



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:44 AM UTC

PDB ID : 3CE6 / pdb_00003ce6
Title : Crystal structure of Mycobacterium tuberculosis S-adenosyl-L-homocysteine hydrolase in ternary complex with NAD and adenosine
Authors : Reddy, M.C.M.; Gokulan, K.; Shetty, N.D.; Owen, J.L.; Ioerger, T.R.; Sacchettini, J.C.
Deposited on : 2008-02-28
Resolution : 1.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

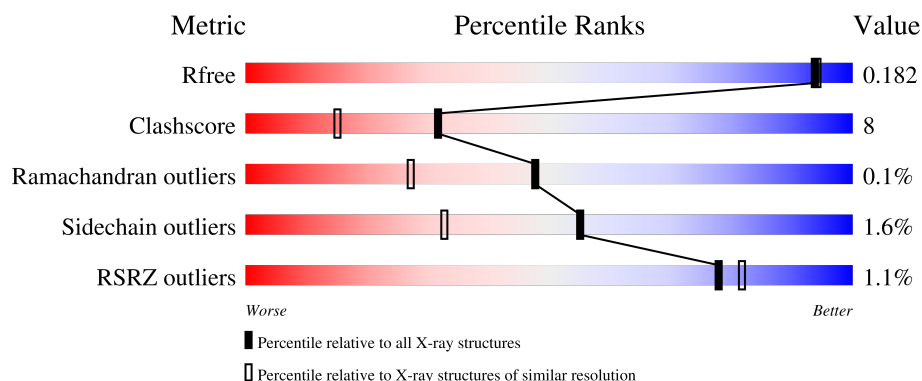
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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

Mol	Chain	Length	Quality of chain
1	A	494	77% 20% ..
1	B	494	76% 22% .
1	C	494	74% 22% ..
1	D	494	76% 19% ..

2 Entry composition [i](#)

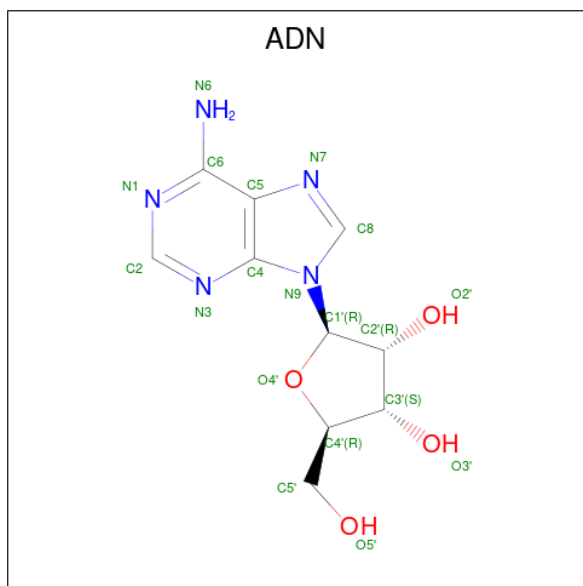
There are 4 unique types of molecules in this entry. The entry contains 16984 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Adenosylhomocysteinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	486	Total	C	N	O	S	0	0	0
			3753	2367	644	725	17			
1	B	485	Total	C	N	O	S	0	0	0
			3748	2364	643	724	17			
1	C	485	Total	C	N	O	S	0	0	0
			3748	2364	643	724	17			
1	D	485	Total	C	N	O	S	0	0	0
			3747	2363	643	724	17			

- Molecule 2 is ADENOSINE (CCD ID: ADN) (formula: $C_{10}H_{13}N_5O_4$).



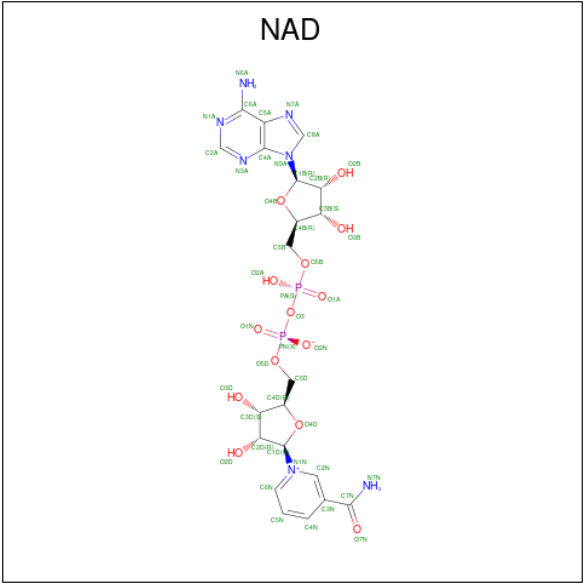
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			19	10	5	4		
2	B	1	Total	C	N	O	0	0
			19	10	5	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			19	10	5	4		
2	D	1	Total	C	N	O	0	0
			19	10	5	4		

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	446	Total	O	0	0
			446	446		
4	B	465	Total	O	0	0
			465	465		
4	C	396	Total	O	0	0
			396	396		

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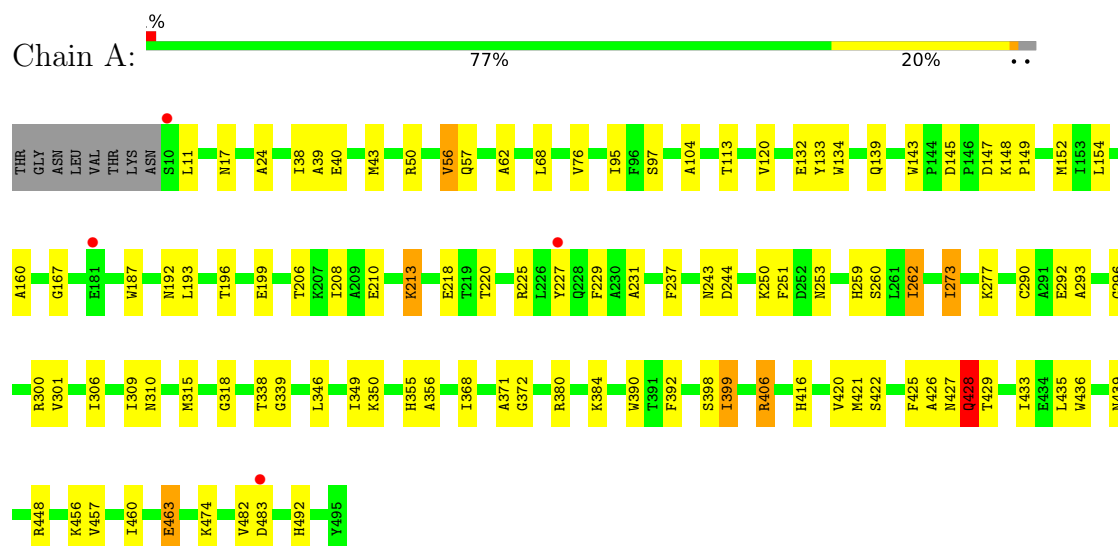
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	429	Total	O	0	0
			429	429		

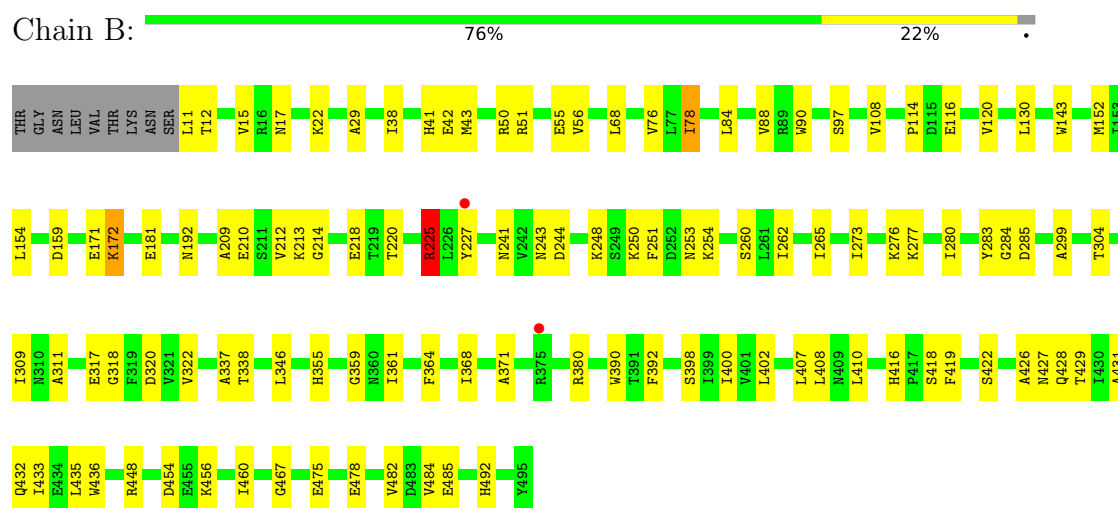
3 Residue-property plots [i](#)

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.

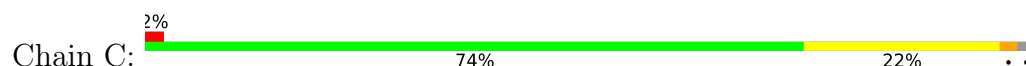
• Molecule 1: Adenosylhomocysteinase

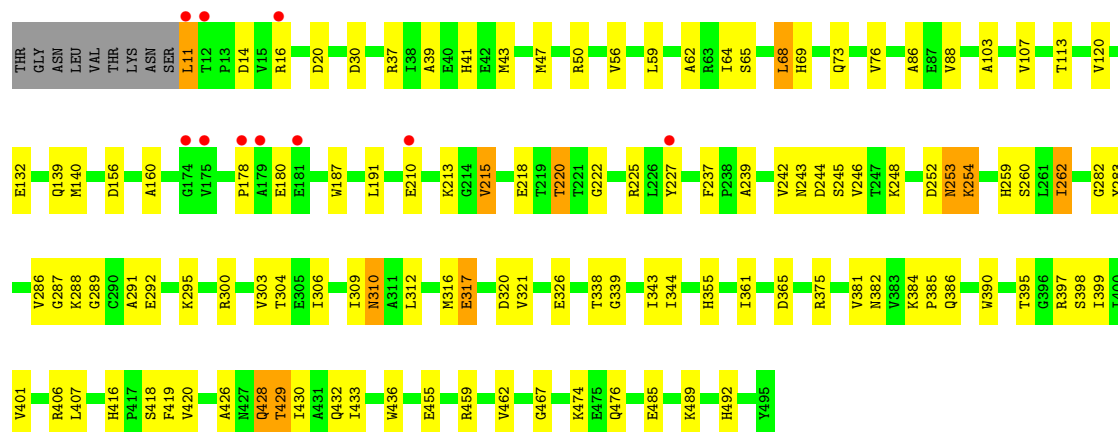


• Molecule 1: Adenosylhomocysteinase

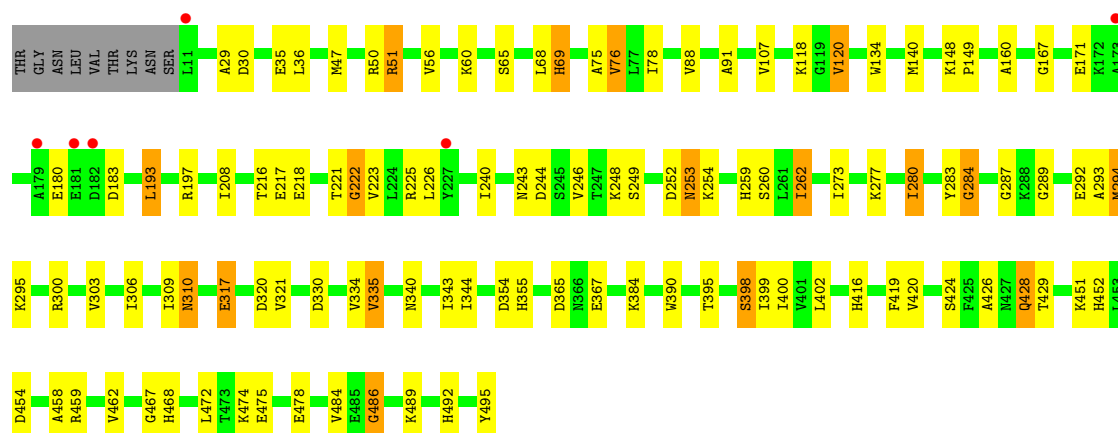
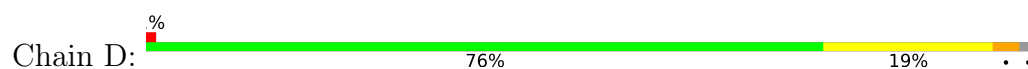


• Molecule 1: Adenosylhomocysteinase





• Molecule 1: Adenosylhomocysteinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	97.04Å 112.13Å 100.23Å 90.00° 92.41° 90.00°	Depositor
Resolution (Å)	30.00 – 1.60 30.00 – 1.60	Depositor EDS
% Data completeness (in resolution range)	97.1 (30.00-1.60) 97.1 (30.00-1.60)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.200 , 0.238 (Not available) , 0.182	Depositor DCC
R_{free} test set	16448 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å ²)	14.7	Xtriage
Anisotropy	0.622	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 40.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for l,k,-h 0.076 for h,-k,-l 0.004 for l,-k,h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16984	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.54% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ADN, 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	1.89	51/3829 (1.3%)	1.53	24/5193 (0.5%)
1	B	1.87	54/3824 (1.4%)	1.51	17/5186 (0.3%)
1	C	1.74	42/3824 (1.1%)	1.44	19/5186 (0.4%)
1	D	1.81	52/3822 (1.4%)	1.44	14/5182 (0.3%)
All	All	1.83	199/15299 (1.3%)	1.48	74/20747 (0.4%)

