

wwPDB X-ray Structure Validation Summary Report (i)

Aug 21, 2023 – 03:14 PM EDT

PDB ID	:	8DR9
Title	:	Crystal structure of human ALDH2 in complex with NAD+ and PEG MME $$
		550
Authors	:	Xu, S.Y.; Weng, J.K.
Deposited on		
Resolution	:	1.50 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 (i) 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 (1)) were used in the production of this report:

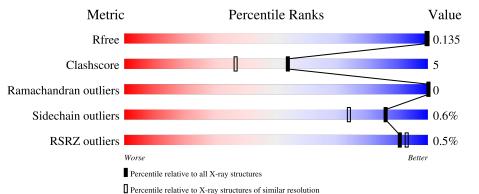
MolProbity	:	4.02b-467 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)		
EDS	:	2.35
buster-report	:	1.1.7(2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\textbf{Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (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 <=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	А	501	% 91%	7% •
1	В	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.

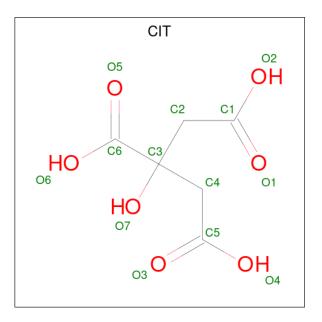
• Molecule 1 is a protein called Aldehyde dehydrogenase, mitochondrial.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	Δ	493	Total	С	Ν	0	\mathbf{S}	0	13	0
		495	3878	2463	661	734	20	0		
1	Р	495	Total	С	Ν	0	S	0	7	0
	D	495	3855	2447	661	728	19	0	1	0

There are 4 discrepancies between the modelled and reference sequences:

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

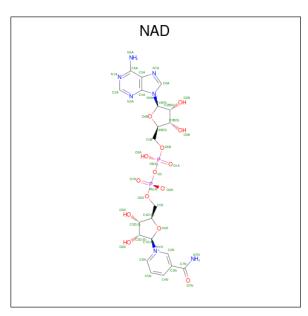
• Molecule 2 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	Total C O 13 6 7	0	0
2	В	1	Total C O 13 6 7	0	0

• Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).



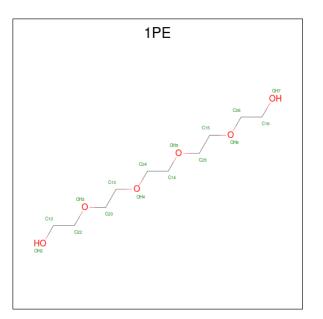
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf		
2	3 A	٨	1	Total	С	Ν	0	Р	0	1
5		1	88	42	14	28	4	0	T	
2	р	D 1	1	Total	С	Ν	0	Р	0	0
0	D		44	21	$\overline{7}$	14	2	0	0	

• Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	1	Total Na 1 1	0	0
4	В	1	Total Na 1 1	0	0

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





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 14 9 5 \end{array}$	0	0
5	А	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 14 9 5 \end{array}$	0	0
5	А	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 14 9 5 \end{array}$	0	0
5	А	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 14 9 5 \end{array}$	0	0
5	В	1	Total C O 11 7 4	0	0
5	В	1	Total C O 14 9 5	0	0
5	В	1	Total C O 11 7 4	0	0
5	В	1	Total C O 14 9 5	0	0
5	В	1	Total C O 14 9 5	0	0

• Molecule 6 is water.

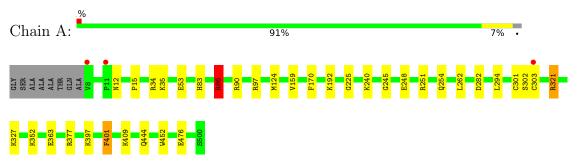
Mo	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	482	Total O 482 482	0	0
6	В	459	Total O 459 459	0	0



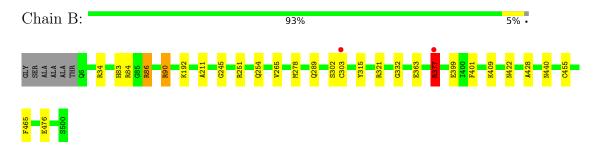
3 Residue-property plots (i)

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: Aldehyde dehydrogenase, mitochondrial



• Molecule 1: Aldehyde dehydrogenase, mitochondrial





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 2 2	Depositor
Cell constants	119.96Å 119.96Å 135.29Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.92 - 1.50	Depositor
Resolution (A)	49.87 - 1.50	EDS
% Data completeness	99.9 (49.92-1.50)	Depositor
(in resolution range)	99.9 (49.87 - 1.50)	EDS
R _{merge}	(Not available)	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.93 (at 1.50 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0352	Depositor
D D.	0.136 , 0.157	Depositor
R, R_{free}	0.136 , 0.135	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 $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.37, 51.8	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.

