



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 08:52 PM UTC

PDB ID : 2ZIZ / pdb_00002ziz
Title : Crystal structure of Mycobacterium tuberculosis S-adenosyl-L-homocysteine hydrolase in ternary complex with NAD and 3-deazaadenosine
Authors : Reddy, M.C.M.; Gokulan, K.; Shetty, N.D.; Owen, J.L.; Ioerger, T.R.; Sacchettini, J.C.
Deposited on : 2008-02-29
Resolution : 2.20 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

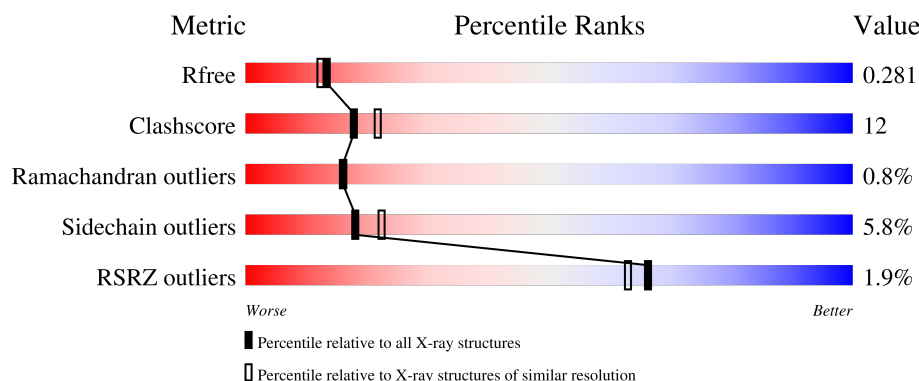
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	495	 71% 24% ..
1	B	495	 3% 68% 26% ...
1	C	495	 % 75% 20% ..
1	D	495	 4% 66% 27% ...

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16004 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.

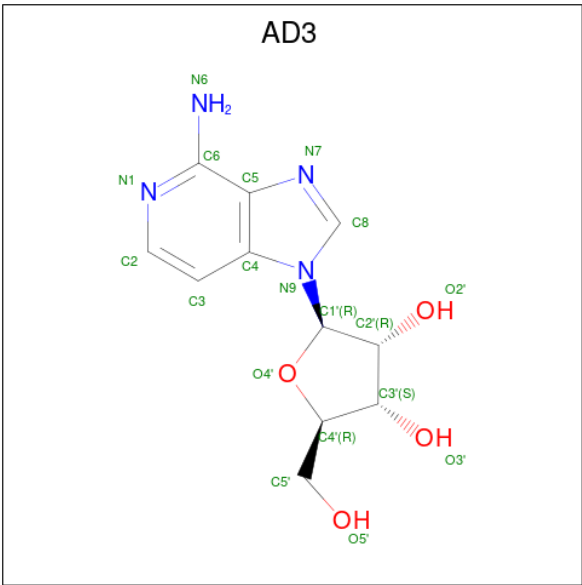
- Molecule 1 is a protein called Adenosylhomocysteinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	485	Total	C	N	O	S	0	0	0
			3748	2364	643	724	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
			3748	2364	643	724	17			

There are 4 discrepancies between the modelled and reference sequences:

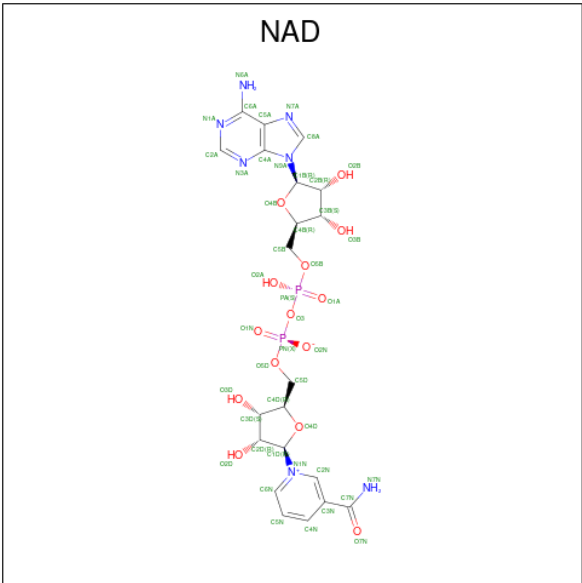
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP P60176
B	1	MET	-	expression tag	UNP P60176
C	1	MET	-	expression tag	UNP P60176
D	1	MET	-	expression tag	UNP P60176

- Molecule 2 is 3-DEAZA-ADENOSINE (CCD ID: AD3) (formula: C₁₁H₁₄N₄O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			19	11	4	4		
2	B	1	Total	C	N	O	0	0
			19	11	4	4		
2	C	1	Total	C	N	O	0	0
			19	11	4	4		
2	D	1	Total	C	N	O	0	0
			19	11	4	4		

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



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

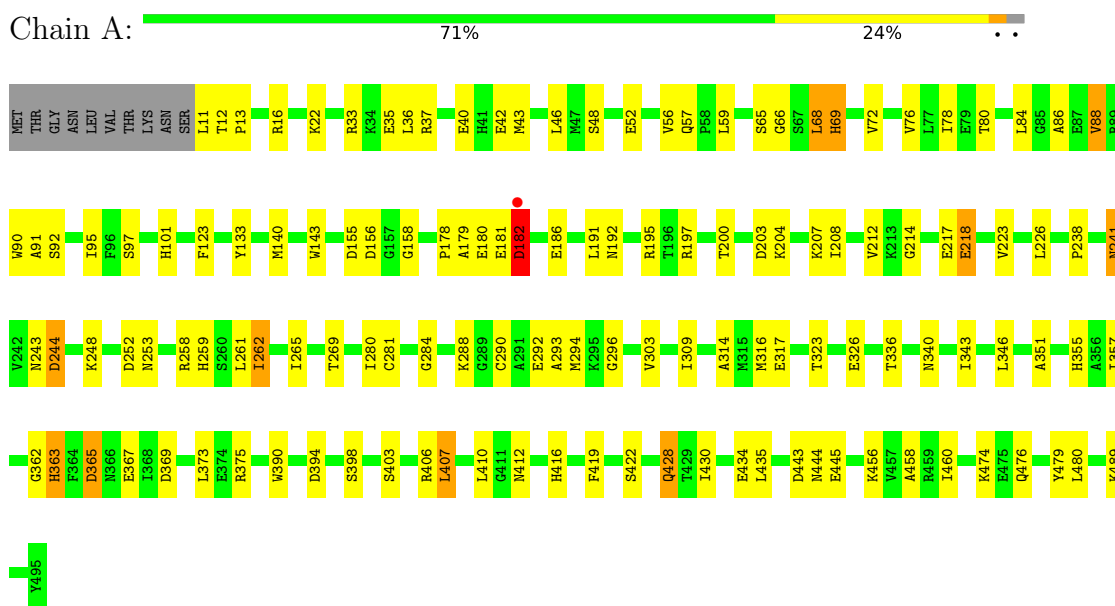
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	209	Total 209	O 209	0	0
4	B	154	Total 154	O 154	0	0
4	C	215	Total 215	O 215	0	0
4	D	182	Total 182	O 182	0	0

