



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:48 PM UTC

PDB ID : 8DR9 / pdb_00008dr9
Title : Crystal structure of human ALDH2 in complex with NAD⁺ and PEG MME 550
Authors : Xu, S.Y.; Weng, J.K.
Deposited on : 2022-07-20
Resolution : 1.50 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

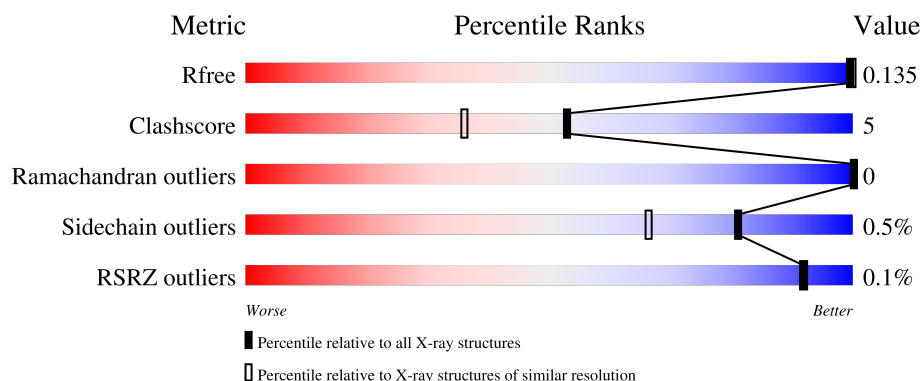
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

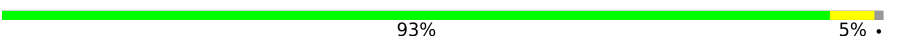
The reported resolution of this entry is 1.50 Å.

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	4037 (1.50-1.50)
Clashscore	190562	4235 (1.50-1.50)
Ramachandran outliers	187476	4153 (1.50-1.50)
Sidechain outliers	187428	4150 (1.50-1.50)
RSRZ outliers	180081	4039 (1.50-1.50)

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	501	 92% 6% ••
1	B	501	 93% 5% •

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 8954 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.

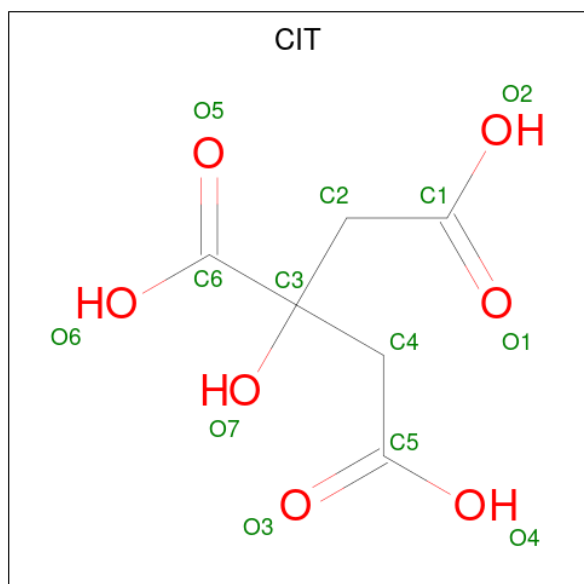
- Molecule 1 is a protein called Aldehyde dehydrogenase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	493	Total	C	N	O	S	0	13	0
			3878	2463	661	734	20			
1	B	495	Total	C	N	O	S	0	7	0
			3855	2447	661	728	19			

There are 4 discrepancies between the modelled and reference sequences:

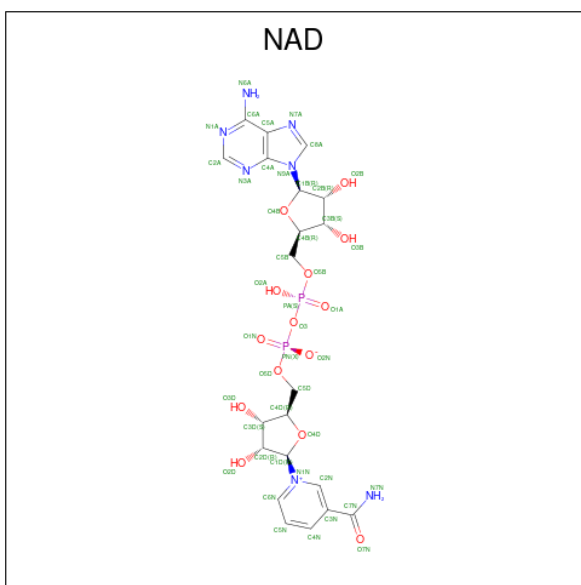
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP P05091
A	302	SER	CYS	engineered mutation	UNP P05091
B	0	GLY	-	expression tag	UNP P05091
B	302	SER	CYS	engineered mutation	UNP P05091

- Molecule 2 is CITRIC ACID (CCD ID: CIT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 13	C 6	O 7	0	0
2	B	1	Total 13	C 6	O 7	0	0

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $\text{C}_{21}\text{H}_{27}\text{N}_7\text{O}_{14}\text{P}_2$) (labeled as "Ligand of Interest" by depositor).

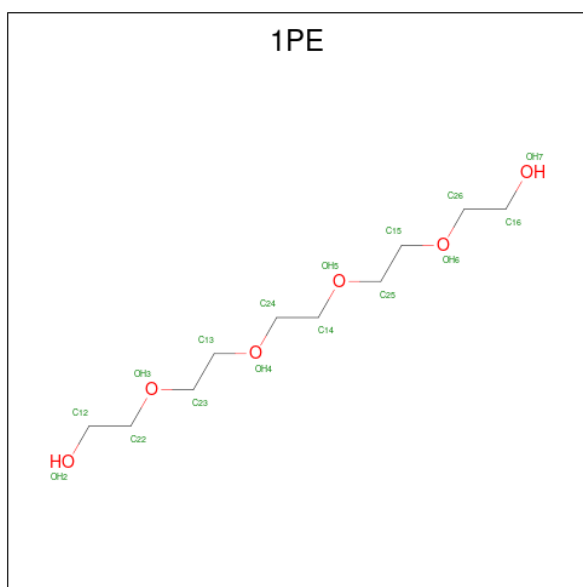


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 88	C 42	N 14	O 28	P 4	0	1
3	B	1	Total 44	C 21	N 7	O 14	P 2	0	0

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 5 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: $C_{10}H_{22}O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			14	9	5		
5	A	1	Total	C	O	0	0
			14	9	5		
5	A	1	Total	C	O	0	0
			14	9	5		
5	A	1	Total	C	O	0	0
			14	9	5		
5	B	1	Total	C	O	0	0
			11	7	4		
5	B	1	Total	C	O	0	0
			14	9	5		
5	B	1	Total	C	O	0	0
			11	7	4		
5	B	1	Total	C	O	0	0
			14	9	5		
5	B	1	Total	C	O	0	0
			14	9	5		

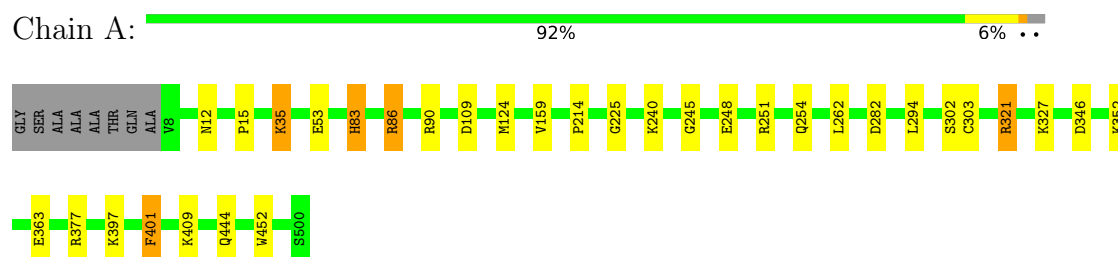
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	482	Total	O	0	0
			482	482		
6	B	459	Total	O	0	0
			459	459		

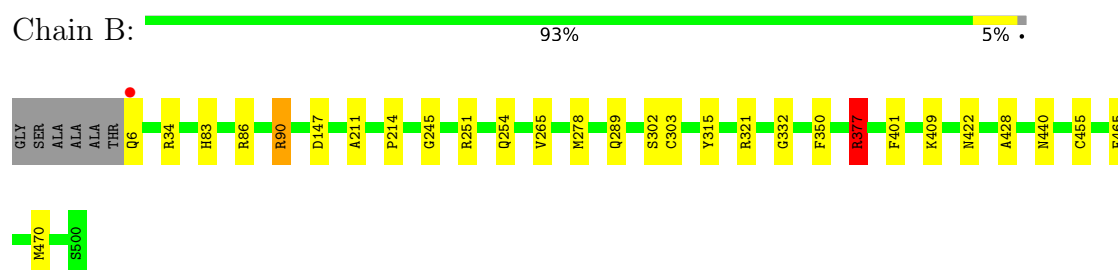
3 Residue-property plots

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, mitochondrial



- Molecule 1: Aldehyde dehydrogenase, mitochondrial



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	119.96Å 119.96Å 135.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.92 – 1.50 49.92 – 1.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.92-1.50) 99.9 (49.92-1.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.93 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.8.0352	Depositor
R, R_{free}	0.136 , 0.157 0.136 , 0.135	Depositor DCC
R_{free} test set	7803 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	15.6	Xtriage
Anisotropy	0.112	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 42.3	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	8954	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.72% 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: 1PE, NAD, NA, CIT

