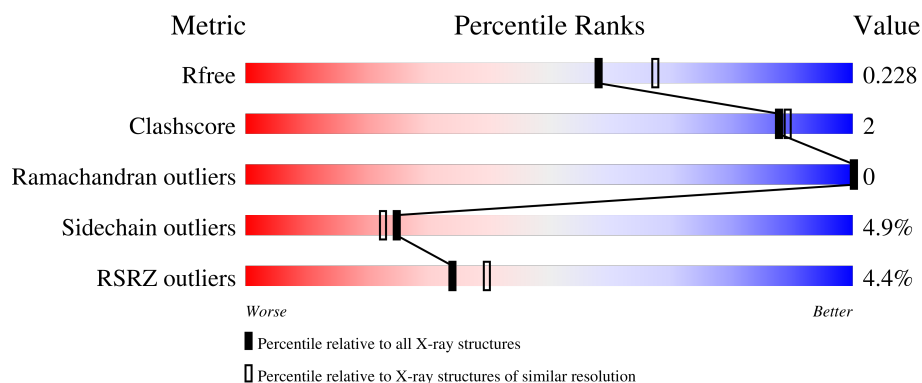
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.12 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}	130704	6241 (2.14-2.10)
Clashscore	141614	6778 (2.14-2.10)
Ramachandran outliers	138981	6705 (2.14-2.10)
Sidechain outliers	138945	6706 (2.14-2.10)
RSRZ outliers	127900	6112 (2.14-2.10)

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	498	<div> <div>3%</div> <div>92%</div> <div>6% ..</div> </div>
1	B	498	<div> <div>6%</div> <div>89%</div> <div>9% ..</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
5	1PE	A	607	-	-	-	X
5	1PE	A	610	-	-	-	X
5	1PE	A	611	-	-	-	X
5	1PE	B	607	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8130 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 Aldehyde dehydrogenase X, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	493	Total	C	N	O	S	0	0	0
			3852	2449	667	719	17			
1	B	493	Total	C	N	O	S	0	0	0
			3852	2449	667	719	17			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	90	ARG	LEU	variant	UNP P30837
A	236	MET	VAL	variant	UNP P30837
B	90	ARG	LEU	variant	UNP P30837
B	236	MET	VAL	variant	UNP P30837

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

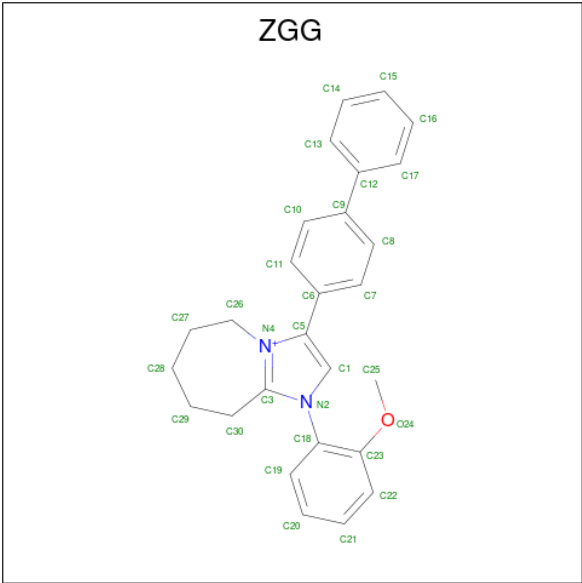
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Na	0	0
			1	1		
2	B	1	Total	Na	0	0
			1	1		

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



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

- Molecule 4 is 8-(2-methoxyphenyl)-10-(4-phenylphenyl)-1 λ^4 ,8-diazabicyclo[5.3.0]deca-1(7),9-diene (three-letter code: ZGG) (formula: C₂₇H₂₇N₂O) (labeled as "Ligand of Interest" by depositor).



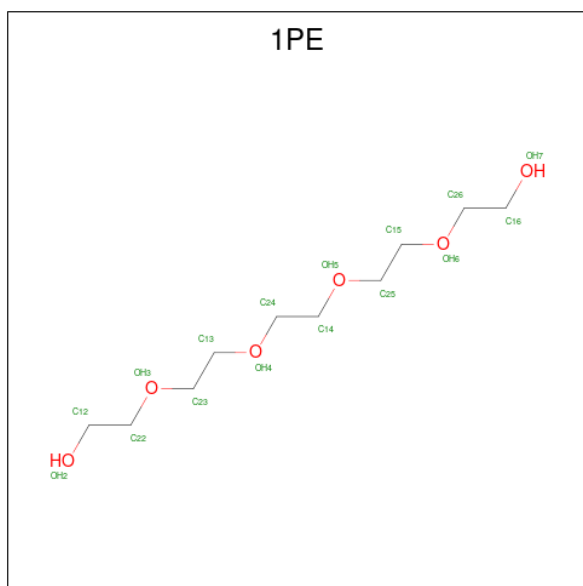
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			30	27	2	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			30	27	2	1		

- Molecule 5 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 7 4 3	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

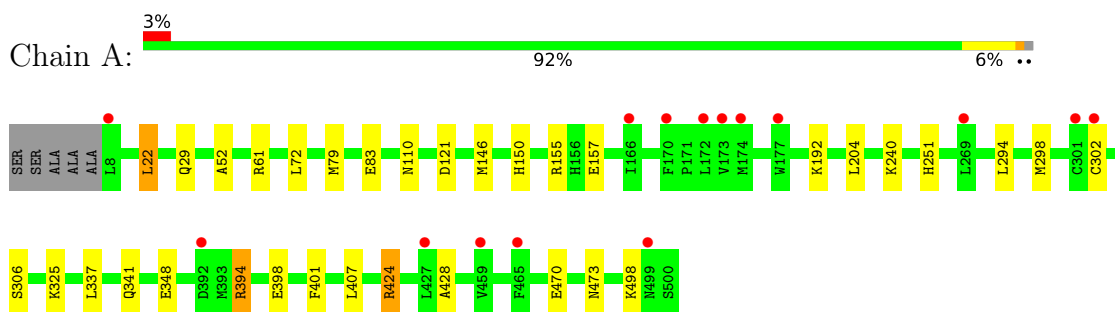
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	111	Total 111	O 111	0	0
7	B	75	Total 75	O 75	0	0

