Full wwPDB X-ray Structure Validation Report ⓘ

Aug 27, 2023 – 04:49 AM EDT

PDB ID	:	3GFB
Title	:	L-Threonine Dehydrogenase (TkTDH) from the hyperthermophilic archaeon Thermococcus kodakaraensis
Authors	:	Bowyer, A.
Deposited on	:	2009-02-26
Resolution	:	2.40 Å(reported)

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

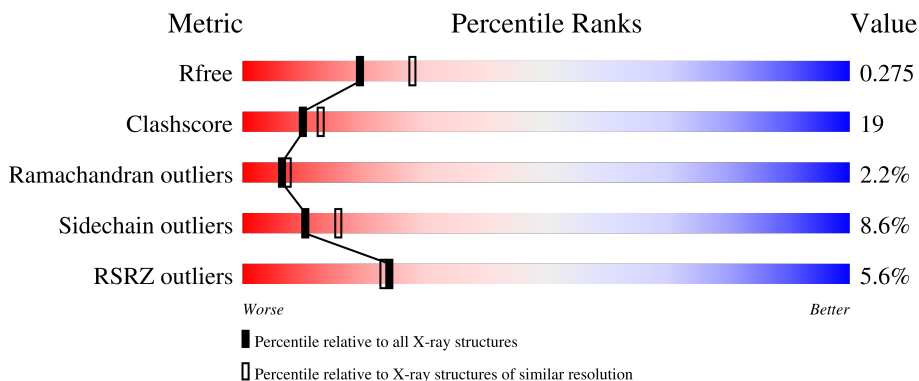|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

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

Metric	Percentile Ranks	Value
Rfree		0.275
Clashscore		19
Ramachandran outliers		2.2%
Sidechain outliers		8.6%
RSRZ outliers		5.6%

Worse — *Better*

▮ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	350	3% / 64% / 27% / 7% ••
1	B	350	6% / 56% / 36% / 6% ••
1	C	350	8% / 57% / 32% / 9% ••
1	D	350	5% / 62% / 29% / 7% ••

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

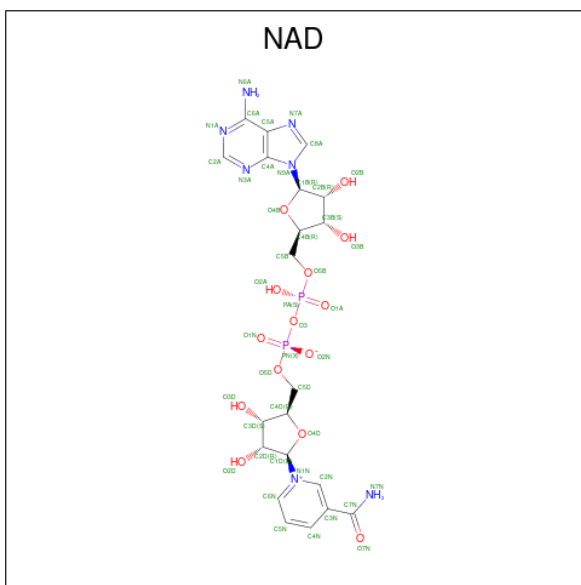| Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAD	A	500	X	-	-	-
2	NAD	B	501	X	-	-	-
2	NAD	C	502	X	-	-	-
2	NAD	D	503	X	-	-	-
3	SO4	B	351	-	-	-	X
3	SO4	C	351	-	-	-	X
3	SO4	D	351	-	-	-	X

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 11389 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 L-threonine 3-dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	347	Total	C	N	O	S	0	0	0
			2668	1726	444	486	12			
1	B	347	Total	C	N	O	S	0	0	0
			2668	1726	444	486	12			
1	C	347	Total	C	N	O	S	0	0	0
			2668	1726	444	486	12			
1	D	347	Total	C	N	O	S	0	0	0
			2668	1726	444	486	12			

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

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

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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 SULFATE ION (three-letter code: SO4) (formula: O_4S).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total 5	O 4	S 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	126	Total 126	O 126	0	0
4	B	119	Total 119	O 119	0	0
4	C	127	Total 127	O 127	0	0
4	D	119	Total 119	O 119	0	0

3 Residue-property plots ⓘ

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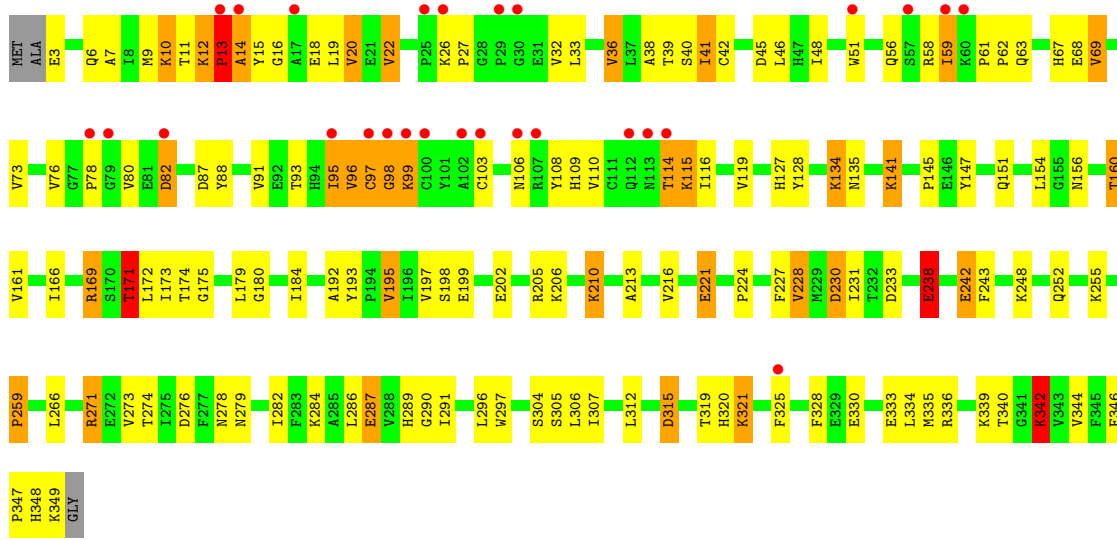
- Molecule 1: L-threonine 3-dehydrogenase
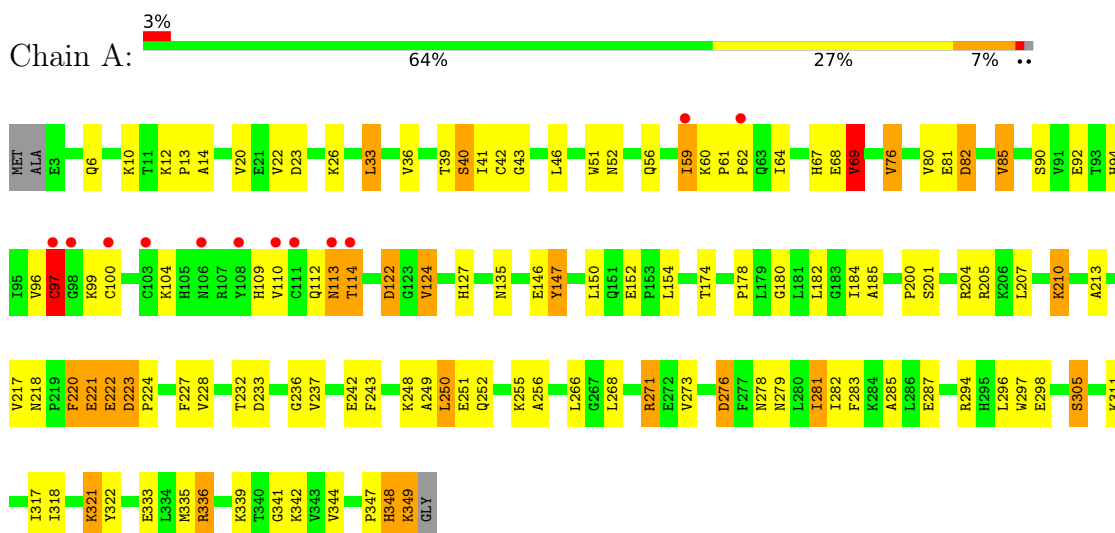
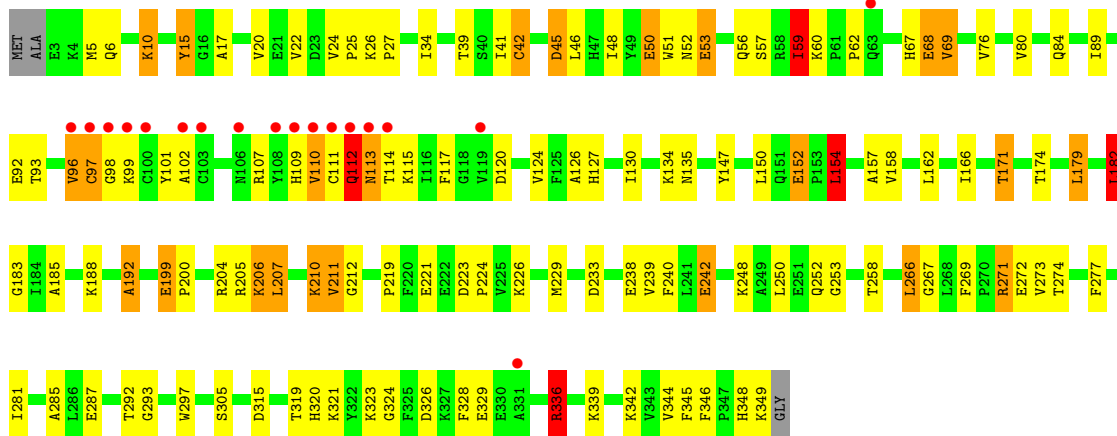- Molecule 1: L-threonine 3-dehydrogenase
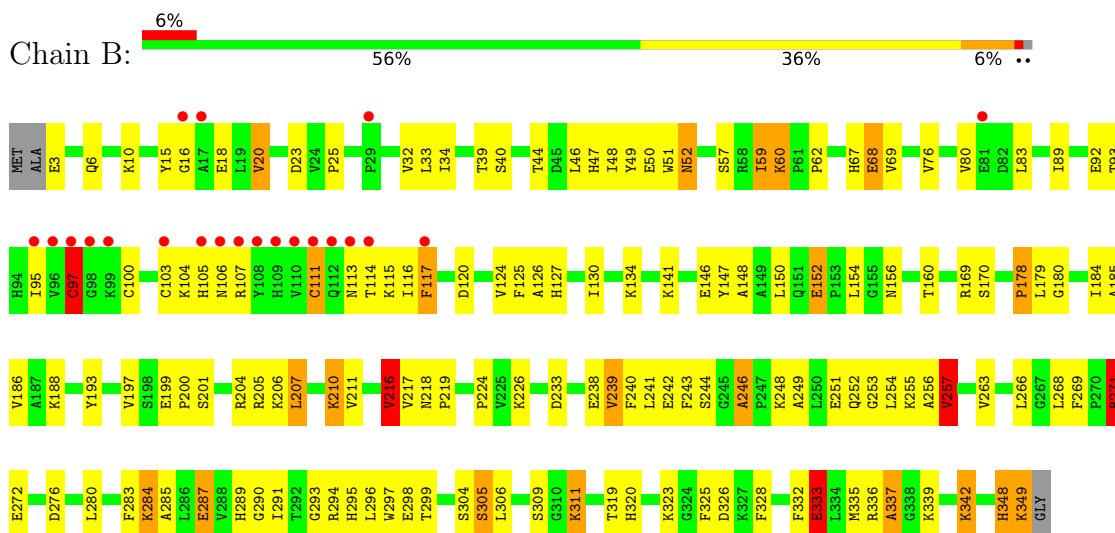
- Molecule 1: L-threonine 3-dehydrogenase

• Molecule 1: L-threonine 3-dehydrogenase

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	124.48Å 124.48Å 271.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	73.92 – 2.40 73.83 – 2.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (73.92-2.40) 100.0 (73.83-2.40)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.85 (at 2.40Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.217 , 0.277 0.217 , 0.275	Depositor DCC
R_{free} test set	4215 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	37.7	Xtriage
Anisotropy	0.117	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 58.4	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	11389	wwPDB-VP
Average B, all atoms (Å^2)	38.0	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 60.44 % 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 1.5213e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: SO4, NAD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z| > 5$	RMSZ	#$|Z| > 5$
1	A	1.52	15/2736 (0.5%)	1.25	15/3716 (0.4%)
1	B	1.54	23/2736 (0.8%)	1.29	13/3716 (0.3%)
1	C	1.57	24/2736 (0.9%)	1.24	13/3716 (0.3%)
1	D	1.58	17/2736 (0.6%)	1.32	17/3716 (0.5%)
All	All	1.55	79/10944 (0.7%)	1.28	58/14864 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	1
1	C	0	1
1	D	0	2
All	All	0	7

