



Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 09:43 am BST

PDB ID : 1LDY
Title : HORSE LIVER ALCOHOL DEHYDROGENASE COMPLEXED TO NADH
AND CYCLOHEXYL FORMAMIDE (CXF)
Authors : Ramaswamy, S.; Plapp, B.V.
Deposited on : 1996-12-23
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

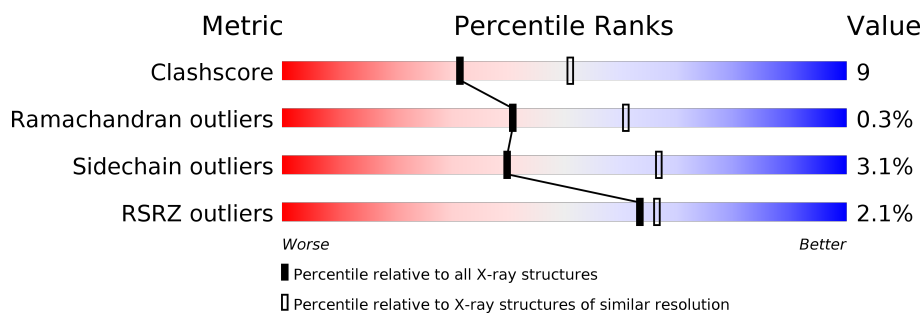
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 on 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	374	
1	B	374	
1	C	374	
1	D	374	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12372 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 ALCOHOL DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	374	Total	C	N	O	S	0	0	0
			2785	1769	472	521	23			
1	B	374	Total	C	N	O	S	0	0	0
			2785	1769	472	521	23			
1	C	374	Total	C	N	O	S	0	0	0
			2785	1769	472	521	23			
1	D	374	Total	C	N	O	S	0	0	0
			2785	1769	472	521	23			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 9 7 1 1	0	0
4	B	1	Total C N O 9 7 1 1	0	0
4	C	1	Total C N O 9 7 1 1	0	0
4	D	1	Total C N O 9 7 1 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	250	Total O 250 250	0	0
5	B	249	Total O 249 249	0	0
5	C	257	Total O 257 257	0	0
5	D	256	Total O 256 256	0	0

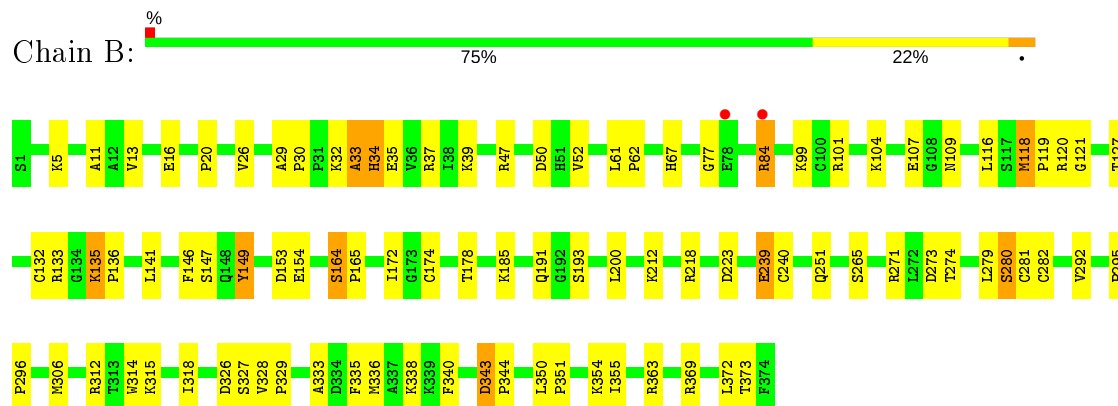
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

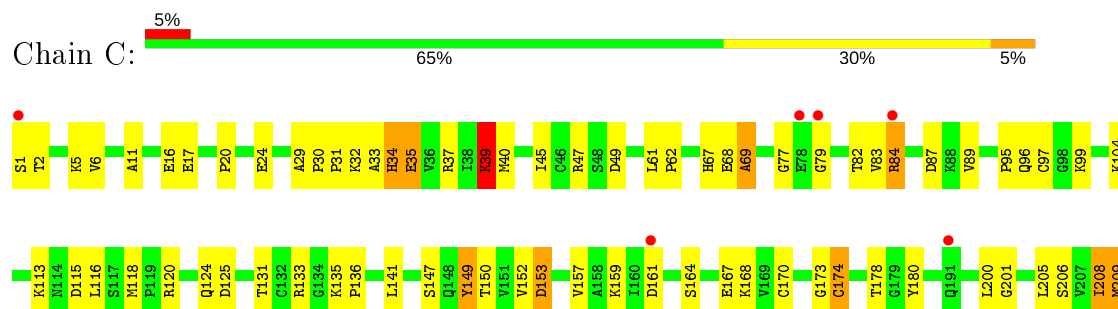
• Molecule 1: ALCOHOL DEHYDROGENASE

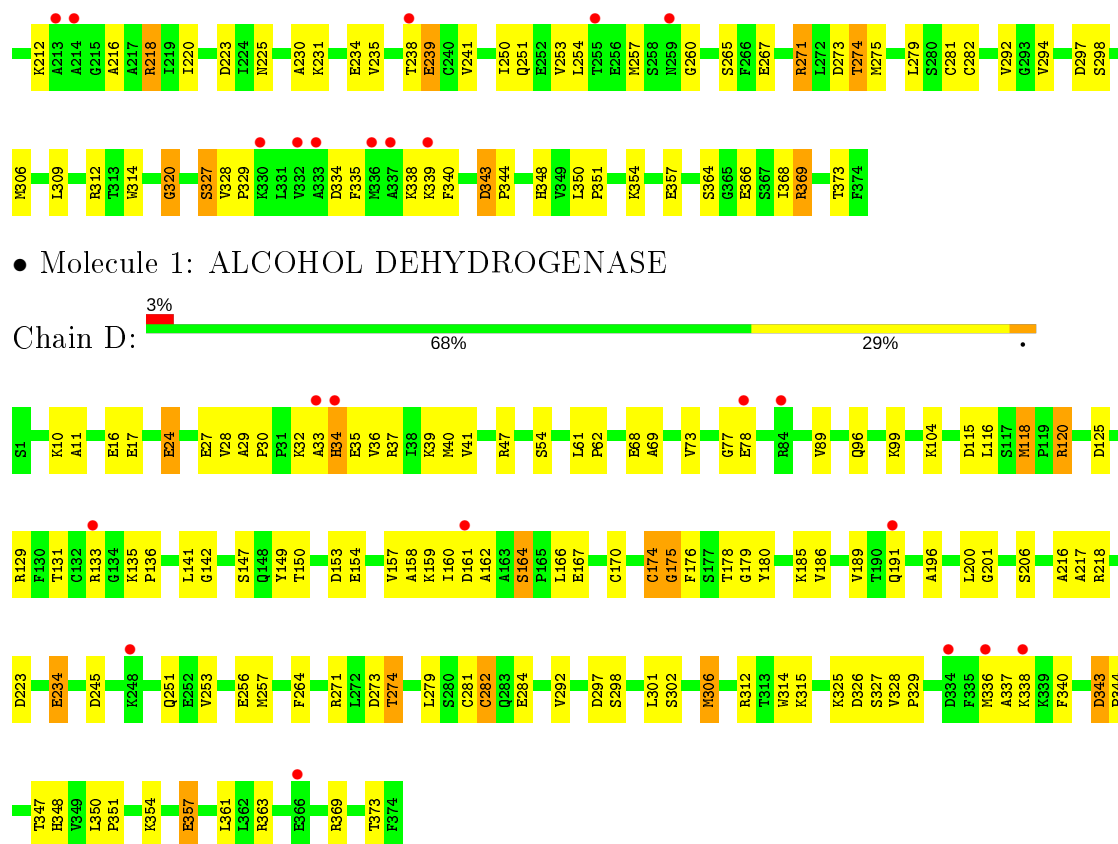


• Molecule 1: ALCOHOL DEHYDROGENASE



• Molecule 1: ALCOHOL DEHYDROGENASE





● Molecule 1: ALCOHOL DEHYDROGENASE

Chain D: 3% 68% 29%

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	49.93Å 180.20Å 86.80Å 90.00° 106.00° 90.00°	Depositor
Resolution (Å)	12.00 – 2.50 12.03 – 2.51	Depositor EDS
% Data completeness (in resolution range)	89.8 (12.00-2.50) 92.5 (12.03-2.51)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	9.40 (at 2.52Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.207 , (Not available) 0.199 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	18.5	Xtriage
Anisotropy	1.109	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 73.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12372	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 87.48 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.7562e-08. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, NAD, CXF

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	0.90	1/2837 (0.0%)	1.74	37/3834 (1.0%)
1	B	0.91	0/2837	1.78	44/3834 (1.1%)
1	C	0.97	0/2837	1.92	64/3834 (1.7%)
1	D	0.97	0/2837	1.92	57/3834 (1.5%)
All	All	0.94	1/11348 (0.0%)	1.84	202/15336 (1.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	234	GLU	CD-OE1	5.25	1.31	1.25