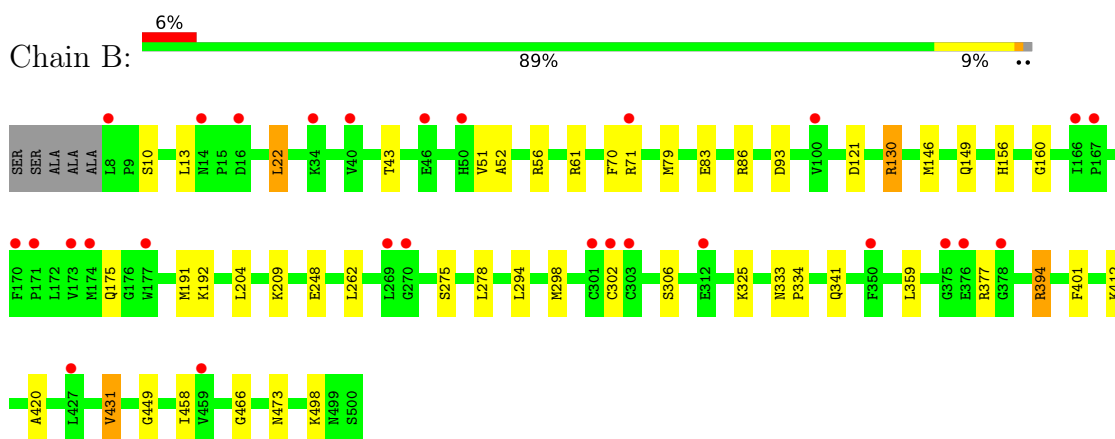
3 Residue-property plots

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 X, mitochondrial



- Molecule 1: Aldehyde dehydrogenase X, mitochondrial



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	102.04Å 102.04Å 186.04Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.37 – 2.12 35.98 – 2.12	Depositor EDS
% Data completeness (in resolution range)	99.7 (30.37-2.12) 99.8 (35.98-2.12)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 2.12Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.180 , 0.219 0.188 , 0.228	Depositor DCC
R_{free} test set	3300 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å ²)	43.3	Xtriage
Anisotropy	0.313	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 45.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.024 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8130	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 1PE, GOL, NAD, ZGG, NA

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	0.57	0/3939	0.72	1/5333 (0.0%)
1	B	0.53	0/3939	0.73	3/5333 (0.1%)
All	All	0.55	0/7878	0.73	4/10666 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	394	ARG	NE-CZ-NH1	6.69	123.64	120.30
1	B	394	ARG	NE-CZ-NH2	-6.10	117.25	120.30
1	B	130	ARG	NE-CZ-NH2	5.70	123.15	120.30
1	B	431	VAL	CB-CA-C	-5.63	100.69	111.40

There are no chirality outliers.

There are no planarity outliers.

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	3852	0	3804	14	0
1	B	3852	0	3803	20	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	44	0	26	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	44	0	26	2	0
4	A	30	0	0	0	0
4	B	30	0	0	0	0
5	A	47	0	58	2	0
5	B	31	0	38	4	0
6	B	12	0	16	1	0
7	A	111	0	0	0	0
7	B	75	0	0	1	0
All	All	8130	0	7771	32	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 2.

All (32) 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:302:CYS:SG	3:A:602:NAD:C4N	2.81	0.69
1:B:93:ASP:OD1	1:B:130:ARG:NH1	2.26	0.68
1:B:302:CYS:SG	3:B:602:NAD:C4N	2.85	0.65
1:A:155:ARG:NH1	1:A:157:GLU:OE2	2.34	0.60
1:A:394:ARG:HD2	1:A:398:GLU:OE1	2.05	0.57
1:A:302:CYS:SG	3:A:602:NAD:C3N	2.94	0.55
1:B:298:MET:HG3	1:B:341:GLN:HG3	1.91	0.53
1:A:22:LEU:HD13	1:A:52:ALA:HB3	1.90	0.52
1:A:294:LEU:HD23	1:A:306:SER:HA	1.91	0.52
1:A:146:MET:CE	1:B:458:ILE:HG22	2.41	0.51
1:B:394:ARG:HH22	5:B:607:1PE:C25	2.25	0.50
1:A:298:MET:HG3	1:A:341:GLN:HG3	1.93	0.49
1:B:156:HIS:H	5:B:608:1PE:H251	1.79	0.48
1:B:302:CYS:SG	3:B:602:NAD:C3N	3.03	0.47
1:B:394:ARG:HH22	5:B:607:1PE:H252	1.78	0.47
1:B:130:ARG:O	5:B:612:1PE:OH7	2.26	0.47
1:A:79:MET:HG2	1:A:83:GLU:HB3	1.97	0.46
1:A:428:ALA:O	5:A:606:1PE:H251	2.17	0.45
1:B:43:THR:HG21	1:B:334:PRO:CD	2.46	0.44
1:B:420:ALA:O	6:B:605:GOL:H2	2.17	0.44
1:B:22:LEU:HD13	1:B:52:ALA:HB3	1.99	0.43
1:A:251:HIS:HA	1:B:262:LEU:HD21	2.01	0.42
1:B:70:PHE:CZ	1:B:160:GLY:HA2	2.55	0.42
1:B:146:MET:HE3	1:B:146:MET:HB2	1.93	0.42
1:A:348:GLU:OE2	5:A:607:1PE:H261	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:HIS:HE1	7:B:706:HOH:O	2.03	0.42
1:B:449:GLY:HA3	1:B:466:GLY:O	2.19	0.42
1:B:175:GLN:HG3	1:B:191:MET:SD	2.61	0.41
1:A:424:ARG:NH1	1:A:470:GLU:OE1	2.54	0.41
1:B:294:LEU:HD23	1:B:306:SER:HA	2.03	0.40
1:B:83:GLU:OE1	1:B:86:ARG:NH1	2.54	0.40
1:B:79:MET:HG3	1:B:83:GLU:HG2	2.02	0.40