All (79) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	238	GLU	CB-CG	-11.32	1.30	1.52
1	B	257	VAL	CB-CG2	-10.54	1.30	1.52
1	B	238	GLU	CB-CG	-9.64	1.33	1.52
1	D	238	GLU	CG-CD	-9.55	1.37	1.51
1	B	238	GLU	CG-CD	-8.92	1.38	1.51
1	C	3	GLU	CG-CD	8.84	1.65	1.51
1	C	88	TYR	CD1-CE1	8.22	1.51	1.39
1	B	287	GLU	CD-OE1	8.02	1.34	1.25
1	C	221	GLU	CG-CD	7.85	1.63	1.51
1	C	287	GLU	CG-CD	7.84	1.63	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	287	GLU	CD-OE2	7.72	1.34	1.25
1	B	333	GLU	CG-CD	7.56	1.63	1.51
1	B	146	GLU	CD-OE1	7.43	1.33	1.25
1	B	311	LYS	CG-CD	6.95	1.76	1.52
1	A	311	LYS	CE-NZ	6.72	1.65	1.49
1	B	125	PHE	CE1-CZ	6.72	1.50	1.37
1	A	322	TYR	CD2-CE2	6.63	1.49	1.39
1	B	246	ALA	C-O	6.56	1.35	1.23
1	A	333	GLU	CD-OE2	6.55	1.32	1.25
1	A	147	TYR	CB-CG	-6.46	1.42	1.51
1	D	158	VAL	CA-CB	6.46	1.68	1.54
1	D	221	GLU	CG-CD	6.33	1.61	1.51
1	B	68	GLU	CG-CD	6.21	1.61	1.51
1	C	238	GLU	CG-CD	-6.21	1.42	1.51
1	B	298	GLU	CG-CD	6.14	1.61	1.51
1	C	22	VAL	CA-CB	6.13	1.67	1.54
1	A	249	ALA	CA-CB	-6.11	1.39	1.52
1	C	175	GLY	C-O	6.03	1.33	1.23
1	A	210	LYS	CD-CE	5.98	1.66	1.51
1	C	221	GLU	CB-CG	5.93	1.63	1.52
1	D	344	VAL	CB-CG2	5.91	1.65	1.52
1	A	69	VAL	CB-CG2	-5.87	1.40	1.52
1	D	42	CYS	CB-SG	-5.77	1.72	1.81
1	D	50	GLU	CB-CG	-5.75	1.41	1.52
1	C	284	LYS	CD-CE	-5.72	1.36	1.51
1	C	193	TYR	CB-CG	5.70	1.60	1.51
1	B	287	GLU	CG-CD	5.65	1.60	1.51
1	C	238	GLU	CD-OE1	5.58	1.31	1.25
1	C	228	VAL	CB-CG1	-5.54	1.41	1.52
1	B	304	SER	CA-CB	-5.50	1.44	1.52
1	A	271	ARG	CG-CD	-5.50	1.38	1.51
1	D	293	GLY	C-O	5.47	1.32	1.23
1	A	236	GLY	N-CA	5.47	1.54	1.46
1	B	185	ALA	CA-CB	5.46	1.64	1.52
1	C	3	GLU	CB-CG	5.44	1.62	1.52
1	A	305	SER	N-CA	-5.44	1.35	1.46
1	C	195	VAL	CB-CG1	5.42	1.64	1.52
1	A	287	GLU	CD-OE1	5.42	1.31	1.25
1	C	242	GLU	CD-OE2	5.37	1.31	1.25
1	C	82	ASP	CB-CG	5.33	1.62	1.51
1	C	36	VAL	CA-CB	5.32	1.66	1.54
1	B	238	GLU	N-CA	-5.32	1.35	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	293	GLY	C-O	5.30	1.32	1.23
1	D	329	GLU	CD-OE2	5.27	1.31	1.25
1	B	186	VAL	C-O	5.21	1.33	1.23
1	D	192	ALA	CA-CB	-5.21	1.41	1.52
1	B	238	GLU	CD-OE2	5.19	1.31	1.25
1	B	216	VAL	CB-CG2	-5.16	1.42	1.52
1	D	185	ALA	CA-CB	5.16	1.63	1.52
1	A	237	VAL	CB-CG2	-5.14	1.42	1.52
1	A	124	VAL	CA-CB	5.14	1.65	1.54
1	C	210	LYS	CD-CE	5.12	1.64	1.51
1	C	259	PRO	CB-CG	5.11	1.75	1.50
1	B	217	VAL	CB-CG2	-5.10	1.42	1.52
1	B	178	PRO	CB-CG	5.10	1.75	1.50
1	C	346	PHE	CE1-CZ	5.10	1.47	1.37
1	C	210	LYS	CE-NZ	5.10	1.61	1.49
1	C	40	SER	C-O	5.09	1.33	1.23
1	D	134	LYS	CD-CE	5.09	1.64	1.51
1	D	199	GLU	CB-CG	5.09	1.61	1.52
1	A	147	TYR	CE1-CZ	-5.09	1.31	1.38
1	B	239	VAL	CA-CB	5.08	1.65	1.54
1	D	277	PHE	CE2-CZ	5.06	1.47	1.37
1	A	90	SER	CA-CB	-5.06	1.45	1.52
1	D	211	VAL	CB-CG1	-5.05	1.42	1.52
1	B	103	CYS	CB-SG	5.04	1.90	1.82
1	C	171	THR	CA-CB	5.03	1.66	1.53
1	D	174	THR	C-O	5.02	1.32	1.23
1	D	15	TYR	CD2-CE2	5.01	1.46	1.39

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	271	ARG	NE-CZ-NH2	-14.27	113.17	120.30
1	B	238	GLU	OE1-CD-OE2	11.38	136.95	123.30
1	D	179	LEU	CB-CG-CD2	-10.14	93.76	111.00
1	C	154	LEU	CA-CB-CG	9.21	136.49	115.30
1	C	230	ASP	CB-CG-OD2	-8.50	110.65	118.30
1	D	238	GLU	OE1-CD-OE2	8.20	133.14	123.30
1	D	315	ASP	CB-CG-OD2	-8.19	110.93	118.30
1	C	238	GLU	OE1-CD-OE2	8.15	133.08	123.30
1	D	154	LEU	CA-CB-CG	7.41	132.34	115.30
1	C	286	LEU	CB-CG-CD1	-7.37	98.47	111.00
1	A	154	LEU	CB-CG-CD1	7.19	123.22	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	154	LEU	CA-CB-CG	7.12	131.67	115.30
1	B	238	GLU	CG-CD-OE1	-7.03	104.23	118.30
1	B	271	ARG	NE-CZ-NH1	7.00	123.80	120.30
1	D	59	ILE	CG1-CB-CG2	-6.90	96.22	111.40
1	C	286	LEU	CB-CG-CD2	6.88	122.69	111.00
1	D	271	ARG	NE-CZ-NH1	6.86	123.73	120.30
1	A	85	VAL	CB-CA-C	-6.77	98.55	111.40
1	A	69	VAL	CB-CA-C	-6.76	98.56	111.40
1	C	306	LEU	CB-CG-CD1	-6.67	99.67	111.00
1	D	266	LEU	CB-CG-CD2	-6.46	100.02	111.00
1	D	111	CYS	CA-CB-SG	6.08	124.94	114.00
1	A	336	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	D	229	MET	CG-SD-CE	5.95	109.72	100.20
1	A	223	ASP	CB-CG-OD1	5.90	123.61	118.30
1	C	284	LYS	CD-CE-NZ	-5.84	98.27	111.70
1	C	10	LYS	CD-CE-NZ	-5.80	98.37	111.70
1	B	23	ASP	CB-CG-OD2	5.79	123.51	118.30
1	C	315	ASP	CB-CG-OD1	5.77	123.49	118.30
1	A	33	LEU	CA-CB-CG	5.74	128.51	115.30
1	C	312	LEU	CB-CG-CD1	-5.70	101.31	111.00
1	C	271	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	D	162	LEU	CB-CG-CD1	5.62	120.55	111.00
1	D	45	ASP	CB-CG-OD1	-5.58	113.28	118.30
1	A	114	THR	N-CA-C	5.56	126.02	111.00
1	D	152	GLU	C-N-CD	5.56	140.08	128.40
1	C	255	LYS	CD-CE-NZ	-5.55	98.93	111.70
1	C	342	LYS	CD-CE-NZ	-5.55	98.93	111.70
1	B	284	LYS	CB-CG-CD	-5.53	97.23	111.60
1	B	107	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	A	223	ASP	CB-CG-OD2	-5.37	113.47	118.30
1	D	326	ASP	CB-CG-OD1	5.32	123.09	118.30
1	D	207	LEU	CA-CB-CG	5.30	127.50	115.30
1	D	182	LEU	CB-CG-CD2	5.30	120.00	111.00
1	B	154	LEU	CB-CG-CD2	5.26	119.95	111.00
1	B	207	LEU	CA-CB-CG	5.24	127.34	115.30
1	B	103	CYS	CA-CB-SG	5.23	123.42	114.00
1	A	23	ASP	CB-CG-OD2	5.22	123.00	118.30
1	A	152	GLU	C-N-CD	5.20	139.31	128.40
1	D	80	VAL	N-CA-C	-5.19	96.98	111.00
1	A	250	LEU	CA-CB-CG	5.18	127.23	115.30
1	B	170	SER	CB-CA-C	5.16	119.91	110.10
1	D	68	GLU	OE1-CD-OE2	-5.15	117.12	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	122	ASP	CB-CG-OD1	5.12	122.91	118.30
1	A	276	ASP	CB-CG-OD2	-5.09	113.72	118.30
1	B	284	LYS	CD-CE-NZ	-5.07	100.04	111.70
1	B	280	LEU	CB-CG-CD1	5.05	119.58	111.00
1	A	113	ASN	N-CA-C	5.04	124.61	111.00

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	112	GLN	Peptide
1	A	113	ASN	Peptide
1	A	348	HIS	Peptide
1	B	348	HIS	Peptide
1	C	12	LYS	Peptide
1	D	112	GLN	Peptide
1	D	113	ASN	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2668	0	2683	89	0
1	B	2668	0	2683	121	0
1	C	2668	0	2684	116	0
1	D	2668	0	2683	101	0
2	A	44	0	26	6	0
2	B	44	0	26	11	0
2	C	44	0	26	4	0
2	D	44	0	26	13	0
3	B	25	0	0	2	0
3	C	15	0	0	1	0
3	D	10	0	0	0	0
4	A	126	0	0	7	0
4	B	119	0	0	14	0
4	C	127	0	0	6	0
4	D	119	0	0	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	11389	0	10837	414	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 19.

