



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:59 AM UTC

PDB ID : 5GTK / pdb_00005gtk
Title : NAD⁺ complex structure of aldehyde dehydrogenase from bacillus cereus
Authors : Ngo, H.P.T.; Hong, S.H.; Ho, T.H.; Oh, D.K.; Kang, L.W.
Deposited on : 2016-08-21
Resolution : 2.60 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

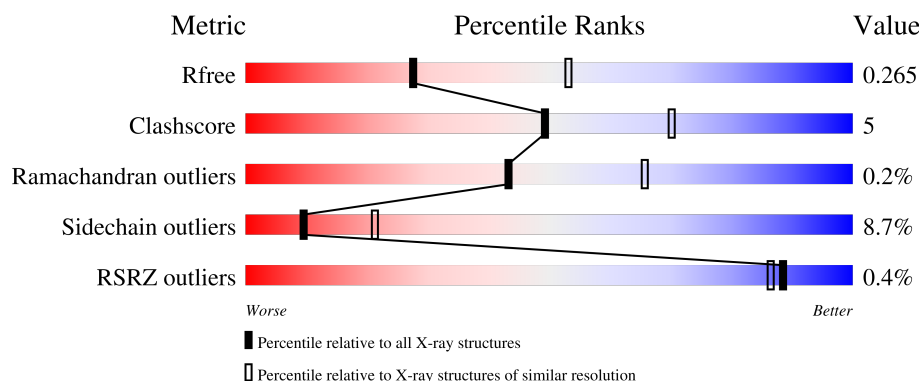
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

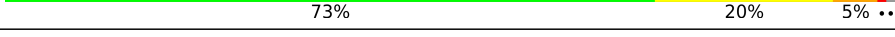
The reported resolution of this entry is 2.60 Å.

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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	494	 71% 24% ..
1	B	494	 74% 22% ..
1	C	494	 69% 24% . ..
1	D	494	 73% 20% 5% ..

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 15843 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 Betaine-aldehyde dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	491	Total	C	N	O	S	0	0	0
			3791	2414	630	733	14			
1	B	488	Total	C	N	O	S	0	1	0
			3771	2402	626	728	15			
1	C	489	Total	C	N	O	S	0	0	0
			3776	2406	627	729	14			
1	D	491	Total	C	N	O	S	0	1	0
			3794	2416	630	733	15			

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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		

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

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

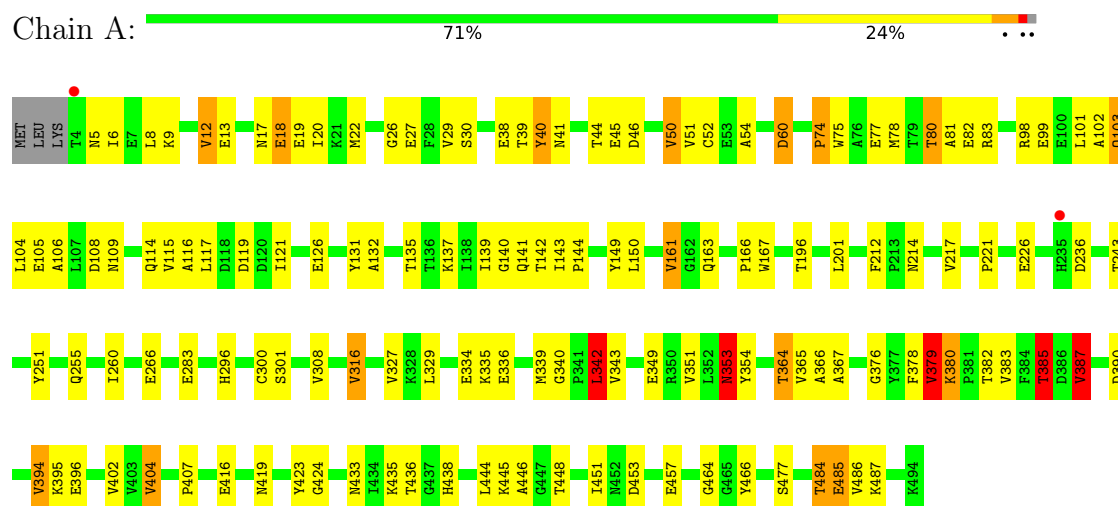
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	140	Total	O	0	0
			140	140		
4	B	141	Total	O	0	0
			141	141		
4	C	126	Total	O	0	0
			126	126		
4	D	125	Total	O	0	0
			125	125		

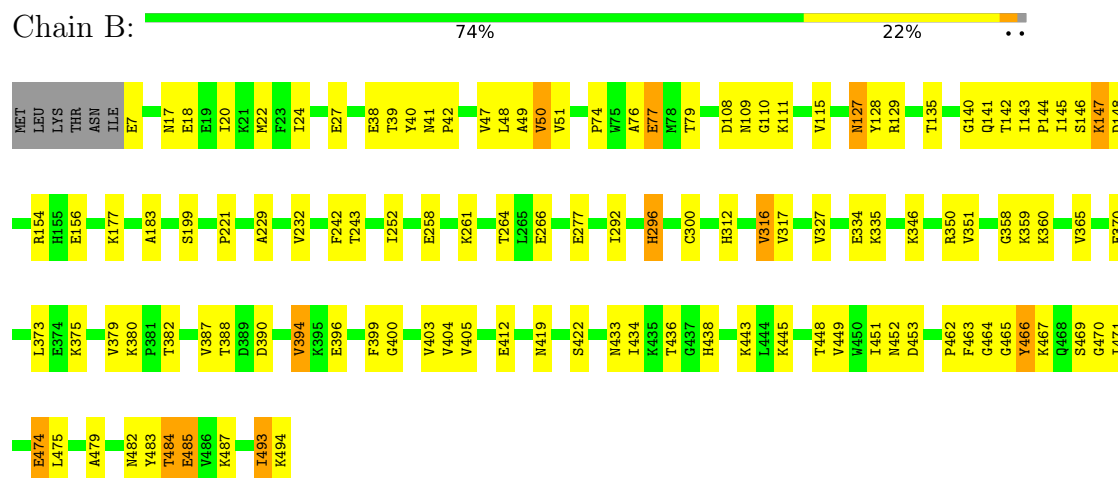
3 Residue-property plots

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: Betaine-aldehyde dehydrogenase

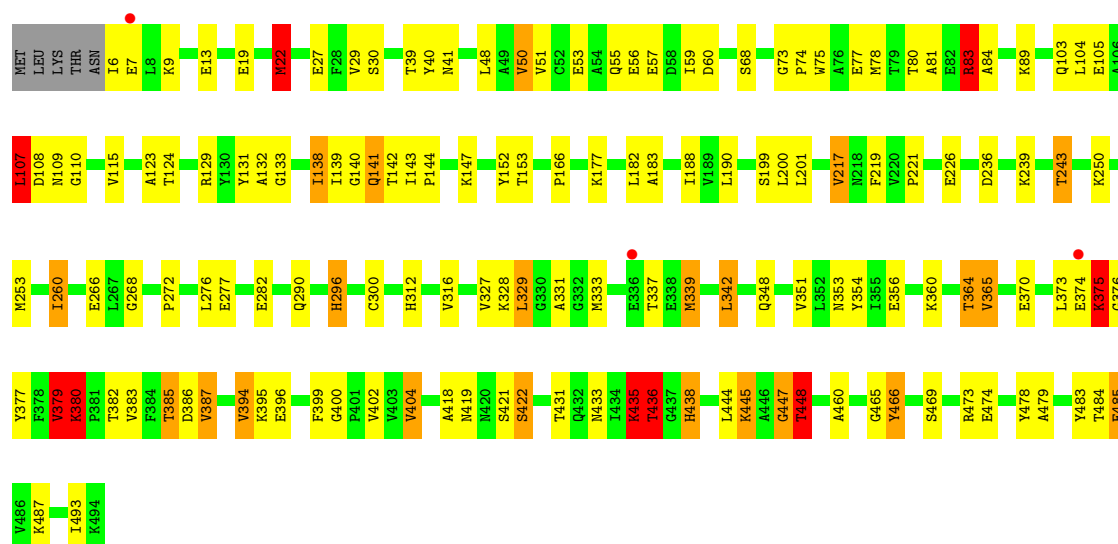


• Molecule 1: Betaine-aldehyde dehydrogenase

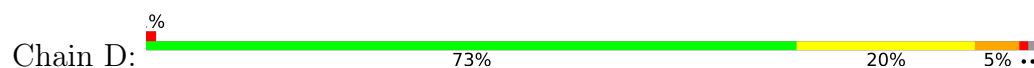


• Molecule 1: Betaine-aldehyde dehydrogenase





• Molecule 1: Betaine-aldehyde dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	83.22Å 93.25Å 145.15Å 90.00° 97.86° 90.00°	Depositor
Resolution (Å)	47.93 – 2.60 47.93 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.4 (47.93-2.60) 99.4 (47.93-2.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	35.35 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.165 , 0.233 (Not available) , 0.265	Depositor DCC
R_{free} test set	3414 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	17.2	Xtriage
Anisotropy	0.151	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 27.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	15843	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.03% 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, NA

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	1.54	57/3870 (1.5%)	1.28	28/5250 (0.5%)
1	B	1.49	52/3853 (1.3%)	1.23	21/5226 (0.4%)
1	C	1.58	62/3855 (1.6%)	1.28	30/5229 (0.6%)
1	D	1.53	63/3876 (1.6%)	1.20	22/5258 (0.4%)
All	All	1.54	234/15454 (1.5%)	1.25	101/20963 (0.5%)