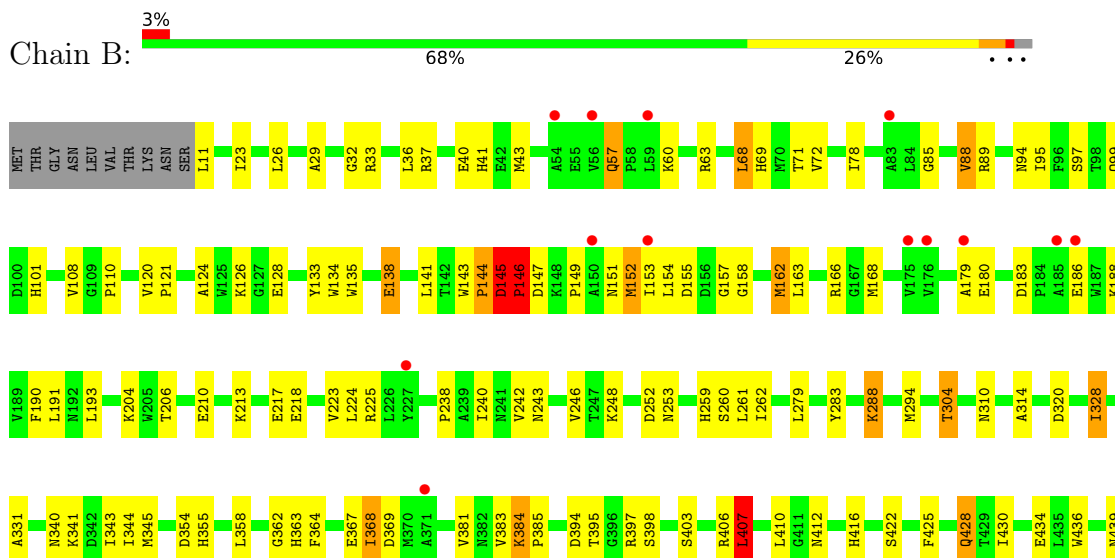
3 Residue-property plots

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

• Molecule 1: Adenosylhomocysteinase

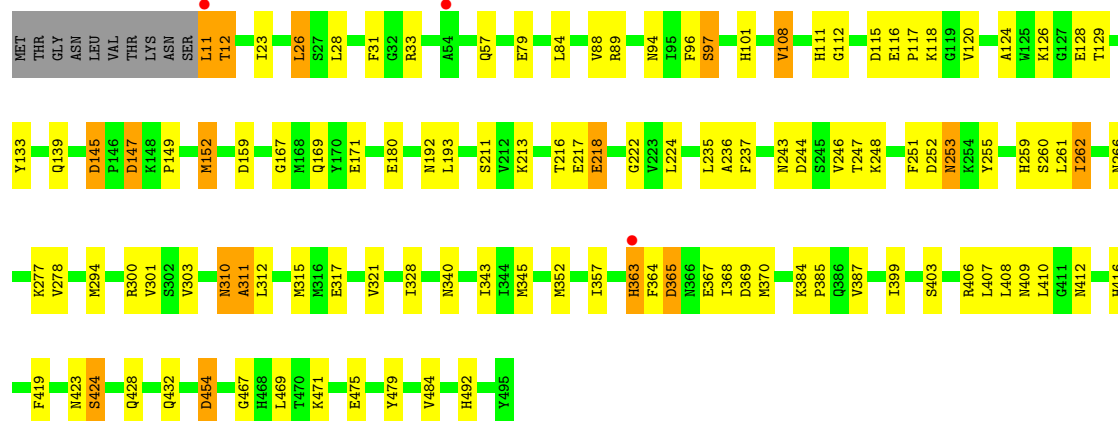
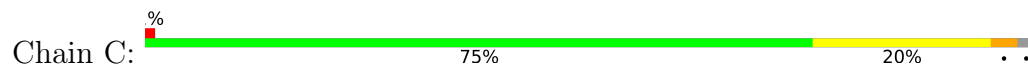


• Molecule 1: Adenosylhomocysteinase

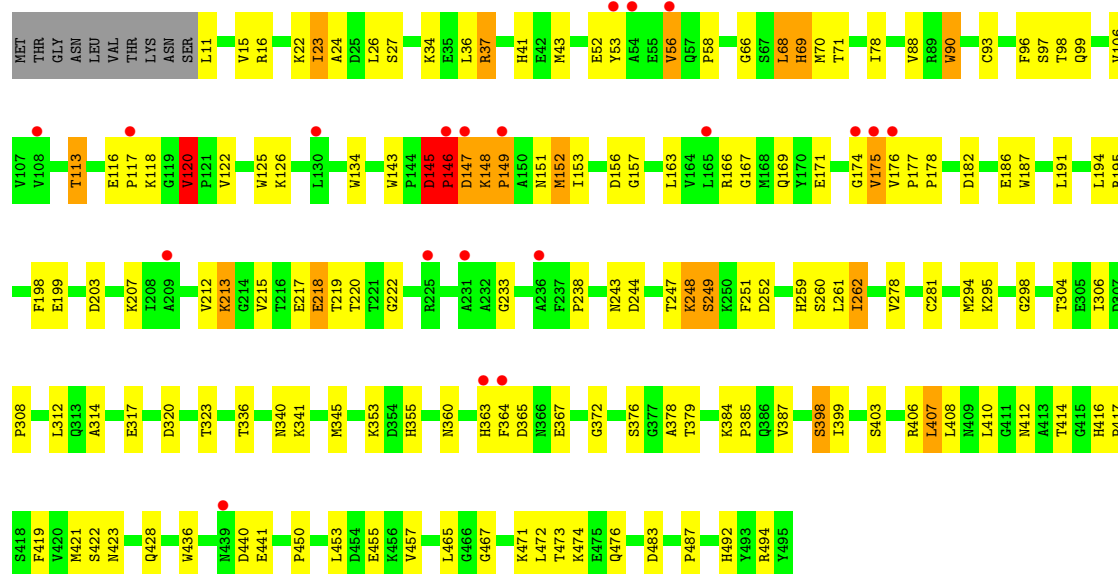




• Molecule 1: Adenosylhomocysteinase



• 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	100.55Å 111.32Å 94.47Å 90.00° 96.77° 90.00°	Depositor
Resolution (Å)	38.18 – 2.20 38.18 – 2.20	Depositor EDS
% Data completeness (in resolution range)	94.4 (38.18-2.20) 94.4 (38.18-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.198 , 0.285 0.195 , 0.281	Depositor DCC
R_{free} test set	4899 reflections (4.69%)	wwPDB-VP
Wilson B-factor (Å ²)	37.2	Xtriage
Anisotropy	0.461	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 53.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16004	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.66% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: AD3, 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	1.23	8/3824 (0.2%)	1.28	15/5186 (0.3%)
1	B	1.11	4/3824 (0.1%)	1.20	13/5186 (0.3%)
1	C	1.11	3/3824 (0.1%)	1.19	10/5186 (0.2%)
1	D	1.05	7/3824 (0.2%)	1.21	17/5186 (0.3%)
All	All	1.13	22/15296 (0.1%)	1.22	55/20744 (0.3%)

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	365	ASP	N-CA	6.63	1.54	1.46
1	A	314	ALA	CA-CB	6.42	1.63	1.53
1	D	314	ALA	CA-CB	6.39	1.63	1.53
1	D	306	ILE	CA-C	6.36	1.60	1.52
1	D	323	THR	CA-CB	5.91	1.63	1.53
1	B	314	ALA	CA-CB	5.79	1.62	1.53
1	A	351	ALA	C-O	5.55	1.31	1.24
1	A	460	ILE	CA-CB	5.50	1.60	1.54
1	A	57	GLN	C-O	-5.45	1.21	1.23
1	A	280	ILE	CA-CB	5.40	1.60	1.54
1	D	320	ASP	N-CA	5.39	1.52	1.46
1	A	57	GLN	N-CA	5.36	1.50	1.46
1	C	419	PHE	N-CA	5.33	1.52	1.46
1	C	343	ILE	CA-CB	5.32	1.62	1.54
1	D	298	GLY	N-CA	5.26	1.53	1.45
1	B	242	VAL	CA-CB	5.25	1.61	1.54
1	D	457	VAL	CA-CB	5.21	1.60	1.54
1	B	153	ILE	CA-CB	5.20	1.61	1.54
1	A	316	MET	N-CA	5.06	1.52	1.46
1	B	331	ALA	CA-CB	-5.04	1.45	1.53
1	D	175	VAL	CA-CB	5.03	1.59	1.53
1	C	454	ASP	CA-C	5.02	1.59	1.52

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	145	ASP	CA-C-N	8.35	130.28	119.84
1	D	145	ASP	C-N-CA	8.35	130.28	119.84
1	C	365	ASP	N-CA-C	8.33	124.87	113.37
1	C	467	GLY	N-CA-C	-7.37	99.34	112.54
1	B	145	ASP	CA-C-N	7.30	128.96	119.84
1	B	145	ASP	C-N-CA	7.30	128.96	119.84
1	A	365	ASP	N-CA-C	7.26	126.27	110.80
1	C	129	THR	N-CA-C	-6.90	101.63	110.53
1	D	365	ASP	N-CA-C	6.69	120.90	113.21
1	C	363	HIS	N-CA-C	6.44	120.34	112.23
1	D	467	GLY	N-CA-C	-6.40	99.11	112.04
1	D	36	LEU	N-CA-C	6.32	118.17	111.28
1	D	473	THR	N-CA-C	-6.30	102.41	110.53
1	A	367	GLU	N-CA-C	-6.29	104.50	111.36
1	B	367	GLU	N-CA-C	-6.17	104.64	111.36
1	C	301	VAL	N-CA-C	6.16	118.23	108.87
1	A	363	HIS	N-CA-C	6.05	118.84	111.82
1	B	120	VAL	CA-C-N	-6.04	113.30	119.83
1	B	120	VAL	C-N-CA	-6.04	113.30	119.83
1	D	120	VAL	CA-C-N	6.01	126.95	119.98
1	D	120	VAL	C-N-CA	6.01	126.95	119.98
1	C	311	ALA	N-CA-C	6.01	117.83	111.28
1	B	459	ARG	N-CA-C	5.96	117.77	111.28
1	A	458	ALA	N-CA-C	5.89	118.46	111.33
1	D	146	PRO	CA-C-N	5.88	132.28	121.70
1	D	146	PRO	C-N-CA	5.88	132.28	121.70
1	D	249	SER	N-CA-C	5.78	118.05	111.11
1	C	97	SER	N-CA-C	5.68	120.05	113.18
1	A	143	TRP	CA-C-N	5.63	125.09	119.24
1	A	143	TRP	C-N-CA	5.63	125.09	119.24
1	D	90	TRP	N-CA-C	5.52	118.73	109.95
1	B	328	ILE	N-CA-C	5.50	117.96	111.09
1	B	57	GLN	CA-C-N	5.49	125.32	119.28
1	B	57	GLN	C-N-CA	5.49	125.32	119.28
1	A	244	ASP	N-CA-C	5.43	119.01	112.93
1	B	384	LYS	CA-C-N	-5.43	113.97	119.83
1	B	384	LYS	C-N-CA	-5.43	113.97	119.83
1	A	182	ASP	N-CA-C	5.35	118.96	111.30
1	B	473	THR	N-CA-C	-5.30	103.69	110.53
1	D	378	ALA	N-CA-C	-5.28	103.56	110.53
1	A	12	THR	CA-C-N	-5.27	114.28	119.92
1	A	12	THR	C-N-CA	-5.27	114.28	119.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	46	LEU	N-CA-C	-5.27	105.21	111.69
1	A	288	LYS	N-CA-C	5.27	116.71	111.07
1	D	56	VAL	N-CA-C	5.23	117.63	111.09
1	D	345	MET	N-CA-C	-5.21	102.81	110.52
1	D	423	ASN	N-CA-C	5.20	116.64	110.97
1	A	296	GLY	N-CA-C	-5.18	108.97	114.67
1	C	328	ILE	N-CA-C	5.17	116.51	110.62
1	C	31	PHE	N-CA-C	-5.13	105.76	111.36
1	B	425	PHE	N-CA-C	5.13	118.70	112.23
1	A	394	ASP	N-CA-C	5.06	117.53	111.71
1	A	362	GLY	N-CA-C	-5.03	104.94	112.89
1	C	108	VAL	N-CA-C	5.01	115.78	110.72
1	D	233	GLY	N-CA-C	-5.00	108.21	115.27

