



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 09:20 AM UTC

PDB ID : 5JFL / pdb_00005jfl
Title : Crystal structure of Rhodopseudomonas palustris propionaldehyde dehydrogenase with bound NAD⁺
Authors : Zarzycki, J.; Sutter, M.; Kerfeld, C.A.
Deposited on : 2016-04-19
Resolution : 2.30 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

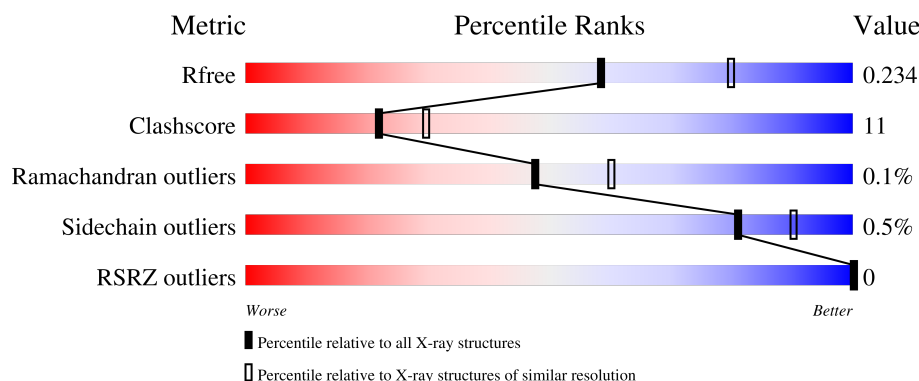
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	524	70% 14% 16%
1	B	524	65% 18% 16%
1	C	524	64% 19% 16%
1	D	524	67% 17% 15%
1	E	524	62% 22% 16%

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Mol	Chain	Length	Quality of chain
1	F	524	 64% 20% 16%
1	G	524	 66% 19% 15%
1	H	524	 61% 23% 16%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 27656 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	440	Total	C	N	O	S	0	0	0
			3291	2072	567	630	22			
1	B	439	Total	C	N	O	S	0	1	0
			3294	2077	566	629	22			
1	C	439	Total	C	N	O	S	0	0	0
			3286	2069	566	629	22			
1	D	445	Total	C	N	O	S	0	0	0
			3326	2092	573	639	22			
1	E	439	Total	C	N	O	S	0	0	0
			3286	2069	566	629	22			
1	F	440	Total	C	N	O	S	0	0	0
			3291	2072	567	630	22			
1	G	445	Total	C	N	O	S	0	0	0
			3326	2092	573	639	22			
1	H	439	Total	C	N	O	S	0	0	0
			3286	2069	566	629	22			

There are 480 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q21A49
A	2	ALA	-	expression tag	UNP Q21A49
A	3	TRP	-	expression tag	UNP Q21A49
A	4	SER	-	expression tag	UNP Q21A49
A	5	HIS	-	expression tag	UNP Q21A49
A	6	PRO	-	expression tag	UNP Q21A49
A	7	GLN	-	expression tag	UNP Q21A49
A	8	PHE	-	expression tag	UNP Q21A49
A	9	GLU	-	expression tag	UNP Q21A49
A	10	LYS	-	expression tag	UNP Q21A49
A	11	GLY	-	expression tag	UNP Q21A49
A	12	HIS	-	expression tag	UNP Q21A49
A	13	MET	-	expression tag	UNP Q21A49

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Chain	Residue	Modelled	Actual	Comment	Reference
A	14	ASN	-	expression tag	UNP Q21A49
A	15	ASP	-	expression tag	UNP Q21A49
A	16	ALA	-	expression tag	UNP Q21A49
A	17	ASN	-	expression tag	UNP Q21A49
A	18	ILE	-	expression tag	UNP Q21A49
A	19	ALA	-	expression tag	UNP Q21A49
A	20	ASP	-	expression tag	UNP Q21A49
A	21	VAL	-	expression tag	UNP Q21A49
A	22	VAL	-	expression tag	UNP Q21A49
A	23	THR	-	expression tag	UNP Q21A49
A	24	LYS	-	expression tag	UNP Q21A49
A	25	VAL	-	expression tag	UNP Q21A49
A	26	LEU	-	expression tag	UNP Q21A49
A	27	GLY	-	expression tag	UNP Q21A49
A	28	GLU	-	expression tag	UNP Q21A49
A	29	TYR	-	expression tag	UNP Q21A49
A	30	GLY	-	expression tag	UNP Q21A49
A	31	ALA	-	expression tag	UNP Q21A49
A	32	PRO	-	expression tag	UNP Q21A49
A	33	GLY	-	expression tag	UNP Q21A49
A	34	ALA	-	expression tag	UNP Q21A49
A	35	VAL	-	expression tag	UNP Q21A49
A	36	SER	-	expression tag	UNP Q21A49
A	37	VAL	-	expression tag	UNP Q21A49
A	38	ALA	-	expression tag	UNP Q21A49
A	39	ALA	-	expression tag	UNP Q21A49
A	40	LEU	-	expression tag	UNP Q21A49
A	41	THR	-	expression tag	UNP Q21A49
A	42	ALA	-	expression tag	UNP Q21A49
A	43	LYS	-	expression tag	UNP Q21A49
A	44	SER	-	expression tag	UNP Q21A49
A	45	PRO	-	expression tag	UNP Q21A49
A	46	ASP	-	expression tag	UNP Q21A49
A	47	GLY	-	expression tag	UNP Q21A49
A	48	LYS	-	expression tag	UNP Q21A49
A	49	SER	-	expression tag	UNP Q21A49
A	50	ASN	-	expression tag	UNP Q21A49
A	51	SER	-	expression tag	UNP Q21A49
A	52	SER	-	expression tag	UNP Q21A49
A	53	ALA	-	expression tag	UNP Q21A49
A	54	ASP	-	expression tag	UNP Q21A49
A	55	ALA	-	expression tag	UNP Q21A49

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Chain	Residue	Modelled	Actual	Comment	Reference
A	56	ASP	-	expression tag	UNP Q21A49
A	57	VAL	-	expression tag	UNP Q21A49
A	58	VAL	-	expression tag	UNP Q21A49
A	59	ALA	-	expression tag	UNP Q21A49
A	60	ARG	-	expression tag	UNP Q21A49
B	1	MET	-	initiating methionine	UNP Q21A49
B	2	ALA	-	expression tag	UNP Q21A49
B	3	TRP	-	expression tag	UNP Q21A49
B	4	SER	-	expression tag	UNP Q21A49
B	5	HIS	-	expression tag	UNP Q21A49
B	6	PRO	-	expression tag	UNP Q21A49
B	7	GLN	-	expression tag	UNP Q21A49
B	8	PHE	-	expression tag	UNP Q21A49
B	9	GLU	-	expression tag	UNP Q21A49
B	10	LYS	-	expression tag	UNP Q21A49
B	11	GLY	-	expression tag	UNP Q21A49
B	12	HIS	-	expression tag	UNP Q21A49
B	13	MET	-	expression tag	UNP Q21A49
B	14	ASN	-	expression tag	UNP Q21A49
B	15	ASP	-	expression tag	UNP Q21A49
B	16	ALA	-	expression tag	UNP Q21A49
B	17	ASN	-	expression tag	UNP Q21A49
B	18	ILE	-	expression tag	UNP Q21A49
B	19	ALA	-	expression tag	UNP Q21A49
B	20	ASP	-	expression tag	UNP Q21A49
B	21	VAL	-	expression tag	UNP Q21A49
B	22	VAL	-	expression tag	UNP Q21A49
B	23	THR	-	expression tag	UNP Q21A49
B	24	LYS	-	expression tag	UNP Q21A49
B	25	VAL	-	expression tag	UNP Q21A49
B	26	LEU	-	expression tag	UNP Q21A49
B	27	GLY	-	expression tag	UNP Q21A49
B	28	GLU	-	expression tag	UNP Q21A49
B	29	TYR	-	expression tag	UNP Q21A49
B	30	GLY	-	expression tag	UNP Q21A49
B	31	ALA	-	expression tag	UNP Q21A49
B	32	PRO	-	expression tag	UNP Q21A49
B	33	GLY	-	expression tag	UNP Q21A49
B	34	ALA	-	expression tag	UNP Q21A49
B	35	VAL	-	expression tag	UNP Q21A49
B	36	SER	-	expression tag	UNP Q21A49
B	37	VAL	-	expression tag	UNP Q21A49

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Chain	Residue	Modelled	Actual	Comment	Reference
B	38	ALA	-	expression tag	UNP Q21A49
B	39	ALA	-	expression tag	UNP Q21A49
B	40	LEU	-	expression tag	UNP Q21A49
B	41	THR	-	expression tag	UNP Q21A49
B	42	ALA	-	expression tag	UNP Q21A49
B	43	LYS	-	expression tag	UNP Q21A49
B	44	SER	-	expression tag	UNP Q21A49
B	45	PRO	-	expression tag	UNP Q21A49
B	46	ASP	-	expression tag	UNP Q21A49
B	47	GLY	-	expression tag	UNP Q21A49
B	48	LYS	-	expression tag	UNP Q21A49
B	49	SER	-	expression tag	UNP Q21A49
B	50	ASN	-	expression tag	UNP Q21A49
B	51	SER	-	expression tag	UNP Q21A49
B	52	SER	-	expression tag	UNP Q21A49
B	53	ALA	-	expression tag	UNP Q21A49
B	54	ASP	-	expression tag	UNP Q21A49
B	55	ALA	-	expression tag	UNP Q21A49
B	56	ASP	-	expression tag	UNP Q21A49
B	57	VAL	-	expression tag	UNP Q21A49
B	58	VAL	-	expression tag	UNP Q21A49
B	59	ALA	-	expression tag	UNP Q21A49
B	60	ARG	-	expression tag	UNP Q21A49
C	1	MET	-	initiating methionine	UNP Q21A49
C	2	ALA	-	expression tag	UNP Q21A49
C	3	TRP	-	expression tag	UNP Q21A49
C	4	SER	-	expression tag	UNP Q21A49
C	5	HIS	-	expression tag	UNP Q21A49
C	6	PRO	-	expression tag	UNP Q21A49
C	7	GLN	-	expression tag	UNP Q21A49
C	8	PHE	-	expression tag	UNP Q21A49
C	9	GLU	-	expression tag	UNP Q21A49
C	10	LYS	-	expression tag	UNP Q21A49
C	11	GLY	-	expression tag	UNP Q21A49
C	12	HIS	-	expression tag	UNP Q21A49
C	13	MET	-	expression tag	UNP Q21A49
C	14	ASN	-	expression tag	UNP Q21A49
C	15	ASP	-	expression tag	UNP Q21A49
C	16	ALA	-	expression tag	UNP Q21A49
C	17	ASN	-	expression tag	UNP Q21A49
C	18	ILE	-	expression tag	UNP Q21A49
C	19	ALA	-	expression tag	UNP Q21A49

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Chain	Residue	Modelled	Actual	Comment	Reference
C	20	ASP	-	expression tag	UNP Q21A49
C	21	VAL	-	expression tag	UNP Q21A49
C	22	VAL	-	expression tag	UNP Q21A49
C	23	THR	-	expression tag	UNP Q21A49
C	24	LYS	-	expression tag	UNP Q21A49
C	25	VAL	-	expression tag	UNP Q21A49
C	26	LEU	-	expression tag	UNP Q21A49
C	27	GLY	-	expression tag	UNP Q21A49
C	28	GLU	-	expression tag	UNP Q21A49
C	29	TYR	-	expression tag	UNP Q21A49
C	30	GLY	-	expression tag	UNP Q21A49
C	31	ALA	-	expression tag	UNP Q21A49
C	32	PRO	-	expression tag	UNP Q21A49
C	33	GLY	-	expression tag	UNP Q21A49
C	34	ALA	-	expression tag	UNP Q21A49
C	35	VAL	-	expression tag	UNP Q21A49
C	36	SER	-	expression tag	UNP Q21A49
C	37	VAL	-	expression tag	UNP Q21A49
C	38	ALA	-	expression tag	UNP Q21A49
C	39	ALA	-	expression tag	UNP Q21A49
C	40	LEU	-	expression tag	UNP Q21A49
C	41	THR	-	expression tag	UNP Q21A49
C	42	ALA	-	expression tag	UNP Q21A49
C	43	LYS	-	expression tag	UNP Q21A49
C	44	SER	-	expression tag	UNP Q21A49
C	45	PRO	-	expression tag	UNP Q21A49
C	46	ASP	-	expression tag	UNP Q21A49
C	47	GLY	-	expression tag	UNP Q21A49
C	48	LYS	-	expression tag	UNP Q21A49
C	49	SER	-	expression tag	UNP Q21A49
C	50	ASN	-	expression tag	UNP Q21A49
C	51	SER	-	expression tag	UNP Q21A49
C	52	SER	-	expression tag	UNP Q21A49
C	53	ALA	-	expression tag	UNP Q21A49
C	54	ASP	-	expression tag	UNP Q21A49
C	55	ALA	-	expression tag	UNP Q21A49
C	56	ASP	-	expression tag	UNP Q21A49
C	57	VAL	-	expression tag	UNP Q21A49
C	58	VAL	-	expression tag	UNP Q21A49
C	59	ALA	-	expression tag	UNP Q21A49
C	60	ARG	-	expression tag	UNP Q21A49
D	1	MET	-	initiating methionine	UNP Q21A49