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	0.73	0/3981	1.01	4/5400 (0.1%)
1	B	0.72	0/3939	1.01	4/5343 (0.1%)
All	All	0.72	0/7920	1.01	8/10743 (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	5
1	B	0	4
All	All	0	9

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	214	PRO	O-C-N	-6.53	118.31	121.31
1	A	346	ASP	CA-CB-CG	6.24	118.84	112.60
1	A	83	HIS	CB-CG-CD2	-6.10	123.27	131.20
1	B	6	GLN	CB-CG-CD	-5.76	102.81	112.60
1	A	109	ASP	CA-CB-CG	5.71	118.31	112.60
1	B	147	ASP	CA-CB-CG	5.56	118.16	112.60
1	B	350	PHE	CA-CB-CG	5.31	119.11	113.80
1	A	214	PRO	O-C-N	-5.24	118.90	121.31

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	251	ARG	Sidechain
1	A	321	ARG	Sidechain
1	A	377	ARG	Sidechain
1	A	86[A]	ARG	Sidechain
1	A	86[B]	ARG	Sidechain
1	B	321	ARG	Sidechain
1	B	34	ARG	Sidechain
1	B	377	ARG	Sidechain
1	B	90	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	3878	0	3826	42	0
1	B	3855	0	3787	31	0
2	A	13	0	5	0	0
2	B	13	0	5	4	0
3	A	88	0	52	12	0
3	B	44	0	26	6	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	56	0	68	5	0
5	B	64	0	77	6	0
6	A	482	0	0	12	0
6	B	459	0	0	7	0
All	All	8954	0	7846	80	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 5.

All (80) 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:248:GLU:HG3	6:A:736:HOH:O	1.61	0.98
1:A:303[B]:CYS:SG	1:A:452:TRP:HH2	1.88	0.97
1:A:321:ARG:HH21	5:A:604:1PE:H122	1.35	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:LYS:HE2	6:A:928:HOH:O	1.69	0.90
3:B:603:NAD:H52N	6:B:829:HOH:O	1.74	0.88
1:A:303[B]:CYS:SG	1:A:452:TRP:CH2	2.70	0.84
1:B:83:HIS:HD2	1:B:86[B]:ARG:HH11	1.27	0.79
1:B:278:MET:HE3	2:B:602:CIT:C1	2.12	0.79
1:A:124[B]:MET:HE3	6:A:1061:HOH:O	1.80	0.79
3:A:602[B]:NAD:H51N	6:A:753:HOH:O	1.83	0.79
1:A:352:LYS:HE3	3:A:602[A]:NAD:H2N	1.64	0.77
1:B:302:SER:OG	3:B:603:NAD:H2D	1.85	0.76
1:B:251:ARG:NH2	1:B:470:MET:HE1	2.02	0.74
1:A:444:GLN:NE2	6:A:701:HOH:O	2.22	0.72
1:B:440:ASN:HB3	6:B:718:HOH:O	1.90	0.71
1:B:83:HIS:HD2	1:B:86[B]:ARG:NH1	1.89	0.69
1:B:303[B]:CYS:SG	1:B:428:ALA:HB2	2.32	0.69
1:A:321:ARG:NH2	5:A:604:1PE:H122	2.10	0.66
1:B:83:HIS:CD2	1:B:86[B]:ARG:HH11	2.12	0.66
1:B:303[B]:CYS:SG	1:B:428:ALA:CB	2.84	0.66
1:A:303[B]:CYS:HG	1:A:452:TRP:HH2	1.40	0.64
1:A:352:LYS:CE	3:A:602[A]:NAD:H2N	2.27	0.64
1:A:245:GLY:O	3:A:602[B]:NAD:H1D	1.98	0.63
1:A:83:HIS:HD2	1:A:86[A]:ARG:HH21	1.46	0.63
1:B:278:MET:HE3	2:B:602:CIT:O2	1.98	0.62
1:B:245:GLY:O	3:B:603:NAD:H1D	2.00	0.61
1:A:302:SER:OG	3:A:602[B]:NAD:H2D	2.01	0.60
1:A:83:HIS:HD2	1:A:86[A]:ARG:NH2	2.00	0.59
1:B:303[B]:CYS:HG	1:B:465:PHE:HZ	1.49	0.58
3:A:602[B]:NAD:C5N	6:A:825:HOH:O	2.50	0.57
5:B:605:1PE:H231	6:B:975:HOH:O	2.04	0.57
1:A:35:LYS:HE2	1:A:53:GLU:OE1	2.05	0.57
1:B:83:HIS:HE1	6:B:1081:HOH:O	1.88	0.56
1:B:289:GLN:NE2	6:B:701:HOH:O	2.20	0.55
1:A:83:HIS:HE1	6:A:1082:HOH:O	1.88	0.55
1:B:377:ARG:HB2	1:B:377:ARG:CZ	2.36	0.55
1:B:422:ASN:HD21	5:B:606:1PE:H141	1.72	0.54
1:B:303[B]:CYS:SG	1:B:465:PHE:CZ	3.00	0.54
1:B:303[B]:CYS:SG	1:B:465:PHE:HZ	2.29	0.54
1:B:422:ASN:ND2	5:B:606:1PE:H132	2.22	0.54
1:B:254[B]:GLN:HA	1:B:254[B]:GLN:OE1	2.08	0.53
1:B:83:HIS:CD2	1:B:86[B]:ARG:NH1	2.74	0.53
1:B:254[B]:GLN:OE1	1:B:265:VAL:HG21	2.09	0.52
1:A:159[B]:VAL:HG11	1:A:240:LYS:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:HIS:CD2	1:A:86[A]:ARG:HH21	2.27	0.51
1:A:294:LEU:C	1:A:294:LEU:HD13	2.36	0.50
1:B:332:GLY:HA2	5:B:607:1PE:H242	1.94	0.49
3:B:603:NAD:C5D	6:B:829:HOH:O	2.44	0.49
1:A:254[B]:GLN:HE21	1:A:254[B]:GLN:HA	1.77	0.49
1:A:90:ARG:NH1	6:A:704:HOH:O	2.44	0.49
1:A:352:LYS:NZ	3:A:602[A]:NAD:C2N	2.76	0.48
1:A:124[B]:MET:CE	6:A:1061:HOH:O	2.48	0.47
1:B:377:ARG:CZ	1:B:377:ARG:CB	2.93	0.46
1:A:225:GLY:HA3	3:A:602[A]:NAD:C8A	2.46	0.46
1:A:302:SER:OG	3:A:602[B]:NAD:C2D	2.64	0.46
1:A:254[B]:GLN:HA	1:A:254[B]:GLN:NE2	2.31	0.45
1:A:83:HIS:CE1	6:A:1082:HOH:O	2.67	0.45
5:A:604:1PE:H122	5:A:604:1PE:H231	1.80	0.45
1:A:401:PHE:CZ	3:A:602[B]:NAD:H3D	2.52	0.44
3:B:603:NAD:C4D	3:B:603:NAD:O1N	2.63	0.43
1:A:321:ARG:NH2	5:A:604:1PE:H231	2.34	0.43
1:A:409:LYS:HD2	5:A:607:1PE:H132	2.01	0.43
1:A:352:LYS:HD3	3:A:602[A]:NAD:O7N	2.19	0.42
1:A:12:ASN:O	1:A:15:PRO:HD3	2.18	0.42
1:A:327:LYS:NZ	6:A:711:HOH:O	2.51	0.42
1:A:245:GLY:C	3:A:602[B]:NAD:H1D	2.44	0.42
1:B:278:MET:CE	2:B:602:CIT:C1	2.91	0.42
1:B:422:ASN:HD21	5:B:606:1PE:H132	1.83	0.42
1:A:83:HIS:HD2	1:A:86[A]:ARG:HE	1.68	0.42
1:A:83:HIS:CD2	1:A:86[A]:ARG:HE	2.38	0.42
1:A:282[B]:ASP:OD2	5:B:601:1PE:H242	2.21	0.41
3:B:603:NAD:C5N	6:B:876:HOH:O	2.68	0.41
1:A:262:LEU:HD21	1:B:251:ARG:HA	2.02	0.41
1:B:315:TYR:CD2	1:B:409:LYS:HE2	2.55	0.41
1:A:397:LYS:HE3	6:A:799:HOH:O	2.20	0.41
1:B:289:GLN:HE21	1:B:455:CYS:HA	1.86	0.41
1:A:83:HIS:CD2	1:A:86[A]:ARG:NH2	2.84	0.41
1:B:278:MET:CE	2:B:602:CIT:H22	2.51	0.41
1:B:90:ARG:HD2	1:B:211:ALA:O	2.21	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	504/501 (101%)	491 (97%)	13 (3%)	0	100	100
1	B	499/501 (100%)	486 (97%)	13 (3%)	0	100	100
All	All	1003/1002 (100%)	977 (97%)	26 (3%)	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	412/402 (102%)	410 (100%)	2 (0%)	81	66
1	B	406/402 (101%)	404 (100%)	2 (0%)	81	66
All	All	818/804 (102%)	814 (100%)	4 (0%)	81	66