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	3748	0	3693	85	0
1	B	3748	0	3693	109	0
1	C	3748	0	3693	84	0
1	D	3748	0	3693	115	0
2	A	19	0	14	3	0
2	B	19	0	14	1	0
2	C	19	0	14	1	0
2	D	19	0	14	1	0
3	A	44	0	26	2	0
3	B	44	0	26	2	0
3	C	44	0	26	1	0
3	D	44	0	26	2	0
4	A	209	0	0	2	0
4	B	154	0	0	4	1
4	C	215	0	0	4	1
4	D	182	0	0	6	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	16004	0	14932	370	2

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 12.

All (370) 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:146:PRO:CB	1:D:147:ASP:HB2	1.52	1.38
1:A:68:LEU:HD22	1:A:156:ASP:HB2	1.35	1.08
1:B:262:ILE:HD11	1:D:262:ILE:HD11	1.09	1.04
1:C:368:ILE:CG2	1:C:370:MET:HE3	1.88	1.02
1:D:146:PRO:HB3	1:D:147:ASP:CB	1.92	1.00
1:D:146:PRO:HB3	1:D:147:ASP:HB2	1.01	0.98
1:B:262:ILE:CD1	1:D:262:ILE:HD11	1.95	0.97
1:D:146:PRO:HB2	1:D:147:ASP:HB2	1.46	0.97
1:D:146:PRO:CB	1:D:147:ASP:CB	2.42	0.96
1:B:358:LEU:HD11	1:B:368:ILE:HD13	1.44	0.95
1:A:218:GLU:HG3	1:A:428:GLN:HE22	1.33	0.93
1:B:262:ILE:HD11	1:D:262:ILE:CD1	1.98	0.92
1:D:259:HIS:HE1	4:D:838:HOH:O	1.53	0.91
1:B:145:ASP:H	1:B:146:PRO:CD	1.84	0.91
1:C:368:ILE:HG21	1:C:370:MET:HE3	1.52	0.90
1:A:262:ILE:HD11	1:C:262:ILE:HD11	1.52	0.90
1:D:218:GLU:HG3	1:D:428:GLN:NE2	1.87	0.90
1:D:145:ASP:OD2	1:D:146:PRO:HD2	1.77	0.84
1:D:384:LYS:HB2	1:D:385:PRO:CD	2.10	0.82
1:B:57:GLN:HE22	1:B:85:GLY:HA2	1.45	0.81
1:C:368:ILE:HG22	1:C:370:MET:HE3	1.61	0.80
3:C:550:NAD:C4N	2:C:500:AD3:H3'	2.10	0.79
1:C:112:GLY:HA2	1:C:118:LYS:HG3	1.64	0.79
1:D:384:LYS:HB2	1:D:385:PRO:HD2	1.64	0.78
1:C:243:ASN:HD21	1:C:253:ASN:HD21	1.31	0.78
1:D:295:LYS:HE3	4:D:736:HOH:O	1.83	0.77
1:B:152:MET:HE3	1:B:213:LYS:HB2	1.68	0.75
1:D:218:GLU:HG3	1:D:428:GLN:HE22	1.49	0.74
1:A:68:LEU:HD22	1:A:156:ASP:CB	2.16	0.73
1:D:450:PRO:HD2	1:D:453:LEU:HD12	1.70	0.73
1:D:70:MET:HB3	1:D:98:THR:HG23	1.70	0.72
1:B:218:GLU:O	1:B:248:LYS:HE3	1.89	0.72
1:C:260:SER:HB2	1:C:409:ASN:HB2	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:358:LEU:CD1	1:B:368:ILE:HD13	2.17	0.72
1:D:218:GLU:CG	1:D:428:GLN:HE22	2.03	0.71
1:D:407:LEU:H	1:D:407:LEU:HD23	1.56	0.71
1:A:265:ILE:CD1	1:A:294:MET:HE1	2.21	0.71
1:A:218:GLU:CG	1:A:428:GLN:HE22	2.02	0.70
1:A:243:ASN:HD21	1:A:253:ASN:HD21	1.37	0.70
1:B:33:ARG:O	1:B:37:ARG:HG3	1.91	0.70
2:A:500:AD3:H3'	3:A:550:NAD:C4N	2.22	0.70
1:C:368:ILE:CG2	1:C:370:MET:CE	2.69	0.69
1:C:218:GLU:HG3	1:C:428:GLN:NE2	2.08	0.68
1:B:68:LEU:O	1:B:69:HIS:C	2.37	0.68
1:B:162:MET:O	1:B:166:ARG:HB2	1.94	0.68
1:C:368:ILE:HG22	1:C:370:MET:CE	2.23	0.68
1:A:241:ASN:HD22	1:A:241:ASN:C	2.02	0.67
2:B:500:AD3:H3'	3:B:550:NAD:C4N	2.23	0.67
1:B:138:GLU:OE2	1:B:204:LYS:NZ	2.28	0.67
1:B:157:GLY:HA3	1:B:363:HIS:NE2	2.10	0.67
1:C:218:GLU:CG	1:C:428:GLN:HE22	2.06	0.67
1:A:479:TYR:CD1	1:B:341:LYS:HD2	2.30	0.67
1:A:22:LYS:HE3	4:A:640:HOH:O	1.94	0.66
1:B:145:ASP:O	1:B:147:ASP:N	2.23	0.66
3:D:550:NAD:C4N	2:D:500:AD3:H3'	2.26	0.66
1:C:11:LEU:HD22	1:C:12:THR:H	1.60	0.65
1:D:153:ILE:O	1:D:215:VAL:HA	1.97	0.65
1:C:216:THR:CG2	1:C:432:GLN:NE2	2.60	0.65
1:B:260:SER:OG	1:B:416:HIS:HD2	1.80	0.64
1:C:236:ALA:O	4:C:869:HOH:O	2.14	0.64
1:B:358:LEU:HD11	1:B:368:ILE:CD1	2.25	0.64
1:B:403:SER:OG	1:B:412:ASN:ND2	2.30	0.64
1:A:252:ASP:OD1	1:A:416:HIS:CE1	2.51	0.64
1:B:145:ASP:H	1:B:146:PRO:HD3	1.62	0.63
1:D:146:PRO:HB2	1:D:147:ASP:CB	2.17	0.62
1:C:57:GLN:HA	1:C:57:GLN:NE2	2.15	0.62
1:D:472:LEU:HD22	1:D:476:GLN:HB3	1.80	0.62
1:C:384:LYS:HB2	1:C:385:PRO:HD2	1.82	0.62
1:C:133:TYR:OH	1:C:159:ASP:OD1	2.12	0.62
1:A:265:ILE:HD13	1:A:294:MET:HE1	1.82	0.61
1:A:252:ASP:OD1	1:A:416:HIS:HE1	1.84	0.61
1:B:213:LYS:HB3	1:B:439:ASN:ND2	2.15	0.61
1:D:187:TRP:NE1	1:D:191:LEU:HD11	2.16	0.61
1:B:381:VAL:HG12	1:D:34:LYS:HE2	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:218:GLU:HG3	1:C:428:GLN:HE22	1.64	0.61
1:B:145:ASP:H	1:B:146:PRO:HD2	1.66	0.61
1:B:168:MET:HG3	1:B:206:THR:HA	1.83	0.60
1:D:403:SER:OG	1:D:412:ASN:ND2	2.34	0.60
1:C:112:GLY:CA	1:C:118:LYS:HG3	2.30	0.60
1:C:365:ASP:HB3	1:C:406:ARG:HG3	1.83	0.60
1:A:33:ARG:O	1:A:37:ARG:HG3	2.02	0.60
1:C:255:TYR:OH	1:D:317:GLU:OE2	2.16	0.60
1:B:213:LYS:HB3	1:B:439:ASN:HD21	1.66	0.60
1:D:145:ASP:HB3	1:D:148:LYS:HG3	1.84	0.59
1:A:340:ASN:HB3	1:A:343:ILE:HD11	1.84	0.59
1:D:96:PHE:O	1:D:126:LYS:NZ	2.28	0.59
1:C:340:ASN:O	1:C:367:GLU:HG2	2.03	0.59
1:B:29:ALA:HB2	1:B:108:VAL:HG21	1.84	0.59
1:B:155:ASP:OD2	1:B:158:GLY:HA2	2.01	0.59
1:D:207:LYS:HE2	4:D:681:HOH:O	2.03	0.58
1:C:152:MET:HE2	1:C:152:MET:HA	1.85	0.58
1:C:167:GLY:O	1:C:171:GLU:HG3	2.02	0.58
1:C:384:LYS:HB2	1:C:385:PRO:CD	2.34	0.58
1:D:23:ILE:HD11	1:D:26:LEU:HD11	1.84	0.58
1:D:152:MET:HE3	1:D:213:LYS:HB2	1.84	0.58
1:C:57:GLN:NE2	1:C:84:LEU:C	2.61	0.58
1:A:403:SER:OG	1:A:412:ASN:ND2	2.37	0.58
1:B:383:VAL:HA	1:D:34:LYS:HD3	1.86	0.58
1:D:260:SER:OG	1:D:416:HIS:HD2	1.87	0.58
1:B:43:MET:HA	1:B:422:SER:HB2	1.86	0.58
1:C:310:ASN:H	1:C:310:ASN:HD22	1.52	0.58
1:D:78:ILE:HG23	1:D:88:VAL:HG21	1.86	0.57
1:C:403:SER:OG	1:C:412:ASN:ND2	2.37	0.57
1:D:167:GLY:O	1:D:171:GLU:HG3	2.04	0.57
1:B:134:TRP:HE1	1:B:186:GLU:HG3	1.69	0.57
1:C:216:THR:HG23	1:C:432:GLN:NE2	2.19	0.57
1:C:115:ASP:C	1:C:117:PRO:HD3	2.30	0.57
1:B:468:HIS:HB3	4:B:660:HOH:O	2.05	0.57
1:B:63:ARG:NH2	1:B:149:PRO:O	2.24	0.57
1:D:248:LYS:HD3	1:D:248:LYS:C	2.29	0.57
1:A:214:GLY:HA3	1:A:435:LEU:HD13	1.86	0.56
1:A:218:GLU:O	1:A:248:LYS:HE3	2.05	0.56
1:C:260:SER:OG	1:C:416:HIS:HD2	1.88	0.56
1:C:368:ILE:HG21	1:C:370:MET:CE	2.32	0.56
1:D:99:GLN:HE22	1:D:414:THR:HB	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:106:VAL:HG12	1:D:120:VAL:HG22	1.87	0.56