All (202) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	133	ARG	NE-CZ-NH2	24.40	132.50	120.30
1	D	218	ARG	NE-CZ-NH2	20.77	130.69	120.30
1	C	312	ARG	NE-CZ-NH2	-18.73	110.93	120.30
1	D	218	ARG	NE-CZ-NH1	-17.32	111.64	120.30
1	D	273	ASP	CB-CG-OD1	16.63	133.26	118.30
1	C	312	ARG	NE-CZ-NH1	16.08	128.34	120.30
1	C	273	ASP	CB-CG-OD1	14.04	130.94	118.30
1	D	129	ARG	NE-CZ-NH2	-13.78	113.41	120.30
1	A	273	ASP	CB-CG-OD1	13.62	130.56	118.30
1	D	312	ARG	NE-CZ-NH2	-13.62	113.49	120.30
1	B	312	ARG	NE-CZ-NH2	-13.42	113.59	120.30
1	C	84	ARG	NE-CZ-NH1	13.23	126.92	120.30
1	C	218	ARG	NE-CZ-NH1	-12.57	114.02	120.30
1	C	218	ARG	NE-CZ-NH2	12.41	126.51	120.30
1	C	369	ARG	NE-CZ-NH2	-12.24	114.18	120.30
1	C	133	ARG	NE-CZ-NH2	11.86	126.23	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	153	ASP	CB-CG-OD2	11.72	128.85	118.30
1	C	115	ASP	CB-CG-OD2	-11.63	107.83	118.30
1	B	153	ASP	CB-CG-OD2	11.44	128.59	118.30
1	A	271	ARG	NE-CZ-NH2	11.14	125.87	120.30
1	A	101	ARG	NE-CZ-NH1	-11.09	114.75	120.30
1	D	133	ARG	NE-CZ-NH2	11.01	125.80	120.30
1	D	369	ARG	NE-CZ-NH2	-10.88	114.86	120.30
1	C	271	ARG	NE-CZ-NH1	10.18	125.39	120.30
1	C	84	ARG	NE-CZ-NH2	-10.02	115.29	120.30
1	D	47	ARG	NE-CZ-NH2	-9.88	115.36	120.30
1	C	125	ASP	CB-CG-OD2	-9.76	109.52	118.30
1	B	37	ARG	NE-CZ-NH2	-9.61	115.50	120.30
1	C	343	ASP	CB-CG-OD2	9.58	126.92	118.30
1	D	120	ARG	NE-CZ-NH2	-9.43	115.58	120.30
1	C	180	TYR	CB-CG-CD2	-9.30	115.42	121.00
1	C	209	MET	CG-SD-CE	-9.17	85.53	100.20
1	A	101	ARG	NE-CZ-NH2	9.16	124.88	120.30
1	B	133	ARG	NE-CZ-NH1	-8.98	115.81	120.30
1	C	47	ARG	NE-CZ-NH2	-8.81	115.89	120.30
1	A	227	ASP	CB-CG-OD2	8.72	126.15	118.30
1	A	153	ASP	CB-CG-OD2	8.59	126.03	118.30
1	C	131	THR	CA-CB-CG2	-8.45	100.56	112.40
1	B	35	GLU	OE1-CD-OE2	-8.14	113.53	123.30
1	B	363	ARG	NE-CZ-NH2	-8.02	116.29	120.30
1	C	115	ASP	CB-CG-OD1	8.02	125.51	118.30
1	A	172	ILE	O-C-N	-7.96	109.67	123.20
1	A	27	GLU	OE1-CD-OE2	-7.84	113.89	123.30
1	D	17	GLU	OE1-CD-OE2	7.81	132.68	123.30
1	D	343	ASP	CB-CG-OD2	-7.80	111.28	118.30
1	A	271	ARG	NH1-CZ-NH2	-7.72	110.91	119.40
1	C	47	ARG	NE-CZ-NH1	7.70	124.15	120.30
1	D	369	ARG	NE-CZ-NH1	7.64	124.12	120.30
1	A	133	ARG	NE-CZ-NH2	7.63	124.11	120.30
1	A	312	ARG	NE-CZ-NH2	-7.59	116.50	120.30
1	D	273	ASP	OD1-CG-OD2	-7.52	109.02	123.30
1	C	161	ASP	CB-CG-OD2	-7.49	111.56	118.30
1	C	17	GLU	OE1-CD-OE2	7.48	132.28	123.30
1	D	363	ARG	NE-CZ-NH1	-7.48	116.56	120.30
1	A	37	ARG	NE-CZ-NH2	-7.46	116.57	120.30
1	B	239	GLU	OE1-CD-OE2	7.39	132.17	123.30
1	B	172	ILE	O-C-N	-7.36	110.70	123.20
1	D	216	ALA	CB-CA-C	-7.34	99.09	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	263	ASP	CB-CG-OD1	-7.28	111.75	118.30
1	D	120	ARG	NH1-CZ-NH2	7.19	127.31	119.40
1	D	131	THR	CA-CB-CG2	-7.17	102.36	112.40
1	A	343	ASP	CB-CG-OD1	7.16	124.74	118.30
1	D	47	ARG	NE-CZ-NH1	7.15	123.88	120.30
1	D	256	GLU	OE1-CD-OE2	7.14	131.87	123.30
1	D	78	GLU	OE1-CD-OE2	7.11	131.83	123.30
1	D	34	HIS	CA-CB-CG	-7.09	101.54	113.60
1	D	343	ASP	CB-CG-OD1	7.07	124.66	118.30
1	C	34	HIS	CA-CB-CG	-7.04	101.63	113.60
1	B	133	ARG	NH1-CZ-NH2	-7.01	111.69	119.40
1	D	16	GLU	OE1-CD-OE2	6.96	131.65	123.30
1	C	369	ARG	CD-NE-CZ	-6.81	114.07	123.60
1	A	353	GLU	OE1-CD-OE2	6.80	131.47	123.30
1	C	153	ASP	CB-CG-OD2	6.80	124.42	118.30
1	D	306	MET	CB-CG-SD	6.70	132.49	112.40
1	C	357	GLU	OE1-CD-OE2	6.67	131.30	123.30
1	C	49	ASP	CB-CG-OD1	6.66	124.29	118.30
1	A	306	MET	CB-CG-SD	6.66	132.38	112.40
1	C	320	GLY	O-C-N	-6.64	111.91	123.20
1	C	35	GLU	OE1-CD-OE2	-6.49	115.51	123.30
1	D	216	ALA	N-CA-CB	6.47	119.16	110.10
1	B	280	SER	N-CA-CB	6.46	120.19	110.50
1	C	238	THR	O-C-N	-6.46	112.36	122.70
1	B	326	ASP	CB-CG-OD2	6.42	124.08	118.30
1	C	216	ALA	CB-CA-C	-6.42	100.47	110.10
1	D	115	ASP	CB-CG-OD1	6.41	124.07	118.30
1	B	34	HIS	CA-CB-CG	-6.38	102.75	113.60
1	D	120	ARG	NE-CZ-NH1	-6.38	117.11	120.30
1	B	154	GLU	OE1-CD-OE2	6.29	130.85	123.30
1	B	273	ASP	CB-CG-OD1	6.26	123.94	118.30
1	C	39	LYS	O-C-N	6.26	132.72	122.70
1	B	218	ARG	NE-CZ-NH2	6.22	123.41	120.30
1	B	13	VAL	CG1-CB-CG2	-6.21	100.96	110.90
1	A	259	ASN	CB-CG-OD1	-6.20	109.19	121.60
1	A	161	ASP	CB-CG-OD1	6.19	123.87	118.30
1	A	34	HIS	CA-CB-CG	-6.18	103.09	113.60
1	A	306	MET	CA-CB-CG	6.12	123.70	113.30
1	A	33	ALA	CB-CA-C	-6.10	100.94	110.10
1	D	125	ASP	CB-CG-OD2	-6.09	112.82	118.30
1	B	33	ALA	CB-CA-C	-6.09	100.97	110.10
1	B	306	MET	CB-CG-SD	6.08	130.65	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	273	ASP	OD1-CG-OD2	-6.04	111.83	123.30
1	D	68	GLU	OE1-CD-OE2	-5.95	116.16	123.30
1	C	180	TYR	CB-CG-CD1	5.88	124.53	121.00
1	B	265	SER	N-CA-CB	5.86	119.29	110.50
1	A	161	ASP	CB-CG-OD2	-5.85	113.03	118.30
1	A	271	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	D	326	ASP	CB-CG-OD1	5.80	123.52	118.30
1	C	37	ARG	NE-CZ-NH2	-5.79	117.41	120.30
1	D	35	GLU	OE1-CD-OE2	-5.78	116.36	123.30
1	B	153	ASP	OD1-CG-OD2	-5.75	112.38	123.30
1	C	306	MET	CB-CG-SD	5.75	129.64	112.40
1	D	176	PHE	O-C-N	5.73	131.87	122.70
1	D	158	ALA	CB-CA-C	-5.73	101.51	110.10
1	D	37	ARG	NE-CZ-NH1	-5.72	117.44	120.30
1	C	24	GLU	CA-CB-CG	5.72	125.98	113.40
1	D	245	ASP	CB-CG-OD2	5.70	123.43	118.30
1	A	67	HIS	CA-CB-CG	-5.68	103.94	113.60
1	C	260	GLY	CA-C-O	-5.61	110.50	120.60
1	D	118	MET	CA-CB-CG	5.61	122.84	113.30
1	A	193	SER	N-CA-CB	-5.60	102.11	110.50
1	A	368	ILE	N-CA-C	-5.60	95.89	111.00
1	B	121	GLY	O-C-N	-5.58	113.77	122.70
1	D	96	GLN	CA-CB-CG	-5.56	101.17	113.40
1	B	20	PRO	N-CA-CB	5.53	109.93	103.30
1	A	372	LEU	O-C-N	5.52	131.53	122.70
1	C	96	GLN	CA-CB-CG	-5.52	101.26	113.40
1	C	320	GLY	CA-C-N	5.50	127.20	116.20
1	D	180	TYR	CB-CG-CD2	-5.48	117.71	121.00
1	D	357	GLU	OE1-CD-OE2	5.48	129.87	123.30
1	D	133	ARG	O-C-N	-5.45	113.94	123.20
1	B	343	ASP	CB-CG-OD1	5.44	123.20	118.30
1	B	369	ARG	N-CA-CB	5.44	120.39	110.60
1	C	69	ALA	N-CA-CB	-5.43	102.49	110.10
1	C	235	VAL	C-N-CA	-5.43	110.90	122.30
1	A	273	ASP	CB-CG-OD2	-5.42	113.42	118.30
1	C	208	ILE	O-C-N	-5.42	114.03	122.70
1	C	265	SER	N-CA-CB	5.41	118.61	110.50
1	B	146	PHE	O-C-N	-5.40	114.05	122.70
1	C	95	PRO	N-CA-CB	5.40	109.78	103.30
1	B	327	SER	O-C-N	5.39	131.33	122.70
1	D	189	VAL	CG1-CB-CG2	-5.37	102.31	110.90
1	D	234	GLU	OE1-CD-OE2	5.34	129.71	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	67	HIS	CA-CB-CG	-5.33	104.53	113.60
1	B	101	ARG	CD-NE-CZ	-5.33	116.14	123.60
1	C	312	ARG	CD-NE-CZ	5.33	131.06	123.60
1	C	133	ARG	NE-CZ-NH1	-5.32	117.64	120.30
1	C	201	GLY	N-CA-C	-5.31	99.82	113.10
1	B	363	ARG	NH1-CZ-NH2	5.31	125.24	119.40
1	C	24	GLU	OE1-CD-OE2	-5.31	116.93	123.30
1	C	334	ASP	CB-CG-OD2	5.29	123.06	118.30
1	A	125	ASP	CB-CG-OD1	5.28	123.05	118.30
1	B	118	MET	CA-CB-CG	5.28	122.27	113.30
1	B	84	ARG	NE-CZ-NH2	-5.27	117.67	120.30
1	B	50	ASP	CB-CG-OD1	5.26	123.03	118.30
1	C	167	GLU	CG-CD-OE1	5.26	128.81	118.30
1	A	16	GLU	CB-CA-C	-5.25	99.91	110.40
1	A	369	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	C	16	GLU	OE1-CD-OE2	5.24	129.59	123.30
1	C	136	PRO	N-CA-CB	5.23	109.57	103.30
1	C	368	ILE	N-CA-C	-5.23	96.89	111.00
1	B	52	VAL	CA-CB-CG1	5.22	118.73	110.90
1	C	309	LEU	O-C-N	-5.22	114.35	122.70
1	B	47	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	B	119	PRO	N-CA-CB	5.21	109.55	103.30
1	B	37	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	D	54	SER	CA-C-O	-5.20	109.19	120.10
1	C	45	ILE	O-C-N	-5.20	114.39	122.70
1	A	280	SER	N-CA-CB	5.19	118.28	110.50
1	D	347	THR	O-C-N	-5.19	114.40	122.70
1	B	16	GLU	CB-CA-C	-5.18	100.03	110.40
1	D	28	VAL	CA-CB-CG1	-5.18	103.13	110.90
1	B	172	ILE	CA-C-O	5.17	130.95	120.10
1	C	343	ASP	OD1-CG-OD2	-5.17	113.48	123.30
1	D	160	ILE	CA-C-O	5.17	130.94	120.10
1	A	16	GLU	OE1-CD-OE2	5.16	129.49	123.30
1	D	282	CYS	CA-CB-SG	5.16	123.29	114.00
1	C	149	TYR	CB-CG-CD1	-5.15	117.91	121.00
1	C	327	SER	CB-CA-C	-5.15	100.32	110.10
1	A	221	GLY	CA-C-O	-5.13	111.36	120.60
1	D	191	GLN	O-C-N	-5.12	114.49	123.20
1	D	24	GLU	CB-CG-CD	-5.12	100.38	114.20
1	D	264	PHE	O-C-N	-5.10	114.54	122.70
1	C	6	VAL	O-C-N	-5.10	114.55	122.70
1	C	212	LYS	O-C-N	-5.09	114.55	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	196	ALA	CB-CA-C	5.09	117.73	110.10
1	C	334	ASP	CB-CG-OD1	5.07	122.86	118.30
1	A	312	ARG	CD-NE-CZ	5.07	130.70	123.60
1	A	245	ASP	CB-CG-OD2	5.06	122.85	118.30
1	D	201	GLY	N-CA-C	-5.06	100.46	113.10
1	B	149	TYR	O-C-N	5.04	130.77	122.70
1	B	193	SER	N-CA-CB	-5.04	102.94	110.50
1	C	239	GLU	CB-CA-C	-5.04	100.32	110.40
1	A	96	GLN	CA-CB-CG	-5.03	102.34	113.40
1	D	28	VAL	CA-CB-CG2	5.03	118.44	110.90
1	D	217	ALA	CB-CA-C	-5.02	102.56	110.10
1	C	79	GLY	CA-C-O	-5.02	111.56	120.60
1	B	109	ASN	CB-CG-OD1	-5.01	111.57	121.60
1	D	153	ASP	CB-CG-OD1	-5.01	113.79	118.30
1	D	136	PRO	N-CA-CB	5.01	109.31	103.30
1	B	240	CYS	N-CA-CB	5.00	119.60	110.60
1	B	306	MET	CA-CB-CG	5.00	121.80	113.30
1	C	225	ASN	N-CA-CB	5.00	119.60	110.60

