



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:49 AM UTC

PDB ID : 3GFB / pdb_00003gfb
Title : L-Threonine Dehydrogenase (TkTDH) from the hyperthermophilic archaeon
Thermococcus kodakaraensis
Authors : Bowyer, A.
Deposited on : 2009-02-26
Resolution : 2.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

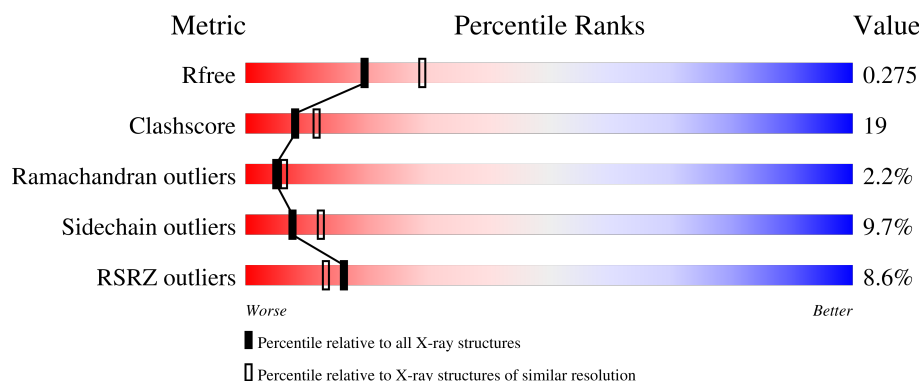
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	350	7% 53% 34% 11% ..
1	B	350	8% 47% 39% 11% ..
1	C	350	11% 47% 37% 12% ..
1	D	350	9% 51% 38% 8% ..

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	-	-	-

2 Entry composition [i](#)

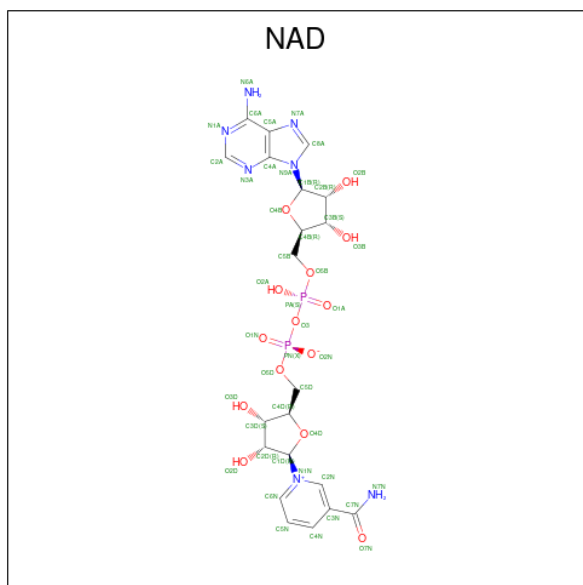
There are 4 unique types of molecules in this entry. The entry contains 11389 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (CCD ID: 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 (CCD ID: SO4) (formula: O₄S).



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	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	O	S	0	0
			5	4	1		

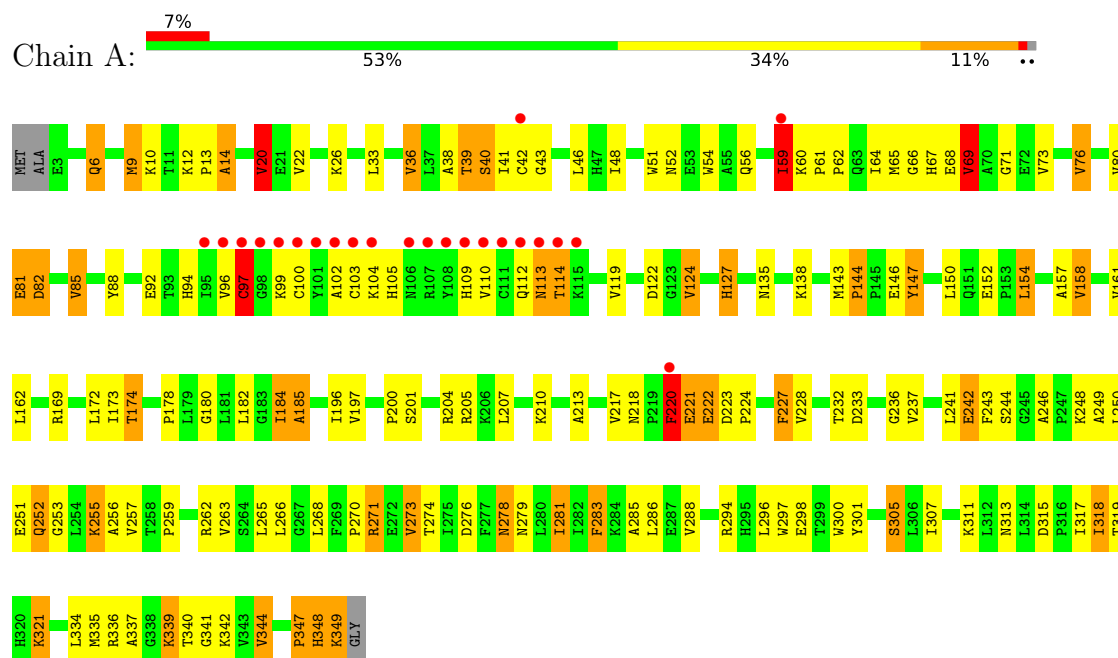
- Molecule 4 is water.

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

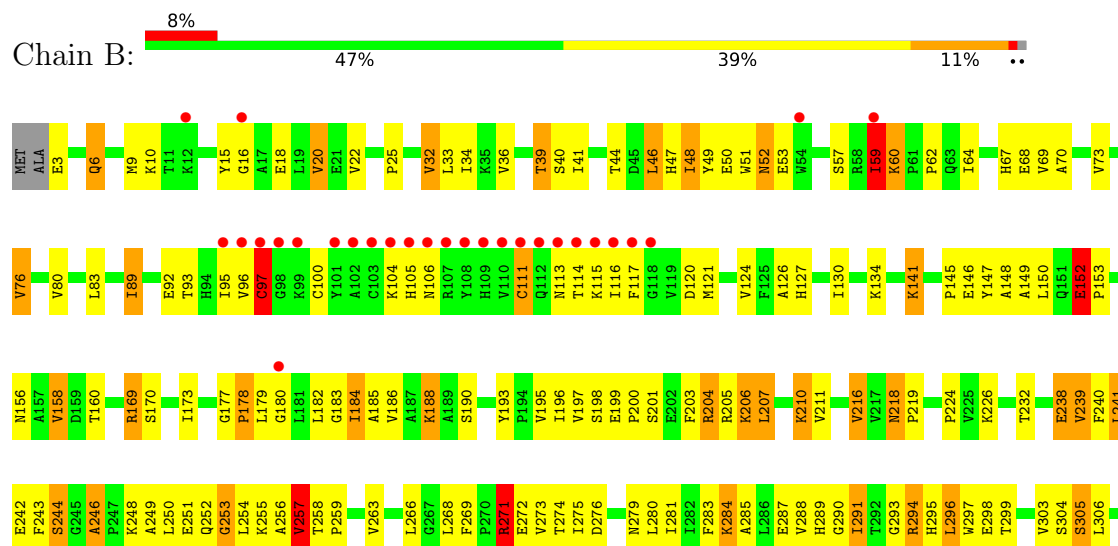
3 Residue-property plots

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

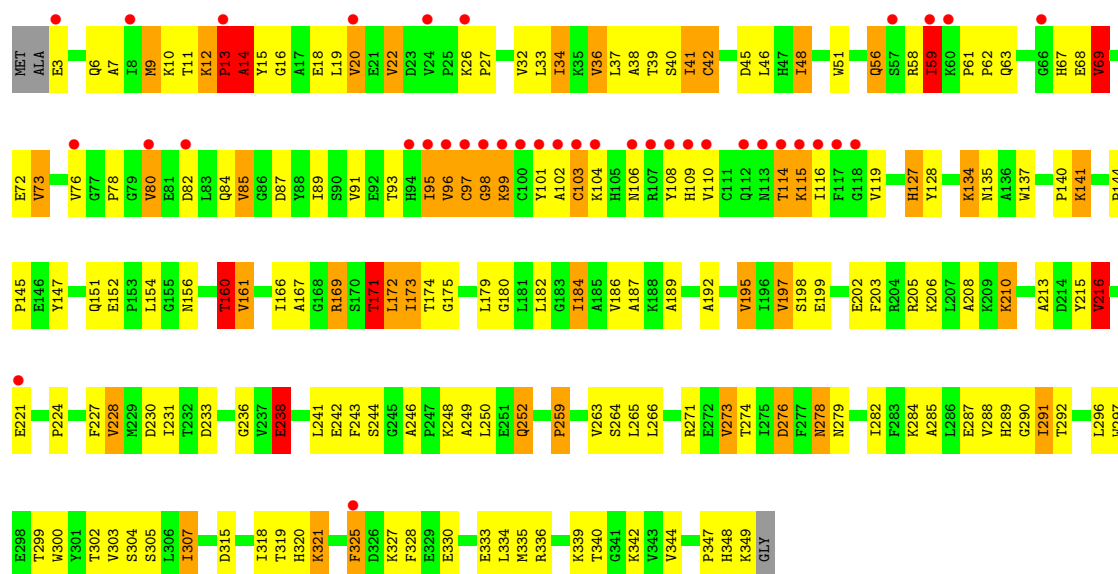


• Molecule 1: L-threonine 3-dehydrogenase

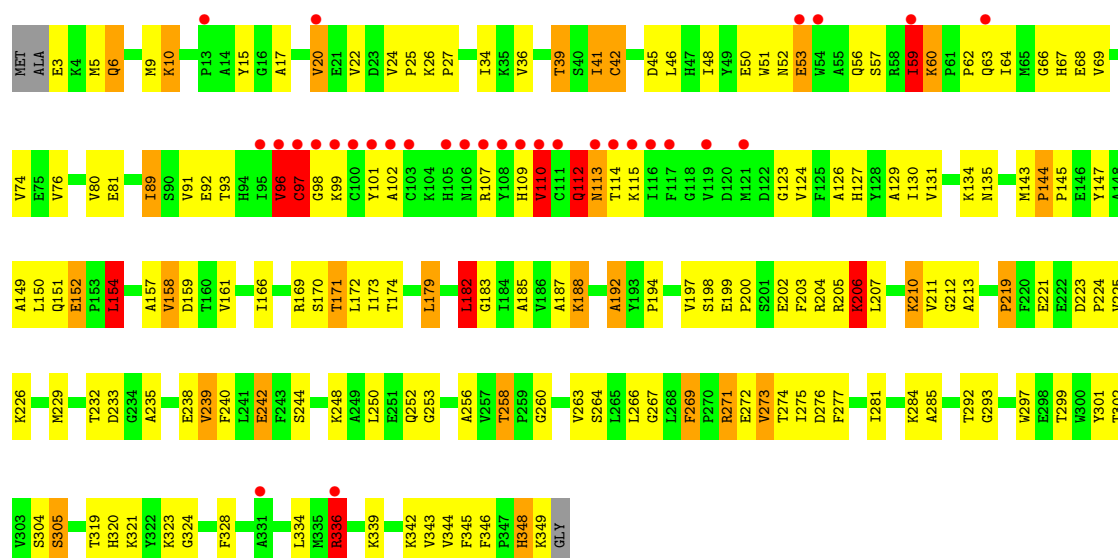




• Molecule 1: L-threonine 3-dehydrogenase



• 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 73.92 – 2.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (73.92-2.40) 100.0 (73.92-2.40)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.85 (at 2.40Å)	Xtrriage
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	Xtrriage
Anisotropy	0.117	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 52.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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.*