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Chain	Residue	Modelled	Actual	Comment	Reference
D	2	ALA	-	expression tag	UNP Q21A49
D	3	TRP	-	expression tag	UNP Q21A49
D	4	SER	-	expression tag	UNP Q21A49
D	5	HIS	-	expression tag	UNP Q21A49
D	6	PRO	-	expression tag	UNP Q21A49
D	7	GLN	-	expression tag	UNP Q21A49
D	8	PHE	-	expression tag	UNP Q21A49
D	9	GLU	-	expression tag	UNP Q21A49
D	10	LYS	-	expression tag	UNP Q21A49
D	11	GLY	-	expression tag	UNP Q21A49
D	12	HIS	-	expression tag	UNP Q21A49
D	13	MET	-	expression tag	UNP Q21A49
D	14	ASN	-	expression tag	UNP Q21A49
D	15	ASP	-	expression tag	UNP Q21A49
D	16	ALA	-	expression tag	UNP Q21A49
D	17	ASN	-	expression tag	UNP Q21A49
D	18	ILE	-	expression tag	UNP Q21A49
D	19	ALA	-	expression tag	UNP Q21A49
D	20	ASP	-	expression tag	UNP Q21A49
D	21	VAL	-	expression tag	UNP Q21A49
D	22	VAL	-	expression tag	UNP Q21A49
D	23	THR	-	expression tag	UNP Q21A49
D	24	LYS	-	expression tag	UNP Q21A49
D	25	VAL	-	expression tag	UNP Q21A49
D	26	LEU	-	expression tag	UNP Q21A49
D	27	GLY	-	expression tag	UNP Q21A49
D	28	GLU	-	expression tag	UNP Q21A49
D	29	TYR	-	expression tag	UNP Q21A49
D	30	GLY	-	expression tag	UNP Q21A49
D	31	ALA	-	expression tag	UNP Q21A49
D	32	PRO	-	expression tag	UNP Q21A49
D	33	GLY	-	expression tag	UNP Q21A49
D	34	ALA	-	expression tag	UNP Q21A49
D	35	VAL	-	expression tag	UNP Q21A49
D	36	SER	-	expression tag	UNP Q21A49
D	37	VAL	-	expression tag	UNP Q21A49
D	38	ALA	-	expression tag	UNP Q21A49
D	39	ALA	-	expression tag	UNP Q21A49
D	40	LEU	-	expression tag	UNP Q21A49
D	41	THR	-	expression tag	UNP Q21A49
D	42	ALA	-	expression tag	UNP Q21A49
D	43	LYS	-	expression tag	UNP Q21A49

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Chain	Residue	Modelled	Actual	Comment	Reference
D	44	SER	-	expression tag	UNP Q21A49
D	45	PRO	-	expression tag	UNP Q21A49
D	46	ASP	-	expression tag	UNP Q21A49
D	47	GLY	-	expression tag	UNP Q21A49
D	48	LYS	-	expression tag	UNP Q21A49
D	49	SER	-	expression tag	UNP Q21A49
D	50	ASN	-	expression tag	UNP Q21A49
D	51	SER	-	expression tag	UNP Q21A49
D	52	SER	-	expression tag	UNP Q21A49
D	53	ALA	-	expression tag	UNP Q21A49
D	54	ASP	-	expression tag	UNP Q21A49
D	55	ALA	-	expression tag	UNP Q21A49
D	56	ASP	-	expression tag	UNP Q21A49
D	57	VAL	-	expression tag	UNP Q21A49
D	58	VAL	-	expression tag	UNP Q21A49
D	59	ALA	-	expression tag	UNP Q21A49
D	60	ARG	-	expression tag	UNP Q21A49
E	1	MET	-	initiating methionine	UNP Q21A49
E	2	ALA	-	expression tag	UNP Q21A49
E	3	TRP	-	expression tag	UNP Q21A49
E	4	SER	-	expression tag	UNP Q21A49
E	5	HIS	-	expression tag	UNP Q21A49
E	6	PRO	-	expression tag	UNP Q21A49
E	7	GLN	-	expression tag	UNP Q21A49
E	8	PHE	-	expression tag	UNP Q21A49
E	9	GLU	-	expression tag	UNP Q21A49
E	10	LYS	-	expression tag	UNP Q21A49
E	11	GLY	-	expression tag	UNP Q21A49
E	12	HIS	-	expression tag	UNP Q21A49
E	13	MET	-	expression tag	UNP Q21A49
E	14	ASN	-	expression tag	UNP Q21A49
E	15	ASP	-	expression tag	UNP Q21A49
E	16	ALA	-	expression tag	UNP Q21A49
E	17	ASN	-	expression tag	UNP Q21A49
E	18	ILE	-	expression tag	UNP Q21A49
E	19	ALA	-	expression tag	UNP Q21A49
E	20	ASP	-	expression tag	UNP Q21A49
E	21	VAL	-	expression tag	UNP Q21A49
E	22	VAL	-	expression tag	UNP Q21A49
E	23	THR	-	expression tag	UNP Q21A49
E	24	LYS	-	expression tag	UNP Q21A49
E	25	VAL	-	expression tag	UNP Q21A49

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Chain	Residue	Modelled	Actual	Comment	Reference
E	26	LEU	-	expression tag	UNP Q21A49
E	27	GLY	-	expression tag	UNP Q21A49
E	28	GLU	-	expression tag	UNP Q21A49
E	29	TYR	-	expression tag	UNP Q21A49
E	30	GLY	-	expression tag	UNP Q21A49
E	31	ALA	-	expression tag	UNP Q21A49
E	32	PRO	-	expression tag	UNP Q21A49
E	33	GLY	-	expression tag	UNP Q21A49
E	34	ALA	-	expression tag	UNP Q21A49
E	35	VAL	-	expression tag	UNP Q21A49
E	36	SER	-	expression tag	UNP Q21A49
E	37	VAL	-	expression tag	UNP Q21A49
E	38	ALA	-	expression tag	UNP Q21A49
E	39	ALA	-	expression tag	UNP Q21A49
E	40	LEU	-	expression tag	UNP Q21A49
E	41	THR	-	expression tag	UNP Q21A49
E	42	ALA	-	expression tag	UNP Q21A49
E	43	LYS	-	expression tag	UNP Q21A49
E	44	SER	-	expression tag	UNP Q21A49
E	45	PRO	-	expression tag	UNP Q21A49
E	46	ASP	-	expression tag	UNP Q21A49
E	47	GLY	-	expression tag	UNP Q21A49
E	48	LYS	-	expression tag	UNP Q21A49
E	49	SER	-	expression tag	UNP Q21A49
E	50	ASN	-	expression tag	UNP Q21A49
E	51	SER	-	expression tag	UNP Q21A49
E	52	SER	-	expression tag	UNP Q21A49
E	53	ALA	-	expression tag	UNP Q21A49
E	54	ASP	-	expression tag	UNP Q21A49
E	55	ALA	-	expression tag	UNP Q21A49
E	56	ASP	-	expression tag	UNP Q21A49
E	57	VAL	-	expression tag	UNP Q21A49
E	58	VAL	-	expression tag	UNP Q21A49
E	59	ALA	-	expression tag	UNP Q21A49
E	60	ARG	-	expression tag	UNP Q21A49
F	1	MET	-	initiating methionine	UNP Q21A49
F	2	ALA	-	expression tag	UNP Q21A49
F	3	TRP	-	expression tag	UNP Q21A49
F	4	SER	-	expression tag	UNP Q21A49
F	5	HIS	-	expression tag	UNP Q21A49
F	6	PRO	-	expression tag	UNP Q21A49
F	7	GLN	-	expression tag	UNP Q21A49

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Chain	Residue	Modelled	Actual	Comment	Reference
F	8	PHE	-	expression tag	UNP Q21A49
F	9	GLU	-	expression tag	UNP Q21A49
F	10	LYS	-	expression tag	UNP Q21A49
F	11	GLY	-	expression tag	UNP Q21A49
F	12	HIS	-	expression tag	UNP Q21A49
F	13	MET	-	expression tag	UNP Q21A49
F	14	ASN	-	expression tag	UNP Q21A49
F	15	ASP	-	expression tag	UNP Q21A49
F	16	ALA	-	expression tag	UNP Q21A49
F	17	ASN	-	expression tag	UNP Q21A49
F	18	ILE	-	expression tag	UNP Q21A49
F	19	ALA	-	expression tag	UNP Q21A49
F	20	ASP	-	expression tag	UNP Q21A49
F	21	VAL	-	expression tag	UNP Q21A49
F	22	VAL	-	expression tag	UNP Q21A49
F	23	THR	-	expression tag	UNP Q21A49
F	24	LYS	-	expression tag	UNP Q21A49
F	25	VAL	-	expression tag	UNP Q21A49
F	26	LEU	-	expression tag	UNP Q21A49
F	27	GLY	-	expression tag	UNP Q21A49
F	28	GLU	-	expression tag	UNP Q21A49
F	29	TYR	-	expression tag	UNP Q21A49
F	30	GLY	-	expression tag	UNP Q21A49
F	31	ALA	-	expression tag	UNP Q21A49
F	32	PRO	-	expression tag	UNP Q21A49
F	33	GLY	-	expression tag	UNP Q21A49
F	34	ALA	-	expression tag	UNP Q21A49
F	35	VAL	-	expression tag	UNP Q21A49
F	36	SER	-	expression tag	UNP Q21A49
F	37	VAL	-	expression tag	UNP Q21A49
F	38	ALA	-	expression tag	UNP Q21A49
F	39	ALA	-	expression tag	UNP Q21A49
F	40	LEU	-	expression tag	UNP Q21A49
F	41	THR	-	expression tag	UNP Q21A49
F	42	ALA	-	expression tag	UNP Q21A49
F	43	LYS	-	expression tag	UNP Q21A49
F	44	SER	-	expression tag	UNP Q21A49
F	45	PRO	-	expression tag	UNP Q21A49
F	46	ASP	-	expression tag	UNP Q21A49
F	47	GLY	-	expression tag	UNP Q21A49
F	48	LYS	-	expression tag	UNP Q21A49
F	49	SER	-	expression tag	UNP Q21A49

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Chain	Residue	Modelled	Actual	Comment	Reference
F	50	ASN	-	expression tag	UNP Q21A49
F	51	SER	-	expression tag	UNP Q21A49
F	52	SER	-	expression tag	UNP Q21A49
F	53	ALA	-	expression tag	UNP Q21A49
F	54	ASP	-	expression tag	UNP Q21A49
F	55	ALA	-	expression tag	UNP Q21A49
F	56	ASP	-	expression tag	UNP Q21A49
F	57	VAL	-	expression tag	UNP Q21A49
F	58	VAL	-	expression tag	UNP Q21A49
F	59	ALA	-	expression tag	UNP Q21A49
F	60	ARG	-	expression tag	UNP Q21A49
G	1	MET	-	initiating methionine	UNP Q21A49
G	2	ALA	-	expression tag	UNP Q21A49
G	3	TRP	-	expression tag	UNP Q21A49
G	4	SER	-	expression tag	UNP Q21A49
G	5	HIS	-	expression tag	UNP Q21A49
G	6	PRO	-	expression tag	UNP Q21A49
G	7	GLN	-	expression tag	UNP Q21A49
G	8	PHE	-	expression tag	UNP Q21A49
G	9	GLU	-	expression tag	UNP Q21A49
G	10	LYS	-	expression tag	UNP Q21A49
G	11	GLY	-	expression tag	UNP Q21A49
G	12	HIS	-	expression tag	UNP Q21A49
G	13	MET	-	expression tag	UNP Q21A49
G	14	ASN	-	expression tag	UNP Q21A49
G	15	ASP	-	expression tag	UNP Q21A49
G	16	ALA	-	expression tag	UNP Q21A49
G	17	ASN	-	expression tag	UNP Q21A49
G	18	ILE	-	expression tag	UNP Q21A49
G	19	ALA	-	expression tag	UNP Q21A49
G	20	ASP	-	expression tag	UNP Q21A49
G	21	VAL	-	expression tag	UNP Q21A49
G	22	VAL	-	expression tag	UNP Q21A49
G	23	THR	-	expression tag	UNP Q21A49
G	24	LYS	-	expression tag	UNP Q21A49
G	25	VAL	-	expression tag	UNP Q21A49
G	26	LEU	-	expression tag	UNP Q21A49
G	27	GLY	-	expression tag	UNP Q21A49
G	28	GLU	-	expression tag	UNP Q21A49
G	29	TYR	-	expression tag	UNP Q21A49
G	30	GLY	-	expression tag	UNP Q21A49
G	31	ALA	-	expression tag	UNP Q21A49