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	491/498 (99%)	476 (97%)	15 (3%)	0	100	100
1	B	491/498 (99%)	476 (97%)	15 (3%)	0	100	100
All	All	982/996 (99%)	952 (97%)	30 (3%)	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	405/407 (100%)	389 (96%)	16 (4%)	31	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	405/407 (100%)	381 (94%)	24 (6%)	19	16
All	All	810/814 (100%)	770 (95%)	40 (5%)	25	22

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	LEU
1	A	29	GLN
1	A	61	ARG
1	A	72	LEU
1	A	110	ASN
1	A	121	ASP
1	A	192	LYS
1	A	204	LEU
1	A	240	LYS
1	A	325	LYS
1	A	337	LEU
1	A	401	PHE
1	A	407	LEU
1	A	424	ARG
1	A	473	ASN
1	A	498	LYS
1	B	10	SER
1	B	13	LEU
1	B	22	LEU
1	B	51	VAL
1	B	56	ARG
1	B	61	ARG
1	B	71	ARG
1	B	121	ASP
1	B	149	GLN
1	B	192	LYS
1	B	204	LEU
1	B	209	LYS
1	B	248	GLU
1	B	275	SER
1	B	278	LEU
1	B	325	LYS
1	B	333	ASN
1	B	359	LEU
1	B	377	ARG
1	B	401	PHE

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Mol	Chain	Res	Type
1	B	412	LYS
1	B	431	VAL
1	B	473	ASN
1	B	498	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	GLN
1	A	150	HIS
1	A	251	HIS
1	B	26	ASN
1	B	29	GLN
1	B	251	HIS
1	B	285	HIS
1	B	333	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 26 ligands modelled in this entry, 2 are monoatomic - leaving 24 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
5	1PE	B	608	-	3,3,15	0.41	0	2,2,14	0.73	0
5	1PE	A	606	-	6,6,15	0.58	0	5,5,14	0.97	0
5	1PE	A	608	-	3,3,15	0.44	0	2,2,14	0.76	0
5	1PE	B	607	-	6,6,15	0.47	0	5,5,14	0.66	0
4	ZGG	B	603	-	30,34,34	1.82	2 (6%)	37,47,47	2.25	8 (21%)
5	1PE	B	612	-	3,3,15	0.42	0	2,2,14	0.67	0
5	1PE	A	607	-	3,3,15	0.50	0	2,2,14	0.28	0
5	1PE	B	609	-	3,3,15	0.45	0	2,2,14	0.41	0
6	GOL	B	605	-	5,5,5	0.78	0	5,5,5	0.86	0
3	NAD	B	602	-	42,48,48	0.96	3 (7%)	50,73,73	1.25	5 (10%)
5	1PE	A	610	-	3,3,15	0.51	0	2,2,14	0.12	0
5	1PE	A	609	-	3,3,15	0.40	0	2,2,14	0.65	0
5	1PE	A	612	-	3,3,15	0.41	0	2,2,14	0.83	0
5	1PE	A	604	-	3,3,15	0.50	0	2,2,14	0.20	0
5	1PE	A	614	-	3,3,15	0.53	0	2,2,14	0.89	0
5	1PE	B	606	-	3,3,15	0.63	0	2,2,14	0.16	0
6	GOL	B	604	-	5,5,5	0.39	0	5,5,5	0.33	0
3	NAD	A	602	-	42,48,48	0.94	3 (7%)	50,73,73	1.21	4 (8%)
4	ZGG	A	603	-	30,34,34	1.76	2 (6%)	37,47,47	1.74	6 (16%)
5	1PE	B	611	-	3,3,15	0.26	0	2,2,14	0.99	0
5	1PE	B	610	-	3,3,15	0.37	0	2,2,14	0.94	0
5	1PE	A	611	-	3,3,15	0.60	0	2,2,14	0.26	0
5	1PE	A	605	-	3,3,15	0.32	0	2,2,14	0.52	0
5	1PE	A	613	-	3,3,15	0.30	0	2,2,14	1.19	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
5	1PE	B	608	-	-	1/1/1/13	-
5	1PE	A	606	-	-	3/4/4/13	-
5	1PE	A	608	-	-	1/1/1/13	-
5	1PE	B	607	-	-	3/4/4/13	-
4	ZGG	B	603	-	-	4/14/22/22	0/4/5/5
5	1PE	B	612	-	-	1/1/1/13	-
5	1PE	A	607	-	-	1/1/1/13	-
5	1PE	B	609	-	-	0/1/1/13	-
6	GOL	B	605	-	-	4/4/4/4	-
3	NAD	B	602	-	-	2/26/62/62	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	1PE	A	610	-	-	1/1/1/13	-
5	1PE	A	609	-	-	1/1/1/13	-
5	1PE	A	612	-	-	1/1/1/13	-
5	1PE	A	604	-	-	1/1/1/13	-
5	1PE	A	614	-	-	0/1/1/13	-
5	1PE	B	606	-	-	1/1/1/13	-
6	GOL	B	604	-	-	0/4/4/4	-
3	NAD	A	602	-	-	3/26/62/62	0/5/5/5
4	ZGG	A	603	-	-	4/14/22/22	0/4/5/5
5	1PE	B	611	-	-	0/1/1/13	-
5	1PE	B	610	-	-	0/1/1/13	-
5	1PE	A	611	-	-	0/1/1/13	-
5	1PE	A	605	-	-	1/1/1/13	-
5	1PE	A	613	-	-	0/1/1/13	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	603	ZGG	C6-C5	-6.58	1.36	1.48
4	B	603	ZGG	C6-C5	-6.55	1.36	1.48
4	B	603	ZGG	C26-N4	6.37	1.53	1.49
4	A	603	ZGG	C26-N4	6.07	1.53	1.49
3	B	602	NAD	C5A-C4A	2.41	1.47	1.40
3	A	602	NAD	PN-O1N	2.33	1.59	1.50
3	A	602	NAD	C5A-C4A	2.32	1.47	1.40
3	B	602	NAD	O4B-C1B	2.30	1.44	1.41
3	B	602	NAD	PN-O1N	2.10	1.58	1.50
3	A	602	NAD	O4B-C1B	2.08	1.44	1.41