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, SO4

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	1.93	62/2736 (2.3%)	1.65	40/3716 (1.1%)
1	B	1.90	53/2736 (1.9%)	1.66	44/3716 (1.2%)
1	C	1.93	59/2736 (2.2%)	1.61	35/3716 (0.9%)
1	D	1.94	57/2736 (2.1%)	1.74	50/3716 (1.3%)
All	All	1.93	231/10944 (2.1%)	1.66	169/14864 (1.1%)

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 (231) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	158	VAL	CA-CB	10.65	1.68	1.54
1	C	36	VAL	CA-CB	9.88	1.66	1.53
1	A	271	ARG	CA-C	8.98	1.63	1.52
1	A	249	ALA	CA-CB	-8.94	1.39	1.53
1	B	239	VAL	CA-CB	8.90	1.65	1.54
1	B	59	ILE	CA-CB	8.81	1.66	1.54
1	B	246	ALA	C-O	8.81	1.35	1.24
1	A	305	SER	N-CA	-8.38	1.35	1.46
1	A	124	VAL	CA-CB	8.15	1.65	1.54
1	B	238	GLU	N-CA	-8.09	1.35	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	96	VAL	CA-C	8.04	1.62	1.52
1	B	96	VAL	CA-CB	8.01	1.63	1.54
1	C	271	ARG	CA-C	7.98	1.62	1.52
1	B	170	SER	C-O	-7.89	1.14	1.24
1	B	311	LYS	CG-CD	7.87	1.76	1.52
1	D	271	ARG	CA-C	7.83	1.62	1.52
1	A	274	THR	CA-CB	7.82	1.64	1.53
1	B	173	ILE	CA-CB	7.80	1.63	1.54
1	C	307	ILE	CA-C	7.72	1.61	1.52
1	C	73	VAL	CA-CB	-7.66	1.44	1.53
1	C	144	PRO	CA-C	7.57	1.59	1.52
1	A	259	PRO	C-O	7.49	1.32	1.23
1	A	263	VAL	N-CA	-7.45	1.37	1.46
1	A	39	THR	CA-C	-7.45	1.43	1.52
1	C	22	VAL	CA-CB	7.43	1.67	1.55
1	B	186	VAL	C-O	7.38	1.33	1.24
1	A	288	VAL	CA-CB	7.37	1.63	1.54
1	D	129	ALA	CA-C	-7.35	1.43	1.52
1	C	285	ALA	CA-C	7.33	1.62	1.53
1	A	246	ALA	CA-C	7.29	1.60	1.52
1	C	238	GLU	CB-CG	-7.27	1.30	1.52
1	D	174	THR	C-O	7.26	1.32	1.24
1	C	228	VAL	CA-CB	-7.25	1.46	1.54
1	C	263	VAL	CA-CB	7.17	1.63	1.54
1	C	276	ASP	CA-C	7.16	1.62	1.52
1	A	88	TYR	CA-C	7.14	1.61	1.52
1	A	265	LEU	C-O	7.14	1.32	1.23
1	B	70	ALA	N-CA	7.07	1.54	1.46
1	D	154	LEU	C-O	-7.07	1.14	1.24
1	A	127	HIS	C-O	-7.06	1.15	1.24
1	D	238	GLU	CA-C	-7.05	1.42	1.52
1	D	192	ALA	CA-CB	-7.02	1.41	1.53
1	B	36	VAL	CA-CB	7.02	1.61	1.53
1	C	40	SER	C-O	6.99	1.33	1.23
1	C	175	GLY	C-O	6.94	1.33	1.23
1	C	34	ILE	N-CA	-6.84	1.38	1.46
1	D	59	ILE	CA-CB	6.84	1.62	1.54
1	C	288	VAL	CA-CB	6.83	1.62	1.54
1	B	185	ALA	CA-CB	6.81	1.64	1.53
1	D	97	CYS	N-CA	6.81	1.54	1.46
1	D	273	VAL	CA-CB	6.79	1.63	1.54
1	D	258	THR	C-N	6.70	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	182	LEU	C-O	-6.69	1.16	1.24
1	C	171	THR	CA-CB	6.67	1.66	1.53
1	A	236	GLY	N-CA	6.66	1.54	1.45
1	B	41	ILE	CA-CB	6.65	1.61	1.54
1	C	250	LEU	C-O	6.63	1.31	1.24
1	B	257	VAL	CB-CG2	-6.62	1.30	1.52
1	A	59	ILE	CA-CB	6.59	1.61	1.54
1	D	232	THR	CA-CB	-6.59	1.44	1.53
1	D	334	LEU	CA-C	6.59	1.61	1.52
1	D	213	ALA	CA-CB	-6.58	1.42	1.53
1	A	278	ASN	CA-C	-6.58	1.44	1.52
1	A	197	VAL	CA-CB	6.55	1.62	1.54
1	B	275	ILE	CA-CB	6.55	1.62	1.54
1	D	305	SER	N-CA	-6.54	1.37	1.46
1	A	300	TRP	C-O	-6.54	1.16	1.24
1	B	22	VAL	CA-CB	6.49	1.64	1.54
1	A	36	VAL	CA-CB	6.43	1.61	1.53
1	B	186	VAL	CA-C	6.42	1.61	1.52
1	D	159	ASP	C-O	-6.38	1.16	1.24
1	C	278	ASN	C-O	-6.36	1.16	1.24
1	A	273	VAL	CA-CB	6.36	1.65	1.54
1	D	96	VAL	N-CA	6.36	1.54	1.46
1	A	255	LYS	CA-C	-6.32	1.44	1.52
1	B	41	ILE	C-O	6.32	1.30	1.24
1	D	192	ALA	C-O	-6.31	1.16	1.23
1	A	315	ASP	CA-C	6.30	1.60	1.52
1	A	36	VAL	C-O	-6.29	1.17	1.23
1	B	259	PRO	CA-C	6.27	1.60	1.52
1	B	294	ARG	CA-C	-6.26	1.44	1.52
1	C	186	VAL	CA-CB	6.26	1.61	1.54
1	D	343	VAL	CA-CB	6.22	1.61	1.54
1	D	277	PHE	C-O	6.21	1.31	1.24
1	B	238	GLU	CB-CG	-6.21	1.33	1.52
1	C	273	VAL	CA-CB	-6.18	1.46	1.54
1	A	66	GLY	N-CA	6.17	1.51	1.45
1	B	312	LEU	C-O	-6.16	1.16	1.24
1	C	127	HIS	C-O	-6.15	1.16	1.24
1	A	196	ILE	C-O	6.13	1.30	1.24
1	D	185	ALA	CA-CB	6.13	1.63	1.53
1	C	80	VAL	CA-CB	6.12	1.61	1.55
1	C	307	ILE	N-CA	6.10	1.53	1.46
1	D	174	THR	N-CA	6.10	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	257	VAL	CA-CB	6.06	1.60	1.54
1	B	331	ALA	CA-C	6.04	1.60	1.52
1	B	46	LEU	CA-C	6.04	1.60	1.52
1	C	292	THR	CA-C	6.03	1.60	1.52
1	A	174	THR	C-O	6.01	1.31	1.24
1	C	246	ALA	CA-C	5.99	1.60	1.52
1	D	145	PRO	CA-C	5.99	1.62	1.52
1	A	313	ASN	CA-C	-5.98	1.45	1.53
1	B	196	ILE	CA-CB	5.97	1.61	1.54
1	A	97	CYS	N-CA	5.96	1.53	1.46
1	D	64	ILE	CA-CB	5.95	1.61	1.54
1	B	158	VAL	CA-CB	5.95	1.62	1.54
1	A	154	LEU	C-O	-5.94	1.16	1.24
1	C	244	SER	N-CA	5.93	1.53	1.46
1	B	141	LYS	N-CA	5.92	1.53	1.46
1	A	162	LEU	N-CA	-5.90	1.39	1.46
1	A	157	ALA	CA-CB	-5.89	1.43	1.53
1	B	64	ILE	CA-CB	5.88	1.61	1.54
1	D	276	ASP	C-O	-5.87	1.16	1.24
1	B	280	LEU	C-O	-5.85	1.16	1.24
1	C	34	ILE	CA-CB	5.85	1.65	1.55
1	D	219	PRO	CA-C	5.84	1.62	1.52
1	A	158	VAL	C-O	-5.82	1.17	1.24
1	A	271	ARG	N-CA	5.80	1.53	1.45
1	D	182	LEU	N-CA	-5.80	1.39	1.46
1	D	187	ALA	CA-CB	5.80	1.62	1.53
1	C	14	ALA	CA-C	5.79	1.60	1.52
1	B	195	VAL	CA-C	5.78	1.59	1.53
1	D	238	GLU	CG-CD	-5.77	1.37	1.52
1	A	281	ILE	C-O	-5.76	1.17	1.24
1	A	6	GLN	CA-C	5.75	1.60	1.52
1	A	262	ARG	CA-C	-5.74	1.45	1.52
1	C	187	ALA	CA-CB	5.74	1.62	1.53
1	A	227	PHE	CA-C	5.73	1.60	1.52
1	A	54	TRP	CA-C	5.73	1.60	1.52
1	D	301	TYR	C-O	-5.72	1.17	1.24
1	A	252	GLN	C-O	-5.71	1.17	1.24
1	A	241	LEU	CA-C	5.69	1.59	1.52
1	D	123	GLY	C-O	-5.69	1.16	1.23
1	C	215	TYR	N-CA	-5.68	1.39	1.46
1	B	146	GLU	N-CA	-5.68	1.38	1.46
1	D	194	PRO	CG-CD	5.68	1.67	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	172	LEU	C-O	5.66	1.30	1.24
1	B	73	VAL	C-O	-5.66	1.18	1.24
1	A	161	VAL	C-O	-5.64	1.17	1.24
1	B	232	THR	CA-CB	-5.63	1.45	1.53
1	D	161	VAL	C-O	-5.62	1.17	1.24
1	D	299	THR	C-O	-5.62	1.17	1.24
1	C	285	ALA	N-CA	-5.62	1.38	1.46
1	B	288	VAL	C-O	-5.61	1.18	1.24
1	D	275	ILE	C-O	-5.61	1.18	1.24
1	A	147	TYR	CA-CB	-5.61	1.44	1.53
1	A	113	ASN	CA-C	5.60	1.60	1.52
1	D	36	VAL	N-CA	-5.60	1.39	1.46
1	D	244	SER	N-CA	5.60	1.53	1.46
1	C	85	VAL	CA-CB	5.59	1.60	1.54
1	C	172	LEU	C-O	5.59	1.30	1.24
1	C	265	LEU	CA-CB	5.59	1.60	1.53
1	C	252	GLN	C-O	-5.58	1.17	1.24
1	B	331	ALA	CA-CB	5.56	1.62	1.53
1	B	253	GLY	N-CA	-5.55	1.39	1.45
1	C	59	ILE	CA-CB	5.54	1.60	1.54
1	A	301	TYR	C-O	-5.54	1.17	1.24
1	B	344	VAL	CA-C	5.53	1.59	1.52
1	C	160	THR	CA-CB	5.52	1.62	1.53
1	D	293	GLY	C-O	5.51	1.32	1.24
1	A	311	LYS	CE-NZ	5.50	1.65	1.49
1	C	236	GLY	N-CA	5.50	1.51	1.45
1	A	172	LEU	CA-C	-5.50	1.46	1.52
1	A	249	ALA	C-O	-5.49	1.17	1.24
1	A	71	GLY	CA-C	5.49	1.57	1.52
1	D	344	VAL	N-CA	5.48	1.53	1.46
1	C	208	ALA	C-O	-5.47	1.17	1.24
1	C	167	ALA	CA-CB	5.47	1.61	1.53
1	D	284	LYS	N-CA	5.45	1.53	1.46
1	A	173	ILE	CA-C	-5.44	1.45	1.52
1	B	183	GLY	CA-C	-5.44	1.46	1.52
1	D	188	LYS	CA-C	5.44	1.59	1.52
1	A	220	PHE	N-CA	5.43	1.53	1.46
1	A	144	PRO	C-O	-5.43	1.18	1.24
1	C	264	SER	CA-C	-5.43	1.46	1.52
1	D	173	ILE	CA-CB	5.42	1.60	1.54
1	A	143	MET	C-O	5.39	1.31	1.24
1	B	238	GLU	CG-CD	-5.39	1.38	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	69	VAL	CA-C	5.37	1.59	1.52
1	D	42	CYS	CA-C	5.37	1.60	1.53
1	A	38	ALA	CA-CB	-5.34	1.45	1.53
1	B	41	ILE	CA-C	5.34	1.59	1.52
1	B	274	THR	CA-CB	5.33	1.60	1.53
1	A	20	VAL	N-CA	-5.33	1.40	1.46
1	D	263	VAL	C-O	5.33	1.29	1.24
1	B	293	GLY	C-O	5.33	1.32	1.24
1	D	89	ILE	C-O	-5.31	1.18	1.24
1	B	170	SER	N-CA	-5.30	1.39	1.46
1	B	298	GLU	CA-C	-5.30	1.45	1.52
1	C	299	THR	CA-CB	5.30	1.61	1.53
1	C	195	VAL	CA-CB	5.28	1.60	1.53
1	B	170	SER	CA-C	-5.27	1.45	1.52
1	C	3	GLU	CG-CD	5.26	1.65	1.52
1	A	242	GLU	N-CA	-5.26	1.39	1.46
1	A	307	ILE	C-O	-5.25	1.18	1.24
1	C	102	ALA	CA-CB	5.25	1.61	1.53
1	B	311	LYS	N-CA	5.23	1.53	1.46
1	B	280	LEU	CA-C	5.23	1.59	1.52
1	A	286	LEU	CA-CB	5.21	1.61	1.53
1	B	273	VAL	N-CA	5.20	1.52	1.46
1	D	144	PRO	C-O	-5.20	1.18	1.24
1	B	304	SER	CA-CB	-5.19	1.44	1.53
1	D	39	THR	CA-CB	-5.19	1.44	1.53
1	D	273	VAL	CA-C	5.19	1.58	1.52
1	C	259	PRO	CB-CG	5.17	1.75	1.49
1	C	161	VAL	C-O	-5.17	1.18	1.24
1	C	284	LYS	CD-CE	-5.17	1.36	1.52
1	C	154	LEU	CA-C	5.17	1.59	1.52
1	C	216	VAL	N-CA	5.17	1.52	1.46
1	B	178	PRO	CB-CG	5.16	1.75	1.49
1	C	189	ALA	CA-C	5.15	1.59	1.52
1	A	114	THR	CA-C	5.14	1.59	1.52
1	C	197	VAL	C-O	5.14	1.29	1.24
1	C	327	LYS	CA-C	5.12	1.59	1.52
1	D	149	ALA	CA-C	5.12	1.59	1.52
1	D	41	ILE	N-CA	5.10	1.52	1.46
1	D	169	ARG	CA-CB	-5.10	1.45	1.53
1	A	257	VAL	C-O	-5.09	1.17	1.24
1	C	318	ILE	CA-C	-5.09	1.48	1.53
1	D	304	SER	CA-CB	-5.07	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	235	ALA	N-CA	5.06	1.52	1.46
1	A	73	VAL	CA-CB	-5.06	1.48	1.54
1	C	48	ILE	N-CA	5.06	1.52	1.46
1	C	173	ILE	CA-CB	-5.05	1.48	1.54
1	C	104	LYS	CA-C	5.05	1.59	1.52
1	B	188	LYS	CA-C	5.04	1.59	1.52
1	C	101	TYR	CA-C	5.04	1.60	1.52
1	D	263	VAL	CA-CB	5.03	1.60	1.54
1	A	318	ILE	C-O	5.03	1.30	1.23
1	A	185	ALA	CA-CB	5.02	1.61	1.53
1	D	36	VAL	CA-C	-5.02	1.46	1.52