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Chain	Residue	Modelled	Actual	Comment	Reference
G	32	PRO	-	expression tag	UNP Q21A49
G	33	GLY	-	expression tag	UNP Q21A49
G	34	ALA	-	expression tag	UNP Q21A49
G	35	VAL	-	expression tag	UNP Q21A49
G	36	SER	-	expression tag	UNP Q21A49
G	37	VAL	-	expression tag	UNP Q21A49
G	38	ALA	-	expression tag	UNP Q21A49
G	39	ALA	-	expression tag	UNP Q21A49
G	40	LEU	-	expression tag	UNP Q21A49
G	41	THR	-	expression tag	UNP Q21A49
G	42	ALA	-	expression tag	UNP Q21A49
G	43	LYS	-	expression tag	UNP Q21A49
G	44	SER	-	expression tag	UNP Q21A49
G	45	PRO	-	expression tag	UNP Q21A49
G	46	ASP	-	expression tag	UNP Q21A49
G	47	GLY	-	expression tag	UNP Q21A49
G	48	LYS	-	expression tag	UNP Q21A49
G	49	SER	-	expression tag	UNP Q21A49
G	50	ASN	-	expression tag	UNP Q21A49
G	51	SER	-	expression tag	UNP Q21A49
G	52	SER	-	expression tag	UNP Q21A49
G	53	ALA	-	expression tag	UNP Q21A49
G	54	ASP	-	expression tag	UNP Q21A49
G	55	ALA	-	expression tag	UNP Q21A49
G	56	ASP	-	expression tag	UNP Q21A49
G	57	VAL	-	expression tag	UNP Q21A49
G	58	VAL	-	expression tag	UNP Q21A49
G	59	ALA	-	expression tag	UNP Q21A49
G	60	ARG	-	expression tag	UNP Q21A49
H	1	MET	-	initiating methionine	UNP Q21A49
H	2	ALA	-	expression tag	UNP Q21A49
H	3	TRP	-	expression tag	UNP Q21A49
H	4	SER	-	expression tag	UNP Q21A49
H	5	HIS	-	expression tag	UNP Q21A49
H	6	PRO	-	expression tag	UNP Q21A49
H	7	GLN	-	expression tag	UNP Q21A49
H	8	PHE	-	expression tag	UNP Q21A49
H	9	GLU	-	expression tag	UNP Q21A49
H	10	LYS	-	expression tag	UNP Q21A49
H	11	GLY	-	expression tag	UNP Q21A49
H	12	HIS	-	expression tag	UNP Q21A49
H	13	MET	-	expression tag	UNP Q21A49

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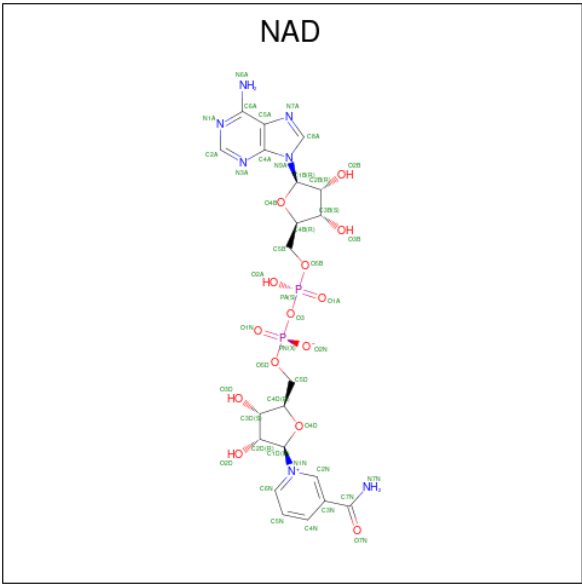
Chain	Residue	Modelled	Actual	Comment	Reference
H	14	ASN	-	expression tag	UNP Q21A49
H	15	ASP	-	expression tag	UNP Q21A49
H	16	ALA	-	expression tag	UNP Q21A49
H	17	ASN	-	expression tag	UNP Q21A49
H	18	ILE	-	expression tag	UNP Q21A49
H	19	ALA	-	expression tag	UNP Q21A49
H	20	ASP	-	expression tag	UNP Q21A49
H	21	VAL	-	expression tag	UNP Q21A49
H	22	VAL	-	expression tag	UNP Q21A49
H	23	THR	-	expression tag	UNP Q21A49
H	24	LYS	-	expression tag	UNP Q21A49
H	25	VAL	-	expression tag	UNP Q21A49
H	26	LEU	-	expression tag	UNP Q21A49
H	27	GLY	-	expression tag	UNP Q21A49
H	28	GLU	-	expression tag	UNP Q21A49
H	29	TYR	-	expression tag	UNP Q21A49
H	30	GLY	-	expression tag	UNP Q21A49
H	31	ALA	-	expression tag	UNP Q21A49
H	32	PRO	-	expression tag	UNP Q21A49
H	33	GLY	-	expression tag	UNP Q21A49
H	34	ALA	-	expression tag	UNP Q21A49
H	35	VAL	-	expression tag	UNP Q21A49
H	36	SER	-	expression tag	UNP Q21A49
H	37	VAL	-	expression tag	UNP Q21A49
H	38	ALA	-	expression tag	UNP Q21A49
H	39	ALA	-	expression tag	UNP Q21A49
H	40	LEU	-	expression tag	UNP Q21A49
H	41	THR	-	expression tag	UNP Q21A49
H	42	ALA	-	expression tag	UNP Q21A49
H	43	LYS	-	expression tag	UNP Q21A49
H	44	SER	-	expression tag	UNP Q21A49
H	45	PRO	-	expression tag	UNP Q21A49
H	46	ASP	-	expression tag	UNP Q21A49
H	47	GLY	-	expression tag	UNP Q21A49
H	48	LYS	-	expression tag	UNP Q21A49
H	49	SER	-	expression tag	UNP Q21A49
H	50	ASN	-	expression tag	UNP Q21A49
H	51	SER	-	expression tag	UNP Q21A49
H	52	SER	-	expression tag	UNP Q21A49
H	53	ALA	-	expression tag	UNP Q21A49
H	54	ASP	-	expression tag	UNP Q21A49
H	55	ALA	-	expression tag	UNP Q21A49

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Chain	Residue	Modelled	Actual	Comment	Reference
H	56	ASP	-	expression tag	UNP Q21A49
H	57	VAL	-	expression tag	UNP Q21A49
H	58	VAL	-	expression tag	UNP Q21A49
H	59	ALA	-	expression tag	UNP Q21A49
H	60	ARG	-	expression tag	UNP Q21A49

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



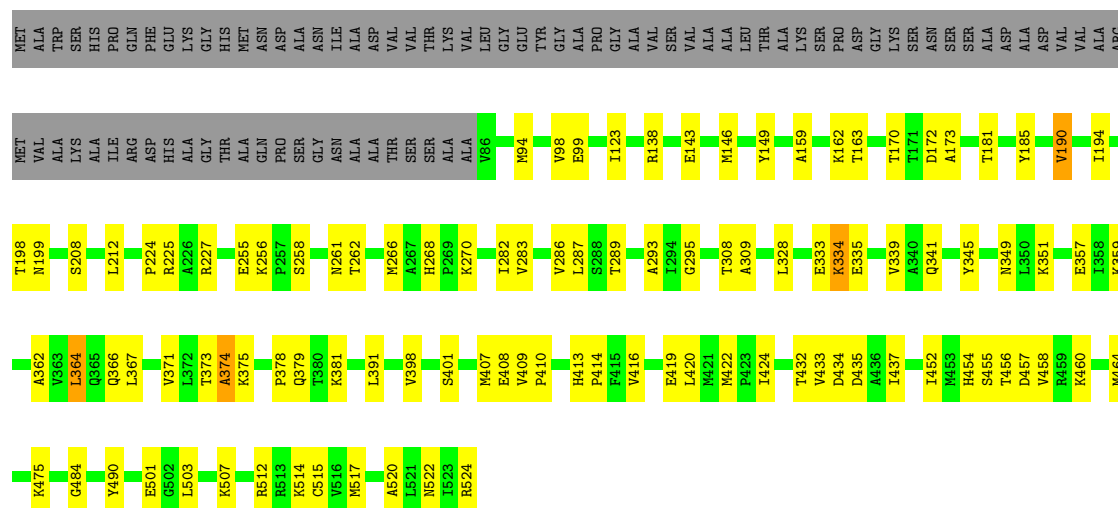
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	E	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	F	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	G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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	121	Total 121	O 121	0	0
3	B	144	Total 144	O 144	0	0
3	C	113	Total 113	O 113	0	0
3	D	113	Total 113	O 113	0	0
3	E	131	Total 131	O 131	0	0
3	F	104	Total 104	O 104	0	0
3	G	123	Total 123	O 123	0	0
3	H	69	Total 69	O 69	0	0