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	2785	0	2848	44	0
1	B	2785	0	2848	44	0
1	C	2785	0	2848	66	0
1	D	2785	0	2848	56	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	44	0	25	1	0
3	B	44	0	25	2	0
3	C	44	0	23	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	44	0	24	2	0
4	A	9	0	13	1	0
4	B	9	0	13	2	0
4	C	9	0	13	3	0
4	D	9	0	13	0	0
5	A	250	0	0	14	0
5	B	249	0	0	12	0
5	C	257	0	0	23	0
5	D	256	0	0	20	0
All	All	12372	0	11541	206	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 9.

All (206) 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:200:LEU:HD12	1:A:223:ASP:HB2	1.56	0.84
1:B:200:LEU:HD12	1:B:223:ASP:HB2	1.61	0.81
1:D:200:LEU:HD12	1:D:223:ASP:HB2	1.68	0.76
1:D:154:GLU:HB3	5:D:556:HOH:O	1.88	0.74
1:C:218:ARG:NH2	5:C:554:HOH:O	2.18	0.72
1:D:32:LYS:HE3	5:D:552:HOH:O	1.91	0.69
1:C:200:LEU:HD12	1:C:223:ASP:HB2	1.74	0.68
1:C:120:ARG:HB2	5:C:562:HOH:O	1.94	0.68
1:A:340:PHE:HB2	5:A:397:HOH:O	1.94	0.67
1:B:99:LYS:O	1:B:104:LYS:HE3	1.94	0.67
1:B:178:THR:HG21	3:B:377:NAD:C4N	2.27	0.65
1:B:340:PHE:HB2	5:B:398:HOH:O	1.94	0.65
1:C:350:LEU:HB3	1:C:351:PRO:HD2	1.79	0.65
1:D:39:LYS:HB2	1:D:149:TYR:CE2	2.31	0.65
1:C:83:VAL:HG12	1:C:159:LYS:HB2	1.79	0.65
1:A:132:CYS:HB3	1:A:137:ILE:HD11	1.80	0.64
1:A:209:MET:SD	5:A:397:HOH:O	2.55	0.64
1:B:191:GLN:HE22	1:D:302:SER:HB3	1.62	0.64
1:B:351:PRO:HG2	1:B:354:LYS:HD2	1.81	0.62
1:C:364:SER:OG	1:C:366:GLU:HG3	2.00	0.62
1:D:162:ALA:HB2	5:D:488:HOH:O	2.01	0.61
1:C:39:LYS:NZ	5:C:559:HOH:O	2.33	0.61
1:A:84:ARG:HD3	5:A:467:HOH:O	2.01	0.61
1:B:39:LYS:HB2	1:B:149:TYR:CE2	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:THR:HG21	3:A:377:NAD:C4N	2.32	0.60
1:C:84:ARG:HD3	5:C:479:HOH:O	2.01	0.59
1:A:32:LYS:HE3	5:A:540:HOH:O	2.01	0.59
1:A:231:LYS:HB3	5:A:538:HOH:O	2.02	0.59
1:B:120:ARG:HB2	5:B:551:HOH:O	2.03	0.58
1:D:340:PHE:HB2	5:D:408:HOH:O	2.03	0.58
1:D:161:ASP:O	1:D:164:SER:OG	2.22	0.58
1:C:173:GLY:HA3	5:C:429:HOH:O	2.02	0.58
1:D:116:LEU:HG	1:D:141:LEU:HD22	1.86	0.57
1:C:338:LYS:HA	5:C:502:HOH:O	2.04	0.57
1:C:1:SER:O	1:C:5:LYS:NZ	2.29	0.57
1:B:32:LYS:HE3	5:B:541:HOH:O	2.05	0.57
1:D:24:GLU:HB2	5:D:474:HOH:O	2.05	0.57
1:C:241:VAL:HA	5:C:402:HOH:O	2.03	0.57
1:B:350:LEU:HB3	1:B:351:PRO:HD2	1.86	0.57
1:C:239:GLU:HA	5:C:403:HOH:O	2.05	0.56
1:D:351:PRO:HG2	1:D:354:LYS:HD2	1.87	0.56
1:C:39:LYS:HB2	1:C:149:TYR:CE2	2.40	0.56
1:B:212:LYS:NZ	5:B:503:HOH:O	2.37	0.55
1:A:99:LYS:O	1:A:104:LYS:HE3	2.06	0.55
1:A:351:PRO:HG2	1:A:354:LYS:HD2	1.87	0.55
1:C:340:PHE:HB2	5:C:408:HOH:O	2.06	0.55
1:A:127:THR:HB	5:A:507:HOH:O	2.06	0.55
1:B:279:LEU:HD13	1:B:314:TRP:CG	2.42	0.55
1:C:116:LEU:HG	1:C:141:LEU:HD22	1.88	0.55
1:D:336:MET:HB2	5:D:557:HOH:O	2.06	0.55
1:C:205:LEU:HD21	5:C:527:HOH:O	2.07	0.55
1:C:339:LYS:HD3	5:C:609:HOH:O	2.05	0.55
1:B:318:ILE:HD12	4:B:378:CXF:H31	1.88	0.54
1:A:17:GLU:OE2	1:B:338:LYS:HE3	2.08	0.54
1:A:116:LEU:HG	1:A:141:LEU:HD22	1.90	0.54
1:D:178:THR:HG21	3:D:377:NAD:C4N	2.37	0.54
1:D:89:VAL:HG12	1:D:159:LYS:HA	1.89	0.54
1:B:116:LEU:HD23	4:B:378:CXF:H41	1.90	0.53
1:B:116:LEU:HG	1:B:141:LEU:HD22	1.91	0.53
1:B:351:PRO:CG	1:B:354:LYS:HD2	2.39	0.53
1:A:157:VAL:O	1:A:325:LYS:HE3	2.09	0.52
1:D:32:LYS:HB3	5:D:592:HOH:O	2.08	0.52
1:D:33:ALA:O	1:D:34:HIS:HB2	2.09	0.52
1:C:11:ALA:HA	1:C:147:SER:HA	1.92	0.51
1:B:61:LEU:HB3	1:B:62:PRO:HA	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:VAL:O	1:A:257:MET:HG3	2.10	0.51
1:C:33:ALA:O	1:C:34:HIS:HB2	2.11	0.50
1:A:295:PRO:HG2	5:A:427:HOH:O	2.12	0.50
1:C:328:VAL:N	1:C:329:PRO:CD	2.73	0.50
1:A:11:ALA:HA	1:A:147:SER:HA	1.93	0.50
1:D:10:LYS:HE3	5:D:532:HOH:O	2.11	0.50
1:D:61:LEU:HB3	1:D:62:PRO:HA	1.94	0.49
1:C:152:VAL:HG21	1:C:157:VAL:HB	1.94	0.49
1:A:32:LYS:O	1:A:77:GLY:HA3	2.12	0.49
1:D:30:PRO:O	5:D:504:HOH:O	2.20	0.49
1:B:33:ALA:O	1:B:34:HIS:HB2	2.11	0.49
1:C:231:LYS:HB3	5:C:411:HOH:O	2.12	0.49
1:D:284:GLU:OE1	5:D:611:HOH:O	2.19	0.49
1:D:39:LYS:NZ	5:D:559:HOH:O	2.45	0.49
1:B:239:GLU:OE1	5:B:513:HOH:O	2.18	0.48
1:D:350:LEU:HB3	1:D:351:PRO:HD2	1.95	0.48
1:A:271:ARG:HB2	1:A:274:THR:OG1	2.13	0.48
1:A:364:SER:OG	1:A:366:GLU:HG3	2.12	0.48
1:B:271:ARG:HB2	1:B:274:THR:OG1	2.14	0.48
1:C:124:GLN:N	1:C:153:ASP:OD2	2.40	0.48
1:C:31:PRO:HD2	5:C:470:HOH:O	2.11	0.48
1:D:157:VAL:O	1:D:325:LYS:HE3	2.12	0.48
1:A:39:LYS:HB2	1:A:149:TYR:CE2	2.48	0.48
1:B:292:VAL:O	3:B:377:NAD:H2N	2.14	0.48
1:B:344:PRO:HA	5:B:400:HOH:O	2.14	0.48
1:A:61:LEU:HB3	1:A:62:PRO:HA	1.95	0.48
1:C:351:PRO:HG2	1:C:354:LYS:HD2	1.96	0.47
1:C:32:LYS:HE3	5:C:552:HOH:O	2.13	0.47
1:A:335:PHE:O	5:A:490:HOH:O	2.20	0.47
1:C:32:LYS:HB2	1:C:35:GLU:CD	2.35	0.47
1:C:271:ARG:HB2	1:C:274:THR:OG1	2.15	0.47
1:D:343:ASP:N	1:D:344:PRO:CD	2.78	0.47
1:B:315:LYS:NZ	5:B:610:HOH:O	2.47	0.47
1:D:337:ALA:O	1:D:338:LYS:CB	2.60	0.47
1:D:27:GLU:HG3	5:D:564:HOH:O	2.15	0.47