All (169) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	281	ILE	N-CA-C	13.44	123.41	112.12
1	A	152	GLU	CA-C-N	-10.40	108.17	119.19
1	A	152	GLU	C-N-CA	-10.40	108.17	119.19
1	D	152	GLU	CA-C-N	-9.91	109.56	119.87
1	D	152	GLU	C-N-CA	-9.91	109.56	119.87
1	B	203	PHE	N-CA-C	-9.50	100.91	111.07
1	A	244	SER	N-CA-C	9.17	122.43	111.33
1	D	269	PHE	CA-C-N	9.14	128.79	119.56
1	D	269	PHE	C-N-CA	9.14	128.79	119.56
1	B	190	SER	N-CA-C	8.85	123.72	113.19
1	B	152	GLU	CA-C-N	-8.82	110.66	119.56
1	B	152	GLU	C-N-CA	-8.82	110.66	119.56
1	D	256	ALA	N-CA-C	8.75	121.97	111.82
1	B	244	SER	N-CA-C	8.30	121.26	111.71
1	B	279	ASN	N-CA-C	8.28	122.67	112.23
1	C	152	GLU	CA-C-N	-8.05	111.43	119.56
1	C	152	GLU	C-N-CA	-8.05	111.43	119.56
1	A	69	VAL	N-CA-C	8.03	121.22	108.85
1	B	182	LEU	CA-C-N	7.99	128.81	119.94
1	B	182	LEU	C-N-CA	7.99	128.81	119.94
1	A	69	VAL	CB-CA-C	-7.96	98.56	110.82
1	A	85	VAL	CB-CA-C	-7.86	98.55	111.51
1	D	173	ILE	CA-C-N	-7.76	112.45	122.77
1	D	173	ILE	C-N-CA	-7.76	112.45	122.77
1	D	197	VAL	N-CA-C	7.73	119.27	107.99
1	A	103	CYS	N-CA-C	7.71	119.32	111.07
1	B	177	GLY	N-CA-C	-7.64	102.98	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	80	VAL	N-CA-C	-7.46	96.98	107.80
1	A	119	VAL	CB-CA-C	-7.45	105.38	111.71
1	C	210	LYS	N-CA-C	-7.37	102.63	111.69
1	D	42	CYS	N-CA-C	7.30	120.40	110.55
1	A	81	GLU	N-CA-C	-7.21	99.54	110.14
1	C	244	SER	N-CA-C	7.19	120.17	111.40
1	C	182	LEU	CA-C-N	7.17	128.06	120.03
1	C	182	LEU	C-N-CA	7.17	128.06	120.03
1	A	114	THR	N-CA-C	7.14	126.02	110.80
1	D	96	VAL	N-CA-C	6.79	123.47	109.34
1	B	271	ARG	NE-CZ-NH2	-6.71	113.17	119.20
1	C	203	PHE	N-CA-C	-6.69	103.92	111.14
1	C	184	ILE	CB-CA-C	-6.66	103.03	112.22
1	D	225	VAL	N-CA-C	6.61	116.76	110.42
1	A	337	ALA	N-CA-C	6.55	120.99	113.19
1	D	91	VAL	N-CA-C	6.52	117.24	108.11
1	D	260	GLY	N-CA-C	-6.50	106.76	115.21
1	A	113	ASN	N-CA-C	6.49	124.61	110.80
1	C	303	VAL	CB-CA-C	-6.48	103.41	111.70
1	D	151	GLN	N-CA-C	-6.48	104.41	112.90
1	A	319	THR	N-CA-C	-6.46	105.22	113.23
1	B	170	SER	CB-CA-C	6.43	119.91	110.26
1	B	183	GLY	N-CA-C	-6.41	105.07	112.50
1	D	185	ALA	N-CA-C	-6.37	103.59	112.45
1	C	37	LEU	N-CA-C	6.36	121.30	112.45
1	C	69	VAL	N-CA-C	6.35	119.21	108.86
1	C	42	CYS	CA-C-N	6.32	128.09	120.13
1	C	42	CYS	C-N-CA	6.32	128.09	120.13
1	C	291	ILE	CB-CA-C	-6.31	101.81	110.77
1	C	171	THR	CB-CA-C	6.25	121.00	109.70
1	D	59	ILE	N-CA-C	6.20	117.08	108.89
1	B	173	ILE	CA-C-N	-6.20	114.52	122.77
1	B	173	ILE	C-N-CA	-6.20	114.52	122.77
1	D	348	HIS	N-CA-C	-6.18	102.46	111.30
1	C	302	THR	CA-C-O	-6.18	114.33	120.82
1	D	182	LEU	CA-C-N	6.17	126.79	119.94
1	D	182	LEU	C-N-CA	6.17	126.79	119.94
1	D	203	PHE	N-CA-C	-6.17	104.48	111.14
1	B	238	GLU	CG-CD-OE1	-6.16	104.23	118.40
1	D	229	MET	N-CA-C	-6.15	104.69	111.82
1	D	239	VAL	CA-C-N	-6.13	114.36	123.00
1	D	239	VAL	C-N-CA	-6.13	114.36	123.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	249	ALA	CA-C-O	-6.13	113.92	120.42
1	C	325	PHE	N-CA-C	6.12	119.78	112.93
1	B	281	ILE	N-CA-C	6.12	116.86	111.90
1	B	284	LYS	CB-CG-CD	-6.12	97.23	111.30
1	B	291	ILE	CB-CA-C	-6.08	102.08	110.96
1	A	283	PHE	N-CA-C	6.07	119.79	112.38
1	D	144	PRO	CA-C-N	-6.07	113.37	119.56
1	D	144	PRO	C-N-CA	-6.07	113.37	119.56
1	C	300	TRP	N-CA-C	6.05	117.88	111.28
1	D	81	GLU	N-CA-C	-6.03	106.06	113.41
1	B	59	ILE	CB-CA-C	6.02	119.46	111.21
1	B	218	ASN	CA-C-N	5.98	126.08	119.87
1	B	218	ASN	C-N-CA	5.98	126.08	119.87
1	A	184	ILE	CB-CA-C	-5.97	102.59	112.26
1	B	96	VAL	N-CA-C	5.95	116.93	110.21
1	B	250	LEU	CA-C-N	5.93	128.22	120.28
1	B	250	LEU	C-N-CA	5.93	128.22	120.28
1	A	347	PRO	N-CA-C	5.91	121.52	113.84
1	D	131	VAL	CA-C-N	-5.86	113.72	119.76
1	D	131	VAL	C-N-CA	-5.86	113.72	119.76
1	B	238	GLU	OE1-CD-OE2	5.86	136.95	122.90
1	A	344	VAL	N-CA-C	5.84	116.27	107.75
1	C	140	PRO	CA-C-O	-5.82	114.56	121.67
1	D	221	GLU	N-CA-C	-5.82	105.44	113.18
1	D	302	THR	N-CA-C	5.81	117.61	111.28
1	D	42	CYS	N-CA-CB	-5.80	101.63	110.45
1	D	110	VAL	CB-CA-C	-5.79	104.49	112.24
1	C	14	ALA	N-CA-C	5.78	123.11	110.80
1	C	154	LEU	CA-CB-CG	5.77	136.49	116.30
1	C	103	CYS	N-CA-C	5.76	117.56	111.28
1	B	238	GLU	N-CA-CB	-5.76	101.69	110.33
1	D	198	SER	N-CA-C	5.73	118.00	108.20
1	A	173	ILE	CA-C-N	-5.69	115.20	122.77
1	A	173	ILE	C-N-CA	-5.69	115.20	122.77
1	C	140	PRO	N-CA-C	-5.68	102.35	111.38
1	A	65	MET	N-CA-C	5.66	117.84	110.53
1	B	170	SER	N-CA-C	-5.65	101.28	109.59
1	D	179	LEU	CB-CG-CD2	-5.64	93.76	110.70
1	A	270	PRO	CA-C-N	5.64	131.50	121.75
1	A	270	PRO	C-N-CA	5.64	131.50	121.75
1	D	202	GLU	N-CA-C	5.64	118.19	111.71
1	D	170	SER	N-CA-C	-5.64	101.30	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	74	VAL	CA-C-O	5.59	123.82	118.90
1	B	198	SER	N-CA-C	5.59	117.40	108.41
1	B	303	VAL	CB-CA-C	-5.55	104.75	112.02
1	B	121	MET	N-CA-C	-5.55	99.24	108.07
1	A	253	GLY	N-CA-C	-5.55	105.67	112.77
1	D	41	ILE	N-CA-C	5.54	116.70	108.23
1	B	39	THR	CB-CA-C	5.51	118.29	110.24
1	A	147	TYR	N-CA-C	5.49	117.72	111.02
1	C	72	GLU	N-CA-C	5.48	117.89	109.07
1	D	41	ILE	CB-CA-C	-5.47	104.34	110.96
1	B	6	GLN	N-CA-C	5.45	118.99	110.32
1	A	14	ALA	N-CA-C	5.44	122.38	110.80
1	D	6	GLN	N-CA-C	5.43	118.77	110.20
1	C	249	ALA	CA-C-N	5.39	128.28	120.79
1	C	249	ALA	C-N-CA	5.39	128.28	120.79
1	B	241	LEU	N-CA-C	5.36	117.37	108.20
1	B	145	PRO	N-CA-C	5.36	121.58	113.81
1	C	56	GLN	N-CA-C	5.35	117.11	111.28
1	B	294	ARG	O-C-N	5.33	129.65	123.41
1	B	188	LYS	N-CA-C	5.32	117.08	111.28
1	C	271	ARG	CB-CG-CD	5.26	123.40	111.30
1	D	206	LYS	N-CA-C	-5.24	105.65	111.36
1	A	169	ARG	N-CA-C	5.23	117.49	109.07
1	B	204	ARG	N-CA-C	5.22	117.72	111.71
1	B	169	ARG	N-CA-C	5.22	117.02	108.52
1	A	102	ALA	CA-C-N	5.21	127.21	120.44
1	A	102	ALA	C-N-CA	5.21	127.21	120.44
1	A	48	ILE	N-CA-C	-5.20	105.65	110.53
1	C	160	THR	N-CA-CB	5.19	117.81	110.13
1	A	138	LYS	N-CA-C	5.18	117.21	109.59
1	D	110	VAL	N-CA-C	5.18	116.65	111.00
1	C	89	ILE	N-CA-C	5.17	117.48	108.95
1	A	339	LYS	CA-CB-CG	-5.15	103.80	114.10
1	B	48	ILE	N-CA-C	-5.15	105.52	110.72
1	B	184	ILE	CB-CA-C	-5.15	105.11	112.22
1	D	154	LEU	N-CA-C	-5.15	106.16	112.90
1	B	207	LEU	N-CA-C	-5.14	105.75	112.23
1	A	249	ALA	N-CA-C	-5.13	106.18	112.90
1	A	249	ALA	CA-C-O	-5.13	113.60	119.60
1	D	264	SER	CA-C-O	5.13	125.97	120.38
1	A	339	LYS	N-CA-C	5.12	119.62	113.17
1	A	237	VAL	CA-C-N	-5.11	112.92	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	237	VAL	C-N-CA	-5.11	112.92	120.28
1	B	169	ARG	CA-CB-CG	-5.11	103.88	114.10
1	B	89	ILE	N-CA-C	5.10	117.37	108.95
1	D	63	GLN	N-CA-C	5.10	117.00	108.99
1	D	89	ILE	N-CA-C	5.10	117.17	108.86
1	A	196	ILE	CA-C-N	-5.08	116.49	123.14
1	A	196	ILE	C-N-CA	-5.08	116.49	123.14
1	C	144	PRO	N-CA-C	5.08	116.89	110.70
1	C	59	ILE	N-CA-C	5.06	115.38	107.99
1	C	137	TRP	N-CA-C	-5.04	100.24	108.76
1	B	314	LEU	N-CA-C	5.03	118.57	112.23
1	A	185	ALA	N-CA-C	-5.01	105.73	111.14
1	D	60	LYS	CA-C-N	5.01	125.54	120.38
1	D	60	LYS	C-N-CA	5.01	125.54	120.38
1	C	238	GLU	N-CA-CB	-5.01	102.59	110.30
1	D	66	GLY	N-CA-C	5.01	118.89	112.18