All (199) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	294	MET	SD-CE	-10.34	1.53	1.79
1	B	309	ILE	CA-CB	-9.83	1.43	1.54
1	B	38	ILE	CA-CB	-9.79	1.43	1.54
1	D	262	ILE	C-O	-9.78	1.12	1.24
1	A	426	ALA	N-CA	8.72	1.56	1.46
1	A	76	VAL	N-CA	8.54	1.56	1.46
1	A	57	GLN	C-O	8.52	1.27	1.23
1	D	246	VAL	C-O	-7.91	1.15	1.24
1	A	120	VAL	N-CA	-7.73	1.39	1.46
1	D	76	VAL	N-CA	7.54	1.55	1.46
1	A	309	ILE	CA-CB	-7.51	1.45	1.54
1	A	293	ALA	CA-CB	-7.50	1.41	1.53
1	D	309	ILE	CA-CB	-7.47	1.46	1.54
1	A	251	PHE	N-CA	7.47	1.53	1.46
1	A	421	MET	C-O	7.47	1.33	1.24
1	D	160	ALA	C-O	7.40	1.32	1.24
1	D	429	THR	N-CA	7.27	1.55	1.46
1	B	304	THR	N-CA	7.24	1.54	1.45
1	A	56	VAL	CA-CB	7.22	1.63	1.54
1	A	38	ILE	CA-CB	-7.21	1.45	1.54
1	C	382	ASN	C-O	-7.19	1.15	1.23
1	D	309	ILE	N-CA	7.12	1.55	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	222	GLY	C-O	7.09	1.32	1.23
1	C	254	LYS	CA-C	7.04	1.59	1.53
1	D	223	VAL	CA-CB	6.99	1.63	1.54
1	C	220	THR	C-O	6.94	1.32	1.24
1	D	287	GLY	N-CA	6.93	1.54	1.45
1	A	62	ALA	CA-CB	6.89	1.63	1.53
1	B	251	PHE	N-CA	6.87	1.54	1.46
1	B	368	ILE	CA-CB	-6.86	1.46	1.54
1	D	262	ILE	CG1-CD1	-6.84	1.25	1.51
1	C	309	ILE	CA-CB	-6.84	1.46	1.54
1	D	107	VAL	CA-CB	-6.82	1.45	1.54
1	C	426	ALA	CA-CB	6.80	1.64	1.53
1	D	222	GLY	C-O	6.75	1.31	1.23
1	B	241	ASN	CA-C	6.73	1.61	1.52
1	C	246	VAL	C-O	-6.71	1.16	1.24
1	B	426	ALA	N-CA	6.68	1.54	1.46
1	D	284	GLY	C-O	6.62	1.30	1.23
1	A	120	VAL	CA-C	6.58	1.58	1.52
1	A	448	ARG	C-O	6.58	1.32	1.23
1	D	29	ALA	CA-CB	6.57	1.63	1.53
1	D	216	THR	N-CA	6.54	1.54	1.46
1	C	429	THR	N-CA	6.52	1.54	1.46
1	B	15	VAL	CA-CB	6.47	1.62	1.54
1	B	120	VAL	CA-C	6.46	1.58	1.52
1	B	448	ARG	C-O	6.44	1.32	1.23
1	C	309	ILE	N-CA	6.42	1.54	1.46
1	B	50	ARG	N-CA	6.40	1.54	1.46
1	B	402	LEU	N-CA	6.40	1.54	1.46
1	C	287	GLY	C-O	6.38	1.31	1.23
1	D	120	VAL	N-CA	6.37	1.52	1.46
1	A	339	GLY	C-O	6.36	1.33	1.24
1	B	454	ASP	N-CA	6.35	1.54	1.46
1	C	430	ILE	N-CA	6.34	1.54	1.46
1	A	371	ALA	CA-C	6.33	1.60	1.52
1	B	410	LEU	N-CA	6.25	1.54	1.46
1	D	287	GLY	C-O	6.24	1.31	1.23
1	D	426	ALA	N-CA	6.24	1.54	1.46
1	C	310	ASN	CG-OD1	6.20	1.35	1.23
1	D	335	VAL	C-O	6.19	1.30	1.24
1	D	402	LEU	CA-CB	6.17	1.62	1.53
1	C	76	VAL	N-CA	6.16	1.53	1.46
1	D	344	ILE	CA-CB	6.16	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	359	GLY	N-CA	6.15	1.50	1.45
1	D	395	THR	C-O	6.15	1.31	1.24
1	B	265	ILE	CA-CB	6.14	1.62	1.54
1	D	160	ALA	N-CA	6.11	1.53	1.46
1	A	456	LYS	C-O	-6.11	1.17	1.24
1	A	76	VAL	CA-C	6.08	1.60	1.52
1	C	395	THR	CA-CB	6.06	1.62	1.54
1	B	76	VAL	N-CA	6.05	1.53	1.46
1	A	104	ALA	N-CA	6.04	1.53	1.46
1	D	424	SER	C-O	6.04	1.31	1.24
1	A	429	THR	N-CA	6.04	1.53	1.46
1	C	215	VAL	N-CA	6.03	1.53	1.46
1	D	197	ARG	CA-C	6.02	1.60	1.52
1	D	398	SER	C-O	5.98	1.31	1.23
1	A	225	ARG	CZ-NH1	5.98	1.41	1.32
1	B	392	PHE	N-CA	5.97	1.53	1.46
1	C	375	ARG	N-CA	5.97	1.53	1.46
1	D	458	ALA	N-CA	5.96	1.53	1.46
1	D	221	THR	CA-CB	-5.96	1.44	1.53
1	A	139	GLN	N-CA	5.94	1.53	1.46
1	B	209	ALA	N-CA	5.93	1.53	1.46
1	C	459	ARG	CB-CG	-5.93	1.34	1.52
1	D	468	HIS	CA-C	-5.93	1.45	1.52
1	B	454	ASP	CA-C	-5.92	1.45	1.52
1	A	192	ASN	N-CA	5.92	1.53	1.46
1	C	120	VAL	N-CA	5.91	1.52	1.46
1	A	160	ALA	CA-CB	5.87	1.62	1.53
1	A	296	GLY	N-CA	5.86	1.53	1.45
1	C	344	ILE	CA-CB	5.84	1.61	1.53
1	D	253	ASN	C-O	-5.84	1.17	1.24
1	B	322	VAL	N-CA	5.81	1.53	1.46
1	D	280	ILE	CA-CB	5.81	1.61	1.54
1	B	482	VAL	CA-CB	5.78	1.63	1.54
1	A	433	ILE	N-CA	5.78	1.53	1.46
1	B	276	LYS	CA-C	5.76	1.60	1.52
1	A	231	ALA	N-CA	5.75	1.53	1.46
1	D	459	ARG	CB-CG	-5.71	1.35	1.52
1	B	280	ILE	CA-CB	5.71	1.61	1.54
1	C	47	MET	CA-C	5.70	1.60	1.52
1	B	299	ALA	CA-CB	5.68	1.62	1.53
1	D	289	GLY	N-CA	5.67	1.52	1.45
1	B	433	ILE	N-CA	5.65	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	489	LYS	C-O	5.65	1.31	1.24
1	A	301	VAL	CA-CB	-5.62	1.47	1.54
1	B	418	SER	C-O	5.61	1.31	1.24
1	A	425	PHE	C-O	5.58	1.31	1.24
1	A	40	GLU	C-O	-5.56	1.17	1.24
1	A	399	ILE	N-CA	5.52	1.52	1.46
1	C	225	ARG	CZ-NH2	5.50	1.40	1.33
1	D	284	GLY	N-CA	5.50	1.51	1.45
1	C	245	SER	N-CA	5.50	1.53	1.46
1	A	24	ALA	CA-C	5.48	1.59	1.52
1	D	91	ALA	N-CA	5.47	1.52	1.45
1	C	476	GLN	N-CA	5.46	1.52	1.46
1	A	460	ILE	N-CA	5.46	1.53	1.46
1	B	114	PRO	CA-C	5.46	1.60	1.52
1	B	364	PHE	C-O	5.45	1.30	1.23
1	C	253	ASN	CG-ND2	5.45	1.44	1.33
1	A	262	ILE	CA-CB	-5.43	1.46	1.54
1	C	381	VAL	C-O	5.42	1.30	1.24
1	C	320	ASP	C-O	5.42	1.30	1.23
1	D	395	THR	CA-CB	5.42	1.62	1.53
1	B	254	LYS	CA-C	5.41	1.58	1.53
1	B	90	TRP	N-CA	5.39	1.52	1.45
1	A	113	THR	CA-C	5.39	1.57	1.52
1	D	300	ARG	CA-CB	5.38	1.59	1.53
1	B	431	ALA	CA-CB	5.37	1.61	1.53
1	B	467	GLY	CA-C	5.37	1.57	1.52
1	B	364	PHE	N-CA	5.36	1.52	1.45
1	C	215	VAL	C-O	5.36	1.29	1.24
1	D	310	ASN	CG-OD1	5.36	1.33	1.23
1	B	143	TRP	CA-C	5.35	1.59	1.53
1	A	483	ASP	CB-CG	5.34	1.65	1.52
1	B	192	ASN	N-CA	5.34	1.52	1.46
1	B	225	ARG	CB-CG	-5.34	1.36	1.52
1	D	400	ILE	C-O	5.34	1.29	1.24
1	B	432	GLN	CA-C	5.32	1.59	1.52
1	C	289	GLY	N-CA	5.32	1.52	1.45
1	A	392	PHE	N-CA	5.32	1.53	1.46
1	A	457	VAL	CA-CB	-5.30	1.48	1.54
1	B	337	ALA	CA-CB	5.30	1.61	1.53
1	D	226	LEU	CG-CD2	5.30	1.70	1.52
1	B	212	VAL	C-O	5.29	1.29	1.24
1	B	172	LYS	N-CA	5.28	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	354	ASP	C-O	5.28	1.30	1.23
1	D	249	SER	CB-OG	5.28	1.52	1.42
1	A	315	MET	CA-C	5.28	1.59	1.52
1	D	320	ASP	N-CA	5.27	1.52	1.46
1	D	451	LYS	N-CA	5.27	1.52	1.46
1	C	365	ASP	N-CA	5.24	1.53	1.46
1	C	237	PHE	C-O	-5.24	1.18	1.24
1	C	312	LEU	CA-C	5.24	1.59	1.52
1	C	107	VAL	CB-CG1	5.23	1.69	1.52
1	A	17	ASN	CG-OD1	5.23	1.33	1.23
1	D	454	ASP	C-O	5.23	1.30	1.24
1	B	456	LYS	CA-C	5.23	1.59	1.52
1	A	368	ILE	CA-C	5.23	1.58	1.52
1	B	460	ILE	C-O	5.23	1.30	1.24
1	A	143	TRP	CA-C	5.22	1.59	1.52
1	C	291	ALA	CA-CB	5.22	1.61	1.53
1	B	159	ASP	N-CA	5.22	1.52	1.46
1	A	482	VAL	C-O	5.21	1.29	1.23
1	D	334	VAL	CA-CB	5.21	1.61	1.54
1	D	208	ILE	N-CA	5.20	1.52	1.46
1	A	97	SER	CA-CB	-5.19	1.45	1.53
1	C	282	GLY	C-O	5.18	1.30	1.23
1	D	484	VAL	C-O	5.17	1.30	1.24
1	C	246	VAL	CA-C	5.15	1.59	1.52
1	A	50	ARG	N-CA	5.15	1.52	1.46
1	B	484	VAL	CA-C	5.14	1.59	1.52
1	C	286	VAL	N-CA	5.14	1.52	1.46
1	D	51	ARG	C-O	5.14	1.30	1.24
1	C	113	THR	N-CA	5.13	1.49	1.46
1	C	304	THR	CA-C	5.13	1.59	1.52
1	B	97	SER	N-CA	5.12	1.52	1.46
1	B	220	THR	CB-OG1	5.11	1.51	1.43
1	C	419	PHE	N-CA	5.10	1.52	1.46
1	B	171	GLU	N-CA	5.09	1.52	1.46
1	A	420	VAL	CA-CB	-5.09	1.48	1.54
1	D	317	GLU	CA-C	5.08	1.60	1.52
1	A	237	PHE	C-O	-5.08	1.18	1.24
1	A	356	ALA	N-CA	5.08	1.52	1.46
1	A	463	GLU	C-O	5.07	1.30	1.24
1	C	62	ALA	CA-CB	5.06	1.61	1.53
1	B	17	ASN	CA-C	5.05	1.59	1.52
1	B	371	ALA	N-CA	5.04	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	160	ALA	N-CA	5.04	1.52	1.46
1	A	346	LEU	CA-C	5.03	1.59	1.52
1	B	12	THR	CA-CB	5.03	1.61	1.54
1	A	229	PHE	N-CA	5.01	1.52	1.46
1	A	187	TRP	CA-C	5.01	1.59	1.52
1	B	78	ILE	N-CA	5.01	1.52	1.46
1	B	346	LEU	CA-C	5.00	1.59	1.52
1	B	309	ILE	N-CA	5.00	1.52	1.46
1	D	419	PHE	N-CA	5.00	1.52	1.46