1:B:32:LYS:O	1:B:77:GLY:HA3	2.15	0.46
1:C:208:ILE:O	1:C:209:MET:C	2.54	0.46
1:D:351:PRO:CG	1:D:354:LYS:HD2	2.44	0.46
1:D:306:MET:HB3	5:D:531:HOH:O	2.14	0.46
1:D:32:LYS:O	1:D:77:GLY:HA3	2.16	0.46
1:A:279:LEU:HD13	1:A:314:TRP:CG	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:LYS:HE2	5:B:415:HOH:O	2.15	0.46
1:D:29:ALA:HB1	1:D:30:PRO:HD2	1.97	0.46
1:C:294:VAL:HG21	4:C:378:CXF:H52	1.97	0.46
1:A:305:PRO:HG3	1:D:301:LEU:HD23	1.96	0.46
1:D:253:VAL:O	1:D:257:MET:HG3	2.16	0.46
1:C:89:VAL:HG12	1:C:159:LYS:HA	1.98	0.46
1:D:11:ALA:HA	1:D:147:SER:HA	1.96	0.46
1:A:350:LEU:HB3	1:A:351:PRO:HD2	1.98	0.46
1:B:11:ALA:HA	1:B:147:SER:HA	1.98	0.45
1:A:120:ARG:HB2	5:A:550:HOH:O	2.16	0.45
1:C:220:ILE:HG21	1:C:254:LEU:HD21	1.99	0.45
1:A:69:ALA:HB3	1:A:145:THR:HG21	1.98	0.45
1:C:294:VAL:CG2	4:C:378:CXF:H32	2.46	0.45
1:D:142:GLY:HA3	5:D:448:HOH:O	2.17	0.45
1:D:120:ARG:HB2	5:D:562:HOH:O	2.17	0.45
1:D:279:LEU:HD13	1:D:314:TRP:CG	2.51	0.45
1:C:32:LYS:CE	5:C:552:HOH:O	2.65	0.44
1:D:167:GLU:HB2	5:D:483:HOH:O	2.16	0.44
1:C:61:LEU:HB3	1:C:62:PRO:HA	2.00	0.44
1:B:164:SER:HA	1:B:165:PRO:HD3	1.81	0.44
1:C:67:HIS:CD2	4:C:378:CXF:H7	2.52	0.44
1:D:271:ARG:HB2	1:D:274:THR:OG1	2.18	0.44
1:D:154:GLU:N	5:D:445:HOH:O	2.50	0.44
1:D:40:MET:HE1	1:D:150:THR:CG2	2.47	0.44
1:B:127:THR:HB	5:B:508:HOH:O	2.17	0.44
1:C:32:LYS:O	1:C:77:GLY:HA3	2.18	0.44
1:C:335:PHE:HB2	1:C:340:PHE:CZ	2.52	0.44
1:C:178:THR:HA	1:C:320:GLY:N	2.33	0.44
1:C:369:ARG:HD3	1:C:369:ARG:HH11	1.63	0.44
1:D:292:VAL:O	3:D:377:NAD:H2N	2.16	0.44
1:C:279:LEU:HD13	1:C:314:TRP:CG	2.53	0.43
1:C:2:THR:HG22	5:C:561:HOH:O	2.17	0.43
1:C:29:ALA:HB1	1:C:30:PRO:HD2	2.00	0.43
1:B:328:VAL:HB	1:B:329:PRO:HD3	1.99	0.43
1:A:351:PRO:CG	1:A:354:LYS:HD2	2.48	0.43
1:B:107:GLU:HG3	5:C:388:HOH:O	2.17	0.43
1:B:343:ASP:N	1:B:344:PRO:CD	2.81	0.43
1:A:361:LEU:HD23	5:A:563:HOH:O	2.18	0.43
1:B:26:VAL:HG12	1:B:132:CYS:HB2	2.00	0.43
1:B:343:ASP:N	1:B:344:PRO:HD2	2.33	0.43
1:D:348:HIS:CD2	1:D:361:LEU:HD13	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:343:ASP:N	1:C:344:PRO:CD	2.81	0.43
1:A:69:ALA:HA	1:A:170:CYS:HB2	2.01	0.43
1:B:296:PRO:HG2	5:B:617:HOH:O	2.19	0.43
1:C:351:PRO:CG	1:C:354:LYS:HD2	2.49	0.43
1:C:97:CYS:HB3	1:C:113:LYS:HG3	2.00	0.43
1:D:328:VAL:HB	1:D:329:PRO:HD3	2.01	0.43
1:D:328:VAL:N	1:D:329:PRO:CD	2.81	0.43
1:C:350:LEU:HB3	1:C:351:PRO:CD	2.47	0.43
1:B:335:PHE:HB2	1:B:340:PHE:CZ	2.54	0.42
1:D:174:CYS:HB3	1:D:175:GLY:H	1.62	0.42
1:D:179:GLY:HA3	1:D:206:SER:HB2	2.00	0.42
1:A:196:ALA:HB2	1:A:262:VAL:HG11	2.01	0.42
1:B:29:ALA:HB1	1:B:30:PRO:HD2	2.00	0.42
1:A:226:LYS:HG2	5:A:473:HOH:O	2.18	0.42
1:A:343:ASP:N	1:A:344:PRO:CD	2.82	0.42
1:C:297:ASP:O	1:C:298:SER:HB2	2.19	0.42
1:D:99:LYS:O	1:D:104:LYS:HE3	2.19	0.42
1:C:253:VAL:O	1:C:257:MET:HG3	2.19	0.42
1:D:41:VAL:HG21	1:D:166:LEU:HD12	2.00	0.42
1:A:185:LYS:HE2	5:A:414:HOH:O	2.19	0.42
1:A:245:ASP:OD2	5:A:390:HOH:O	2.22	0.42
1:A:230:ALA:O	1:A:234:GLU:HG3	2.20	0.42
1:A:302:SER:HA	1:D:301:LEU:O	2.20	0.42
1:C:231:LYS:NZ	1:C:344:PRO:O	2.39	0.42
1:A:318:ILE:HD12	4:A:378:CXF:H31	2.02	0.42
1:D:234:GLU:OE1	5:D:617:HOH:O	2.22	0.41
1:C:20:PRO:HD2	5:C:581:HOH:O	2.20	0.41
1:B:120:ARG:NH1	5:B:605:HOH:O	2.46	0.41
1:C:68:GLU:OE2	1:C:174:CYS:HB3	2.21	0.41
1:A:53:VAL:HG11	5:A:449:HOH:O	2.20	0.41
1:B:333:ALA:O	1:B:336:MET:HB2	2.21	0.41
1:B:84:ARG:HG3	5:B:547:HOH:O	2.20	0.41
1:D:120:ARG:NH1	5:D:619:HOH:O	2.41	0.41
1:C:250:ILE:HG22	5:C:399:HOH:O	2.20	0.41
1:C:343:ASP:N	1:C:344:PRO:HD2	2.36	0.41
1:D:186:VAL:HG12	1:D:315:LYS:HE2	2.02	0.41
1:C:82:THR:HB	5:C:573:HOH:O	2.19	0.41
1:B:295:PRO:HG2	5:C:383:HOH:O	2.21	0.41
1:C:292:VAL:O	3:C:377:NAD:H2N	2.20	0.41
1:D:69:ALA:HA	1:D:170:CYS:HB2	2.02	0.41
1:C:267:GLU:HG3	1:C:275:MET:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:185:LYS:HE2	5:D:425:HOH:O	2.20	0.41
1:A:29:ALA:HB1	1:A:30:PRO:HD2	2.02	0.41
1:B:328:VAL:N	1:B:329:PRO:CD	2.83	0.41
1:B:355:ILE:HG13	1:B:372:LEU:HD11	2.02	0.41
1:C:348:HIS:HA	5:C:530:HOH:O	2.20	0.41
1:C:84:ARG:N	1:C:87:ASP:OD2	2.47	0.41
1:A:328:VAL:HB	1:A:329:PRO:HD3	2.03	0.40
1:C:230:ALA:O	1:C:234:GLU:HG3	2.21	0.40
1:A:335:PHE:HB2	1:A:340:PHE:CZ	2.56	0.40
1:B:135:LYS:HA	1:B:136:PRO:HD3	1.99	0.40
1:C:69:ALA:HA	1:C:170:CYS:HB2	2.02	0.40
1:D:297:ASP:O	1:D:298:SER:HB2	2.21	0.40
1:A:83:VAL:HG12	1:A:159:LYS:HB2	2.04	0.40
1:C:40:MET:HE1	1:C:150:THR:CG2	2.51	0.40
1:C:99:LYS:O	1:C:104:LYS:HE3	2.21	0.40
1:D:36:VAL:HG13	1:D:73:VAL:HG13	2.04	0.40
1:C:168:LYS:HE3	5:C:608:HOH:O	2.22	0.40
1:C:328:VAL:HB	1:C:329:PRO:HD3	2.03	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	372/374 (100%)	353 (95%)	18 (5%)	1 (0%)	41	61
1	B	372/374 (100%)	353 (95%)	18 (5%)	1 (0%)	41	61
1	C	372/374 (100%)	355 (95%)	16 (4%)	1 (0%)	41	61
1	D	372/374 (100%)	357 (96%)	13 (4%)	2 (0%)	29	48
All	All	1488/1496 (100%)	1418 (95%)	65 (4%)	5 (0%)	41	61