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	90	0
1	B	2668	0	2683	126	0
1	C	2668	0	2684	118	0
1	D	2668	0	2683	102	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	44	0	26	5	0
2	B	44	0	26	11	0
2	C	44	0	26	4	0
2	D	44	0	26	12	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	5	0
4	D	119	0	0	14	0
All	All	11389	0	10837	421	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 (421) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:B:9:MET:HE2	1:B:62:PRO:HB2	1.66	0.76
1:D:5:MET:HE2	1:D:24:VAL:HA	1.67	0.75
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:97:CYS:C	1:D:99:LYS:H	2.00	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:C:10:LYS:NZ	1:C:16:GLY:O	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
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:9:MET:HE2	1:C:62:PRO:HB2	1.77	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:210:LYS:NZ	4:C:415:HOH:O	2.34	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
1:C:46:LEU:HD22	1:C:335:MET:HE2	1.84	0.59
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:B:59:ILE:HD12	1:B:59:ILE:C	2.28	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: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:A:348:HIS:O	1:A:349:LYS:C	2.47	0.56
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:B:193:TYR:C	1:B:193:TYR:CD2	2.85	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: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:5:MET:HE2	1:D:25:PRO:CD	2.39	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:250:LEU:O	1:A:251:GLU:C	2.52	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
1:A:218:ASN:CG	1:A:221:GLU:HB3	2.36	0.51
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: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:B:52:ASN:OD1	1:B:52:ASN:C	2.54	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:C:13:PRO:O	1:C:14:ALA:C	2.54	0.49
1:B:333:GLU:CD	4:B:425:HOH:O	2.55	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:50:GLU:O	1:B:51:TRP:HB3	2.13	0.48
1:B:68:GLU:OE1	1:B:342:LYS:NZ	2.47	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
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:D:53:GLU:CD	1:D:53:GLU:H	2.20	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:D:5:MET:HE2	1:D:25:PRO:HD2	1.96	0.47
1:D:9:MET:HE2	1:D:62:PRO:HB2	1.96	0.47
1:C:26:LYS:O	1:C:27:PRO:C	2.55	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:39:THR:HA	1:A:68:GLU:O	2.15	0.46
1:B:15:TYR:CD1	1:B:50:GLU:HA	2.51	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:A:9:MET:HE2	1:A:62:PRO:HB2	1.96	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
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:B:53:GLU:CD	1:B:53:GLU:H	2.23	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: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
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:A:59:ILE:O	1:A:61:PRO:HD3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:147:TYR:O	1:B:148:ALA:C	2.59	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: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: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
1:C:58:ARG:HH22	1:C:116:ILE:HD12	1.83	0.44
1:C:97:CYS:C	1:C:99:LYS:H	2.25	0.44
1:A:51:TRP:NE1	1:A:56:GLN:HG2	2.32	0.44
1:B:97:CYS:HB3	1:B:111:CYS:HB3	1.74	0.43
1:D:97:CYS:C	1:D:99:LYS:N	2.65	0.43
1:A:184:ILE:O	1:A:184:ILE:HG22	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:147:TYR:C	1:B:149:ALA:N	2.75	0.42
1:B:150:LEU:C	1:B:153:PRO:HD2	2.44	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: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: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
1:D:250:LEU:HD23	1:D:273:VAL:HG11	2.02	0.42
1:B:295:HIS:C	1:B:296:LEU:HD23	2.45	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: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:143:MET:O	1:D:144:PRO:C	2.64	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:334:LEU:C	1:A:340:THR:HG23	2.45	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: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: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
1:C:84:GLN:O	1:C:85:VAL:C	2.64	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%)	3	3
1	B	345/350 (99%)	308 (89%)	31 (9%)	6 (2%)	7	10
1	C	345/350 (99%)	311 (90%)	26 (8%)	8 (2%)	5	6
1	D	345/350 (99%)	312 (90%)	27 (8%)	6 (2%)	7	10
All	All	1380/1400 (99%)	1244 (90%)	105 (8%)	31 (2%)	5	6

All (31) Ramachandran outliers are listed below:

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

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Mol	Chain	Res	Type
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%)	256 (90%)	27 (10%)	8	13
1	B	283/284 (100%)	254 (90%)	29 (10%)	7	11
1	C	283/284 (100%)	256 (90%)	27 (10%)	8	13
1	D	283/284 (100%)	256 (90%)	27 (10%)	8	13
All	All	1132/1136 (100%)	1022 (90%)	110 (10%)	8	12

All (110) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	MET
1	A	12	LYS
1	A	20	VAL
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	105	HIS
1	A	144	PRO
1	A	154	LEU
1	A	158	VAL
1	A	210	LYS
1	A	221	GLU
1	A	222	GLU
1	A	242	GLU

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Mol	Chain	Res	Type
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	32	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	76	VAL
1	B	97	CYS
1	B	111	CYS
1	B	134	LYS
1	B	152	GLU
1	B	158	VAL
1	B	206	LYS
1	B	210	LYS
1	B	216	VAL
1	B	226	LYS
1	B	238	GLU
1	B	242	GLU
1	B	257	VAL
1	B	258	THR
1	B	271	ARG
1	B	296	LEU
1	B	305	SER
1	B	306	LEU
1	B	333	GLU
1	B	335	MET
1	B	349	LYS
1	C	9	MET
1	C	12	LYS
1	C	13	PRO
1	C	20	VAL
1	C	34	ILE
1	C	41	ILE

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Mol	Chain	Res	Type
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	216	VAL
1	C	221	GLU
1	C	230	ASP
1	C	238	GLU
1	C	241	LEU
1	C	242	GLU
1	C	304	SER
1	C	305	SER
1	C	321	LYS
1	C	339	LYS
1	D	3	GLU
1	D	10	LYS
1	D	20	VAL
1	D	41	ILE
1	D	53	GLU
1	D	57	SER
1	D	59	ILE
1	D	60	LYS
1	D	69	VAL
1	D	76	VAL
1	D	97	CYS
1	D	110	VAL
1	D	112	GLN
1	D	114	THR
1	D	134	LYS
1	D	154	LEU
1	D	158	VAL
1	D	171	THR
1	D	182	LEU
1	D	206	LYS
1	D	210	LYS

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Mol	Chain	Res	Type
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 (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	47	HIS
1	A	94	HIS
1	A	106	ASN
1	A	112	GLN
1	A	139	ASN
1	A	156	ASN
1	A	218	ASN
1	A	289	HIS
1	A	308	GLN
1	A	348	HIS
1	B	6	GLN
1	B	63	GLN
1	B	94	HIS
1	B	112	GLN
1	B	113	ASN
1	B	139	ASN
1	B	151	GLN
1	B	279	ASN
1	B	289	HIS
1	B	320	HIS
1	B	348	HIS
1	C	6	GLN
1	C	94	HIS
1	C	106	ASN
1	C	109	HIS
1	C	113	ASN
1	C	139	ASN
1	C	156	ASN
1	C	252	GLN
1	C	289	HIS
1	C	308	GLN

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Mol	Chain	Res	Type
1	C	320	HIS
1	C	348	HIS
1	D	47	HIS
1	D	63	GLN
1	D	67	HIS
1	D	106	ASN
1	D	109	HIS
1	D	113	ASN
1	D	139	ASN
1	D	151	GLN
1	D	279	ASN
1	D	308	GLN
1	D	320	HIS
1	D	348	HIS

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](#)