All (234) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	144	PRO	C-O	-10.21	1.15	1.24
1	D	119	ASP	CA-C	-8.76	1.46	1.52
1	C	144	PRO	C-O	-8.49	1.17	1.24
1	B	467	LYS	C-O	-8.23	1.16	1.24
1	B	453	ASP	C-O	-8.18	1.15	1.24
1	B	449	VAL	C-O	-7.94	1.15	1.24
1	A	379	VAL	C-O	-7.82	1.16	1.24
1	D	449	VAL	C-O	-7.78	1.16	1.24
1	A	106	ALA	C-O	-7.71	1.15	1.24
1	D	85	HIS	C-O	-7.55	1.15	1.24
1	A	385	THR	C-O	-7.53	1.14	1.23
1	A	141	GLN	C-O	-7.49	1.14	1.23
1	B	144	PRO	C-O	-7.49	1.18	1.24
1	A	378	PHE	C-O	-7.49	1.14	1.23
1	C	83	ARG	C-O	-7.48	1.15	1.24
1	D	463	PHE	C-O	-7.42	1.15	1.23
1	D	491	VAL	C-O	-7.22	1.16	1.24
1	D	133	GLY	C-O	-7.16	1.15	1.24
1	C	141	GLN	C-O	-7.14	1.14	1.23
1	A	131	TYR	C-O	-7.11	1.14	1.24
1	B	140	GLY	C-O	-7.10	1.17	1.23
1	C	140	GLY	C-O	-7.06	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	485	GLU	C-O	-6.96	1.16	1.23
1	C	123	ALA	C-O	-6.92	1.15	1.24
1	C	80	THR	C-O	-6.90	1.15	1.24
1	D	484	THR	C-O	-6.90	1.15	1.23
1	A	402	VAL	C-O	-6.87	1.16	1.24
1	A	6	ILE	C-O	-6.85	1.17	1.24
1	B	448	THR	C-O	-6.82	1.16	1.24
1	C	53	GLU	C-O	-6.82	1.15	1.24
1	D	450	TRP	C-O	-6.80	1.15	1.24
1	C	143	ILE	C-O	-6.78	1.16	1.24
1	A	39	THR	C-O	-6.74	1.15	1.23
1	D	50	VAL	C-O	-6.71	1.16	1.24
1	A	81	ALA	C-O	-6.68	1.15	1.24
1	C	394	VAL	C-O	-6.68	1.17	1.24
1	A	451	ILE	C-O	-6.65	1.17	1.24
1	B	474	GLU	CA-C	-6.61	1.44	1.52
1	D	131	TYR	C-O	-6.58	1.15	1.24
1	B	145	ILE	C-O	-6.56	1.16	1.24
1	C	379	VAL	C-O	-6.55	1.17	1.24
1	D	59	ILE	C-O	-6.54	1.16	1.24
1	C	50	VAL	C-O	-6.52	1.17	1.24
1	C	374	GLU	C-O	-6.45	1.15	1.24
1	B	127	ASN	C-O	-6.42	1.16	1.24
1	A	150	LEU	C-O	-6.41	1.16	1.24
1	D	134	TRP	C-O	-6.41	1.15	1.24
1	D	54	ALA	C-O	-6.38	1.16	1.24
1	C	22	MET	C-O	-6.34	1.15	1.23
1	B	400	GLY	C-O	-6.34	1.15	1.24
1	C	74	PRO	C-O	-6.33	1.15	1.24
1	B	128	TYR	C-O	-6.32	1.16	1.24
1	A	383	VAL	C-O	-6.32	1.17	1.24
1	C	469	SER	C-O	-6.25	1.15	1.24
1	A	50	VAL	C-O	-6.22	1.17	1.24
1	A	80	THR	C-O	-6.22	1.16	1.24
1	D	31	ALA	C-O	-6.21	1.16	1.23
1	C	19	GLU	C-O	-6.20	1.16	1.23
1	A	20	ILE	C-O	-6.16	1.17	1.24
1	C	55	GLN	C-O	-6.14	1.15	1.23
1	B	394	VAL	C-O	-6.14	1.17	1.24
1	C	129	ARG	C-O	-6.12	1.17	1.24
1	A	82	GLU	C-O	-6.12	1.16	1.24
1	A	40	TYR	C-O	-6.12	1.15	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	447	GLY	C-O	-6.11	1.16	1.23
1	C	365	VAL	C-O	-6.09	1.16	1.23
1	A	105	GLU	C-O	-6.09	1.16	1.24
1	A	364	THR	C-O	-6.09	1.16	1.24
1	A	396	GLU	C-O	-6.09	1.16	1.23
1	C	421	SER	C-O	-6.09	1.16	1.23
1	C	438	HIS	C-O	-6.08	1.16	1.24
1	B	474	GLU	C-O	-6.08	1.16	1.23
1	D	329	LEU	C-O	-6.07	1.16	1.23
1	C	354	TYR	C-O	-6.07	1.16	1.24
1	D	19	GLU	C-O	-6.06	1.16	1.23
1	B	463	PHE	C-O	-6.06	1.17	1.24
1	A	387	VAL	C-O	-6.05	1.16	1.24
1	B	485	GLU	C-O	-6.04	1.17	1.24
1	D	387	VAL	N-CA	-6.03	1.39	1.46
1	B	379	VAL	C-O	-6.03	1.18	1.24
1	D	365	VAL	C-O	-6.03	1.16	1.23
1	D	39	THR	C-O	-6.02	1.16	1.23
1	D	379	VAL	C-O	-6.02	1.18	1.24
1	B	451	ILE	C-O	-6.02	1.17	1.24
1	D	56	GLU	C-O	-6.01	1.16	1.24
1	C	485	GLU	C-O	-5.98	1.17	1.24
1	B	49	ALA	C-O	-5.98	1.16	1.23
1	B	51	VAL	C-O	-5.97	1.18	1.24
1	D	120	ASP	C-O	-5.95	1.17	1.24
1	C	339	MET	C-O	-5.92	1.16	1.23
1	D	347	GLN	C-O	-5.89	1.17	1.24
1	B	146	SER	C-O	-5.88	1.16	1.23
1	C	377	TYR	C-O	-5.88	1.15	1.23
1	D	378	PHE	C-O	-5.88	1.16	1.23
1	D	129	ARG	C-O	-5.83	1.17	1.24
1	C	402	VAL	C-O	-5.80	1.17	1.24
1	C	133	GLY	C-O	-5.79	1.17	1.24
1	B	41	ASN	C-N	5.79	1.39	1.34
1	D	53	GLU	C-O	-5.79	1.17	1.24
1	A	367	ALA	C-O	-5.78	1.16	1.23
1	D	465	GLY	C-O	-5.78	1.16	1.23
1	B	483	TYR	C-O	-5.77	1.16	1.24
1	D	445	LYS	C-O	-5.77	1.16	1.23
1	C	436	THR	C-O	-5.76	1.16	1.24
1	D	448	THR	C-O	-5.76	1.17	1.23
1	A	486	VAL	C-O	-5.76	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	119	ASP	C-O	-5.74	1.16	1.23
1	B	452	ASN	C-O	-5.74	1.16	1.23
1	C	51	VAL	C-O	-5.74	1.18	1.24
1	C	387	VAL	C-O	-5.72	1.18	1.24
1	B	471	ILE	C-O	-5.70	1.18	1.24
1	B	147	LYS	C-O	-5.69	1.16	1.24
1	C	131	TYR	C-O	-5.66	1.16	1.24
1	D	422	SER	C-O	-5.66	1.16	1.24
1	A	74	PRO	C-O	-5.65	1.16	1.24
1	C	396	GLU	C-O	-5.65	1.17	1.23
1	D	380	LYS	C-O	-5.64	1.16	1.23
1	A	477	SER	C-O	-5.64	1.16	1.24
1	D	348	GLN	C-O	-5.63	1.17	1.24
1	D	435	LYS	C-O	-5.63	1.17	1.24
1	C	104	LEU	C-O	-5.62	1.16	1.24
1	B	47	VAL	C-O	-5.62	1.18	1.24
1	A	366	ALA	C-O	-5.61	1.16	1.24
1	B	50	VAL	C-O	-5.61	1.18	1.24
1	A	38	GLU	C-O	-5.61	1.17	1.23
1	D	27	GLU	C-O	-5.60	1.16	1.23
1	D	490	TRP	C-O	-5.60	1.17	1.24
1	C	41	ASN	C-O	-5.59	1.17	1.24
1	D	49	ALA	C-O	-5.59	1.17	1.23
1	A	46	ASP	C-O	-5.58	1.16	1.23
1	C	40	TYR	C-O	-5.58	1.16	1.23
1	B	399	PHE	C-O	-5.58	1.17	1.24
1	C	77	GLU	C-O	-5.57	1.16	1.24
1	D	466	TYR	C-O	-5.56	1.16	1.23
1	C	75	TRP	C-O	-5.55	1.17	1.24
1	C	448	THR	C-O	-5.55	1.17	1.23
1	B	334	GLU	C-O	-5.54	1.17	1.24
1	A	365	VAL	C-O	-5.54	1.17	1.23
1	A	51	VAL	C-O	-5.54	1.18	1.24
1	D	364	THR	C-O	-5.54	1.17	1.24
1	C	124	THR	C-O	-5.54	1.17	1.24
1	D	382	THR	C-O	-5.54	1.17	1.24
1	B	74	PRO	C-O	-5.53	1.17	1.24
1	D	384	PHE	C-O	-5.53	1.17	1.24
1	D	35	LYS	C-O	-5.52	1.16	1.23
1	B	464	GLY	C-O	-5.52	1.16	1.23
1	D	328	LYS	C-O	-5.52	1.16	1.23
1	B	20	ILE	C-O	-5.51	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	383	VAL	C-O	-5.50	1.18	1.24
1	C	81	ALA	C-O	-5.50	1.17	1.24
1	C	138	ILE	C-O	-5.47	1.17	1.24
1	D	57	GLU	C-O	-5.46	1.17	1.24
1	B	77	GLU	C-O	-5.46	1.17	1.23
1	A	226	GLU	CA-C	5.45	1.56	1.52
1	C	142	THR	C-O	-5.45	1.17	1.24
1	B	143	ILE	C-O	-5.43	1.18	1.24
1	C	419	ASN	C-O	-5.42	1.16	1.24
1	A	334	GLU	C-O	-5.40	1.17	1.23
1	D	451	ILE	C-O	-5.40	1.17	1.24
1	B	396	GLU	C-O	-5.39	1.17	1.23
1	C	89	LYS	C-O	-5.39	1.17	1.24
1	D	447	GLY	C-O	-5.38	1.17	1.23
1	B	108	ASP	CG-OD2	-5.38	1.15	1.25
1	B	39	THR	C-O	-5.37	1.17	1.24
1	A	143	ILE	C-O	-5.36	1.18	1.24
1	C	30	SER	C-O	-5.35	1.16	1.23
1	C	382	THR	C-O	-5.35	1.17	1.24
1	D	404	VAL	C-O	-5.35	1.18	1.24
1	B	419	ASN	C-O	-5.34	1.17	1.24
1	A	376	GLY	C-O	-5.34	1.17	1.23
1	C	39	THR	C-O	-5.34	1.17	1.24
1	D	474	GLU	CA-C	-5.34	1.46	1.52
1	A	342	LEU	C-O	-5.33	1.16	1.23
1	A	149	TYR	CA-C	-5.32	1.46	1.52
1	A	140	GLY	C-O	-5.32	1.18	1.23
1	A	149	TYR	C-O	-5.32	1.17	1.23
1	C	56	GLU	C-O	-5.32	1.18	1.24
1	C	27	GLU	C-O	-5.28	1.17	1.23
1	A	29	VAL	C-O	-5.28	1.18	1.23
1	C	84	ALA	C-O	-5.28	1.17	1.24
1	D	36	THR	C-O	-5.27	1.17	1.23
1	A	41	ASN	C-O	-5.27	1.17	1.24
1	A	448	THR	C-O	-5.26	1.18	1.24
1	C	435	LYS	C-O	-5.25	1.18	1.24
1	D	79	THR	C-O	-5.25	1.16	1.23
1	D	407	PRO	C-O	-5.25	1.17	1.23
1	A	353	ASN	C-O	-5.24	1.17	1.24
1	D	18	GLU	CA-C	-5.24	1.46	1.52
1	B	358	GLY	C-O	-5.24	1.17	1.23
1	C	84	ALA	CA-C	-5.23	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	18	GLU	C-O	-5.23	1.17	1.23
1	D	22	MET	C-O	-5.23	1.17	1.23
1	B	76	ALA	C-O	-5.22	1.17	1.24
1	B	48	LEU	C-O	-5.21	1.17	1.24
1	B	452	ASN	CG-OD1	-5.20	1.13	1.23
1	B	110	GLY	C-O	-5.19	1.17	1.24
1	B	38	GLU	C-O	-5.18	1.17	1.23
1	B	469	SER	C-O	-5.18	1.17	1.24
1	D	119	ASP	C-O	-5.18	1.17	1.23
1	C	483	TYR	C-O	-5.18	1.17	1.24
1	B	41	ASN	C-O	-5.18	1.17	1.24
1	C	108	ASP	CG-OD2	-5.17	1.15	1.25
1	D	403	VAL	C-O	-5.16	1.18	1.24
1	A	446	ALA	C-O	-5.16	1.17	1.23
1	A	423	TYR	C-O	-5.15	1.17	1.23
1	A	464	GLY	C-O	-5.13	1.16	1.24
1	B	42	PRO	C-O	-5.13	1.17	1.24
1	B	493	ILE	C-O	-5.13	1.18	1.24
1	A	18	GLU	C-O	-5.12	1.17	1.23
1	D	107	LEU	C-O	-5.11	1.18	1.24
1	A	380	LYS	C-N	5.11	1.39	1.33
1	D	26	GLY	C-O	-5.11	1.17	1.24
1	D	483	TYR	C-O	-5.11	1.17	1.24
1	B	484	THR	C-O	-5.10	1.17	1.23
1	A	419	ASN	C-O	-5.08	1.17	1.24
1	D	405	VAL	C-O	-5.08	1.18	1.24
1	B	422	SER	C-O	-5.07	1.17	1.24
1	A	137	LYS	C-O	-5.07	1.16	1.24
1	C	48	LEU	C-O	-5.07	1.17	1.24
1	C	107	LEU	C-O	-5.06	1.18	1.24
1	A	19	GLU	C-O	-5.05	1.17	1.23
1	C	445	LYS	C-O	-5.05	1.17	1.23
1	C	473	ARG	C-O	-5.05	1.17	1.23
1	C	226	GLU	CA-C	5.05	1.56	1.52
1	D	51	VAL	C-O	-5.05	1.18	1.24
1	A	453	ASP	N-CA	-5.04	1.40	1.46
1	C	59	ILE	C-O	-5.04	1.17	1.24
1	B	129	ARG	C-O	-5.03	1.18	1.24
1	D	464	GLY	C-O	-5.03	1.18	1.24
1	B	462	PRO	C-O	-5.02	1.18	1.23
1	A	54	ALA	C-O	-5.02	1.18	1.23
1	D	34	GLY	C-O	-5.01	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	29	VAL	C-O	-5.01	1.17	1.23
1	A	102	ALA	C-O	-5.01	1.17	1.24