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	174	CYS
1	C	174	CYS
1	D	174	CYS
1	B	174	CYS
1	D	175	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	308/308 (100%)	300 (97%)	8 (3%)	46	72
1	B	308/308 (100%)	299 (97%)	9 (3%)	42	69
1	C	308/308 (100%)	297 (96%)	11 (4%)	35	61
1	D	308/308 (100%)	298 (97%)	10 (3%)	39	65
All	All	1232/1232 (100%)	1194 (97%)	38 (3%)	40	67

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LYS
1	A	118	MET
1	A	135	LYS
1	A	164	SER
1	A	281	CYS
1	A	282	CYS
1	A	327	SER
1	A	373	THR
1	B	5	LYS
1	B	118	MET
1	B	135	LYS
1	B	164	SER
1	B	251	GLN
1	B	280	SER
1	B	281	CYS
1	B	282	CYS
1	B	373	THR

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Mol	Chain	Res	Type
1	C	39	LYS
1	C	118	MET
1	C	135	LYS
1	C	164	SER
1	C	206	SER
1	C	251	GLN
1	C	274	THR
1	C	281	CYS
1	C	282	CYS
1	C	327	SER
1	C	373	THR
1	D	118	MET
1	D	135	LYS
1	D	164	SER
1	D	251	GLN
1	D	274	THR
1	D	281	CYS
1	D	282	CYS
1	D	327	SER
1	D	357	GLU
1	D	373	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	191	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 carbohydrates in this entry.

5.6 Ligand geometry

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 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
4	CXF	A	378	2	9,9,9	1.41	1 (11%)	9,10,10	1.96	4 (44%)
4	CXF	D	378	2	9,9,9	1.66	2 (22%)	9,10,10	2.75	5 (55%)
4	CXF	B	378	2	9,9,9	1.67	2 (22%)	9,10,10	2.25	4 (44%)
4	CXF	C	378	2	9,9,9	1.31	0	9,10,10	1.40	2 (22%)
3	NAD	C	377	-	42,48,48	1.97	12 (28%)	50,73,73	2.88	19 (38%)
3	NAD	D	377	-	42,48,48	2.27	13 (30%)	50,73,73	2.87	19 (38%)
3	NAD	A	377	-	42,48,48	2.07	11 (26%)	50,73,73	2.23	13 (26%)
3	NAD	B	377	-	42,48,48	1.96	13 (30%)	50,73,73	2.72	17 (34%)

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
4	CXF	A	378	2	-	1/3/11/11	0/1/1/1
4	CXF	D	378	2	-	0/3/11/11	0/1/1/1
4	CXF	B	378	2	-	1/3/11/11	0/1/1/1
4	CXF	C	378	2	-	0/3/11/11	0/1/1/1
3	NAD	C	377	-	-	9/26/62/62	0/5/5/5
3	NAD	D	377	-	-	6/26/62/62	0/5/5/5
3	NAD	A	377	-	-	8/26/62/62	0/5/5/5
3	NAD	B	377	-	-	10/26/62/62	0/5/5/5

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	377	NAD	C3N-C7N	5.19	1.58	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	377	NAD	O4D-C4D	5.15	1.56	1.45
3	C	377	NAD	C3N-C7N	5.09	1.58	1.50
3	A	377	NAD	C2A-N3A	4.57	1.39	1.32
3	D	377	NAD	O2B-C2B	-4.53	1.32	1.43
3	D	377	NAD	O4D-C1D	4.47	1.47	1.41
3	D	377	NAD	C2A-N3A	4.43	1.39	1.32
3	B	377	NAD	C2D-C1D	4.29	1.60	1.53
3	B	377	NAD	C2A-N3A	4.08	1.38	1.32
3	A	377	NAD	C3N-C7N	4.06	1.56	1.50
3	C	377	NAD	C2A-N3A	4.05	1.38	1.32
3	C	377	NAD	O4D-C1D	4.02	1.46	1.41
3	C	377	NAD	O2B-C2B	-4.00	1.33	1.43
3	A	377	NAD	C4A-N3A	3.88	1.41	1.35
3	A	377	NAD	O2B-C2B	-3.76	1.34	1.43
3	A	377	NAD	O4B-C1B	-3.66	1.36	1.41
3	B	377	NAD	C3N-C7N	3.51	1.55	1.50
3	B	377	NAD	O4D-C4D	3.51	1.52	1.45
3	B	377	NAD	O2B-C2B	-3.49	1.34	1.43
3	D	377	NAD	C2N-C3N	-3.43	1.33	1.39
4	D	378	CXF	C6-C1	3.38	1.59	1.52
3	A	377	NAD	O4D-C4D	3.32	1.52	1.45
3	A	377	NAD	C2N-C3N	-3.25	1.34	1.39
3	C	377	NAD	O4D-C4D	3.17	1.52	1.45
3	D	377	NAD	C2N-N1N	3.12	1.38	1.35
3	A	377	NAD	O4D-C1D	3.12	1.45	1.41
3	D	377	NAD	C2D-C1D	3.08	1.58	1.53
3	B	377	NAD	C4A-N3A	3.06	1.39	1.35
3	C	377	NAD	O3D-C3D	-3.03	1.35	1.43
3	B	377	NAD	C8A-N7A	-3.01	1.29	1.34
3	C	377	NAD	C2D-C1D	3.00	1.58	1.53
4	B	378	CXF	C6-C1	2.99	1.59	1.52
3	A	377	NAD	C2D-C1D	2.87	1.58	1.53
3	D	377	NAD	C3B-C4B	2.86	1.60	1.53
3	C	377	NAD	O3B-C3B	2.84	1.49	1.43
3	A	377	NAD	O3B-C3B	2.83	1.49	1.43
3	B	377	NAD	O4D-C1D	2.80	1.45	1.41
3	D	377	NAD	C5N-C4N	2.76	1.44	1.38
4	B	378	CXF	C2-C1	2.75	1.58	1.52
3	A	377	NAD	C5N-C4N	2.74	1.44	1.38
3	D	377	NAD	O3D-C3D	-2.68	1.36	1.43
3	B	377	NAD	C2N-N1N	2.53	1.38	1.35
3	B	377	NAD	O3B-C3B	2.53	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	378	CXF	C2-C1	2.48	1.57	1.52
3	B	377	NAD	C5N-C4N	2.43	1.44	1.38
4	A	378	CXF	C2-C1	2.41	1.57	1.52
3	D	377	NAD	O3B-C3B	2.37	1.48	1.43
3	C	377	NAD	O4B-C1B	-2.32	1.37	1.41
3	C	377	NAD	C8A-N7A	-2.27	1.30	1.34
3	D	377	NAD	C3D-C4D	2.26	1.58	1.53
3	B	377	NAD	O3D-C3D	-2.15	1.37	1.43
3	C	377	NAD	C5D-C4D	-2.09	1.45	1.51
3	B	377	NAD	C5B-C4B	-2.05	1.45	1.51
3	C	377	NAD	C3B-C4B	2.03	1.58	1.53

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	377	NAD	C2N-C3N-C4N	9.40	128.92	118.26
3	C	377	NAD	C2N-C3N-C4N	9.37	128.88	118.26
3	C	377	NAD	C3N-C2N-N1N	-8.72	111.91	120.43
3	B	377	NAD	C2N-C3N-C4N	8.57	127.97	118.26
3	D	377	NAD	C5N-C4N-C3N	-7.65	111.29	120.34
3	A	377	NAD	C2N-C3N-C4N	7.65	126.93	118.26
3	B	377	NAD	C3N-C2N-N1N	-7.31	113.28	120.43
3	D	377	NAD	C3N-C2N-N1N	-6.84	113.75	120.43
3	C	377	NAD	C5N-C4N-C3N	-6.33	112.85	120.34
3	B	377	NAD	C5N-C4N-C3N	-6.26	112.94	120.34
3	A	377	NAD	C5N-C4N-C3N	-6.17	113.05	120.34
4	D	378	CXF	O9-C7-N8	-5.56	110.62	125.27
3	B	377	NAD	C2A-N1A-C6A	5.52	128.20	118.75
3	D	377	NAD	C2A-N1A-C6A	5.45	128.07	118.75
3	C	377	NAD	C6N-N1N-C2N	5.29	126.80	121.97
3	A	377	NAD	C2A-N1A-C6A	5.18	127.62	118.75
3	C	377	NAD	C2A-N1A-C6A	4.89	127.12	118.75
4	B	378	CXF	C6-C1-N8	-4.61	102.00	110.57
3	D	377	NAD	C6N-N1N-C2N	4.26	125.86	121.97
3	A	377	NAD	C3N-C2N-N1N	-4.26	116.26	120.43
3	B	377	NAD	O2B-C2B-C3B	4.18	125.35	111.82
3	D	377	NAD	N6A-C6A-N1A	4.12	127.13	118.57
3	B	377	NAD	C6N-N1N-C2N	4.11	125.73	121.97
3	D	377	NAD	C5A-C6A-N1A	-4.06	111.16	120.35
3	D	377	NAD	C3N-C7N-N7N	4.04	122.60	117.75
3	B	377	NAD	C5A-C6A-N1A	-4.03	111.22	120.35
3	B	377	NAD	C3D-C2D-C1D	-4.02	94.92	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	377	NAD	C5A-C6A-N1A	-4.02	111.24	120.35
3	C	377	NAD	O2A-PA-O1A	3.80	131.03	112.24
3	C	377	NAD	N3A-C2A-N1A	-3.72	122.86	128.68
3	A	377	NAD	O2B-C2B-C3B	3.63	123.58	111.82
3	A	377	NAD	N3A-C2A-N1A	-3.48	123.24	128.68
3	A	377	NAD	C5A-C6A-N1A	-3.36	112.72	120.35
4	B	378	CXF	C2-C1-N8	-3.28	104.47	110.57
3	C	377	NAD	O4B-C1B-C2B	3.27	111.71	106.93
3	D	377	NAD	N3A-C2A-N1A	-3.24	123.62	128.68
3	C	377	NAD	N6A-C6A-N1A	3.21	125.24	118.57
4	A	378	CXF	O9-C7-N8	-3.21	116.82	125.27
3	B	377	NAD	N3A-C2A-N1A	-3.21	123.67	128.68
4	D	378	CXF	C6-C1-N8	-3.17	104.66	110.57
3	D	377	NAD	C6N-C5N-C4N	3.07	123.90	119.44
3	B	377	NAD	C2B-C3B-C4B	3.06	108.59	102.64
3	C	377	NAD	C3D-C2D-C1D	-3.05	96.39	100.98
3	C	377	NAD	C2D-C3D-C4D	3.04	108.55	102.64
3	C	377	NAD	C2N-C3N-C7N	-3.03	110.68	119.46
3	B	377	NAD	N6A-C6A-N1A	3.02	124.83	118.57
3	D	377	NAD	C2N-C3N-C7N	-2.96	110.89	119.46
3	D	377	NAD	O7N-C7N-C3N	-2.93	116.13	119.63
3	D	377	NAD	O2B-C2B-C3B	2.91	121.25	111.82
3	C	377	NAD	C5D-C4D-C3D	2.88	125.96	115.18
3	D	377	NAD	C5N-C6N-N1N	-2.87	116.28	120.40
4	D	378	CXF	C6-C1-C2	-2.87	105.84	110.82
3	D	377	NAD	C2B-C3B-C4B	2.86	108.19	102.64
3	B	377	NAD	C2N-C3N-C7N	-2.71	111.60	119.46
4	C	378	CXF	C6-C1-C2	2.64	115.39	110.82
3	D	377	NAD	O4B-C1B-C2B	2.60	110.73	106.93
3	D	377	NAD	O3B-C3B-C4B	-2.59	103.57	111.05
4	B	378	CXF	O9-C7-N8	-2.54	118.58	125.27
3	A	377	NAD	C2N-C3N-C7N	-2.54	112.10	119.46
4	D	378	CXF	C5-C6-C1	-2.50	106.39	111.11
3	B	377	NAD	C5D-C4D-C3D	2.49	124.51	115.18
3	A	377	NAD	C2B-C3B-C4B	2.47	107.45	102.64
3	A	377	NAD	O4B-C1B-C2B	2.43	110.48	106.93
4	B	378	CXF	C6-C1-C2	-2.43	106.61	110.82
4	A	378	CXF	C6-C1-N8	-2.42	106.07	110.57
3	C	377	NAD	C2B-C3B-C4B	2.39	107.29	102.64
3	C	377	NAD	O4D-C4D-C3D	-2.38	100.39	105.11
3	B	377	NAD	C5A-C6A-N6A	2.36	123.94	120.35
4	D	378	CXF	C2-C1-N8	-2.36	106.18	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	377	NAD	O2A-PA-O1A	2.35	123.86	112.24
3	A	377	NAD	C5A-C6A-N6A	2.34	123.91	120.35
4	C	378	CXF	C2-C1-N8	-2.34	106.22	110.57
3	A	377	NAD	N6A-C6A-N1A	2.31	123.37	118.57
3	C	377	NAD	O3B-C3B-C4B	-2.24	104.56	111.05
4	A	378	CXF	C6-C1-C2	-2.23	106.96	110.82
4	A	378	CXF	C4-C3-C2	-2.19	106.94	111.42
3	D	377	NAD	C2D-C3D-C4D	2.18	106.88	102.64
3	B	377	NAD	O4B-C1B-C2B	2.14	110.05	106.93
3	C	377	NAD	C5A-C6A-N6A	2.08	123.52	120.35
3	B	377	NAD	C2D-C3D-C4D	2.07	106.67	102.64
3	D	377	NAD	O2A-PA-O1A	2.07	122.48	112.24
3	B	377	NAD	O3B-C3B-C4B	-2.06	105.08	111.05
3	C	377	NAD	O2B-C2B-C3B	2.04	118.44	111.82