1:B:354:ASP:HB2	1:B:397:ARG:HG2	1.87	0.56
1:D:145:ASP:CB	1:D:146:PRO:HD2	2.35	0.56
1:D:384:LYS:CB	1:D:385:PRO:CD	2.78	0.56
1:C:370:MET:HE2	1:C:370:MET:HA	1.87	0.56
1:C:97:SER:HB3	1:C:410:LEU:HB3	1.88	0.56
1:B:340:ASN:HB3	1:B:343:ILE:HD11	1.86	0.56
1:D:213:LYS:O	1:D:238:PRO:HD2	2.06	0.55
1:B:95:ILE:HG22	1:B:133:TYR:HB2	1.86	0.55
1:B:261:LEU:HD21	1:B:294:MET:HE2	1.86	0.55
1:A:489:LYS:NZ	3:B:550:NAD:O3B	2.35	0.55
1:B:36:LEU:HD12	1:B:72:VAL:HG13	1.88	0.55
1:D:37:ARG:NH2	4:D:764:HOH:O	2.40	0.55
1:D:203:ASP:O	1:D:207:LYS:HG2	2.07	0.55
1:D:145:ASP:CG	1:D:146:PRO:HD2	2.30	0.55
1:D:261:LEU:HD21	1:D:294:MET:HE2	1.89	0.55
1:A:241:ASN:C	1:A:241:ASN:ND2	2.65	0.54
1:A:80:THR:O	1:A:84:LEU:HG	2.08	0.54
1:C:262:ILE:HD12	1:C:266:ASN:ND2	2.22	0.54
1:C:244:ASP:OD2	1:D:492:HIS:HE1	1.91	0.54
1:C:246:VAL:HG22	1:D:494:ARG:CZ	2.38	0.54
1:C:252:ASP:OD2	1:C:416:HIS:HE1	1.90	0.54
1:B:57:GLN:HE22	1:B:85:GLY:CA	2.19	0.53
1:C:152:MET:HE3	1:C:213:LYS:HB2	1.89	0.53
1:A:42:GLU:O	1:A:419:PHE:HA	2.07	0.53
1:A:262:ILE:CD1	1:C:262:ILE:HD11	2.32	0.53
1:B:358:LEU:CD1	1:B:368:ILE:CD1	2.86	0.53
1:D:384:LYS:HE3	1:D:387:VAL:HG21	1.91	0.53
1:A:197:ARG:HD2	1:A:204:LYS:HD2	1.91	0.53
1:D:78:ILE:HD11	1:D:90:TRP:CD2	2.43	0.53
1:B:145:ASP:N	1:B:146:PRO:CD	2.60	0.53
1:D:23:ILE:O	1:D:24:ALA:C	2.52	0.53
1:B:252:ASP:OD1	1:B:416:HIS:CE1	2.62	0.52
1:A:65:SER:HB3	1:A:140:MET:SD	2.49	0.52
1:B:407:LEU:HD22	1:B:410:LEU:HD12	1.91	0.52
1:C:492:HIS:HE1	1:D:244:ASP:OD2	1.92	0.52
1:A:223:VAL:HG21	1:A:241:ASN:ND2	2.25	0.52
1:B:450:PRO:HD2	1:B:453:LEU:HD12	1.91	0.52
1:D:11:LEU:HD22	1:D:22:LYS:HE3	1.92	0.52
1:B:243:ASN:HD21	1:B:253:ASN:HD21	1.58	0.51
1:C:261:LEU:HD12	1:C:408:LEU:HD11	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:489:LYS:HE2	1:B:310:ASN:HD21	1.75	0.51
1:A:35:GLU:OE1	1:A:101:HIS:HE1	1.94	0.51
1:A:261:LEU:CD2	1:A:294:MET:HE2	2.40	0.51
1:A:178:PRO:HA	1:A:195:ARG:NH2	2.26	0.51
1:A:363:HIS:ND1	2:A:500:AD3:O5'	2.34	0.51
4:A:732:HOH:O	1:C:259:HIS:HE1	1.92	0.51
1:A:261:LEU:HD21	1:A:294:MET:HE2	1.92	0.51
1:D:243:ASN:O	1:D:249:SER:HB3	2.10	0.51
1:B:240:ILE:HG12	1:B:447:TYR:HB2	1.93	0.51
1:B:381:VAL:CG1	1:D:34:LYS:HE2	2.41	0.51
1:A:59:LEU:HB3	1:A:86:ALA:HB2	1.92	0.51
1:A:179:ALA:HB2	1:A:191:LEU:HD12	1.92	0.51
1:A:309:ILE:HG21	1:B:246:VAL:HG11	1.93	0.51
1:A:269:THR:HG21	1:A:357:ILE:HD13	1.93	0.51
1:B:218:GLU:HG3	1:B:428:GLN:HE22	1.75	0.51
1:D:455:GLU:OE2	1:D:487:PRO:HA	2.10	0.50
1:B:206:THR:O	1:B:210:GLU:HG3	2.10	0.50
1:D:406:ARG:O	1:D:407:LEU:C	2.52	0.50
1:B:78:ILE:HG23	1:B:88:VAL:HG21	1.93	0.50
1:D:408:LEU:HD12	1:D:408:LEU:C	2.37	0.50
1:B:144:PRO:O	1:B:145:ASP:HB2	2.12	0.49
1:B:283:TYR:CE2	1:B:288:LYS:HE3	2.47	0.49
1:D:23:ILE:HD11	1:D:26:LEU:CD1	2.42	0.49
1:B:141:LEU:HD12	1:B:163:LEU:HD23	1.95	0.49
1:B:283:TYR:CD2	1:B:288:LYS:HE3	2.47	0.49
1:D:69:HIS:CE1	1:D:93:CYS:SG	3.05	0.49
1:A:43:MET:HA	1:A:422:SER:HB2	1.94	0.49
1:D:178:PRO:HA	1:D:195:ARG:HH21	1.76	0.49
1:C:23:ILE:HD11	1:C:26:LEU:HD13	1.94	0.49
1:D:407:LEU:HD12	1:D:410:LEU:HD12	1.94	0.49
1:D:53:TYR:HD2	1:D:58:PRO:HG3	1.77	0.49
1:D:143:TRP:HB2	1:D:149:PRO:HA	1.93	0.49
1:D:146:PRO:HB2	1:D:147:ASP:CA	2.42	0.49
1:D:166:ARG:HA	1:D:169:GLN:HB3	1.95	0.49
1:B:145:ASP:C	1:B:147:ASP:H	2.15	0.49
1:C:145:ASP:OD1	1:C:147:ASP:HB2	2.13	0.49
1:D:43:MET:HA	1:D:422:SER:HB2	1.95	0.49
1:C:218:GLU:HG2	1:C:428:GLN:HE22	1.77	0.49
1:A:192:ASN:OD1	1:A:195:ARG:NH1	2.45	0.48
1:B:163:LEU:HD13	1:B:190:PHE:CE1	2.48	0.48
1:C:124:ALA:HA	1:C:128:GLU:OE2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:68:LEU:HB2	1:D:156:ASP:HB3	1.96	0.48
1:B:252:ASP:OD1	1:B:416:HIS:HE1	1.96	0.48
1:D:218:GLU:CG	1:D:428:GLN:NE2	2.63	0.48
1:A:78:ILE:HG23	1:A:88:VAL:HG21	1.96	0.48
1:A:155:ASP:OD2	1:A:158:GLY:HA2	2.13	0.48
1:A:284:GLY:HA3	3:A:550:NAD:O5B	2.14	0.48
1:B:430:ILE:O	1:B:434:GLU:HG2	2.13	0.48
1:C:247:THR:HA	1:C:251:PHE:CD2	2.49	0.48
1:D:15:VAL:O	1:D:16:ARG:NH1	2.47	0.48
1:A:238:PRO:HB2	1:A:435:LEU:HD21	1.94	0.47
1:B:457:VAL:O	1:B:461:HIS:ND1	2.38	0.47
1:C:471:LYS:NZ	1:C:484:VAL:HG11	2.29	0.47
1:A:340:ASN:HD21	1:B:476:GLN:HB3	1.79	0.47
1:B:71:THR:HG22	1:B:99:GLN:NE2	2.30	0.47
1:C:28:LEU:HB3	1:C:101:HIS:HA	1.97	0.47
1:B:29:ALA:CB	1:B:108:VAL:HG21	2.44	0.47
1:B:41:HIS:HD2	4:B:685:HOH:O	1.96	0.47
1:B:57:GLN:NE2	1:B:85:GLY:HA2	2.22	0.47
1:B:384:LYS:HB2	1:B:385:PRO:CD	2.44	0.47
1:D:52:GLU:HB3	1:D:53:TYR:CD1	2.50	0.47
1:B:57:GLN:HB3	1:B:60:LYS:HG3	1.97	0.47
1:B:23:ILE:HD11	1:B:26:LEU:HD13	1.97	0.47
1:B:394:ASP:OD1	1:B:395:THR:HG23	2.15	0.47
1:A:281:CYS:HB2	1:A:336:THR:HA	1.96	0.46
1:B:124:ALA:HA	1:B:128:GLU:OE2	2.15	0.46
1:B:213:LYS:HG3	1:B:436:TRP:CZ3	2.51	0.46
1:C:252:ASP:OD2	1:C:416:HIS:CE1	2.67	0.46
1:D:151:ASN:HA	1:D:212:VAL:HA	1.97	0.46
1:B:179:ALA:HB2	1:B:191:LEU:HD12	1.97	0.46
1:C:479:TYR:CD1	1:D:341:LYS:HD2	2.50	0.46
1:A:406:ARG:O	1:A:407:LEU:C	2.58	0.46
1:C:57:GLN:HE22	1:C:84:LEU:C	2.23	0.46
1:D:360:ASN:ND2	1:D:364:PHE:O	2.48	0.46
1:B:68:LEU:HD22	1:B:154:LEU:CD2	2.46	0.46
1:C:363:HIS:CD2	1:C:364:PHE:CE1	3.04	0.46
1:C:423:ASN:HD21	1:D:312:LEU:CD2	2.28	0.46
1:C:469:LEU:HD11	1:D:308:PRO:HB3	1.98	0.46
1:A:95:ILE:HG22	1:A:133:TYR:HB2	1.98	0.46
1:A:197:ARG:O	1:A:197:ARG:HG3	2.16	0.46
1:D:22:LYS:HG3	1:D:125:TRP:CZ3	2.51	0.46
1:D:146:PRO:CB	1:D:147:ASP:CA	2.94	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:ILE:HD11	1:C:262:ILE:CD1	2.34	0.46
1:B:442:TYR:CD1	1:B:442:TYR:N	2.84	0.46
1:C:57:GLN:HA	1:C:57:GLN:HE21	1.81	0.46
1:C:345:MET:HA	1:C:369:ASP:HB2	1.97	0.46
1:B:69:HIS:CE1	1:B:410:LEU:HD13	2.51	0.45
1:C:33:ARG:NH2	1:C:79:GLU:OE2	2.23	0.45