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	152	MET	CG-SD-CE	-18.23	60.80	100.90
1	A	406	ARG	CD-NE-CZ	13.49	143.28	124.40
1	A	406	ARG	CG-CD-NE	-12.57	84.34	112.00
1	A	406	ARG	CB-CG-CD	12.32	139.63	111.30
1	A	406	ARG	NE-CZ-NH2	-8.34	111.69	119.20
1	A	338	THR	N-CA-C	7.55	122.62	113.41
1	C	225	ARG	NE-CZ-NH1	-7.51	113.99	121.50
1	C	262	ILE	CB-CG1-CD1	-7.50	98.06	113.80
1	C	489	LYS	O-C-N	7.36	128.13	121.80
1	B	429	THR	N-CA-C	-7.19	103.38	111.14
1	D	489	LYS	O-C-N	7.12	127.92	121.80
1	A	225	ARG	NE-CZ-NH2	-6.89	113.00	119.20
1	A	220	THR	CA-C-O	-6.70	113.44	120.55
1	A	309	ILE	N-CA-C	-6.65	104.28	110.53
1	C	50	ARG	N-CA-C	-6.57	104.04	111.07
1	D	50	ARG	N-CA-C	-6.53	104.16	111.28
1	D	384	LYS	CA-C-N	-6.38	113.19	119.76
1	D	384	LYS	C-N-CA	-6.38	113.19	119.76
1	D	317	GLU	CB-CG-CD	6.35	123.40	112.60
1	C	103	ALA	N-CA-C	-6.30	104.33	111.07
1	D	462	VAL	N-CA-C	-6.29	104.38	110.42
1	A	292	GLU	N-CA-C	-6.18	104.62	111.36
1	A	384	LYS	CA-C-N	-6.16	113.41	119.76
1	A	384	LYS	C-N-CA	-6.16	113.41	119.76
1	C	76	VAL	N-CA-C	-6.11	104.55	110.72
1	D	294	MET	CG-SD-CE	-6.11	87.46	100.90
1	C	406	ARG	NE-CZ-NH1	-6.09	115.41	121.50
1	C	365	ASP	N-CA-C	6.02	120.09	112.87
1	D	240	ILE	O-C-N	5.98	129.46	123.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	361	ILE	CB-CA-C	5.96	117.49	110.93
1	B	400	ILE	N-CA-C	-5.92	99.34	107.99
1	C	225	ARG	NE-CZ-NH2	5.87	124.48	119.20
1	D	426	ALA	N-CA-C	-5.79	105.04	111.36
1	A	273	ILE	N-CA-C	-5.71	106.90	111.81
1	D	486	GLY	C-N-CA	5.67	125.57	119.85
1	B	361	ILE	CB-CA-C	5.66	117.16	110.93
1	C	386	GLN	CA-C-N	-5.64	115.15	122.99
1	C	386	GLN	C-N-CA	-5.64	115.15	122.99
1	C	467	GLY	N-CA-C	-5.62	105.06	112.82
1	D	35	GLU	N-CA-C	5.61	117.48	111.36
1	A	349	ILE	N-CA-C	5.60	116.33	110.62
1	C	326	GLU	N-CA-C	5.56	118.27	111.82
1	A	315	MET	CA-CB-CG	-5.53	103.04	114.10
1	B	426	ALA	N-CA-C	-5.53	105.16	111.07
1	A	372	GLY	O-C-N	-5.51	116.90	122.19
1	B	51	ARG	N-CA-C	-5.48	105.39	111.36
1	B	318	GLY	CA-C-N	-5.47	115.28	122.99
1	B	318	GLY	C-N-CA	-5.47	115.28	122.99
1	C	309	ILE	N-CA-C	-5.45	105.40	110.53
1	B	154	LEU	N-CA-C	-5.44	98.33	108.02
1	A	426	ALA	N-CA-C	-5.44	105.25	111.07
1	B	210	GLU	N-CA-C	5.38	117.14	111.28
1	C	317	GLU	CA-CB-CG	-5.35	103.40	114.10
1	B	311	ALA	O-C-N	5.34	127.57	122.07
1	B	116	GLU	CB-CG-CD	5.33	121.66	112.60
1	C	407	LEU	CB-CA-C	5.28	118.14	109.90
1	B	338	THR	N-CA-C	5.27	119.84	113.41
1	A	318	GLY	CA-C-N	-5.22	115.62	122.99
1	A	318	GLY	C-N-CA	-5.22	115.62	122.99
1	D	225	ARG	CG-CD-NE	-5.22	100.52	112.00
1	A	167	GLY	N-CA-C	-5.21	106.47	112.73
1	D	148	LYS	O-C-N	5.19	125.44	121.23
1	A	428	GLN	CA-CB-CG	-5.18	103.75	114.10
1	A	439	ASN	N-CA-C	5.16	117.57	111.33
1	A	300	ARG	NE-CZ-NH1	5.15	126.65	121.50
1	A	208	ILE	O-C-N	5.13	126.94	121.91
1	B	130	LEU	N-CA-C	5.12	116.86	111.28
1	C	462	VAL	N-CA-C	-5.12	105.50	110.42
1	D	365	ASP	N-CA-C	5.07	118.95	112.87
1	B	284	GLY	CA-C-N	-5.04	113.14	120.29
1	B	284	GLY	C-N-CA	-5.04	113.14	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	242	VAL	N-CA-C	-5.02	105.28	112.35
1	A	290	CYS	N-CA-C	-5.01	105.71	111.07
1	B	346	LEU	N-CA-C	5.00	117.11	111.11

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3753	0	3695	41	0
1	B	3748	0	3693	43	0
1	C	3748	0	3693	81	0
1	D	3747	0	3690	78	0
2	A	19	0	13	1	0
2	B	19	0	13	1	0
2	C	19	0	13	1	0
2	D	19	0	13	1	0
3	A	44	0	26	1	0
3	B	44	0	26	1	0
3	C	44	0	26	6	0
3	D	44	0	26	2	0
4	A	446	0	0	20	0
4	B	465	0	0	25	0
4	C	396	0	0	40	0
4	D	429	0	0	45	0
All	All	16984	0	14927	245	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 8.

All (245) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:343:ILE:HG21	4:D:1453:HOH:O	1.26	1.35