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

Mol	Chain	Res	Type
1	A	35	LYS
1	A	401	PHE
1	B	377	ARG
1	B	401	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	ASN
1	A	71	GLN
1	A	83	HIS
1	A	444	GLN
1	B	13	GLN
1	B	83	HIS
1	B	289	GLN
1	B	358	ASN
1	B	390	GLN
1	B	422	ASN
1	B	483	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 16 ligands modelled in this entry, 2 are monoatomic - leaving 14 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	$\# Z > 2$
2	CIT	B	602	-	12,12,12	1.29	2 (16%)	17,17,17	1.18	2 (11%)
5	1PE	B	607	-	13,13,15	0.28	0	12,12,14	0.29	0
5	1PE	A	606	-	13,13,15	0.31	0	12,12,14	0.25	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAD	A	602[A]	-	46,48,48	0.90	2 (4%)	64,73,73	0.71	2 (3%)
5	1PE	A	607	-	13,13,15	0.42	0	12,12,14	0.28	0
5	1PE	B	606	-	10,10,15	0.30	0	9,9,14	0.19	0
5	1PE	A	604	-	13,13,15	0.35	0	12,12,14	0.48	0
3	NAD	A	602[B]	-	46,48,48	1.16	3 (6%)	64,73,73	1.29	10 (15%)
3	NAD	B	603	-	46,48,48	1.01	2 (4%)	64,73,73	1.29	8 (12%)
5	1PE	A	605	-	13,13,15	0.21	0	12,12,14	0.30	0
5	1PE	B	608	-	13,13,15	0.26	0	12,12,14	0.14	0
2	CIT	A	601	-	12,12,12	1.31	3 (25%)	17,17,17	1.41	3 (17%)
5	1PE	B	601	-	10,10,15	0.16	0	9,9,14	0.15	0
5	1PE	B	605	-	13,13,15	0.34	0	12,12,14	0.39	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CIT	B	602	-	-	8/16/16/16	-
5	1PE	B	607	-	-	7/11/11/13	-
5	1PE	A	606	-	-	5/11/11/13	-
3	NAD	A	602[A]	-	-	9/30/62/62	0/5/5/5
5	1PE	A	607	-	-	6/11/11/13	-
5	1PE	B	606	-	-	3/8/8/13	-
5	1PE	A	604	-	-	5/11/11/13	-
3	NAD	A	602[B]	-	-	8/30/62/62	0/5/5/5
3	NAD	B	603	-	-	10/30/62/62	0/5/5/5
5	1PE	A	605	-	-	2/11/11/13	-
5	1PE	B	608	-	-	6/11/11/13	-
2	CIT	A	601	-	-	0/16/16/16	-
5	1PE	B	601	-	-	3/8/8/13	-
5	1PE	B	605	-	-	6/11/11/13	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602[B]	NAD	PN-O3	4.59	1.64	1.59
3	A	602[A]	NAD	PN-O3	4.05	1.63	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	603	NAD	C2N-N1N	3.84	1.39	1.35
3	A	602[B]	NAD	C2N-N1N	3.73	1.39	1.35
3	B	603	NAD	PA-O3	-3.25	1.56	1.59
2	A	601	CIT	O4-C5	-2.54	1.22	1.30
3	A	602[A]	NAD	C2N-N1N	2.53	1.37	1.35
2	B	602	CIT	C3-C6	2.26	1.55	1.53
2	A	601	CIT	O2-C1	-2.16	1.23	1.30
2	B	602	CIT	O4-C5	-2.13	1.23	1.30
3	A	602[B]	NAD	PA-O3	2.12	1.61	1.59
2	A	601	CIT	O5-C6	2.10	1.28	1.22

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602[B]	NAD	O2A-PA-O3	3.78	117.50	107.27
3	B	603	NAD	O2D-C2D-C3D	-3.71	99.92	111.82
3	B	603	NAD	C6N-N1N-C2N	-3.56	118.85	121.88
3	A	602[B]	NAD	O4D-C4D-C3D	-3.30	98.59	105.15
3	B	603	NAD	O2N-PN-O3	3.07	115.57	107.27
2	A	601	CIT	O3-C5-C4	-2.90	114.75	122.95
3	A	602[A]	NAD	C6N-N1N-C2N	-2.76	119.53	121.88
2	B	602	CIT	O5-C6-C3	-2.72	116.82	122.09
3	A	602[B]	NAD	O2D-C2D-C3D	-2.72	103.11	111.82
3	A	602[B]	NAD	C2N-C3N-C4N	2.70	121.39	118.26
3	A	602[B]	NAD	C6N-N1N-C2N	-2.64	119.63	121.88
3	A	602[B]	NAD	O4D-C4D-C5D	-2.60	101.01	109.33
3	A	602[B]	NAD	C5D-C4D-C3D	2.56	124.44	115.21
2	B	602	CIT	O6-C6-C3	2.51	117.96	113.14
3	B	603	NAD	PN-O5D-C5D	-2.51	106.98	121.35
3	B	603	NAD	C2N-N1N-C1D	2.39	124.42	119.13
3	A	602[B]	NAD	C2N-N1N-C1D	2.38	124.39	119.13
2	A	601	CIT	O4-C5-C4	2.35	121.78	114.35
3	A	602[B]	NAD	C4N-C3N-C7N	-2.29	114.81	121.06
3	A	602[B]	NAD	C6N-N1N-C1D	-2.28	115.26	119.73
2	A	601	CIT	O5-C6-C3	-2.27	117.69	122.09
3	A	602[A]	NAD	O2N-PN-O1N	2.16	122.48	112.44
3	B	603	NAD	O3-PN-O1N	-2.15	104.24	110.70
3	B	603	NAD	O2B-C2B-C3B	2.12	118.60	111.82
3	B	603	NAD	O2N-PN-O5D	2.03	116.76	107.57

There are no chirality outliers.

All (78) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	602	CIT	C2-C3-C6-O5
2	B	602	CIT	C2-C3-C6-O6
2	B	602	CIT	O7-C3-C6-O5
2	B	602	CIT	O7-C3-C6-O6
3	A	602[A]	NAD	C5D-O5D-PN-O3
3	A	602[A]	NAD	C5D-O5D-PN-O1N
3	A	602[A]	NAD	O4D-C1D-N1N-C6N
3	A	602[B]	NAD	C5D-O5D-PN-O3
3	A	602[B]	NAD	C5D-O5D-PN-O2N
3	A	602[B]	NAD	C4D-C5D-O5D-PN
3	B	603	NAD	C5D-O5D-PN-O3
3	B	603	NAD	C5D-O5D-PN-O1N
3	B	603	NAD	C5D-O5D-PN-O2N
3	B	603	NAD	C4D-C5D-O5D-PN
5	A	606	1PE	C24-C14-OH5-C25
5	B	605	1PE	C23-C13-OH4-C24
5	A	606	1PE	C23-C13-OH4-C24
3	B	603	NAD	C3D-C4D-C5D-O5D
5	B	608	1PE	OH6-C15-C25-OH5
5	A	607	1PE	OH5-C14-C24-OH4
5	B	607	1PE	OH5-C14-C24-OH4
5	A	606	1PE	OH6-C15-C25-OH5
5	A	607	1PE	OH4-C13-C23-OH3
3	B	603	NAD	O4D-C4D-C5D-O5D
5	A	607	1PE	OH2-C12-C22-OH3
5	B	606	1PE	OH2-C12-C22-OH3
5	A	604	1PE	OH6-C15-C25-OH5
5	B	605	1PE	OH5-C14-C24-OH4
5	A	605	1PE	OH6-C15-C25-OH5
5	A	606	1PE	OH7-C16-C26-OH6
5	B	607	1PE	OH7-C16-C26-OH6
5	A	604	1PE	OH4-C13-C23-OH3
2	B	602	CIT	C1-C2-C3-O7
2	B	602	CIT	C1-C2-C3-C6
5	B	607	1PE	OH6-C15-C25-OH5
3	A	602[B]	NAD	O4D-C4D-C5D-O5D
2	B	602	CIT	C1-C2-C3-C4
5	B	608	1PE	OH4-C13-C23-OH3
5	B	605	1PE	OH6-C15-C25-OH5
5	B	601	1PE	OH2-C12-C22-OH3
2	B	602	CIT	O7-C3-C4-C5
5	B	601	1PE	C24-C14-OH5-C25
5	A	604	1PE	OH5-C14-C24-OH4

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Mol	Chain	Res	Type	Atoms
5	A	607	1PE	C25-C15-OH6-C26
3	B	603	NAD	C2B-C1B-N9A-C8A
5	B	607	1PE	C25-C15-OH6-C26
3	A	602[A]	NAD	C2B-C1B-N9A-C8A
3	A	602[B]	NAD	C2B-C1B-N9A-C8A
5	A	604	1PE	OH2-C12-C22-OH3
5	A	606	1PE	C16-C26-OH6-C15
5	B	608	1PE	C16-C26-OH6-C15
5	B	607	1PE	C23-C13-OH4-C24
5	B	607	1PE	C13-C23-OH3-C22
3	A	602[A]	NAD	C5B-O5B-PA-O1A
3	A	602[B]	NAD	C5D-O5D-PN-O1N
5	B	608	1PE	OH7-C16-C26-OH6
5	A	607	1PE	C24-C14-OH5-C25
5	A	607	1PE	C23-C13-OH4-C24
3	A	602[A]	NAD	PN-O3-PA-O1A
5	B	601	1PE	C12-C22-OH3-C23
5	B	605	1PE	OH4-C13-C23-OH3
5	B	608	1PE	C14-C24-OH4-C13
5	B	606	1PE	C24-C14-OH5-C25
3	A	602[A]	NAD	O4D-C1D-N1N-C2N
5	B	605	1PE	C14-C24-OH4-C13
3	B	603	NAD	PA-O3-PN-O2N
3	B	603	NAD	O4B-C1B-N9A-C8A
3	A	602[A]	NAD	O4B-C1B-N9A-C8A
3	A	602[B]	NAD	O4B-C1B-N9A-C8A
5	B	606	1PE	C12-C22-OH3-C23
3	B	603	NAD	PA-O3-PN-O1N
5	A	605	1PE	OH5-C14-C24-OH4
5	B	605	1PE	C16-C26-OH6-C15
5	B	607	1PE	OH4-C13-C23-OH3
5	A	604	1PE	C12-C22-OH3-C23
3	A	602[A]	NAD	PN-O3-PA-O2A
3	A	602[B]	NAD	PN-O3-PA-O2A
5	B	608	1PE	C13-C23-OH3-C22

There are no ring outliers.