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	603	ZGG	C25-O24-C23	7.70	129.16	117.53
4	B	603	ZGG	C27-C26-N4	7.65	117.18	111.18
4	A	603	ZGG	C25-O24-C23	7.49	128.83	117.53
3	B	602	NAD	N3A-C2A-N1A	-4.45	121.72	128.68
3	A	602	NAD	N3A-C2A-N1A	-3.83	122.69	128.68
4	B	603	ZGG	C1-C5-C6	-3.65	124.07	128.47
4	A	603	ZGG	C1-C5-C6	-3.65	124.07	128.47
3	A	602	NAD	O4D-C1D-C2D	-3.59	101.69	106.93
4	B	603	ZGG	C28-C29-C30	3.55	119.94	114.23
4	A	603	ZGG	C27-C26-N4	2.86	113.42	111.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	602	NAD	C1B-N9A-C4A	-2.75	121.80	126.64
3	A	602	NAD	C1B-N9A-C4A	-2.70	121.89	126.64
4	B	603	ZGG	C10-C11-C6	2.59	124.86	121.13
3	B	602	NAD	C4A-C5A-N7A	-2.51	106.78	109.40
3	A	602	NAD	C4A-C5A-N7A	-2.45	106.84	109.40
3	B	602	NAD	O4D-C1D-C2D	-2.44	103.36	106.93
4	B	603	ZGG	N2-C3-N4	2.43	108.80	106.52
4	A	603	ZGG	C30-C3-N4	2.39	128.00	123.13
3	B	602	NAD	O5B-PA-O1A	2.32	118.12	109.07
4	A	603	ZGG	C7-C6-C5	2.29	124.82	120.74
4	B	603	ZGG	C7-C6-C11	-2.22	113.16	117.59
4	B	603	ZGG	O24-C23-C18	-2.19	116.16	118.47
4	A	603	ZGG	C29-C30-C3	2.15	116.25	113.96

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	605	GOL	C1-C2-C3-O3
5	B	607	1PE	OH7-C16-C26-OH6
5	B	607	1PE	OH6-C15-C25-OH5
6	B	605	GOL	O1-C1-C2-C3
6	B	605	GOL	O1-C1-C2-O2
6	B	605	GOL	O2-C2-C3-O3
5	A	608	1PE	OH7-C16-C26-OH6
5	B	612	1PE	OH7-C16-C26-OH6
5	A	606	1PE	OH7-C16-C26-OH6
5	A	604	1PE	OH7-C16-C26-OH6
5	B	606	1PE	OH7-C16-C26-OH6
4	A	603	ZGG	C1-C5-C6-C7
4	B	603	ZGG	C1-C5-C6-C7
5	A	605	1PE	OH6-C15-C25-OH5
5	A	612	1PE	OH7-C16-C26-OH6
5	B	608	1PE	OH6-C15-C25-OH5
3	A	602	NAD	PN-O3-PA-O5B
3	B	602	NAD	PN-O3-PA-O5B
3	A	602	NAD	C4D-C5D-O5D-PN
3	B	602	NAD	C4D-C5D-O5D-PN
5	A	607	1PE	OH7-C16-C26-OH6
5	B	607	1PE	C16-C26-OH6-C15
5	A	606	1PE	C16-C26-OH6-C15
5	A	606	1PE	OH6-C15-C25-OH5