All (101) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	335	LYS	N-CA-C	9.34	121.46	111.28
1	C	422	SER	N-CA-C	-8.49	102.70	113.23
1	C	466	TYR	N-CA-C	-8.20	98.70	110.59
1	C	376	GLY	N-CA-C	7.76	121.87	112.48
1	A	378	PHE	N-CA-C	7.66	121.62	110.28
1	B	143	ILE	N-CA-C	7.56	116.35	107.73
1	C	143	ILE	N-CA-C	7.48	116.26	107.73
1	A	143	ILE	N-CA-C	7.36	116.02	107.77
1	C	139	ILE	N-CA-C	7.26	120.60	109.12
1	B	466	TYR	N-CA-C	-7.22	99.23	110.42
1	A	382	THR	N-CA-C	7.16	120.60	109.07
1	B	467	LYS	N-CA-C	7.14	119.17	108.31
1	C	141	GLN	N-CA-C	7.03	121.03	110.14
1	D	343	VAL	N-CA-C	7.03	119.87	111.09
1	B	465	GLY	N-CA-C	6.94	125.69	112.51
1	A	354	TYR	N-CA-C	-6.82	103.63	112.23
1	B	141	GLN	N-CA-C	6.82	120.72	110.14
1	D	382	THR	N-CA-C	6.81	120.03	109.07
1	D	337	THR	N-CA-C	6.58	120.17	110.30
1	D	335	LYS	N-CA-C	6.53	119.22	111.71
1	C	478	TYR	N-CA-C	6.53	118.39	111.28
1	D	21	LYS	N-CA-C	6.52	120.68	110.32
1	C	382	THR	N-CA-C	6.49	119.48	108.90
1	D	387	VAL	N-CA-CB	-6.47	101.61	112.47
1	B	50	VAL	CB-CA-C	6.42	120.12	110.63
1	D	40	TYR	N-CA-C	6.41	119.56	110.14
1	A	142	THR	N-CA-CB	6.39	120.75	110.65
1	A	466	TYR	N-CA-C	-6.34	101.14	110.52
1	B	470	GLY	N-CA-C	6.30	119.33	110.38
1	A	29	VAL	N-CA-C	6.28	118.99	108.81
1	B	382	THR	N-CA-C	6.28	119.13	108.90
1	D	120	ASP	N-CA-C	6.24	118.63	111.02
1	C	400	GLY	CA-C-N	-6.17	113.58	121.91
1	C	400	GLY	C-N-CA	-6.17	113.58	121.91
1	C	29	VAL	N-CA-C	6.16	117.58	108.65
1	A	340	GLY	CA-C-N	-6.12	114.25	120.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	340	GLY	C-N-CA	-6.12	114.25	120.85
1	C	465	GLY	N-CA-C	6.11	122.67	111.12
1	D	466	TYR	N-CA-C	-6.03	101.54	110.46
1	A	132	ALA	N-CA-C	-6.01	104.73	111.28
1	D	470	GLY	N-CA-C	5.96	119.70	110.88
1	A	114	GLN	N-CA-C	5.92	117.73	111.28
1	C	77	GLU	CA-C-N	5.90	129.22	120.90
1	C	77	GLU	C-N-CA	5.90	129.22	120.90
1	D	365	VAL	CB-CA-C	5.88	118.72	111.25
1	B	74	PRO	N-CA-C	5.87	121.57	113.65
1	A	51	VAL	N-CA-C	5.85	116.90	108.48
1	A	116	ALA	N-CA-C	-5.84	104.99	111.36
1	B	40	TYR	N-CA-C	5.84	118.72	110.14
1	C	375	LYS	N-CA-C	-5.68	100.71	109.52
1	D	448	THR	CB-CA-C	5.65	119.53	109.65
1	D	59	ILE	N-CA-C	-5.62	105.04	110.72
1	C	460	ALA	N-CA-C	5.54	119.88	113.18
1	D	41	ASN	N-CA-C	-5.52	98.76	108.69
1	B	434	ILE	N-CA-C	5.50	115.70	110.53
1	B	177	LYS	N-CA-C	5.49	116.94	111.07
1	D	406	LEU	CA-C-N	-5.48	114.94	120.31
1	D	406	LEU	C-N-CA	-5.48	114.94	120.31
1	C	108	ASP	N-CA-C	5.47	118.42	111.69
1	D	117	LEU	N-CA-C	5.47	117.32	111.36
1	D	351	VAL	N-CA-CB	5.46	118.77	110.58
1	C	41	ASN	N-CA-C	-5.39	98.99	108.69
1	C	73	GLY	O-C-N	5.38	127.16	121.77
1	A	40	TYR	N-CA-C	5.38	118.05	109.81
1	C	110	GLY	N-CA-C	5.35	122.13	114.64
1	B	467	LYS	CB-CA-C	-5.34	110.40	116.54
1	A	5	ASN	N-CA-C	5.33	118.62	110.20
1	B	18	GLU	N-CA-C	-5.33	101.31	109.41
1	A	141	GLN	N-CA-C	5.33	118.39	110.14
1	A	103	GLN	N-CA-C	-5.32	105.56	111.36
1	C	380	LYS	N-CA-C	5.32	116.59	109.83
1	A	137	LYS	N-CA-C	5.32	119.53	112.30
1	A	60	ASP	N-CA-C	5.32	117.49	111.11
1	C	342	LEU	N-CA-C	-5.29	103.54	110.53
1	C	78	MET	N-CA-CB	-5.29	101.28	109.69
1	D	6	ILE	N-CA-C	-5.29	101.91	108.89
1	B	41	ASN	CB-CA-C	5.27	115.39	110.17
1	B	316	VAL	N-CA-CB	5.27	118.49	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	29	VAL	N-CA-C	5.27	116.50	108.80
1	B	142	THR	N-CA-CB	5.27	118.87	110.65
1	A	212	PHE	CA-C-N	-5.23	114.85	120.03
1	A	212	PHE	C-N-CA	-5.23	114.85	120.03
1	A	101	LEU	N-CA-C	5.23	116.98	111.28
1	B	127	ASN	N-CA-C	5.17	116.60	111.07
1	A	74	PRO	N-CA-C	5.16	121.44	113.75
1	A	236	ASP	N-CA-C	5.14	119.19	113.02
1	C	236	ASP	N-CA-C	5.14	119.53	113.16
1	D	224	GLY	CA-C-N	-5.13	114.50	120.04
1	D	224	GLY	C-N-CA	-5.13	114.50	120.04
1	C	404	VAL	N-CA-CB	-5.11	104.99	111.64
1	C	337	THR	N-CA-C	5.11	117.71	110.10
1	B	140	GLY	N-CA-C	-5.09	105.78	112.81
1	A	6	ILE	N-CA-C	-5.09	101.01	108.54
1	B	474	GLU	N-CA-C	-5.06	101.62	109.72
1	C	331	ALA	CA-C-N	5.04	126.44	120.14
1	C	331	ALA	C-N-CA	5.04	126.44	120.14
1	A	50	VAL	CB-CA-C	5.04	118.08	110.63
1	B	464	GLY	N-CA-C	5.03	117.93	110.63
1	A	19	GLU	N-CA-C	-5.03	103.51	110.35
1	C	50	VAL	CB-CA-C	5.01	118.04	110.63
1	C	132	ALA	N-CA-C	-5.00	106.69	112.89