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	377	NAD	O4D-C1D-N1N-C2N
3	C	377	NAD	O4D-C1D-N1N-C6N
3	C	377	NAD	C2D-C1D-N1N-C2N
3	C	377	NAD	C2D-C1D-N1N-C6N
3	D	377	NAD	O4D-C1D-N1N-C2N
3	D	377	NAD	O4D-C1D-N1N-C6N
3	D	377	NAD	C2D-C1D-N1N-C2N
3	D	377	NAD	C2D-C1D-N1N-C6N
3	A	377	NAD	C5B-O5B-PA-O1A
3	A	377	NAD	O4D-C1D-N1N-C2N
3	A	377	NAD	O4D-C1D-N1N-C6N
3	A	377	NAD	C2D-C1D-N1N-C2N
3	A	377	NAD	C2D-C1D-N1N-C6N
3	B	377	NAD	C5B-O5B-PA-O1A
3	B	377	NAD	O4D-C1D-N1N-C2N
3	B	377	NAD	O4D-C1D-N1N-C6N
3	B	377	NAD	C2D-C1D-N1N-C2N
3	B	377	NAD	C2D-C1D-N1N-C6N
3	C	377	NAD	O4D-C4D-C5D-O5D
3	A	377	NAD	C5B-O5B-PA-O3
3	B	377	NAD	C5B-O5B-PA-O3
3	C	377	NAD	C3D-C4D-C5D-O5D
3	B	377	NAD	C3D-C4D-C5D-O5D

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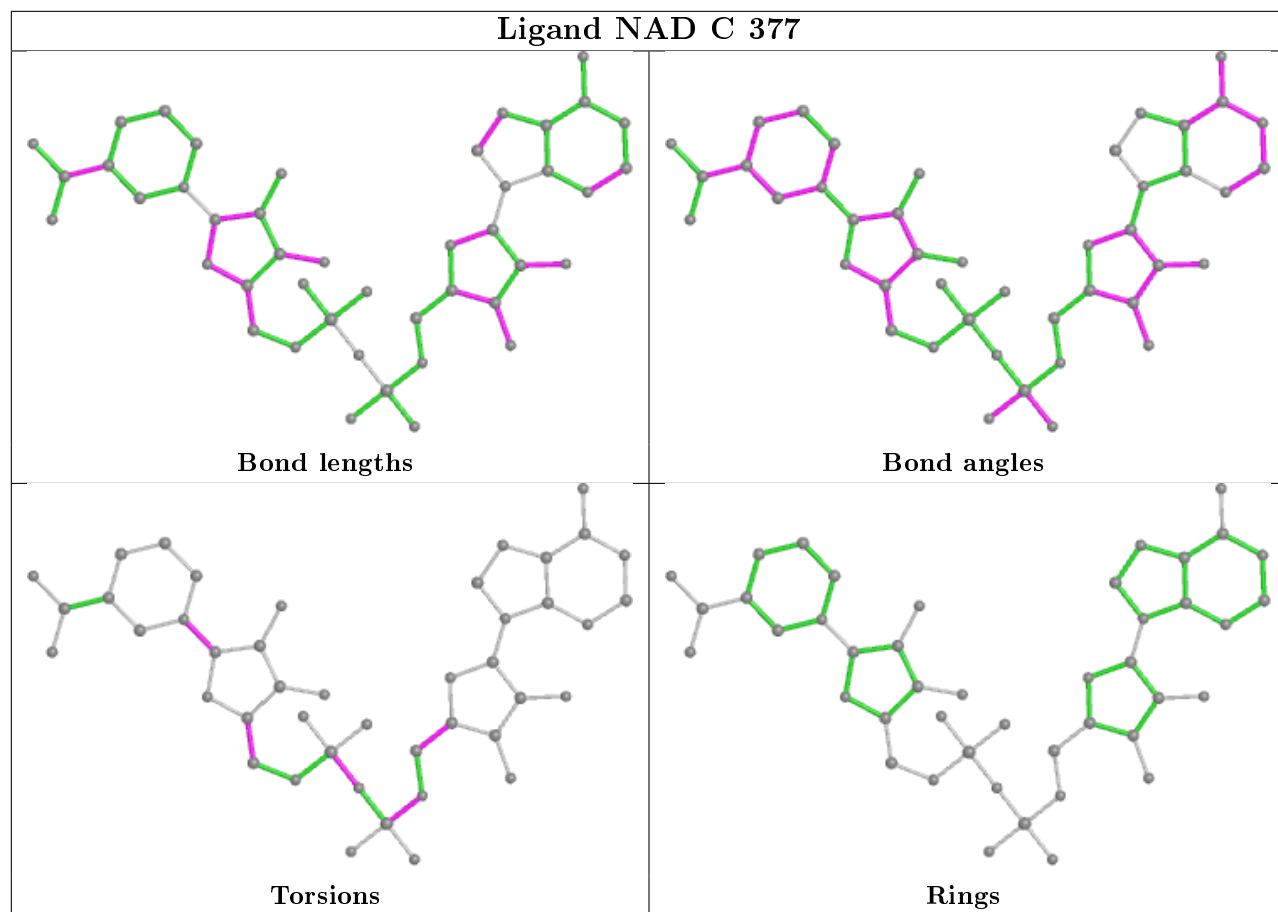
Mol	Chain	Res	Type	Atoms
3	D	377	NAD	C3D-C4D-C5D-O5D
3	B	377	NAD	O4D-C4D-C5D-O5D
4	B	378	CXF	C2-C1-N8-C7
4	A	378	CXF	C2-C1-N8-C7
3	C	377	NAD	C5B-O5B-PA-O3
3	D	377	NAD	O4B-C4B-C5B-O5B
3	B	377	NAD	O4B-C4B-C5B-O5B
3	C	377	NAD	PA-O3-PN-O1N
3	A	377	NAD	PA-O3-PN-O1N
3	B	377	NAD	C5B-O5B-PA-O2A
3	C	377	NAD	O4B-C4B-C5B-O5B
3	A	377	NAD	O4B-C4B-C5B-O5B