All (414) 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:B:311:LYS:CG	1:B:311:LYS:CD	1.76	1.60
1:C:259:PRO:CG	1:C:259:PRO:CB	1.75	1.43
1:B:178:PRO:CG	1:B:178:PRO:CB	1.75	1.42
1:A:110:VAL:HG11	1:B:285:ALA:CB	1.80	1.11
1:D:67:HIS:HB2	1:D:93:THR:HG21	1.22	1.11
1:A:251:GLU:HB2	4:A:433:HOH:O	1.51	1.08
1:A:110:VAL:HG11	1:B:285:ALA:HB3	1.07	1.05
1:C:259:PRO:HB3	1:D:110:VAL:HG11	1.36	1.05
1:B:204:ARG:NH1	2:B:501:NAD:O3B	1.91	1.04
1:C:259:PRO:HB3	1:D:110:VAL:CG1	1.88	1.03
2:D:503:NAD:H4N	4:D:633:HOH:O	1.57	1.03
1:A:349:LYS:CE	1:A:349:LYS:H	1.71	1.03
1:B:67:HIS:HB2	1:B:93:THR:HG21	1.38	1.01
1:B:289:HIS:HD2	4:B:495:HOH:O	1.45	0.99
1:D:67:HIS:HB2	1:D:93:THR:CG2	1.92	0.99
1:C:110:VAL:HG11	1:D:285:ALA:HB3	1.48	0.95
1:D:349:LYS:H	1:D:349:LYS:HD2	1.33	0.94
1:C:289:HIS:HD2	4:D:492:HOH:O	1.49	0.94
1:A:81:GLU:O	1:A:82:ASP:HB2	1.66	0.93
1:A:349:LYS:H	1:A:349:LYS:HE2	1.31	0.91
1:B:207:LEU:O	1:B:211:VAL:HG23	1.71	0.91
1:D:323:LYS:HB3	1:D:349:LYS:HG3	1.53	0.90
1:D:349:LYS:HD2	1:D:349:LYS:N	1.86	0.90
1:C:248:LYS:O	1:C:252:GLN:HG3	1.72	0.89
1:A:110:VAL:CG1	1:B:285:ALA:HB3	1.99	0.87
1:C:141:LYS:HE3	1:C:141:LYS:N	1.91	0.85
1:C:171:THR:HG21	1:C:192:ALA:HB1	1.57	0.85
1:C:96:VAL:HG23	1:C:97:CYS:H	1.43	0.84
1:A:97:CYS:HA	4:A:368:HOH:O	1.78	0.83
1:A:276:ASP:OD2	1:A:279:ASN:HB2	1.79	0.83
1:A:110:VAL:CG1	1:B:285:ALA:CB	2.55	0.83
1:D:109:HIS:HB2	1:D:292:THR:O	1.77	0.83
1:A:13:PRO:O	1:A:51:TRP:CD1	2.33	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:ASN:HB3	1:B:114:THR:HA	1.62	0.82
1:C:259:PRO:CB	1:D:110:VAL:HG11	2.10	0.81
2:D:503:NAD:O1N	4:D:444:HOH:O	1.98	0.81
1:C:110:VAL:HG11	1:D:285:ALA:CB	2.11	0.81
1:D:97:CYS:O	1:D:99:LYS:N	2.12	0.81
1:C:179:LEU:HD12	2:C:502:NAD:H4D	1.63	0.81
1:B:254:LEU:O	1:B:284:LYS:NZ	2.13	0.80
1:D:204:ARG:NH1	2:D:503:NAD:O3B	2.13	0.80
1:D:349:LYS:N	1:D:349:LYS:CD	2.45	0.80
1:D:67:HIS:CB	1:D:93:THR:HG21	2.10	0.79
1:A:228:VAL:HG11	1:A:256:ALA:HB1	1.64	0.78
1:B:323:LYS:HB3	1:B:349:LYS:HB2	1.64	0.77
1:A:46:LEU:HD11	1:A:336:ARG:HG3	1.67	0.77
1:C:141:LYS:HE3	1:C:141:LYS:H	1.50	0.76
3:B:353:SO4:O3	4:B:527:HOH:O	2.06	0.74
2:A:500:NAD:O1N	4:A:449:HOH:O	2.06	0.74
1:D:319:THR:OG1	1:D:320:HIS:HD2	1.70	0.74
1:C:180:GLY:O	1:C:184:ILE:HG13	1.87	0.73
1:B:311:LYS:CD	1:B:311:LYS:CB	2.66	0.73
1:B:319:THR:OG1	1:B:320:HIS:HD2	1.70	0.73
1:B:67:HIS:CB	1:B:93:THR:HG21	2.18	0.72
1:B:47:HIS:HB3	1:B:52:ASN:ND2	2.03	0.72
1:C:68:GLU:OE1	1:C:342:LYS:NZ	2.22	0.72
1:A:224:PRO:CG	1:A:252:GLN:OE1	2.37	0.72
1:B:76:VAL:HG13	1:B:80:VAL:HB	1.71	0.72
1:D:5:MET:HE2	1:D:24:VAL:HA	1.71	0.71
1:C:289:HIS:CD2	4:D:492:HOH:O	2.31	0.71
1:B:113:ASN:HB3	1:B:114:THR:CA	2.20	0.71
1:C:171:THR:HG23	1:C:195:VAL:HG22	1.71	0.70
1:C:173:ILE:HD12	1:C:195:VAL:HG13	1.73	0.70
2:C:502:NAD:H4N	4:C:451:HOH:O	1.90	0.70
1:B:251:GLU:O	1:B:255:LYS:HG3	1.91	0.70
1:A:349:LYS:HE2	1:A:349:LYS:N	2.05	0.69
1:B:323:LYS:HB3	1:B:349:LYS:CB	2.21	0.68
1:C:259:PRO:HB3	1:D:110:VAL:HG12	1.76	0.68
1:C:46:LEU:HD11	1:C:336:ARG:HG2	1.73	0.68
1:C:171:THR:CG2	1:C:192:ALA:HB1	2.24	0.68
1:B:113:ASN:CB	1:B:114:THR:HA	2.24	0.68
2:D:503:NAD:C3D	4:D:634:HOH:O	2.40	0.67
1:B:67:HIS:HB2	1:B:93:THR:CG2	2.21	0.67
1:A:200:PRO:O	1:A:205:ARG:NH1	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:266:LEU:O	2:D:503:NAD:H2N	1.93	0.67
1:A:182:LEU:HD23	1:A:317:ILE:HD13	1.77	0.67
1:B:333:GLU:HG3	4:B:425:HOH:O	1.94	0.67
1:C:10:LYS:O	1:C:62:PRO:HA	1.95	0.67
2:A:500:NAD:H4N	4:A:404:HOH:O	1.95	0.66
1:B:244:SER:HA	2:B:501:NAD:H52A	1.78	0.66
2:D:503:NAD:O2N	4:D:443:HOH:O	2.14	0.66
1:A:321:LYS:HA	1:A:344:VAL:O	1.94	0.66
1:D:97:CYS:C	1:D:99:LYS:H	2.00	0.65
1:D:223:ASP:OD1	1:D:224:PRO:HD2	1.97	0.65
1:B:257:VAL:O	1:B:284:LYS:HE2	1.96	0.65
1:A:283:PHE:CE1	1:B:268:LEU:HD21	2.32	0.65
1:C:63:GLN:NE2	1:C:119:VAL:O	2.25	0.64
1:A:94:HIS:HE1	4:A:427:HOH:O	1.79	0.64
1:A:178:PRO:HD2	2:A:500:NAD:O2N	1.97	0.64
1:D:93:THR:N	1:D:152:GLU:OE2	2.27	0.64
1:C:38:ALA:HB3	1:C:145:PRO:O	1.97	0.64
1:C:51:TRP:HZ3	1:C:59:ILE:HG12	1.63	0.64
1:A:6:GLN:HB2	1:A:127:HIS:CE1	2.32	0.64
1:B:59:ILE:HD12	1:B:60:LYS:N	2.12	0.63
1:C:67:HIS:HB2	1:C:93:THR:HG21	1.81	0.63
1:A:318:ILE:HG23	1:A:344:VAL:HG23	1.81	0.62
1:C:15:TYR:OH	1:C:333:GLU:OE1	2.17	0.62
1:C:151:GLN:HG2	1:C:307:ILE:HD11	1.82	0.62
1:B:206:LYS:HE2	1:B:210:LYS:HE3	1.80	0.62
1:A:110:VAL:CG1	1:B:285:ALA:HB2	2.30	0.62
1:B:3:GLU:HA	4:B:388:HOH:O	2.00	0.62
2:B:501:NAD:H2D	4:B:446:HOH:O	2.00	0.61
1:A:52:ASN:O	1:A:56:GLN:HG3	2.01	0.61
1:B:266:LEU:O	2:B:501:NAD:H2N	2.00	0.61
1:A:222:GLU:HG3	1:A:223:ASP:N	2.14	0.61
1:B:115:LYS:O	1:B:116:ILE:HD13	2.00	0.61
1:A:82:ASP:OD2	1:C:99:LYS:HE2	2.01	0.60
1:C:51:TRP:CZ3	1:C:59:ILE:HG12	2.36	0.60
1:C:147:TYR:OH	1:C:315:ASP:OD1	2.14	0.60
1:B:328:PHE:O	1:B:332:PHE:HD2	1.85	0.60
1:D:267:GLY:HA2	2:D:503:NAD:H1D	1.83	0.60
1:B:97:CYS:SG	1:B:100:CYS:HB2	2.42	0.60
1:C:173:ILE:HD12	1:C:195:VAL:CG1	2.32	0.59
1:A:10:LYS:O	1:A:62:PRO:HA	2.02	0.59
1:C:46:LEU:HD11	1:C:336:ARG:CG	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:LEU:O	2:A:500:NAD:H2N	2.02	0.59
2:D:503:NAD:H3D	4:D:634:HOH:O	2.00	0.59
1:A:349:LYS:CE	1:A:349:LYS:N	2.56	0.59
1:C:276:ASP:OD2	1:C:279:ASN:HB2	2.02	0.59
1:C:166:ILE:HG12	1:C:192:ALA:HB2	1.85	0.58
1:D:52:ASN:O	1:D:56:GLN:HG3	2.02	0.58
1:C:7:ALA:O	1:C:19:LEU:HD12	2.04	0.58
2:D:503:NAD:O3D	4:D:634:HOH:O	2.17	0.58
1:A:20:VAL:HG12	1:A:22:VAL:HG13	1.84	0.58
1:C:342:LYS:HE3	4:C:385:HOH:O	2.03	0.58
1:B:95:ILE:O	1:B:114:THR:HG22	2.04	0.58
1:C:10:LYS:NZ	1:C:16:GLY:O	2.24	0.58
1:D:154:LEU:HD13	1:D:182:LEU:HG	1.85	0.58
1:A:13:PRO:O	1:A:51:TRP:CG	2.57	0.57
1:C:210:LYS:NZ	4:C:415:HOH:O	2.34	0.57
1:C:36:VAL:HG12	1:C:347:PRO:HG2	1.85	0.57
1:C:110:VAL:CG1	1:D:285:ALA:CB	2.80	0.57
1:A:68:GLU:OE1	1:A:342:LYS:NZ	2.37	0.57
1:C:42:CYS:HB3	1:C:68:GLU:OE2	2.04	0.57
1:A:81:GLU:O	1:A:82:ASP:CB	2.41	0.57
1:B:305:SER:O	1:B:309:SER:HB3	2.03	0.57
1:D:5:MET:CE	1:D:25:PRO:HD3	2.34	0.57
1:D:68:GLU:OE1	1:D:342:LYS:NZ	2.38	0.56
1:B:239:VAL:CG1	1:B:241:LEU:HD21	2.35	0.56
1:C:13:PRO:O	1:C:14:ALA:O	2.24	0.56
1:B:243:PHE:O	2:B:501:NAD:H51N	2.05	0.56
2:B:501:NAD:O5D	4:B:441:HOH:O	2.18	0.56
1:C:9:MET:HE1	4:C:399:HOH:O	2.05	0.56
1:A:224:PRO:HG2	1:A:252:GLN:OE1	2.05	0.56
1:D:10:LYS:O	1:D:62:PRO:HA	2.06	0.56
1:D:248:LYS:O	1:D:252:GLN:HG3	2.06	0.56
1:A:147:TYR:CD1	1:A:147:TYR:N	2.65	0.55
1:A:251:GLU:HG2	1:A:255:LYS:HE3	1.88	0.55
1:A:220:PHE:CD1	1:A:220:PHE:N	2.73	0.55
1:D:20:VAL:HG23	1:D:22:VAL:HG13	1.88	0.55
1:D:48:ILE:HG23	1:D:59:ILE:HD11	1.88	0.55
1:A:217:VAL:HB	1:A:227:PHE:CD2	2.42	0.55
1:C:171:THR:CG2	1:C:195:VAL:HG22	2.37	0.55
1:C:179:LEU:HD12	2:C:502:NAD:C4D	2.35	0.55
1:C:325:PHE:O	1:C:328:PHE:HB3	2.07	0.55
1:D:42:CYS:SG	1:D:67:HIS:CE1	2.99	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:GLU:OE2	1:B:336:ARG:HG2	2.08	0.54
1:A:41:ILE:O	4:A:561:HOH:O	2.18	0.54
1:B:179:LEU:HD11	4:B:542:HOH:O	2.06	0.54
1:B:240:PHE:CZ	1:B:253:GLY:HA3	2.42	0.54
1:A:127:HIS:CD2	1:A:347:PRO:O	2.59	0.54
1:C:156:ASN:O	1:C:160:THR:HG23	2.07	0.54
1:A:97:CYS:HB3	1:A:100:CYS:SG	2.48	0.54
1:C:98:GLY:HA2	1:C:103:CYS:HB3	1.89	0.54
1:C:348:HIS:O	1:C:349:LYS:CG	2.56	0.54
1:B:156:ASN:HB2	1:B:179:LEU:CD2	2.37	0.54
1:D:171:THR:HB	1:D:239:VAL:HB	1.90	0.54
1:C:319:THR:OG1	1:C:320:HIS:HD2	1.91	0.53
1:C:115:LYS:H	1:C:115:LYS:HD2	1.73	0.53
1:B:59:ILE:HD12	1:B:59:ILE:C	2.28	0.53
1:B:295:HIS:HB2	1:B:299:THR:OG1	2.08	0.53
1:D:199:GLU:O	1:D:205:ARG:HD3	2.09	0.53
1:C:51:TRP:NE1	1:C:56:GLN:HG2	2.25	0.52
1:D:96:VAL:HG21	4:D:421:HOH:O	2.09	0.52
1:D:42:CYS:SG	1:D:67:HIS:HE1	2.33	0.52
2:B:501:NAD:N6A	4:B:414:HOH:O	2.24	0.52
1:D:200:PRO:HD2	2:D:503:NAD:H1B	1.91	0.52
1:A:348:HIS:O	1:A:349:LYS:C	2.47	0.52
1:B:10:LYS:O	1:B:62:PRO:HA	2.10	0.52
1:C:151:GLN:HG2	1:C:307:ILE:CD1	2.39	0.52
1:D:42:CYS:CB	1:D:45:ASP:OD2	2.57	0.52
1:C:319:THR:OG1	1:C:320:HIS:CD2	2.62	0.52
1:D:271:ARG:HG3	4:D:610:HOH:O	2.08	0.52
1:A:250:LEU:HD23	1:A:273:VAL:HG11	1.92	0.52
1:B:240:PHE:O	1:B:263:VAL:HA	2.09	0.52
1:A:268:LEU:HD21	1:B:283:PHE:CE1	2.45	0.51
1:B:47:HIS:HB3	1:B:52:ASN:HD21	1.72	0.51
1:D:321:LYS:HB3	1:D:346:PHE:HE1	1.75	0.51
1:C:39:THR:HA	1:C:68:GLU:O	2.11	0.51
1:A:182:LEU:HD23	1:A:317:ILE:CD1	2.39	0.51
1:B:180:GLY:O	1:B:184:ILE:HG13	2.11	0.51
1:A:294:ARG:O	1:A:296:LEU:HD13	2.11	0.51
1:C:110:VAL:CG1	1:D:285:ALA:HB3	2.31	0.51
1:D:102:ALA:O	1:D:107:ARG:HB2	2.11	0.51
1:A:92:GLU:OE2	1:A:294:ARG:NH2	2.38	0.51
1:B:39:THR:HA	1:B:68:GLU:O	2.11	0.51
1:C:114:THR:HG22	1:C:115:LYS:HD2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:THR:O	1:A:243:PHE:HB2	2.11	0.50
1:C:273:VAL:HG12	1:C:274:THR:N	2.26	0.50
1:D:6:GLN:O	1:D:126:ALA:HA	2.11	0.50
1:C:13:PRO:HD3	1:C:61:PRO:HG2	1.93	0.50
1:D:5:MET:HE1	1:D:25:PRO:CD	2.41	0.50
1:A:94:HIS:CE1	4:A:427:HOH:O	2.57	0.50
1:C:78:PRO:HA	3:C:351:SO4:O2	2.12	0.50
1:D:5:MET:CE	1:D:25:PRO:CD	2.89	0.50
1:A:92:GLU:O	1:A:135:ASN:OD1	2.29	0.50
1:B:199:GLU:OE2	1:B:201:SER:N	2.43	0.50
1:A:6:GLN:HB2	1:A:127:HIS:HE1	1.77	0.50
1:B:92:GLU:OE2	1:B:294:ARG:NH2	2.33	0.50
1:C:96:VAL:O	1:C:97:CYS:CB	2.59	0.50
1:D:199:GLU:HB3	1:D:205:ARG:HG2	1.94	0.50