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
2	NAD	D	503	-	46,48,48	2.33	13 (28%)	64,73,73	3.06	34 (53%)
3	SO4	C	351	-	4,4,4	0.23	0	6,6,6	0.44	0
3	SO4	B	354	-	4,4,4	0.79	0	6,6,6	1.12	1 (16%)
3	SO4	D	352	-	4,4,4	0.57	0	6,6,6	0.96	1 (16%)
2	NAD	C	502	-	46,48,48	2.38	13 (28%)	64,73,73	3.49	26 (40%)
3	SO4	B	351	-	4,4,4	2.25	1 (25%)	6,6,6	1.51	2 (33%)
3	SO4	C	353	-	4,4,4	0.48	0	6,6,6	1.05	1 (16%)
3	SO4	C	352	-	4,4,4	0.36	0	6,6,6	0.12	0
3	SO4	B	355	-	4,4,4	0.54	0	6,6,6	0.77	0
3	SO4	B	353	-	4,4,4	2.87	2 (50%)	6,6,6	0.86	0
2	NAD	A	500	-	46,48,48	2.53	8 (17%)	64,73,73	2.78	24 (37%)
2	NAD	B	501	-	46,48,48	3.06	12 (26%)	64,73,73	2.86	25 (39%)
3	SO4	B	352	-	4,4,4	1.53	1 (25%)	6,6,6	1.07	0
3	SO4	D	351	-	4,4,4	0.25	0	6,6,6	0.51	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	D	503	-	2/2/11/11	13/30/62/62	0/5/5/5
2	NAD	A	500	-	2/2/11/11	13/30/62/62	0/5/5/5
2	NAD	B	501	-	2/2/11/11	16/30/62/62	0/5/5/5
2	NAD	C	502	-	2/2/11/11	12/30/62/62	0/5/5/5

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	NAD	O4D-C1D	16.17	1.62	1.40
2	A	500	NAD	PN-O3	13.22	1.73	1.59
2	C	502	NAD	O4D-C1D	11.84	1.56	1.40
2	D	503	NAD	O4D-C1D	10.17	1.54	1.40
2	B	501	NAD	C2N-N1N	6.65	1.42	1.35
2	A	500	NAD	O4D-C1D	4.85	1.47	1.40
3	B	353	SO4	O1-S	4.77	1.73	1.44
2	D	503	NAD	C2N-N1N	4.37	1.39	1.35
2	B	501	NAD	C3N-C7N	4.16	1.56	1.50
2	C	502	NAD	O4D-C4D	-3.97	1.36	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	351	SO4	O1-S	3.81	1.67	1.44
2	B	501	NAD	PA-O3	3.79	1.63	1.59
2	C	502	NAD	PN-O5D	-3.45	1.45	1.59
2	B	501	NAD	PA-O1A	3.43	1.62	1.50
2	D	503	NAD	C5A-N7A	-3.40	1.32	1.39
2	C	502	NAD	PA-O3	-3.39	1.55	1.59
2	D	503	NAD	C3N-C7N	-3.34	1.45	1.50
2	A	500	NAD	PN-O5D	-3.33	1.46	1.59
2	D	503	NAD	PN-O1N	3.31	1.62	1.50
2	A	500	NAD	PA-O1A	3.14	1.61	1.50
2	C	502	NAD	C5A-N7A	-3.13	1.33	1.39
2	A	500	NAD	C1B-N9A	3.13	1.55	1.46
2	D	503	NAD	C5B-C4B	3.12	1.61	1.51
2	B	501	NAD	C5A-N7A	-3.11	1.33	1.39
2	A	500	NAD	O4D-C4D	-3.04	1.38	1.45
2	D	503	NAD	C2D-C3D	-2.85	1.45	1.53
2	D	503	NAD	C1B-N9A	2.79	1.54	1.46
3	B	353	SO4	O4-S	2.76	1.70	1.48
2	D	503	NAD	C6N-N1N	2.74	1.41	1.35
2	D	503	NAD	C2B-C1B	2.74	1.62	1.53
2	A	500	NAD	C5A-N7A	-2.72	1.34	1.39
2	D	503	NAD	O2B-C2B	2.62	1.49	1.43
2	B	501	NAD	C4A-N3A	2.59	1.39	1.34
2	C	502	NAD	C2N-N1N	2.55	1.37	1.35
2	D	503	NAD	O4D-C4D	-2.52	1.39	1.45
2	C	502	NAD	PN-O3	2.45	1.62	1.59
2	B	501	NAD	C1B-N9A	2.38	1.52	1.46
2	C	502	NAD	C2A-N1A	-2.34	1.29	1.33
2	A	500	NAD	C5B-C4B	2.23	1.58	1.51
3	B	352	SO4	O2-S	2.12	1.57	1.44
2	C	502	NAD	O7N-C7N	2.11	1.28	1.24
2	D	503	NAD	PN-O5D	-2.07	1.51	1.59
2	C	502	NAD	PN-O1N	2.05	1.57	1.50
2	B	501	NAD	C2B-C1B	2.04	1.59	1.53
2	C	502	NAD	C6N-N1N	2.04	1.40	1.35
2	C	502	NAD	PA-O1A	2.03	1.57	1.50
2	B	501	NAD	O2D-C2D	-2.02	1.38	1.43
2	B	501	NAD	O4B-C1B	-2.02	1.37	1.42
2	C	502	NAD	O2B-C2B	2.02	1.47	1.43
2	B	501	NAD	C6N-N1N	2.02	1.39	1.35

All (114) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	503	NAD	C4D-O4D-C1D	-13.21	97.83	109.92
2	C	502	NAD	C4D-O4D-C1D	-11.90	99.03	109.92
2	A	500	NAD	C4D-O4D-C1D	-11.40	99.48	109.92
2	C	502	NAD	C3N-C7N-N7N	-10.28	105.07	117.74
2	B	501	NAD	C6N-N1N-C2N	-9.01	114.22	121.88
2	C	502	NAD	C6N-N1N-C2N	-8.70	114.48	121.88
2	B	501	NAD	C4D-O4D-C1D	-8.60	102.05	109.92
2	C	502	NAD	N3A-C2A-N1A	-7.66	116.99	128.58
2	C	502	NAD	C5A-C4A-N3A	-6.69	117.50	126.72
2	B	501	NAD	N3A-C2A-N1A	-6.26	119.10	128.58
2	D	503	NAD	O2N-PN-O3	6.26	124.18	107.27
2	C	502	NAD	C2A-N3A-C4A	5.89	126.22	111.83
2	A	500	NAD	O4B-C1B-N9A	5.55	118.75	108.09
2	D	503	NAD	O4B-C1B-N9A	5.54	118.73	108.09
2	D	503	NAD	C5A-C4A-N3A	-5.42	119.26	126.72
2	A	500	NAD	N3A-C2A-N1A	-5.31	120.54	128.58
2	C	502	NAD	O2N-PN-O3	5.21	121.35	107.27
2	C	502	NAD	O7N-C7N-C3N	5.17	125.92	119.60
2	A	500	NAD	C5A-C4A-N3A	-5.17	119.60	126.72
2	A	500	NAD	O2D-C2D-C3D	-5.16	95.27	111.82
2	B	501	NAD	C5A-C4A-N3A	-5.06	119.75	126.72
2	D	503	NAD	O3-PA-O1A	-4.99	95.68	110.70
2	D	503	NAD	N3A-C4A-N9A	4.89	135.49	127.17
2	C	502	NAD	O2D-C2D-C3D	-4.89	96.15	111.82
2	C	502	NAD	N3A-C4A-N9A	4.87	135.46	127.17
2	B	501	NAD	N3A-C4A-N9A	4.72	135.20	127.17
2	C	502	NAD	C5N-C4N-C3N	-4.69	115.75	120.36
2	D	503	NAD	N3A-C2A-N1A	-4.65	121.55	128.58
2	B	501	NAD	C6N-C5N-C4N	4.64	126.14	119.45
2	B	501	NAD	O2N-PN-O3	4.54	119.55	107.27
2	B	501	NAD	O5D-PN-O1N	-4.51	91.05	108.94
2	A	500	NAD	C6N-N1N-C2N	-4.44	118.10	121.88
2	A	500	NAD	N3A-C4A-N9A	4.44	134.72	127.17
2	C	502	NAD	O7N-C7N-N7N	4.37	128.93	122.62
2	C	502	NAD	O4D-C4D-C5D	4.22	122.86	109.33
2	A	500	NAD	C2A-N3A-C4A	4.21	122.12	111.83
2	C	502	NAD	O4B-C1B-N9A	4.19	116.14	108.09
2	A	500	NAD	C3N-C7N-N7N	-4.17	112.60	117.74
2	B	501	NAD	O2D-C2D-C3D	-4.07	98.78	111.82
2	B	501	NAD	C5A-N7A-C8A	4.04	109.80	103.45
2	B	501	NAD	C5N-C4N-C3N	-4.01	116.43	120.36
2	A	500	NAD	O2N-PN-O3	3.92	117.86	107.27
2	B	501	NAD	C6N-N1N-C1D	3.81	127.21	119.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	503	NAD	C2A-N3A-C4A	3.73	120.93	111.83
2	B	501	NAD	C2A-N3A-C4A	3.71	120.90	111.83
2	D	503	NAD	C2N-C3N-C4N	3.69	122.55	118.26
2	A	500	NAD	C2D-C3D-C4D	-3.67	95.52	102.61
2	C	502	NAD	C5D-C4D-C3D	-3.65	102.06	115.21
2	D	503	NAD	O5D-C5D-C4D	-3.62	96.67	108.99
2	D	503	NAD	N9A-C8A-N7A	-3.61	108.81	113.94
2	B	501	NAD	N9A-C8A-N7A	-3.53	108.93	113.94
2	A	500	NAD	O5D-C5D-C4D	-3.50	97.08	108.99
2	A	500	NAD	O4B-C4B-C3B	-3.47	98.26	105.15
2	B	501	NAD	O4B-C1B-N9A	3.46	114.74	108.09
2	D	503	NAD	C3N-C7N-N7N	-3.41	113.54	117.74
2	B	501	NAD	C2A-N1A-C6A	3.39	124.31	118.73
2	B	501	NAD	O4B-C4B-C3B	-3.33	98.54	105.15
2	A	500	NAD	C6N-N1N-C1D	3.24	126.08	119.73
2	B	501	NAD	C3N-C7N-N7N	-3.21	113.78	117.74
2	D	503	NAD	O3D-C3D-C2D	-3.19	101.58	111.82
2	B	501	NAD	O3D-C3D-C2D	-3.19	101.60	111.82
2	D	503	NAD	O4D-C4D-C5D	3.15	119.41	109.33
2	D	503	NAD	O2D-C2D-C3D	-3.12	101.80	111.82
2	C	502	NAD	N9A-C8A-N7A	-3.12	109.51	113.94
2	D	503	NAD	N6A-C6A-N1A	3.08	125.23	118.38
2	C	502	NAD	C6N-N1N-C1D	3.06	125.72	119.73
2	D	503	NAD	C6N-N1N-C1D	3.02	125.65	119.73
2	A	500	NAD	C5A-N7A-C8A	3.01	108.18	103.45
2	A	500	NAD	N9A-C8A-N7A	-2.98	109.71	113.94
2	D	503	NAD	C5A-N7A-C8A	2.97	108.12	103.45
2	D	503	NAD	C5A-C6A-N6A	-2.96	115.96	123.29
2	D	503	NAD	C2D-C3D-C4D	-2.90	97.01	102.61
2	D	503	NAD	C5N-C4N-C3N	-2.87	117.55	120.36
2	A	500	NAD	C5N-C4N-C3N	-2.77	117.64	120.36
2	D	503	NAD	O2A-PA-O3	2.71	114.59	107.27
2	C	502	NAD	O3B-C3B-C2B	-2.69	103.19	111.82
2	C	502	NAD	C5A-N7A-C8A	2.68	107.66	103.45
2	D	503	NAD	C4B-O4B-C1B	-2.60	103.72	109.47
2	D	503	NAD	O2B-C2B-C1B	2.60	119.07	110.10
2	C	502	NAD	C2D-C3D-C4D	-2.58	97.63	102.61
2	D	503	NAD	C5N-C6N-N1N	-2.56	116.89	120.38
2	B	501	NAD	O5B-PA-O1A	-2.56	98.79	108.94
2	A	500	NAD	N6A-C6A-N1A	2.52	123.99	118.38
2	A	500	NAD	O7N-C7N-C3N	2.47	122.62	119.60
2	B	501	NAD	C4A-N9A-C8A	2.45	108.31	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	503	NAD	C2N-N1N-C1D	-2.45	113.73	119.13
3	B	351	SO4	O3-S-O2	-2.42	96.92	109.56
2	C	502	NAD	C5A-C6A-N6A	-2.38	117.39	123.29
2	C	502	NAD	O5D-C5D-C4D	-2.34	101.01	108.99
2	B	501	NAD	C4A-C5A-N7A	-2.34	107.90	110.58
2	A	500	NAD	C2B-C1B-N9A	-2.33	107.52	113.30
2	D	503	NAD	PA-O5B-C5B	2.33	134.68	121.35
2	C	502	NAD	C6N-C5N-C4N	2.30	122.77	119.45
2	D	503	NAD	C4A-N9A-C8A	2.30	108.15	105.74
2	D	503	NAD	O2N-PN-O5D	-2.28	97.21	107.57
2	C	502	NAD	O2A-PA-O5B	2.26	117.80	107.57
3	B	354	SO4	O3-S-O1	-2.25	97.77	109.56
2	A	500	NAD	O3D-C3D-C2D	-2.24	104.62	111.82
2	B	501	NAD	O3B-C3B-C4B	-2.24	104.64	111.08
2	D	503	NAD	C2N-C3N-C7N	-2.21	113.07	119.46
2	A	500	NAD	O3-PA-O1A	2.19	117.28	110.70
2	A	500	NAD	C5A-C6A-N6A	-2.18	117.89	123.29
2	D	503	NAD	O4B-C4B-C3B	-2.18	100.83	105.15
2	B	501	NAD	O7N-C7N-C3N	2.14	122.22	119.60
2	D	503	NAD	O2N-PN-O1N	2.13	122.34	112.44
3	B	351	SO4	O2-S-O1	2.12	123.98	109.06
2	D	503	NAD	C6N-C5N-C4N	2.11	122.49	119.45
2	C	502	NAD	C2A-N1A-C6A	2.11	122.19	118.73
2	B	501	NAD	C4B-O4B-C1B	-2.08	104.87	109.47
3	C	353	SO4	O4-S-O2	2.08	120.44	109.56
2	C	502	NAD	C2N-C3N-C4N	2.06	120.66	118.26
2	D	503	NAD	O7N-C7N-N7N	2.06	125.59	122.62
2	A	500	NAD	O2A-PA-O5B	2.04	116.81	107.57
3	D	352	SO4	O3-S-O1	2.02	120.14	109.56

