



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:31 AM UTC

PDB ID : 4PZ2 / pdb_00004pz2
Title : Structure of Zm ALDH2-6 (RF2F) in complex with NAD
Authors : Morera, S.; Vigouroux, A.; Kopečný, D.
Deposited on : 2014-03-28
Resolution : 2.40 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

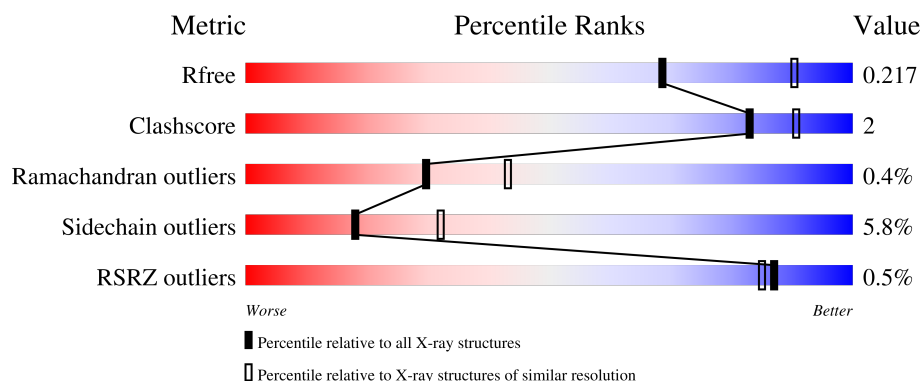
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

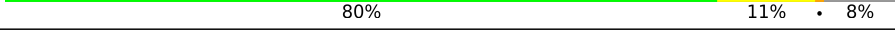
The reported resolution of this entry is 2.40 Å.

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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	534	
1	B	534	
1	C	534	
1	D	534	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15179 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 ZmALDH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	491	Total	C	N	O	S	0	0	0
			3713	2350	650	692	21			
1	B	494	Total	C	N	O	S	0	0	0
			3734	2363	653	697	21			
1	C	491	Total	C	N	O	S	0	0	0
			3713	2350	650	692	21			
1	D	491	Total	C	N	O	S	0	0	0
			3712	2350	649	692	21			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	GLY	-	expression tag	UNP K7VEU7
A	-13	SER	-	expression tag	UNP K7VEU7
A	-12	SER	-	expression tag	UNP K7VEU7
A	-11	HIS	-	expression tag	UNP K7VEU7
A	-10	HIS	-	expression tag	UNP K7VEU7
A	-9	HIS	-	expression tag	UNP K7VEU7
A	-8	HIS	-	expression tag	UNP K7VEU7
A	-7	HIS	-	expression tag	UNP K7VEU7
A	-6	HIS	-	expression tag	UNP K7VEU7
A	-5	SER	-	expression tag	UNP K7VEU7
A	-4	GLN	-	expression tag	UNP K7VEU7
A	-3	ASP	-	expression tag	UNP K7VEU7
A	-2	PRO	-	expression tag	UNP K7VEU7
A	-1	ASN	-	expression tag	UNP K7VEU7
A	0	SER	-	expression tag	UNP K7VEU7
A	18	GLU	-	expression tag	UNP K7VEU7
A	19	GLU	-	expression tag	UNP K7VEU7
A	20	LYS	-	expression tag	UNP K7VEU7
A	54	ASP	GLU	SEE REMARK 999	UNP K7VEU7
A	113	HIS	ARG	SEE REMARK 999	UNP K7VEU7
A	115	GLY	ASP	SEE REMARK 999	UNP K7VEU7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	354	ARG	SER	SEE REMARK 999	UNP K7VEU7
A	391	ALA	GLY	SEE REMARK 999	UNP K7VEU7
B	-14	GLY	-	expression tag	UNP K7VEU7
B	-13	SER	-	expression tag	UNP K7VEU7
B	-12	SER	-	expression tag	UNP K7VEU7
B	-11	HIS	-	expression tag	UNP K7VEU7
B	-10	HIS	-	expression tag	UNP K7VEU7
B	-9	HIS	-	expression tag	UNP K7VEU7
B	-8	HIS	-	expression tag	UNP K7VEU7
B	-7	HIS	-	expression tag	UNP K7VEU7
B	-6	HIS	-	expression tag	UNP K7VEU7
B	-5	SER	-	expression tag	UNP K7VEU7
B	-4	GLN	-	expression tag	UNP K7VEU7
B	-3	ASP	-	expression tag	UNP K7VEU7
B	-2	PRO	-	expression tag	UNP K7VEU7
B	-1	ASN	-	expression tag	UNP K7VEU7
B	0	SER	-	expression tag	UNP K7VEU7
B	18	GLU	-	expression tag	UNP K7VEU7
B	19	GLU	-	expression tag	UNP K7VEU7
B	20	LYS	-	expression tag	UNP K7VEU7
B	54	ASP	GLU	SEE REMARK 999	UNP K7VEU7
B	113	HIS	ARG	SEE REMARK 999	UNP K7VEU7
B	115	GLY	ASP	SEE REMARK 999	UNP K7VEU7
B	354	ARG	SER	SEE REMARK 999	UNP K7VEU7
B	391	ALA	GLY	SEE REMARK 999	UNP K7VEU7
C	-14	GLY	-	expression tag	UNP K7VEU7
C	-13	SER	-	expression tag	UNP K7VEU7
C	-12	SER	-	expression tag	UNP K7VEU7
C	-11	HIS	-	expression tag	UNP K7VEU7
C	-10	HIS	-	expression tag	UNP K7VEU7
C	-9	HIS	-	expression tag	UNP K7VEU7
C	-8	HIS	-	expression tag	UNP K7VEU7
C	-7	HIS	-	expression tag	UNP K7VEU7
C	-6	HIS	-	expression tag	UNP K7VEU7
C	-5	SER	-	expression tag	UNP K7VEU7
C	-4	GLN	-	expression tag	UNP K7VEU7
C	-3	ASP	-	expression tag	UNP K7VEU7
C	-2	PRO	-	expression tag	UNP K7VEU7
C	-1	ASN	-	expression tag	UNP K7VEU7
C	0	SER	-	expression tag	UNP K7VEU7
C	18	GLU	-	expression tag	UNP K7VEU7
C	19	GLU	-	expression tag	UNP K7VEU7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	20	LYS	-	expression tag	UNP K7VEU7
C	54	ASP	GLU	SEE REMARK 999	UNP K7VEU7
C	113	HIS	ARG	SEE REMARK 999	UNP K7VEU7
C	115	GLY	ASP	SEE REMARK 999	UNP K7VEU7
C	354	ARG	SER	SEE REMARK 999	UNP K7VEU7
C	391	ALA	GLY	SEE REMARK 999	UNP K7VEU7
D	-14	GLY	-	expression tag	UNP K7VEU7
D	-13	SER	-	expression tag	UNP K7VEU7
D	-12	SER	-	expression tag	UNP K7VEU7
D	-11	HIS	-	expression tag	UNP K7VEU7
D	-10	HIS	-	expression tag	UNP K7VEU7
D	-9	HIS	-	expression tag	UNP K7VEU7
D	-8	HIS	-	expression tag	UNP K7VEU7
D	-7	HIS	-	expression tag	UNP K7VEU7
D	-6	HIS	-	expression tag	UNP K7VEU7
D	-5	SER	-	expression tag	UNP K7VEU7
D	-4	GLN	-	expression tag	UNP K7VEU7
D	-3	ASP	-	expression tag	UNP K7VEU7
D	-2	PRO	-	expression tag	UNP K7VEU7
D	-1	ASN	-	expression tag	UNP K7VEU7
D	0	SER	-	expression tag	UNP K7VEU7
D	18	GLU	-	expression tag	UNP K7VEU7
D	19	GLU	-	expression tag	UNP K7VEU7
D	20	LYS	-	expression tag	UNP K7VEU7
D	54	ASP	GLU	SEE REMARK 999	UNP K7VEU7
D	113	HIS	ARG	SEE REMARK 999	UNP K7VEU7
D	115	GLY	ASP	SEE REMARK 999	UNP K7VEU7
D	354	ARG	SER	SEE REMARK 999	UNP K7VEU7
D	391	ALA	GLY	SEE REMARK 999	UNP K7VEU7

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 3 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	N	O	P	
			44	21	7	14	2	
4	D	1	Total	C	N	O	P	
			44	21	7	14	2	

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

- Molecule 6 is water.