1:C:174:THR:HG22	1:C:198:SER:HB3	1.94	0.49
1:A:180:GLY:O	1:A:184:ILE:HG13	2.12	0.49
1:B:92:GLU:HG2	1:B:296:LEU:HD11	1.92	0.49
1:C:109:HIS:H	1:C:109:HIS:CD2	2.30	0.49
1:A:69:VAL:HG13	1:A:124:VAL:HG21	1.93	0.49
1:C:282:ILE:CG2	2:D:503:NAD:H72N	2.25	0.49
1:D:113:ASN:ND2	1:D:115:LYS:H	2.10	0.49
1:C:11:THR:OG1	1:C:18:GLU:HG3	2.12	0.49
1:B:105:HIS:O	1:B:106:ASN:HB2	2.13	0.49
1:C:287:GLU:HB3	4:C:354:HOH:O	2.12	0.49
1:B:25:PRO:HB2	1:B:130:ILE:HG12	1.94	0.49
1:B:193:TYR:C	1:B:193:TYR:CD2	2.85	0.49
1:C:227:PHE:CE2	1:C:231:ILE:HD11	2.48	0.49
1:A:36:VAL:HG13	1:A:69:VAL:HG12	1.95	0.49
1:B:150:LEU:HD22	1:B:342:LYS:HD3	1.95	0.49
1:C:41:ILE:HG22	1:C:45:ASP:HB2	1.95	0.49
1:C:296:LEU:HA	1:C:297:TRP:HA	1.48	0.49
1:D:51:TRP:CZ3	1:D:59:ILE:HG12	2.48	0.49
1:C:73:VAL:HG23	1:C:87:ASP:O	2.14	0.48
1:C:259:PRO:CB	1:D:110:VAL:CG1	2.74	0.48
1:C:32:VAL:HG12	1:C:76:VAL:HG22	1.94	0.48
1:C:172:LEU:HD22	1:C:228:VAL:HG21	1.95	0.48
1:A:201:SER:HB3	1:A:204:ARG:HB2	1.95	0.48
1:A:281:ILE:HG13	1:A:282:ILE:N	2.26	0.48
1:B:50:GLU:O	1:B:51:TRP:HB3	2.13	0.48
1:B:246:ALA:O	1:B:249:ALA:N	2.47	0.48
1:D:272:GLU:O	4:D:610:HOH:O	2.19	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:HIS:O	1:A:96:VAL:HG13	2.14	0.48
1:C:20:VAL:HG23	1:C:22:VAL:HG13	1.96	0.48
1:C:348:HIS:O	1:C:349:LYS:HG3	2.13	0.48
1:B:253:GLY:O	1:B:256:ALA:HB3	2.13	0.48
1:D:48:ILE:HG23	1:D:59:ILE:CD1	2.43	0.47
1:D:166:ILE:HD11	1:D:171:THR:HG21	1.96	0.47
1:D:171:THR:CG2	1:D:192:ALA:HB1	2.43	0.47
1:C:243:PHE:CD1	1:C:266:LEU:HD23	2.49	0.47
1:B:204:ARG:HH12	2:B:501:NAD:C3B	2.28	0.47
1:D:150:LEU:O	1:D:154:LEU:HB2	2.15	0.47
1:D:219:PRO:HB3	1:D:224:PRO:HG3	1.96	0.47
1:A:268:LEU:CD2	1:B:283:PHE:CE1	2.98	0.47
1:B:117:PHE:HE2	1:B:124:VAL:HG13	1.80	0.47
1:C:80:VAL:O	1:C:82:ASP:N	2.41	0.47
1:C:110:VAL:CG1	1:D:285:ALA:HB2	2.45	0.47
1:C:161:VAL:HG13	1:C:166:ILE:HD13	1.97	0.47
1:C:95:ILE:HG12	1:C:135:ASN:OD1	2.15	0.47
1:D:59:ILE:HG23	1:D:59:ILE:HD13	1.42	0.47
1:B:160:THR:OG1	1:B:291:ILE:HG21	2.15	0.46
1:C:160:THR:HG22	1:C:291:ILE:HG21	1.96	0.46
1:D:107:ARG:HB3	1:D:110:VAL:HG23	1.97	0.46
1:C:67:HIS:HB2	1:C:93:THR:CG2	2.45	0.46
1:C:169:ARG:HG2	1:C:238:GLU:HG2	1.95	0.46
1:A:40:SER:HB3	1:A:68:GLU:OE1	2.16	0.46
1:A:296:LEU:HA	1:A:297:TRP:HA	1.66	0.46
1:B:219:PRO:HB3	1:B:224:PRO:HG3	1.96	0.46
1:C:197:VAL:O	1:C:216:VAL:HA	2.15	0.46
1:D:51:TRP:HZ3	1:D:59:ILE:HG12	1.80	0.46
2:D:503:NAD:H6N	2:D:503:NAD:H2D	1.79	0.46
1:A:39:THR:HA	1:A:68:GLU:O	2.15	0.46
1:A:250:LEU:O	1:A:251:GLU:C	2.52	0.46
1:B:15:TYR:CD1	1:B:50:GLU:HA	2.51	0.46
1:A:218:ASN:CG	1:A:221:GLU:HB3	2.36	0.46
1:A:298:GLU:OE1	1:C:106:ASN:ND2	2.45	0.46
1:B:115:LYS:HD3	1:B:120:ASP:HB3	1.98	0.46
1:C:330:GLU:O	1:C:334:LEU:HG	2.15	0.46
1:B:93:THR:HG22	1:B:117:PHE:HB3	1.98	0.46
1:B:200:PRO:HA	1:B:218:ASN:OD1	2.16	0.46
1:C:15:TYR:CD2	1:C:16:GLY:N	2.84	0.46
1:D:46:LEU:HD11	1:D:336:ARG:HG3	1.97	0.46
1:B:3:GLU:CA	4:B:388:HOH:O	2.62	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:39:THR:CG2	1:D:345:PHE:HB2	2.45	0.46
1:D:51:TRP:NE1	1:D:56:GLN:HG2	2.31	0.46
1:D:109:HIS:CD2	1:D:109:HIS:H	2.32	0.46
1:A:109:HIS:CD2	1:A:109:HIS:H	2.34	0.45
1:D:96:VAL:CG2	4:D:421:HOH:O	2.62	0.45
1:B:32:VAL:HG21	1:B:83:LEU:HD13	1.98	0.45
1:B:47:HIS:CB	1:B:52:ASN:ND2	2.78	0.45
1:C:69:VAL:CG1	1:C:91:VAL:HG23	2.46	0.45
1:D:127:HIS:O	1:D:348:HIS:HE1	1.99	0.45
1:A:99:LYS:CD	1:A:104:LYS:HE2	2.46	0.45
1:B:6:GLN:HB2	1:B:127:HIS:CE1	2.52	0.45
1:B:52:ASN:OD1	1:B:52:ASN:C	2.54	0.45
1:D:188:LYS:HD2	1:D:188:LYS:HA	1.55	0.45
1:A:69:VAL:HG13	1:A:124:VAL:CG2	2.46	0.45
1:A:317:ILE:O	1:A:342:LYS:N	2.41	0.45
2:A:500:NAD:H8A	2:A:500:NAD:H2B	1.84	0.45
1:B:93:THR:HG22	1:B:117:PHE:CB	2.46	0.45
1:C:160:THR:HB	1:C:291:ILE:HG13	1.99	0.45
1:D:157:ALA:HB1	1:D:183:GLY:HA2	1.97	0.45
1:A:146:GLU:HG2	1:A:147:TYR:H	1.80	0.45
1:B:6:GLN:O	1:B:126:ALA:HA	2.17	0.45
1:C:13:PRO:O	1:C:14:ALA:C	2.54	0.45
1:A:59:ILE:O	1:A:61:PRO:HD3	2.17	0.45
1:B:289:HIS:CD2	4:B:495:HOH:O	2.34	0.45
1:B:296:LEU:N	1:B:296:LEU:HD23	2.31	0.45
1:D:26:LYS:HB2	1:D:26:LYS:HE3	1.77	0.45
1:D:42:CYS:HB3	1:D:45:ASP:OD2	2.15	0.45
1:B:104:LYS:O	1:D:297:TRP:HB2	2.17	0.45
1:D:59:ILE:HG21	1:D:59:ILE:HD12	1.42	0.45
1:B:333:GLU:CD	4:B:425:HOH:O	2.55	0.44
1:B:50:GLU:O	1:B:51:TRP:CB	2.63	0.44
1:C:238:GLU:OE2	1:D:101:TYR:OH	2.34	0.44
1:D:339:LYS:HG2	4:D:546:HOH:O	2.16	0.44
1:D:53:GLU:CD	1:D:53:GLU:H	2.20	0.44
1:B:51:TRP:HZ3	1:B:59:ILE:HG13	1.83	0.44
1:C:42:CYS:SG	1:C:67:HIS:NE2	2.91	0.44
1:D:240:PHE:CZ	1:D:253:GLY:HA3	2.53	0.44
1:A:146:GLU:HG2	1:A:147:TYR:N	2.32	0.44
1:B:47:HIS:CG	1:B:52:ASN:ND2	2.86	0.44
1:D:179:LEU:HA	1:D:179:LEU:HD23	1.78	0.44
1:B:271:ARG:HA	3:B:355:SO4:O2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:58:ARG:HH22	1:C:116:ILE:HD12	1.83	0.44
1:A:51:TRP:NE1	1:A:56:GLN:HG2	2.32	0.44
1:B:68:GLU:OE1	1:B:342:LYS:NZ	2.47	0.43
1:B:97:CYS:HB3	1:B:111:CYS:HB3	1.74	0.43
1:A:184:ILE:O	1:A:184:ILE:HG22	2.19	0.43
1:C:46:LEU:HB2	1:C:335:MET:HE1	1.99	0.43
1:D:34:ILE:HG21	1:D:89:ILE:HD11	2.00	0.43
1:D:207:LEU:O	1:D:211:VAL:HG23	2.19	0.43
1:B:115:LYS:CD	1:B:120:ASP:HB3	2.49	0.43
1:B:296:LEU:HA	1:B:297:TRP:HA	1.79	0.43
1:B:348:HIS:HD2	4:B:411:HOH:O	2.01	0.43
1:C:166:ILE:O	1:C:169:ARG:HB2	2.18	0.43
1:A:204:ARG:NH1	2:A:500:NAD:O3B	2.46	0.43
1:B:248:LYS:O	1:B:252:GLN:HG3	2.18	0.43
1:C:199:GLU:O	1:C:205:ARG:HD3	2.18	0.43
1:A:349:LYS:H	1:A:349:LYS:CD	2.22	0.43
1:B:243:PHE:CD1	1:B:266:LEU:HD23	2.54	0.43
1:B:127:HIS:O	1:B:348:HIS:HE1	2.01	0.43
1:B:266:LEU:HD12	2:B:501:NAD:N7N	2.33	0.43
1:B:199:GLU:OE1	2:B:501:NAD:H1B	2.19	0.43
1:D:319:THR:CB	1:D:320:HIS:HD2	2.31	0.43
1:A:182:LEU:O	1:A:185:ALA:HB3	2.19	0.42
1:A:224:PRO:HG3	1:A:252:GLN:OE1	2.16	0.42
1:B:325:PHE:O	1:B:328:PHE:HB3	2.19	0.42
1:C:41:ILE:CG2	1:C:45:ASP:HB2	2.49	0.42
1:D:39:THR:O	1:D:39:THR:HG23	2.19	0.42
1:B:337:ALA:HB1	1:B:339:LYS:HE2	2.01	0.42
1:D:92:GLU:O	1:D:135:ASN:OD1	2.37	0.42
1:D:130:ILE:HA	1:D:130:ILE:HD13	1.72	0.42
1:B:3:GLU:N	4:B:388:HOH:O	2.51	0.42
1:B:156:ASN:HB2	1:B:179:LEU:HD22	2.02	0.42
1:C:160:THR:HG21	1:C:266:LEU:HD22	2.00	0.42
1:A:278:ASN:ND2	1:B:269:PHE:O	2.45	0.42
1:C:276:ASP:HB2	1:D:272:GLU:HG2	2.01	0.42
1:C:321:LYS:HA	1:C:344:VAL:O	2.19	0.42
1:D:69:VAL:O	1:D:69:VAL:CG1	2.67	0.42
1:B:130:ILE:HD13	1:B:130:ILE:HA	1.76	0.42
1:B:141:LYS:HA	1:B:141:LYS:HD3	1.90	0.42
1:C:26:LYS:O	1:C:27:PRO:C	2.55	0.42
1:C:274:THR:OG1	1:D:274:THR:OG1	2.17	0.42
1:C:278:ASN:ND2	1:D:269:PHE:O	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:250:LEU:HD23	1:D:273:VAL:HG11	2.02	0.42
1:C:156:ASN:O	1:C:160:THR:CG2	2.67	0.42
1:C:197:VAL:HG23	1:C:213:ALA:HB1	2.01	0.42
1:A:42:CYS:SG	1:A:67:HIS:NE2	2.92	0.42
1:B:349:LYS:HB3	1:B:349:LYS:HE3	1.61	0.42
1:D:97:CYS:C	1:D:99:LYS:N	2.65	0.42
1:D:147:TYR:N	1:D:147:TYR:CD1	2.80	0.42
1:D:324:GLY:HA3	1:D:349:LYS:HE3	2.02	0.42
1:B:152:GLU:HG2	1:B:294:ARG:CZ	2.50	0.42
1:C:320:HIS:CD2	1:C:340:THR:HG22	2.55	0.42
1:B:287:GLU:OE1	1:B:289:HIS:HE1	2.03	0.41
1:C:224:PRO:O	1:C:227:PHE:HB3	2.20	0.41
1:C:290:GLY:HA3	1:D:281:ILE:O	2.20	0.41
1:D:15:TYR:CD1	1:D:50:GLU:HA	2.55	0.41
1:C:33:LEU:HD11	1:C:128:TYR:HB3	2.01	0.41
1:D:51:TRP:HZ3	1:D:59:ILE:CG1	2.33	0.41
1:A:285:ALA:HA	1:B:290:GLY:O	2.20	0.41
1:A:207:LEU:HD23	1:A:207:LEU:HA	1.79	0.41
1:B:188:LYS:HA	1:B:188:LYS:HD2	1.81	0.41
1:B:156:ASN:CB	1:B:179:LEU:HD22	2.51	0.41
1:B:204:ARG:NH1	2:B:501:NAD:C3B	2.78	0.41
1:D:48:ILE:HG12	1:D:59:ILE:CD1	2.51	0.41
1:D:179:LEU:HD12	2:D:503:NAD:H4D	2.03	0.41
1:A:64:ILE:HB	1:A:122:ASP:HB3	2.03	0.41
1:B:34:ILE:HG21	1:B:89:ILE:HD11	2.02	0.41
1:B:46:LEU:O	1:B:46:LEU:HD12	2.21	0.41
1:B:93:THR:CG2	1:B:117:PHE:HB3	2.50	0.41
1:B:200:PRO:O	1:B:205:ARG:NH1	2.51	0.41
1:C:20:VAL:CG2	1:C:22:VAL:HG13	2.50	0.41
1:D:17:ALA:HB3	1:D:328:PHE:CE2	2.56	0.41
1:D:26:LYS:HA	1:D:27:PRO:HD2	1.87	0.41
1:D:242:GLU:HB3	4:D:362:HOH:O	2.20	0.41
1:C:103:CYS:SG	1:C:108:TYR:CD1	3.14	0.41
1:A:42:CYS:HB3	1:A:68:GLU:OE2	2.21	0.40
1:A:76:VAL:HG13	1:A:80:VAL:HB	2.03	0.40
1:A:248:LYS:O	1:A:252:GLN:HG3	2.20	0.40
1:B:18:GLU:HB3	1:B:20:VAL:HG12	2.02	0.40
1:B:197:VAL:O	1:B:216:VAL:HA	2.21	0.40
1:A:51:TRP:CZ3	1:A:59:ILE:HG13	2.57	0.40
1:A:218:ASN:ND2	1:A:221:GLU:HB3	2.36	0.40
1:D:5:MET:HE1	1:D:25:PRO:HD2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:206:LYS:NZ	1:D:210:LYS:HE2	2.35	0.40
1:B:16:GLY:HA2	1:B:49:TYR:CE1	2.56	0.40
1:B:199:GLU:OE2	1:B:200:PRO:HD2	2.21	0.40
1:C:48:ILE:HG12	1:C:59:ILE:HG21	2.03	0.40
1:C:134:LYS:HG2	4:C:379:HOH:O	2.21	0.40
1:A:127:HIS:NE2	1:A:347:PRO:O	2.55	0.40
1:B:44:THR:O	1:B:48:ILE:HG13	2.21	0.40
1:B:147:TYR:O	1:B:148:ALA:C	2.59	0.40
1:B:169:ARG:HH11	1:B:169:ARG:HD3	1.68	0.40
1:B:326:ASP:HB2	4:B:393:HOH:O	2.20	0.40
1:C:179:LEU:HD11	2:C:502:NAD:H6N	2.03	0.40
1:C:6:GLN:HB2	1:C:127:HIS:CE1	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	345/350 (99%)	313 (91%)	21 (6%)	11 (3%)	4	3
1	B	345/350 (99%)	308 (89%)	31 (9%)	6 (2%)	9	11
1	C	345/350 (99%)	311 (90%)	26 (8%)	8 (2%)	6	7
1	D	345/350 (99%)	312 (90%)	27 (8%)	6 (2%)	9	11
All	All	1380/1400 (99%)	1244 (90%)	105 (8%)	31 (2%)	6	7