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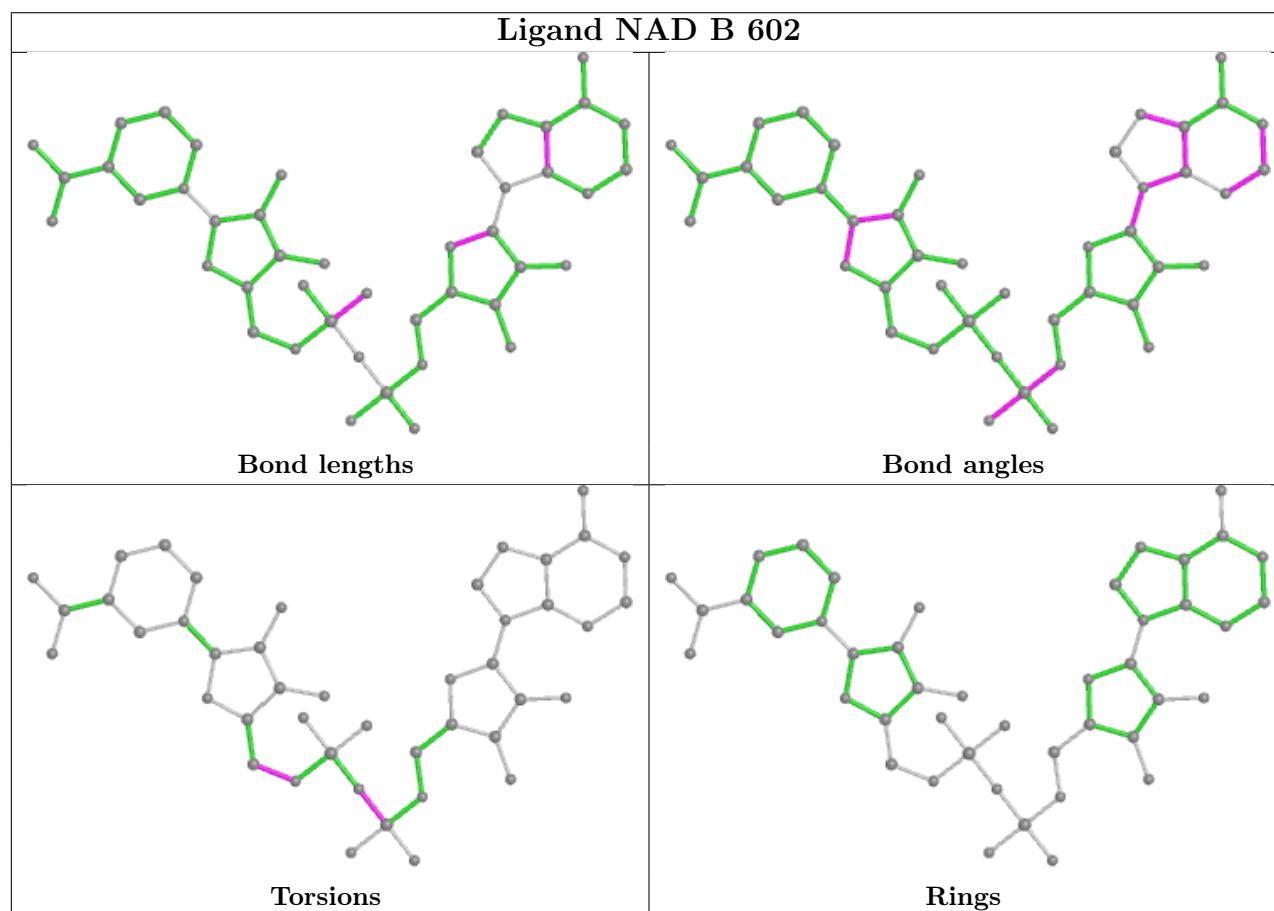
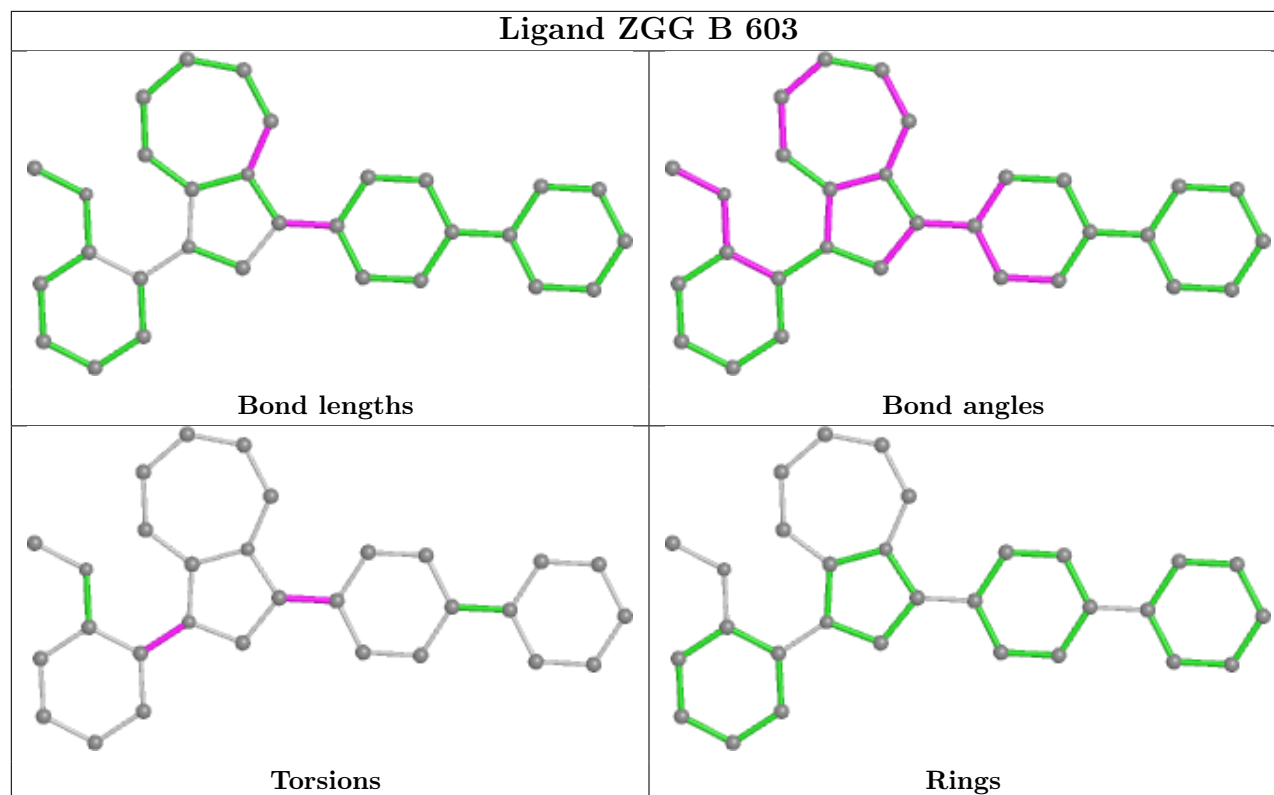
Mol	Chain	Res	Type	Atoms
5	A	610	1PE	OH7-C16-C26-OH6
4	A	603	ZGG	C1-C5-C6-C11
4	B	603	ZGG	C1-C5-C6-C11
4	A	603	ZGG	C23-C18-N2-C3
4	B	603	ZGG	C23-C18-N2-C3
4	A	603	ZGG	C23-C18-N2-C1
4	B	603	ZGG	C23-C18-N2-C1
3	A	602	NAD	C5B-O5B-PA-O1A
5	A	609	1PE	OH7-C16-C26-OH6