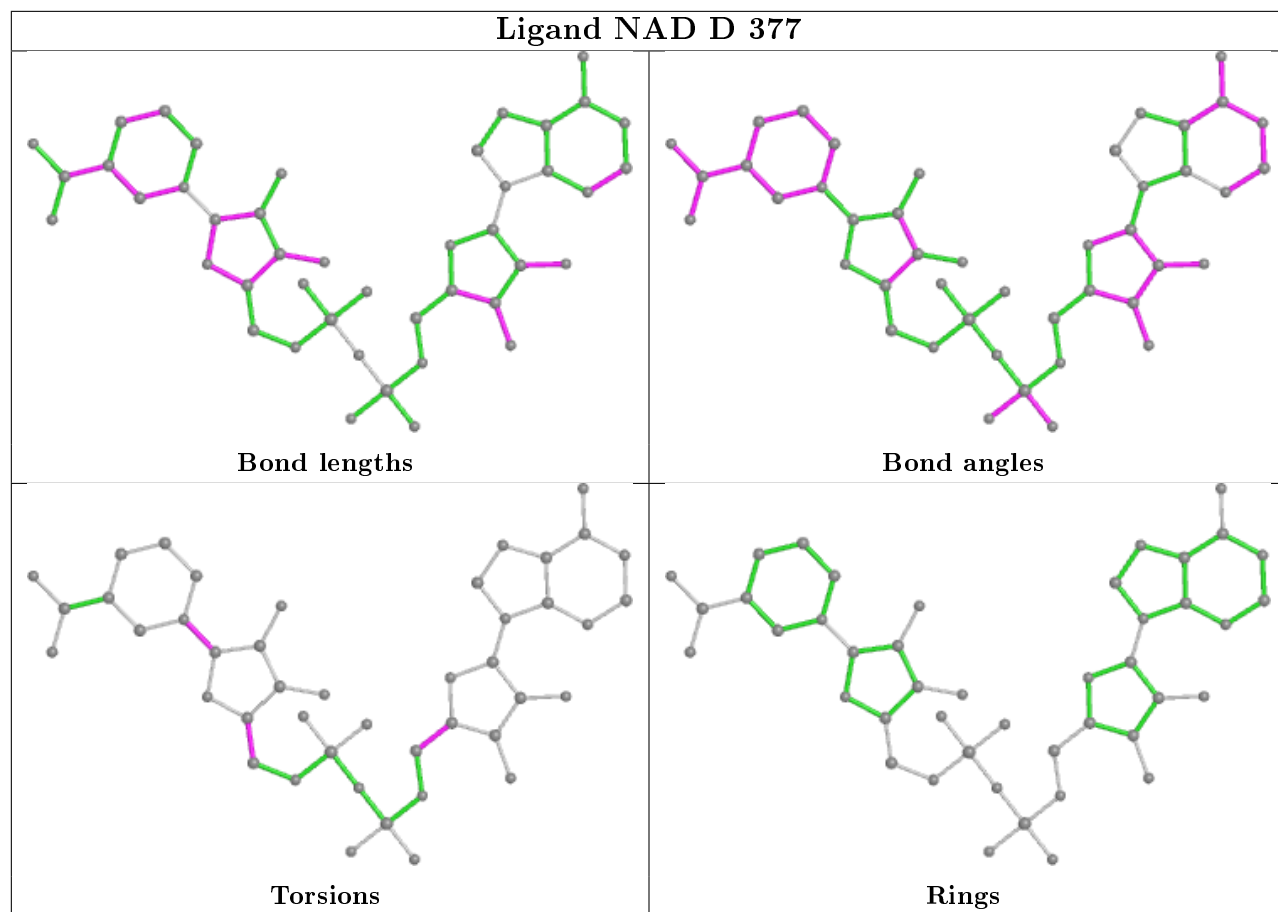
There are no ring outliers.

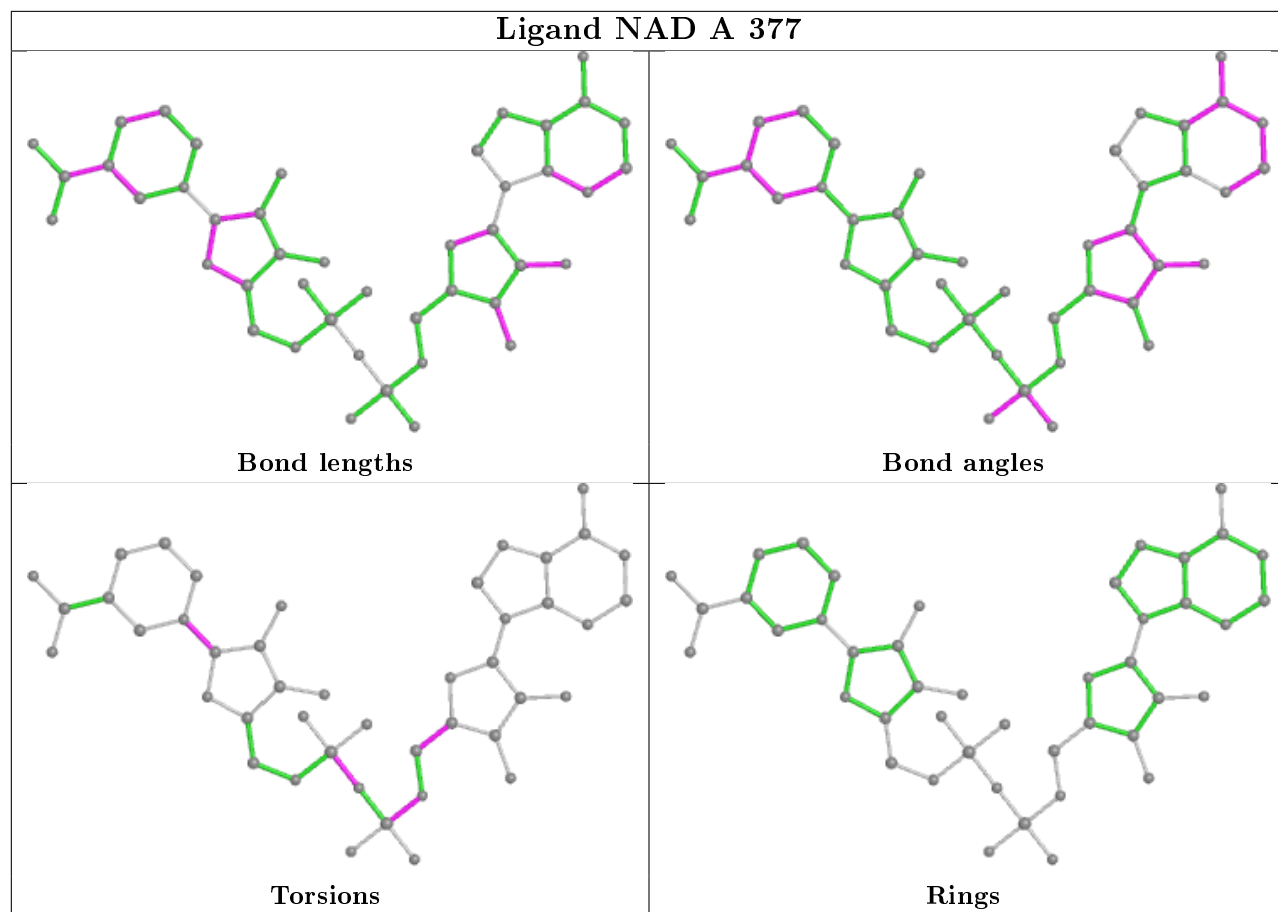
7 monomers are involved in 12 short contacts:

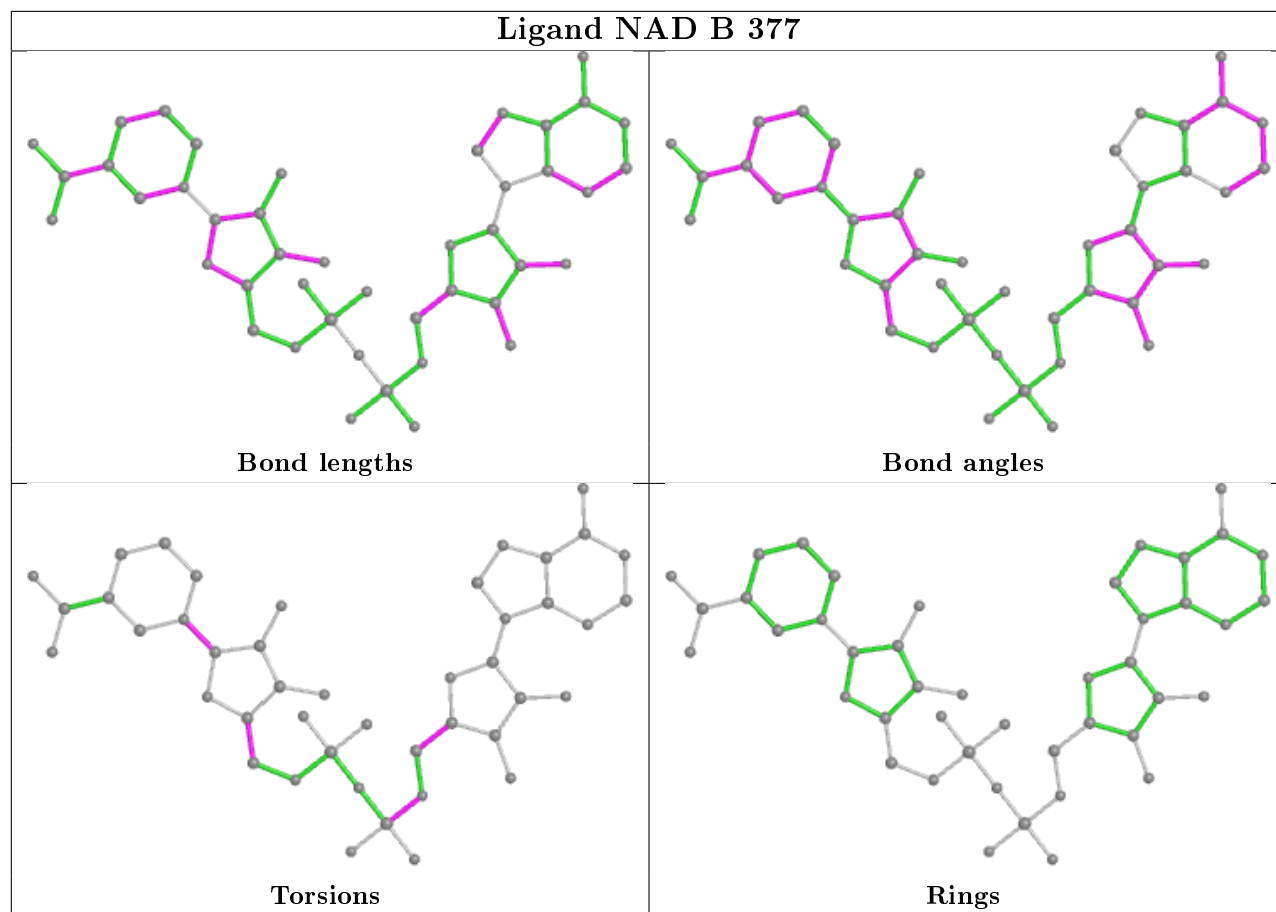
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	378	CXF	1	0
4	B	378	CXF	2	0
4	C	378	CXF	3	0
3	C	377	NAD	1	0
3	D	377	NAD	2	0
3	A	377	NAD	1	0
3	B	377	NAD	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	374/374 (100%)	-0.33	0 100 100	17, 26, 38, 46	0
1	B	374/374 (100%)	-0.32	2 (0%) 91 91	17, 25, 38, 46	0
1	C	374/374 (100%)	0.04	17 (4%) 33 36	17, 26, 38, 46	0
1	D	374/374 (100%)	-0.03	12 (3%) 47 51	17, 26, 38, 47	0
All	All	1496/1496 (100%)	-0.16	31 (2%) 63 66	17, 26, 38, 47	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	336	MET	3.9
1	C	191	GLN	3.9
1	D	84	ARG	3.6
1	C	213	ALA	3.2
1	C	339	LYS	3.0
1	D	334	ASP	2.9
1	D	191	GLN	2.8
1	C	330	LYS	2.7
1	D	338	LYS	2.6
1	C	79	GLY	2.6
1	D	34	HIS	2.5
1	B	78	GLU	2.5
1	C	84	ARG	2.5
1	C	333	ALA	2.5
1	C	214	ALA	2.5
1	D	161	ASP	2.5
1	C	336	MET	2.4
1	C	337	ALA	2.4
1	C	1	SER	2.4
1	D	248	LYS	2.3
1	C	78	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	78	GLU	2.3
1	D	366	GLU	2.2
1	C	161	ASP	2.1
1	D	33	ALA	2.1
1	D	133	ARG	2.1
1	C	238	THR	2.1
1	C	255	THR	2.1
1	C	332	VAL	2.1
1	C	259	ASN	2.1
1	B	84	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	CXF	C	378	9/9	0.93	0.12	23,26,27,27	0
4	CXF	D	378	9/9	0.95	0.14	24,26,27,27	0
4	CXF	B	378	9/9	0.95	0.12	23,26,27,27	0
4	CXF	A	378	9/9	0.96	0.12	23,25,27,27	0
3	NAD	C	377	44/44	0.97	0.10	13,21,27,28	0
3	NAD	D	377	44/44	0.97	0.10	13,21,27,28	0
3	NAD	A	377	44/44	0.97	0.11	14,21,27,28	0
3	NAD	B	377	44/44	0.97	0.11	14,21,27,28	0
2	ZN	D	376	1/1	0.99	0.05	24,24,24,24	0
2	ZN	B	376	1/1	0.99	0.03	22,22,22,22	0
2	ZN	A	376	1/1	0.99	0.02	23,23,23,23	0
2	ZN	C	375	1/1	0.99	0.03	18,18,18,18	0
2	ZN	C	376	1/1	0.99	0.03	26,26,26,26	0