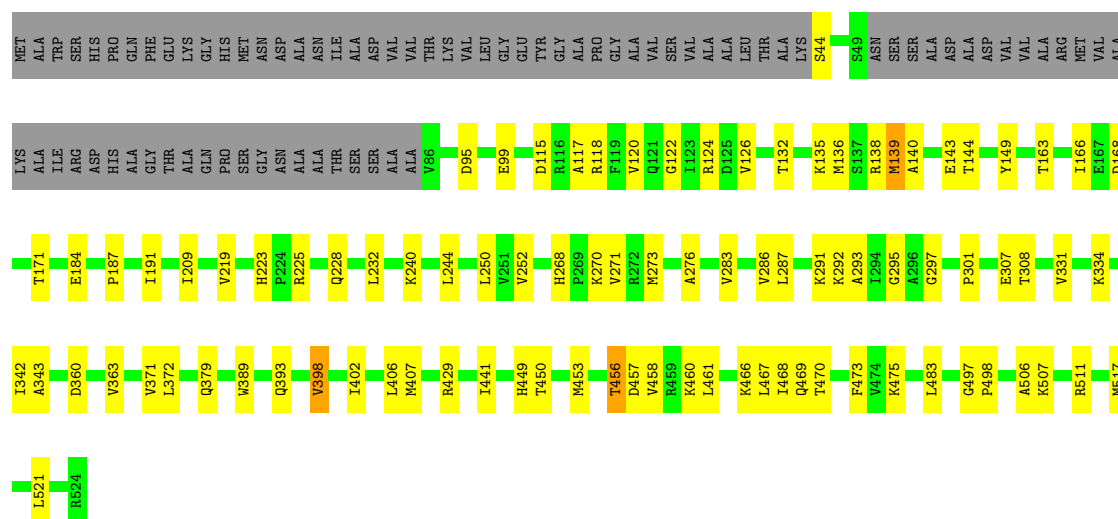
- Molecule 1: Aldehyde dehydrogenase





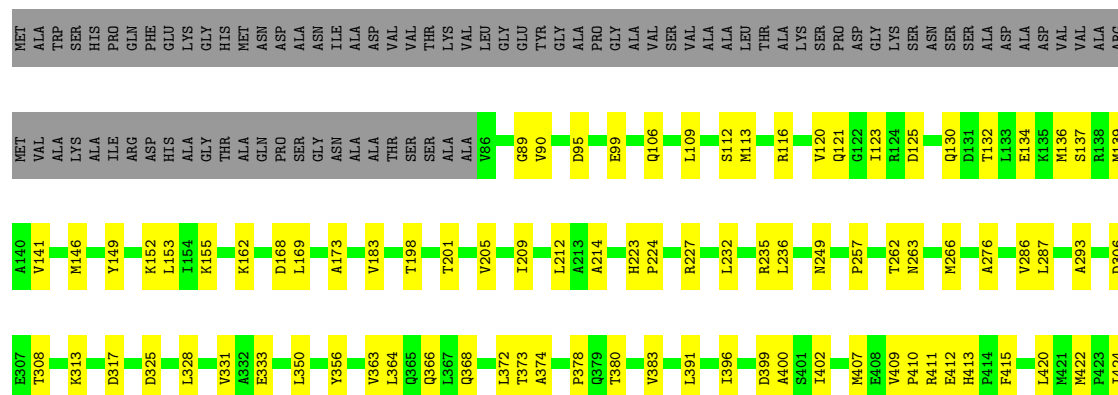
• Molecule 1: Aldehyde dehydrogenase

Chain D: 67% 17% 15%



• Molecule 1: Aldehyde dehydrogenase

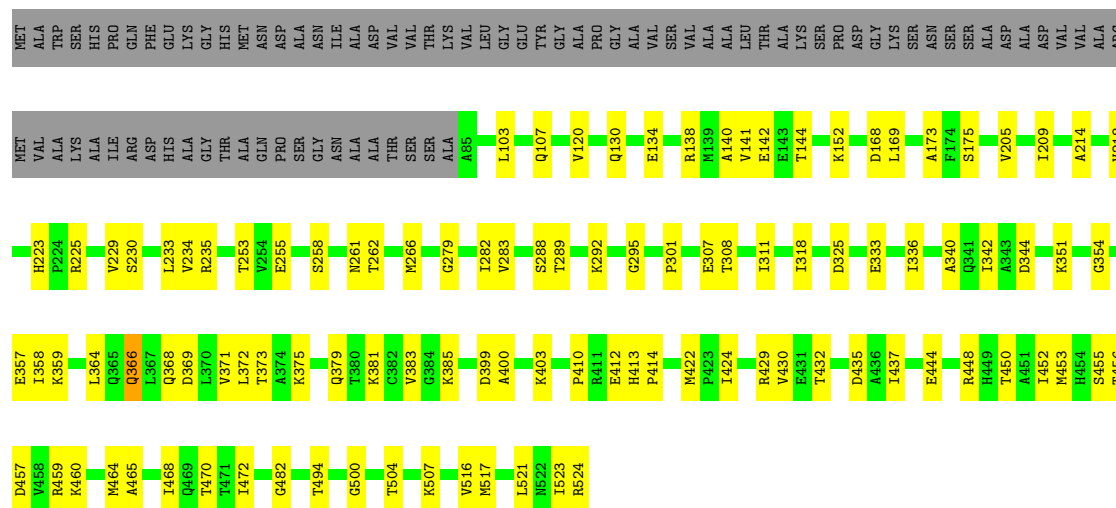
Chain E: 62% 22% 16%





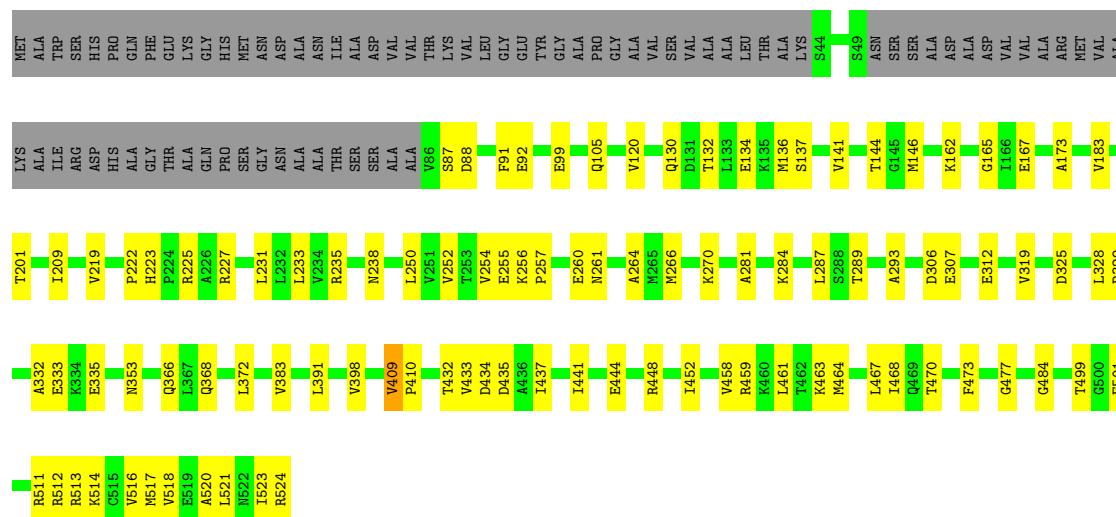
• Molecule 1: Aldehyde dehydrogenase

Chain F: 64% 20% 16%



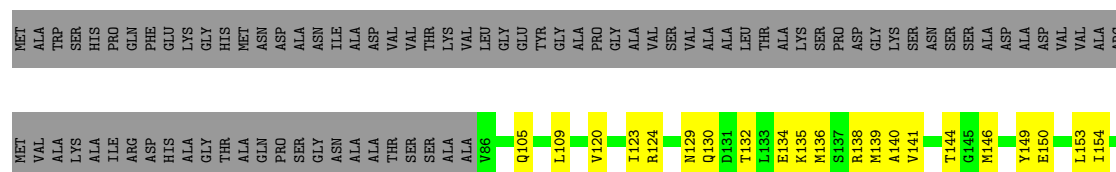
• Molecule 1: Aldehyde dehydrogenase

Chain G: 66% 19% 15%



• Molecule 1: Aldehyde dehydrogenase

Chain H: 61% 23% 16%



L158	I311	M421
T163	E312	M422
L169	K313	P423
D172	A314	I424
A173	A315	L425
F174	C316	P426
G179	D317	V430
	I318	A436
	V319	R448
Y185	D325	I452
S186	L328	S455
T195	P329	T456
P196	E333	D457
T197	K334	L461
T198	E335	I472
N199	A340	K475
E202	Y345	G482
T203	L346	L483
I204	N349	G484
V205	N353	A485
I209	K359	I495
A214	Q366	T499
P222	T373	G500
H223	A374	E501
P224	G362	R511
R227	L380	R512
Q228	L391	R513
V229	I394	K514
L232	G395	V518
L233	I396	E519
L236	I405	V522
P257	L406	I523
H268	M407	R524
V283	E408	
S288	V409	
	P410	
K291	R411	
G295	E412	
A296	H413	
G297	P414	
	F415	
P301	E418	
T308	E419	
	L420	

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	107.39Å 154.80Å 126.59Å 90.00° 90.13° 90.00°	Depositor
Resolution (Å)	33.64 – 2.30 33.64 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.7 (33.64-2.30) 97.1 (33.64-2.30)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 2.29Å)	Xtriage
Refinement program	PHENIX (1.10_2152: ???)	Depositor
R, R_{free}	0.189 , 0.228 (Not available) , 0.234	Depositor DCC
R_{free} test set	2005 reflections (1.11%)	wwPDB-VP
Wilson B-factor (Å ²)	31.7	Xtriage
Anisotropy	0.876	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 31.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.358 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	27656	wwPDB-VP
Average B, all atoms (Å ²)	38.0	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: NAD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.11	0/3338	0.32	0/4528
1	B	0.18	0/3345	0.35	0/4537
1	C	0.16	0/3333	0.39	0/4521
1	D	0.16	0/3373	0.35	1/4573 (0.0%)
1	E	0.16	0/3333	0.35	0/4521
1	F	0.14	0/3338	0.36	0/4528
1	G	0.15	0/3373	0.34	0/4573
1	H	0.22	0/3333	0.40	0/4521
All	All	0.16	0/26766	0.36	1/36302 (0.0%)

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	F	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	139	MET	CB-CG-SD	-5.30	96.79	112.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	366	GLN	Peptide

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	3291	0	3382	50	0
1	B	3294	0	3386	72	0
1	C	3286	0	3377	80	0
1	D	3326	0	3413	63	0
1	E	3286	0	3377	92	0
1	F	3291	0	3382	74	0
1	G	3326	0	3413	67	0
1	H	3286	0	3377	108	0
2	A	44	0	24	2	0
2	B	44	0	24	3	0
2	C	44	0	24	3	0
2	D	44	0	24	3	0
2	E	44	0	24	0	0
2	F	44	0	24	2	0
2	G	44	0	24	2	0
2	H	44	0	24	4	0
3	A	121	0	0	7	0
3	B	144	0	0	4	0
3	C	113	0	0	5	0
3	D	113	0	0	2	0
3	E	131	0	0	5	0
3	F	104	0	0	5	0
3	G	123	0	0	3	0
3	H	69	0	0	8	0
All	All	27656	0	27299	576	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 11.

The worst 5 of 576 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:H:366:GLN:HE22	1:H:394:ILE:CD1	1.20	1.50
1:H:366:GLN:NE2	1:H:394:ILE:HD12	0.95	1.28
1:H:366:GLN:CD	1:H:394:ILE:HD12	1.65	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:366:GLN:NE2	1:H:394:ILE:CD1	1.88	1.09
1:B:515:CYS:SG	1:D:475:LYS:NZ	2.31	1.03

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	438/524 (84%)	425 (97%)	13 (3%)	0	100	100
1	B	438/524 (84%)	420 (96%)	18 (4%)	0	100	100
1	C	437/524 (83%)	423 (97%)	12 (3%)	2 (0%)	24	31
1	D	441/524 (84%)	432 (98%)	9 (2%)	0	100	100
1	E	437/524 (83%)	417 (95%)	20 (5%)	0	100	100
1	F	438/524 (84%)	421 (96%)	15 (3%)	2 (0%)	24	31
1	G	441/524 (84%)	426 (97%)	15 (3%)	0	100	100
1	H	437/524 (83%)	417 (95%)	19 (4%)	1 (0%)	43	55
All	All	3507/4192 (84%)	3381 (96%)	121 (4%)	5 (0%)	48	60

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	374	ALA
1	F	410	PRO
1	C	419	GLU
1	H	373	THR
1	F	354	GLY

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	358/417 (86%)	356 (99%)	2 (1%)	78	89
1	B	359/417 (86%)	358 (100%)	1 (0%)	86	93
1	C	358/417 (86%)	355 (99%)	3 (1%)	73	86
1	D	363/417 (87%)	360 (99%)	3 (1%)	73	86
1	E	358/417 (86%)	357 (100%)	1 (0%)	86	93
1	F	358/417 (86%)	357 (100%)	1 (0%)	86	93
1	G	363/417 (87%)	360 (99%)	3 (1%)	73	86
1	H	358/417 (86%)	358 (100%)	0	100	100
All	All	2875/3336 (86%)	2861 (100%)	14 (0%)	81	90

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	398	VAL
1	D	456	THR
1	G	409	VAL
1	G	312	GLU
1	G	335	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	368	GLN
1	H	326	ASN
1	F	178	ASN
1	H	368	GLN
1	H	105	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 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
2	NAD	H	600	-	46,48,48	3.69	15 (32%)	64,73,73	1.59	11 (17%)
2	NAD	E	600	-	46,48,48	3.66	15 (32%)	64,73,73	1.57	10 (15%)
2	NAD	C	600	-	46,48,48	3.65	15 (32%)	64,73,73	1.60	11 (17%)
2	NAD	F	600	-	46,48,48	3.66	15 (32%)	64,73,73	1.63	12 (18%)
2	NAD	D	600	-	46,48,48	3.66	15 (32%)	64,73,73	1.60	9 (14%)
2	NAD	G	600	-	46,48,48	3.67	15 (32%)	64,73,73	1.59	10 (15%)
2	NAD	B	600	-	46,48,48	3.64	15 (32%)	64,73,73	1.57	10 (15%)
2	NAD	A	600	-	46,48,48	3.65	15 (32%)	64,73,73	1.65	9 (14%)

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	NAD	H	600	-	-	11/30/62/62	0/5/5/5
2	NAD	E	600	-	-	4/30/62/62	0/5/5/5
2	NAD	C	600	-	-	5/30/62/62	0/5/5/5
2	NAD	F	600	-	-	8/30/62/62	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	D	600	-	-	11/30/62/62	0/5/5/5
2	NAD	G	600	-	-	2/30/62/62	0/5/5/5
2	NAD	B	600	-	-	4/30/62/62	0/5/5/5
2	NAD	A	600	-	-	6/30/62/62	0/5/5/5

The worst 5 of 120 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	600	NAD	O4D-C1D	16.18	1.62	1.40
2	G	600	NAD	O4D-C1D	16.04	1.61	1.40
2	E	600	NAD	O4D-C1D	15.93	1.61	1.40
2	C	600	NAD	O4D-C1D	15.91	1.61	1.40
2	F	600	NAD	O4D-C1D	15.90	1.61	1.40

The worst 5 of 82 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	600	NAD	N3A-C2A-N1A	-5.75	119.88	128.58
2	G	600	NAD	N3A-C2A-N1A	-5.67	120.00	128.58
2	D	600	NAD	N3A-C2A-N1A	-5.64	120.04	128.58
2	C	600	NAD	N3A-C2A-N1A	-5.63	120.06	128.58
2	H	600	NAD	N3A-C2A-N1A	-5.63	120.06	128.58

There are no chirality outliers.