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 (54) 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
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	C	502	NAD	O4B-C4B-C5B-O5B
2	C	502	NAD	C2N-C3N-C7N-O7N
2	C	502	NAD	C4N-C3N-C7N-N7N
2	A	500	NAD	O4B-C4B-C5B-O5B
2	A	500	NAD	C3B-C4B-C5B-O5B
2	A	500	NAD	O4D-C4D-C5D-O5D
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	C3D-C4D-C5D-O5D
2	A	500	NAD	C4N-C3N-C7N-O7N
2	A	500	NAD	C4N-C3N-C7N-N7N
2	C	502	NAD	C3D-C4D-C5D-O5D
2	D	503	NAD	C2B-C1B-N9A-C8A
2	A	500	NAD	C2B-C1B-N9A-C8A
2	C	502	NAD	C2B-C1B-N9A-C8A
2	B	501	NAD	C5B-O5B-PA-O2A
2	D	503	NAD	C5B-O5B-PA-O1A
2	D	503	NAD	C5D-O5D-PN-O2N
2	A	500	NAD	C4B-C5B-O5B-PA
2	B	501	NAD	C2B-C1B-N9A-C8A
2	A	500	NAD	C2N-C3N-C7N-O7N
2	D	503	NAD	C2B-C1B-N9A-C4A
2	B	501	NAD	C3B-C4B-C5B-O5B

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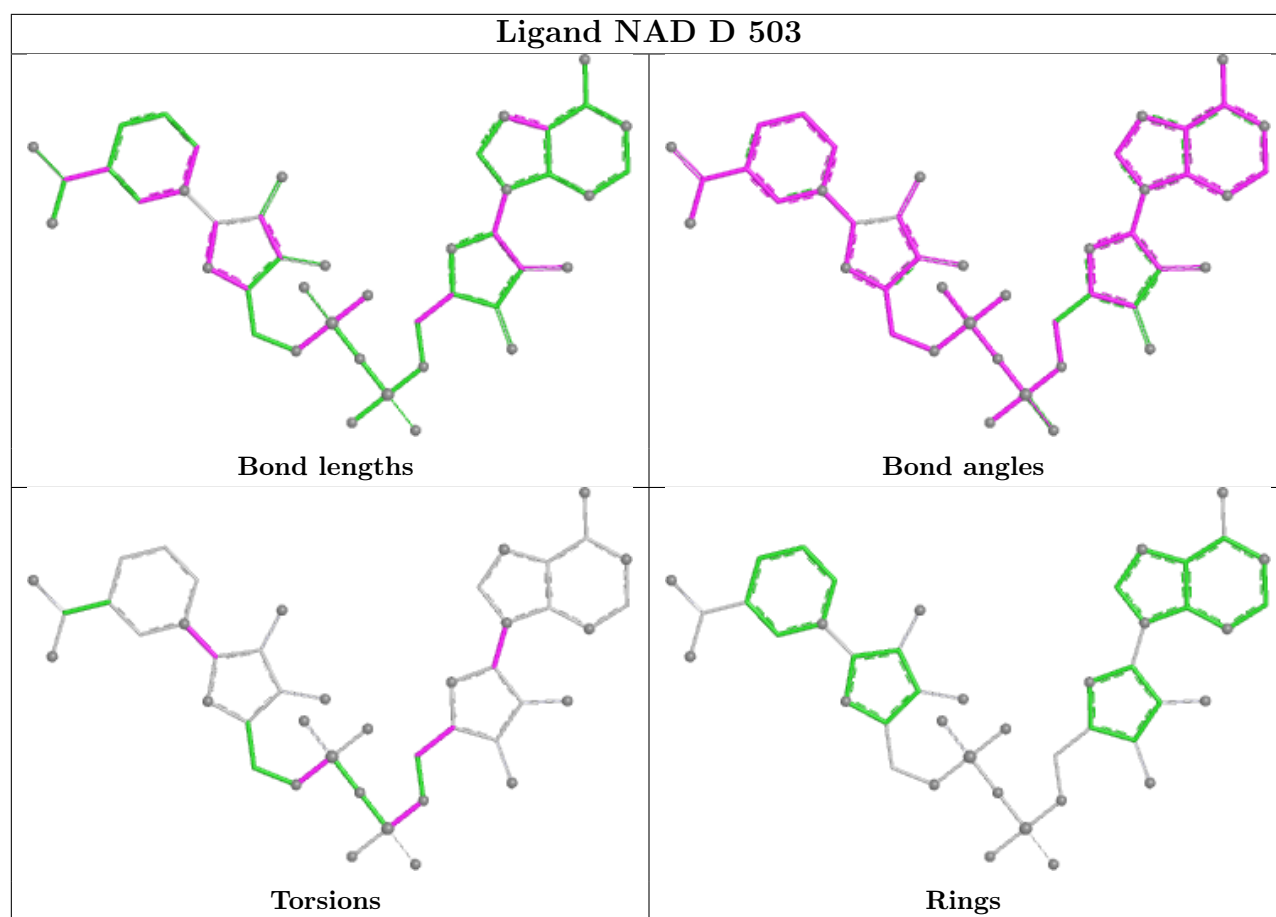
Mol	Chain	Res	Type	Atoms
2	B	501	NAD	C2D-C1D-N1N-C2N
2	C	502	NAD	O4D-C4D-C5D-O5D
2	B	501	NAD	C4B-C5B-O5B-PA
2	A	500	NAD	O4D-C1D-N1N-C2N
2	A	500	NAD	O4D-C1D-N1N-C6N
2	C	502	NAD	O4D-C1D-N1N-C2N
2	C	502	NAD	O4B-C1B-N9A-C8A
2	A	500	NAD	C2N-C3N-C7N-N7N
2	A	500	NAD	O4B-C1B-N9A-C8A
2	B	501	NAD	O4B-C1B-N9A-C8A
2	D	503	NAD	O4B-C1B-N9A-C8A
2	B	501	NAD	PA-O3-PN-O2N