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.



¹Intensities estimated from amplitudes.

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: CIT, NA, 1PE, 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).

Mal	Mol Chain		nd lengths	Bond angles		
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.61	2/3981~(0.1%)	0.92	6/5400~(0.1%)	
1	В	0.61	3/3939~(0.1%)	0.87	3/5343~(0.1%)	
All	All	0.61	5/7920~(0.1%)	0.90	9/10743~(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	А	0	5
1	В	0	4
All	All	0	9

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(Å)
1	В	399	GLU	CD-OE2	5.42	1.31	1.25
1	А	476	GLU	CD-OE2	5.18	1.31	1.25
1	А	476	GLU	CD-OE1	-5.16	1.20	1.25
1	В	476	GLU	CD-OE1	-5.14	1.20	1.25
1	В	363	GLU	CD-OE1	5.14	1.31	1.25

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	86[A]	ARG	NE-CZ-NH1	11.03	125.81	120.30
1	А	86[B]	ARG	NE-CZ-NH1	11.03	125.81	120.30
1	В	84	ARG	NE-CZ-NH2	-9.86	115.37	120.30
1	А	86[A]	ARG	NE-CZ-NH2	-9.58	115.51	120.30

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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	86[B]	ARG	NE-CZ-NH2	-9.58	115.51	120.30

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	А	251	ARG	Sidechain
1	А	321	ARG	Sidechain
1	А	377	ARG	Sidechain
1	А	86[A]	ARG	Sidechain
1	А	86[B]	ARG	Sidechain

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	А	3878	0	3826	43	0
1	В	3855	0	3787	30	0
2	А	13	0	5	0	0
2	В	13	0	5	4	0
3	А	88	0	52	11	0
3	В	44	0	26	6	0
4	А	1	0	0	0	0
4	В	1	0	0	0	0
5	А	56	0	68	9	0
5	В	64	0	77	6	0
6	А	482	0	0	13	0
6	В	459	0	0	7	0
All	All	8954	0	7846	84	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.

The worst 5 of 84 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
5:A:606:1PE:C24	5:A:606:1PE:OH3	2.15	0.94
1:A:321:ARG:HH21	5:A:604:1PE:H122	1.35	0.92
1:A:352:LYS:HE2	6:A:928:HOH:O	1.69	0.90

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	Percer	ntiles
1	А	504/501~(101%)	491~(97%)	13 (3%)	0	100	100
1	В	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 (i)

In the following table, the Percentiles column shows the percent side chain 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	Analysed Rotameric Outliers		Percentiles		
1	А	412/402~(102%)	410 (100%)	2~(0%)		88	78
1	В	406/402~(101%)	403 (99%)	3 (1%)		84	69
All	All	818/804 (102%)	813~(99%)	5 (1%)		86	74



All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	192	LYS
1	А	401	PHE
1	В	192	LYS
1	В	377	ARG
1	В	401	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	В	422	ASN
1	В	358	ASN
1	В	83	HIS
1	В	13	GLN
1	В	289	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 monosaccharides 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	Turne	Chain	Res	Link	Bo	ond leng	ths	Bond angles		
10101	Type	Unam	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
5	1PE	В	608	-	$13,\!13,\!15$	0.26	0	12,12,14	0.14	0
5	1PE	А	605	-	$13,\!13,\!15$	0.21	0	12,12,14	0.31	0
5	1PE	А	606	-	$13,\!13,\!15$	0.31	0	12,12,14	0.25	0
5	1PE	В	606	-	10, 10, 15	0.30	0	9,9,14	0.19	0
5	1PE	А	604	-	$13,\!13,\!15$	0.35	0	12,12,14	0.48	0
5	1PE	В	601	-	10,10,15	0.16	0	9,9,14	0.15	0
3	NAD	В	603	-	42,48,48	0.90	1 (2%)	50,73,73	1.43	8 (16%)
5	1PE	В	605	-	$13,\!13,\!15$	0.33	0	12,12,14	0.39	0
2	CIT	А	601	-	12,12,12	1.28	3 (25%)	17,17,17	1.51	3 (17%)
5	1PE	В	607	_	$13,\!13,\!15$	0.28	0	12,12,14	0.29	0
5	1PE	А	607	-	$13,\!13,\!15$	0.42	0	12,12,14	0.28	0
2	CIT	В	602	-	12,12,12	1.27	2 (16%)	17,17,17	1.39	2 (11%)
3	NAD	А	602[B]	-	42,48,48	0.95	1 (2%)	50,73,73	1.62	11 (22%)
3	NAD	А	602[A]	-	42,48,48	0.74	1 (2%)	50,73,73	0.83	3 (6%)