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	3791	0	3740	49	0
1	B	3771	0	3721	38	0
1	C	3776	0	3727	59	0
1	D	3794	0	3745	39	0
2	A	44	0	26	1	0
2	B	44	0	26	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	44	0	26	1	0
2	D	44	0	26	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
4	A	140	0	0	0	0
4	B	141	0	0	1	0
4	C	126	0	0	4	0
4	D	125	0	0	0	0
All	All	15843	0	15037	164	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (164) 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:C:364:THR:HG21	1:C:386:ASP:OD2	1.44	1.18
1:C:364:THR:CG2	1:C:386:ASP:OD2	2.01	1.08
1:D:364:THR:HB	1:D:385:THR:HG22	1.53	0.88
1:D:387:VAL:HG11	1:D:404:VAL:HG13	1.58	0.86
1:C:433:ASN:HB3	1:C:436:THR:HG23	1.59	0.85
1:D:300[A]:CYS:SG	2:D:501:NAD:C7N	2.69	0.81
1:B:300[B]:CYS:SG	2:B:501:NAD:C7N	2.70	0.80
1:A:387:VAL:HG11	1:A:404:VAL:HG13	1.65	0.78
1:D:22:MET:HE3	1:D:220:VAL:HG12	1.66	0.76
1:D:243:THR:HB	1:D:266:GLU:HB2	1.68	0.76
1:C:243:THR:HB	1:C:266:GLU:HB2	1.69	0.75
1:A:438:HIS:HE1	1:C:438:HIS:HE1	1.35	0.74
1:D:22:MET:HG2	1:D:221:PRO:HD2	1.71	0.73
1:C:300:CYS:SG	2:C:501:NAD:C7N	2.77	0.72
1:C:435:LYS:HG3	1:D:493:ILE:HA	1.74	0.68
1:A:438:HIS:CE1	1:C:438:HIS:HE1	2.13	0.67
1:A:9:LYS:H	1:A:103:GLN:HE22	1.42	0.66
1:A:349:GLU:O	1:A:353:ASN:HB2	1.96	0.66
1:A:300:CYS:SG	2:A:501:NAD:C7N	2.84	0.66
1:A:387:VAL:HG13	1:A:394:VAL:HG11	1.78	0.65
1:B:22:MET:HE3	1:B:24:ILE:HD11	1.76	0.65
1:C:342:LEU:HD12	1:C:348:GLN:HA	1.79	0.64
1:D:4:THR:HB	1:D:335:LYS:HB2	1.77	0.64
1:B:264:THR:HG21	1:B:482:ASN:CG	2.23	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:356:GLU:O	1:C:360:LYS:HG2	1.99	0.63
1:C:448:THR:CG2	4:C:653:HOH:O	2.47	0.63
1:C:107:LEU:HD13	1:C:333:MET:HG3	1.81	0.62
1:A:166:PRO:HD3	1:A:243:THR:HG23	1.81	0.62
1:A:9:LYS:HB2	1:A:12:VAL:HG13	1.83	0.61
1:A:201:LEU:HD11	1:A:221:PRO:HG3	1.82	0.61
1:D:433:ASN:HD22	1:D:436:THR:H	1.48	0.61
1:B:109:ASN:OD1	1:B:111:LYS:HE2	2.00	0.61
1:A:329:LEU:HD21	1:A:339:MET:HE2	1.83	0.61
1:B:387:VAL:HG21	1:B:404:VAL:HG13	1.84	0.59
1:C:436:THR:HG21	4:C:613:HOH:O	2.02	0.59
1:D:9:LYS:H	1:D:103:GLN:HE22	1.49	0.58
1:C:493:ILE:HA	1:D:435:LYS:HG3	1.85	0.58
1:D:372:ALA:HB2	1:D:380:LYS:HG3	1.86	0.57
1:A:487:LYS:NZ	1:D:444:LEU:O	2.38	0.57
1:B:300[B]:CYS:SG	2:B:501:NAD:N7N	2.78	0.57
1:C:22:MET:CG	1:C:221:PRO:HD2	2.36	0.56
1:C:276:LEU:HD12	1:C:431:THR:HB	1.87	0.56
1:A:438:HIS:HE1	1:C:438:HIS:CE1	2.20	0.55
1:D:78:MET:HG2	1:D:82:GLU:HB2	1.88	0.55
1:A:9:LYS:H	1:A:103:GLN:NE2	2.03	0.55
1:A:364:THR:HB	1:A:385:THR:HG22	1.87	0.55
1:C:370:GLU:HG2	1:C:380:LYS:HE2	1.89	0.55
1:B:438:HIS:HE1	1:D:438:HIS:HE1	1.53	0.55
1:A:22:MET:HG2	1:A:221:PRO:HD2	1.89	0.54
1:D:342:LEU:HD22	1:D:379:VAL:CG1	2.38	0.54
1:A:22:MET:HG2	1:A:221:PRO:CD	2.37	0.54
1:D:268:GLY:HA2	1:D:300[A]:CYS:SG	2.47	0.54
1:A:201:LEU:HD11	1:A:221:PRO:CG	2.37	0.54
1:D:448:THR:HG21	1:D:463:PHE:CD2	2.43	0.54
1:D:464:GLY:HA3	1:D:473:ARG:HD3	1.91	0.53
1:A:433:ASN:HD22	1:A:436:THR:H	1.56	0.53
1:B:485:GLU:HG3	1:C:466:TYR:CE1	2.44	0.53
1:A:108:ASP:OD2	1:A:196:THR:HA	2.09	0.53
1:C:370:GLU:CG	1:C:380:LYS:HE2	2.39	0.52
1:A:435:LYS:HG2	1:B:493:ILE:HA	1.91	0.52
1:C:277:GLU:O	1:C:312:HIS:HE1	1.92	0.51
1:D:342:LEU:HD21	1:D:351:VAL:HG11	1.93	0.51
1:B:438:HIS:HD2	1:C:152:TYR:OH	1.93	0.51
1:A:390:ASP:O	1:A:395:LYS:HE2	2.11	0.51
1:D:22:MET:CE	1:D:24:ILE:HD11	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:487:LYS:NZ	1:C:444:LEU:O	2.44	0.51
1:A:40:TYR:CD1	1:A:40:TYR:N	2.78	0.51
1:C:260:ILE:O	1:C:260:ILE:HG22	2.11	0.51
1:C:448:THR:HG23	4:C:653:HOH:O	2.10	0.50
1:B:317:VAL:HG22	1:B:405:VAL:HG11	1.94	0.50
1:C:22:MET:HG2	1:C:221:PRO:HD2	1.93	0.50
1:C:342:LEU:HD11	1:C:379:VAL:HG11	1.93	0.50
1:A:387:VAL:HG11	1:A:404:VAL:CG1	2.38	0.50
1:C:6:ILE:HD12	1:C:333:MET:O	2.10	0.50
1:C:138:ILE:HG22	1:C:138:ILE:O	2.11	0.50
1:B:261:LYS:O	1:C:253:MET:HE1	2.12	0.50
1:D:296:HIS:CD2	1:D:296:HIS:N	2.80	0.49
1:A:251:TYR:O	1:A:255:GLN:HG2	2.12	0.49
1:B:258:GLU:O	1:C:250:LYS:HE2	2.13	0.49
1:A:342:LEU:HD22	1:A:379:VAL:CG1	2.43	0.49
1:B:22:MET:HG2	1:B:221:PRO:HD2	1.95	0.48
1:D:277:GLU:O	1:D:312:HIS:HE1	1.96	0.48
1:A:243:THR:HB	1:A:266:GLU:HB2	1.95	0.48
1:C:153:THR:HA	1:C:487:LYS:O	2.14	0.47
1:D:169:PHE:HB3	1:D:172:VAL:CG1	2.43	0.47
1:B:370:GLU:OE2	1:B:380:LYS:NZ	2.38	0.47
1:A:342:LEU:HD22	1:A:379:VAL:HG13	1.97	0.47
1:C:201:LEU:HD11	1:C:221:PRO:HG3	1.96	0.47
1:A:139:ILE:HD12	1:C:141:GLN:HG2	1.97	0.47
1:B:433:ASN:HD22	1:B:436:THR:H	1.63	0.46
1:C:83:ARG:NH2	1:C:183:ALA:O	2.47	0.46
1:B:350:ARG:NH1	2:B:501:NAD:O3D	2.48	0.46
1:A:8:LEU:HA	1:A:103:GLN:HE22	1.80	0.46
1:B:292:ILE:HG21	1:B:403:VAL:HB	1.98	0.46
1:D:153:THR:HA	1:D:487:LYS:O	2.15	0.46
1:C:364:THR:CG2	1:C:386:ASP:CG	2.84	0.46
1:A:30:SER:HA	1:A:52:CYS:SG	2.55	0.46
1:C:364:THR:HG23	1:C:385:THR:HG22	1.97	0.45
1:C:268:GLY:HA2	1:C:300:CYS:SG	2.57	0.45
1:B:147:LYS:HG2	4:B:709:HOH:O	2.15	0.45
1:B:264:THR:HG21	1:B:482:ASN:ND2	2.32	0.45
1:D:260:ILE:HG22	1:D:260:ILE:O	2.17	0.45
1:D:300[A]:CYS:SG	2:D:501:NAD:N7N	2.90	0.45
1:D:308:VAL:HG11	1:D:316:VAL:HG13	1.99	0.45
1:B:387:VAL:HG21	1:B:404:VAL:CG1	2.47	0.44
1:C:22:MET:HG3	1:C:221:PRO:HD2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:375:LYS:HD3	1:C:375:LYS:HA	1.80	0.44
1:C:9:LYS:H	1:C:103:GLN:HE22	1.65	0.44
1:A:44:THR:O	1:A:45:GLU:HB2	2.17	0.44
1:B:79:THR:HG22	1:D:146:SER:HB2	1.99	0.44
1:C:199:SER:HB2	4:C:616:HOH:O	2.18	0.44
1:B:300[B]:CYS:SG	2:B:501:NAD:C2N	3.06	0.44
1:A:80:THR:HB	1:A:135:THR:HG22	1.99	0.43
1:D:190:LEU:C	1:D:190:LEU:HD23	2.43	0.43
1:B:135:THR:HG22	1:B:183:ALA:HA	1.99	0.43
1:A:395:LYS:HE3	1:A:395:LYS:HB2	1.71	0.43
1:A:444:LEU:O	1:D:487:LYS:NZ	2.50	0.43
1:C:329:LEU:HD12	1:C:339:MET:HB3	1.99	0.43
1:A:77:GLU:HG2	1:C:147:LYS:HE3	2.00	0.43
1:B:466:TYR:CE1	1:C:485:GLU:HG3	2.53	0.43
1:B:242:PHE:CD1	1:B:252:ILE:CD1	3.01	0.43
1:B:154:ARG:NH2	1:B:156:GLU:OE2	2.48	0.43
1:A:99:GLU:O	1:A:103:GLN:HG3	2.18	0.43
1:B:300[B]:CYS:SG	2:B:501:NAD:C3N	3.07	0.43
1:B:229:ALA:HA	1:B:232:VAL:HG12	2.00	0.42
1:D:22:MET:HE1	1:D:24:ILE:HD11	1.99	0.42
1:C:190:LEU:HD12	1:C:200:LEU:HD21	2.00	0.42
1:A:75:TRP:CH2	1:A:83:ARG:HD2	2.54	0.42
1:A:98:ARG:CZ	1:A:117:LEU:HD11	2.49	0.42
1:C:190:LEU:HD12	1:C:200:LEU:CD2	2.50	0.42
1:D:217:VAL:HG13	1:D:219:PHE:CE1	2.55	0.42
1:A:26:GLY:HA3	1:A:214:ASN:HD22	1.85	0.42
1:C:474:GLU:HA	1:C:479:ALA:HB2	2.01	0.42
1:C:272:PRO:HG3	1:C:418:ALA:HB1	2.02	0.42
1:C:296:HIS:N	1:C:296:HIS:CD2	2.88	0.42
1:D:403:VAL:HG22	1:D:404:VAL:N	2.35	0.42
1:A:308:VAL:HG11	1:A:316:VAL:HG13	2.02	0.41
1:B:148:ASP:HB3	1:B:494:LYS:HE2	2.00	0.41
1:D:345:LYS:HE2	1:D:349:GLU:OE2	2.20	0.41
1:A:438:HIS:CE1	1:C:438:HIS:CE1	3.01	0.41
1:B:277:GLU:O	1:B:312:HIS:HE1	2.03	0.41
1:B:296:HIS:CD2	1:B:296:HIS:N	2.88	0.41
1:A:484:THR:CG2	1:A:485:GLU:N	2.83	0.41
1:D:217:VAL:CG1	1:D:219:PHE:CZ	3.03	0.41
1:A:308:VAL:O	1:A:407:PRO:HA	2.21	0.41
1:A:260:ILE:HG22	1:A:260:ILE:O	2.20	0.41
1:C:217:VAL:HG13	1:C:219:PHE:CZ	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:PRO:O	1:A:78:MET:HB2	2.21	0.41
1:A:109:ASN:ND2	1:A:167:TRP:O	2.52	0.41
1:C:364:THR:CG2	1:C:386:ASP:HB2	2.50	0.41
1:D:84:ALA:HB2	1:D:135:THR:OG1	2.21	0.41
1:B:243:THR:HA	1:B:266:GLU:O	2.21	0.41
1:B:388:THR:OG1	1:B:390:ASP:OD1	2.19	0.41
1:B:474:GLU:O	1:B:475:LEU:HB2	2.21	0.41
1:B:475:LEU:N	1:B:479:ALA:HB2	2.36	0.41
1:C:177:LYS:NZ	1:C:474:GLU:OE2	2.49	0.41
1:C:266:GLU:HG3	1:C:474:GLU:OE1	2.21	0.41
1:C:364:THR:HG22	1:C:386:ASP:HB2	2.03	0.41
1:C:182:LEU:HD21	1:C:188:ILE:HD12	2.02	0.40
1:A:485:GLU:HG3	1:D:466:TYR:CE1	2.56	0.40
1:A:161:VAL:HG23	1:A:163:GLN:HG3	2.04	0.40
1:D:190:LEU:HD22	1:D:200:LEU:CD2	2.52	0.40
1:B:487:LYS:HA	1:C:447:GLY:O	2.22	0.40
1:C:6:ILE:HD12	1:C:333:MET:C	2.47	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	489/494 (99%)	472 (96%)	16 (3%)	1 (0%)	43	66
1	B	487/494 (99%)	471 (97%)	16 (3%)	0	100	100
1	C	487/494 (99%)	467 (96%)	19 (4%)	1 (0%)	43	66
1	D	490/494 (99%)	475 (97%)	14 (3%)	1 (0%)	43	66
All	All	1953/1976 (99%)	1885 (96%)	65 (3%)	3 (0%)	43	66