5 of 51 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	600	NAD	PN-O3-PA-O5B
2	C	600	NAD	O4B-C4B-C5B-O5B
2	D	600	NAD	C5B-O5B-PA-O1A
2	D	600	NAD	C5B-O5B-PA-O2A
2	D	600	NAD	C5B-O5B-PA-O3

There are no ring outliers.

7 monomers are involved in 19 short contacts:

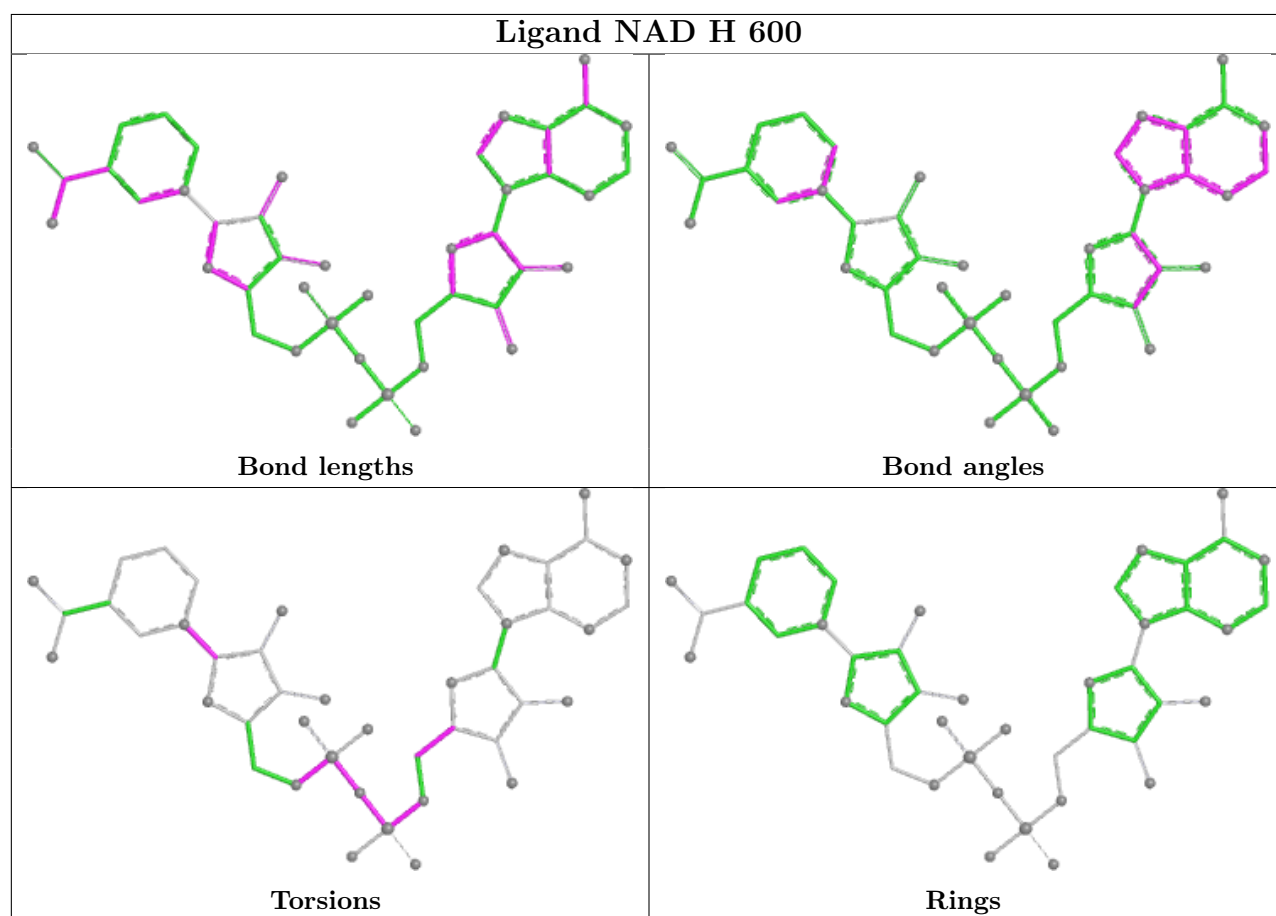
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	600	NAD	4	0
2	C	600	NAD	3	0
2	F	600	NAD	2	0

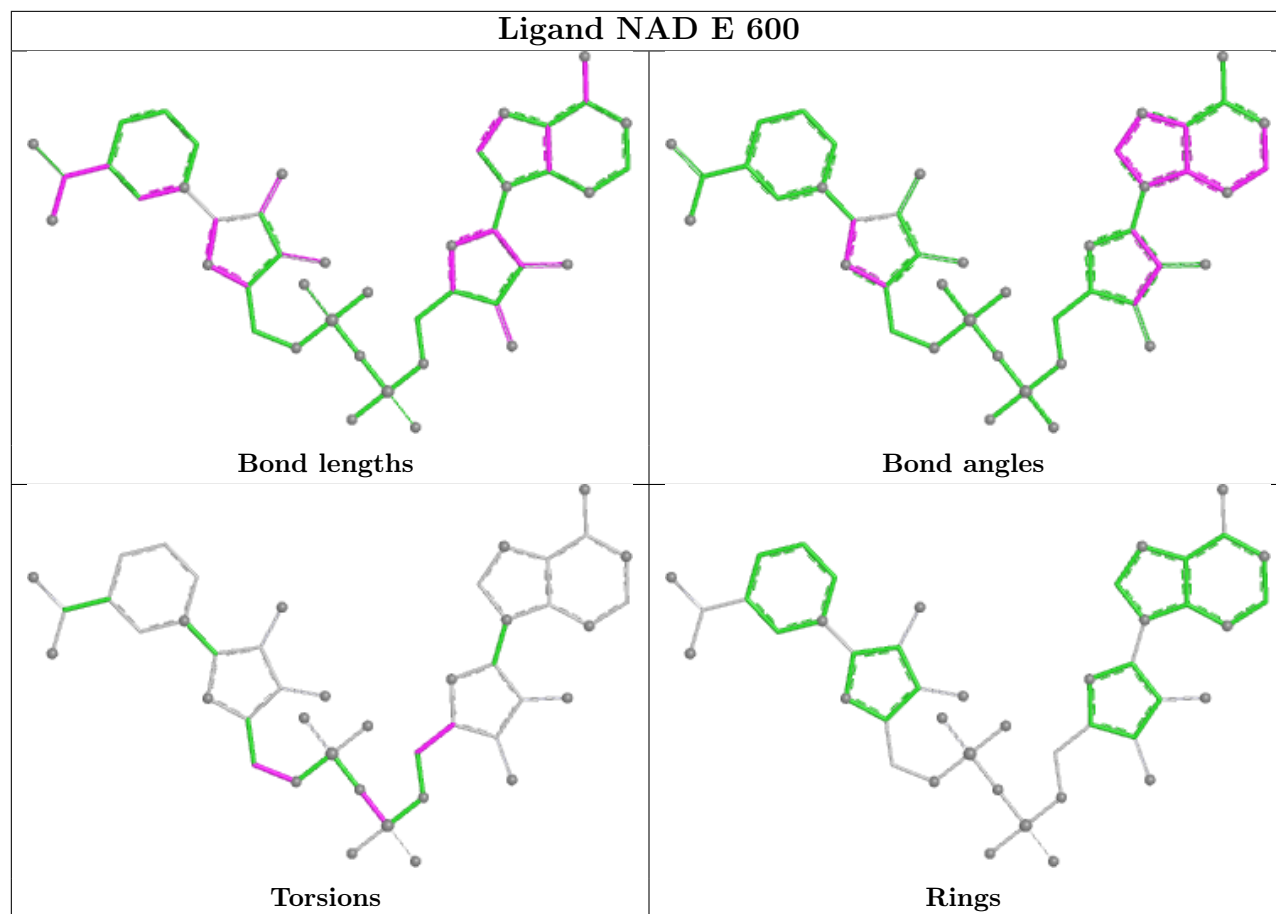
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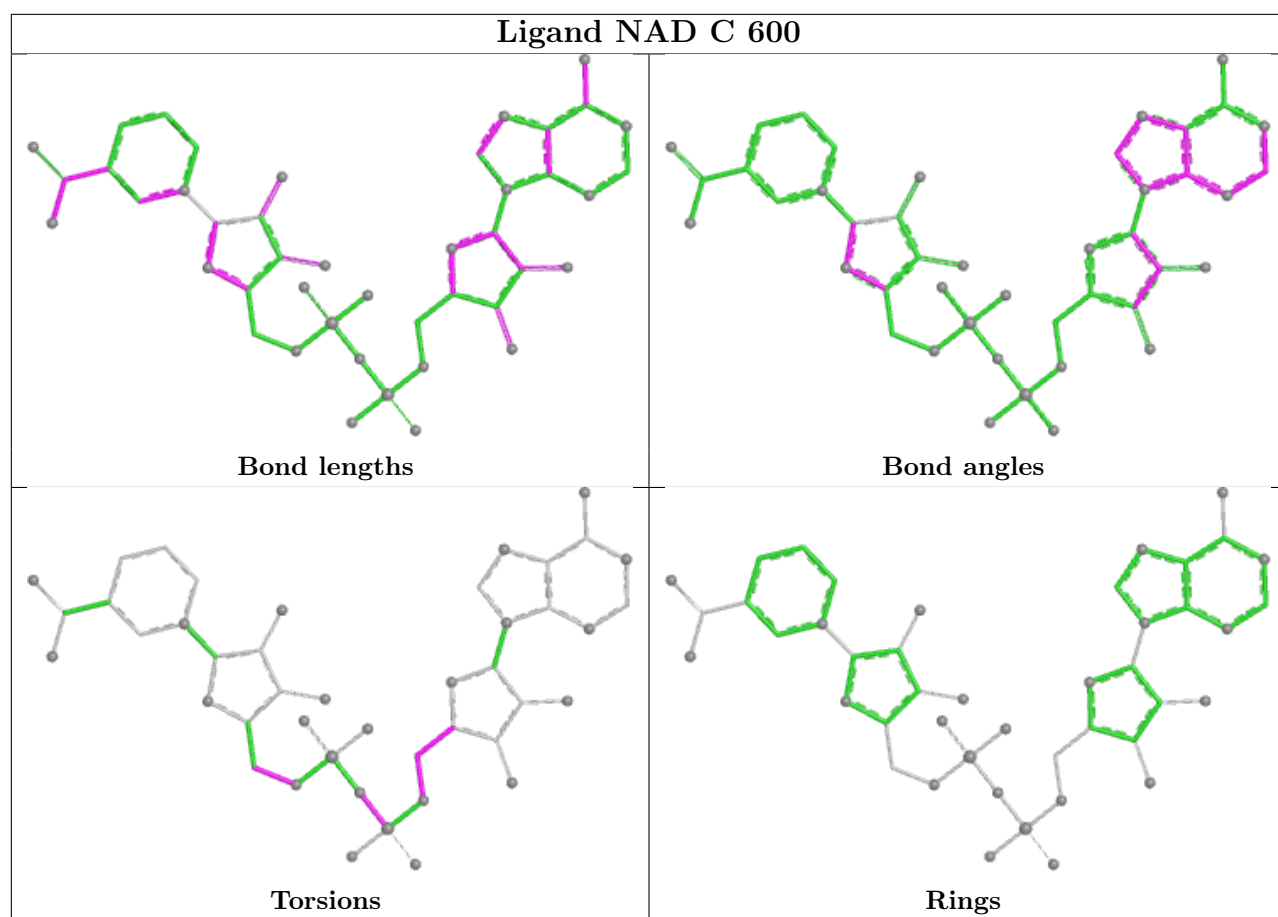
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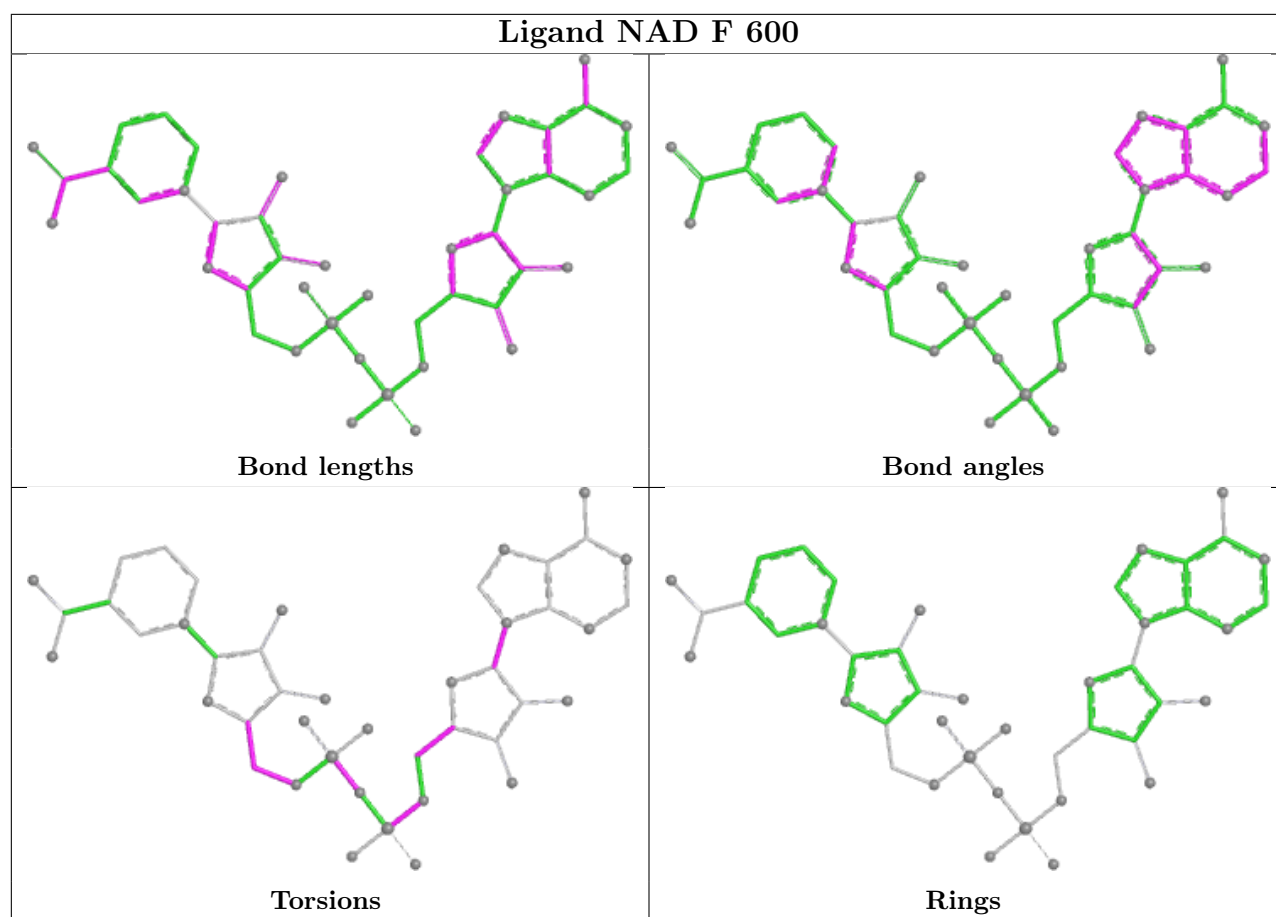
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	600	NAD	3	0
2	G	600	NAD	2	0
2	B	600	NAD	3	0
2	A	600	NAD	2	0