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:306:ILE:HG12	4:C:1347:HOH:O	1.21	1.31
1:C:321:VAL:CG1	4:D:1454:HOH:O	1.74	1.29
3:C:550:NAD:C3D	4:C:1355:HOH:O	1.81	1.26
3:C:550:NAD:H3D	4:C:1355:HOH:O	1.33	1.26
1:B:78:ILE:HG23	4:B:1024:HOH:O	1.33	1.26
1:B:84:LEU:HG	4:B:1025:HOH:O	1.07	1.24
1:D:306:ILE:HG12	4:D:1447:HOH:O	1.34	1.23
1:D:317:GLU:HG2	4:D:1340:HOH:O	1.34	1.21
1:A:463:GLU:HG2	4:A:946:HOH:O	1.40	1.21
1:D:306:ILE:CD1	4:D:1447:HOH:O	1.86	1.20
1:C:37:ARG:HD3	4:C:1280:HOH:O	1.38	1.18
1:B:227:TYR:OH	4:B:1006:HOH:O	1.59	1.17
1:D:452:HIS:HB2	4:D:1468:HOH:O	1.44	1.14
1:C:16:ARG:HD3	4:C:1276:HOH:O	1.51	1.10
1:C:401:VAL:HG23	4:C:1357:HOH:O	0.93	1.10
1:D:254:LYS:HD3	4:D:1448:HOH:O	1.48	1.09
1:C:474:LYS:HD2	4:C:1325:HOH:O	1.53	1.09
1:A:227:TYR:OH	4:A:976:HOH:O	1.60	1.07
1:D:306:ILE:CG1	4:D:1447:HOH:O	1.87	1.06
1:C:39:ALA:HB1	1:C:43:MET:HE3	1.06	1.04
1:C:39:ALA:HB1	1:C:43:MET:CE	1.88	1.04
1:D:474:LYS:HD2	4:D:1384:HOH:O	1.60	1.00
1:B:262:ILE:HD13	4:B:936:HOH:O	1.64	0.97
1:C:56:VAL:HG23	4:C:1265:HOH:O	1.62	0.97
1:A:250:LYS:NZ	4:A:970:HOH:O	1.82	0.96
1:C:288:LYS:HE3	4:C:1283:HOH:O	0.75	0.92
1:D:280:ILE:HG23	4:D:1449:HOH:O	1.69	0.91
1:D:262:ILE:HD11	1:D:294:MET:HE2	1.50	0.91
1:A:56:VAL:HG23	4:A:851:HOH:O	1.72	0.88
1:D:474:LYS:CD	4:D:1384:HOH:O	2.19	0.87
1:B:84:LEU:CD2	4:B:1025:HOH:O	2.17	0.87
1:C:474:LYS:CD	4:C:1325:HOH:O	2.16	0.87
1:C:398:SER:O	1:C:399:ILE:HD13	1.75	0.86
1:D:262:ILE:HD11	1:D:294:MET:CE	2.04	0.86
1:D:262:ILE:CD1	1:D:294:MET:CE	2.55	0.84
1:C:338:THR:HG23	4:C:1354:HOH:O	1.78	0.83
1:C:306:ILE:CG1	4:C:1347:HOH:O	1.95	0.83
1:C:39:ALA:CB	1:C:43:MET:HE3	2.01	0.83
1:D:343:ILE:CG2	4:D:1453:HOH:O	2.00	0.82
1:C:43:MET:HE2	1:C:418:SER:HB3	1.62	0.81
1:D:56:VAL:HG23	4:D:1317:HOH:O	1.79	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:478:GLU:HG3	4:D:1421:HOH:O	1.79	0.81
1:D:467:GLY:O	4:D:1452:HOH:O	2.00	0.80
1:D:262:ILE:CD1	1:D:294:MET:HE1	2.11	0.79
1:D:149:PRO:HG3	4:D:1354:HOH:O	1.82	0.78
1:C:399:ILE:HD11	4:C:1248:HOH:O	1.83	0.78
1:D:486:GLY:C	1:D:486:GLY:N	2.42	0.78
1:C:213:LYS:HD3	1:C:436:TRP:CZ3	2.19	0.77
1:A:206:THR:O	1:A:210:GLU:HG3	1.83	0.77
1:C:339:GLY:HA3	4:C:1355:HOH:O	1.83	0.77
1:C:455:GLU:OE2	4:C:1379:HOH:O	2.03	0.77
1:A:277:LYS:HE2	4:A:881:HOH:O	1.83	0.76
1:C:306:ILE:CD1	4:C:1347:HOH:O	2.27	0.76
1:C:321:VAL:HG11	4:D:1454:HOH:O	1.52	0.75
1:C:43:MET:HE2	1:C:418:SER:CB	2.15	0.74
1:A:250:LYS:NZ	4:A:903:HOH:O	2.19	0.73
1:D:118:LYS:HE2	4:D:1289:HOH:O	1.88	0.73
1:C:321:VAL:HG12	4:D:1454:HOH:O	1.59	0.72
3:C:550:NAD:C4D	4:C:1355:HOH:O	2.21	0.72
1:B:172:LYS:HE3	4:B:986:HOH:O	1.89	0.72
1:A:262:ILE:HD11	4:A:848:HOH:O	1.92	0.70
1:D:295:LYS:HE3	4:D:1235:HOH:O	1.91	0.70
1:B:262:ILE:HD11	4:B:907:HOH:O	1.91	0.70
1:D:398:SER:O	1:D:399:ILE:HD13	1.92	0.69
1:B:88:VAL:HG21	4:B:1024:HOH:O	1.92	0.69
1:C:343:ILE:HG21	4:C:1354:HOH:O	1.92	0.68
1:D:292:GLU:OE1	4:D:1464:HOH:O	2.12	0.68
1:C:401:VAL:CG2	4:C:1357:HOH:O	1.72	0.67
1:C:338:THR:CG2	4:C:1354:HOH:O	2.38	0.67
1:D:474:LYS:HE2	4:D:1433:HOH:O	1.93	0.67
1:D:399:ILE:HD11	4:D:1305:HOH:O	1.95	0.67
1:C:213:LYS:HD3	1:C:436:TRP:HZ3	1.61	0.66
1:B:285:ASP:OD2	4:B:960:HOH:O	2.13	0.66
1:D:474:LYS:CE	4:D:1384:HOH:O	2.43	0.66
1:C:292:GLU:OE1	4:C:1337:HOH:O	2.14	0.65
1:C:474:LYS:HE2	4:C:1281:HOH:O	1.95	0.64
1:B:56:VAL:HG23	4:B:874:HOH:O	1.96	0.64
1:A:492:HIS:HE1	1:B:244:ASP:OD2	1.82	0.63
1:B:88:VAL:HG11	4:B:1024:HOH:O	1.97	0.63
3:C:550:NAD:C5D	4:C:1355:HOH:O	2.47	0.62
1:C:218:GLU:HG3	1:C:428:GLN:HE22	1.64	0.61
1:C:492:HIS:HE1	1:D:244:ASP:OD2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:285:ASP:CG	4:B:960:HOH:O	2.42	0.61
1:B:243:ASN:HD21	1:B:253:ASN:HD21	1.49	0.61
1:C:254:LYS:HD3	4:C:1167:HOH:O	2.02	0.60
1:C:178:PRO:HD3	4:C:1266:HOH:O	2.00	0.60
1:A:250:LYS:CE	4:A:903:HOH:O	2.50	0.60
1:D:218:GLU:HG3	1:D:428:GLN:HE22	1.67	0.60
1:C:243:ASN:HD21	1:C:253:ASN:HD21	1.49	0.59
1:C:492:HIS:HD2	4:C:1359:HOH:O	1.85	0.59
1:C:43:MET:HE1	1:C:73:GLN:HA	1.85	0.58
3:C:550:NAD:H52N	4:C:1355:HOH:O	2.04	0.58
1:A:244:ASP:OD2	1:B:492:HIS:HE1	1.87	0.58
1:B:380:ARG:NH1	4:B:1009:HOH:O	2.37	0.57
4:C:1347:HOH:O	1:D:472:LEU:HD21	2.05	0.57
1:C:310:ASN:HD22	1:C:310:ASN:H	1.52	0.56
1:C:30:ASP:OD1	4:C:1351:HOH:O	2.17	0.56
1:D:355:HIS:HE1	4:D:1290:HOH:O	1.89	0.56
1:A:11:LEU:HD11	1:A:132:GLU:HG2	1.87	0.56
1:B:485:GLU:HG2	4:B:925:HOH:O	2.06	0.56
1:C:11:LEU:HD11	1:C:132:GLU:HG2	1.88	0.55
1:A:243:ASN:HD21	1:A:253:ASN:HD21	1.52	0.55
1:A:152:MET:HE1	1:A:435:LEU:HB3	1.88	0.55
1:D:262:ILE:HD12	1:D:273:ILE:HD13	1.89	0.55
1:B:213:LYS:HD3	1:B:436:TRP:CZ3	2.42	0.55
1:C:65:SER:HB3	1:C:140:MET:SD	2.46	0.55
1:D:243:ASN:HD21	1:D:253:ASN:HD21	1.54	0.54
1:D:280:ILE:HA	4:D:1449:HOH:O	2.07	0.54
1:C:43:MET:CE	1:C:418:SER:HB3	2.34	0.54
1:D:56:VAL:HG21	4:D:1381:HOH:O	2.07	0.54
1:A:463:GLU:CG	4:A:946:HOH:O	2.21	0.54
1:D:335:VAL:O	4:D:1449:HOH:O	2.18	0.54
1:C:384:LYS:HB2	1:C:385:PRO:CD	2.37	0.53
1:D:343:ILE:CG1	4:D:1453:HOH:O	2.57	0.53
1:C:474:LYS:CE	4:C:1325:HOH:O	2.51	0.53
1:D:51:ARG:HG3	4:D:1417:HOH:O	2.09	0.53
1:B:273:ILE:HD12	4:B:939:HOH:O	2.08	0.52
1:C:187:TRP:NE1	1:C:191:LEU:HD11	2.24	0.52
1:A:380:ARG:HD3	1:A:390:TRP:CZ2	2.45	0.52
2:C:500:ADN:H3'	3:C:550:NAD:C4N	2.39	0.52
1:B:78:ILE:CG2	4:B:1024:HOH:O	2.17	0.52
1:D:492:HIS:HD2	4:D:1401:HOH:O	1.91	0.52
1:C:64:ILE:HD13	1:C:432:GLN:OE1	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:295:LYS:HE3	4:C:1187:HOH:O	2.08	0.52
1:C:485:GLU:CD	4:C:1369:HOH:O	2.53	0.51
1:D:134:TRP:HB3	1:D:193:LEU:HD12	1.92	0.51
2:D:500:ADN:H3'	3:D:550:NAD:C4N	2.41	0.51
1:A:277:LYS:NZ	4:A:894:HOH:O	2.34	0.50
1:D:218:GLU:HG3	1:D:428:GLN:NE2	2.27	0.50
1:D:36:LEU:HD21	1:D:75:ALA:HB1	1.94	0.49
1:D:283:TYR:OH	1:D:317:GLU:OE1	2.23	0.49
1:C:218:GLU:HG3	1:C:428:GLN:NE2	2.26	0.49
1:C:355:HIS:HE1	4:C:1178:HOH:O	1.95	0.49
1:D:343:ILE:HG13	4:D:1453:HOH:O	2.13	0.49
2:A:500:ADN:H3'	3:A:550:NAD:C4N	2.42	0.49
1:A:463:GLU:CD	4:A:946:HOH:O	2.54	0.49
1:C:390:TRP:O	1:C:398:SER:HA	2.13	0.49
1:C:227:TYR:CE2	4:D:1053:HOH:O	2.65	0.48
1:B:478:GLU:CD	4:B:964:HOH:O	2.56	0.48
1:D:65:SER:HB3	1:D:140:MET:SD	2.53	0.48
1:D:68:LEU:O	1:D:69:HIS:C	2.56	0.48
1:B:475:GLU:HG3	4:B:921:HOH:O	2.12	0.48
1:C:16:ARG:CD	4:C:1276:HOH:O	2.30	0.48
1:D:262:ILE:HG12	1:D:293:ALA:HB1	1.96	0.48
1:B:218:GLU:O	1:B:248:LYS:HE3	2.14	0.48
1:D:262:ILE:HD13	1:D:294:MET:HE1	1.93	0.48
1:C:316:MET:HE2	4:D:1271:HOH:O	2.14	0.47
4:A:987:HOH:O	1:C:41:HIS:HD2	1.96	0.47
1:C:244:ASP:OD2	1:D:492:HIS:HE1	1.97	0.47
1:D:262:ILE:HD13	1:D:294:MET:CE	2.43	0.47
1:C:252:ASP:HA	1:C:420:VAL:CG1	2.44	0.47
1:D:167:GLY:O	1:D:171:GLU:HG3	2.14	0.47
1:A:148:LYS:N	1:A:149:PRO:HD3	2.30	0.47
1:A:196:THR:O	1:A:199:GLU:HB2	2.14	0.47
1:C:288:LYS:NZ	1:D:495:TYR:OXT	2.45	0.47
1:C:492:HIS:CD2	4:C:1359:HOH:O	2.63	0.47
1:D:180:GLU:O	1:D:183:ASP:HB2	2.15	0.47
1:C:384:LYS:HB2	1:C:385:PRO:HD2	1.96	0.46
1:D:306:ILE:HD13	4:D:1447:HOH:O	1.82	0.46
1:C:139:GLN:HG2	4:C:1240:HOH:O	2.14	0.46
1:C:343:ILE:HG13	4:C:1354:HOH:O	2.15	0.46
1:B:427:ASN:ND2	4:B:937:HOH:O	2.48	0.46
1:B:355:HIS:HE1	4:D:1049:HOH:O	1.99	0.46
1:B:408:LEU:C	1:B:408:LEU:HD12	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:478:GLU:CG	4:D:1421:HOH:O	2.51	0.45
1:D:248:LYS:HD3	1:D:248:LYS:C	2.41	0.45
1:D:478:GLU:CD	4:D:1309:HOH:O	2.60	0.45
4:A:844:HOH:O	1:C:259:HIS:HE1	1.99	0.45
2:B:500:ADN:H3'	3:B:550:NAD:C4N	2.46	0.45
1:D:47:MET:CE	1:D:76:VAL:CG1	2.95	0.45
1:D:260:SER:OG	1:D:416:HIS:HD2	2.00	0.45
1:D:280:ILE:CG2	4:D:1449:HOH:O	2.45	0.45
1:A:39:ALA:O	1:A:43:MET:HG3	2.16	0.45
1:C:339:GLY:CA	4:C:1355:HOH:O	2.52	0.45
1:C:283:TYR:OH	1:C:317:GLU:OE1	2.22	0.45
1:C:215:VAL:O	1:C:239:ALA:HA	2.16	0.45
1:A:398:SER:O	1:A:399:ILE:HD13	2.16	0.44
1:A:218:GLU:HG3	1:A:428:GLN:HE22	1.82	0.44
1:B:492:HIS:H	1:B:492:HIS:CD2	2.36	0.44
4:B:903:HOH:O	1:D:259:HIS:HD2	2.00	0.44
1:A:492:HIS:HD2	4:A:758:HOH:O	1.99	0.44
1:C:227:TYR:HD2	4:D:1053:HOH:O	1.98	0.44
1:C:397:ARG:HB3	4:C:1248:HOH:O	2.17	0.44
1:A:492:HIS:CE1	1:B:244:ASP:OD2	2.68	0.44
1:B:42:GLU:O	1:B:419:PHE:HA	2.17	0.44
1:A:310:ASN:H	1:A:310:ASN:HD22	1.66	0.44
1:A:427:ASN:ND2	4:A:879:HOH:O	2.45	0.44
1:D:390:TRP:O	1:D:398:SER:HA	2.18	0.44
1:B:260:SER:OG	1:B:416:HIS:HD2	2.00	0.44
1:D:47:MET:HE1	1:D:76:VAL:CG1	2.48	0.44
1:A:95:ILE:HG12	1:A:406:ARG:HD2	1.99	0.44
1:A:95:ILE:HG22	1:A:133:TYR:HB2	1.99	0.44
1:A:355:HIS:HE1	4:A:829:HOH:O	2.00	0.44
1:C:260:SER:OG	1:C:416:HIS:HD2	2.01	0.43
1:A:145:ASP:HB3	1:A:148:LYS:HB2	2.00	0.43
1:A:154:LEU:C	1:A:154:LEU:HD23	2.44	0.43
1:A:474:LYS:HE3	4:A:974:HOH:O	2.18	0.43
4:C:1164:HOH:O	1:D:475:GLU:HG2	2.18	0.43
1:C:429:THR:O	1:C:433:ILE:HG13	2.19	0.43
1:A:134:TRP:HB3	1:A:193:LEU:HD13	2.00	0.43
1:A:147:ASP:C	1:A:149:PRO:HD3	2.43	0.43
1:A:259:HIS:HE1	4:A:820:HOH:O	2.01	0.43
1:B:43:MET:HA	1:B:422:SER:HB2	1.99	0.43
4:B:897:HOH:O	1:D:259:HIS:HE1	2.02	0.43
1:B:320:ASP:OD1	1:C:300:ARG:HD2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:14:ASP:O	1:C:20:ASP:HA	2.18	0.42
1:C:248:LYS:HD3	1:C:248:LYS:C	2.44	0.42
1:B:29:ALA:CB	1:B:108:VAL:HG21	2.49	0.42
1:B:390:TRP:O	1:B:398:SER:HA	2.19	0.42
1:C:398:SER:C	1:C:399:ILE:HD13	2.42	0.42
1:C:68:LEU:HG	1:C:156:ASP:HB2	2.01	0.42
1:D:252:ASP:HA	1:D:420:VAL:CG1	2.49	0.42
1:D:284:GLY:HA3	3:D:550:NAD:O5B	2.19	0.42
1:D:399:ILE:HD12	1:D:399:ILE:HG23	1.79	0.42
1:A:218:GLU:HG3	1:A:428:GLN:NE2	2.35	0.42
1:D:277:LYS:HE2	4:D:1249:HOH:O	2.18	0.42
1:D:310:ASN:HD22	1:D:310:ASN:H	1.67	0.42
1:A:43:MET:HA	1:A:422:SER:HB2	2.02	0.42
1:B:243:ASN:HD22	1:B:248:LYS:HZ1	1.68	0.42
1:A:273:ILE:HD12	4:A:906:HOH:O	2.20	0.42
1:B:84:LEU:CG	4:B:1025:HOH:O	1.85	0.42
1:D:306:ILE:HD11	4:D:1447:HOH:O	1.82	0.42
1:B:41:HIS:HD2	4:D:1245:HOH:O	2.02	0.42
1:B:277:LYS:HE3	4:B:951:HOH:O	2.20	0.41
1:A:260:SER:OG	1:A:416:HIS:HD2	2.02	0.41
1:B:492:HIS:HD2	4:B:755:HOH:O	2.02	0.41
1:D:303:VAL:O	1:D:321:VAL:HA	2.21	0.41
1:C:303:VAL:O	1:C:321:VAL:HA	2.20	0.41
1:A:213:LYS:HE2	1:A:436:TRP:CE3	2.56	0.41
4:A:987:HOH:O	1:C:41:HIS:CD2	2.73	0.41
1:D:340:ASN:O	1:D:367:GLU:HG2	2.21	0.41
1:B:11:LEU:HD22	1:B:22:LYS:HE2	2.03	0.41
1:B:225:ARG:NH2	4:B:780:HOH:O	2.40	0.41
1:B:283:TYR:OH	1:B:317:GLU:OE1	2.32	0.41
1:D:88:VAL:CG2	1:D:120:VAL:HG21	2.51	0.41
1:C:59:LEU:HB3	1:C:86:ALA:HB2	2.03	0.40
1:C:227:TYR:CD2	4:D:1053:HOH:O	2.57	0.40
1:C:310:ASN:H	1:C:310:ASN:ND2	2.18	0.40
1:D:78:ILE:HG23	1:D:88:VAL:HG21	2.03	0.40
1:D:217:GLU:CD	1:D:222:GLY:HA3	2.46	0.40
1:D:218:GLU:CG	1:D:428:GLN:HE22	2.31	0.40
1:D:280:ILE:CA	4:D:1449:HOH:O	2.66	0.40
1:B:214:GLY:HA3	1:B:435:LEU:HD13	2.03	0.40
1:C:73:GLN:H	1:C:73:GLN:CD	2.30	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	484/494 (98%)	473 (98%)	11 (2%)	0	100	100
1	B	483/494 (98%)	470 (97%)	13 (3%)	0	100	100
1	C	483/494 (98%)	471 (98%)	11 (2%)	1 (0%)	43	24
1	D	482/494 (98%)	472 (98%)	9 (2%)	1 (0%)	43	24
All	All	1932/1976 (98%)	1886 (98%)	44 (2%)	2 (0%)	48	27

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	69	HIS
1	C	69	HIS

5.3.2 Protein sidechains [i](#)

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	395/403 (98%)	390 (99%)	5 (1%)	61	40
1	B	395/403 (98%)	388 (98%)	7 (2%)	51	28
1	C	395/403 (98%)	387 (98%)	8 (2%)	48	24
1	D	395/403 (98%)	390 (99%)	5 (1%)	61	40
All	All	1580/1612 (98%)	1555 (98%)	25 (2%)	55	33

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	LEU
1	A	213	LYS
1	A	306	ILE
1	A	350	LYS
1	A	428	GLN
1	B	55	GLU
1	B	68	LEU
1	B	181	GLU
1	B	225	ARG
1	B	250	LYS
1	B	407	LEU
1	B	428	GLN
1	C	11	LEU
1	C	68	LEU
1	C	88	VAL
1	C	180	GLU
1	C	210	GLU
1	C	220	THR
1	C	262	ILE
1	C	428	GLN
1	D	30	ASP
1	D	60	LYS
1	D	193	LEU
1	D	330	ASP
1	D	428	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	243	ASN
1	A	259	HIS
1	A	310	ASN
1	A	355	HIS
1	A	386	GLN
1	A	412	ASN
1	A	416	HIS
1	A	428	GLN
1	A	492	HIS
1	B	41	HIS
1	B	243	ASN
1	B	259	HIS
1	B	310	ASN
1	B	355	HIS