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	В	608	-	-	5/11/11/13	-
5	1PE	А	605	-	-	2/11/11/13	-
5	1PE	А	606	-	-	6/11/11/13	-
5	1PE	В	606	-	-	4/8/8/13	-
5	1PE	А	604	-	-	5/11/11/13	-
5	1PE	В	601	-	-	3/8/8/13	-
3	NAD	В	603	-	-	8/26/62/62	0/5/5/5
5	1PE	В	605	-	-	6/11/11/13	-
2	CIT	А	601	-	-	0/16/16/16	-
5	1PE	В	607	-	-	7/11/11/13	-
5	1PE	А	607	-	-	6/11/11/13	-
2	CIT	В	602	-	-	8/16/16/16	-
3	NAD	А	602[B]	-	-	5/26/62/62	0/5/5/5
3	NAD	А	602[A]	-	-	5/26/62/62	0/5/5/5

The worst 5 of 8 bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
3	В	603	NAD	C2N-N1N	3.48	1.39	1.35
3	А	602[B]	NAD	C2N-N1N	3.39	1.39	1.35
2	А	601	CIT	O4-C5	-2.48	1.22	1.30
2	В	602	CIT	C3-C6	2.31	1.55	1.53
3	А	602[A]	NAD	C2N-N1N	2.30	1.37	1.35

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	А	602[B]	NAD	O4D-C1D-C2D	-5.77	98.49	106.93
2	В	602	CIT	O5-C6-C3	-3.84	116.82	122.25
3	В	603	NAD	O2D-C2D-C3D	-3.68	99.92	111.82
3	В	603	NAD	O4D-C1D-C2D	-3.57	101.70	106.93
3	В	603	NAD	C6N-N1N-C2N	-3.43	118.85	121.97

There are no chirality outliers.

5 of 70 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	В	602	CIT	C2-C3-C6-O5
2	В	602	CIT	C2-C3-C6-O6
2	В	602	CIT	O7-C3-C6-O5
2	В	602	CIT	O7-C3-C6-O6
3	А	602[A]	NAD	C5D-O5D-PN-O3

There are no ring outliers.

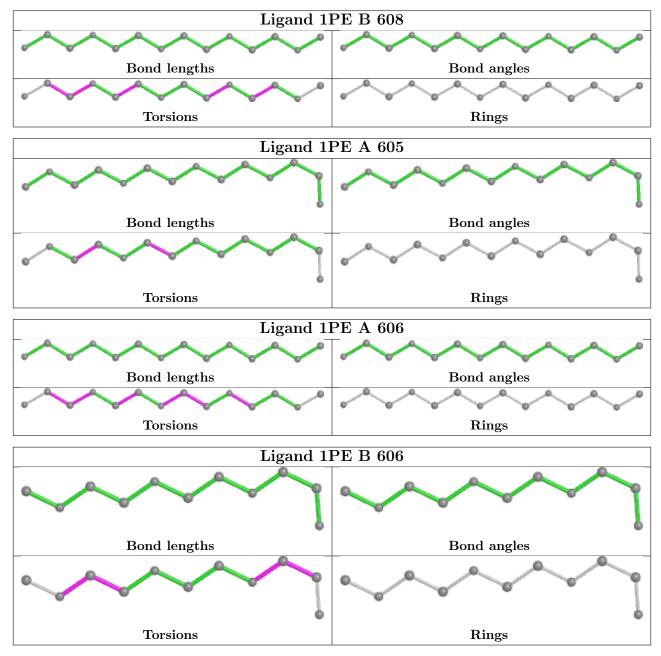
11 monomers are involved in 36 short contacts:

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

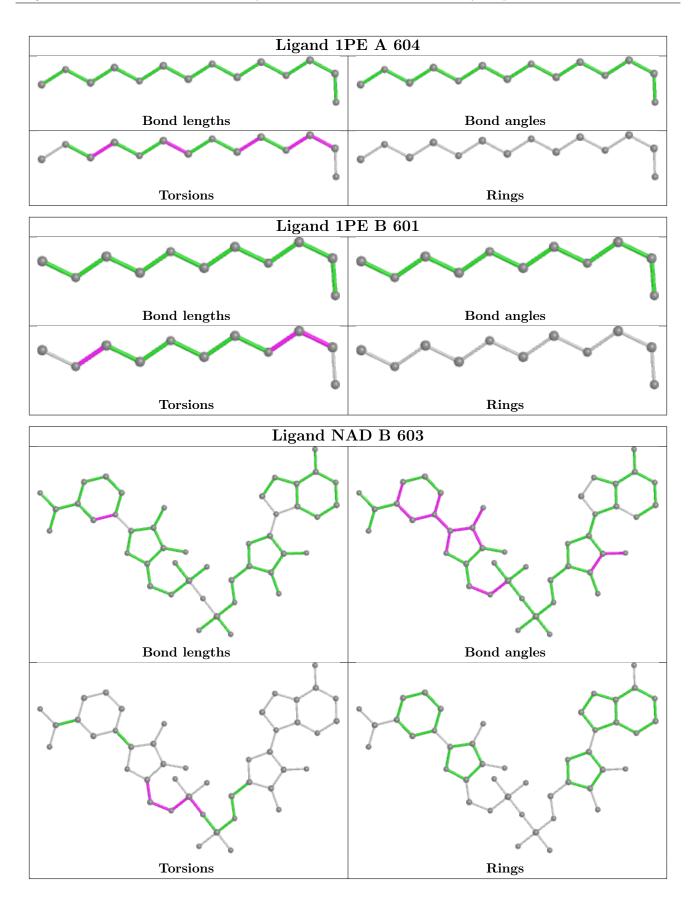
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,



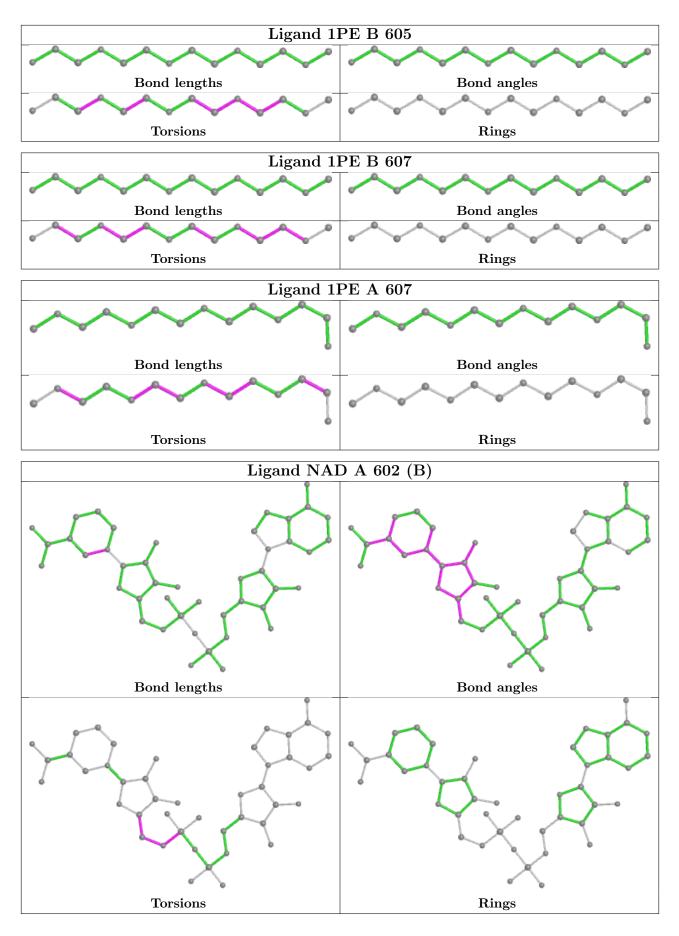
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 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.