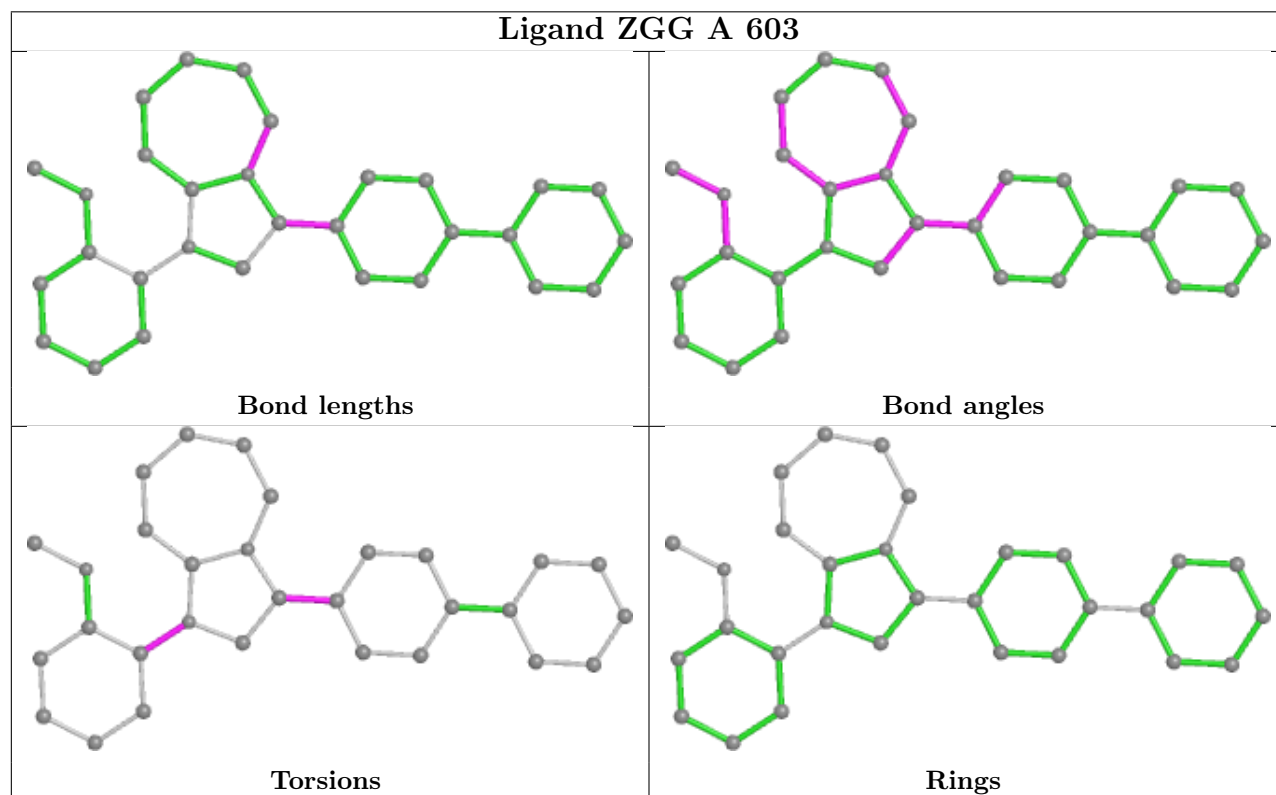
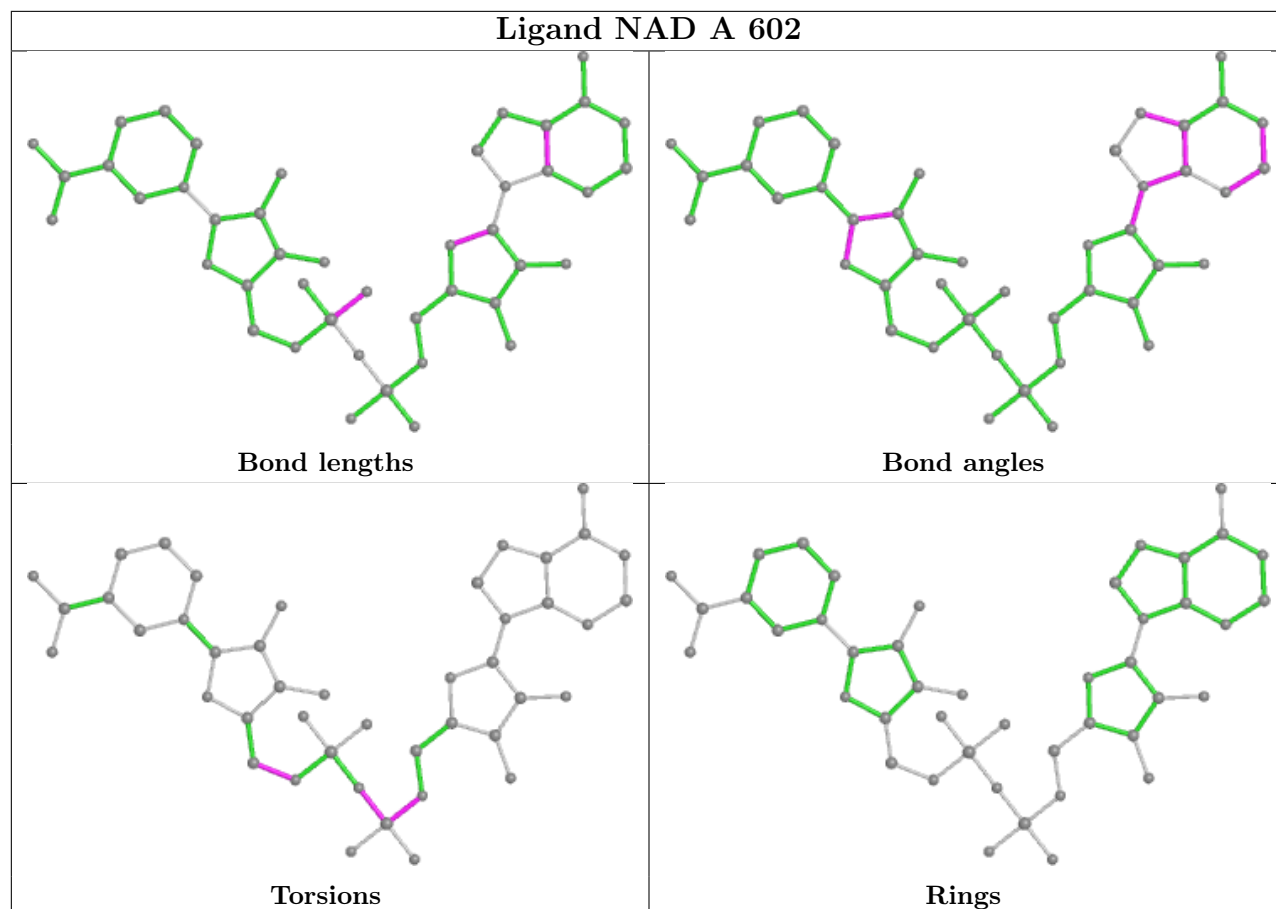
There are no ring outliers.