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Mol	Chain	Res	Type
1	B	386	GLN
1	B	412	ASN
1	B	416	HIS
1	B	428	GLN
1	B	432	GLN
1	B	492	HIS
1	C	41	HIS
1	C	111	HIS
1	C	243	ASN
1	C	259	HIS
1	C	266	ASN
1	C	310	ASN
1	C	355	HIS
1	C	386	GLN
1	C	412	ASN
1	C	416	HIS
1	C	427	ASN
1	C	428	GLN
1	C	492	HIS
1	D	41	HIS
1	D	111	HIS
1	D	243	ASN
1	D	259	HIS
1	D	310	ASN
1	D	355	HIS
1	D	386	GLN
1	D	412	ASN
1	D	416	HIS
1	D	428	GLN
1	D	492	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

8 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	ADN	B	500	-	21,21,21	1.42	3 (14%)	31,31,31	2.00	12 (38%)
3	NAD	D	550	-	46,48,48	1.45	7 (15%)	64,73,73	1.95	16 (25%)
2	ADN	C	500	-	21,21,21	1.55	4 (19%)	31,31,31	2.01	10 (32%)
2	ADN	A	500	-	21,21,21	1.48	4 (19%)	31,31,31	1.79	9 (29%)
3	NAD	C	550	-	46,48,48	1.41	6 (13%)	64,73,73	1.72	15 (23%)
3	NAD	B	550	-	46,48,48	1.41	7 (15%)	64,73,73	2.03	15 (23%)
3	NAD	A	550	-	46,48,48	1.45	7 (15%)	64,73,73	1.94	15 (23%)
2	ADN	D	500	-	21,21,21	1.41	4 (19%)	31,31,31	1.92	12 (38%)

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	ADN	B	500	-	-	0/6/22/22	0/3/3/3
3	NAD	D	550	-	-	4/30/62/62	0/5/5/5
2	ADN	C	500	-	-	0/6/22/22	0/3/3/3
2	ADN	A	500	-	-	0/6/22/22	0/3/3/3
3	NAD	C	550	-	-	5/30/62/62	0/5/5/5
3	NAD	B	550	-	-	4/30/62/62	0/5/5/5
3	NAD	A	550	-	-	4/30/62/62	0/5/5/5
2	ADN	D	500	-	-	0/6/22/22	0/3/3/3

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	500	ADN	C5-C4	4.95	1.47	1.39
3	C	550	NAD	C5A-C4A	4.81	1.47	1.39
2	A	500	ADN	C5-C4	4.44	1.47	1.39
3	D	550	NAD	C5A-C4A	4.43	1.47	1.39
3	A	550	NAD	C5A-C4A	4.42	1.47	1.39
3	B	550	NAD	C5A-C4A	4.33	1.46	1.39
2	D	500	ADN	C5-C4	4.13	1.46	1.39
3	A	550	NAD	O7N-C7N	4.13	1.31	1.24
3	D	550	NAD	O7N-C7N	4.13	1.31	1.24
2	B	500	ADN	C5-C4	4.11	1.46	1.39
3	C	550	NAD	O7N-C7N	3.91	1.31	1.24
3	C	550	NAD	PN-O3	3.63	1.63	1.59
3	B	550	NAD	O7N-C7N	3.45	1.30	1.24
3	B	550	NAD	O4D-C1D	3.30	1.45	1.40
3	A	550	NAD	PN-O3	3.14	1.62	1.59
3	D	550	NAD	PN-O3	3.13	1.62	1.59
3	B	550	NAD	C7N-N7N	-3.10	1.27	1.33
3	B	550	NAD	PN-O3	2.98	1.62	1.59
3	D	550	NAD	C7N-N7N	-2.71	1.28	1.33
3	C	550	NAD	C8A-N7A	2.70	1.36	1.31
3	A	550	NAD	C7N-N7N	-2.70	1.28	1.33
2	B	500	ADN	C4-N9	-2.58	1.32	1.37
2	C	500	ADN	C5-N7	-2.56	1.34	1.39
2	A	500	ADN	C4-N9	-2.53	1.32	1.37
2	C	500	ADN	C5-C6	2.35	1.47	1.41
3	C	550	NAD	O4D-C1D	2.35	1.44	1.40
3	D	550	NAD	C8A-N7A	2.30	1.36	1.31
3	A	550	NAD	C8A-N7A	2.29	1.36	1.31
3	A	550	NAD	C4A-N9A	-2.27	1.33	1.37
3	C	550	NAD	C4A-N9A	-2.27	1.33	1.37
3	D	550	NAD	C4A-N9A	-2.26	1.33	1.37
3	B	550	NAD	C8A-N7A	2.24	1.36	1.31
2	D	500	ADN	C5-C6	2.19	1.47	1.41
3	A	550	NAD	PA-O3	2.19	1.61	1.59
2	D	500	ADN	C4-N9	-2.17	1.33	1.37
3	D	550	NAD	PA-O3	2.17	1.61	1.59
2	D	500	ADN	C5-N7	-2.14	1.35	1.39
3	B	550	NAD	C4A-N9A	-2.11	1.33	1.37
2	C	500	ADN	C4-N9	-2.06	1.33	1.37
2	A	500	ADN	C5-N7	-2.04	1.35	1.39
2	A	500	ADN	C5-C6	2.02	1.46	1.41
2	B	500	ADN	C5-C6	2.02	1.46	1.41

All (104) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	550	NAD	C5A-C4A-N3A	-6.01	118.44	126.72
3	D	550	NAD	C5A-C4A-N3A	-5.89	118.61	126.72
3	A	550	NAD	C5A-C4A-N3A	-5.85	118.66	126.72
3	B	550	NAD	C3N-C7N-N7N	5.07	123.99	117.74
3	B	550	NAD	N3A-C4A-N9A	4.87	135.45	127.17
3	D	550	NAD	N3A-C4A-N9A	4.82	135.36	127.17
3	A	550	NAD	N3A-C4A-N9A	4.81	135.34	127.17
3	B	550	NAD	N3A-C2A-N1A	-4.78	121.34	128.58
2	C	500	ADN	C5-C4-N3	-4.65	120.31	126.72
3	D	550	NAD	O7N-C7N-C3N	-4.49	114.11	119.60
3	A	550	NAD	O7N-C7N-C3N	-4.47	114.13	119.60
3	C	550	NAD	C3N-C7N-N7N	4.43	123.20	117.74
3	A	550	NAD	C3N-C7N-N7N	4.43	123.20	117.74
3	C	550	NAD	C5A-C4A-N3A	-4.42	120.63	126.72
3	D	550	NAD	C3N-C7N-N7N	4.41	123.17	117.74
2	B	500	ADN	C5-C4-N3	-4.29	120.82	126.72
3	B	550	NAD	O7N-C7N-C3N	-4.22	114.44	119.60
3	D	550	NAD	C4A-N9A-C8A	4.21	110.16	105.74
3	A	550	NAD	C4A-N9A-C8A	4.20	110.15	105.74
3	C	550	NAD	N3A-C2A-N1A	-4.20	122.22	128.58
3	B	550	NAD	C5N-C4N-C3N	-4.11	116.33	120.36
3	A	550	NAD	N3A-C2A-N1A	-4.09	122.40	128.58
3	D	550	NAD	N3A-C2A-N1A	-4.09	122.40	128.58
2	A	500	ADN	C5-C4-N3	-4.08	121.09	126.72
2	C	500	ADN	C4-C5-N7	-4.06	105.94	110.58
2	D	500	ADN	C5-C4-N3	-3.93	121.31	126.72
3	B	550	NAD	C2A-N3A-C4A	3.93	121.42	111.83
3	C	550	NAD	C4A-C5A-N7A	-3.73	106.32	110.58
2	B	500	ADN	C4-C5-N7	-3.71	106.34	110.58
3	D	550	NAD	C4A-C5A-N7A	-3.68	106.38	110.58
3	B	550	NAD	C4A-N9A-C8A	3.64	109.56	105.74
3	A	550	NAD	C4A-C5A-N7A	-3.63	106.43	110.58
2	C	500	ADN	N3-C4-N9	3.62	133.32	127.17
2	D	500	ADN	N3-C2-N1	-3.58	123.17	128.58
2	D	500	ADN	N3-C4-N9	3.51	133.13	127.17
3	D	550	NAD	C2A-N3A-C4A	3.51	120.40	111.83
3	A	550	NAD	C2A-N3A-C4A	3.50	120.37	111.83
2	A	500	ADN	N3-C4-N9	3.48	133.09	127.17
2	B	500	ADN	N3-C4-N9	3.47	133.07	127.17
2	D	500	ADN	C4-N9-C8	3.46	109.37	105.74
3	B	550	NAD	C4A-C5A-N7A	-3.42	106.67	110.58
3	C	550	NAD	O7N-C7N-C3N	-3.42	115.42	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	ADN	C4'-O4'-C1'	-3.42	101.92	109.47
2	C	500	ADN	C5-N7-C8	3.39	108.78	103.45
3	C	550	NAD	C5N-C4N-C3N	-3.31	117.11	120.36
3	D	550	NAD	N9A-C8A-N7A	-3.31	109.24	113.94
3	A	550	NAD	N9A-C8A-N7A	-3.29	109.27	113.94
2	B	500	ADN	N3-C2-N1	-3.17	123.78	128.58
3	C	550	NAD	C2A-N3A-C4A	3.16	119.55	111.83
2	B	500	ADN	C4-N9-C8	3.08	108.97	105.74
3	B	550	NAD	N9A-C8A-N7A	-3.06	109.59	113.94
2	D	500	ADN	C4-C5-N7	-3.05	107.09	110.58
3	C	550	NAD	N3A-C4A-N9A	3.05	132.36	127.17
3	D	550	NAD	C5A-N7A-C8A	3.01	108.17	103.45
3	A	550	NAD	C5A-N7A-C8A	2.97	108.12	103.45
2	C	500	ADN	C2-N3-C4	2.94	119.01	111.83
2	B	500	ADN	C4'-O4'-C1'	-2.94	102.97	109.47
3	D	550	NAD	C5N-C4N-C3N	-2.92	117.49	120.36
3	B	550	NAD	C5A-N7A-C8A	2.92	108.04	103.45
2	D	500	ADN	C2-N1-C6	2.89	123.48	118.73
3	A	550	NAD	C5N-C4N-C3N	-2.88	117.53	120.36
2	A	500	ADN	C4-C5-N7	-2.86	107.31	110.58
2	C	500	ADN	N3-C2-N1	-2.78	124.37	128.58
3	C	550	NAD	C4A-N9A-C8A	2.75	108.63	105.74
2	A	500	ADN	C4-N9-C8	2.73	108.60	105.74
2	C	500	ADN	C4-N9-C8	2.70	108.57	105.74
2	D	500	ADN	C5-N7-C8	2.70	107.69	103.45
2	C	500	ADN	C6-C5-N7	2.63	137.16	132.09
2	D	500	ADN	C2-N3-C4	2.61	118.21	111.83
3	C	550	NAD	C6A-C5A-N7A	2.59	137.09	132.09
2	B	500	ADN	C2-N3-C4	2.59	118.15	111.83
2	D	500	ADN	N9-C8-N7	-2.58	110.27	113.94
3	D	550	NAD	C6N-N1N-C1D	2.57	124.76	119.73
2	A	500	ADN	N6-C6-N1	2.56	124.08	118.38
3	A	550	NAD	C6N-N1N-C1D	2.56	124.75	119.73
2	C	500	ADN	N9-C8-N7	-2.53	110.35	113.94
2	B	500	ADN	C5-N7-C8	2.51	107.40	103.45
2	A	500	ADN	N3-C2-N1	-2.50	124.80	128.58
3	B	550	NAD	O3-PA-O1A	-2.47	103.27	110.70
2	B	500	ADN	C2-N1-C6	2.46	122.77	118.73
3	D	550	NAD	C2N-N1N-C1D	-2.44	113.76	119.13
2	B	500	ADN	C6-C5-N7	2.44	136.78	132.09
3	A	550	NAD	C2N-N1N-C1D	-2.43	113.77	119.13
2	A	500	ADN	C2-N1-C6	2.42	122.70	118.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	550	NAD	C2N-C3N-C4N	2.38	121.02	118.26
3	C	550	NAD	C5A-N7A-C8A	2.38	107.18	103.45
2	C	500	ADN	C4'-O4'-C1'	-2.38	104.22	109.47
2	D	500	ADN	C4'-O4'-C1'	-2.36	104.26	109.47
2	B	500	ADN	N6-C6-N1	2.34	123.60	118.38
3	C	550	NAD	C2N-C3N-C4N	2.30	120.94	118.26
3	B	550	NAD	C6N-N1N-C1D	2.28	124.19	119.73
3	D	550	NAD	O3-PA-O1A	-2.22	104.02	110.70
3	A	550	NAD	O3-PA-O1A	-2.22	104.03	110.70
2	D	500	ADN	C6-C5-N7	2.21	136.35	132.09
3	C	550	NAD	C6N-N1N-C1D	2.20	124.04	119.73
3	C	550	NAD	N9A-C8A-N7A	-2.19	110.83	113.94
3	D	550	NAD	C6A-C5A-N7A	2.15	136.23	132.09
3	A	550	NAD	C6A-C5A-N7A	2.12	136.18	132.09
2	D	500	ADN	C4-N9-C1'	-2.10	121.73	126.63
2	A	500	ADN	C2-N3-C4	2.06	116.86	111.83
3	B	550	NAD	C4B-O4B-C1B	-2.05	104.95	109.47
2	B	500	ADN	O4'-C1'-N9	2.04	112.00	108.09
3	C	550	NAD	C2N-N1N-C1D	-2.02	114.68	119.13
3	D	550	NAD	C4A-N9A-C1B	-2.00	121.95	126.63

There are no chirality outliers.