1:D:483:ASP:HB3	4:D:733:HOH:O	2.14	0.45
1:A:13:PRO:HB3	1:A:123:PHE:HE1	1.80	0.45
1:C:216:THR:HG23	1:C:432:GLN:HE22	1.80	0.45
1:D:113:THR:HG23	1:D:116:GLU:HB3	1.98	0.45
1:D:88:VAL:CG2	1:D:120:VAL:HG21	2.46	0.45
1:D:16:ARG:HB2	1:D:117:PRO:HG2	1.98	0.45
1:A:182:ASP:OD1	1:A:375:ARG:NH1	2.49	0.45
1:B:248:LYS:HD3	1:B:252:ASP:HB3	1.99	0.45
1:B:320:ASP:OD1	1:C:300:ARG:HD2	2.16	0.45
1:C:311:ALA:O	1:C:315:MET:HG3	2.17	0.45
1:D:106:VAL:CG1	1:D:120:VAL:HG22	2.47	0.45
1:A:241:ASN:ND2	1:A:244:ASP:H	2.15	0.45
1:D:157:GLY:HA3	1:D:363:HIS:NE2	2.32	0.45
1:A:323:THR:OG1	1:A:326:GLU:HG2	2.17	0.45
1:D:259:HIS:ND1	1:D:417:PRO:HD3	2.32	0.45
1:B:225:ARG:HE	1:B:364:PHE:HE2	1.64	0.44
1:B:246:VAL:HG21	1:B:495:TYR:CE1	2.52	0.44
1:B:259:HIS:HE1	4:D:673:HOH:O	2.00	0.44
1:B:32:GLY:HA2	1:B:101:HIS:HD2	1.82	0.44
1:C:217:GLU:OE2	1:C:222:GLY:HA3	2.18	0.44
1:C:312:LEU:HG	1:D:251:PHE:CE2	2.52	0.44
1:A:72:VAL:O	1:A:76:VAL:HG23	2.17	0.44
1:A:259:HIS:HE1	4:C:850:HOH:O	2.00	0.44
1:C:96:PHE:O	1:C:126:LYS:NZ	2.44	0.44
1:C:216:THR:CG2	1:C:432:GLN:HE21	2.29	0.44
1:D:97:SER:HB2	1:D:410:LEU:HB3	1.98	0.44
1:D:340:ASN:O	1:D:367:GLU:HG2	2.17	0.44
1:B:213:LYS:O	1:B:238:PRO:HD2	2.17	0.44
1:D:88:VAL:HG23	1:D:120:VAL:HG21	2.00	0.44
1:A:261:LEU:HD22	1:A:290:CYS:SG	2.58	0.44
1:B:406:ARG:O	1:B:407:LEU:C	2.61	0.44
1:C:89:ARG:NH2	1:C:139:GLN:O	2.37	0.44
1:C:278:VAL:HG11	1:C:294:MET:HG3	2.00	0.44
1:D:416:HIS:HB2	1:D:421:MET:SD	2.58	0.44
1:B:88:VAL:O	1:B:121:PRO:HD2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:235:LEU:HG	1:C:237:PHE:O	2.16	0.44
1:C:352:MET:HB2	1:C:399:ILE:HD11	1.99	0.44
1:A:52:GLU:OE1	1:A:456:LYS:NZ	2.32	0.43
1:A:59:LEU:HD23	1:A:59:LEU:HA	1.84	0.43
1:D:68:LEU:O	1:D:69:HIS:C	2.62	0.43
1:A:91:ALA:HB2	1:A:140:MET:HB2	2.00	0.43
1:D:252:ASP:OD1	1:D:416:HIS:CE1	2.71	0.43
1:A:248:LYS:HD3	1:A:252:ASP:HB3	1.99	0.43
1:A:363:HIS:CE1	2:A:500:AD3:HO5'	2.31	0.43
1:D:217:GLU:CD	1:D:222:GLY:HA3	2.43	0.43
1:D:218:GLU:HG3	1:D:428:GLN:HE21	1.74	0.43
1:B:95:ILE:CG2	1:B:133:TYR:HB2	2.49	0.43
1:A:69:HIS:ND1	1:A:97:SER:CB	2.82	0.43
1:B:57:GLN:NE2	1:B:85:GLY:CA	2.80	0.43
1:B:345:MET:HA	1:B:369:ASP:HB3	2.00	0.43
1:C:423:ASN:HD21	1:D:312:LEU:HD21	1.84	0.43
1:D:71:THR:HA	1:D:99:GLN:HG3	1.99	0.43
1:D:281:CYS:HB2	1:D:336:THR:HA	2.01	0.43
1:A:390:TRP:O	1:A:398:SER:HA	2.19	0.43
1:B:145:ASP:C	1:B:147:ASP:N	2.76	0.43
1:B:394:ASP:OD1	1:B:395:THR:N	2.52	0.43
1:D:134:TRP:CZ3	1:D:163:LEU:HD22	2.54	0.43
1:A:428:GLN:HE21	1:A:428:GLN:HB2	1.55	0.43
1:A:258:ARG:HD3	1:A:292:GLU:CD	2.44	0.42
1:D:99:GLN:NE2	1:D:414:THR:HB	2.33	0.42
1:B:89:ARG:HD3	1:B:143:TRP:CE2	2.54	0.42
1:A:258:ARG:HA	1:A:293:ALA:HB2	2.00	0.42
1:D:23:ILE:HG23	1:D:122:VAL:O	2.19	0.42
1:A:36:LEU:HD12	1:A:72:VAL:HG13	2.01	0.42
1:A:36:LEU:O	1:A:40:GLU:HG3	2.19	0.42
1:A:69:HIS:CD2	1:A:410:LEU:HD13	2.55	0.42
1:A:203:ASP:O	1:A:207:LYS:HG3	2.20	0.42
1:A:217:GLU:HG3	1:A:223:VAL:HG23	2.01	0.42
1:D:213:LYS:HG3	1:D:436:TRP:HZ3	1.85	0.42
1:A:476:GLN:HB3	1:B:340:ASN:HD21	1.83	0.42
1:A:480:LEU:HA	1:B:224:LEU:HD21	2.01	0.42
1:A:252:ASP:OD1	1:A:252:ASP:C	2.61	0.42
1:A:346:LEU:HD13	1:A:373:LEU:HA	2.02	0.42
1:B:94:ASN:ND2	1:B:407:LEU:CD1	2.83	0.42
1:B:126:LYS:HE2	4:B:697:HOH:O	2.18	0.42
1:C:108:VAL:O	1:C:112:GLY:HA3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:357:ILE:HD11	4:C:849:HOH:O	2.19	0.42
1:B:36:LEU:O	1:B:40:GLU:HG3	2.20	0.42
1:C:218:GLU:CG	1:C:428:GLN:NE2	2.73	0.42
1:D:163:LEU:HD12	1:D:194:LEU:HD21	2.01	0.42
1:D:471:LYS:HG2	1:D:472:LEU:O	2.20	0.42
1:A:244:ASP:OD2	1:B:492:HIS:HE1	2.03	0.42
1:B:355:HIS:NE2	1:D:41:HIS:ND1	2.68	0.42
1:D:419:PHE:CZ	1:D:465:LEU:HG	2.55	0.42
1:A:68:LEU:O	1:A:69:HIS:C	2.63	0.41
1:C:248:LYS:HG2	1:C:424:SER:HB3	2.02	0.41
1:C:115:ASP:HB3	4:C:779:HOH:O	2.19	0.41
1:C:149:PRO:HG2	1:C:211:SER:HB2	2.02	0.41
1:D:174:GLY:O	1:D:198:PHE:CE2	2.74	0.41
1:B:328:ILE:CD1	1:B:344:ILE:HD12	2.50	0.41
1:C:216:THR:HG21	1:C:432:GLN:NE2	2.32	0.41
1:A:66:GLY:HA3	1:A:90:TRP:CZ3	2.55	0.41
1:A:403:SER:O	1:A:406:ARG:CG	2.68	0.41
1:B:151:ASN:O	1:B:152:MET:HG2	2.20	0.41
1:B:477:ALA:HB1	1:B:482:VAL:O	2.21	0.41
1:D:278:VAL:HG11	1:D:294:MET:HG3	2.01	0.41
1:D:355:HIS:N	1:D:398:SER:O	2.47	0.41
1:A:430:ILE:O	1:A:434:GLU:HG2	2.21	0.41
1:D:163:LEU:CD1	1:D:194:LEU:HD21	2.50	0.41
1:D:176:VAL:HA	1:D:177:PRO:HD3	1.85	0.41
1:C:217:GLU:CD	1:C:222:GLY:HA3	2.45	0.41
1:C:303:VAL:O	1:C:321:VAL:HA	2.20	0.41
1:B:490:PRO:HD2	1:B:493:TYR:HB2	2.02	0.41
1:C:94:ASN:HB3	1:C:97:SER:OG	2.21	0.41
1:D:66:GLY:HA3	1:D:90:TRP:CZ3	2.55	0.41
1:A:66:GLY:HA3	1:A:90:TRP:CE3	2.56	0.41
1:B:279:LEU:HD11	1:B:304:THR:CG2	2.51	0.41
1:B:473:THR:OG1	1:B:476:GLN:HG3	2.21	0.41
1:D:26:LEU:HD12	1:D:26:LEU:N	2.36	0.41
1:D:252:ASP:OD1	1:D:416:HIS:HE1	2.03	0.41
1:D:372:GLY:O	1:D:376:SER:HB3	2.21	0.41
1:B:94:ASN:HB3	1:B:97:SER:HB3	2.04	0.40
1:B:110:PRO:HD2	4:B:598:HOH:O	2.20	0.40
1:B:217:GLU:HG3	1:B:223:VAL:HG23	2.01	0.40
1:B:260:SER:OG	1:B:416:HIS:CD2	2.66	0.40
1:A:223:VAL:O	1:A:226:LEU:HB2	2.21	0.40
1:B:213:LYS:HG3	1:B:436:TRP:HZ3	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:443:ASP:CG	1:A:444:ASN:N	2.80	0.40
1:C:97:SER:CB	1:C:410:LEU:HB3	2.50	0.40
1:A:208:ILE:O	1:A:212:VAL:HG23	2.21	0.40
1:A:355:HIS:N	1:A:398:SER:O	2.40	0.40
1:B:135:TRP:O	1:B:138:GLU:HB3	2.21	0.40
1:C:384:LYS:HE3	1:C:387:VAL:HG21	2.02	0.40
1:D:304:THR:OG1	3:D:550:NAD:H2A	2.21	0.40
1:A:133:TYR:CD1	1:A:133:TYR:C	3.00	0.40
1:D:247:THR:HA	1:D:251:PHE:CD1	2.56	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:847:HOH:O	4:D:691:HOH:O[1_455]	2.08	0.12
4:B:679:HOH:O	4:D:689:HOH:O[1_556]	2.16	0.04