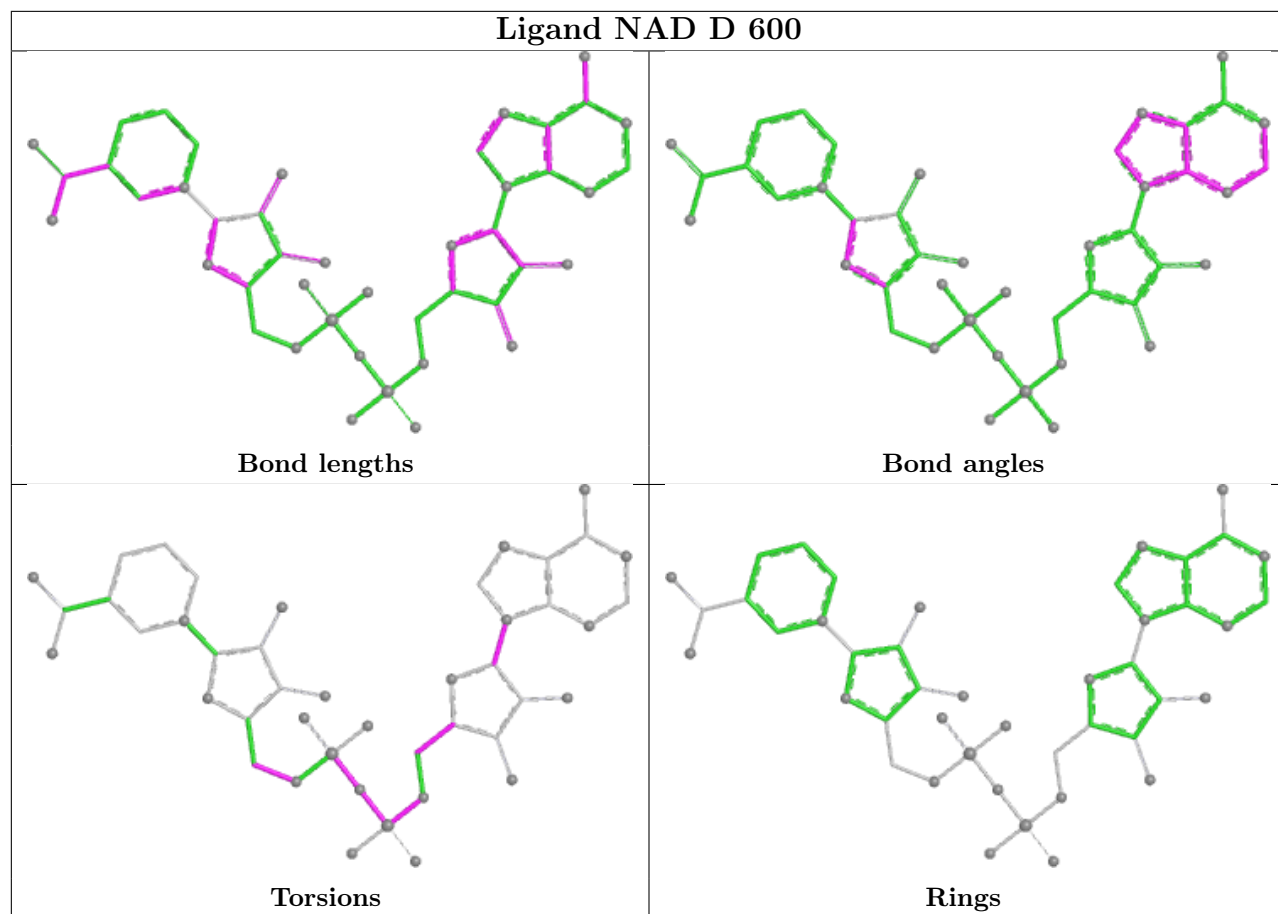
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