8 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	608	1PE	1	0
5	A	606	1PE	1	0
5	B	607	1PE	2	0
5	B	612	1PE	1	0
5	A	607	1PE	1	0
6	B	605	GOL	1	0
3	B	602	NAD	2	0
3	A	602	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 [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

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	493/498 (98%)	-0.01	15 (3%) 50 56	32, 44, 63, 78	0
1	B	493/498 (98%)	0.11	28 (5%) 23 28	33, 49, 69, 88	0
All	All	986/996 (98%)	0.05	43 (4%) 34 40	32, 46, 67, 88	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	170	PHE	4.0
1	A	170	PHE	3.9
1	A	166	ILE	3.8
1	B	174	MET	3.6
1	A	301	CYS	3.5
1	A	427	LEU	3.4
1	A	173	VAL	3.4
1	B	376	GLU	3.3
1	A	8	LEU	3.3
1	B	173	VAL	3.2
1	A	459	VAL	3.0
1	B	177	TRP	2.9
1	A	174	MET	2.9
1	A	392	ASP	2.8
1	A	177	TRP	2.7
1	B	14	ASN	2.7
1	B	427	LEU	2.7
1	B	40	VAL	2.6
1	B	50	HIS	2.6
1	B	100	VAL	2.6
1	B	171	PRO	2.6
1	B	459	VAL	2.5
1	B	34	LYS	2.5
1	A	499	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	172	LEU	2.5
1	A	269	LEU	2.4
1	A	302	CYS	2.4
1	B	303	CYS	2.4
1	B	301	CYS	2.4
1	B	166	ILE	2.4
1	B	16	ASP	2.4
1	A	465	PHE	2.3
1	B	167	PRO	2.2
1	B	270	GLY	2.2
1	B	71	ARG	2.2
1	B	302	CYS	2.1
1	B	46	GLU	2.1
1	B	8	LEU	2.1
1	B	269	LEU	2.1
1	B	350	PHE	2.1
1	B	375	GLY	2.1
1	B	312	GLU	2.0
1	B	378	GLY	2.0

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 monosaccharides 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(\AA^2)	Q<0.9
5	1PE	A	607	4/16	0.61	0.81	39,40,41,41	4
5	1PE	B	607	7/16	0.73	0.54	43,49,52,54	7
5	1PE	A	610	4/16	0.74	0.57	29,32,33,34	4
6	GOL	B	604	6/6	0.76	0.20	62,72,75,77	0

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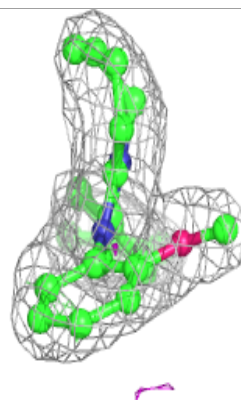
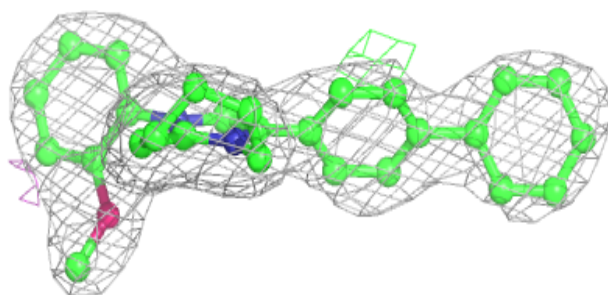
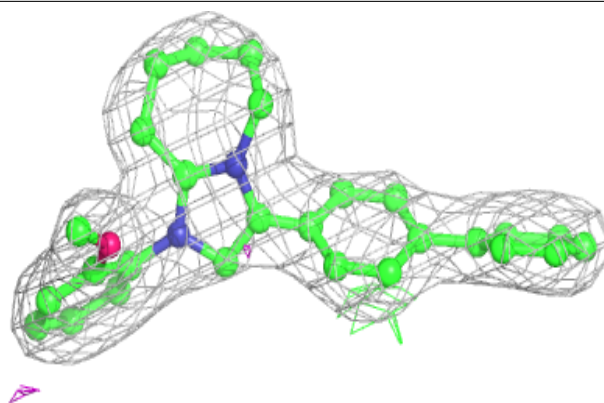
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	1PE	A	611	4/16	0.77	0.83	40,40,41,46	4
5	1PE	A	614	4/16	0.80	0.36	25,25,26,28	4
4	ZGG	A	603	30/30	0.80	0.20	55,59,62,63	0
5	1PE	A	613	4/16	0.80	0.46	35,36,36,40	4
5	1PE	A	606	7/16	0.83	0.56	23,30,30,34	7
5	1PE	B	611	4/16	0.84	0.43	26,26,26,28	4
5	1PE	B	610	4/16	0.85	0.24	35,36,37,38	4
5	1PE	A	604	4/16	0.85	0.90	43,47,49,50	4
4	ZGG	B	603	30/30	0.85	0.17	54,64,73,74	0
5	1PE	A	608	4/16	0.90	0.69	30,35,37,43	4
5	1PE	B	612	4/16	0.90	0.28	25,25,25,25	4
5	1PE	A	612	4/16	0.90	0.86	34,35,35,36	4
6	GOL	B	605	6/6	0.90	0.17	50,52,55,56	0
5	1PE	B	608	4/16	0.91	0.56	29,31,32,34	4
5	1PE	A	605	4/16	0.92	0.59	27,28,30,36	4
5	1PE	B	609	4/16	0.93	0.25	36,39,40,41	4
2	NA	B	601	1/1	0.93	0.05	53,53,53,53	0
5	1PE	B	606	4/16	0.95	0.19	54,60,61,62	0
5	1PE	A	609	4/16	0.95	0.29	31,31,32,32	4
2	NA	A	601	1/1	0.95	0.07	44,44,44,44	0
3	NAD	A	602	44/44	0.96	0.11	36,45,50,51	0
3	NAD	B	602	44/44	0.97	0.13	37,43,47,50	0