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	166	PRO
1	A	424	GLY
1	D	166	PRO

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	398/401 (99%)	365 (92%)	33 (8%)	10	23
1	B	396/401 (99%)	372 (94%)	24 (6%)	17	37
1	C	396/401 (99%)	353 (89%)	43 (11%)	6	13
1	D	399/401 (100%)	361 (90%)	38 (10%)	8	18
All	All	1589/1604 (99%)	1451 (91%)	138 (9%)	9	21

All (138) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	VAL
1	A	13	GLU
1	A	17	ASN
1	A	18	GLU
1	A	27	GLU
1	A	50	VAL
1	A	60	ASP
1	A	104	LEU
1	A	115	VAL
1	A	121	ILE
1	A	126	GLU
1	A	161	VAL
1	A	217	VAL
1	A	283	GLU
1	A	296	HIS
1	A	301	SER
1	A	316	VAL
1	A	327	VAL
1	A	336	GLU

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Mol	Chain	Res	Type
1	A	342	LEU
1	A	343	VAL
1	A	351	VAL
1	A	353	ASN
1	A	379	VAL
1	A	380	LYS
1	A	385	THR
1	A	387	VAL
1	A	394	VAL
1	A	404	VAL
1	A	416	GLU
1	A	445	LYS
1	A	457	GLU
1	A	484	THR
1	B	7	GLU
1	B	17	ASN
1	B	27	GLU
1	B	50	VAL
1	B	77	GLU
1	B	115	VAL
1	B	127	ASN
1	B	199	SER
1	B	296	HIS
1	B	316	VAL
1	B	327	VAL
1	B	335	LYS
1	B	346	LYS
1	B	351	VAL
1	B	359	LYS
1	B	360	LYS
1	B	365	VAL
1	B	373	LEU
1	B	375	LYS
1	B	394	VAL
1	B	412	GLU
1	B	443	LYS
1	B	445	LYS
1	B	484	THR
1	C	7	GLU
1	C	13	GLU
1	C	22	MET
1	C	50	VAL

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Mol	Chain	Res	Type
1	C	57	GLU
1	C	60	ASP
1	C	68	SER
1	C	83	ARG
1	C	105	GLU
1	C	107	LEU
1	C	109	ASN
1	C	115	VAL
1	C	217	VAL
1	C	239	LYS
1	C	243	THR
1	C	260	ILE
1	C	282	GLU
1	C	290	GLN
1	C	296	HIS
1	C	316	VAL
1	C	327	VAL
1	C	328	LYS
1	C	329	LEU
1	C	351	VAL
1	C	353	ASN
1	C	364	THR
1	C	365	VAL
1	C	373	LEU
1	C	375	LYS
1	C	379	VAL
1	C	380	LYS
1	C	385	THR
1	C	387	VAL
1	C	394	VAL
1	C	395	LYS
1	C	399	PHE
1	C	404	VAL
1	C	422	SER
1	C	435	LYS
1	C	436	THR
1	C	445	LYS
1	C	448	THR
1	C	484	THR
1	D	4	THR
1	D	7	GLU
1	D	12	VAL

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Mol	Chain	Res	Type
1	D	18	GLU
1	D	21	LYS
1	D	50	VAL
1	D	109	ASN
1	D	115	VAL
1	D	146	SER
1	D	161	VAL
1	D	191	LYS
1	D	217	VAL
1	D	220	VAL
1	D	239	LYS
1	D	243	THR
1	D	264	THR
1	D	283	GLU
1	D	296	HIS
1	D	311	LYS
1	D	316	VAL
1	D	327	VAL
1	D	328	LYS
1	D	335	LYS
1	D	342	LEU
1	D	343	VAL
1	D	351	VAL
1	D	365	VAL
1	D	371	ARG
1	D	379	VAL
1	D	385	THR
1	D	387	VAL
1	D	394	VAL
1	D	404	VAL
1	D	405	VAL
1	D	435	LYS
1	D	443	LYS
1	D	448	THR
1	D	484	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	GLN
1	A	114	GLN
1	A	214	ASN

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Mol	Chain	Res	Type
1	A	262	HIS
1	A	299	ASN
1	A	326	ASN
1	A	357	GLN
1	A	432	GLN
1	A	433	ASN
1	A	438	HIS
1	B	85	HIS
1	B	114	GLN
1	B	141	GLN
1	B	214	ASN
1	B	233	ASN
1	B	255	GLN
1	B	312	HIS
1	B	326	ASN
1	B	357	GLN
1	B	432	GLN
1	B	433	ASN
1	B	438	HIS
1	B	482	ASN
1	C	85	HIS
1	C	103	GLN
1	C	163	GLN
1	C	233	ASN
1	C	255	GLN
1	C	312	HIS
1	C	325	ASN
1	C	326	ASN
1	C	357	GLN
1	C	432	GLN
1	C	433	ASN
1	C	438	HIS
1	C	482	ASN
1	D	85	HIS
1	D	103	GLN
1	D	114	GLN
1	D	214	ASN
1	D	299	ASN
1	D	312	HIS
1	D	325	ASN
1	D	326	ASN
1	D	347	GLN

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Mol	Chain	Res	Type
1	D	432	GLN
1	D	433	ASN
1	D	438	HIS
1	D	482	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	NAD	C	501	-	46,48,48	1.43	6 (13%)	64,73,73	1.88	15 (23%)
2	NAD	A	501	-	46,48,48	1.24	4 (8%)	64,73,73	1.56	9 (14%)
2	NAD	D	501	-	46,48,48	1.33	8 (17%)	64,73,73	1.67	13 (20%)
2	NAD	B	501	-	46,48,48	1.44	7 (15%)	64,73,73	1.63	14 (21%)

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	C	501	-	-	7/30/62/62	0/5/5/5
2	NAD	A	501	-	-	13/30/62/62	0/5/5/5
2	NAD	D	501	-	-	13/30/62/62	0/5/5/5
2	NAD	B	501	-	-	9/30/62/62	0/5/5/5