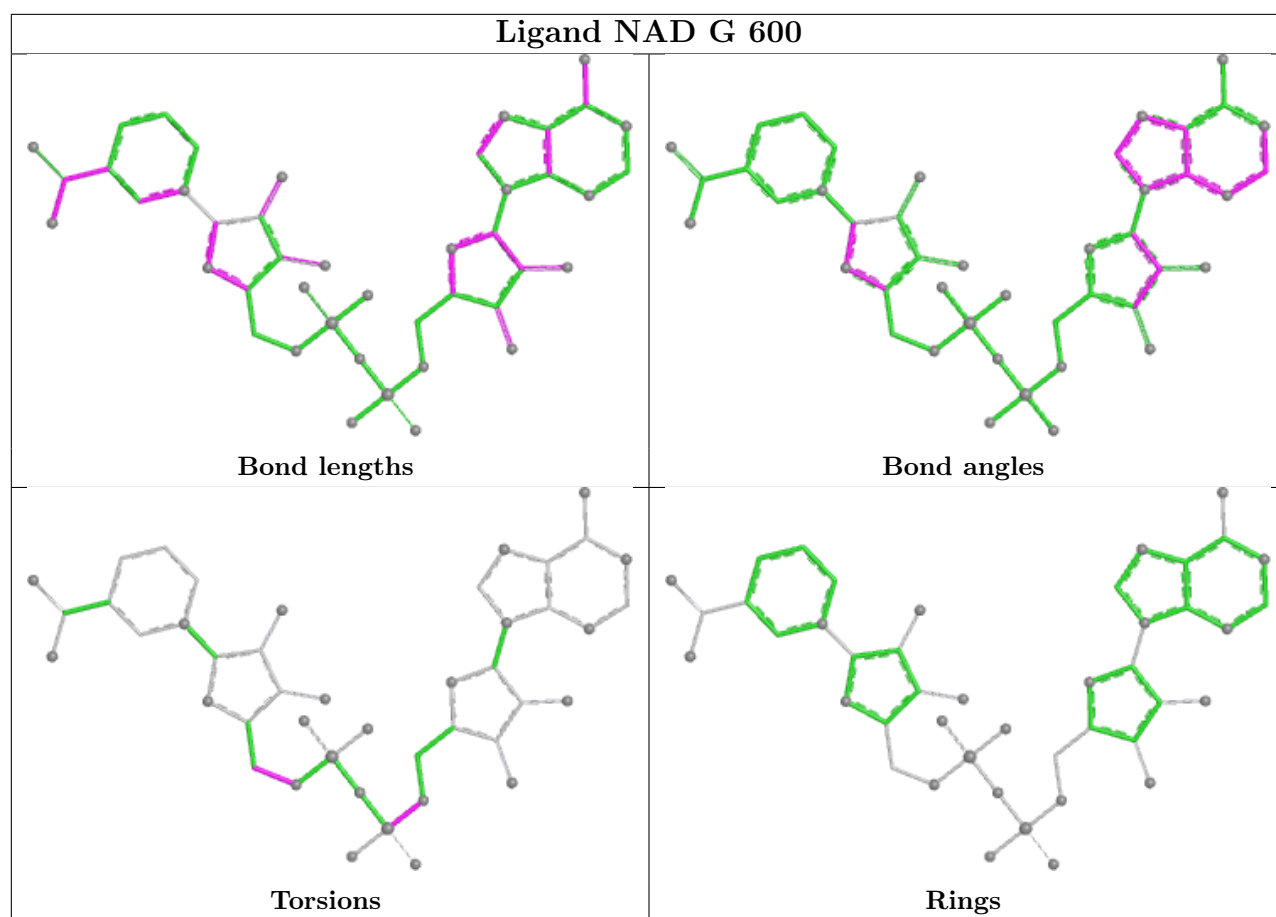


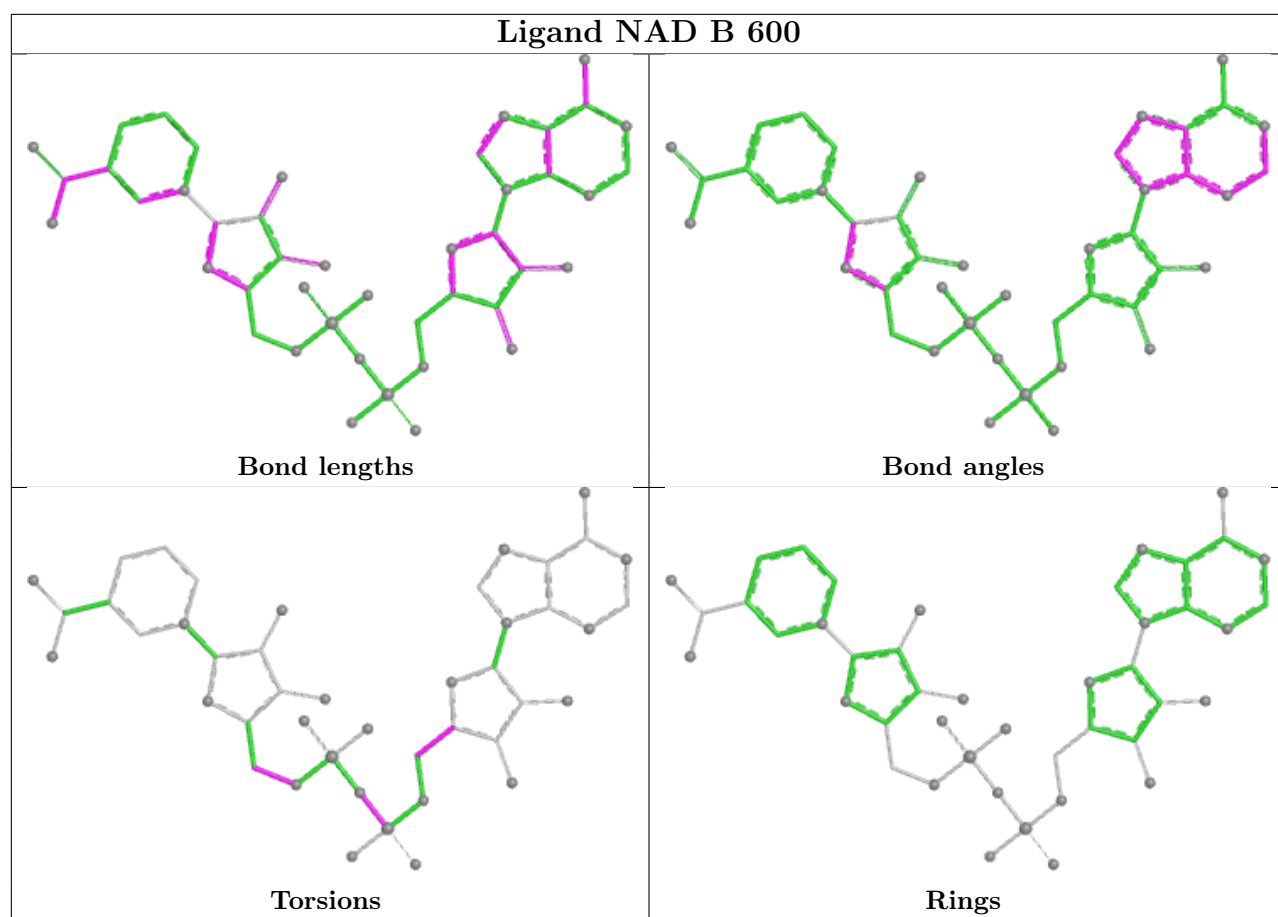


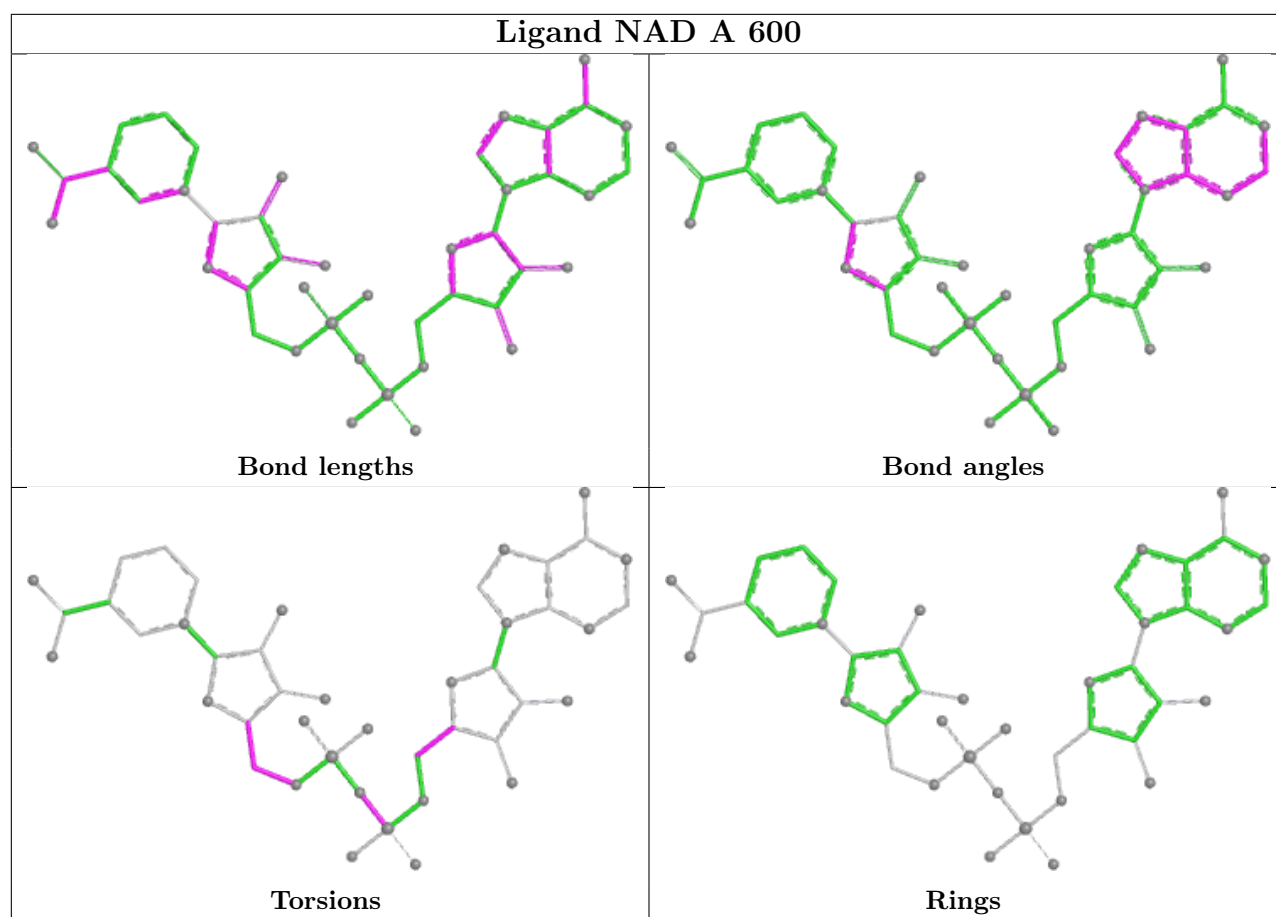












5.7 Other polymers [i](#)

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 [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	440/524 (83%)	-1.39	0 100 100	23, 34, 47, 61	0
1	B	439/524 (83%)	-1.38	0 100 100	22, 33, 49, 62	1 (0%)
1	C	439/524 (83%)	-1.33	0 100 100	24, 40, 54, 73	0
1	D	445/524 (84%)	-1.38	0 100 100	22, 36, 49, 57	0
1	E	439/524 (83%)	-1.37	0 100 100	24, 34, 49, 61	0
1	F	440/524 (83%)	-1.33	0 100 100	24, 37, 64, 85	0
1	G	445/524 (84%)	-1.37	0 100 100	24, 37, 51, 66	0
1	H	439/524 (83%)	-1.24	0 100 100	25, 50, 74, 90	0
All	All	3526/4192 (84%)	-1.35	0 100 100	22, 36, 58, 90	1 (0%)

There are no RSRZ outliers to report.

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](#)

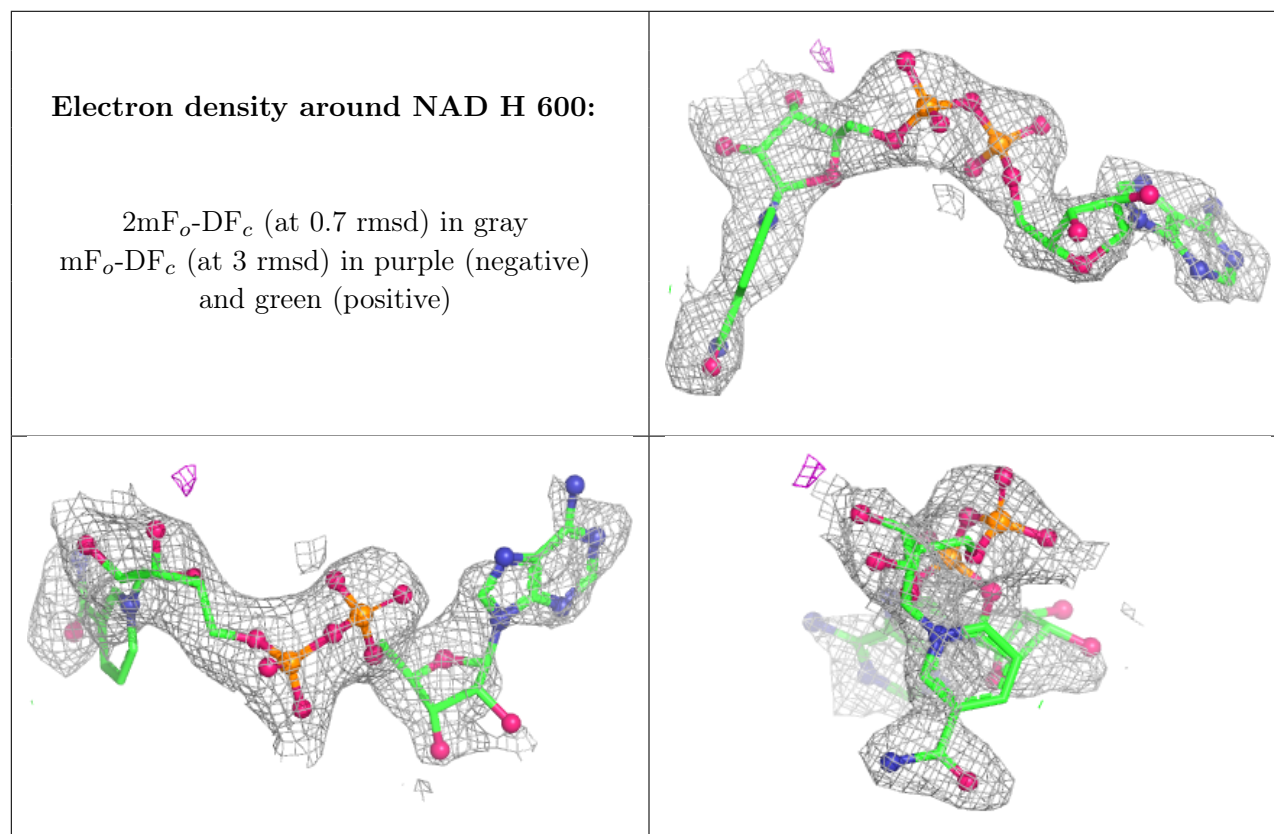
There are no oligosaccharides in this entry.

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.

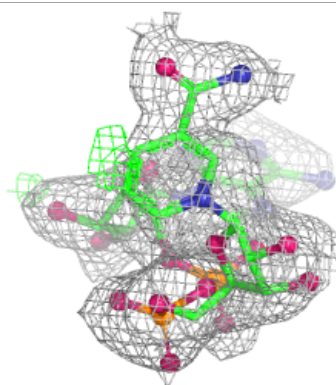
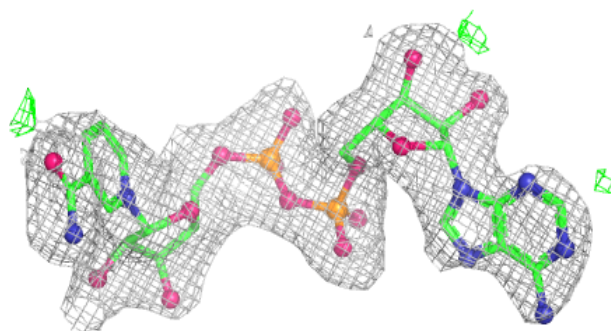
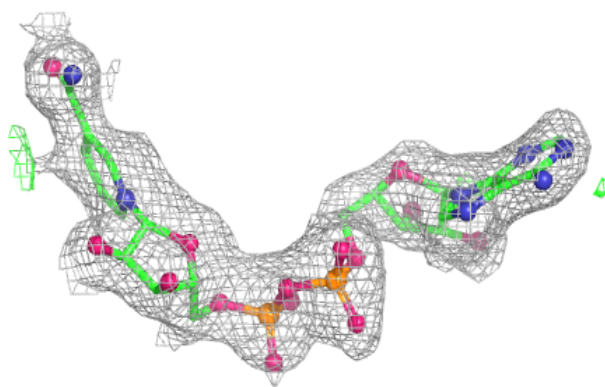
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAD	H	600	44/44	0.98	0.05	43,62,67,68	44
2	NAD	B	600	44/44	0.99	0.04	31,44,49,52	0
2	NAD	C	600	44/44	0.99	0.04	39,47,59,62	44
2	NAD	D	600	44/44	0.99	0.03	29,42,45,46	0
2	NAD	E	600	44/44	0.99	0.04	30,38,45,48	44
2	NAD	F	600	44/44	0.99	0.04	38,44,48,50	44
2	NAD	G	600	44/44	0.99	0.04	31,41,44,49	44
2	NAD	A	600	44/44	0.99	0.03	32,43,47,50	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.