10 monomers are involved in 33 short contacts:

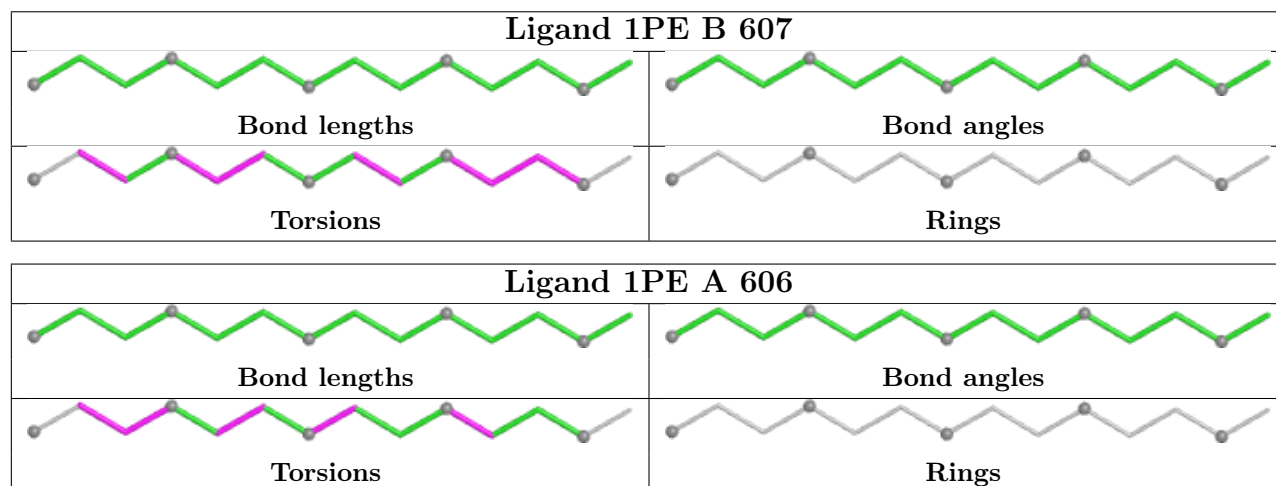
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	602	CIT	4	0
5	B	607	1PE	1	0