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	NAD	PN-O3	5.11	1.65	1.59
2	D	501	NAD	C5A-C4A	4.90	1.47	1.39
2	B	501	NAD	PN-O3	4.78	1.64	1.59
2	C	501	NAD	C5A-C4A	4.74	1.47	1.39
2	B	501	NAD	C5A-C4A	4.61	1.47	1.39
2	A	501	NAD	PN-O3	3.79	1.63	1.59
2	A	501	NAD	C5A-C4A	3.67	1.45	1.39
2	C	501	NAD	C8A-N7A	3.08	1.37	1.31
2	A	501	NAD	C5A-N7A	-3.04	1.33	1.39
2	D	501	NAD	O4D-C1D	2.82	1.44	1.40
2	D	501	NAD	C8A-N7A	2.57	1.36	1.31
2	B	501	NAD	O4D-C1D	2.57	1.44	1.40
2	D	501	NAD	C5A-N7A	-2.55	1.34	1.39
2	C	501	NAD	C5A-C6A	2.53	1.48	1.41
2	A	501	NAD	O4D-C1D	2.50	1.44	1.40
2	D	501	NAD	C5A-C6A	2.45	1.47	1.41
2	D	501	NAD	C4A-N9A	-2.42	1.32	1.37
2	B	501	NAD	C8A-N7A	2.38	1.36	1.31
2	D	501	NAD	PN-O3	2.36	1.62	1.59
2	B	501	NAD	C5A-N7A	-2.31	1.34	1.39
2	B	501	NAD	C5A-C6A	2.30	1.47	1.41
2	B	501	NAD	PA-O3	2.24	1.61	1.59
2	D	501	NAD	PA-O3	2.15	1.61	1.59
2	C	501	NAD	C4A-N3A	2.05	1.38	1.34
2	C	501	NAD	PA-O3	2.04	1.61	1.59

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	NAD	C5A-C4A-N3A	-5.90	118.59	126.72
2	A	501	NAD	C5A-C4A-N3A	-5.66	118.93	126.72
2	D	501	NAD	C5A-C4A-N3A	-5.56	119.06	126.72
2	C	501	NAD	N3A-C4A-N9A	5.51	136.53	127.17
2	B	501	NAD	C5A-C4A-N3A	-5.11	119.69	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	NAD	N3A-C2A-N1A	-4.55	121.70	128.58
2	C	501	NAD	C2A-N3A-C4A	4.53	122.89	111.83
2	B	501	NAD	N3A-C4A-N9A	4.43	134.71	127.17
2	A	501	NAD	N3A-C4A-N9A	4.21	134.32	127.17
2	D	501	NAD	O3-PA-O1A	-4.10	98.36	110.70
2	D	501	NAD	N3A-C4A-N9A	4.08	134.11	127.17
2	C	501	NAD	C6N-N1N-C2N	-3.99	118.48	121.88
2	D	501	NAD	C2A-N3A-C4A	3.99	121.58	111.83
2	C	501	NAD	C4A-N9A-C8A	3.77	109.70	105.74
2	D	501	NAD	N3A-C2A-N1A	-3.65	123.05	128.58
2	A	501	NAD	C2A-N3A-C4A	3.62	120.68	111.83
2	B	501	NAD	N3A-C2A-N1A	-3.58	123.16	128.58
2	B	501	NAD	C2A-N3A-C4A	3.56	120.52	111.83
2	A	501	NAD	C4A-C5A-N7A	-3.20	106.92	110.58
2	A	501	NAD	N3A-C2A-N1A	-2.92	124.16	128.58
2	B	501	NAD	C4A-N9A-C8A	2.90	108.78	105.74
2	A	501	NAD	C5A-N7A-C8A	2.79	107.83	103.45
2	D	501	NAD	O2A-PA-O3	2.73	114.64	107.27
2	C	501	NAD	C6A-C5A-N7A	2.63	137.17	132.09
2	B	501	NAD	C4A-C5A-N7A	-2.58	107.63	110.58
2	C	501	NAD	C5A-C6A-N6A	-2.58	116.91	123.29
2	B	501	NAD	C5A-N7A-C8A	2.55	107.45	103.45
2	D	501	NAD	C2N-C3N-C4N	2.52	121.19	118.26
2	C	501	NAD	O2A-PA-O3	2.52	114.08	107.27
2	B	501	NAD	N9A-C8A-N7A	-2.42	110.51	113.94
2	C	501	NAD	N9A-C8A-N7A	-2.42	110.51	113.94
2	D	501	NAD	C4A-C5A-N7A	-2.41	107.83	110.58
2	B	501	NAD	O5B-PA-O1A	-2.40	99.41	108.94
2	B	501	NAD	O7N-C7N-N7N	-2.34	119.23	122.62
2	D	501	NAD	C6A-C5A-N7A	2.31	136.54	132.09
2	C	501	NAD	O4B-C1B-N9A	2.30	112.50	108.09
2	A	501	NAD	O2N-PN-O5D	2.29	117.95	107.57
2	B	501	NAD	C4A-N9A-C1B	-2.27	121.33	126.63
2	D	501	NAD	O2N-PN-O1N	2.26	122.95	112.44
2	A	501	NAD	N9A-C8A-N7A	-2.17	110.86	113.94
2	C	501	NAD	O3D-C3D-C4D	2.15	117.27	111.08
2	B	501	NAD	O4B-C1B-N9A	2.14	112.20	108.09
2	B	501	NAD	C3N-C7N-N7N	2.14	120.37	117.74
2	B	501	NAD	C2B-C3B-C4B	-2.13	98.49	102.61
2	D	501	NAD	C2A-N1A-C6A	2.11	122.20	118.73
2	D	501	NAD	C4D-O4D-C1D	2.08	111.83	109.92
2	C	501	NAD	C5N-C4N-C3N	-2.08	118.32	120.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	NAD	C4A-C5A-N7A	-2.05	108.23	110.58
2	D	501	NAD	C5N-C4N-C3N	-2.05	118.35	120.36
2	C	501	NAD	C5A-N7A-C8A	2.05	106.67	103.45
2	A	501	NAD	O2B-C2B-C1B	2.03	117.08	110.10

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	NAD	C5B-O5B-PA-O1A
2	A	501	NAD	C5B-O5B-PA-O3
2	A	501	NAD	C5D-O5D-PN-O3
2	A	501	NAD	C5D-O5D-PN-O1N
2	A	501	NAD	C5D-O5D-PN-O2N
2	B	501	NAD	O4B-C4B-C5B-O5B
2	B	501	NAD	C5D-O5D-PN-O3
2	B	501	NAD	C5D-O5D-PN-O1N
2	C	501	NAD	C5D-O5D-PN-O3
2	C	501	NAD	C5D-O5D-PN-O1N
2	C	501	NAD	C5D-O5D-PN-O2N
2	D	501	NAD	C5B-O5B-PA-O1A
2	D	501	NAD	C5B-O5B-PA-O2A
2	D	501	NAD	C5B-O5B-PA-O3
2	D	501	NAD	C5D-O5D-PN-O1N
2	B	501	NAD	C3B-C4B-C5B-O5B
2	A	501	NAD	C5B-O5B-PA-O2A
2	B	501	NAD	C5D-O5D-PN-O2N
2	D	501	NAD	C4N-C3N-C7N-O7N
2	D	501	NAD	C4N-C3N-C7N-N7N
2	A	501	NAD	C3D-C4D-C5D-O5D
2	C	501	NAD	PN-O3-PA-O1A
2	D	501	NAD	PA-O3-PN-O1N
2	D	501	NAD	O4D-C4D-C5D-O5D
2	D	501	NAD	C3D-C4D-C5D-O5D
2	D	501	NAD	C2N-C3N-C7N-O7N
2	A	501	NAD	C4N-C3N-C7N-N7N
2	D	501	NAD	C2N-C3N-C7N-N7N
2	A	501	NAD	O4D-C4D-C5D-O5D
2	B	501	NAD	O4D-C4D-C5D-O5D
2	A	501	NAD	C2B-C1B-N9A-C8A
2	B	501	NAD	C2B-C1B-N9A-C8A
2	D	501	NAD	C2B-C1B-N9A-C8A

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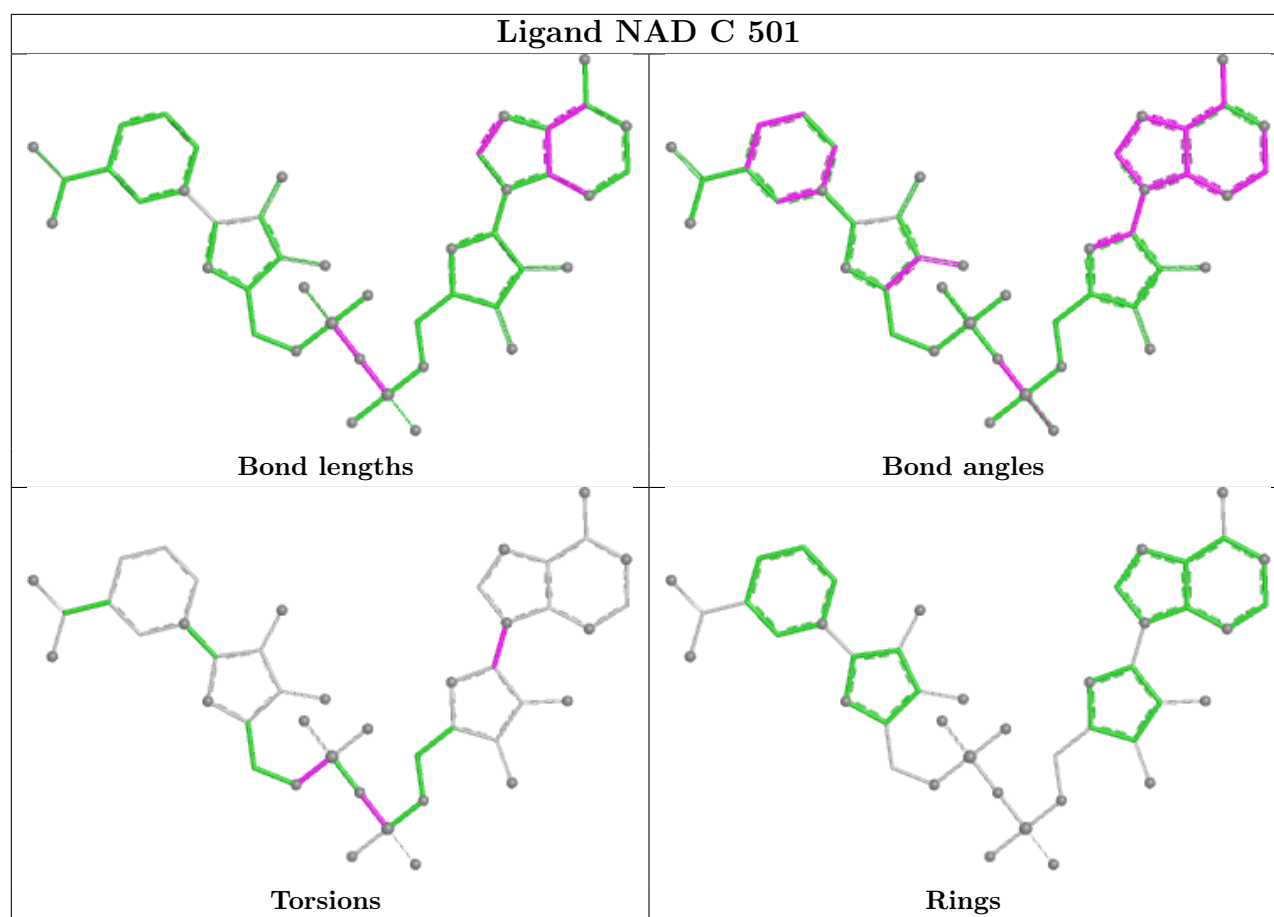
Mol	Chain	Res	Type	Atoms
2	B	501	NAD	PN-O3-PA-O1A
2	C	501	NAD	PN-O3-PA-O2A
2	D	501	NAD	PA-O3-PN-O2N
2	A	501	NAD	C4N-C3N-C7N-O7N
2	C	501	NAD	C2B-C1B-N9A-C8A
2	C	501	NAD	O4B-C1B-N9A-C8A
2	A	501	NAD	C4B-C5B-O5B-PA
2	A	501	NAD	C2N-C3N-C7N-N7N
2	B	501	NAD	PN-O3-PA-O2A