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	483/495 (98%)	456 (94%)	22 (5%)	5 (1%)	12	11
1	B	483/495 (98%)	455 (94%)	23 (5%)	5 (1%)	12	11
1	C	483/495 (98%)	456 (94%)	25 (5%)	2 (0%)	30	34
1	D	483/495 (98%)	454 (94%)	25 (5%)	4 (1%)	16	16
All	All	1932/1980 (98%)	1821 (94%)	95 (5%)	16 (1%)	16	16

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	365	ASP
1	B	145	ASP
1	B	146	PRO
1	D	146	PRO
1	A	181	GLU
1	B	362	GLY
1	D	69	HIS
1	D	149	PRO
1	A	369	ASP
1	B	407	LEU
1	C	145	ASP
1	A	69	HIS
1	A	474	LYS
1	D	147	ASP
1	C	116	GLU
1	B	144	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	395/404 (98%)	376 (95%)	19 (5%)	23	30
1	B	395/404 (98%)	374 (95%)	21 (5%)	20	26
1	C	395/404 (98%)	372 (94%)	23 (6%)	18	22
1	D	395/404 (98%)	366 (93%)	29 (7%)	13	15
All	All	1580/1616 (98%)	1488 (94%)	92 (6%)	18	22

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LEU
1	A	16	ARG
1	A	48	SER
1	A	56	VAL
1	A	68	LEU
1	A	88	VAL

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Mol	Chain	Res	Type
1	A	92	SER
1	A	180	GLU
1	A	182	ASP
1	A	186	GLU
1	A	200	THR
1	A	218	GLU
1	A	241	ASN
1	A	262	ILE
1	A	303	VAL
1	A	317	GLU
1	A	407	LEU
1	A	428	GLN
1	A	445	GLU
1	B	11	LEU
1	B	68	LEU
1	B	88	VAL
1	B	138	GLU
1	B	146	PRO
1	B	152	MET
1	B	162	MET
1	B	180	GLU
1	B	183	ASP
1	B	188	LYS
1	B	193	LEU
1	B	288	LYS
1	B	304	THR
1	B	368	ILE
1	B	398	SER
1	B	407	LEU
1	B	428	GLN
1	B	440	ASP
1	B	442	TYR
1	B	469	LEU
1	B	475	GLU
1	C	11	LEU
1	C	12	THR
1	C	26	LEU
1	C	88	VAL
1	C	111	HIS
1	C	120	VAL
1	C	147	ASP
1	C	152	MET

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Mol	Chain	Res	Type
1	C	169	GLN
1	C	180	GLU
1	C	192	ASN
1	C	193	LEU
1	C	218	GLU
1	C	224	LEU
1	C	253	ASN
1	C	262	ILE
1	C	277	LYS
1	C	310	ASN
1	C	317	GLU
1	C	407	LEU
1	C	424	SER
1	C	454	ASP
1	C	475	GLU
1	D	23	ILE
1	D	27	SER
1	D	37	ARG
1	D	56	VAL
1	D	68	LEU
1	D	113	THR
1	D	118	LYS
1	D	120	VAL
1	D	145	ASP
1	D	148	LYS
1	D	152	MET
1	D	175	VAL
1	D	182	ASP
1	D	186	GLU
1	D	199	GLU
1	D	213	LYS
1	D	218	GLU
1	D	219	THR
1	D	220	THR
1	D	248	LYS
1	D	262	ILE
1	D	353	LYS
1	D	379	THR
1	D	398	SER
1	D	399	ILE
1	D	407	LEU
1	D	440	ASP

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Mol	Chain	Res	Type
1	D	441	GLU
1	D	474	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	GLN
1	A	101	HIS
1	A	241	ASN
1	A	243	ASN
1	A	259	HIS
1	A	310	ASN
1	A	412	ASN
1	A	416	HIS
1	A	423	ASN
1	A	428	GLN
1	A	492	HIS
1	B	41	HIS
1	B	57	GLN
1	B	101	HIS
1	B	111	HIS
1	B	228	GLN
1	B	243	ASN
1	B	259	HIS
1	B	310	ASN
1	B	340	ASN
1	B	386	GLN
1	B	412	ASN
1	B	416	HIS
1	B	439	ASN
1	B	492	HIS
1	C	57	GLN
1	C	192	ASN
1	C	228	GLN
1	C	243	ASN
1	C	259	HIS
1	C	310	ASN
1	C	355	HIS
1	C	360	ASN
1	C	412	ASN
1	C	416	HIS
1	C	427	ASN