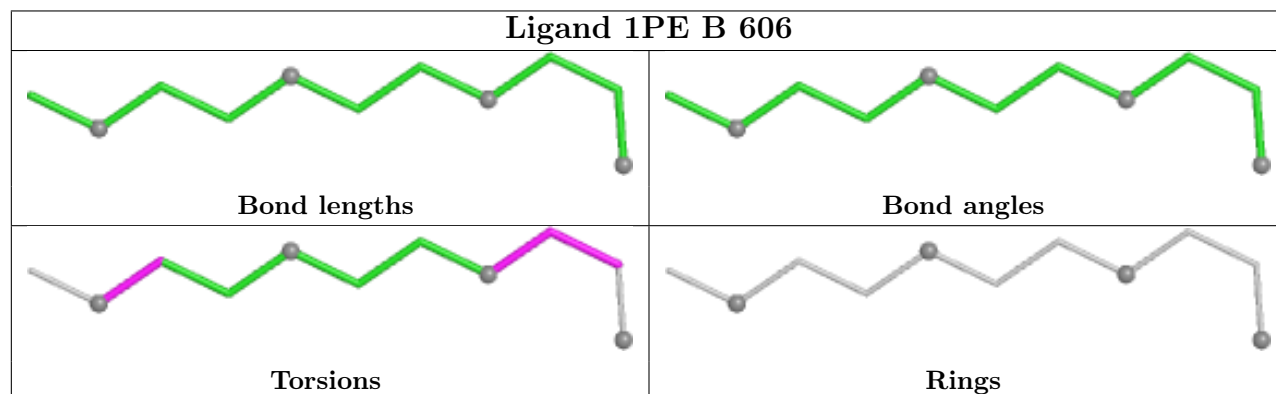
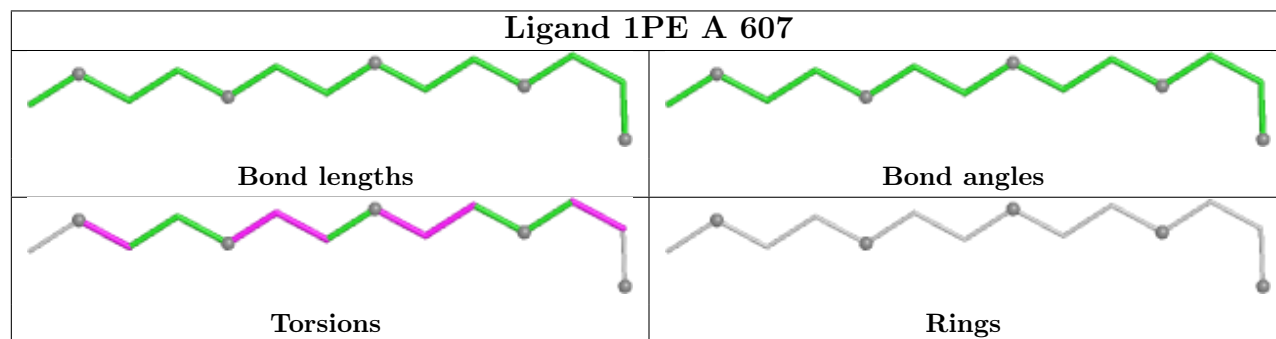
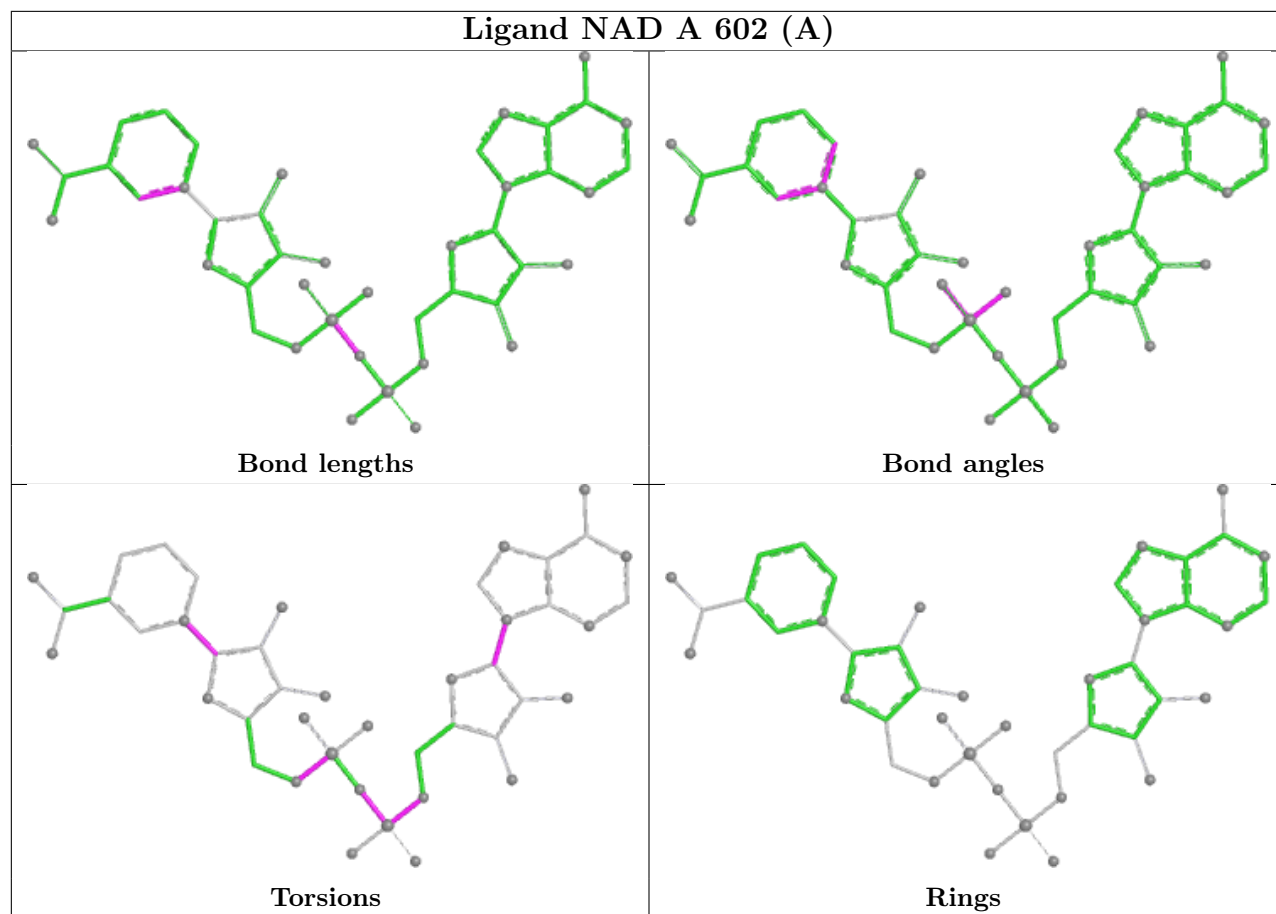
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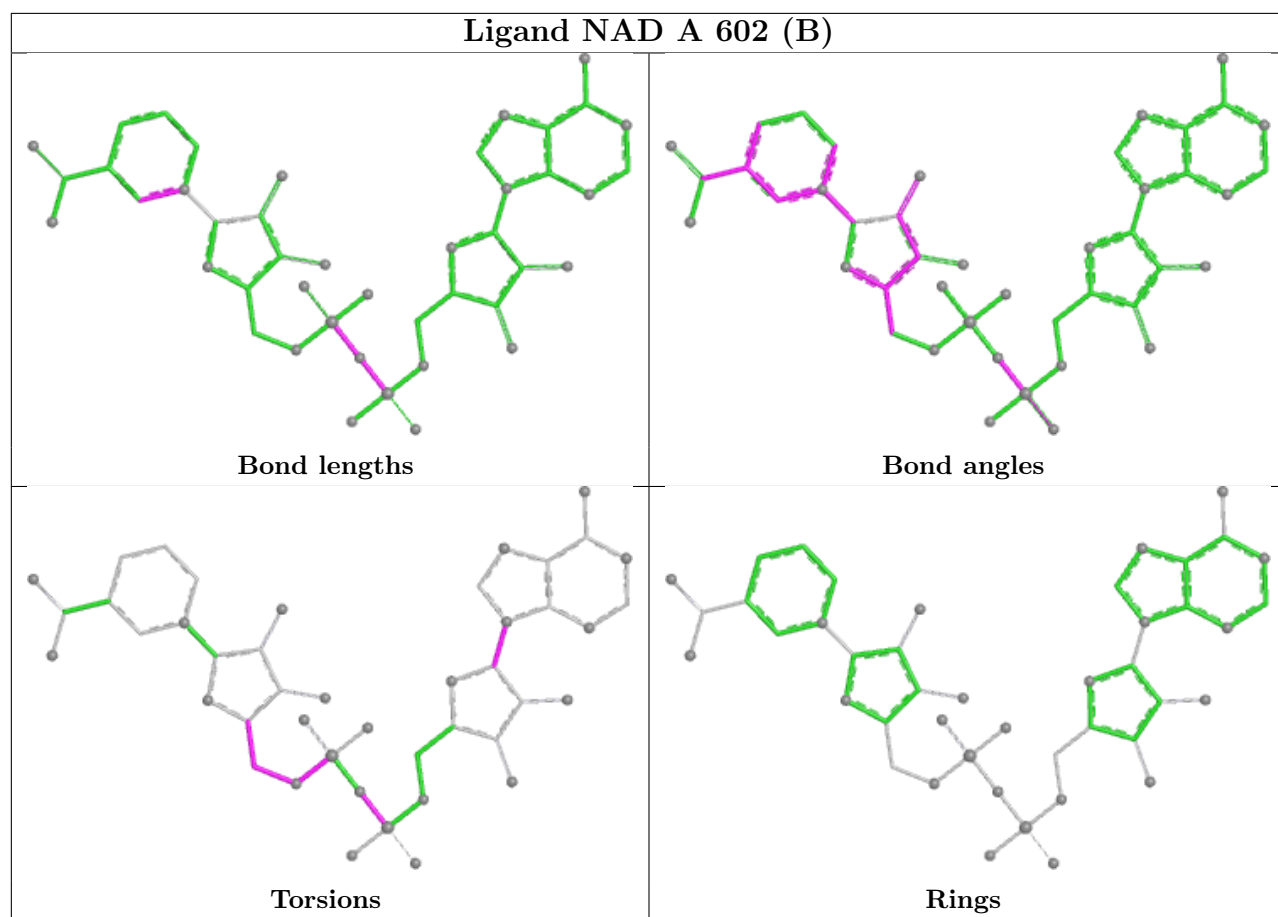
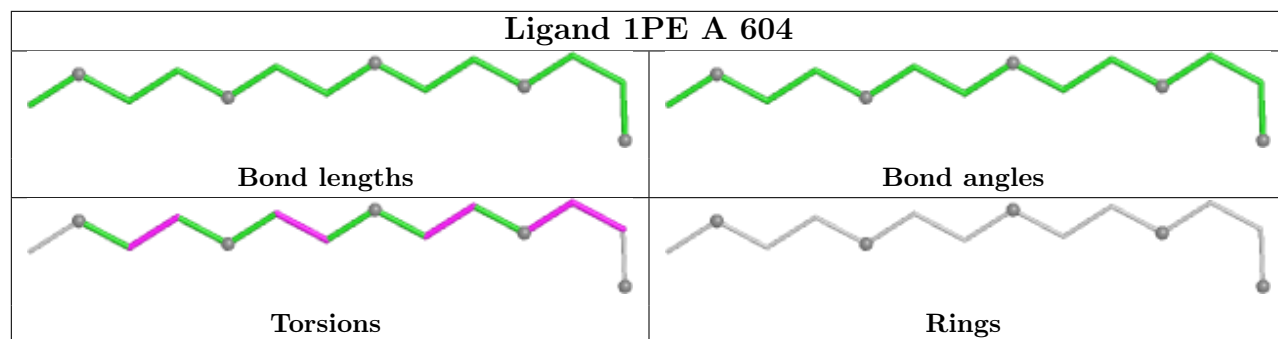
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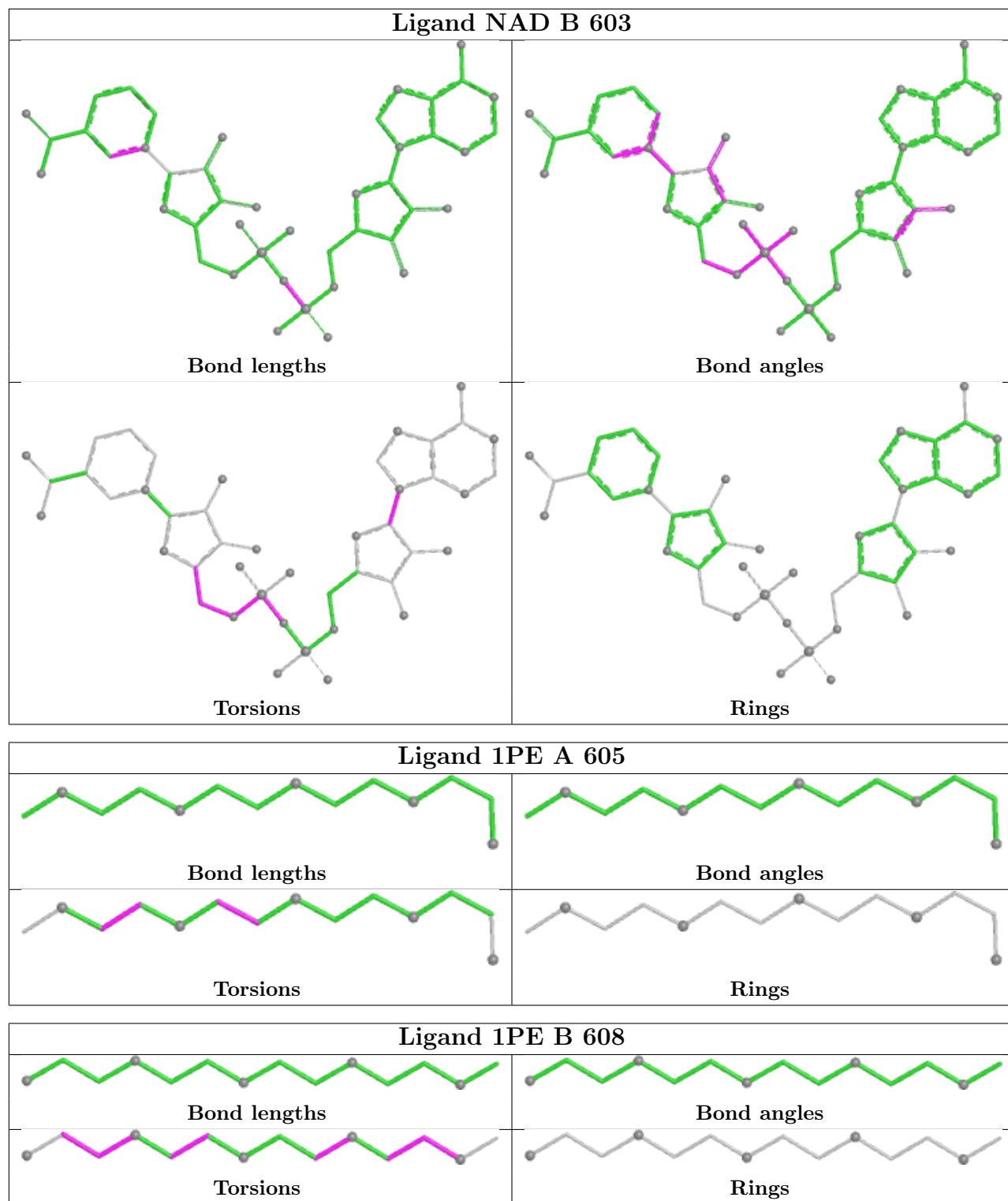
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	602[A]	NAD	5	0
5	A	607	1PE	1	0
5	B	606	1PE	3	0
5	A	604	1PE	4	0
3	A	602[B]	NAD	7	0
3	B	603	NAD	6	0
5	B	601	1PE	1	0
5	B	605	1PE	1	0