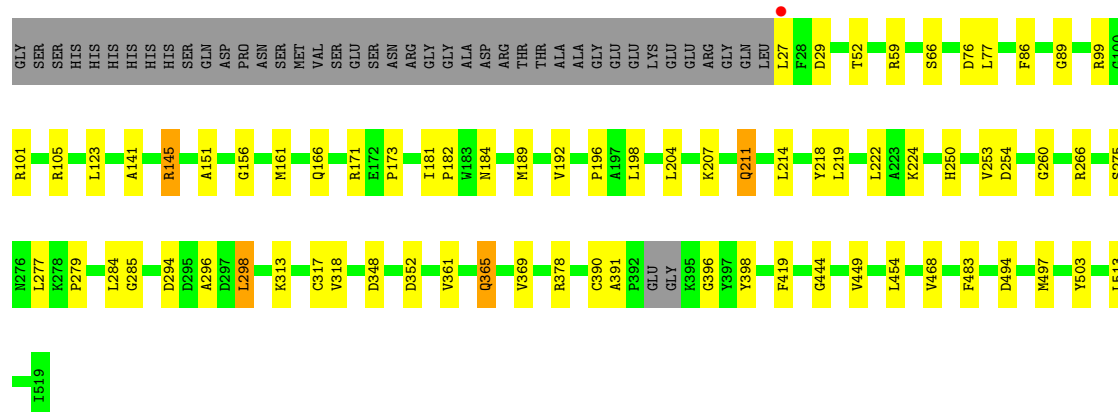
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	25	Total 25	O 25	0	0
6	B	22	Total 22	O 22	0	0
6	C	23	Total 23	O 23	0	0
6	D	18	Total 18	O 18	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

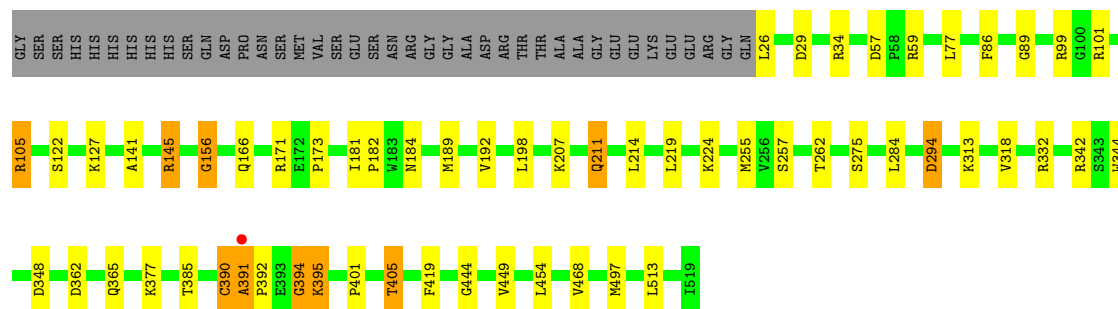
• Molecule 1: ZmALDH

Chain A: 



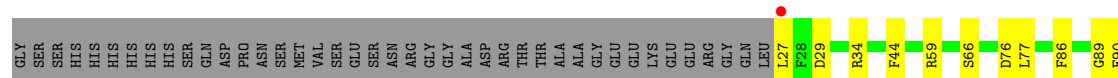
• Molecule 1: ZmALDH

Chain B: 



• Molecule 1: ZmALDH

Chain C: 





4 Data and refinement statistics

Property	Value	Source
Space group	I 41	Depositor
Cell constants a, b, c, α , β , γ	233.88Å 233.88Å 82.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.81 – 2.40 46.81 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (46.81-2.40) 99.8 (46.81-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.11 (at 2.39Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.190 , 0.213 0.191 , 0.217	Depositor DCC
R_{free} test set	4381 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	67.5	Xtriage
Anisotropy	0.377	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 48.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.019 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	15179	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.84% 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, EDO, NA, PEG

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	0.81	0/3790	1.41	30/5133 (0.6%)
1	B	0.80	2/3812 (0.1%)	1.44	24/5164 (0.5%)
1	C	0.80	1/3790 (0.0%)	1.39	23/5133 (0.4%)
1	D	0.80	0/3789	1.42	22/5133 (0.4%)
All	All	0.80	3/15181 (0.0%)	1.42	99/20563 (0.5%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	390	CYS	CA-C	5.89	1.59	1.53
1	C	275	SER	CA-C	5.48	1.55	1.52
1	B	275	SER	CA-C	5.37	1.54	1.52