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Mol	Chain	Res	Type
1	C	428	GLN
1	C	432	GLN
1	C	492	HIS
1	D	57	GLN
1	D	192	ASN
1	D	259	HIS
1	D	310	ASN
1	D	412	ASN
1	D	416	HIS
1	D	427	ASN
1	D	428	GLN
1	D	492	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](#)

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	AD3	A	500	-	21,21,21	2.00	3 (14%)	30,31,31	2.29	10 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAD	A	550	-	46,48,48	1.55	8 (17%)	64,73,73	2.33	19 (29%)
3	NAD	C	550	-	46,48,48	1.44	9 (19%)	64,73,73	2.19	14 (21%)
3	NAD	B	550	-	46,48,48	1.93	10 (21%)	64,73,73	2.68	23 (35%)
2	AD3	B	500	-	21,21,21	1.67	3 (14%)	30,31,31	1.95	8 (26%)
3	NAD	D	550	-	46,48,48	1.51	6 (13%)	64,73,73	2.32	19 (29%)
2	AD3	D	500	-	21,21,21	1.77	5 (23%)	30,31,31	2.37	10 (33%)
2	AD3	C	500	-	21,21,21	1.62	2 (9%)	30,31,31	2.13	9 (30%)

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	AD3	A	500	-	-	4/6/22/22	0/3/3/3
3	NAD	A	550	-	-	4/30/62/62	0/5/5/5
3	NAD	C	550	-	-	5/30/62/62	0/5/5/5
3	NAD	B	550	-	-	7/30/62/62	0/5/5/5
2	AD3	B	500	-	-	4/6/22/22	0/3/3/3
3	NAD	D	550	-	-	6/30/62/62	0/5/5/5
2	AD3	D	500	-	-	4/6/22/22	0/3/3/3
2	AD3	C	500	-	-	4/6/22/22	0/3/3/3

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	550	NAD	PA-O3	7.71	1.67	1.59
2	A	500	AD3	C4-C5	6.50	1.48	1.40
2	B	500	AD3	C4-C5	6.07	1.48	1.40
2	C	500	AD3	C4-C5	5.67	1.47	1.40
2	D	500	AD3	C4-C5	5.61	1.47	1.40
3	A	550	NAD	O7N-C7N	5.59	1.34	1.24
3	D	550	NAD	O4D-C1D	5.20	1.47	1.40
3	C	550	NAD	O7N-C7N	5.04	1.33	1.24
3	B	550	NAD	O7N-C7N	4.65	1.32	1.24
3	D	550	NAD	O7N-C7N	4.37	1.32	1.24
2	A	500	AD3	C4-N9	-4.18	1.31	1.39
3	B	550	NAD	C5A-C4A	3.72	1.45	1.39
3	A	550	NAD	O4D-C1D	3.49	1.45	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	550	NAD	PA-O3	3.48	1.63	1.59
3	B	550	NAD	PN-O3	3.48	1.63	1.59
3	B	550	NAD	O4D-C1D	3.22	1.45	1.40
2	C	500	AD3	C4-N9	-2.99	1.33	1.39
3	D	550	NAD	C5A-C4A	2.93	1.44	1.39
3	B	550	NAD	C2A-N3A	2.82	1.39	1.33
3	C	550	NAD	C4A-N9A	-2.80	1.31	1.37
3	C	550	NAD	C7N-N7N	-2.76	1.27	1.33
3	A	550	NAD	C2N-N1N	-2.70	1.32	1.35
3	A	550	NAD	C6A-N6A	2.63	1.40	1.34
2	D	500	AD3	C4-N9	-2.62	1.34	1.39
2	D	500	AD3	C8-N7	2.59	1.36	1.31
3	A	550	NAD	C7N-N7N	-2.58	1.28	1.33
3	B	550	NAD	C7N-N7N	-2.51	1.28	1.33
3	A	550	NAD	PA-O3	2.50	1.62	1.59
3	A	550	NAD	C1B-N9A	2.32	1.52	1.46
3	C	550	NAD	C5A-C4A	2.31	1.43	1.39
2	A	500	AD3	C8-N7	2.31	1.36	1.31
3	A	550	NAD	C5A-C4A	2.29	1.43	1.39
2	D	500	AD3	C8-N9	-2.28	1.33	1.37
2	D	500	AD3	C3-C4	2.27	1.43	1.39
3	B	550	NAD	C4A-N3A	2.25	1.38	1.34
3	B	550	NAD	C8A-N7A	2.21	1.35	1.31
3	D	550	NAD	C7N-N7N	-2.21	1.28	1.33
3	C	550	NAD	C2N-C3N	2.19	1.42	1.39
3	C	550	NAD	O4D-C1D	2.18	1.43	1.40
2	B	500	AD3	C8-N7	2.18	1.35	1.31
3	C	550	NAD	O3D-C3D	2.18	1.48	1.43
3	C	550	NAD	C3N-C7N	2.17	1.53	1.50
3	B	550	NAD	O2B-C2B	2.15	1.48	1.43
3	D	550	NAD	C2N-N1N	-2.13	1.32	1.35
2	B	500	AD3	C4-N9	-2.07	1.35	1.39
3	C	550	NAD	C5D-C4D	2.02	1.57	1.51