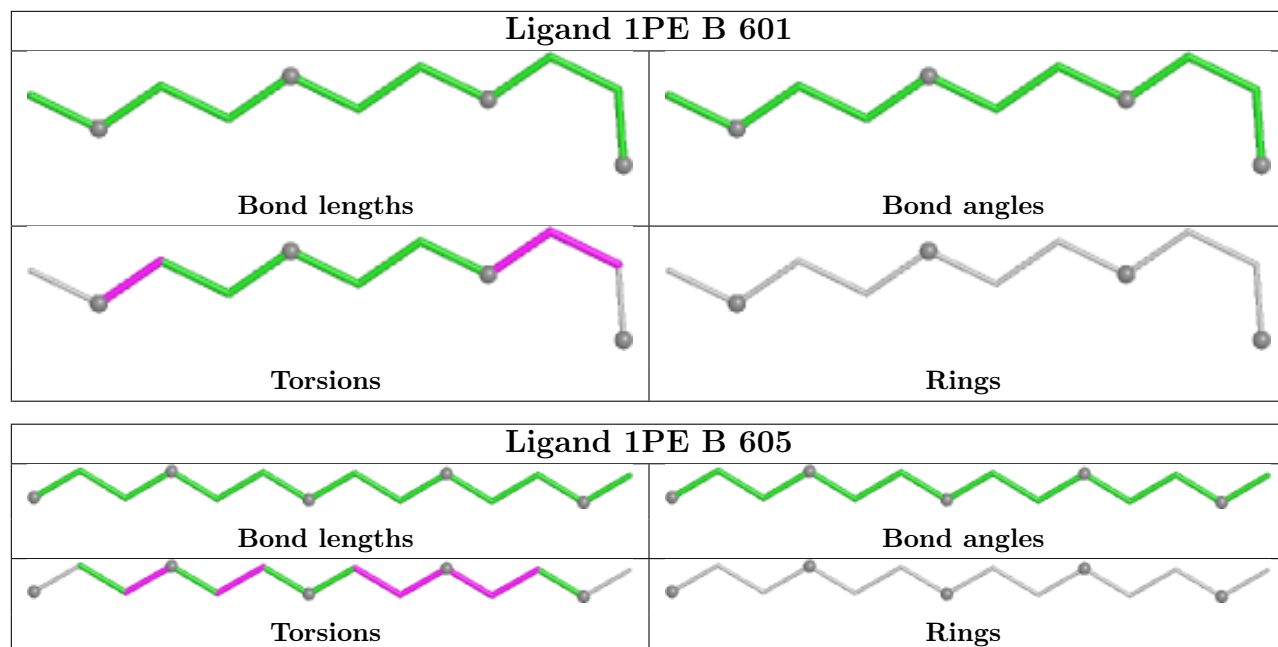
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 [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	493/501 (98%)	-0.43	0 100 100	7, 14, 25, 43	13 (2%)
1	B	495/501 (98%)	-0.29	1 (0%) 91 92	8, 16, 29, 51	6 (1%)
All	All	988/1002 (98%)	-0.36	1 (0%) 92 92	7, 15, 26, 51	19 (1%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	6	GLN	2.3

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
3	NAD	A	602[A]	44/44	0.65	0.24	4,7,10,11	44
3	NAD	A	602[B]	44/44	0.65	0.24	13,22,51,63	44
2	CIT	B	602	13/13	0.71	0.16	40,56,75,79	0
5	1PE	A	607	14/16	0.74	0.18	45,51,63,64	0

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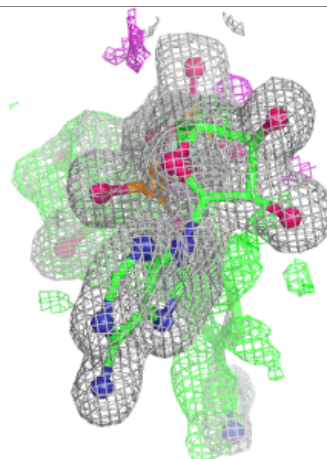
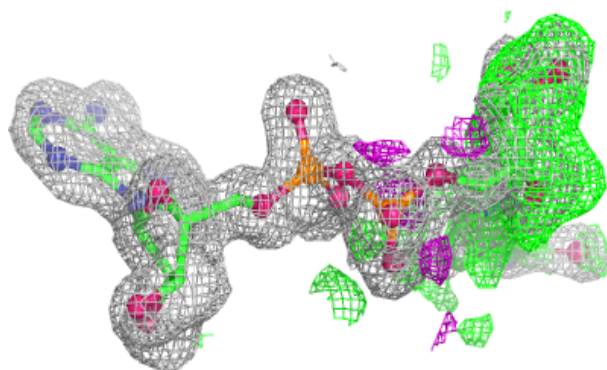
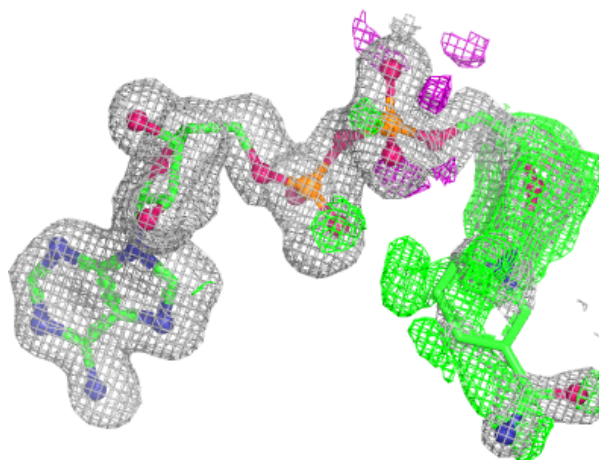
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	1PE	B	607	14/16	0.81	0.17	45,54,64,67	0
5	1PE	B	605	14/16	0.82	0.17	32,39,47,56	0
5	1PE	B	606	11/16	0.84	0.15	48,52,57,65	0
5	1PE	B	608	14/16	0.84	0.17	34,42,58,60	14
5	1PE	A	606	14/16	0.85	0.14	34,38,39,41	14
5	1PE	B	601	11/16	0.85	0.14	42,48,61,66	0
5	1PE	A	604	14/16	0.89	0.15	20,38,61,66	0
5	1PE	A	605	14/16	0.91	0.11	25,34,44,46	0
3	NAD	B	603	44/44	0.95	0.10	13,21,49,63	0
2	CIT	A	601	13/13	0.96	0.06	17,21,28,28	0
4	NA	B	604	1/1	0.99	0.03	16,16,16,16	0
4	NA	A	603	1/1	0.99	0.04	14,14,14,14	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.

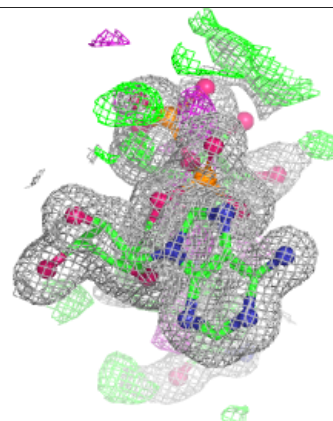
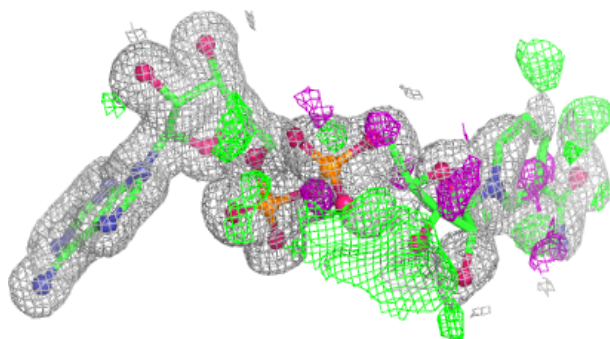
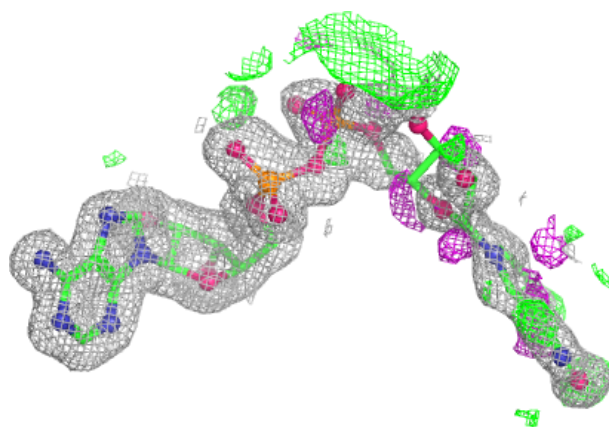
Electron density around NAD A 602 (A):