All (99) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	294	ASP	CA-C-N	8.54	132.09	120.38
1	A	294	ASP	C-N-CA	8.54	132.09	120.38
1	C	214	LEU	N-CA-C	7.67	119.27	111.07
1	D	214	LEU	N-CA-C	7.31	119.03	111.14
1	B	294	ASP	CA-CB-CG	7.29	119.89	112.60
1	C	497	MET	CA-C-N	7.14	129.85	120.28
1	C	497	MET	C-N-CA	7.14	129.85	120.28
1	C	397	TYR	N-CA-C	7.00	121.06	111.54
1	B	181	ILE	N-CA-C	6.86	116.68	108.45
1	A	497	MET	CA-C-N	6.72	129.29	120.28
1	A	497	MET	C-N-CA	6.72	129.29	120.28
1	D	181	ILE	N-CA-C	6.67	116.45	108.45
1	A	214	LEU	N-CA-C	6.54	118.48	111.36
1	B	99	ARG	CA-C-N	6.50	127.19	119.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	99	ARG	C-N-CA	6.50	127.19	119.98
1	C	181	ILE	N-CA-C	6.50	116.25	108.45
1	D	184	ASN	N-CA-C	6.49	118.43	111.36
1	A	181	ILE	N-CA-C	6.48	116.23	108.45
1	C	184	ASN	N-CA-C	6.47	118.42	111.36
1	B	184	ASN	N-CA-C	6.44	118.38	111.36
1	B	214	LEU	N-CA-C	6.44	118.38	111.36
1	A	99	ARG	CA-C-N	6.23	126.90	119.98
1	A	99	ARG	C-N-CA	6.23	126.90	119.98
1	A	184	ASN	N-CA-C	6.12	118.04	111.36
1	A	494	ASP	N-CA-C	-5.97	100.46	109.95
1	D	497	MET	CA-C-N	5.93	128.82	120.28
1	D	497	MET	C-N-CA	5.93	128.82	120.28
1	B	405	THR	CB-CA-C	5.91	120.35	109.71
1	B	497	MET	CA-C-N	5.88	128.74	120.28
1	B	497	MET	C-N-CA	5.88	128.74	120.28
1	B	89	GLY	CA-C-N	5.83	128.56	120.29
1	B	89	GLY	C-N-CA	5.83	128.56	120.29
1	B	394	GLY	CA-C-N	5.75	132.06	121.70
1	B	394	GLY	C-N-CA	5.75	132.06	121.70
1	B	390	CYS	CA-C-N	5.69	131.94	121.70
1	B	390	CYS	C-N-CA	5.69	131.94	121.70
1	C	161	MET	N-CA-C	5.67	118.12	110.29
1	C	76	ASP	CA-C-N	5.67	127.81	120.44
1	C	76	ASP	C-N-CA	5.67	127.81	120.44
1	A	156	GLY	N-CA-C	-5.66	104.81	112.57
1	B	57	ASP	CA-CB-CG	5.63	118.23	112.60
1	C	156	GLY	N-CA-C	-5.62	104.87	112.57
1	A	89	GLY	CA-C-N	5.59	128.23	120.29
1	A	89	GLY	C-N-CA	5.59	128.23	120.29
1	C	89	GLY	CA-C-N	5.59	128.22	120.29
1	C	89	GLY	C-N-CA	5.59	128.22	120.29
1	A	123	LEU	CA-C-N	5.55	128.17	120.29
1	A	123	LEU	C-N-CA	5.55	128.17	120.29
1	C	362	ASP	CA-CB-CG	5.55	118.15	112.60
1	D	293	PHE	CA-C-N	5.52	127.67	120.28
1	D	293	PHE	C-N-CA	5.52	127.67	120.28
1	A	365	GLN	CA-C-N	5.50	127.58	120.44
1	A	365	GLN	C-N-CA	5.50	127.58	120.44
1	D	353	PRO	CA-C-N	5.47	127.93	120.54
1	D	353	PRO	C-N-CA	5.47	127.93	120.54
1	A	396	GLY	N-CA-C	5.47	117.14	111.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	76	ASP	CA-C-N	5.45	127.52	120.44
1	A	76	ASP	C-N-CA	5.45	127.52	120.44
1	A	161	MET	N-CA-C	5.44	117.80	110.29
1	B	362	ASP	CA-CB-CG	5.38	117.98	112.60
1	A	296	ALA	N-CA-C	5.32	118.00	110.50
1	C	90	GLU	N-CA-C	5.31	117.15	111.36
1	B	156	GLY	N-CA-C	-5.29	105.33	112.57
1	D	151	ALA	N-CA-C	5.28	117.72	111.33
1	D	89	GLY	CA-C-N	5.26	127.76	120.29
1	D	89	GLY	C-N-CA	5.26	127.76	120.29
1	D	156	GLY	N-CA-C	-5.23	105.41	112.57
1	C	123	LEU	CA-C-N	5.22	127.70	120.29
1	C	123	LEU	C-N-CA	5.22	127.70	120.29
1	B	365	GLN	CA-C-N	5.21	127.21	120.44
1	B	365	GLN	C-N-CA	5.21	127.21	120.44
1	B	141	ALA	CA-C-N	5.20	125.75	119.98
1	B	141	ALA	C-N-CA	5.20	125.75	119.98
1	C	377	LYS	CA-C-N	5.17	127.21	120.28
1	C	377	LYS	C-N-CA	5.17	127.21	120.28
1	C	151	ALA	N-CA-C	5.17	117.58	111.33
1	C	141	ALA	CA-C-N	5.14	125.69	119.98
1	C	141	ALA	C-N-CA	5.14	125.69	119.98
1	A	151	ALA	N-CA-C	5.13	117.53	111.33
1	D	119	ALA	CA-C-N	5.12	127.14	120.28
1	D	119	ALA	C-N-CA	5.12	127.14	120.28
1	A	141	ALA	CA-C-N	5.10	125.64	119.98
1	A	141	ALA	C-N-CA	5.10	125.64	119.98
1	D	141	ALA	CA-C-N	5.10	125.64	119.98
1	D	141	ALA	C-N-CA	5.10	125.64	119.98
1	A	204	LEU	N-CA-C	5.10	117.88	109.72
1	D	411	MET	CA-C-N	5.09	126.98	120.56
1	D	411	MET	C-N-CA	5.09	126.98	120.56
1	C	197	ALA	CA-C-N	5.08	127.05	120.44
1	C	197	ALA	C-N-CA	5.08	127.05	120.44
1	D	158	THR	N-CA-C	-5.08	100.24	108.52
1	A	218	TYR	CA-C-N	5.08	127.08	120.28
1	A	218	TYR	C-N-CA	5.08	127.08	120.28
1	A	352	ASP	CA-CB-CG	5.06	117.66	112.60
1	A	494	ASP	CA-CB-CG	5.06	117.66	112.60
1	D	388	ARG	N-CA-C	5.05	112.77	108.22
1	B	377	LYS	CA-C-N	5.04	127.53	120.28
1	B	377	LYS	C-N-CA	5.04	127.53	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	352	ASP	CA-CB-CG	5.02	117.62	112.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3713	0	3693	23	0
1	B	3734	0	3714	21	0
1	C	3713	0	3693	16	0
1	D	3712	0	3691	18	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	7	0	10	1	0
4	A	44	0	26	5	0
4	B	44	0	26	1	0
4	C	44	0	26	1	0
4	D	44	0	26	2	0
5	A	12	0	18	0	0
5	C	16	0	24	0	0
5	D	4	0	6	0	0
6	A	25	0	0	0	0
6	B	22	0	0	0	0
6	C	23	0	0	0	0
6	D	18	0	0	1	0
All	All	15179	0	14953	72	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (72) 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:D:57:ASP:HB2	1:D:64:ILE:HD11	1.53	0.88
1:A:211:GLN:HE21	1:A:211:GLN:H	1.28	0.79
1:B:211:GLN:HE21	1:B:211:GLN:H	1.30	0.78
1:C:211:GLN:HE21	1:C:211:GLN:H	1.31	0.77
1:B:391:ALA:HB3	1:B:392:PRO:HD3	1.71	0.72
1:D:326:GLN:HG2	6:D:711:HOH:O	1.97	0.64
1:A:101:ARG:HD3	1:B:145:ARG:HD3	1.83	0.59
1:B:394:GLY:CA	1:B:395:LYS:HB3	2.32	0.59
1:C:391:ALA:HB1	1:C:395:LYS:HA	1.88	0.56
1:A:145:ARG:HD3	1:B:101:ARG:HD3	1.88	0.55
1:B:390:CYS:HB2	1:B:391:ALA:HA	1.88	0.55
1:B:390:CYS:HB2	1:B:391:ALA:CA	2.39	0.53
1:D:171:ARG:HG3	1:D:504:LEU:HD13	1.90	0.52
1:D:26:LEU:HD13	1:D:350:PHE:HB3	1.92	0.52
1:C:101:ARG:HD3	1:D:145:ARG:HD3	1.92	0.51
1:A:52:THR:H	3:A:602:PEG:H12	1.74	0.51
1:D:90:GLU:HB3	1:D:94:MET:HE3	1.93	0.50
1:B:394:GLY:HA3	1:B:395:LYS:HB3	1.94	0.49
1:A:391:ALA:H	1:A:398:TYR:HB2	1.78	0.48
1:D:182:PRO:HD2	1:D:189:MET:HG3	1.95	0.48
1:A:182:PRO:HD2	1:A:189:MET:HG3	1.96	0.48
1:C:182:PRO:HD2	1:C:189:MET:HG3	1.96	0.47
1:B:156:GLY:HA2	1:B:171:ARG:HH11	1.79	0.47
1:A:59:ARG:HD2	1:A:348:ASP:OD1	2.15	0.47
1:B:166:GLN:HB2	1:B:513:LEU:HD21	1.97	0.47
1:C:391:ALA:H	1:C:398:TYR:HB2	1.80	0.47
1:A:317:CYS:SG	4:A:603:NAD:C4N	3.03	0.46
1:A:483:PHE:HE2	4:A:603:NAD:H72N	1.63	0.46
1:D:125:ALA:HB3	1:D:127:LYS:HD3	1.96	0.46
1:B:390:CYS:HB2	1:B:391:ALA:HB2	1.96	0.46
1:B:59:ARG:HD2	1:B:348:ASP:OD1	2.15	0.46
1:D:44:PHE:HE2	1:D:221:GLN:HE21	1.63	0.45
1:D:388:ARG:O	1:D:400:GLU:HG2	2.16	0.45
1:C:166:GLN:HB2	1:C:513:LEU:HD21	1.99	0.45
1:D:59:ARG:HD2	1:D:348:ASP:OD1	2.17	0.45
1:C:44:PHE:HE2	1:C:221:GLN:HE21	1.64	0.44
1:A:285:GLY:HA2	4:A:603:NAD:O2D	2.17	0.44
1:A:196:PRO:HG2	1:A:503:TYR:HE2	1.82	0.44
1:B:255:MET:HE1	1:B:257:SER:HB2	1.98	0.44
1:C:86:PHE:HE1	1:C:173:PRO:HB2	1.83	0.44
1:D:166:GLN:HB2	1:D:513:LEU:HD21	2.00	0.44
1:A:166:GLN:HB2	1:A:513:LEU:HD21	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:PHE:CE1	4:A:603:NAD:H2D	2.53	0.44
1:B:182:PRO:HD2	1:B:189:MET:HG3	1.99	0.44
1:A:86:PHE:HE1	1:A:173:PRO:HB2	1.82	0.43
1:D:344:TRP:CD1	1:D:401:PRO:HG3	2.54	0.43
1:C:317:CYS:SG	4:C:606:NAD:C4N	3.06	0.43
1:A:275:SER:O	1:C:266:ARG:NH2	2.52	0.43
1:A:277:LEU:HD21	1:C:266:ARG:HA	1.99	0.43
1:A:266:ARG:NH2	1:C:275:SER:O	2.51	0.43
1:B:86:PHE:HE1	1:B:173:PRO:HB2	1.83	0.43
1:A:483:PHE:HE2	4:A:603:NAD:N7N	2.17	0.43
1:D:419:PHE:CE1	4:D:603:NAD:H2D	2.54	0.43
1:C:288:SER:HA	1:C:289:PRO:HD3	1.99	0.42
1:C:59:ARG:HD2	1:C:348:ASP:OD1	2.19	0.42
1:C:250:HIS:HB3	1:C:253:VAL:HG23	2.02	0.42
1:A:365:GLN:O	1:A:369:VAL:HG23	2.20	0.42
1:A:298:LEU:HD12	1:A:298:LEU:HA	1.91	0.42
1:A:254:ASP:O	1:A:279:PRO:HD2	2.20	0.41
1:D:250:HIS:HB3	1:D:253:VAL:HG23	2.02	0.41
1:A:260:GLY:O	1:A:284:LEU:HA	2.20	0.41
1:B:390:CYS:HB2	1:B:391:ALA:CB	2.50	0.41
1:D:86:PHE:HE1	1:D:173:PRO:HB2	1.85	0.41
1:D:483:PHE:HE2	4:D:603:NAD:H72N	1.69	0.41
1:B:262:THR:HA	1:B:284:LEU:HD13	2.03	0.41
1:C:255:MET:HE1	1:C:257:SER:HB2	2.02	0.41
1:D:255:MET:HE1	1:D:257:SER:HB2	2.03	0.41
1:B:122:SER:HA	1:B:127:LYS:HB2	2.03	0.41
1:A:250:HIS:HB3	1:A:253:VAL:HG23	2.02	0.40
1:B:105:ARG:HA	1:B:105:ARG:HD2	1.86	0.40
1:B:344:TRP:CD1	1:B:401:PRO:HG3	2.56	0.40
1:B:419:PHE:CE1	4:B:602:NAD:H2D	2.57	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	487/534 (91%)	468 (96%)	18 (4%)	1 (0%)	43	58
1	B	492/534 (92%)	470 (96%)	19 (4%)	3 (1%)	21	32
1	C	487/534 (91%)	468 (96%)	16 (3%)	3 (1%)	21	32
1	D	487/534 (91%)	470 (96%)	16 (3%)	1 (0%)	43	58
All	All	1953/2136 (91%)	1876 (96%)	69 (4%)	8 (0%)	30	43