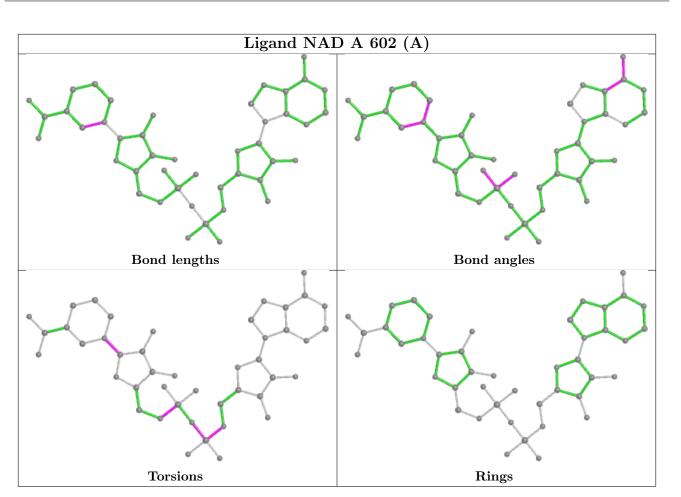












5.7 Other polymers (i)

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, 95^{th} 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	$\langle RSRZ \rangle$	#RSRZ>2		$\mathbf{OWAB}(\mathrm{\AA}^2)$	Q < 0.9
1	А	493/501~(98%)	-0.54	3 (0%) 89	91	11, 15, 25, 43	0
1	В	495/501~(98%)	-0.44	2 (0%) 92	94	11, 16, 29, 51	0
All	All	988/1002~(98%)	-0.49	5 (0%) 91	93	11, 15, 26, 51	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	303[A]	CYS	2.8
1	В	377	ARG	2.3
1	В	303[A]	CYS	2.3
1	А	11	PRO	2.1
1	А	8	VAL	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 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, 95^{th} 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.