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	14	ALA
1	A	97	CYS
1	B	97	CYS

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Mol	Chain	Res	Type
1	B	271	ARG
1	C	13	PRO
1	C	14	ALA
1	C	97	CYS
1	C	115	LYS
1	D	96	VAL
1	D	98	GLY
1	A	43	GLY
1	A	114	THR
1	A	220	PHE
1	B	52	ASN
1	B	272	GLU
1	C	98	GLY
1	C	233	ASP
1	A	82	ASP
1	A	233	ASP
1	B	276	ASP
1	C	95	ILE
1	A	150	LEU
1	B	337	ALA
1	A	213	ALA
1	C	96	VAL
1	D	336	ARG
1	A	232	THR
1	D	112	GLN
1	D	212	GLY
1	A	341	GLY
1	D	124	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	283/284 (100%)	262 (93%)	21 (7%)	13	22
1	B	283/284 (100%)	258 (91%)	25 (9%)	10	15
1	C	283/284 (100%)	258 (91%)	25 (9%)	10	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	283/284 (100%)	257 (91%)	26 (9%)	9	13
All	All	1132/1136 (100%)	1035 (91%)	97 (9%)	10	16

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LYS
1	A	26	LYS
1	A	33	LEU
1	A	40	SER
1	A	59	ILE
1	A	60	LYS
1	A	69	VAL
1	A	76	VAL
1	A	85	VAL
1	A	97	CYS
1	A	210	LYS
1	A	221	GLU
1	A	222	GLU
1	A	242	GLU
1	A	271	ARG
1	A	281	ILE
1	A	305	SER
1	A	321	LYS
1	A	335	MET
1	A	339	LYS
1	A	349	LYS
1	B	20	VAL
1	B	33	LEU
1	B	40	SER
1	B	57	SER
1	B	59	ILE
1	B	60	LYS
1	B	69	VAL
1	B	97	CYS
1	B	111	CYS
1	B	117	PHE
1	B	134	LYS
1	B	152	GLU
1	B	210	LYS
1	B	216	VAL
1	B	226	LYS

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Mol	Chain	Res	Type
1	B	233	ASP
1	B	242	GLU
1	B	257	VAL
1	B	271	ARG
1	B	305	SER
1	B	306	LEU
1	B	333	GLU
1	B	335	MET
1	B	342	LYS
1	B	349	LYS
1	C	12	LYS
1	C	13	PRO
1	C	20	VAL
1	C	41	ILE
1	C	59	ILE
1	C	69	VAL
1	C	99	LYS
1	C	114	THR
1	C	134	LYS
1	C	141	LYS
1	C	160	THR
1	C	169	ARG
1	C	171	THR
1	C	202	GLU
1	C	206	LYS
1	C	221	GLU
1	C	230	ASP
1	C	238	GLU
1	C	242	GLU
1	C	271	ARG
1	C	304	SER
1	C	305	SER
1	C	321	LYS
1	C	339	LYS
1	C	342	LYS
1	D	10	LYS
1	D	41	ILE
1	D	53	GLU
1	D	57	SER
1	D	59	ILE
1	D	60	LYS
1	D	69	VAL

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Mol	Chain	Res	Type
1	D	76	VAL
1	D	84	GLN
1	D	97	CYS
1	D	110	VAL
1	D	112	GLN
1	D	114	THR
1	D	117	PHE
1	D	120	ASP
1	D	154	LEU
1	D	171	THR
1	D	182	LEU
1	D	206	LYS
1	D	210	LYS
1	D	226	LYS
1	D	233	ASP
1	D	242	GLU
1	D	258	THR
1	D	305	SER
1	D	336	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	HIS
1	A	135	ASN
1	A	139	ASN
1	A	151	GLN
1	A	156	ASN
1	A	289	HIS
1	A	308	GLN
1	A	348	HIS
1	B	94	HIS
1	B	106	ASN
1	B	113	ASN
1	B	139	ASN
1	B	151	GLN
1	B	289	HIS
1	B	320	HIS
1	B	348	HIS
1	C	94	HIS
1	C	109	HIS
1	C	139	ASN

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Mol	Chain	Res	Type
1	C	151	GLN
1	C	289	HIS
1	C	308	GLN
1	C	320	HIS
1	D	47	HIS
1	D	67	HIS
1	D	109	HIS
1	D	112	GLN
1	D	113	ASN
1	D	135	ASN
1	D	156	ASN
1	D	308	GLN
1	D	320	HIS
1	D	348	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

14 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
3	SO4	B	354	-	4,4,4	0.76	0	6,6,6	1.12	1 (16%)
2	NAD	D	503	-	42,48,48	2.35	10 (23%)	50,73,73	2.04	21 (42%)
2	NAD	A	500	-	42,48,48	1.59	7 (16%)	50,73,73	2.10	14 (28%)
3	SO4	B	355	-	4,4,4	0.51	0	6,6,6	0.82	0
3	SO4	C	351	-	4,4,4	0.13	0	6,6,6	0.46	0
2	NAD	C	502	-	42,48,48	2.32	9 (21%)	50,73,73	3.03	20 (40%)
3	SO4	D	351	-	4,4,4	0.13	0	6,6,6	0.60	0
3	SO4	B	353	-	4,4,4	2.97	2 (50%)	6,6,6	0.88	0
3	SO4	C	352	-	4,4,4	0.25	0	6,6,6	0.09	0
3	SO4	D	352	-	4,4,4	0.49	0	6,6,6	1.00	1 (16%)
2	NAD	B	501	-	42,48,48	2.96	8 (19%)	50,73,73	2.55	16 (32%)
3	SO4	B	351	-	4,4,4	2.31	1 (25%)	6,6,6	1.52	1 (16%)
3	SO4	B	352	-	4,4,4	1.52	1 (25%)	6,6,6	1.20	1 (16%)
3	SO4	C	353	-	4,4,4	0.42	0	6,6,6	1.13	1 (16%)

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	A	500	-	2/2/11/11	9/26/62/62	0/5/5/5
2	NAD	C	502	-	2/2/11/11	9/26/62/62	0/5/5/5
2	NAD	B	501	-	2/2/11/11	13/26/62/62	0/5/5/5
2	NAD	D	503	-	2/2/11/11	11/26/62/62	0/5/5/5

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	NAD	O4D-C1D	15.08	1.62	1.41
2	C	502	NAD	O4D-C1D	11.00	1.56	1.41
2	D	503	NAD	O4D-C1D	9.43	1.54	1.41
2	B	501	NAD	C2N-N1N	6.01	1.42	1.35
2	D	503	NAD	C2B-C1B	5.50	1.62	1.53
3	B	353	SO4	O1-S	5.00	1.73	1.46
2	A	500	NAD	O4D-C1D	4.43	1.47	1.41
2	B	501	NAD	C3N-C7N	4.13	1.56	1.50
2	B	501	NAD	C2B-C1B	4.05	1.59	1.53
2	D	503	NAD	C2N-N1N	3.96	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	351	SO4	O1-S	3.96	1.67	1.46
2	C	502	NAD	O4D-C4D	-3.95	1.36	1.45
2	C	502	NAD	C2B-C1B	3.51	1.59	1.53
2	B	501	NAD	PA-O1A	3.33	1.62	1.50
2	C	502	NAD	PN-O5D	-3.32	1.45	1.59
2	D	503	NAD	C3N-C7N	-3.30	1.45	1.50
2	D	503	NAD	PN-O1N	3.21	1.62	1.50
2	A	500	NAD	PN-O5D	-3.19	1.46	1.59
2	A	500	NAD	PA-O1A	3.05	1.61	1.50
2	A	500	NAD	O4D-C4D	-3.02	1.38	1.45
2	D	503	NAD	C5B-C4B	3.00	1.61	1.51
2	C	502	NAD	O4B-C1B	2.82	1.45	1.41
2	D	503	NAD	C2D-C3D	-2.81	1.45	1.53
3	B	353	SO4	O4-S	2.78	1.70	1.47
2	D	503	NAD	O2B-C2B	2.74	1.49	1.43
2	B	501	NAD	O4B-C1B	-2.68	1.37	1.41
2	A	500	NAD	C2D-C1D	2.65	1.57	1.53
2	B	501	NAD	C4A-N3A	2.61	1.39	1.35
2	D	503	NAD	C6N-N1N	2.53	1.41	1.35
2	D	503	NAD	O4D-C4D	-2.51	1.39	1.45
2	C	502	NAD	C2N-N1N	2.32	1.37	1.35
2	C	502	NAD	C2A-N1A	-2.21	1.29	1.33
2	A	500	NAD	C5B-C4B	2.14	1.58	1.51
2	B	501	NAD	O2D-C2D	-2.13	1.38	1.43
2	C	502	NAD	O2B-C2B	2.11	1.47	1.43
3	B	352	SO4	O2-S	2.11	1.57	1.46
2	A	500	NAD	C2B-C1B	2.08	1.56	1.53
2	C	502	NAD	O7N-C7N	2.04	1.28	1.24