All (17) torsion outliers are listed below:

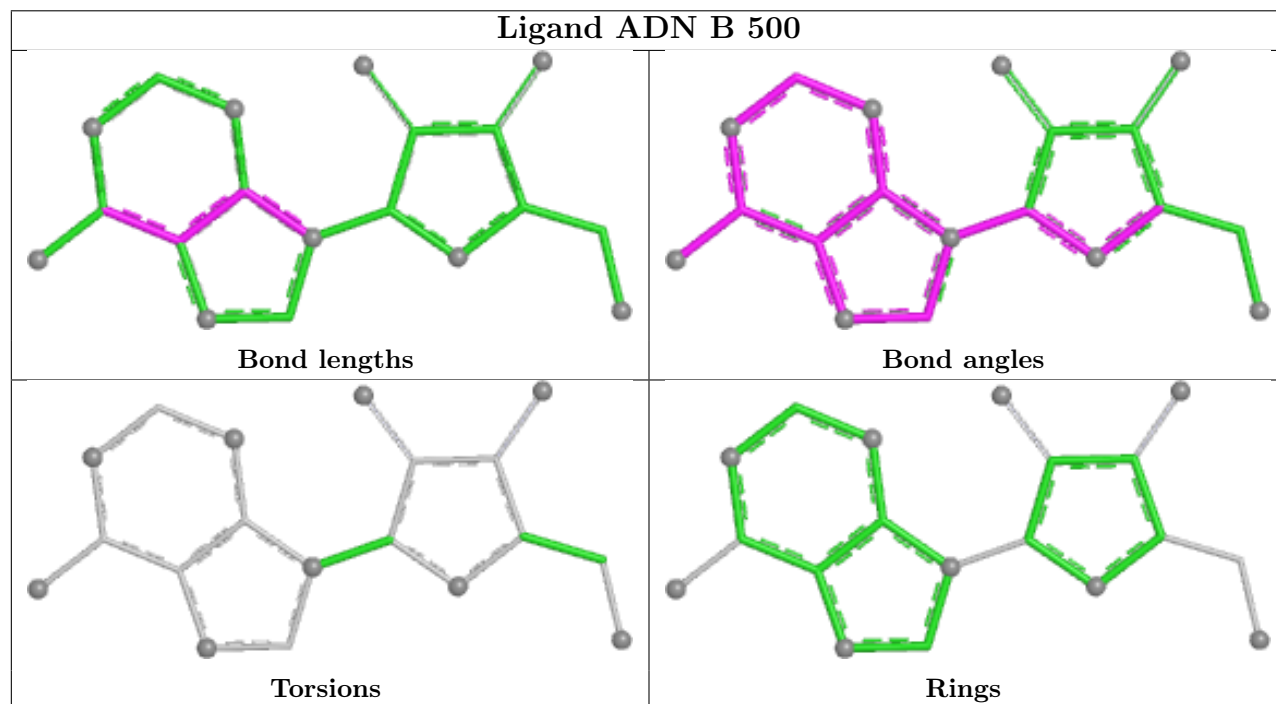
Mol	Chain	Res	Type	Atoms
3	A	550	NAD	O4D-C1D-N1N-C2N
3	A	550	NAD	O4D-C1D-N1N-C6N
3	A	550	NAD	C2D-C1D-N1N-C2N
3	A	550	NAD	C2D-C1D-N1N-C6N
3	B	550	NAD	O4D-C1D-N1N-C2N
3	B	550	NAD	O4D-C1D-N1N-C6N
3	B	550	NAD	C2D-C1D-N1N-C2N
3	B	550	NAD	C2D-C1D-N1N-C6N
3	C	550	NAD	O4D-C1D-N1N-C2N
3	C	550	NAD	O4D-C1D-N1N-C6N
3	C	550	NAD	C2D-C1D-N1N-C2N
3	C	550	NAD	C2D-C1D-N1N-C6N
3	D	550	NAD	O4D-C1D-N1N-C2N
3	D	550	NAD	O4D-C1D-N1N-C6N
3	D	550	NAD	C2D-C1D-N1N-C2N
3	D	550	NAD	C2D-C1D-N1N-C6N
3	C	550	NAD	O4B-C4B-C5B-O5B

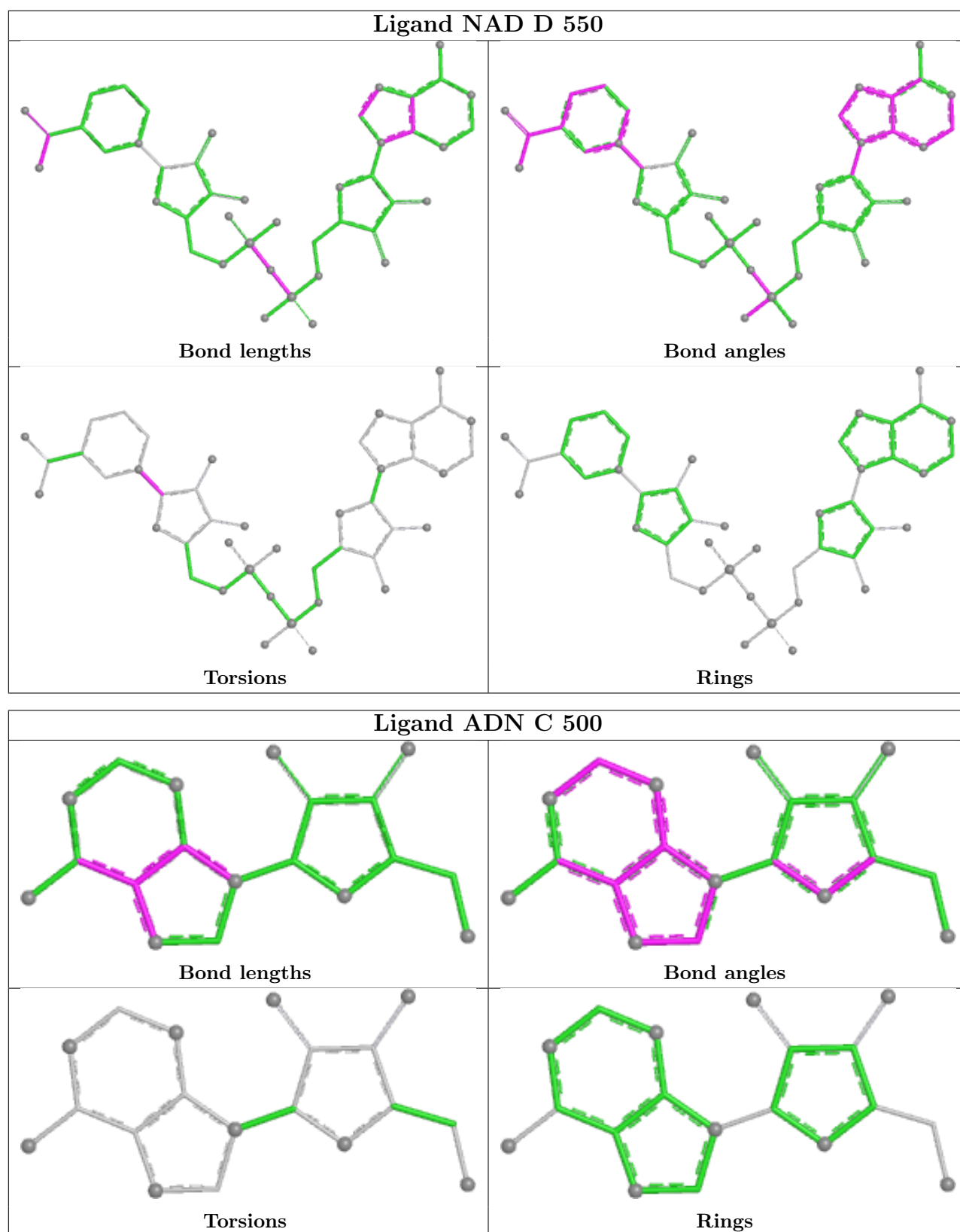
There are no ring outliers.

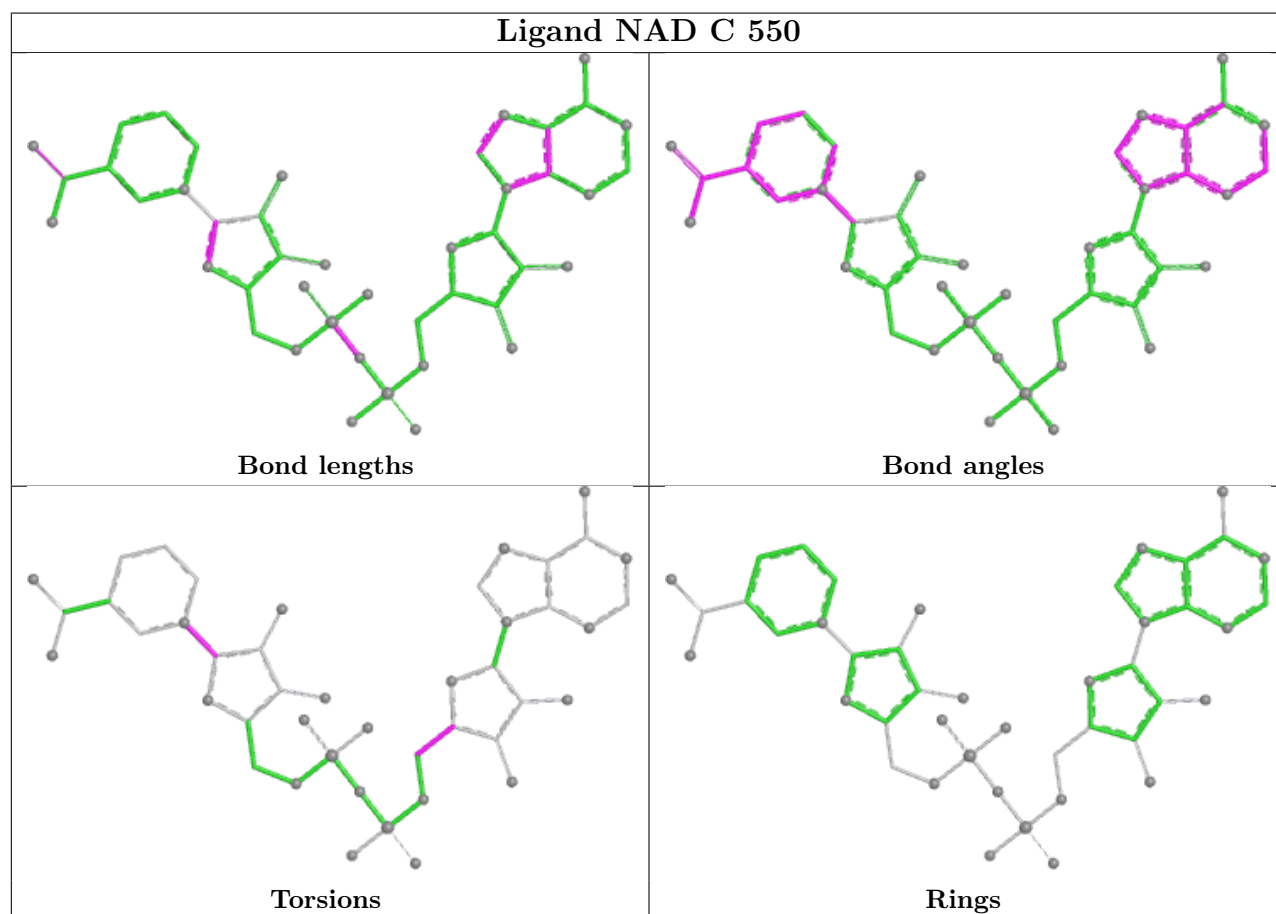
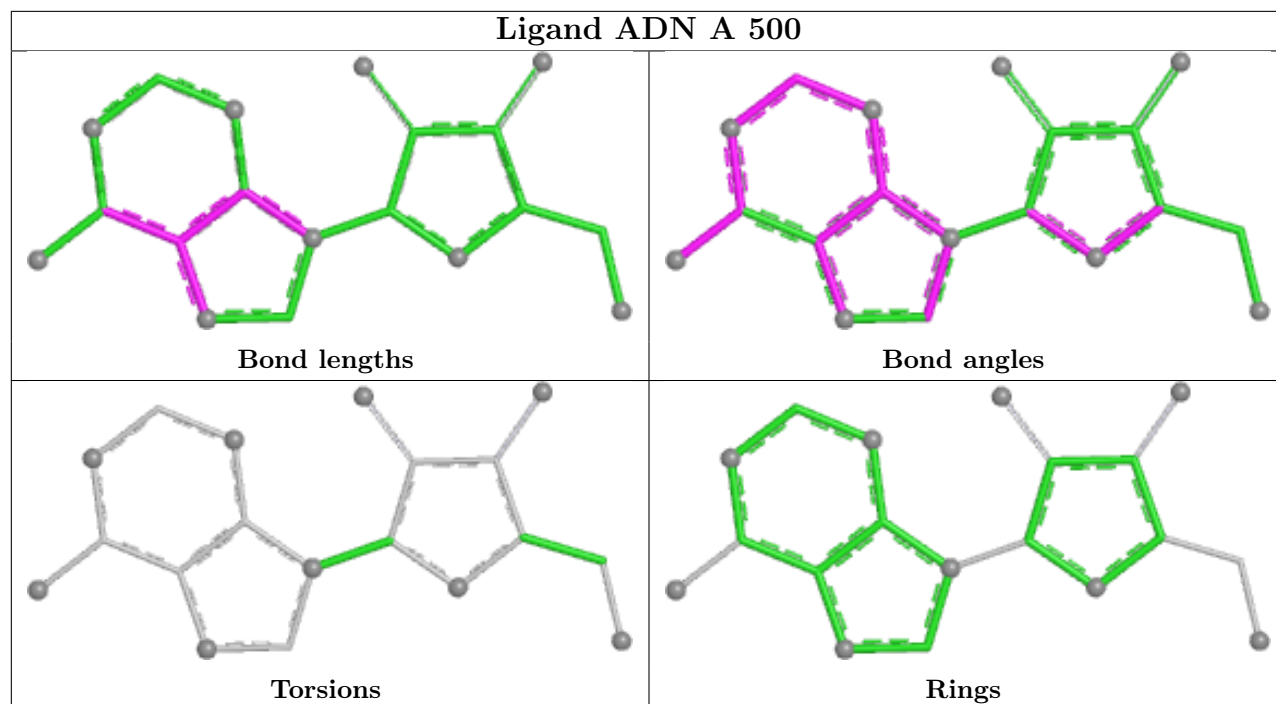
8 monomers are involved in 10 short contacts:

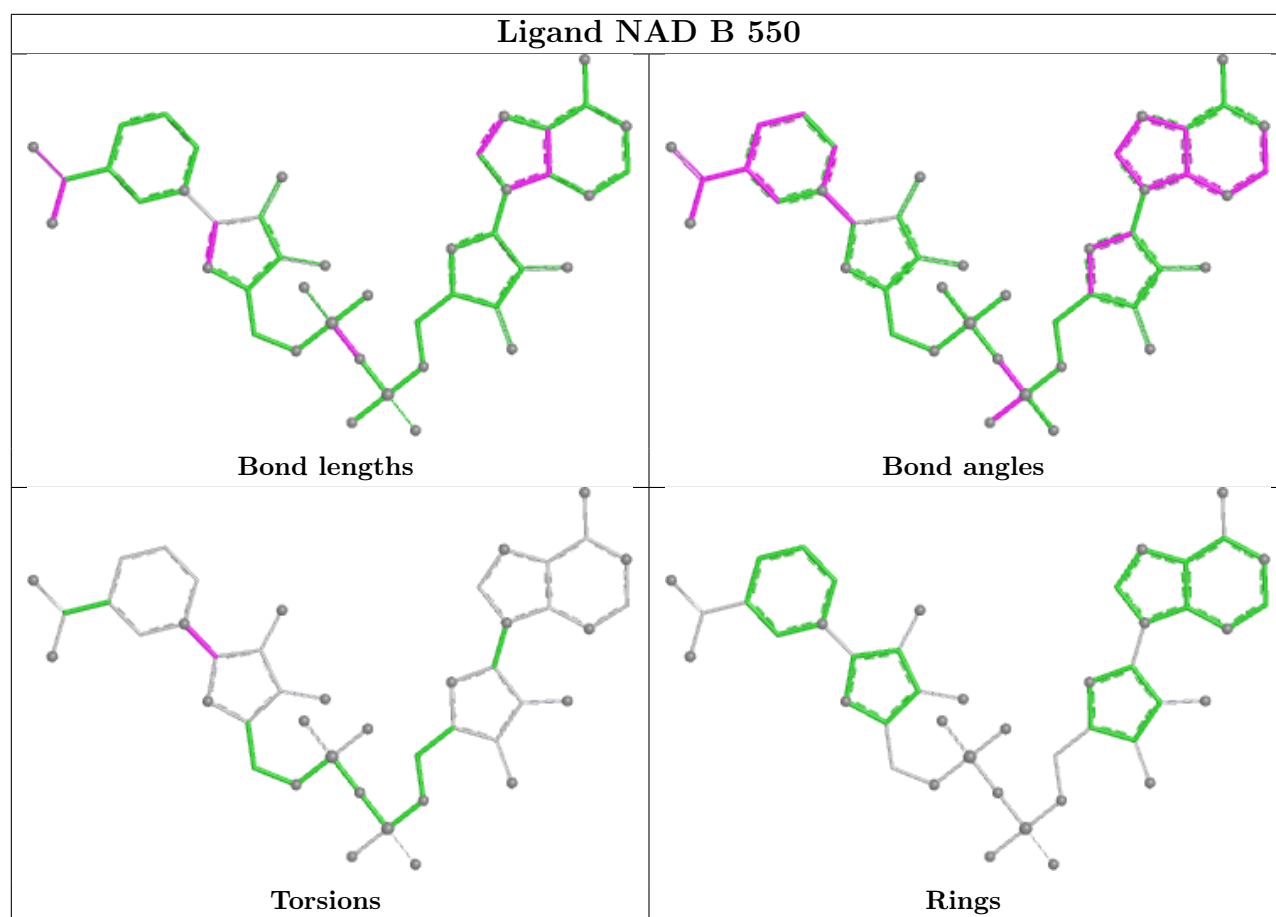
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	500	ADN	1	0
3	D	550	NAD	2	0
2	C	500	ADN	1	0
2	A	500	ADN	1	0
3	C	550	NAD	6	0
3	B	550	NAD	1	0
3	A	550	NAD	1	0
2	D	500	ADN	1	0

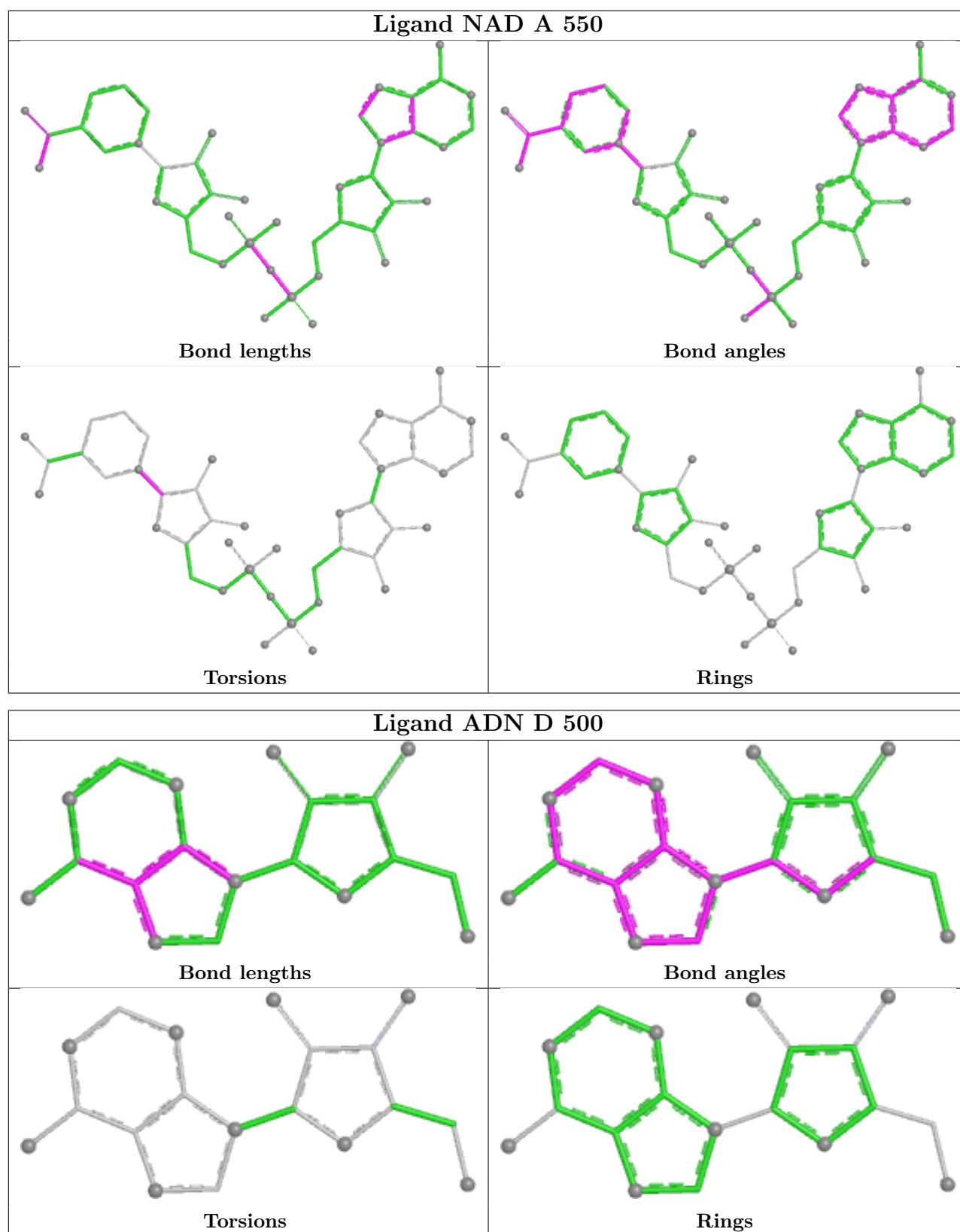
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











5.7 Other polymers ⓘ

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(Å ²)	Q<0.9
1	A	486/494 (98%)	-0.23	4 (0%) 82 86	8, 14, 30, 49	0
1	B	485/494 (98%)	-0.33	2 (0%) 88 91	8, 14, 28, 44	0
1	C	485/494 (98%)	-0.08	10 (2%) 63 67	7, 16, 36, 88	0
1	D	485/494 (98%)	-0.11	6 (1%) 76 80	8, 16, 34, 80	0
All	All	1941/1976 (98%)	-0.19	22 (1%) 78 82	7, 15, 32, 88	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	10	SER	3.9
1	D	11	LEU	3.7
1	C	11	LEU	3.3
1	D	182	ASP	3.1
1	C	179	ALA	3.1
1	D	181	GLU	3.0
1	A	227	TYR	2.9
1	C	175	VAL	2.6
1	D	227	TYR	2.5
1	A	483	ASP	2.5
1	C	181	GLU	2.5
1	A	181	GLU	2.4
1	C	227	TYR	2.4
1	C	16	ARG	2.4
1	B	227	TYR	2.4
1	C	12	THR	2.3
1	C	210	GLU	2.2
1	C	178	PRO	2.2
1	D	179	ALA	2.2
1	C	174	GLY	2.2
1	B	375	ARG	2.2
1	D	173	ALA	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

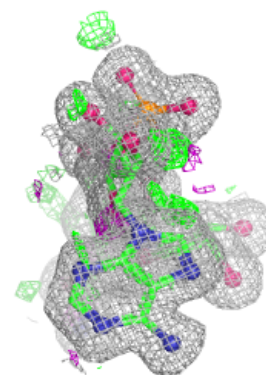
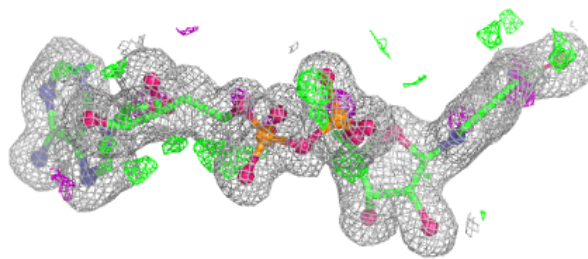
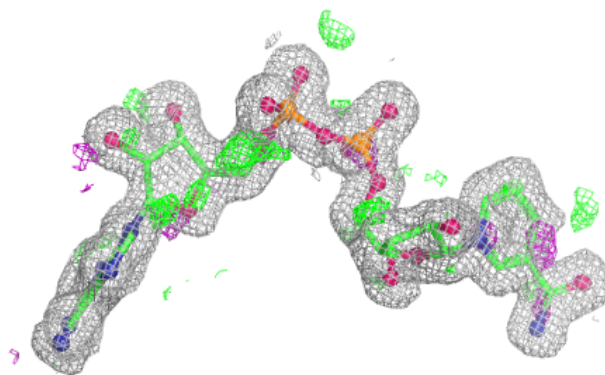
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAD	D	550	44/44	0.96	0.06	8,10,11,13	0
2	ADN	B	500	19/19	0.97	0.05	6,9,11,11	0
2	ADN	C	500	19/19	0.97	0.05	10,11,12,13	0
2	ADN	D	500	19/19	0.97	0.05	9,10,12,13	0
3	NAD	A	550	44/44	0.97	0.05	8,10,11,13	0
3	NAD	B	550	44/44	0.97	0.05	7,10,11,13	0
3	NAD	C	550	44/44	0.97	0.05	8,11,12,14	0
2	ADN	A	500	19/19	0.97	0.05	7,9,12,12	0

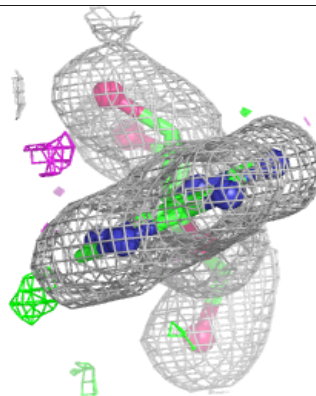
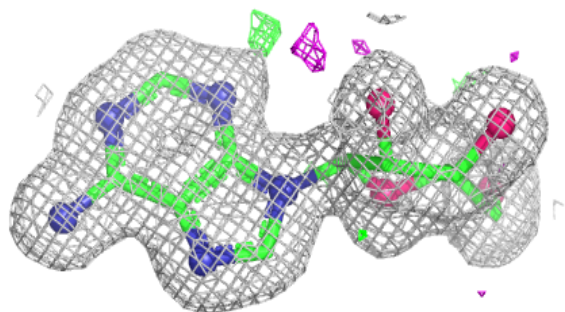
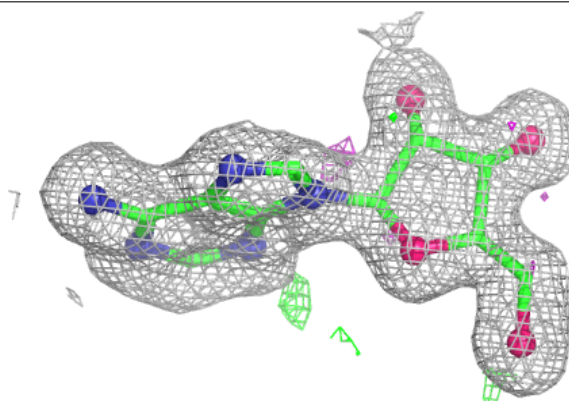
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAD D 550:

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

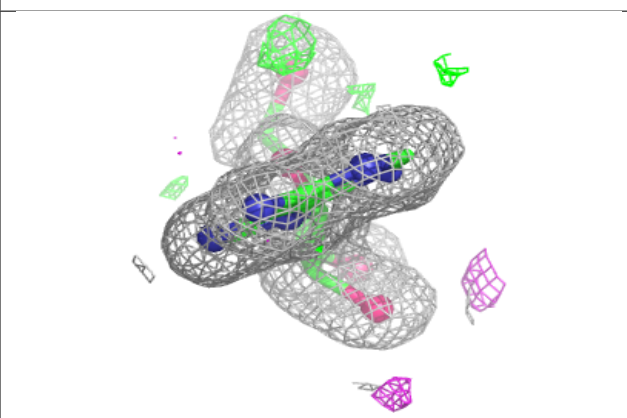
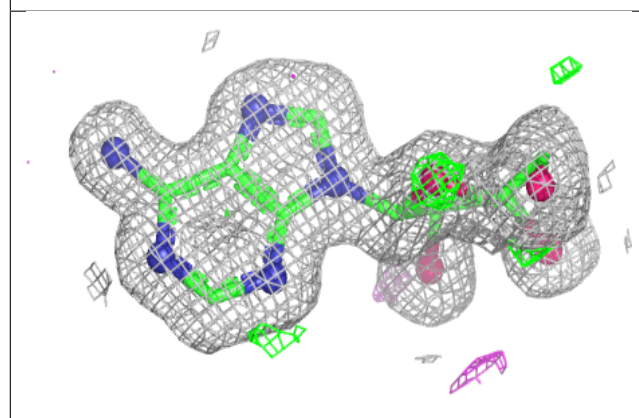
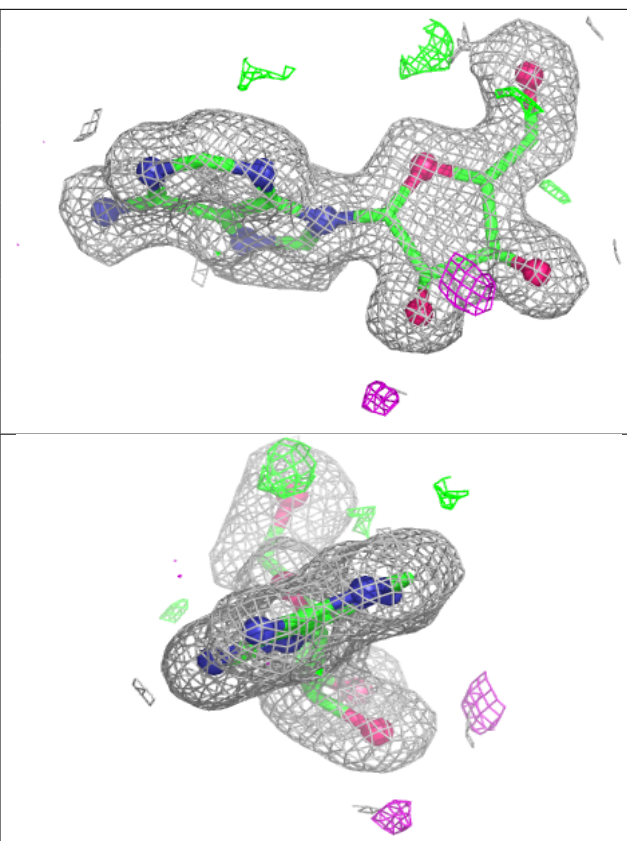
**Electron density around ADN B 500:**

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

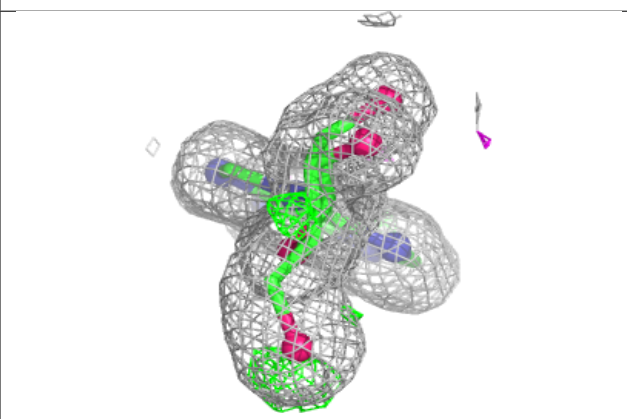
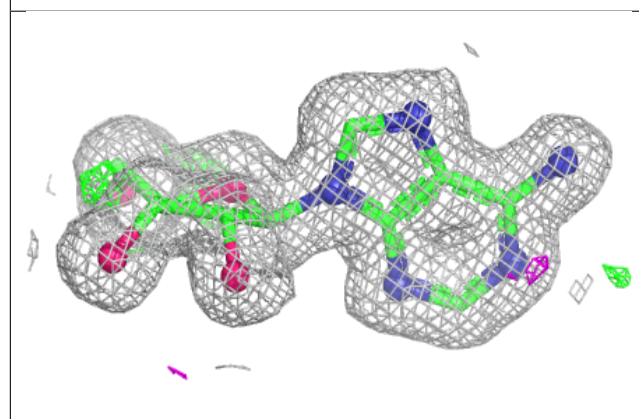
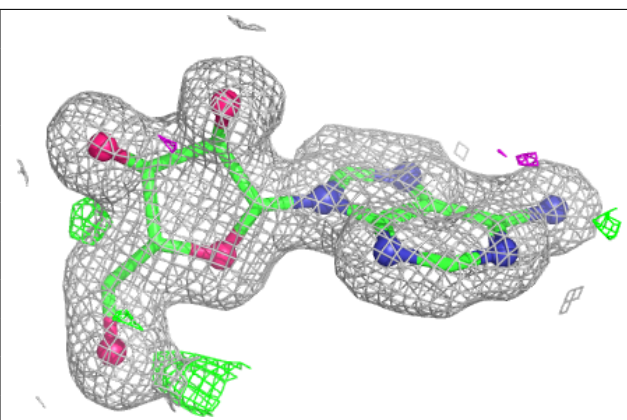


Electron density around ADN C 500:

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

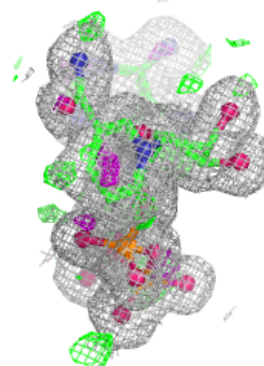
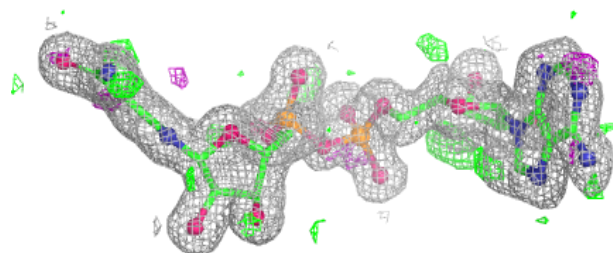
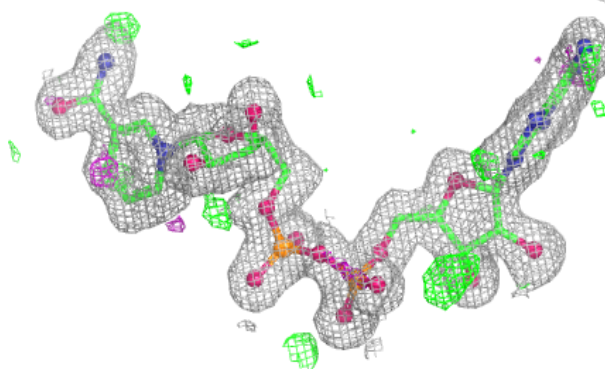
**Electron density around ADN D 500:**

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

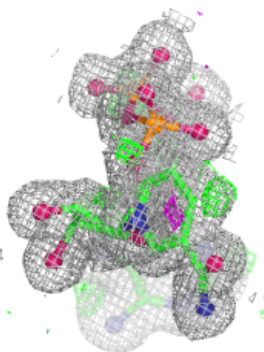
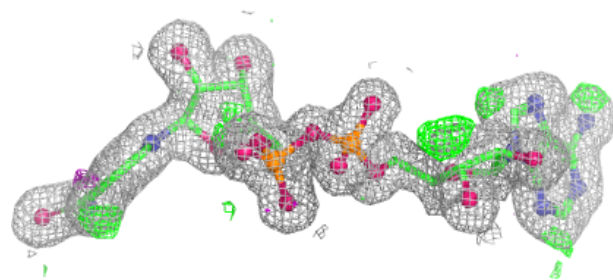
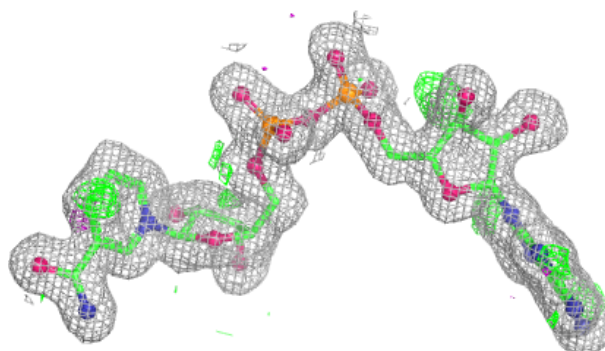


Electron density around NAD A 550:

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

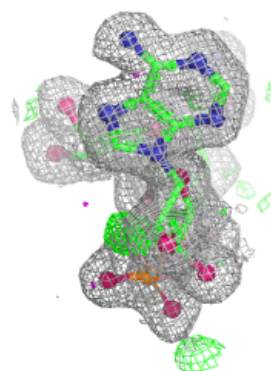
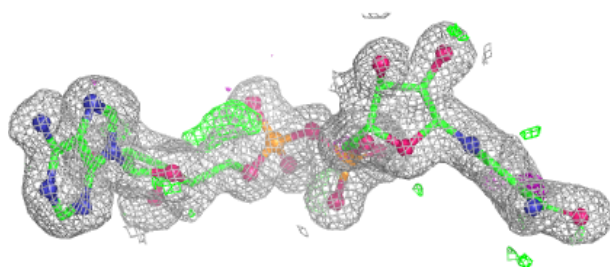
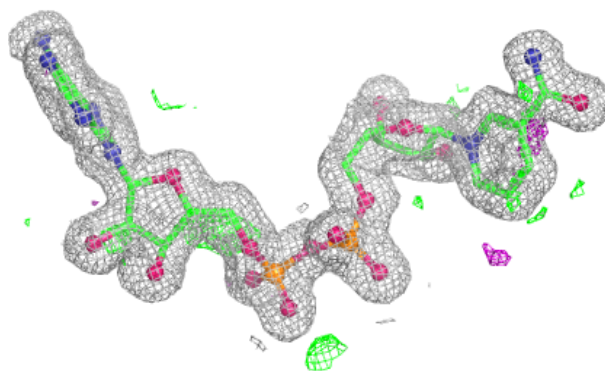
**Electron density around NAD B 550:**

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

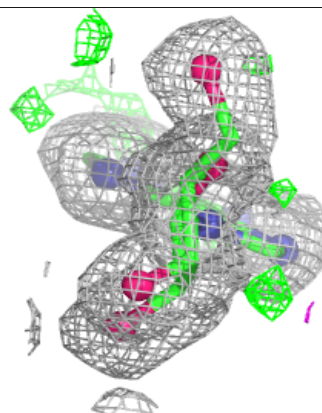
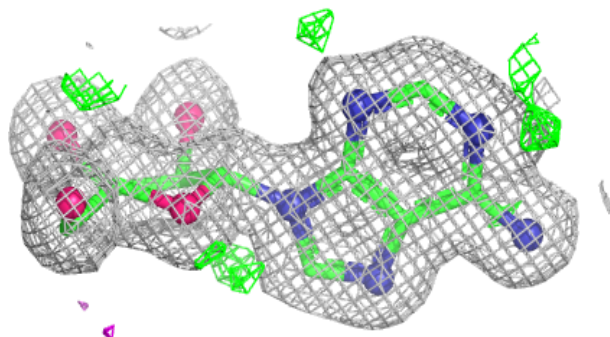
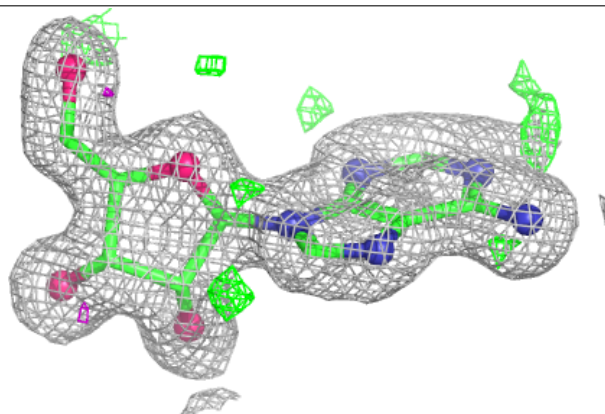


Electron density around NAD C 550:

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

**Electron density around ADN 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.