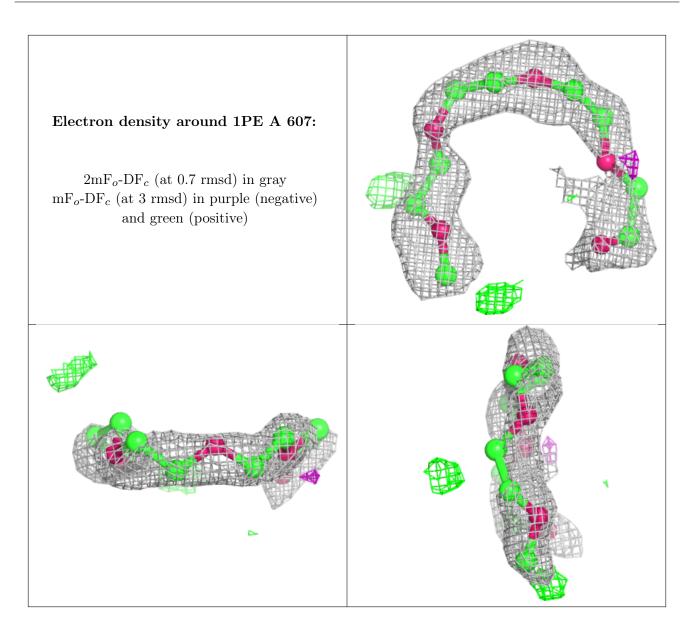


8DR9

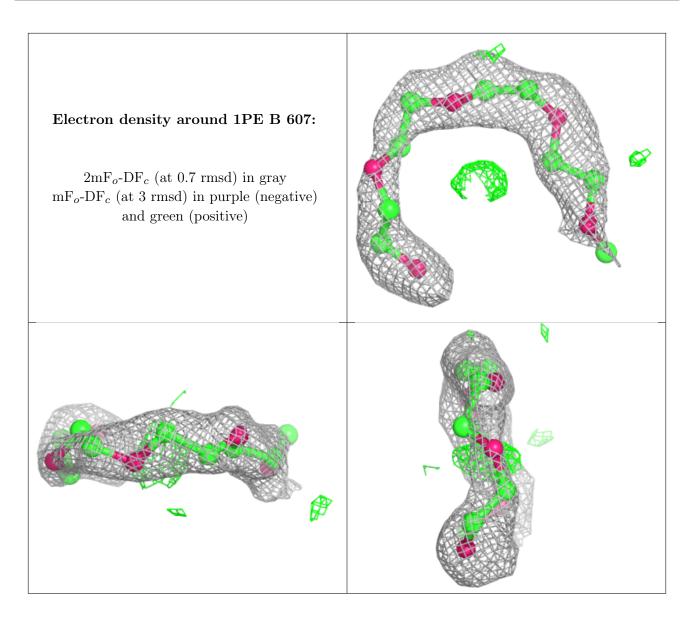
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B -factors($Å^2$)	Q<0.9
5	1PE	А	607	14/16	0.75	0.18	45,51,63,64	0
2	CIT	В	602	13/13	0.80	0.16	40,56,75,79	0
5	1PE	В	607	14/16	0.81	0.14	45,54,64,67	0
5	1PE	В	605	14/16	0.86	0.13	32,39,47,56	0
5	1PE	В	606	11/16	0.88	0.14	48,52,57,65	0
5	1PE	В	601	11/16	0.89	0.14	42,48,61,66	0
5	1PE	А	606	14/16	0.89	0.13	34,38,39,41	14
5	1PE	В	608	14/16	0.89	0.17	34,42,58,60	14
5	1PE	А	605	14/16	0.92	0.10	25,34,44,46	0
3	NAD	А	602[A]	44/44	0.92	0.16	4,7,10,11	44
3	NAD	А	602[B]	44/44	0.92	0.16	13,22,51,63	44
5	1PE	А	604	14/16	0.92	0.12	20,38,61,66	0
3	NAD	В	603	44/44	0.96	0.10	13,21,49,63	0
2	CIT	А	601	13/13	0.96	0.08	17,21,28,28	0
4	NA	В	604	1/1	0.99	0.03	16,16,16,16	0
4	NA	А	603	1/1	0.99	0.03	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.