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	391	ALA
1	B	395	LYS
1	C	391	ALA
1	C	396	GLY
1	A	444	GLY
1	D	444	GLY
1	B	444	GLY
1	C	361	VAL

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	381/415 (92%)	358 (94%)	23 (6%)	17	31
1	B	383/415 (92%)	361 (94%)	22 (6%)	18	33
1	C	381/415 (92%)	358 (94%)	23 (6%)	17	31
1	D	381/415 (92%)	360 (94%)	21 (6%)	19	34
All	All	1526/1660 (92%)	1437 (94%)	89 (6%)	18	32

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	LEU
1	A	29	ASP
1	A	66	SER
1	A	77	LEU
1	A	105	ARG
1	A	145	ARG
1	A	171	ARG
1	A	192	VAL
1	A	198	LEU
1	A	207	LYS
1	A	211	GLN
1	A	219	LEU
1	A	222	LEU
1	A	224	LYS
1	A	298	LEU
1	A	313	LYS
1	A	318	VAL
1	A	361	VAL
1	A	378	ARG
1	A	390	CYS
1	A	449	VAL
1	A	454	LEU
1	A	468	VAL
1	B	26	LEU
1	B	29	ASP
1	B	34	ARG
1	B	77	LEU
1	B	105	ARG
1	B	145	ARG
1	B	192	VAL
1	B	198	LEU
1	B	207	LYS
1	B	211	GLN
1	B	219	LEU
1	B	224	LYS
1	B	294	ASP
1	B	313	LYS
1	B	318	VAL
1	B	332	ARG
1	B	342	ARG
1	B	385	THR
1	B	405	THR
1	B	449	VAL

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Mol	Chain	Res	Type
1	B	454	LEU
1	B	468	VAL
1	C	27	LEU
1	C	29	ASP
1	C	34	ARG
1	C	66	SER
1	C	77	LEU
1	C	145	ARG
1	C	171	ARG
1	C	192	VAL
1	C	198	LEU
1	C	207	LYS
1	C	211	GLN
1	C	219	LEU
1	C	224	LYS
1	C	298	LEU
1	C	313	LYS
1	C	318	VAL
1	C	361	VAL
1	C	385	THR
1	C	390	CYS
1	C	408	LYS
1	C	426	MET
1	C	449	VAL
1	C	468	VAL
1	D	29	ASP
1	D	66	SER
1	D	101	ARG
1	D	116	GLU
1	D	127	LYS
1	D	145	ARG
1	D	157	GLU
1	D	171	ARG
1	D	192	VAL
1	D	198	LEU
1	D	207	LYS
1	D	224	LYS
1	D	298	LEU
1	D	313	LYS
1	D	318	VAL
1	D	385	THR
1	D	415	LYS