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



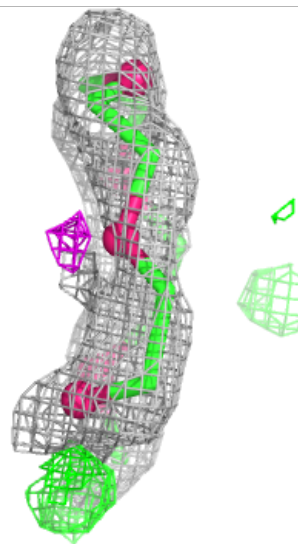
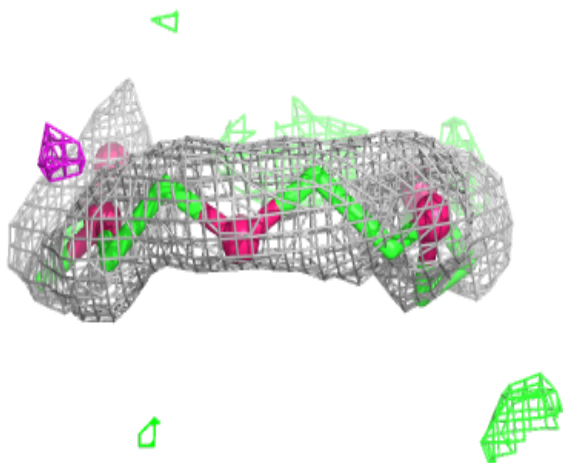
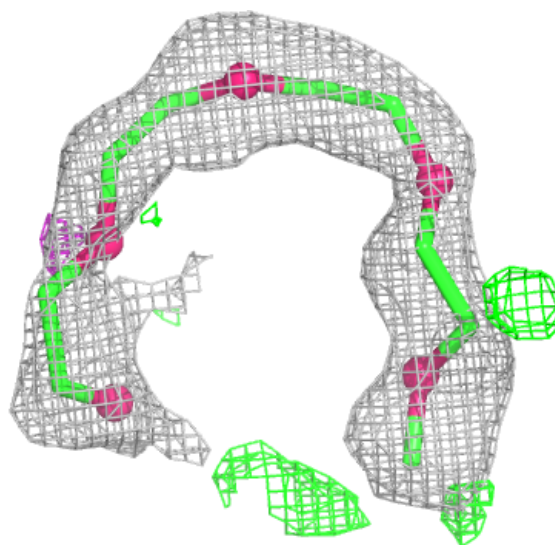
Electron density around NAD A 602 (B):

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



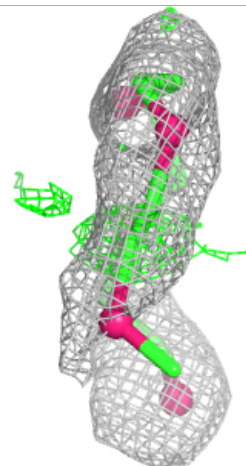
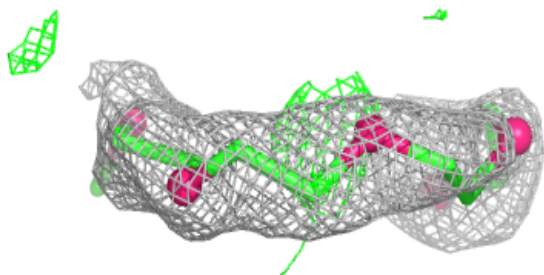
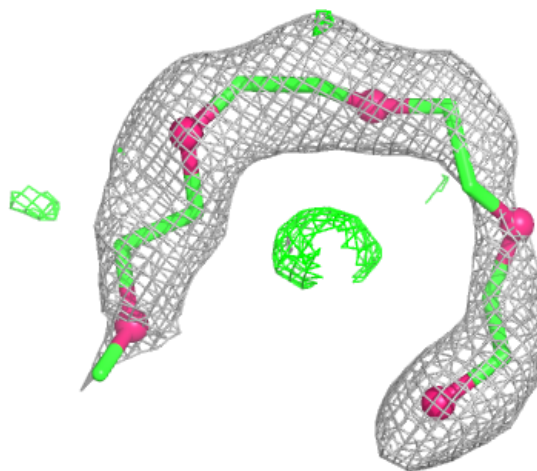
Electron density around 1PE A 607:

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



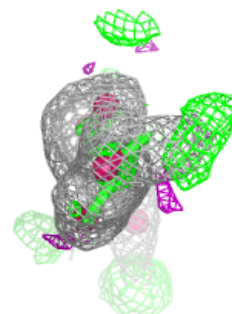
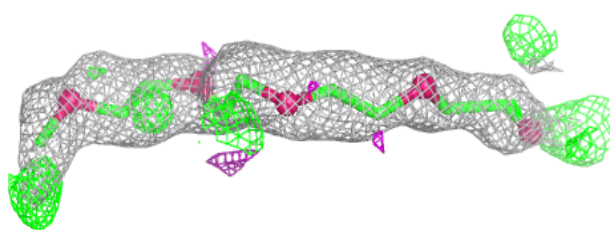
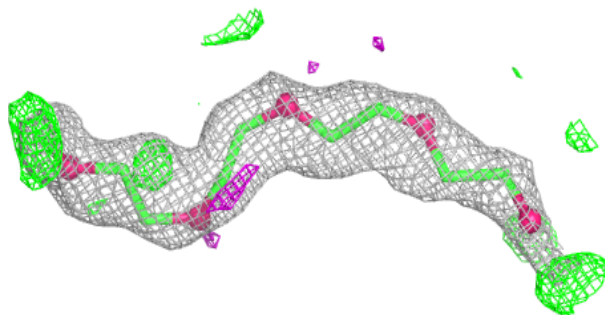
Electron density around 1PE B 607:

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

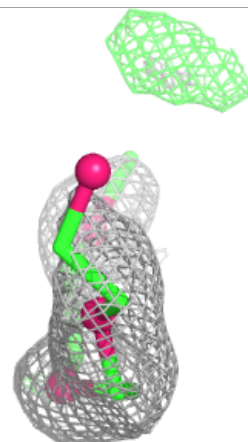
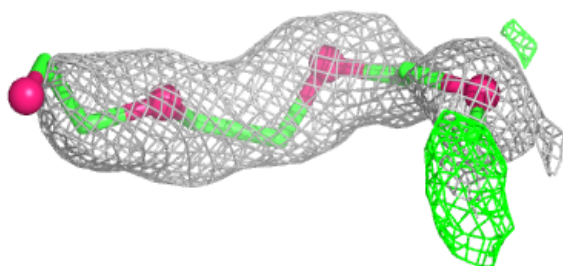
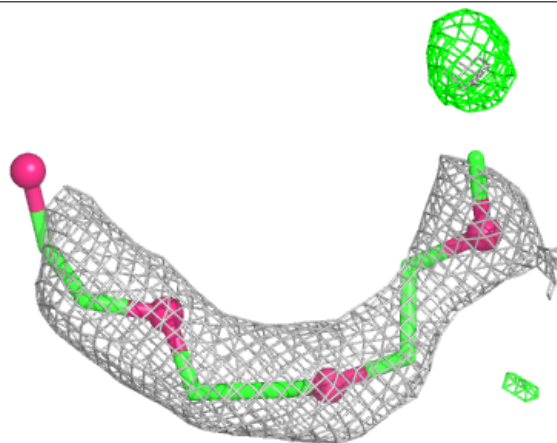


Electron density around 1PE B 605:

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

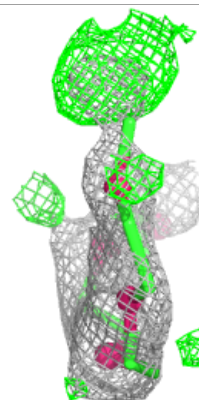
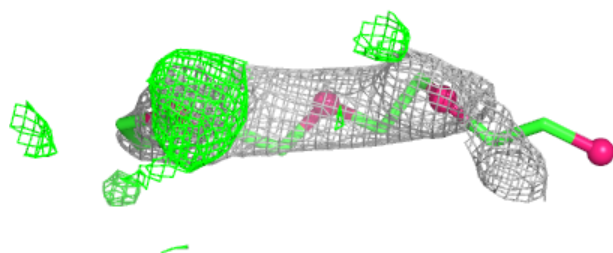
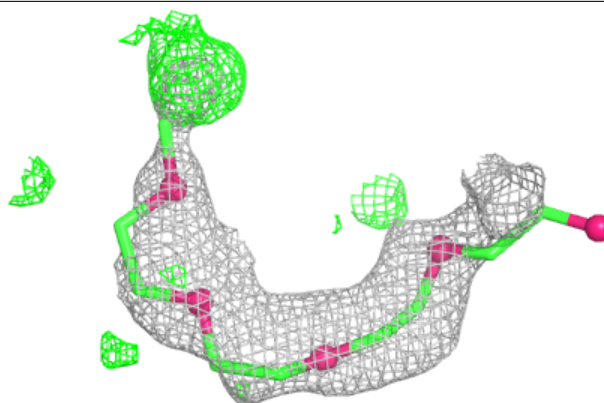
**Electron density around 1PE B 606:**