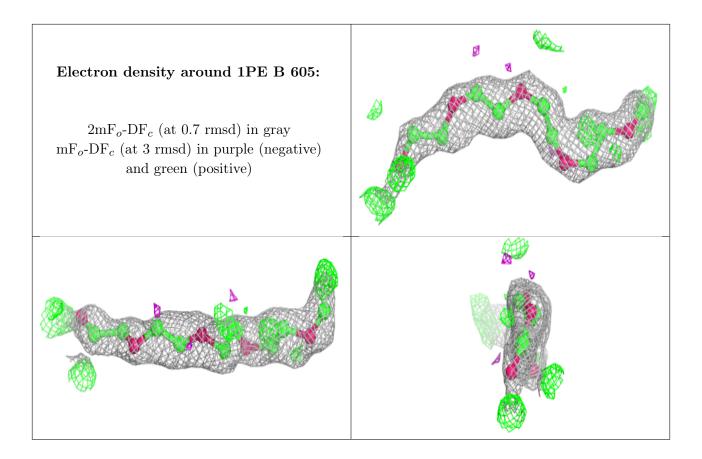




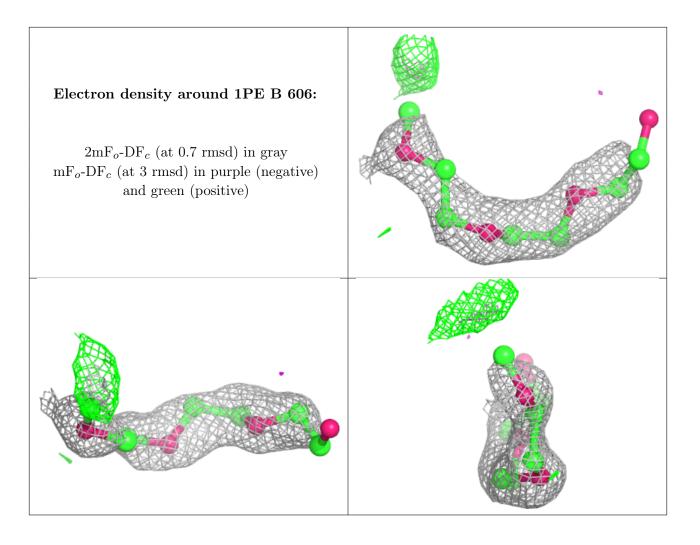




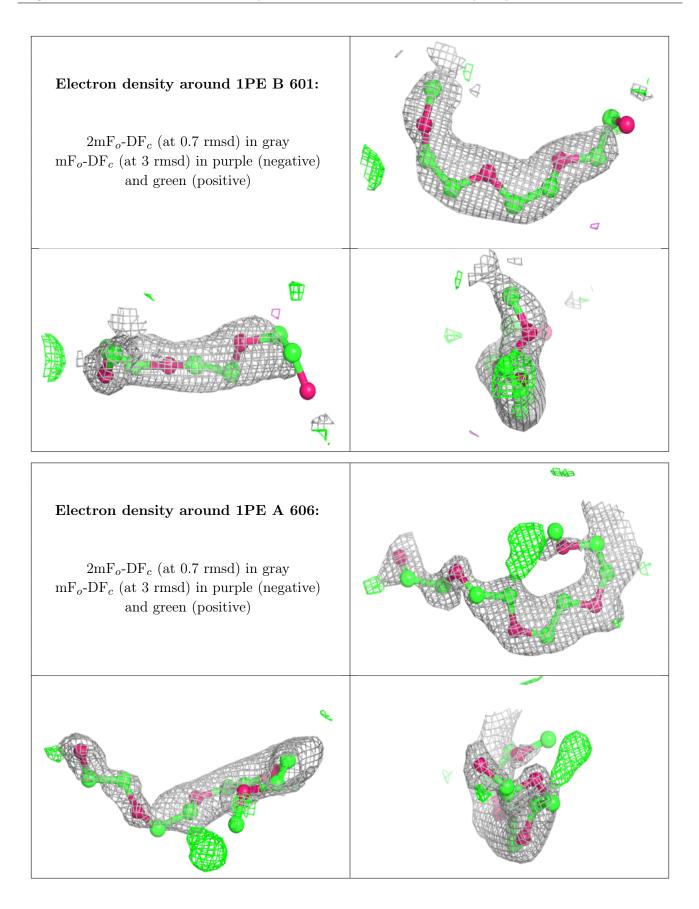




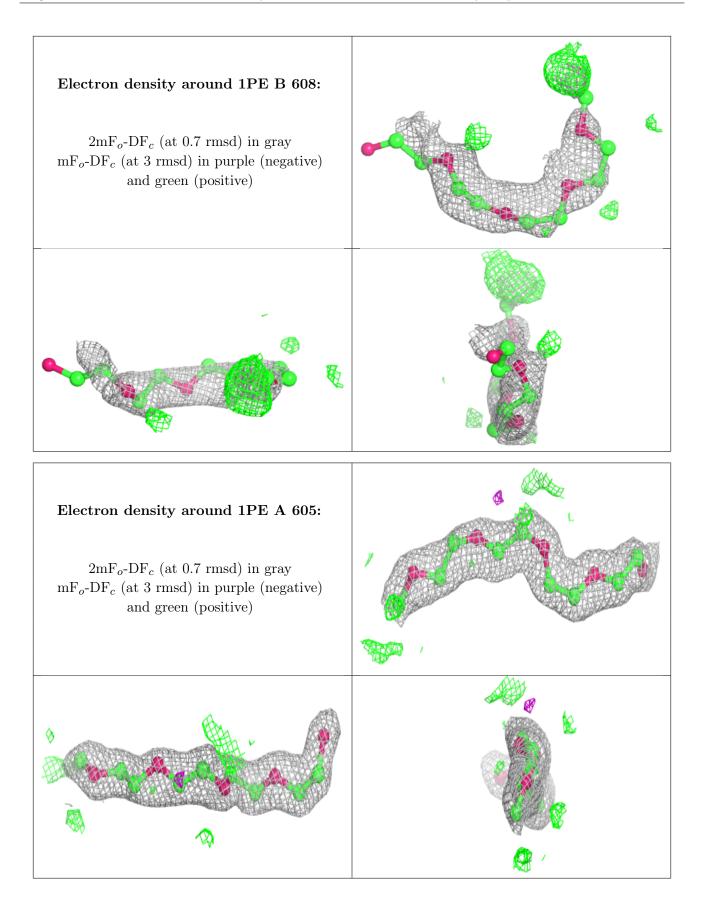