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Mol	Chain	Res	Type
1	D	426	MET
1	D	449	VAL
1	D	454	LEU
1	D	468	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	HIS
1	A	168	HIS
1	A	211	GLN
1	A	225	GLN
1	A	360	GLN
1	B	41	ASN
1	B	88	HIS
1	B	211	GLN
1	B	225	GLN
1	C	41	ASN
1	C	211	GLN
1	C	221	GLN
1	C	225	GLN
1	D	88	HIS
1	D	221	GLN
1	D	225	GLN
1	D	365	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 17 ligands modelled in this entry, 4 are monoatomic - leaving 13 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	EDO	A	604	-	3,3,3	0.61	0	2,2,2	0.33	0
3	PEG	A	602	-	6,6,6	0.17	0	5,5,5	0.06	0
5	EDO	C	604	-	3,3,3	0.59	0	2,2,2	0.29	0
5	EDO	C	605	-	3,3,3	0.52	0	2,2,2	0.37	0
5	EDO	A	605	-	3,3,3	0.52	0	2,2,2	0.44	0
5	EDO	A	606	-	3,3,3	0.58	0	2,2,2	0.35	0
5	EDO	C	602	-	3,3,3	0.53	0	2,2,2	0.18	0
4	NAD	A	603	-	46,48,48	1.07	1 (2%)	64,73,73	0.69	2 (3%)
4	NAD	C	606	-	46,48,48	1.11	1 (2%)	64,73,73	0.70	1 (1%)
4	NAD	D	603	-	46,48,48	1.08	1 (2%)	64,73,73	0.66	2 (3%)
5	EDO	C	603	-	3,3,3	0.49	0	2,2,2	0.45	0
4	NAD	B	602	-	46,48,48	0.95	1 (2%)	64,73,73	0.63	1 (1%)
5	EDO	D	602	-	3,3,3	0.55	0	2,2,2	0.33	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	A	604	-	-	0/1/1/1	-
3	PEG	A	602	-	-	2/4/4/4	-
5	EDO	C	604	-	-	0/1/1/1	-
5	EDO	C	605	-	-	0/1/1/1	-
5	EDO	A	605	-	-	0/1/1/1	-
5	EDO	A	606	-	-	0/1/1/1	-
5	EDO	C	602	-	-	1/1/1/1	-
4	NAD	A	603	-	-	4/30/62/62	0/5/5/5
4	NAD	C	606	-	-	4/30/62/62	0/5/5/5
4	NAD	D	603	-	-	4/30/62/62	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	C	603	-	-	0/1/1/1	-
4	NAD	B	602	-	-	4/30/62/62	0/5/5/5
5	EDO	D	602	-	-	0/1/1/1	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	606	NAD	C2N-N1N	6.73	1.42	1.35
4	D	603	NAD	C2N-N1N	6.56	1.42	1.35
4	A	603	NAD	C2N-N1N	6.46	1.42	1.35
4	B	602	NAD	C2N-N1N	5.65	1.41	1.35

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	603	NAD	C4D-O4D-C1D	2.49	112.20	109.92
4	B	602	NAD	C6N-N1N-C1D	2.24	124.13	119.73
4	A	603	NAD	C6N-N1N-C1D	2.19	124.02	119.73
4	D	603	NAD	C6N-N1N-C1D	2.16	123.96	119.73
4	D	603	NAD	C4D-O4D-C1D	2.06	111.81	109.92
4	C	606	NAD	C4D-O4D-C1D	2.05	111.80	109.92

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	602	NAD	C5B-O5B-PA-O1A
4	A	603	NAD	C2B-C1B-N9A-C8A
4	B	602	NAD	C2B-C1B-N9A-C8A
4	C	606	NAD	C2B-C1B-N9A-C8A
4	D	603	NAD	C2B-C1B-N9A-C8A
4	A	603	NAD	C5B-O5B-PA-O1A
4	C	606	NAD	C5B-O5B-PA-O1A
4	D	603	NAD	C5B-O5B-PA-O1A
4	A	603	NAD	C4D-C5D-O5D-PN
4	B	602	NAD	C4D-C5D-O5D-PN
4	D	603	NAD	C4D-C5D-O5D-PN
4	C	606	NAD	C4D-C5D-O5D-PN
4	A	603	NAD	O4B-C1B-N9A-C8A
4	B	602	NAD	O4B-C1B-N9A-C8A
4	C	606	NAD	O4B-C1B-N9A-C8A

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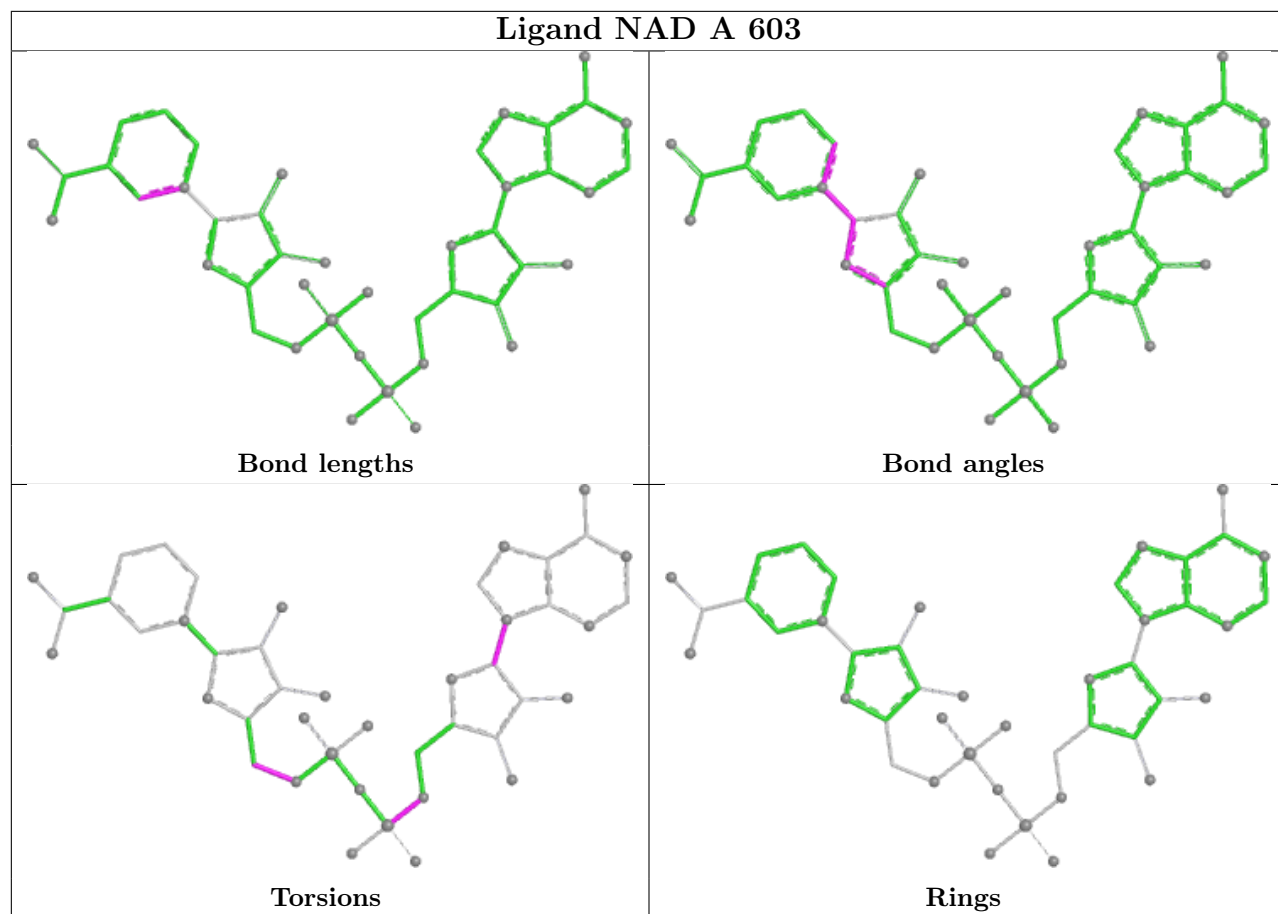
Mol	Chain	Res	Type	Atoms
4	D	603	NAD	O4B-C1B-N9A-C8A
5	C	602	EDO	O1-C1-C2-O2
3	A	602	PEG	O1-C1-C2-O2
3	A	602	PEG	C1-C2-O2-C3