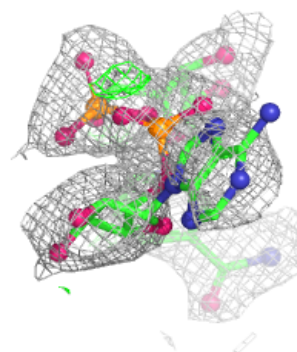
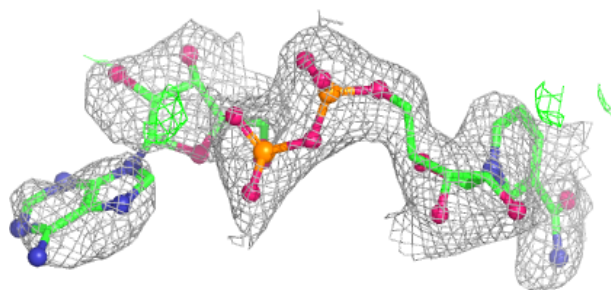
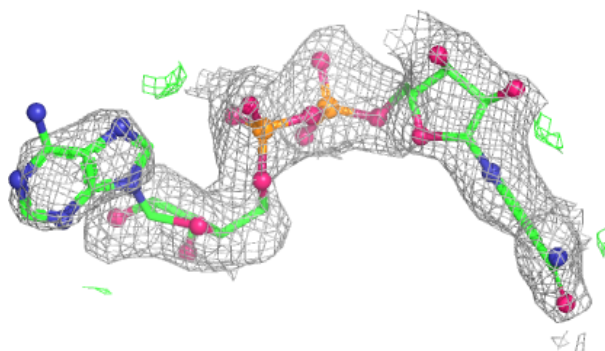


Electron density around NAD B 600:

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

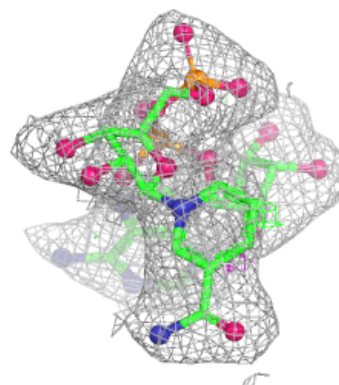
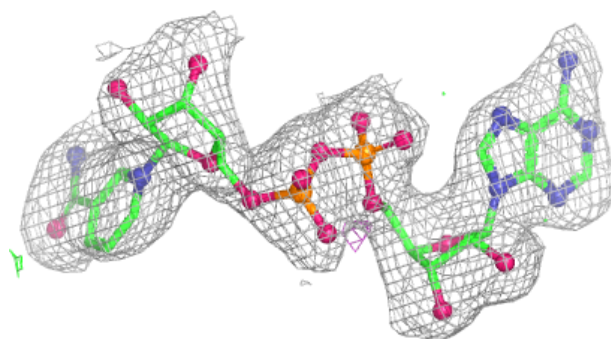
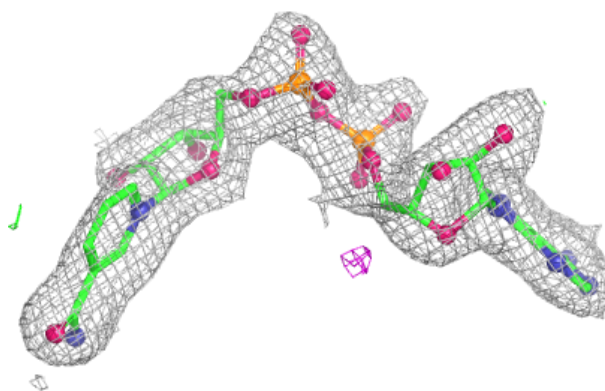
**Electron density around NAD C 600:**

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

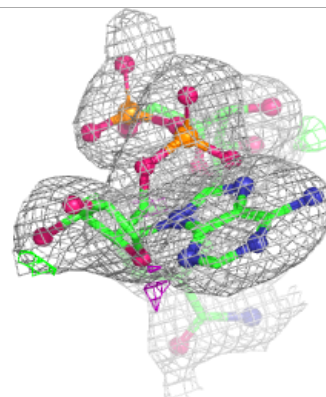
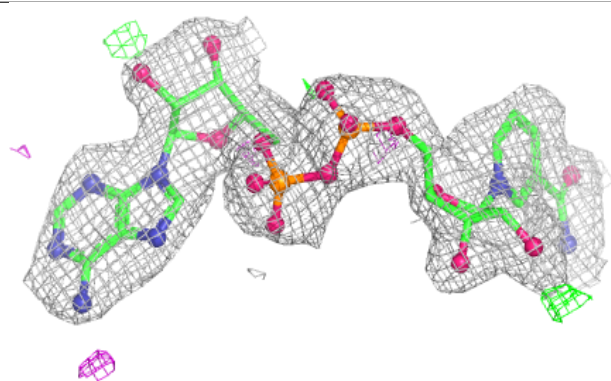
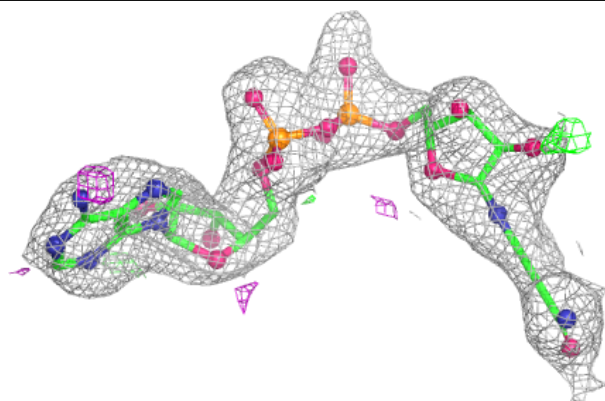


Electron density around NAD D 600:

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

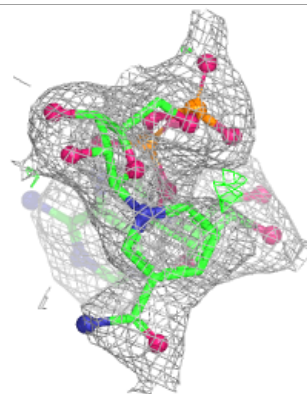
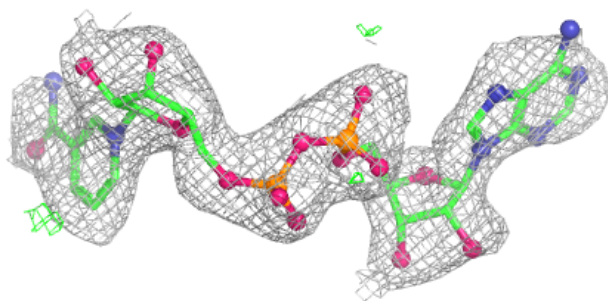
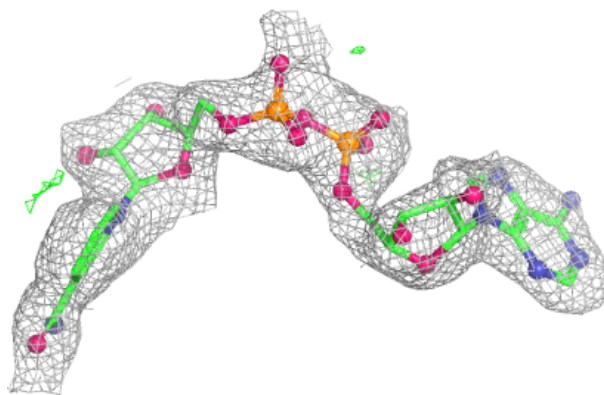
**Electron density around NAD E 600:**

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

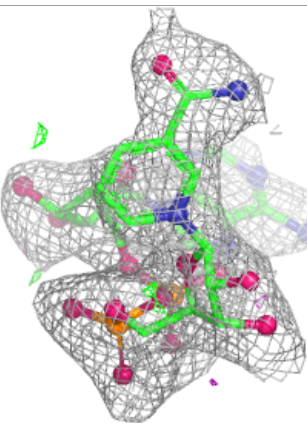
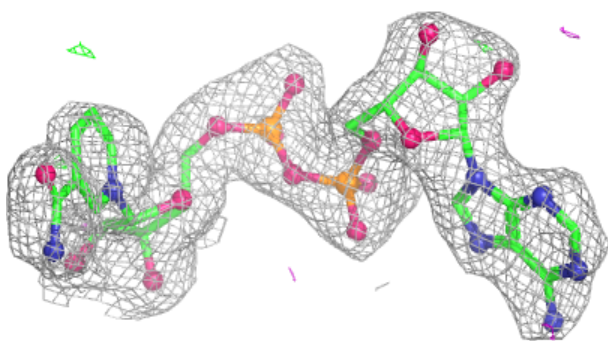
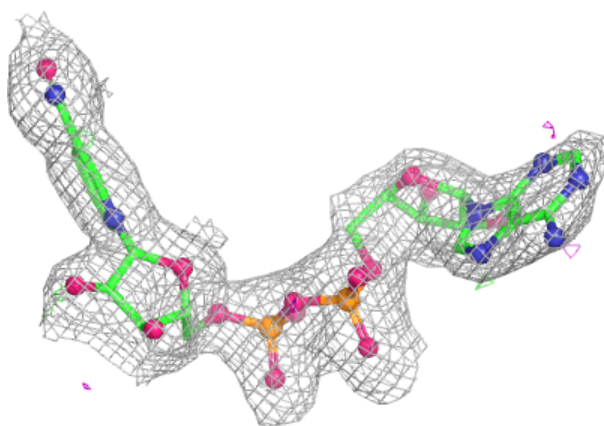


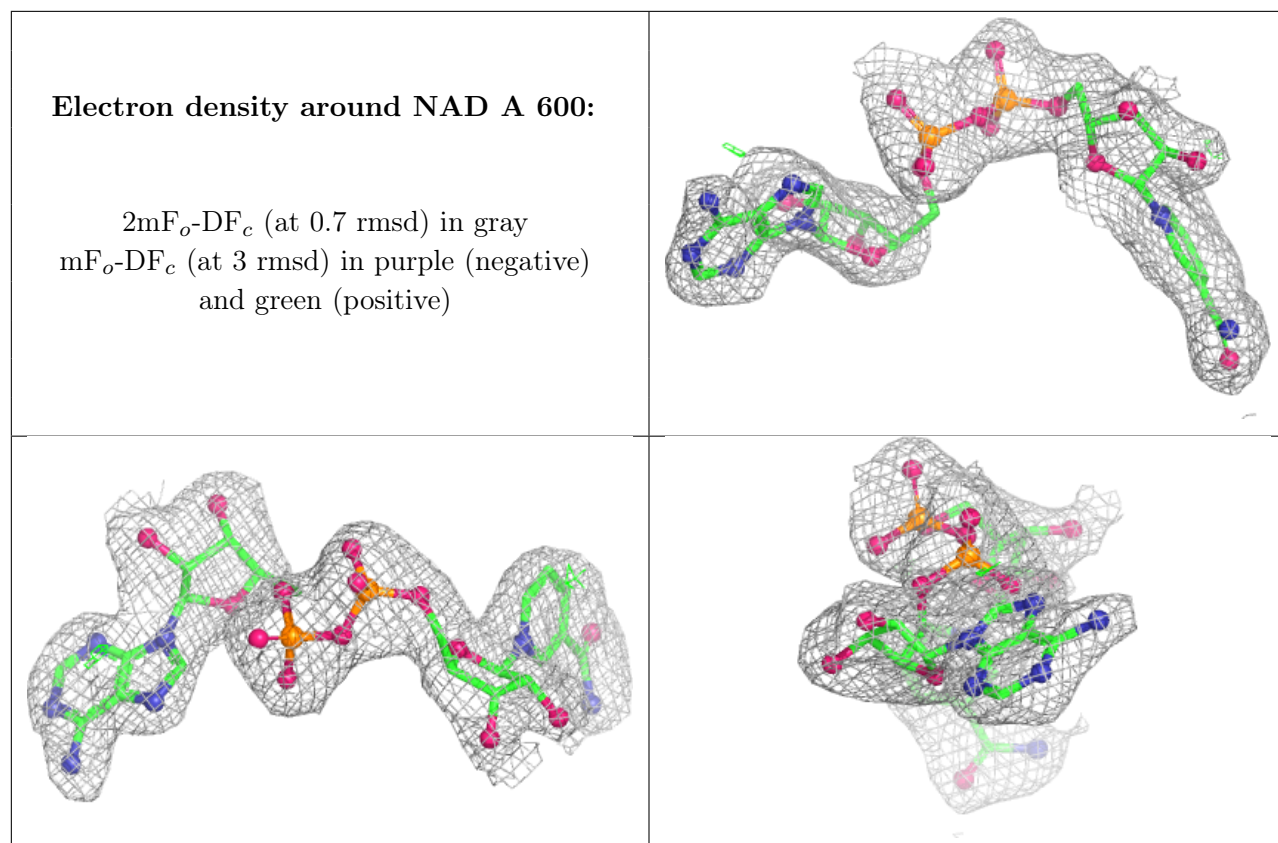
Electron density around NAD F 600:

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

**Electron density around NAD G 600:**

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





6.5 Other polymers ⓘ

There are no such residues in this entry.