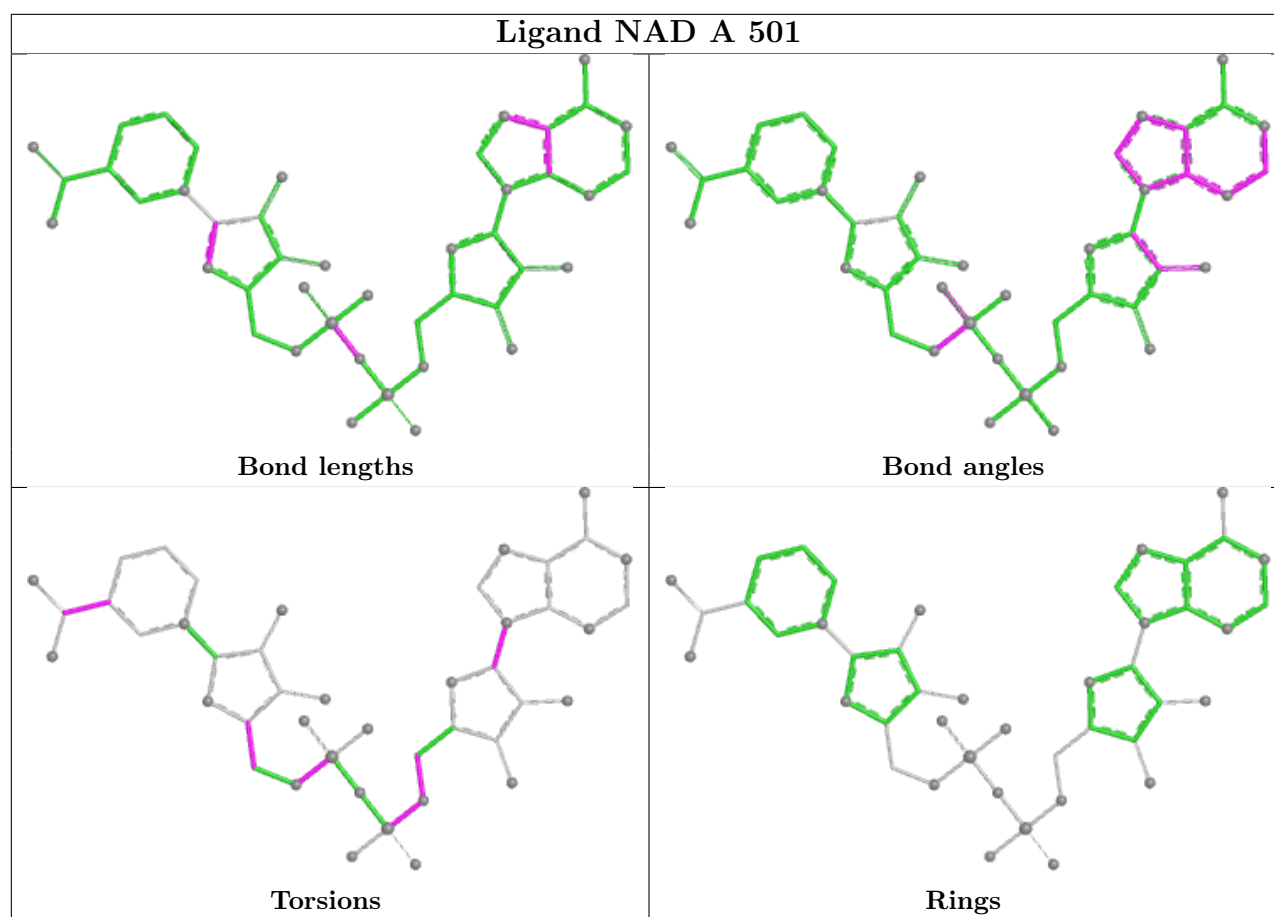
There are no ring outliers.

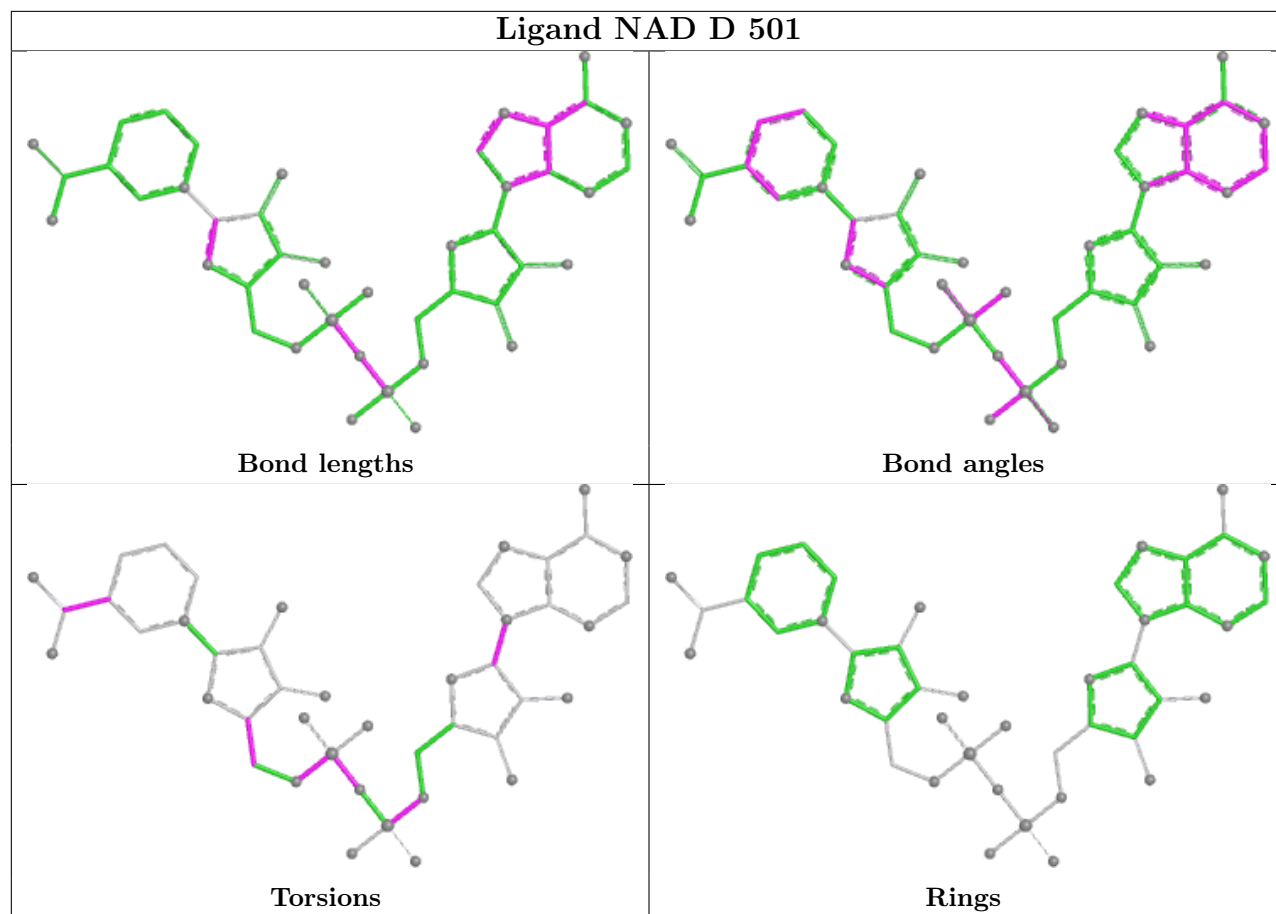
4 monomers are involved in 9 short contacts:

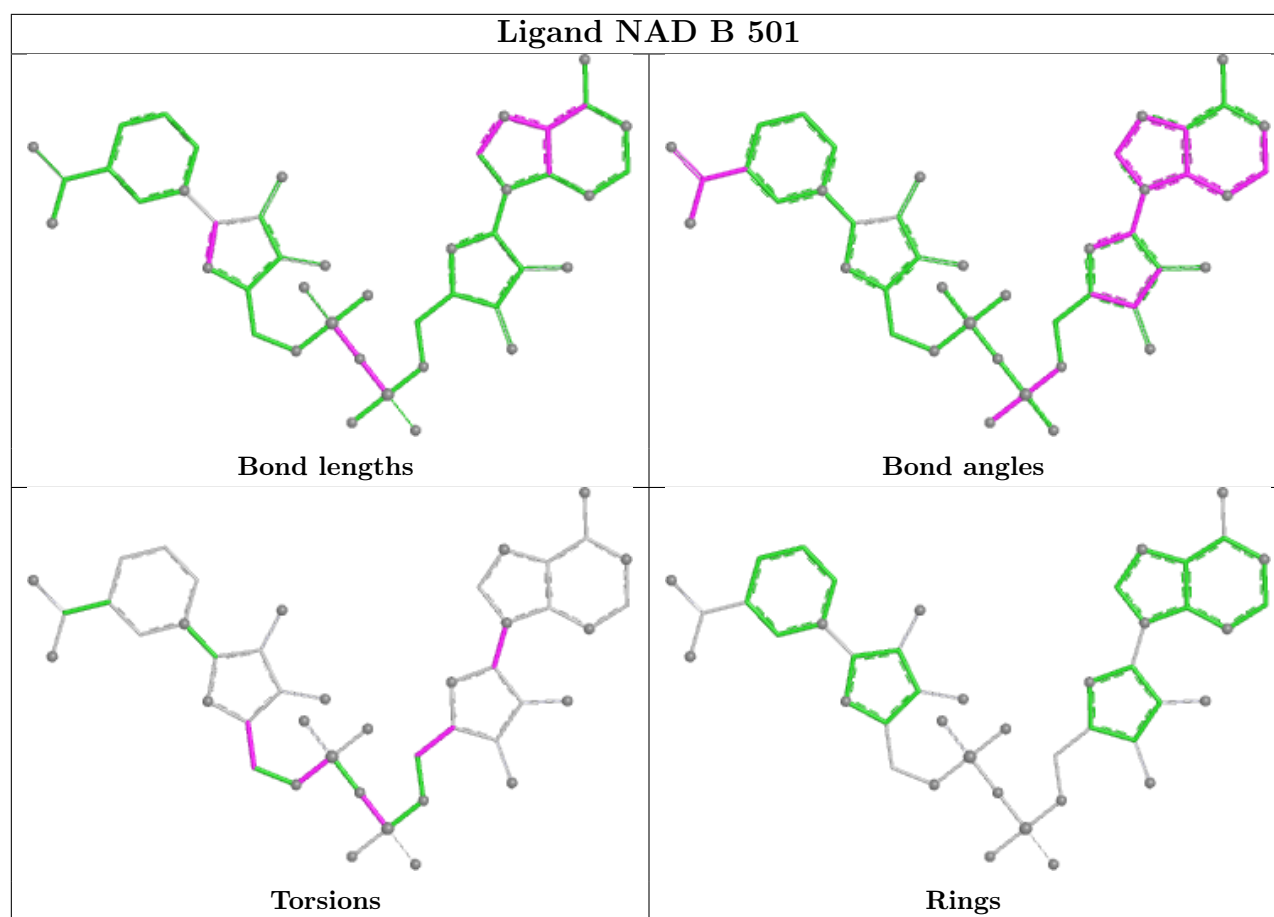
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	501	NAD	1	0
2	A	501	NAD	1	0
2	D	501	NAD	2	0
2	B	501	NAD	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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	491/494 (99%)	-0.40	2 (0%) 88 86	8, 14, 26, 42	0
1	B	488/494 (98%)	-0.41	0 100 100	6, 14, 26, 41	1 (0%)
1	C	489/494 (98%)	-0.37	3 (0%) 85 83	7, 13, 26, 50	0
1	D	491/494 (99%)	-0.34	3 (0%) 85 83	8, 16, 31, 46	1 (0%)
All	All	1959/1976 (99%)	-0.38	8 (0%) 88 86	6, 14, 27, 50	2 (0%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	7	GLU	4.0
1	D	4	THR	3.0
1	C	336	GLU	2.8
1	A	4	THR	2.7
1	D	412	GLU	2.5
1	A	235	HIS	2.4
1	C	374	GLU	2.2
1	D	494	LYS	2.2

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

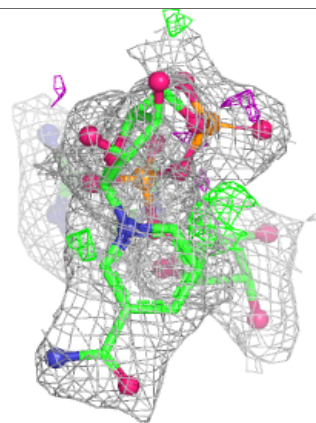
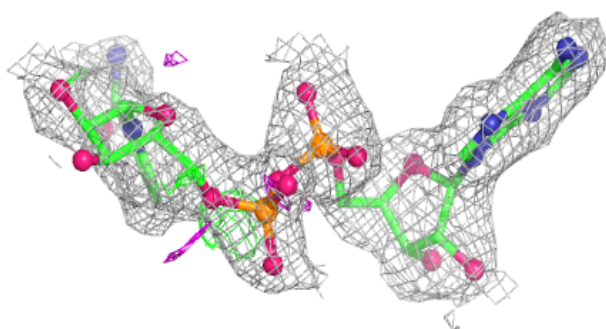
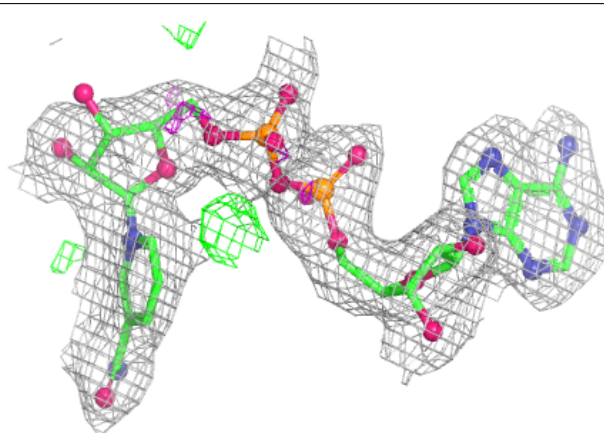
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NA	B	502	1/1	0.88	0.08	17,17,17,17	0
3	NA	A	502	1/1	0.90	0.06	14,14,14,14	0
2	NAD	B	501	44/44	0.94	0.09	17,26,44,48	0
2	NAD	D	501	44/44	0.95	0.08	16,27,40,41	0
2	NAD	A	501	44/44	0.95	0.08	16,21,30,31	0
2	NAD	C	501	44/44	0.95	0.08	18,25,30,33	0
3	NA	D	502	1/1	0.95	0.05	21,21,21,21	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.

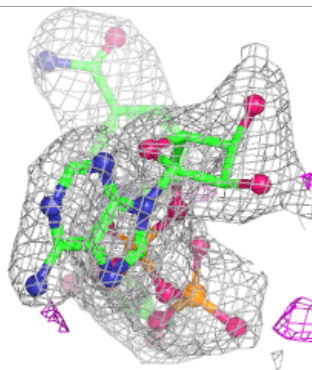
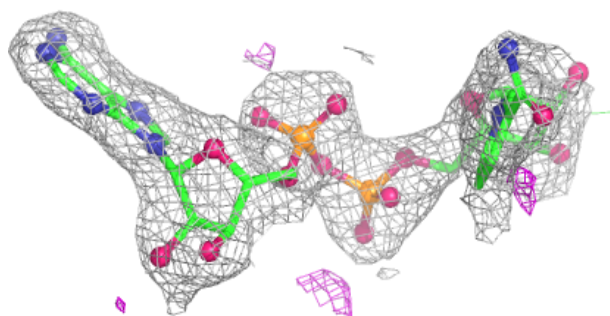
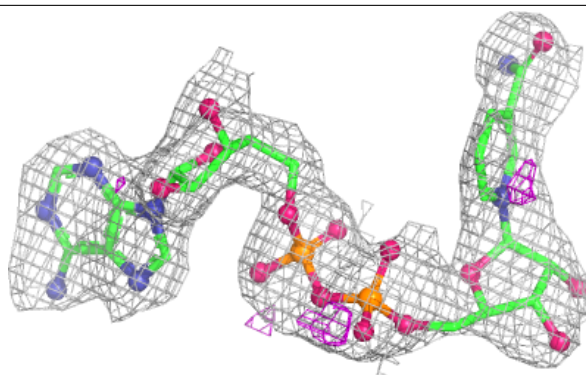
Electron density around NAD B 501:

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

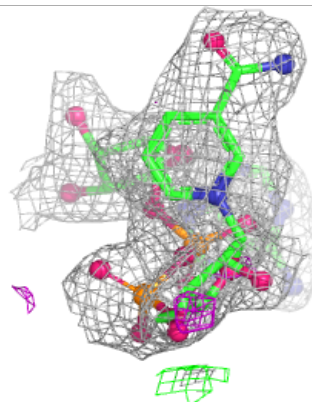
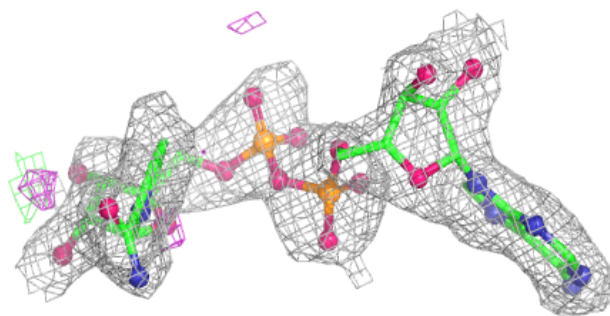
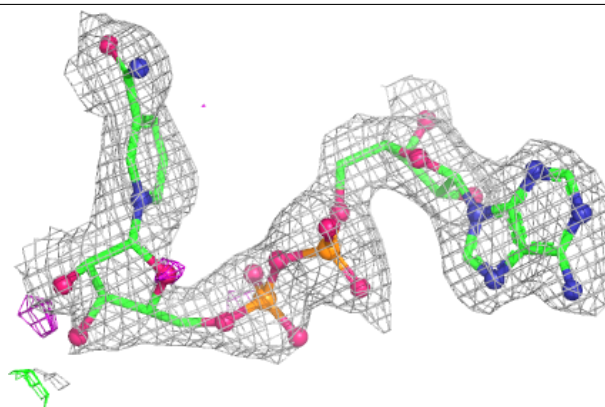


Electron density around NAD D 501:

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

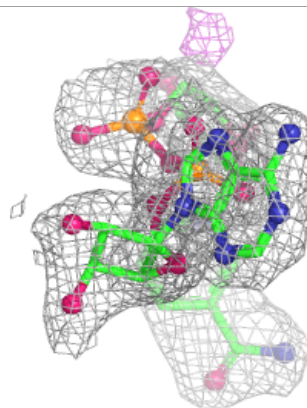
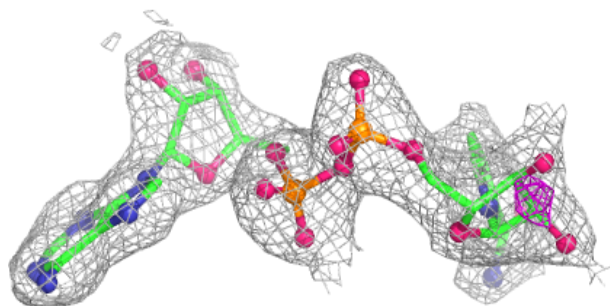
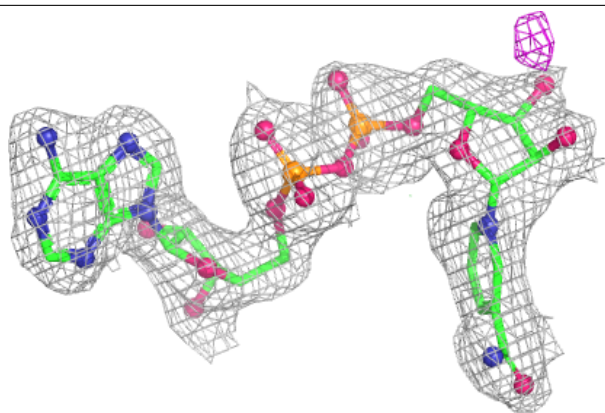
**Electron density around NAD A 501:**

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



Electron density around NAD C 501:

$2mF_o-DF_c$ (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.