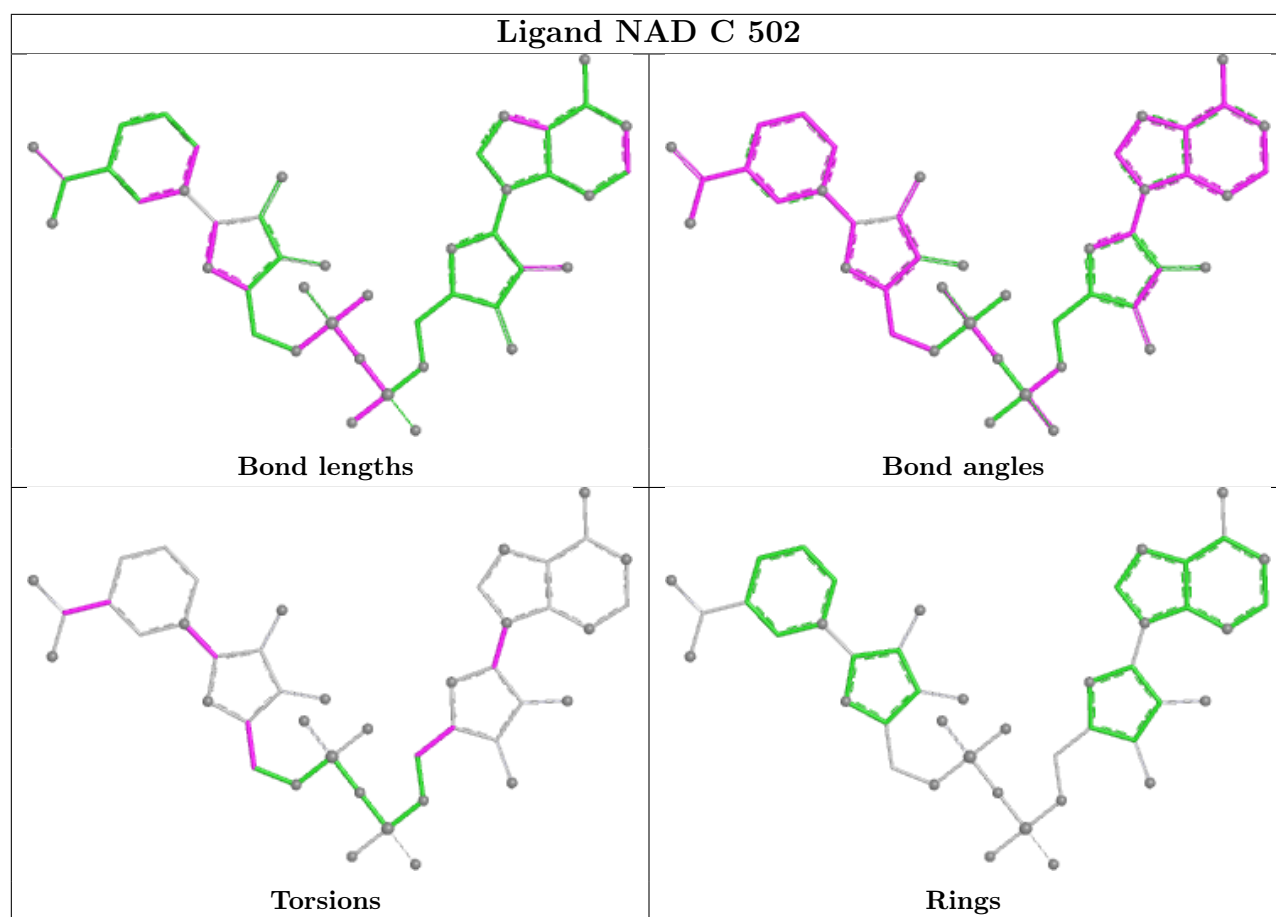
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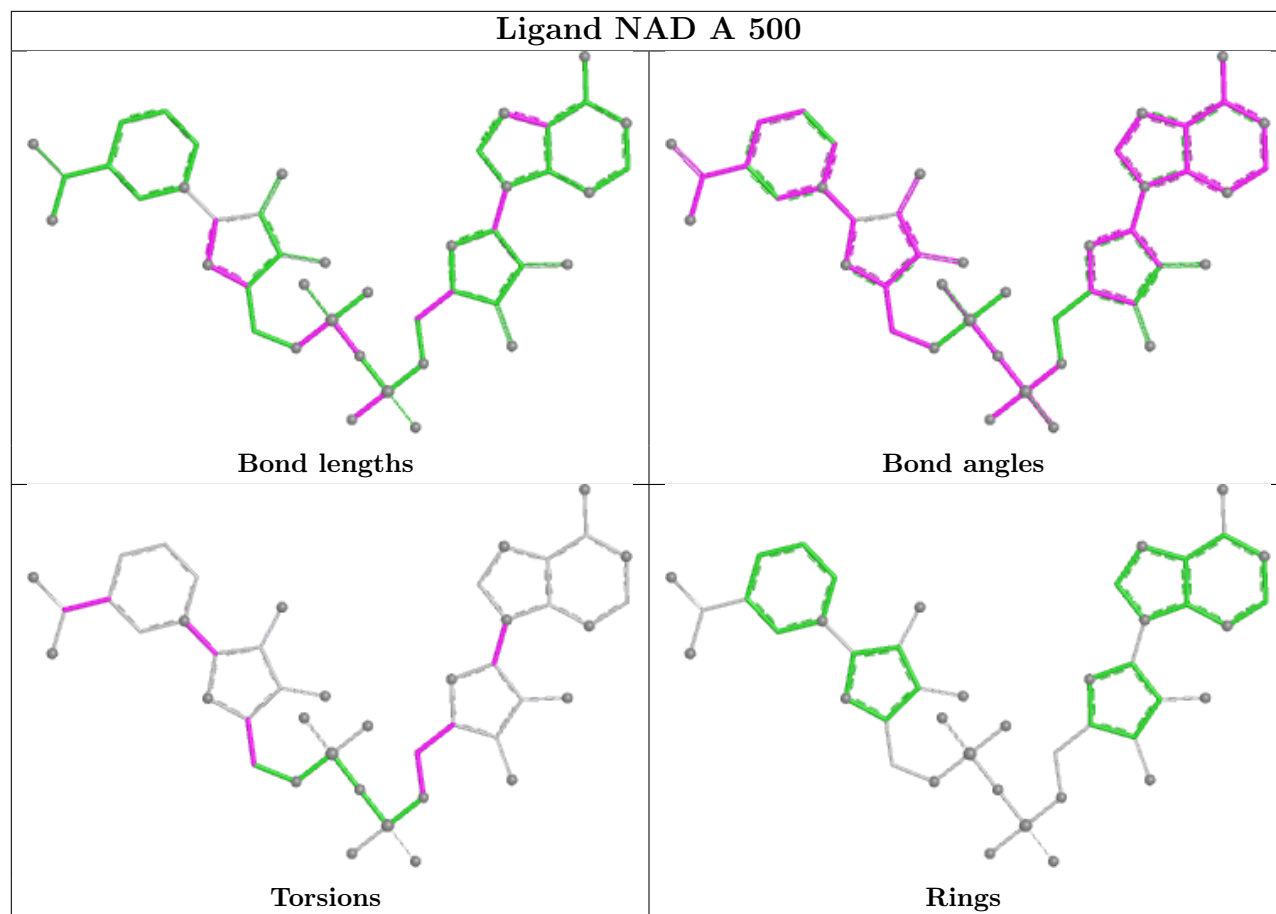
7 monomers are involved in 35 short contacts:

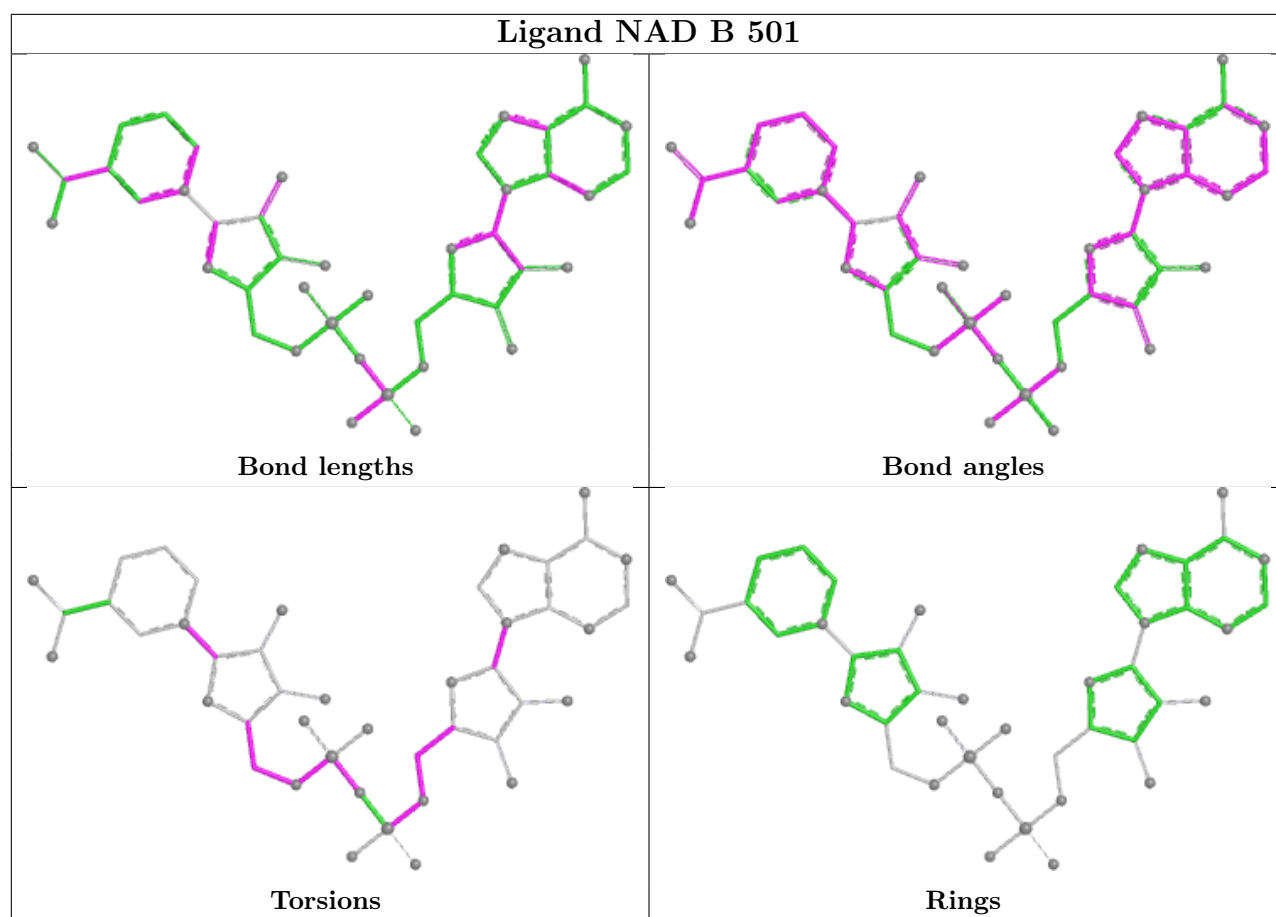
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	503	NAD	12	0
3	C	351	SO4	1	0
2	C	502	NAD	4	0
3	B	355	SO4	1	0
3	B	353	SO4	1	0
2	A	500	NAD	5	0
2	B	501	NAD	11	0

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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	347/350 (99%)	0.37	23 (6%)	24	20	15, 33, 63, 88	1 (0%)
1	B	347/350 (99%)	0.45	28 (8%)	18	14	17, 35, 76, 100	1 (0%)
1	C	347/350 (99%)	0.59	38 (10%)	10	8	17, 36, 67, 88	1 (0%)
1	D	347/350 (99%)	0.48	31 (8%)	15	12	15, 33, 72, 97	1 (0%)
All	All	1388/1400 (99%)	0.47	120 (8%)	16	13	15, 34, 69, 100	4 (0%)

All (120) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	96	VAL	8.9
1	D	96	VAL	8.7
1	A	97	CYS	7.2
1	D	97	CYS	7.2
1	B	97	CYS	6.7
1	D	106	ASN	6.6
1	D	102	ALA	6.6
1	B	106	ASN	6.3
1	D	110	VAL	6.3
1	D	114	THR	6.1
1	D	99	LYS	5.7
1	A	113	ASN	5.6
1	B	110	VAL	5.4
1	A	110	VAL	5.4
1	B	111	CYS	5.3
1	A	108	TYR	5.3
1	A	106	ASN	5.3
1	D	108	TYR	5.2
1	D	103	CYS	5.1
1	B	99	LYS	5.1
1	C	98	GLY	5.0

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Mol	Chain	Res	Type	RSRZ
1	A	103	CYS	4.9
1	D	98	GLY	4.9
1	D	111	CYS	4.8
1	A	99	LYS	4.7
1	D	101	TYR	4.7
1	B	108	TYR	4.6
1	D	109	HIS	4.6
1	A	114	THR	4.4
1	B	109	HIS	4.4
1	C	97	CYS	4.4
1	A	100	CYS	4.3
1	C	102	ALA	4.3
1	D	113	ASN	4.2
1	A	98	GLY	4.0
1	A	102	ALA	3.9
1	C	106	ASN	3.9
1	C	109	HIS	3.8
1	A	111	CYS	3.8
1	C	113	ASN	3.8
1	B	98	GLY	3.7
1	C	99	LYS	3.7
1	A	96	VAL	3.7
1	C	110	VAL	3.7
1	B	105	HIS	3.6
1	C	108	TYR	3.6
1	B	103	CYS	3.5
1	B	102	ALA	3.5
1	C	82	ASP	3.4
1	D	95	ILE	3.4
1	C	115	LYS	3.4
1	A	112	GLN	3.3
1	B	112	GLN	3.3
1	C	114	THR	3.3
1	C	59	ILE	3.3
1	D	115	LYS	3.3
1	D	105	HIS	3.3
1	B	115	LYS	3.2
1	B	107	ARG	3.1
1	D	20	VAL	3.1
1	A	109	HIS	3.0
1	B	104	LYS	3.0
1	C	116	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	117	PHE	3.0
1	C	100	CYS	3.0
1	A	115	LYS	3.0
1	B	113	ASN	2.9
1	D	119	VAL	2.9
1	C	60	LYS	2.9
1	A	59	ILE	2.9
1	D	116	ILE	2.8
1	C	80	VAL	2.8
1	C	103	CYS	2.8
1	A	107	ARG	2.8
1	C	13	PRO	2.7
1	C	76	VAL	2.7
1	B	114	THR	2.7
1	B	116	ILE	2.7
1	C	107	ARG	2.7
1	D	53	GLU	2.7
1	C	112	GLN	2.6
1	B	16	GLY	2.6
1	C	118	GLY	2.6
1	D	331	ALA	2.6
1	D	54	TRP	2.5
1	C	24	VAL	2.5
1	A	101	TYR	2.5
1	B	101	TYR	2.5
1	D	117	PHE	2.5
1	C	26	LYS	2.5
1	D	336	ARG	2.5
1	C	101	TYR	2.5
1	A	95	ILE	2.5
1	B	54	TRP	2.5
1	D	59	ILE	2.4
1	B	59	ILE	2.4
1	C	325	PHE	2.4
1	C	221	GLU	2.4
1	D	100	CYS	2.3
1	C	104	LYS	2.3
1	C	3	GLU	2.3
1	C	94	HIS	2.3
1	C	96	VAL	2.3
1	D	63	GLN	2.3
1	B	118	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	104	LYS	2.2
1	C	8	ILE	2.2
1	A	220	PHE	2.2
1	C	20	VAL	2.1
1	C	95	ILE	2.1
1	D	107	ARG	2.1
1	C	57	SER	2.1
1	C	117	PHE	2.1
1	D	121	MET	2.1
1	C	66	GLY	2.1
1	B	12	LYS	2.1
1	A	42	CYS	2.1
1	B	95	ILE	2.1
1	D	13	PRO	2.0
1	B	180	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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.