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

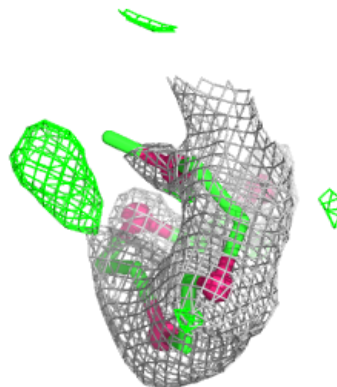
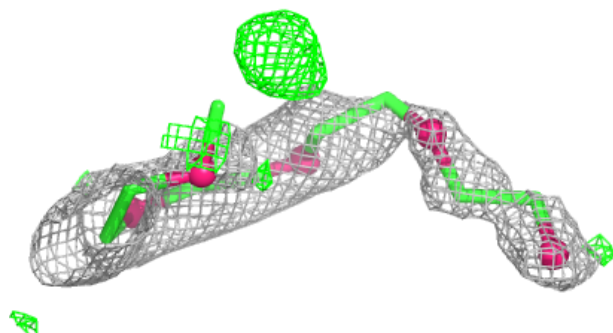
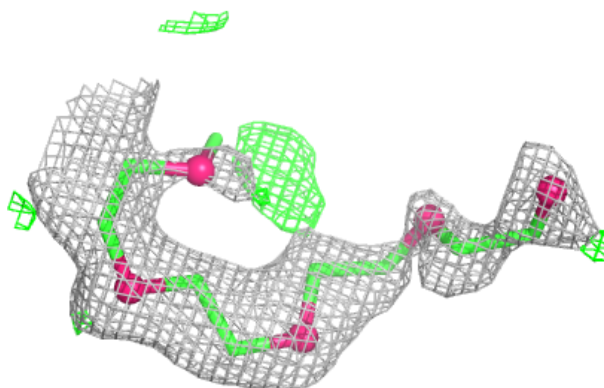


Electron density around 1PE B 608:

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

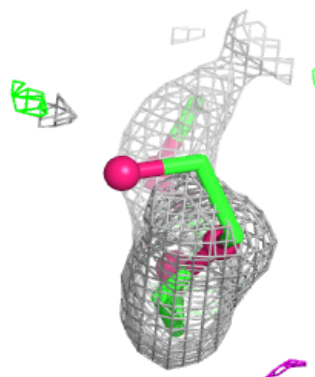
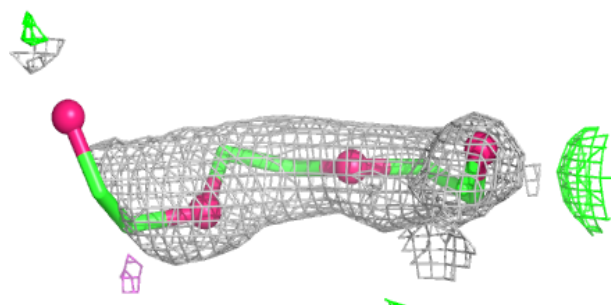
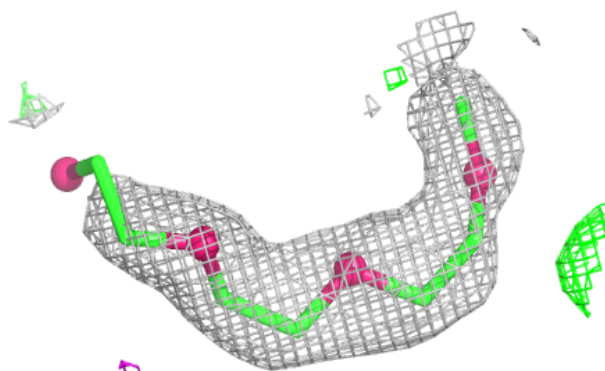
**Electron density around 1PE A 606:**

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

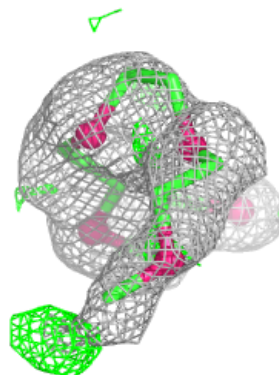
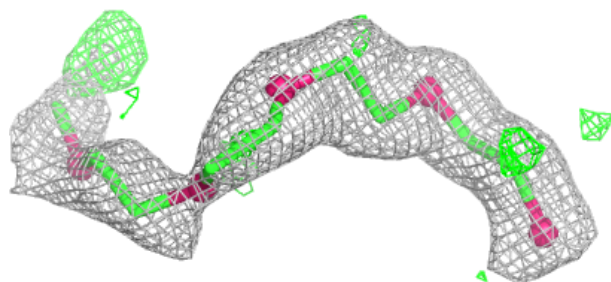
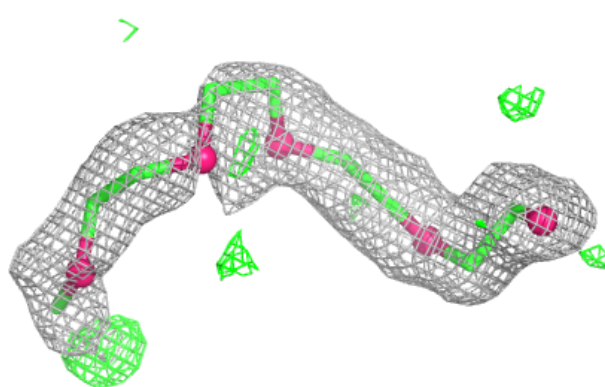


Electron density around 1PE B 601:

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

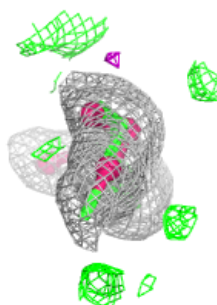
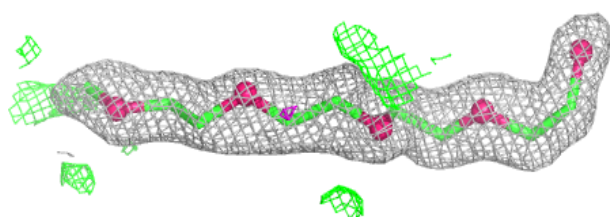
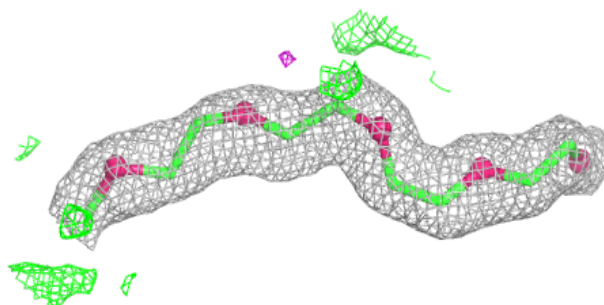
**Electron density around 1PE A 604:**

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

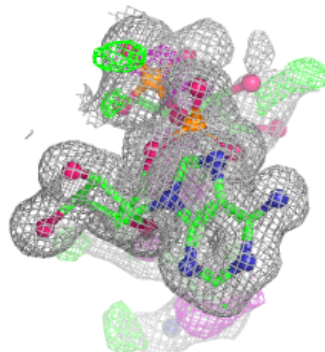
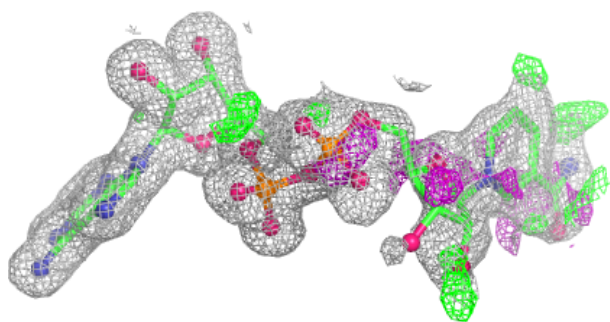
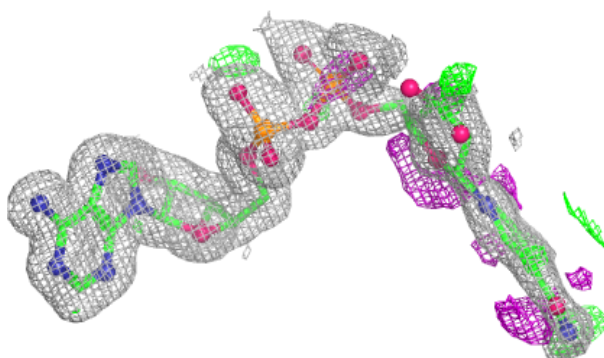


Electron density around 1PE A 605:

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

**Electron density around NAD B 603:**

$2mF_o-DF_c$ (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.