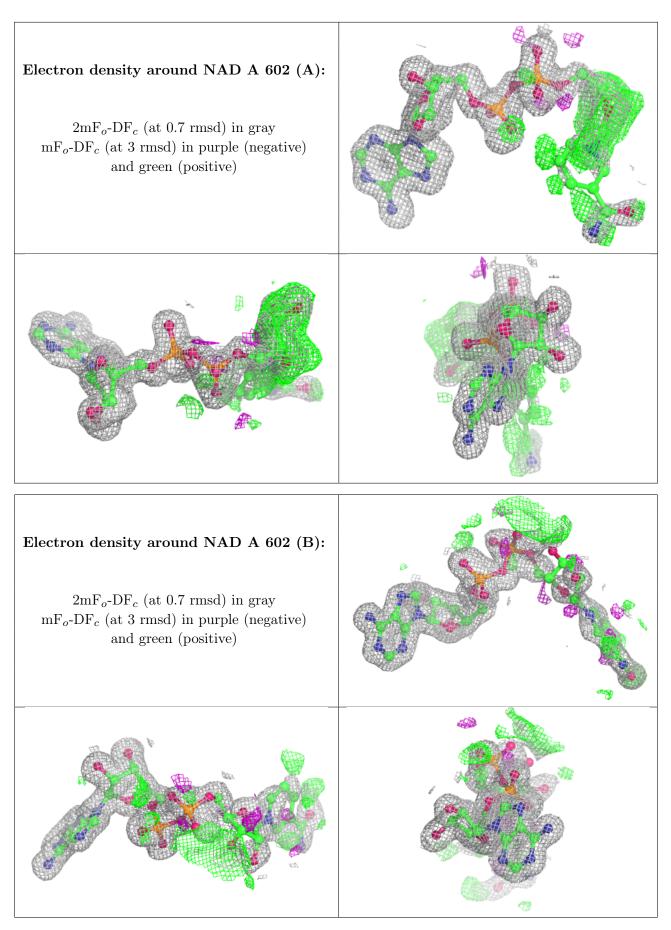




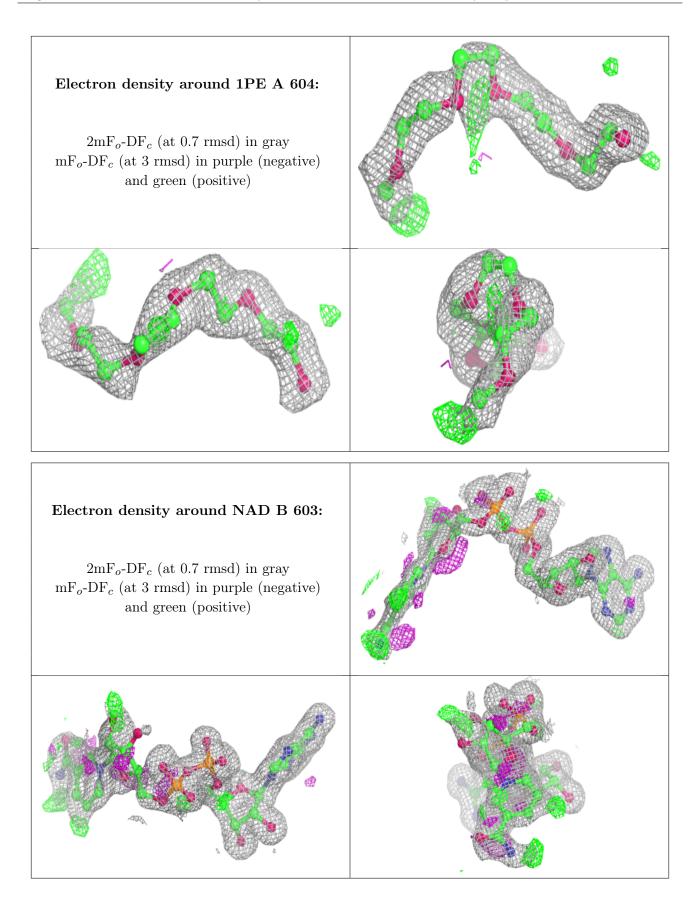














6.5 Other polymers (i)

There are no such residues in this entry.