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	502	NAD	C3N-C7N-N7N	-10.57	105.07	117.75
2	B	501	NAD	C6N-N1N-C2N	-8.51	114.22	121.97
2	C	502	NAD	C6N-N1N-C2N	-8.22	114.48	121.97
2	C	502	NAD	N3A-C2A-N1A	-7.48	116.99	128.68
2	B	501	NAD	C3N-C2N-N1N	6.14	126.43	120.43
2	B	501	NAD	N3A-C2A-N1A	-6.13	119.10	128.68
2	C	502	NAD	O7N-C7N-C3N	5.25	125.92	119.63
2	A	500	NAD	N3A-C2A-N1A	-5.21	120.54	128.68
2	A	500	NAD	O2D-C2D-C3D	-5.12	95.27	111.82
2	C	502	NAD	O2D-C2D-C3D	-4.84	96.15	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	501	NAD	O5D-PN-O1N	-4.61	91.05	109.07
2	B	501	NAD	C6N-C5N-C4N	4.61	126.14	119.44
2	D	503	NAD	N3A-C2A-N1A	-4.56	121.55	128.68
2	C	502	NAD	O7N-C7N-N7N	4.47	128.93	122.58
2	A	500	NAD	C3N-C7N-N7N	-4.29	112.60	117.75
2	A	500	NAD	C6N-N1N-C2N	-4.25	118.10	121.97
2	C	502	NAD	O4D-C4D-C5D	4.10	122.86	109.37
2	B	501	NAD	O2D-C2D-C3D	-4.03	98.78	111.82
2	C	502	NAD	C3N-C2N-N1N	4.01	124.35	120.43
2	C	502	NAD	C5N-C4N-C3N	-3.88	115.75	120.34
2	A	500	NAD	PN-O3-PA	-3.81	119.74	132.83
2	D	503	NAD	C2N-C3N-C4N	3.78	122.55	118.26
2	A	500	NAD	C2D-C3D-C4D	-3.66	95.52	102.64
2	D	503	NAD	O5D-C5D-C4D	-3.58	96.67	108.99
2	D	503	NAD	C3N-C7N-N7N	-3.51	113.54	117.75
2	C	502	NAD	C5D-C4D-C3D	-3.50	102.06	115.18
2	A	500	NAD	O4B-C4B-C3B	-3.47	98.26	105.11
2	A	500	NAD	O5D-C5D-C4D	-3.46	97.08	108.99
2	B	501	NAD	O4B-C4B-C3B	-3.32	98.54	105.11
2	B	501	NAD	C5N-C4N-C3N	-3.31	116.43	120.34
2	B	501	NAD	C3N-C7N-N7N	-3.30	113.78	117.75
2	B	501	NAD	C2A-N1A-C6A	3.25	124.31	118.75
2	D	503	NAD	N6A-C6A-N1A	3.21	125.23	118.57
2	D	503	NAD	O3D-C3D-C2D	-3.16	101.58	111.82
2	B	501	NAD	O3D-C3D-C2D	-3.16	101.60	111.82
2	D	503	NAD	O2D-C2D-C3D	-3.10	101.80	111.82
2	D	503	NAD	O4D-C4D-C5D	3.05	119.41	109.37
2	B	501	NAD	PN-O3-PA	-2.95	122.69	132.83
2	D	503	NAD	C2D-C3D-C4D	-2.90	97.01	102.64
2	D	503	NAD	C5A-C6A-N6A	-2.89	115.96	120.35
2	C	502	NAD	O3B-C3B-C2B	-2.67	103.19	111.82
2	B	501	NAD	O5B-PA-O1A	-2.63	98.79	109.07
2	A	500	NAD	N6A-C6A-N1A	2.61	123.99	118.57
2	C	502	NAD	PN-O3-PA	-2.60	123.91	132.83
2	C	502	NAD	C2D-C3D-C4D	-2.58	97.63	102.64
2	A	500	NAD	O4B-C1B-C2B	-2.51	103.26	106.93
2	A	500	NAD	O7N-C7N-C3N	2.50	122.62	119.63
2	D	503	NAD	C5N-C6N-N1N	-2.45	116.89	120.40
2	D	503	NAD	C2N-N1N-C1D	-2.43	113.73	119.14
3	B	351	SO4	O3-S-O2	-2.37	96.92	109.31
2	D	503	NAD	C5N-C4N-C3N	-2.36	117.55	120.34
2	C	502	NAD	O4D-C1D-C2D	-2.33	103.52	106.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	502	NAD	O5D-C5D-C4D	-2.32	101.01	108.99
3	B	352	SO4	O4-S-O3	2.31	118.94	109.06
2	C	502	NAD	C6N-C5N-C4N	2.29	122.77	119.44
2	A	500	NAD	C5N-C4N-C3N	-2.29	117.64	120.34
2	D	503	NAD	O2N-PN-O5D	-2.27	97.21	107.75
2	A	500	NAD	O3D-C3D-C2D	-2.23	104.62	111.82
2	D	503	NAD	O2B-C2B-C1B	2.23	119.07	110.85
2	D	503	NAD	PA-O5B-C5B	2.22	134.68	121.68
2	B	501	NAD	O3B-C3B-C4B	-2.22	104.64	111.05
3	B	354	SO4	O3-S-O1	-2.21	97.77	109.31
2	D	503	NAD	C2N-C3N-C7N	-2.20	113.07	119.46
2	D	503	NAD	O4B-C4B-C3B	-2.16	100.83	105.11
2	C	502	NAD	O2A-PA-O5B	2.16	117.80	107.75
2	B	501	NAD	O7N-C7N-C3N	2.16	122.22	119.63
3	C	353	SO4	O4-S-O2	2.13	120.44	109.31
2	D	503	NAD	O7N-C7N-N7N	2.12	125.59	122.58
2	C	502	NAD	C2N-C3N-C4N	2.12	120.66	118.26
2	D	503	NAD	C6N-C5N-C4N	2.10	122.49	119.44
3	D	352	SO4	O3-S-O1	2.08	120.14	109.31
2	C	502	NAD	O5B-PA-O1A	-2.05	101.05	109.07
2	B	501	NAD	C3D-C2D-C1D	2.05	104.06	100.98
2	D	503	NAD	O2N-PN-O1N	2.04	122.34	112.24
2	C	502	NAD	C2A-N1A-C6A	2.01	122.19	118.75
2	A	500	NAD	C3N-C2N-N1N	2.00	122.39	120.43

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	500	NAD	C4B
2	A	500	NAD	C4D
2	B	501	NAD	C4B
2	B	501	NAD	C4D
2	C	502	NAD	C4B
2	C	502	NAD	C4D
2	D	503	NAD	C4B
2	D	503	NAD	C4D

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	501	NAD	C5D-O5D-PN-O3
2	B	501	NAD	C5D-O5D-PN-O1N

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Mol	Chain	Res	Type	Atoms
2	B	501	NAD	C5D-O5D-PN-O2N
2	B	501	NAD	C3D-C4D-C5D-O5D
2	B	501	NAD	O4D-C1D-N1N-C2N
2	B	501	NAD	O4D-C1D-N1N-C6N
2	B	501	NAD	C2D-C1D-N1N-C6N
2	C	502	NAD	O4D-C1D-N1N-C6N
2	D	503	NAD	C5B-O5B-PA-O3
2	D	503	NAD	O4B-C4B-C5B-O5B
2	D	503	NAD	C5D-O5D-PN-O1N
2	D	503	NAD	O4D-C1D-N1N-C2N
2	D	503	NAD	O4D-C1D-N1N-C6N
2	D	503	NAD	C2D-C1D-N1N-C2N
2	D	503	NAD	C2D-C1D-N1N-C6N
2	C	502	NAD	C4N-C3N-C7N-O7N
2	A	500	NAD	O4D-C4D-C5D-O5D
2	A	500	NAD	C3D-C4D-C5D-O5D
2	C	502	NAD	O4B-C4B-C5B-O5B
2	C	502	NAD	C4N-C3N-C7N-N7N
2	C	502	NAD	C2N-C3N-C7N-O7N
2	A	500	NAD	O4B-C4B-C5B-O5B
2	A	500	NAD	C3B-C4B-C5B-O5B
2	B	501	NAD	O4D-C4D-C5D-O5D
2	C	502	NAD	C3B-C4B-C5B-O5B
2	D	503	NAD	C3B-C4B-C5B-O5B
2	C	502	NAD	C2N-C3N-C7N-N7N
2	B	501	NAD	C4D-C5D-O5D-PN
2	A	500	NAD	C4N-C3N-C7N-O7N
2	C	502	NAD	C3D-C4D-C5D-O5D
2	A	500	NAD	C4N-C3N-C7N-N7N
2	A	500	NAD	C4B-C5B-O5B-PA
2	C	502	NAD	O4D-C4D-C5D-O5D
2	B	501	NAD	C5B-O5B-PA-O2A
2	D	503	NAD	C5D-O5D-PN-O2N
2	A	500	NAD	C2N-C3N-C7N-O7N
2	B	501	NAD	C4B-C5B-O5B-PA
2	B	501	NAD	C3B-C4B-C5B-O5B
2	A	500	NAD	C2N-C3N-C7N-N7N
2	B	501	NAD	C2D-C1D-N1N-C2N
2	D	503	NAD	C5B-O5B-PA-O1A
2	D	503	NAD	O4D-C4D-C5D-O5D

There are no ring outliers.
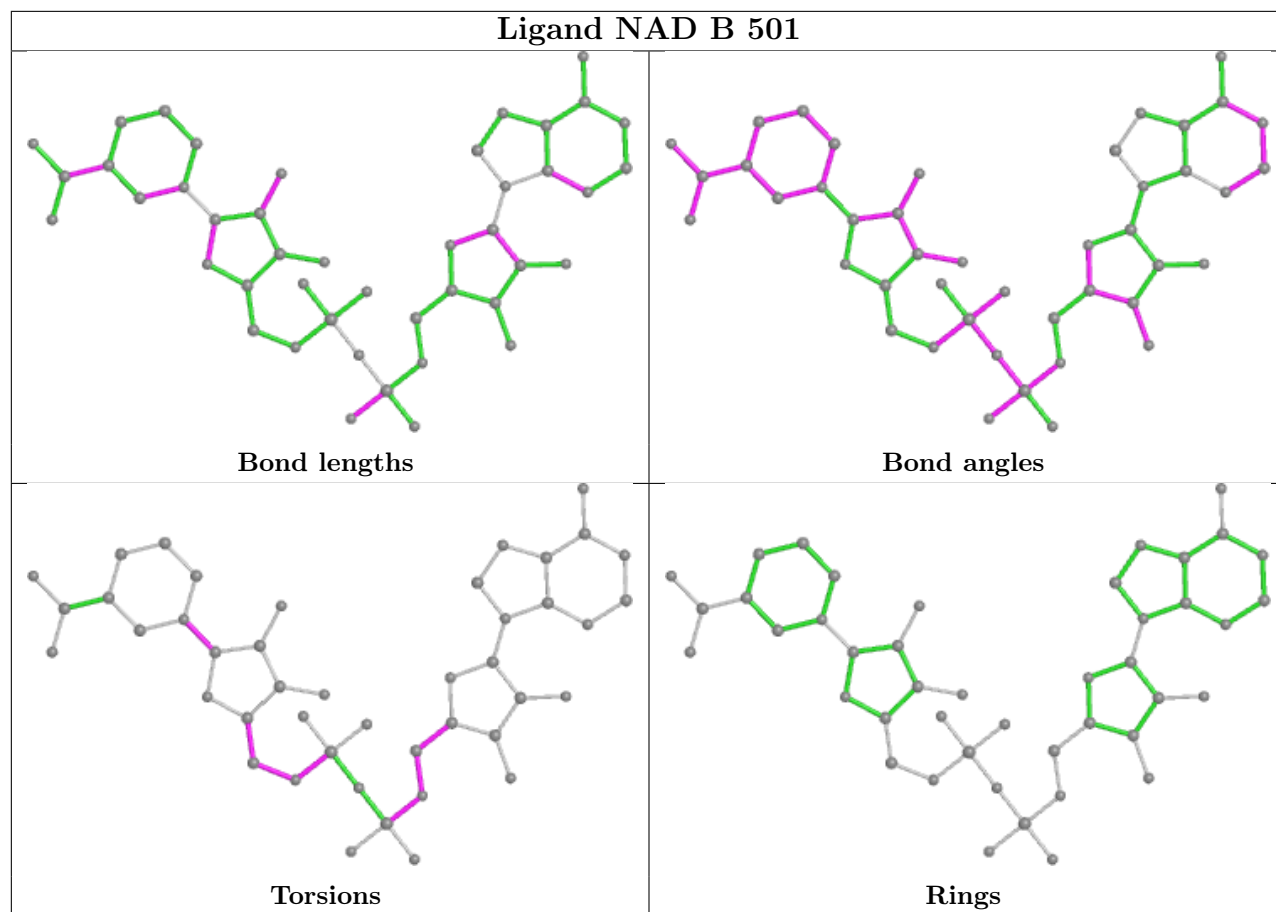
7 monomers are involved in 37 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	503	NAD	13	0
2	A	500	NAD	6	0
3	B	355	SO4	1	0
3	C	351	SO4	1	0
2	C	502	NAD	4	0
3	B	353	SO4	1	0
2	B	501	NAD	11	0