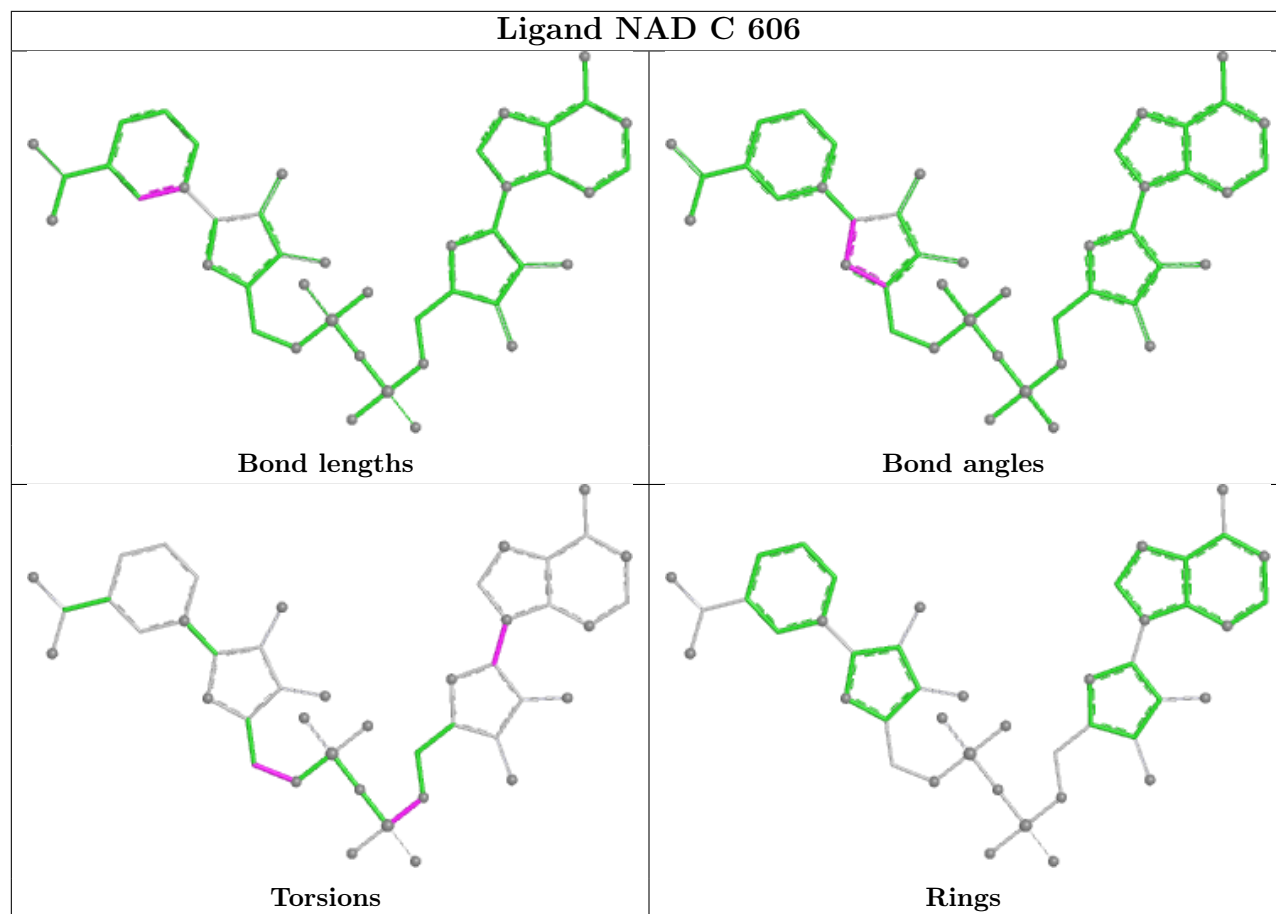
There are no ring outliers.

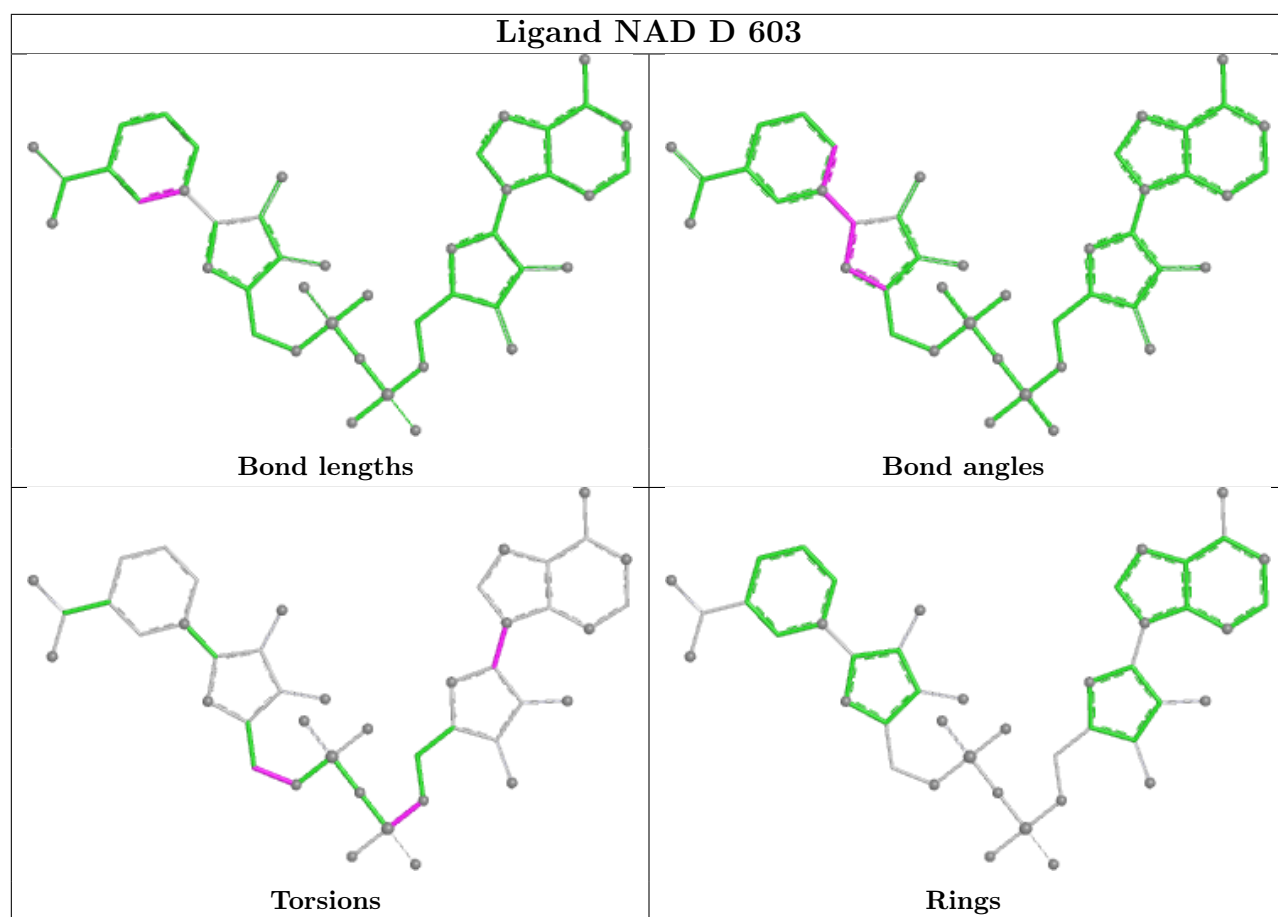
5 monomers are involved in 10 short contacts:

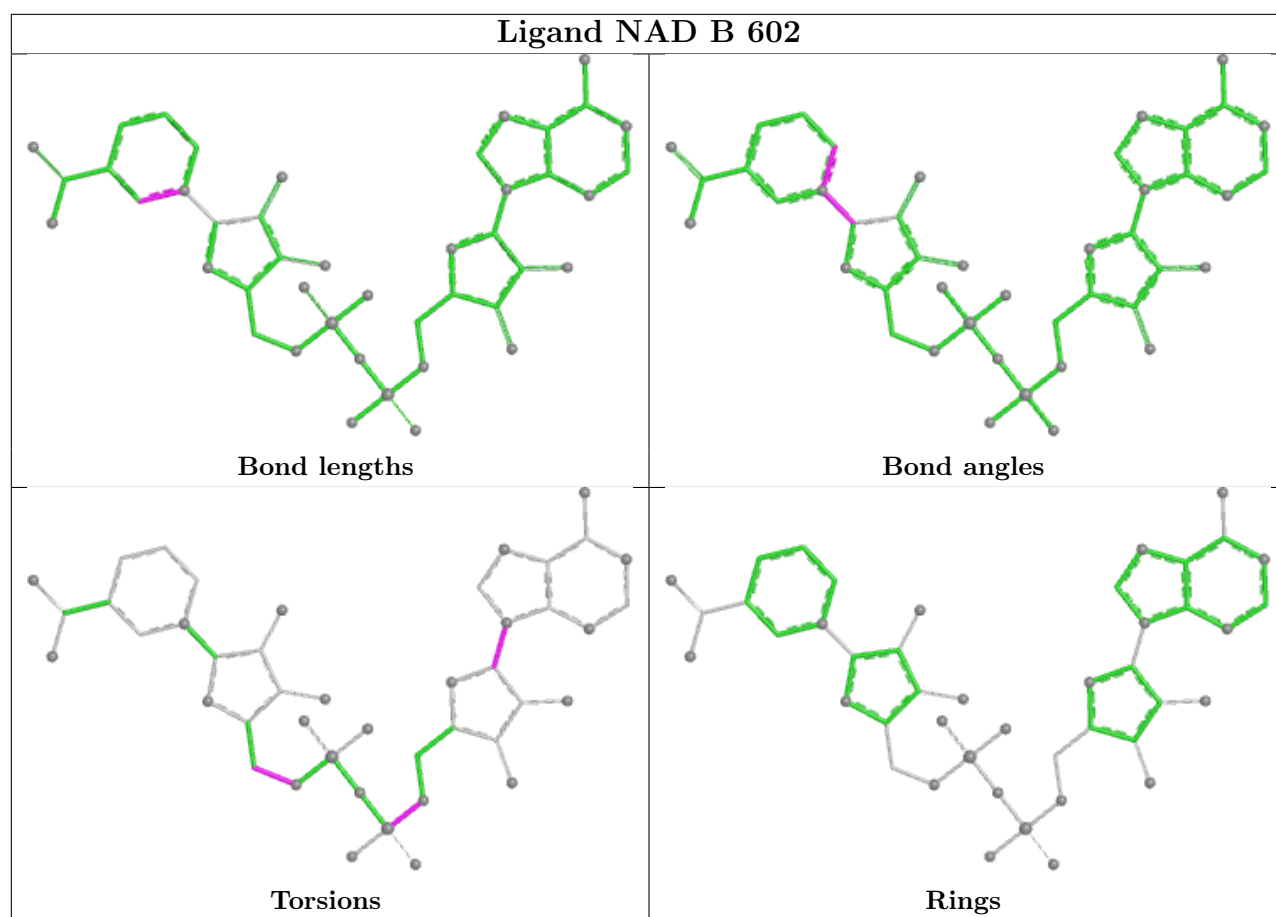
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	602	PEG	1	0
4	A	603	NAD	5	0
4	C	606	NAD	1	0
4	D	603	NAD	2	0
4	B	602	NAD	1	0

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	491/534 (91%)	-0.21	1 (0%) 91 89	53, 70, 97, 124	0
1	B	494/534 (92%)	-0.12	1 (0%) 91 89	58, 80, 110, 131	0
1	C	491/534 (91%)	-0.14	3 (0%) 85 83	56, 78, 102, 132	0
1	D	491/534 (91%)	0.04	4 (0%) 82 80	59, 95, 131, 156	0
All	All	1967/2136 (92%)	-0.11	9 (0%) 87 85	53, 80, 118, 156	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	27	LEU	3.7
1	D	35	PHE	3.6
1	B	391	ALA	3.0
1	C	27	LEU	2.9
1	C	396	GLY	2.4
1	C	395	LYS	2.4
1	D	26	LEU	2.1
1	D	396	GLY	2.1
1	D	392	PRO	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

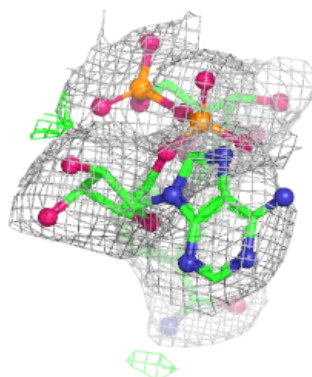
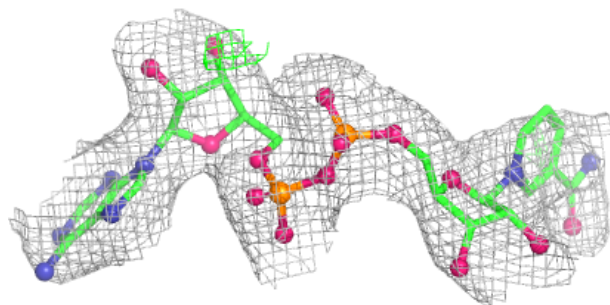
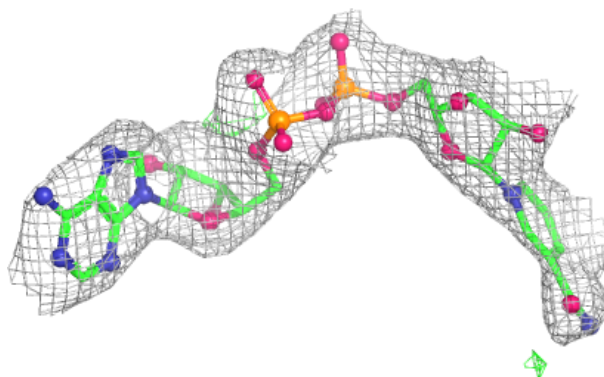
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	EDO	C	604	4/4	0.80	0.18	88,90,92,93	0
5	EDO	A	606	4/4	0.81	0.24	104,105,105,106	0
2	NA	B	601	1/1	0.81	0.09	84,84,84,84	0
5	EDO	C	603	4/4	0.83	0.20	108,109,109,109	0
3	PEG	A	602	7/7	0.83	0.13	102,103,107,108	0
2	NA	D	601	1/1	0.85	0.09	104,104,104,104	0
2	NA	C	601	1/1	0.85	0.08	84,84,84,84	0
5	EDO	A	605	4/4	0.85	0.16	100,101,101,102	0
5	EDO	A	604	4/4	0.89	0.26	82,83,85,86	0
4	NAD	D	603	44/44	0.91	0.09	94,105,116,121	0
5	EDO	C	605	4/4	0.91	0.19	91,93,95,97	0
5	EDO	D	602	4/4	0.91	0.18	92,97,100,100	0
5	EDO	C	602	4/4	0.92	0.19	82,83,83,85	0
4	NAD	A	603	44/44	0.95	0.08	66,73,82,86	0
4	NAD	B	602	44/44	0.96	0.07	76,85,89,93	0
4	NAD	C	606	44/44	0.97	0.06	63,71,81,84	0
2	NA	A	601	1/1	0.97	0.07	79,79,79,79	0