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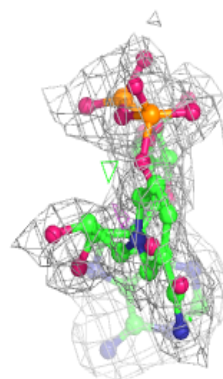
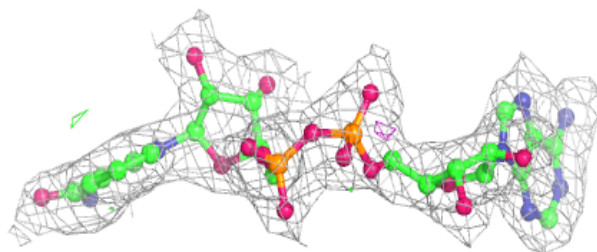
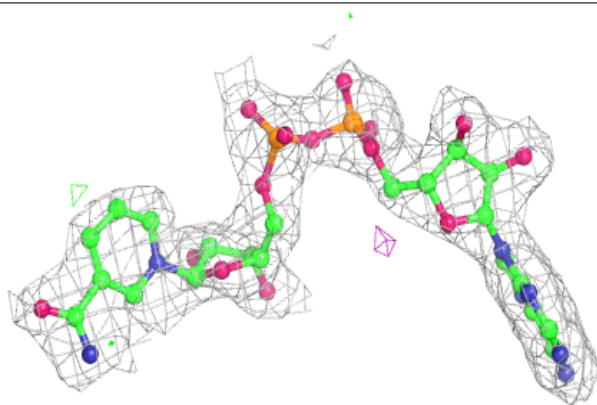
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	ZN	A	375	1/1	1.00	0.02	13,13,13,13	0
2	ZN	B	375	1/1	1.00	0.02	13,13,13,13	0
2	ZN	D	375	1/1	1.00	0.03	17,17,17,17	0

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.

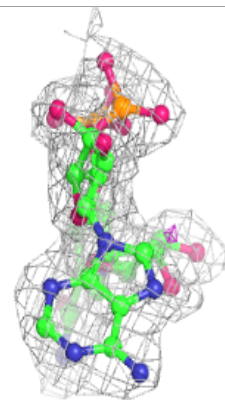
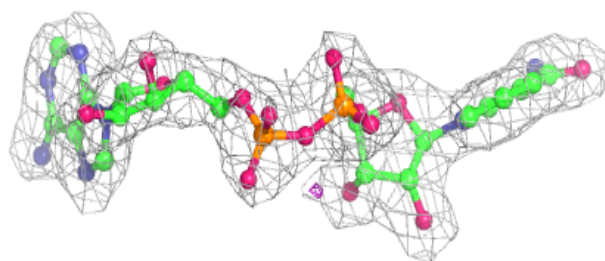
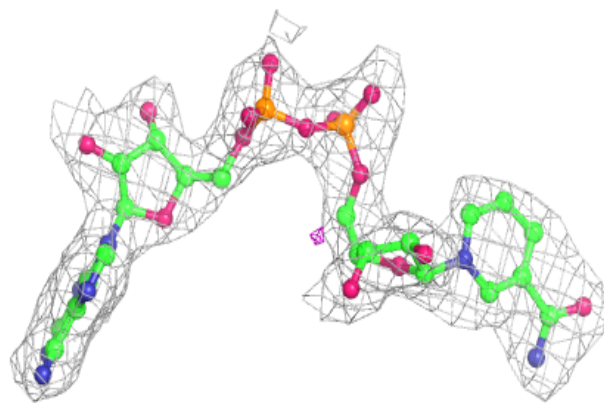
Electron density around NAD C 377:

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

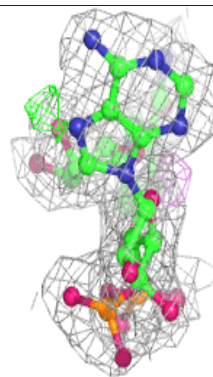
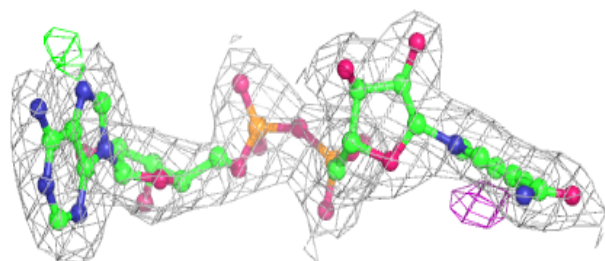
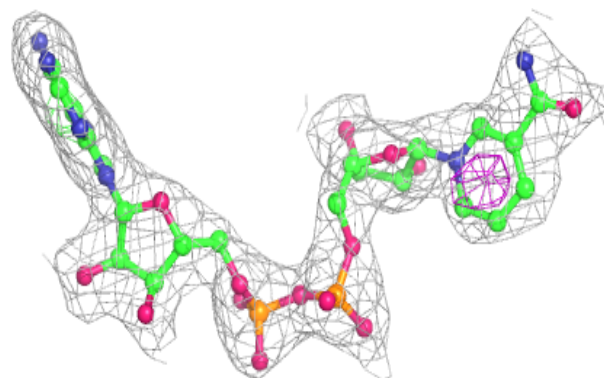


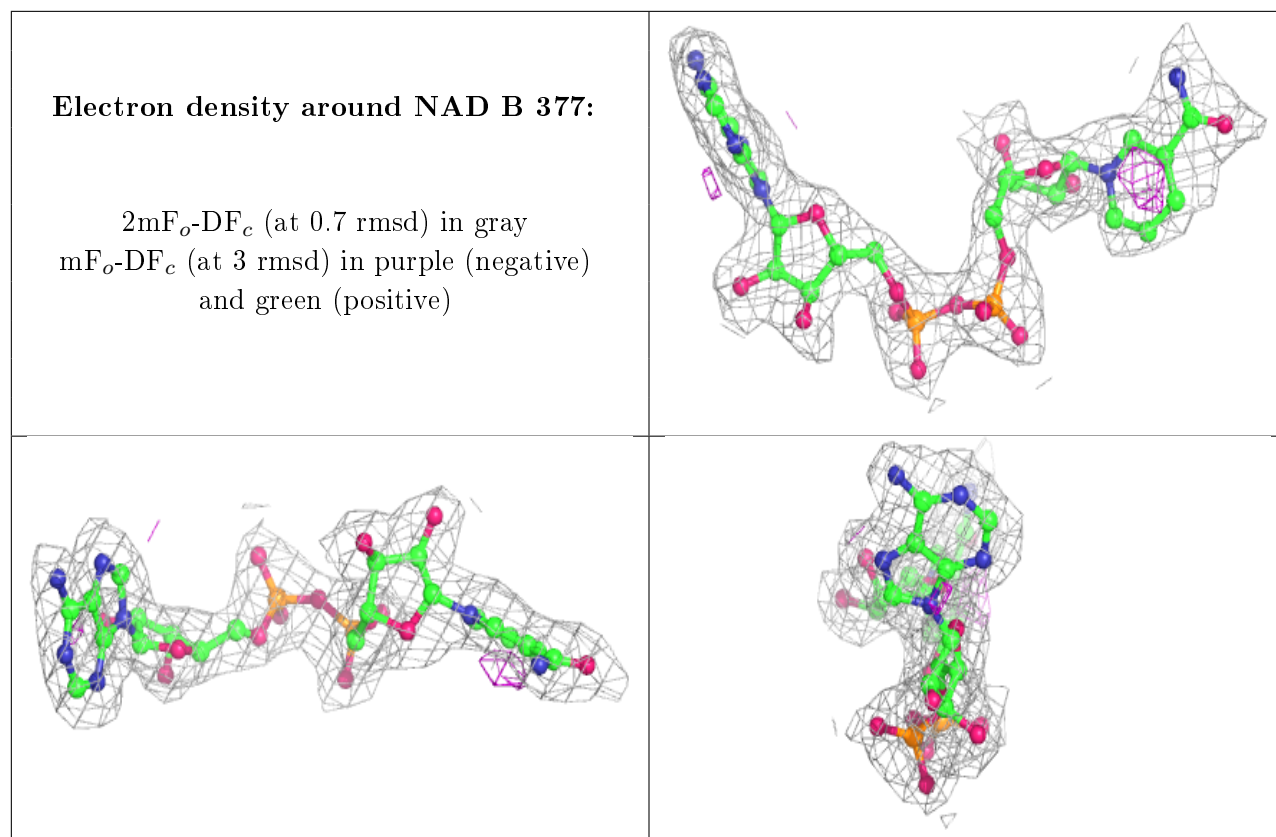
Electron density around NAD D 377:

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

**Electron density around NAD A 377:**

$2mF_o-DF_c$ (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.