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

Ligand NAD D 503

Bond lengths

Bond angles

Torsions

Rings

Ligand NAD A 500

Bond lengths

Bond angles

Torsions

Rings

Ligand NAD C 502

Bond lengths

Bond angles

Torsions

Rings

Ligand NAD B 501

Bond lengths

Bond angles

Torsions

Rings
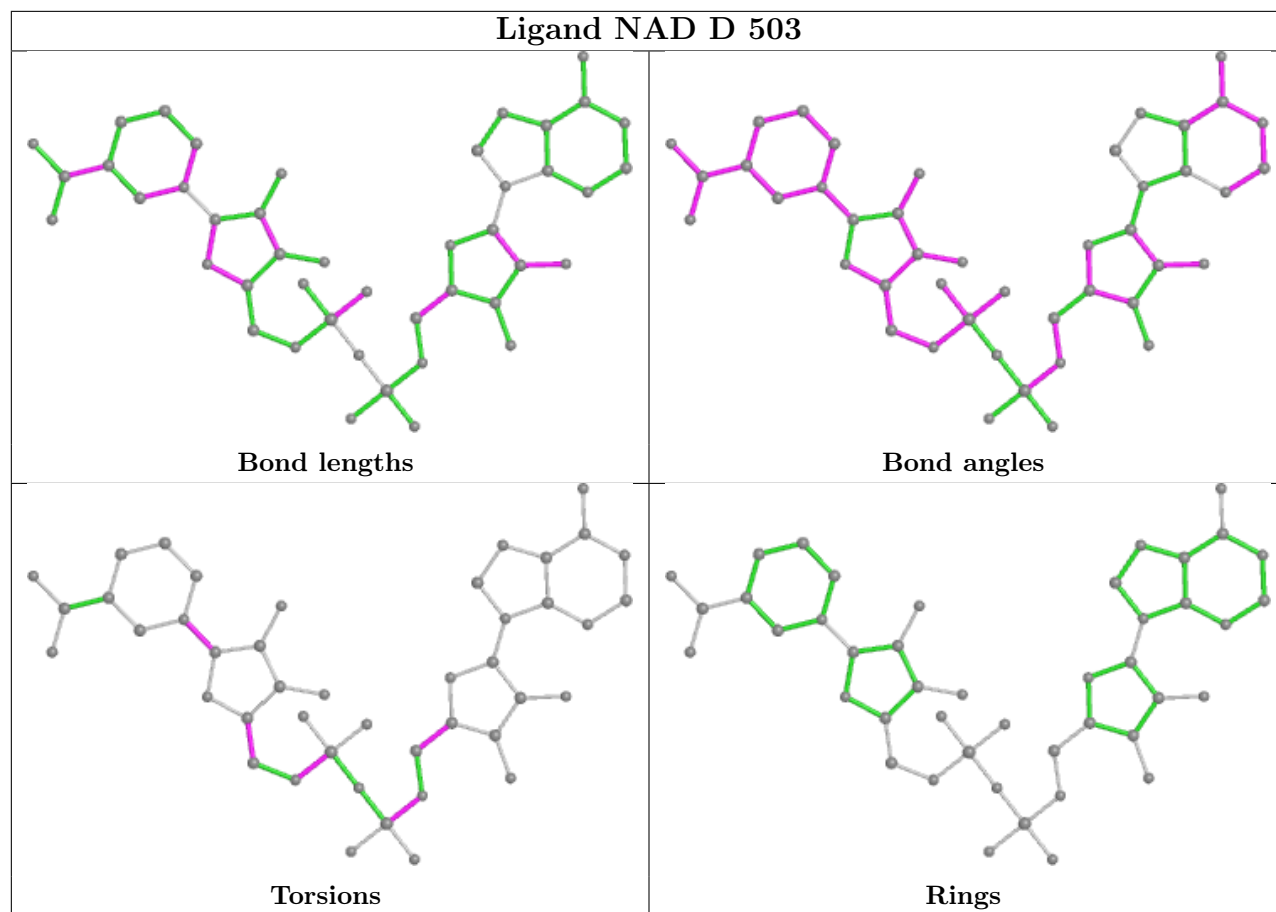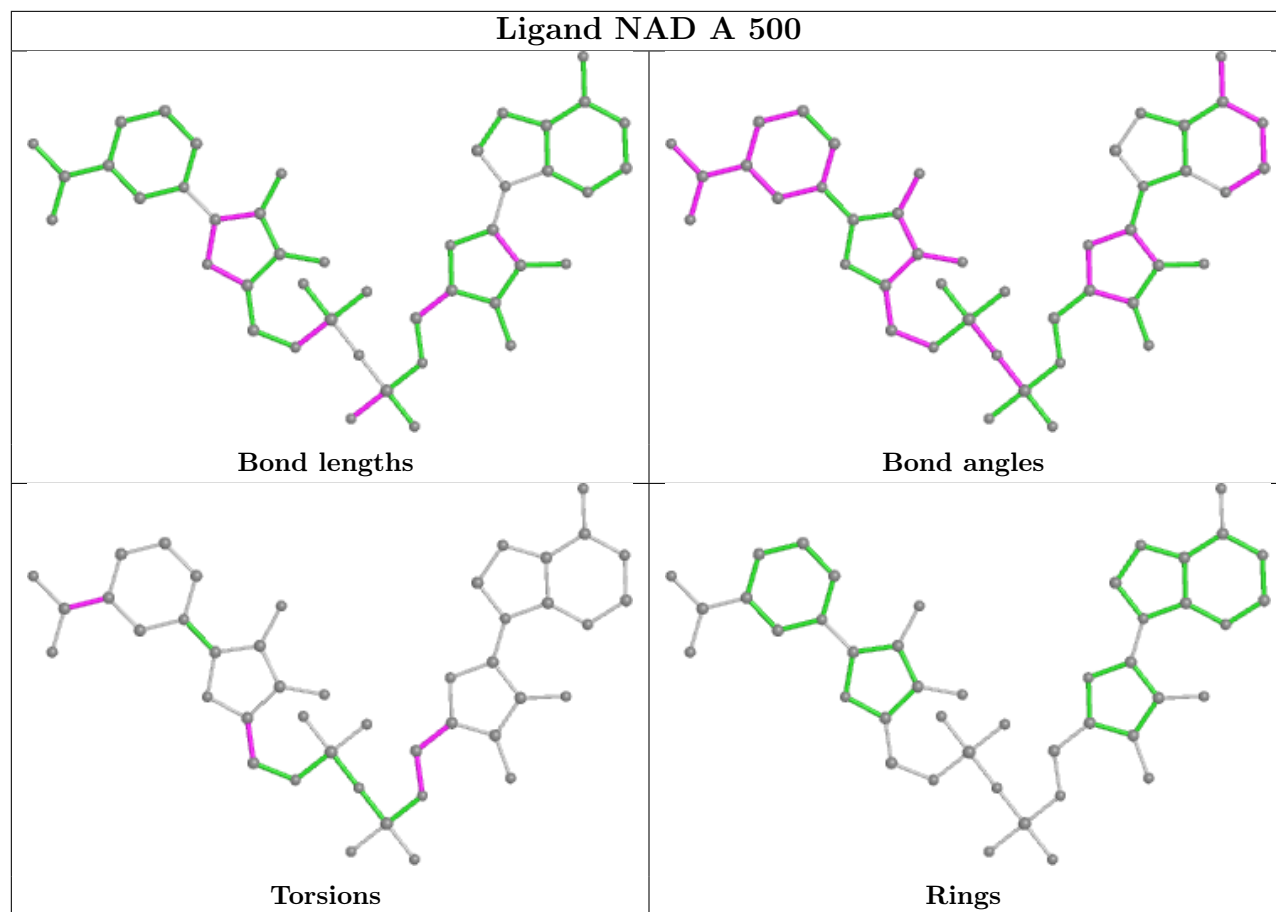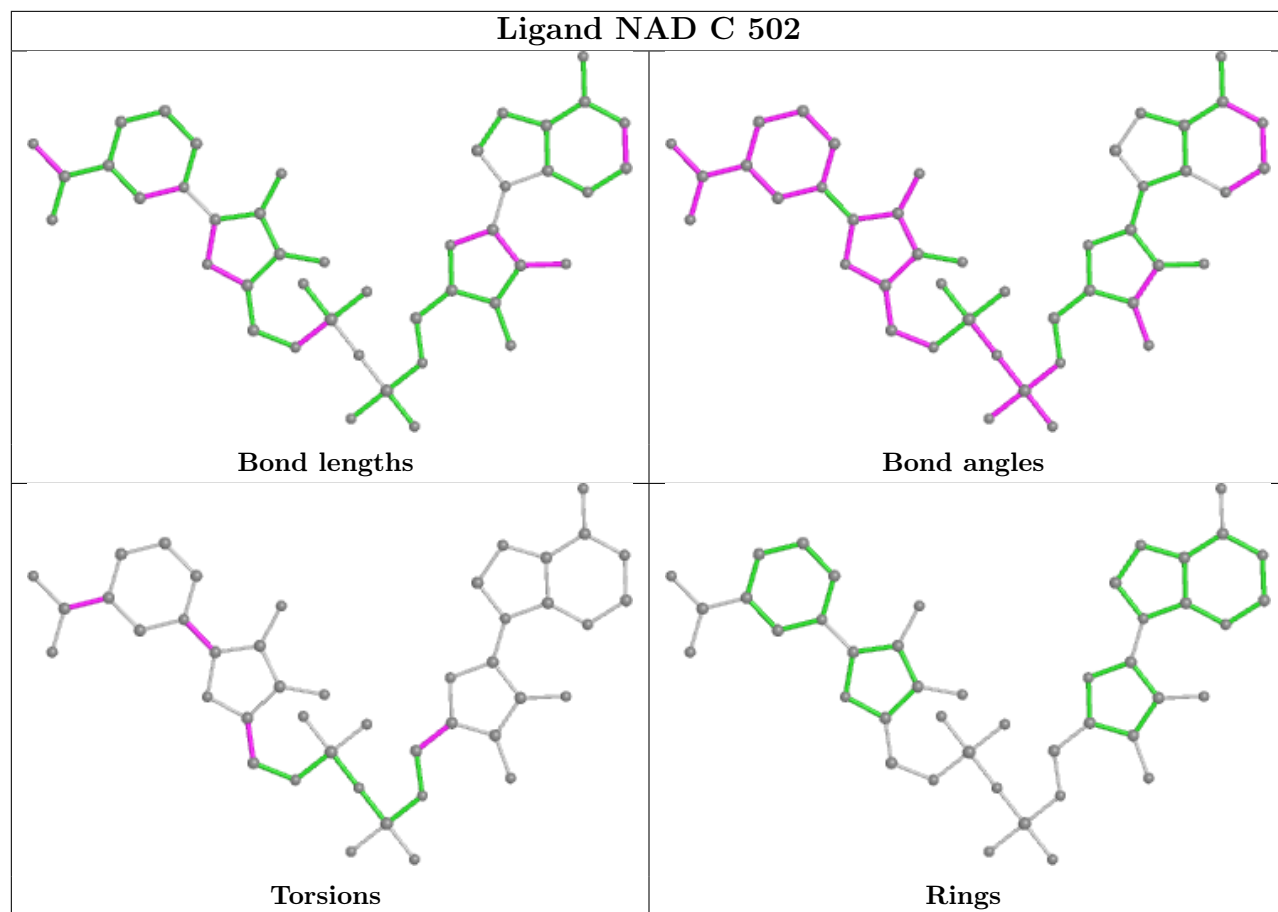
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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(Å²)	Q<0.9
1	A	347/350 (99%)	0.09	12 (3%)	44	43	15, 33, 63, 88	1 (0%)
1	B	347/350 (99%)	0.21	21 (6%)	21	20	17, 35, 76, 100	1 (0%)
1	C	347/350 (99%)	0.27	27 (7%)	13	11	17, 36, 67, 88	1 (0%)
1	D	347/350 (99%)	0.12	18 (5%)	27	26	15, 33, 72, 97	1 (0%)
All	All	1388/1400 (99%)	0.17	78 (5%)	24	23	15, 34, 69, 100	4 (0%)