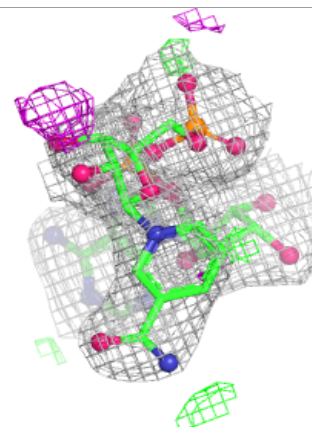
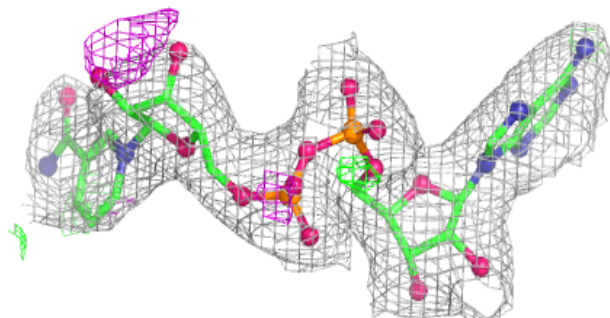
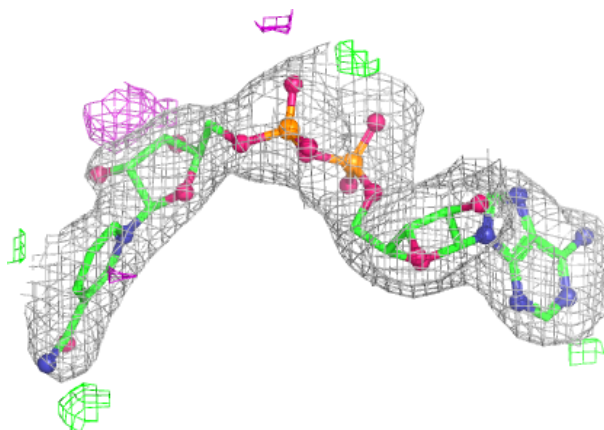
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAD D 603:

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

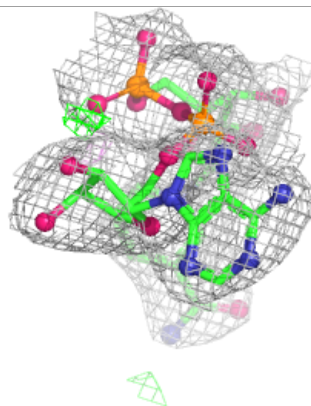
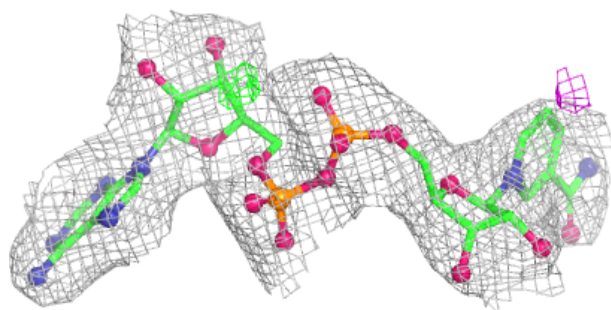
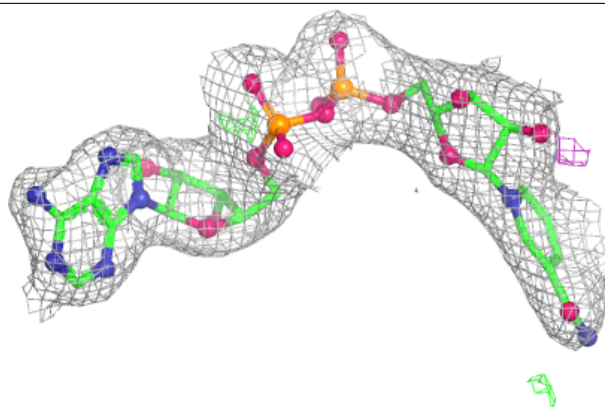
**Electron density around NAD A 603:**

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

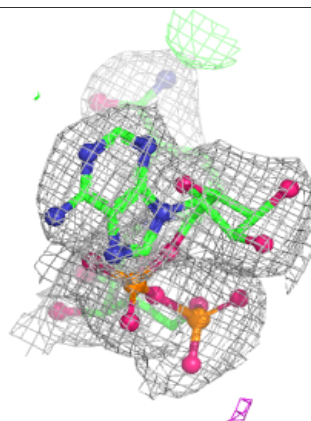
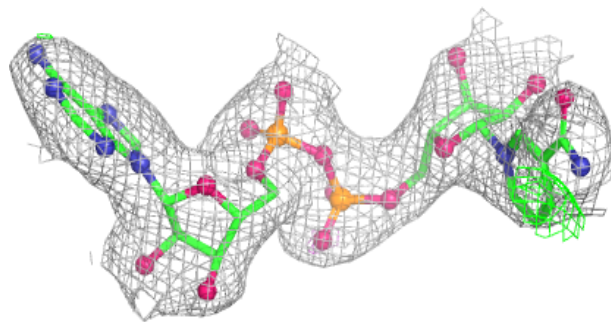
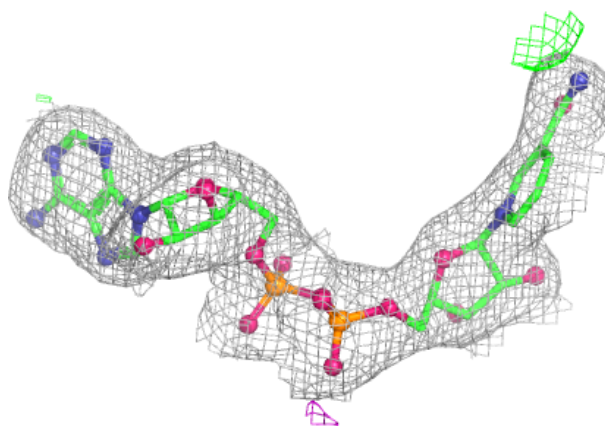


Electron density around NAD B 602:

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

**Electron density around NAD C 606:**

$2mF_o-DF_c$ (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.