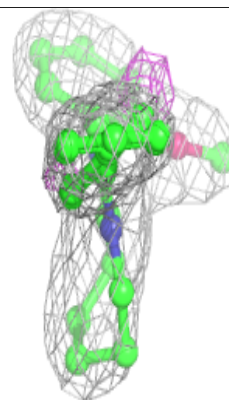
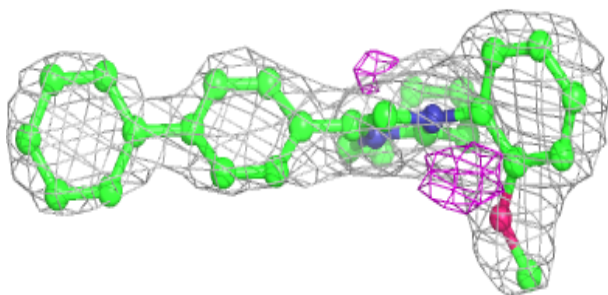
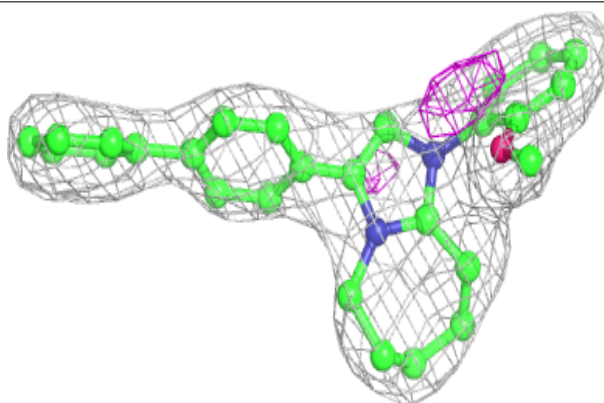
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ZGG A 603:

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

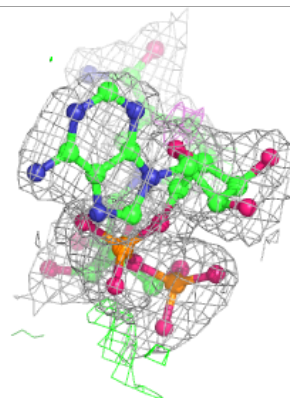
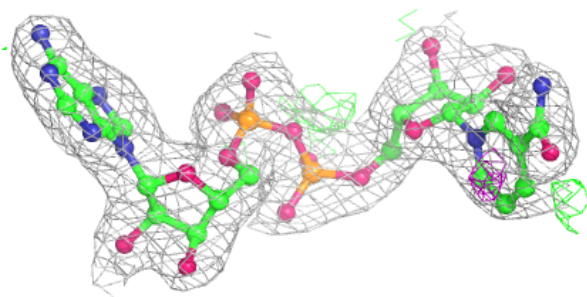
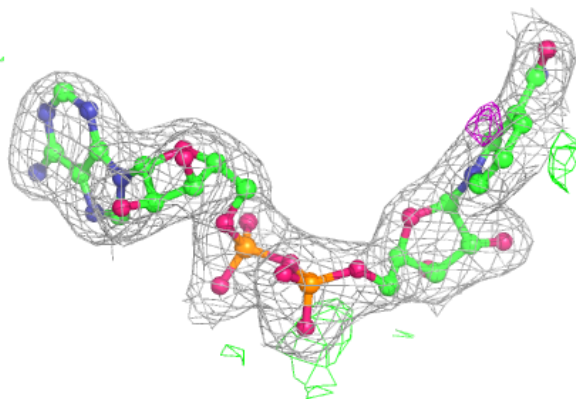
**Electron density around ZGG B 603:**

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

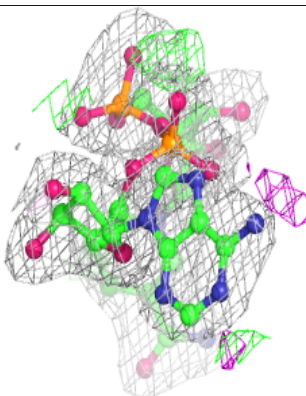
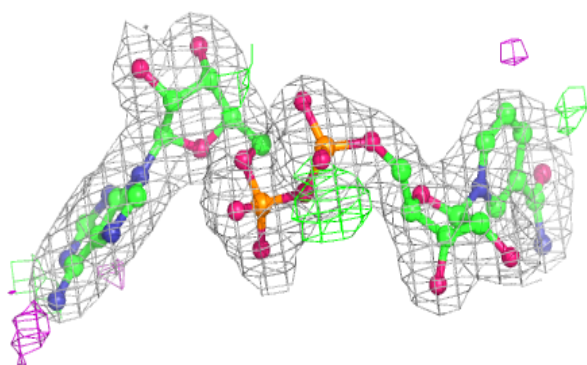
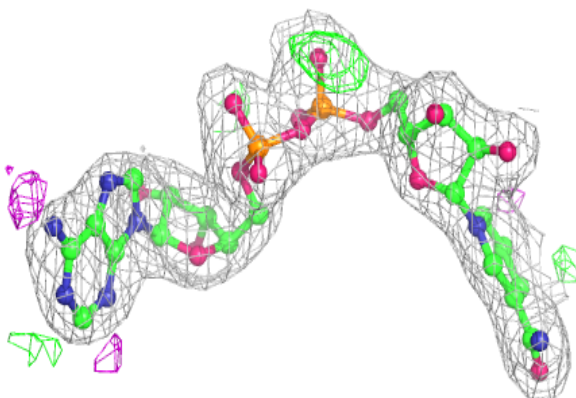


Electron density around NAD A 602:

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

**Electron density around NAD B 602:**

$2mF_o-DF_c$ (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.