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	97	CYS	13.1
1	B	96	VAL	10.4
1	A	113	ASN	8.2
1	A	97	CYS	8.2
1	B	111	CYS	7.9
1	D	97	CYS	7.5
1	C	97	CYS	7.3
1	D	113	ASN	6.0
1	D	114	THR	5.6
1	B	113	ASN	5.4
1	B	106	ASN	5.3
1	C	100	CYS	5.1
1	B	114	THR	4.8
1	D	96	VAL	4.4
1	A	100	CYS	4.2
1	D	102	ALA	4.2
1	B	108	TYR	4.1
1	C	113	ASN	4.1
1	B	110	VAL	4.0
1	B	99	LYS	3.9
1	A	114	THR	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	98	GLY	3.8
1	C	29	PRO	3.8
1	B	112	GLN	3.7
1	D	106	ASN	3.7
1	C	59	ILE	3.7
1	D	108	TYR	3.6
1	D	111	CYS	3.5
1	A	103	CYS	3.4
1	A	59	ILE	3.3
1	B	81	GLU	3.3
1	D	110	VAL	3.3
1	B	16	GLY	3.2
1	C	79	GLY	3.1
1	C	114	THR	3.1
1	C	99	LYS	3.0
1	B	109	HIS	3.0
1	D	119	VAL	2.9
1	A	108	TYR	2.9
1	A	106	ASN	2.9
1	C	30	GLY	2.9
1	C	51	TRP	2.9
1	D	109	HIS	2.8
1	C	98	GLY	2.7
1	C	26	LYS	2.7
1	D	103	CYS	2.6
1	A	62	PRO	2.6
1	B	107	ARG	2.5
1	C	103	CYS	2.5
1	D	331	ALA	2.5
1	A	110	VAL	2.5
1	C	14	ALA	2.5
1	B	95	ILE	2.4
1	A	98	GLY	2.4
1	D	99	LYS	2.4
1	C	13	PRO	2.4
1	C	102	ALA	2.3
1	B	98	GLY	2.3
1	B	103	CYS	2.3
1	C	17	ALA	2.3
1	C	95	ILE	2.3
1	A	111	CYS	2.3
1	C	78	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	325	PHE	2.2
1	C	112	GLN	2.2
1	B	17	ALA	2.2
1	D	100	CYS	2.2
1	C	82	ASP	2.1
1	C	106	ASN	2.1
1	B	29	PRO	2.1
1	C	60	LYS	2.1
1	B	117	PHE	2.1
1	B	105	HIS	2.0
1	C	57	SER	2.0
1	D	63	GLN	2.0
1	C	107	ARG	2.0
1	D	112	GLN	2.0
1	C	25	PRO	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SO4	B	353	5/5	0.50	0.35	114,115,117,117	0
3	SO4	B	351	5/5	0.55	0.47	116,117,118,118	0
3	SO4	D	351	5/5	0.67	0.48	127,128,129,131	0
3	SO4	B	352	5/5	0.76	0.31	105,106,108,109	0
3	SO4	C	353	5/5	0.78	0.32	87,88,90,90	0
3	SO4	B	354	5/5	0.78	0.23	95,96,98,99	0
3	SO4	C	351	5/5	0.80	0.41	112,112,112,113	0
2	NAD	B	501	44/44	0.82	0.31	6,26,34,37	44

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SO4	C	352	5/5	0.84	0.34	101,101,102,102	0
2	NAD	A	500	44/44	0.86	0.33	9,28,32,33	44
2	NAD	C	502	44/44	0.89	0.32	6,26,31,35	44
2	NAD	D	503	44/44	0.92	0.27	8,23,27,29	44
3	SO4	B	355	5/5	0.96	0.15	38,47,50,53	0
3	SO4	D	352	5/5	0.99	0.10	30,44,46,49	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:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
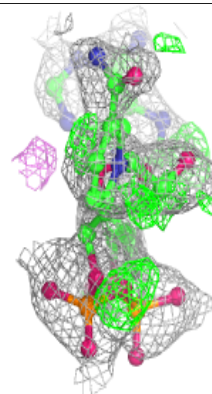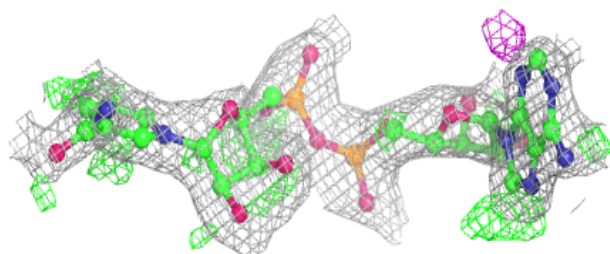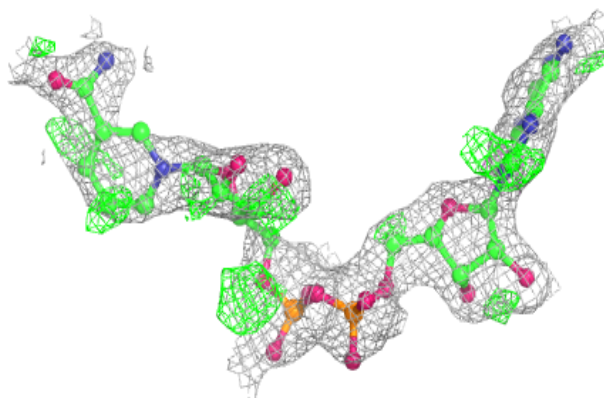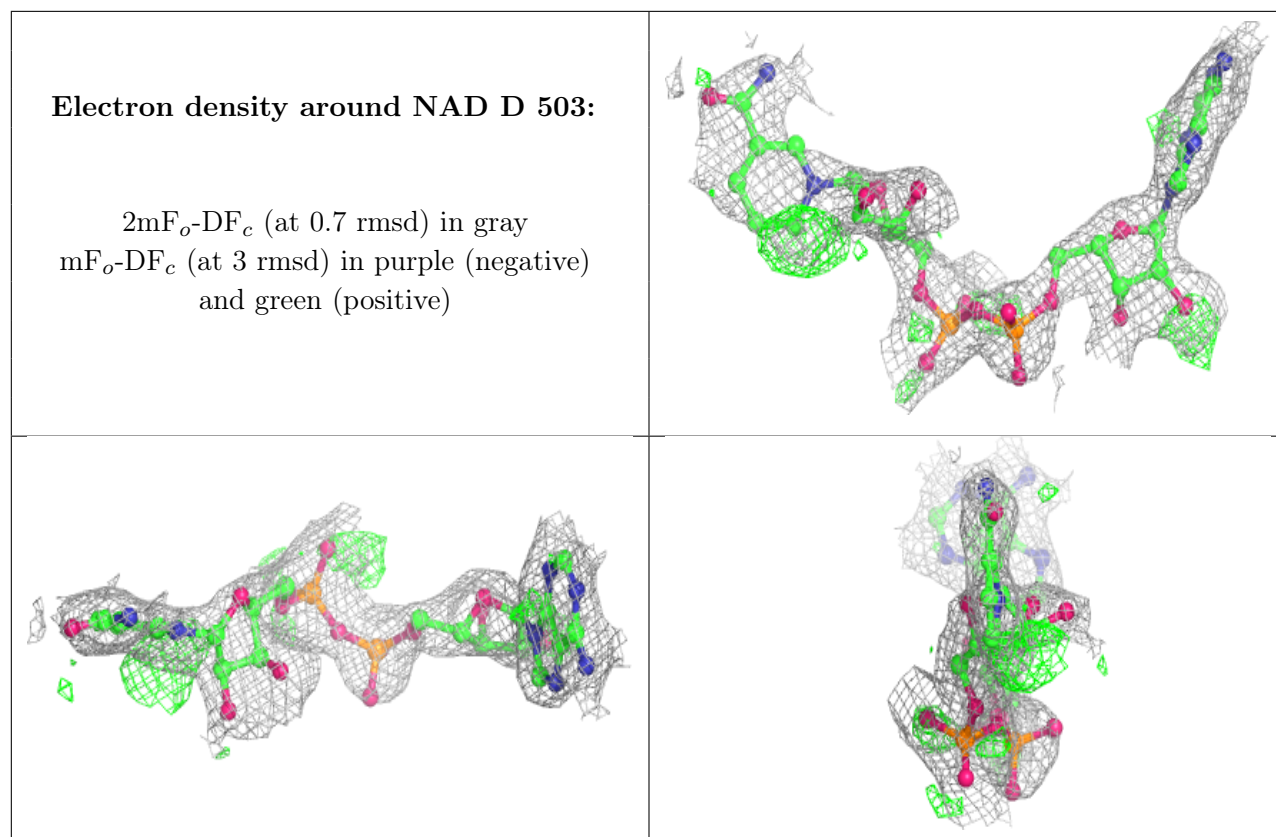$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative) and green (positive)
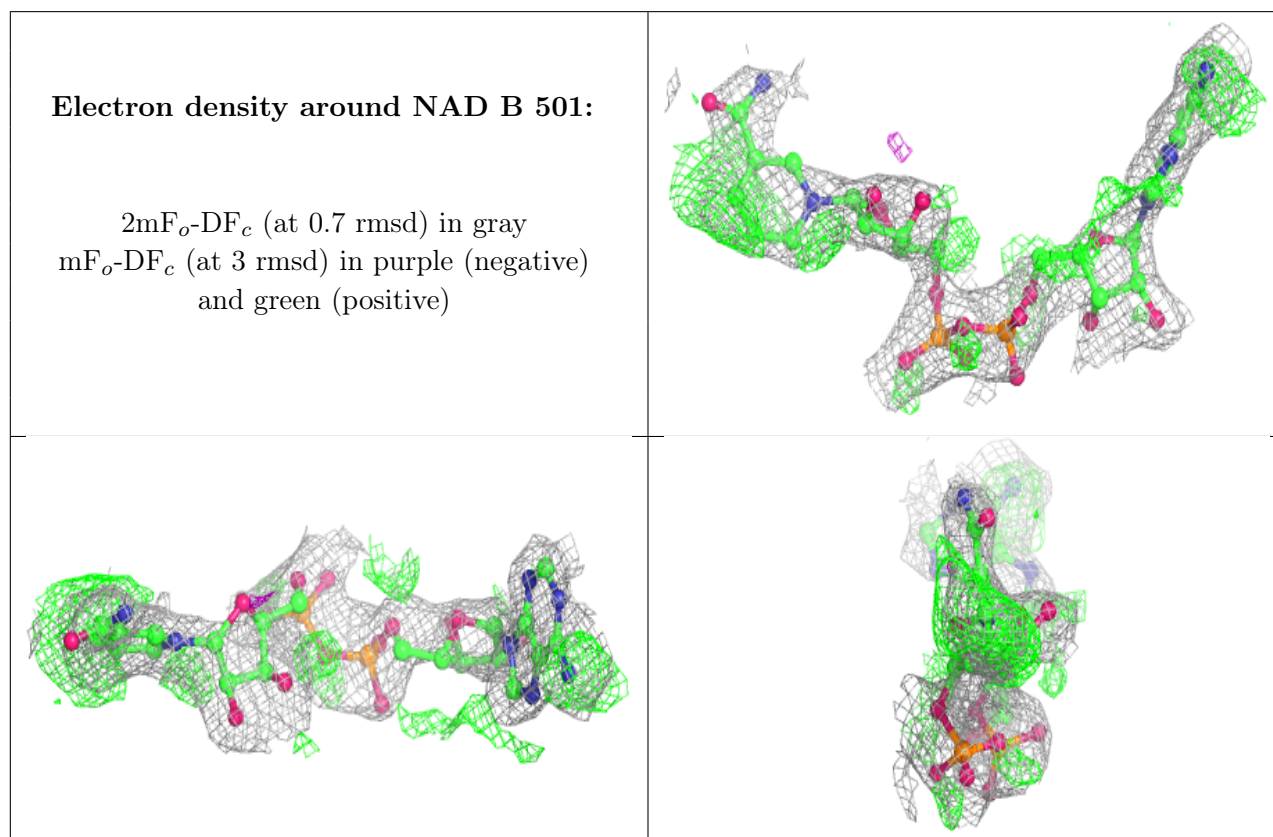
Electron density around NAD A 500:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
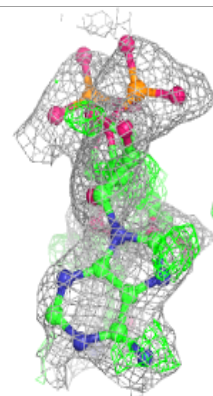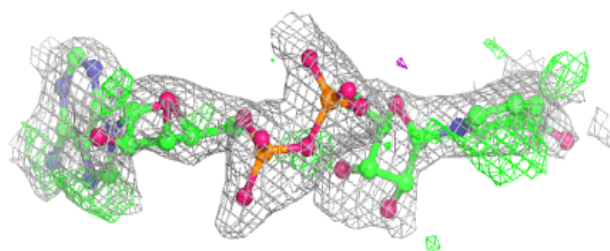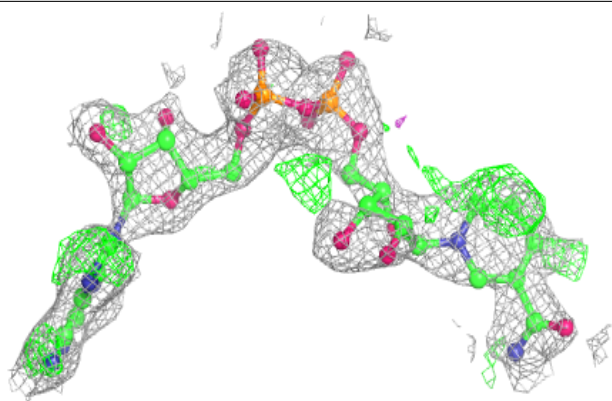
Electron density around NAD C 502:

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

Electron density around NAD D 503:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.