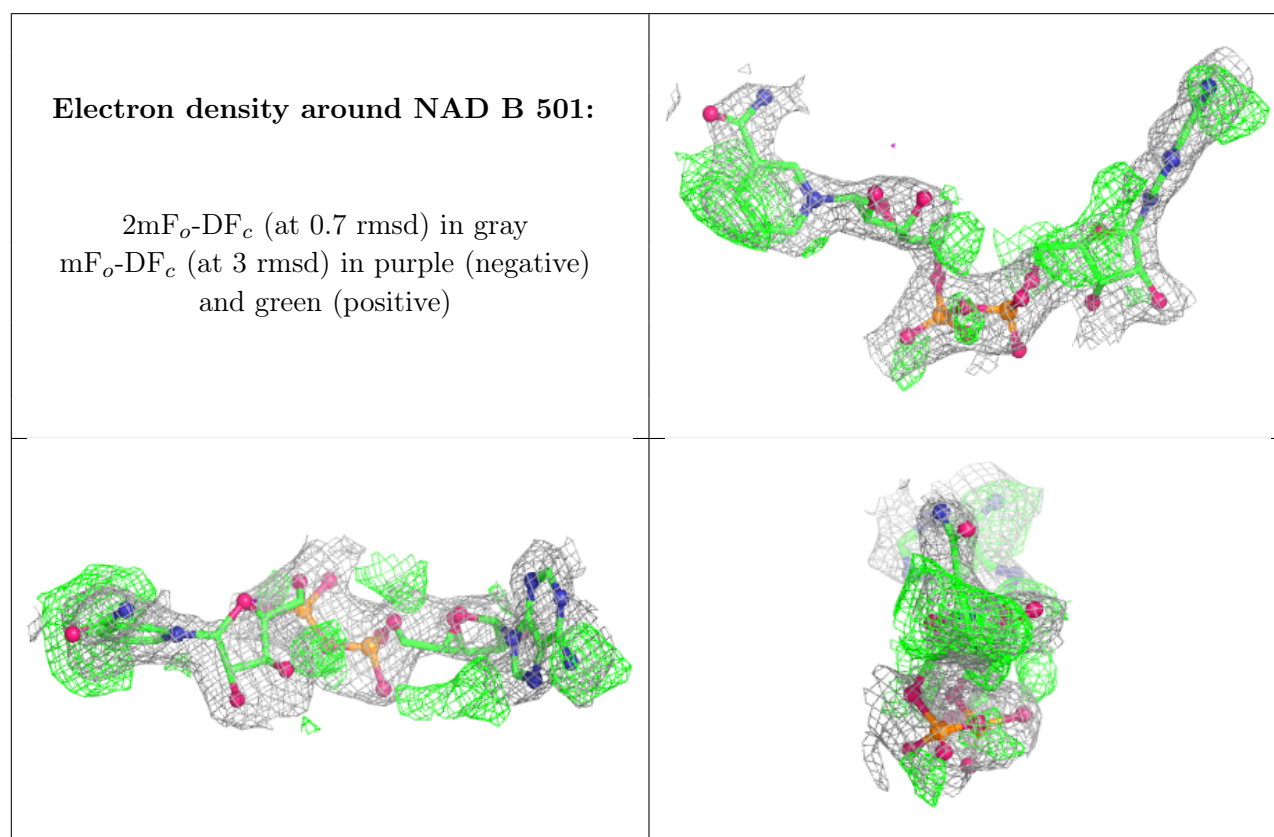
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SO4	C	351	5/5	0.63	0.13	112,112,112,113	0
3	SO4	B	354	5/5	0.69	0.28	95,96,98,99	0
3	SO4	B	351	5/5	0.70	0.34	116,117,118,118	0
3	SO4	C	353	5/5	0.70	0.23	87,88,90,90	0
3	SO4	B	353	5/5	0.74	0.27	114,115,117,117	0
3	SO4	B	352	5/5	0.74	0.25	105,106,108,109	0
3	SO4	C	352	5/5	0.75	0.18	101,101,102,102	0
3	SO4	D	351	5/5	0.79	0.23	127,128,129,131	0

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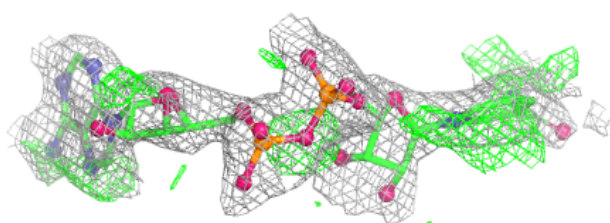
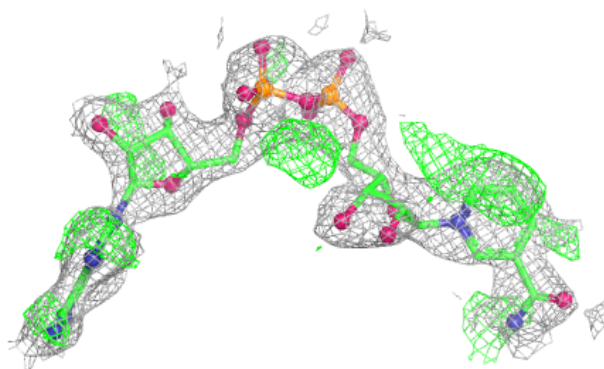
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAD	B	501	44/44	0.83	0.22	6,26,34,37	44
2	NAD	A	500	44/44	0.89	0.18	9,28,32,33	44
2	NAD	C	502	44/44	0.90	0.18	6,26,31,35	44
2	NAD	D	503	44/44	0.90	0.16	8,23,27,29	44
3	SO4	B	355	5/5	0.94	0.10	38,47,50,53	0
3	SO4	D	352	5/5	0.97	0.11	30,44,46,49	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.

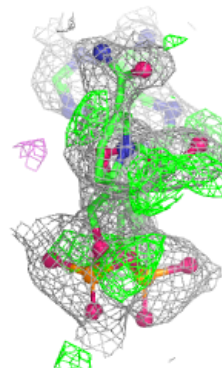
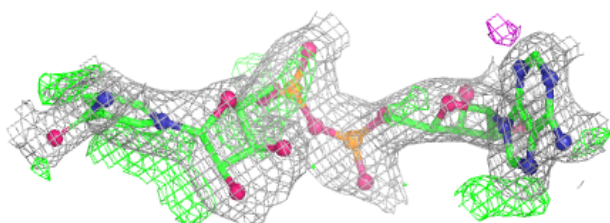
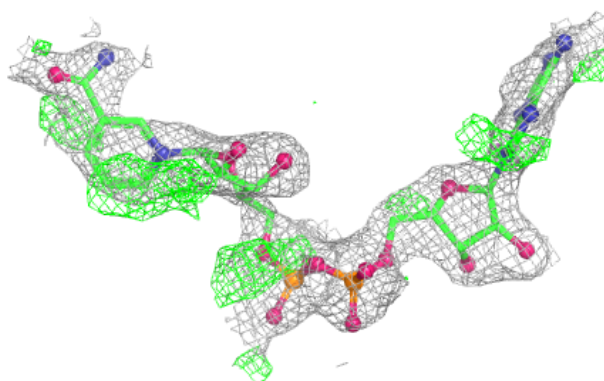


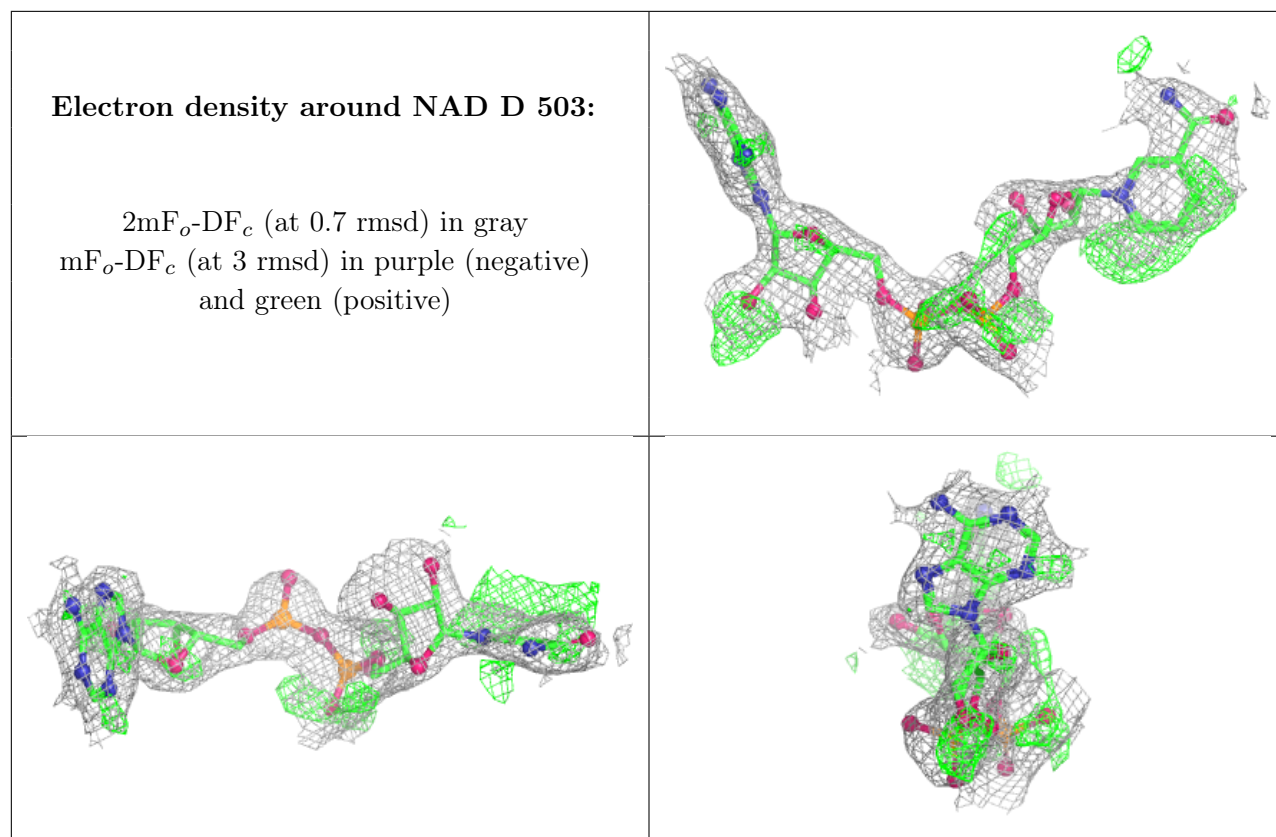
Electron density around NAD A 500:

$2mF_o-DF_c$ (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)





6.5 Other polymers ⓘ

There are no such residues in this entry.