All (112) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	550	NAD	N3A-C2A-N1A	-8.01	116.46	128.58
3	A	550	NAD	N3A-C2A-N1A	-7.37	117.43	128.58
3	D	550	NAD	N3A-C2A-N1A	-7.09	117.85	128.58
3	D	550	NAD	C4A-N9A-C8A	6.58	112.64	105.74
2	D	500	AD3	C4-C5-N7	-6.46	105.61	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	550	NAD	C4A-N9A-C8A	6.45	112.51	105.74
3	B	550	NAD	C5A-C4A-N3A	-6.26	118.09	126.72
3	C	550	NAD	N3A-C2A-N1A	-6.22	119.17	128.58
2	A	500	AD3	C2-N1-C6	6.05	126.30	117.62
3	C	550	NAD	C4A-N9A-C8A	6.02	112.06	105.74
3	B	550	NAD	N3A-C4A-N9A	5.93	137.25	127.17
2	C	500	AD3	C4-C5-N7	-5.71	106.17	110.44
3	C	550	NAD	C5A-C4A-N3A	-5.69	118.89	126.72
3	B	550	NAD	N9A-C8A-N7A	-5.65	105.92	113.94
3	D	550	NAD	N9A-C8A-N7A	-5.62	105.97	113.94
3	B	550	NAD	C2A-N3A-C4A	5.50	125.27	111.83
3	C	550	NAD	N3A-C4A-N9A	5.41	136.37	127.17
3	C	550	NAD	N9A-C8A-N7A	-5.29	106.42	113.94
2	B	500	AD3	C4-C5-N7	-5.16	106.58	110.44
2	D	500	AD3	C2-N1-C6	5.15	125.01	117.62
3	A	550	NAD	C2A-N3A-C4A	4.80	123.54	111.83
2	D	500	AD3	C4-N9-C8	4.76	110.58	106.26
3	A	550	NAD	N9A-C8A-N7A	-4.74	107.22	113.94
3	B	550	NAD	C5A-N7A-C8A	4.73	110.88	103.45
3	A	550	NAD	C4A-N9A-C8A	4.66	110.63	105.74
2	A	500	AD3	C4-N9-C8	4.65	110.48	106.26
3	C	550	NAD	C2A-N3A-C4A	4.61	123.08	111.83
3	C	550	NAD	C5A-N7A-C8A	4.53	110.57	103.45
2	A	500	AD3	C3-C2-N1	-4.51	118.44	123.97
3	A	550	NAD	C5A-C4A-N3A	-4.43	120.62	126.72
3	D	550	NAD	C5A-N7A-C8A	4.42	110.39	103.45
3	B	550	NAD	C5N-C4N-C3N	-4.40	116.03	120.36
3	A	550	NAD	O3-PA-O1A	-4.38	97.54	110.70
2	C	500	AD3	C4-N9-C8	4.33	110.19	106.26
3	A	550	NAD	C4A-C5A-N7A	-4.24	105.73	110.58
3	B	550	NAD	C3N-C7N-N7N	4.22	122.94	117.74
3	D	550	NAD	N3A-C4A-N9A	4.22	134.34	127.17
3	B	550	NAD	C4A-C5A-N7A	-4.20	105.78	110.58
2	B	500	AD3	C3-C4-C5	-4.17	118.20	122.62
3	A	550	NAD	C5A-N7A-C8A	4.15	109.97	103.45
3	D	550	NAD	C5A-C4A-N3A	-4.11	121.06	126.72
3	D	550	NAD	C2A-N3A-C4A	4.09	121.81	111.83
3	A	550	NAD	C4D-O4D-C1D	4.02	113.61	109.92
3	D	550	NAD	C2A-N1A-C6A	3.94	125.20	118.73
3	C	550	NAD	C4A-C5A-N7A	-3.90	106.12	110.58
3	B	550	NAD	O4B-C1B-N9A	3.89	115.57	108.09
3	A	550	NAD	C2A-N1A-C6A	3.75	124.90	118.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	550	NAD	C2N-C3N-C4N	3.75	122.62	118.26
3	D	550	NAD	C4A-C5A-N7A	-3.69	106.37	110.58
2	B	500	AD3	C2-N1-C6	3.64	122.84	117.62
2	C	500	AD3	O5'-C5'-C4'	-3.60	99.07	111.33
2	D	500	AD3	C5-N7-C8	3.56	109.04	103.45
3	A	550	NAD	C6A-C5A-N7A	3.42	138.68	132.09
3	A	550	NAD	N3A-C4A-N9A	3.40	132.96	127.17
2	C	500	AD3	C5-N7-C8	3.38	108.76	103.45
2	D	500	AD3	N9-C8-N7	-3.37	109.16	113.94
3	B	550	NAD	C6A-C5A-N7A	3.36	138.56	132.09
2	D	500	AD3	C4'-O4'-C1'	-3.35	102.08	109.47
2	A	500	AD3	C4-N9-C1'	-3.33	119.77	125.41
3	D	550	NAD	C6N-N1N-C2N	-3.24	119.12	121.88
2	C	500	AD3	N9-C8-N7	-3.22	109.36	113.94
2	C	500	AD3	C3-C4-C5	-3.17	119.26	122.62
3	D	550	NAD	C5N-C4N-C3N	-3.13	117.29	120.36
3	B	550	NAD	C2B-C3B-C4B	3.08	108.56	102.61
3	C	550	NAD	O7N-C7N-N7N	-3.05	118.20	122.62
2	C	500	AD3	C4'-O4'-C1'	-2.99	102.86	109.47
3	A	550	NAD	C4A-N9A-C1B	-2.99	119.64	126.63
3	A	550	NAD	O2A-PA-O1A	2.94	126.13	112.44
3	D	550	NAD	O3-PA-O1A	-2.94	101.86	110.70
3	B	550	NAD	O7N-C7N-N7N	-2.93	118.38	122.62
3	A	550	NAD	C5N-C4N-C3N	-2.93	117.48	120.36
2	A	500	AD3	O4'-C1'-N9	2.93	113.72	108.09
3	D	550	NAD	C6A-C5A-N7A	2.92	137.71	132.09
3	D	550	NAD	C5B-C4B-C3B	-2.89	104.82	115.21
2	A	500	AD3	C5-C6-N6	-2.88	116.14	123.29
2	A	500	AD3	N6-C6-N1	2.88	124.79	118.38
2	D	500	AD3	O2'-C2'-C3'	-2.87	102.63	111.82
3	B	550	NAD	O5B-PA-O1A	2.86	120.26	108.94
2	B	500	AD3	C3-C4-N9	2.81	136.18	130.61
3	B	550	NAD	O4B-C1B-C2B	2.80	112.61	106.62
3	B	550	NAD	C2N-C3N-C4N	2.80	121.51	118.26
2	B	500	AD3	C4-N9-C8	2.79	108.79	106.26
3	C	550	NAD	C6A-C5A-N7A	2.72	137.33	132.09
3	D	550	NAD	O4B-C4B-C3B	2.66	110.44	105.15
3	D	550	NAD	C4D-O4D-C1D	2.64	112.34	109.92
2	A	500	AD3	C5-C4-N9	-2.63	104.24	105.24
3	C	550	NAD	O2N-PN-O1N	2.58	124.43	112.44
3	D	550	NAD	C3N-C7N-N7N	2.57	120.90	117.74
2	C	500	AD3	C2-N1-C6	2.56	121.29	117.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	500	AD3	C5-N7-C8	2.54	107.44	103.45
2	D	500	AD3	C3-C4-C5	-2.52	119.95	122.62
2	D	500	AD3	C3-C2-N1	-2.48	120.94	123.97
3	B	550	NAD	C4A-N9A-C1B	-2.46	120.87	126.63
2	B	500	AD3	C3-C2-N1	-2.45	120.97	123.97
3	C	550	NAD	O7N-C7N-C3N	2.41	122.55	119.60
3	A	550	NAD	C2B-C1B-N9A	2.40	119.26	113.30
2	C	500	AD3	C3-C4-N9	2.38	135.32	130.61
2	A	500	AD3	N9-C8-N7	-2.37	110.58	113.94
3	B	550	NAD	C2A-N1A-C6A	2.35	122.59	118.73
3	A	550	NAD	C5N-C6N-N1N	2.30	123.52	120.38
3	D	550	NAD	C4A-N9A-C1B	-2.28	121.30	126.63
3	B	550	NAD	O2A-PA-O3	-2.26	101.17	107.27
3	B	550	NAD	C5D-C4D-C3D	-2.25	107.10	115.21
2	D	500	AD3	C6-C5-N7	2.22	136.37	132.09
3	C	550	NAD	O3-PA-O1A	-2.20	104.09	110.70
3	B	550	NAD	C5A-C6A-N6A	-2.18	117.90	123.29
2	A	500	AD3	O2'-C2'-C1'	-2.17	102.64	110.10
3	A	550	NAD	C6N-N1N-C2N	-2.16	120.04	121.88
2	B	500	AD3	C4'-O4'-C1'	-2.16	104.70	109.47
3	C	550	NAD	C1B-N9A-C8A	-2.09	122.46	127.09
3	B	550	NAD	C4D-O4D-C1D	2.01	111.77	109.92
3	D	550	NAD	O2N-PN-O1N	2.00	121.76	112.44

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	500	AD3	O4'-C1'-N9-C4
2	D	500	AD3	O4'-C4'-C5'-O5'
2	D	500	AD3	O4'-C1'-N9-C4
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

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Mol	Chain	Res	Type	Atoms
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
2	D	500	AD3	C3'-C4'-C5'-O5'
2	B	500	AD3	C3'-C4'-C5'-O5'
2	A	500	AD3	O4'-C4'-C5'-O5'
2	A	500	AD3	C3'-C4'-C5'-O5'
2	C	500	AD3	C3'-C4'-C5'-O5'
2	B	500	AD3	O4'-C4'-C5'-O5'
2	A	500	AD3	O4'-C1'-N9-C4
2	A	500	AD3	C2'-C1'-N9-C4
2	B	500	AD3	O4'-C1'-N9-C4
2	B	500	AD3	C2'-C1'-N9-C4
2	C	500	AD3	C2'-C1'-N9-C4
2	D	500	AD3	C2'-C1'-N9-C4
3	D	550	NAD	O4B-C4B-C5B-O5B
3	D	550	NAD	C3B-C4B-C5B-O5B
2	C	500	AD3	O4'-C4'-C5'-O5'
3	B	550	NAD	O4B-C4B-C5B-O5B
3	B	550	NAD	O4B-C1B-N9A-C8A
3	B	550	NAD	C2B-C1B-N9A-C8A
3	C	550	NAD	O4B-C4B-C5B-O5B

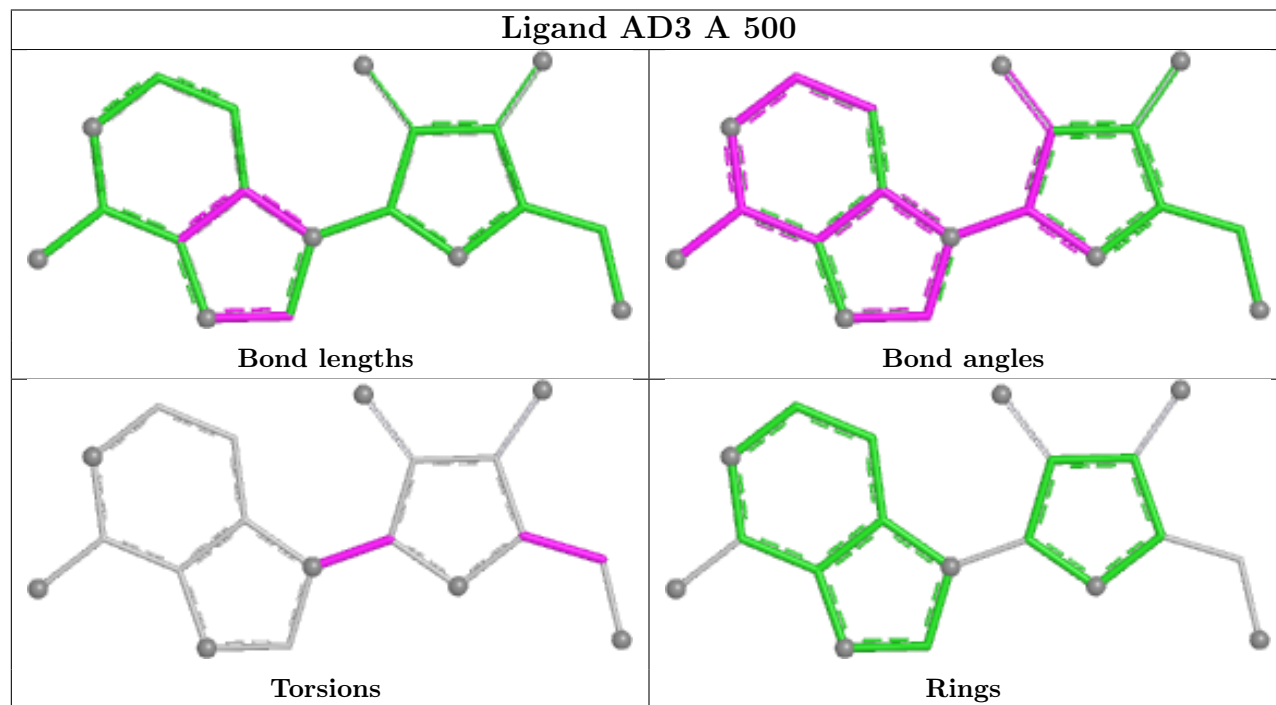
There are no ring outliers.

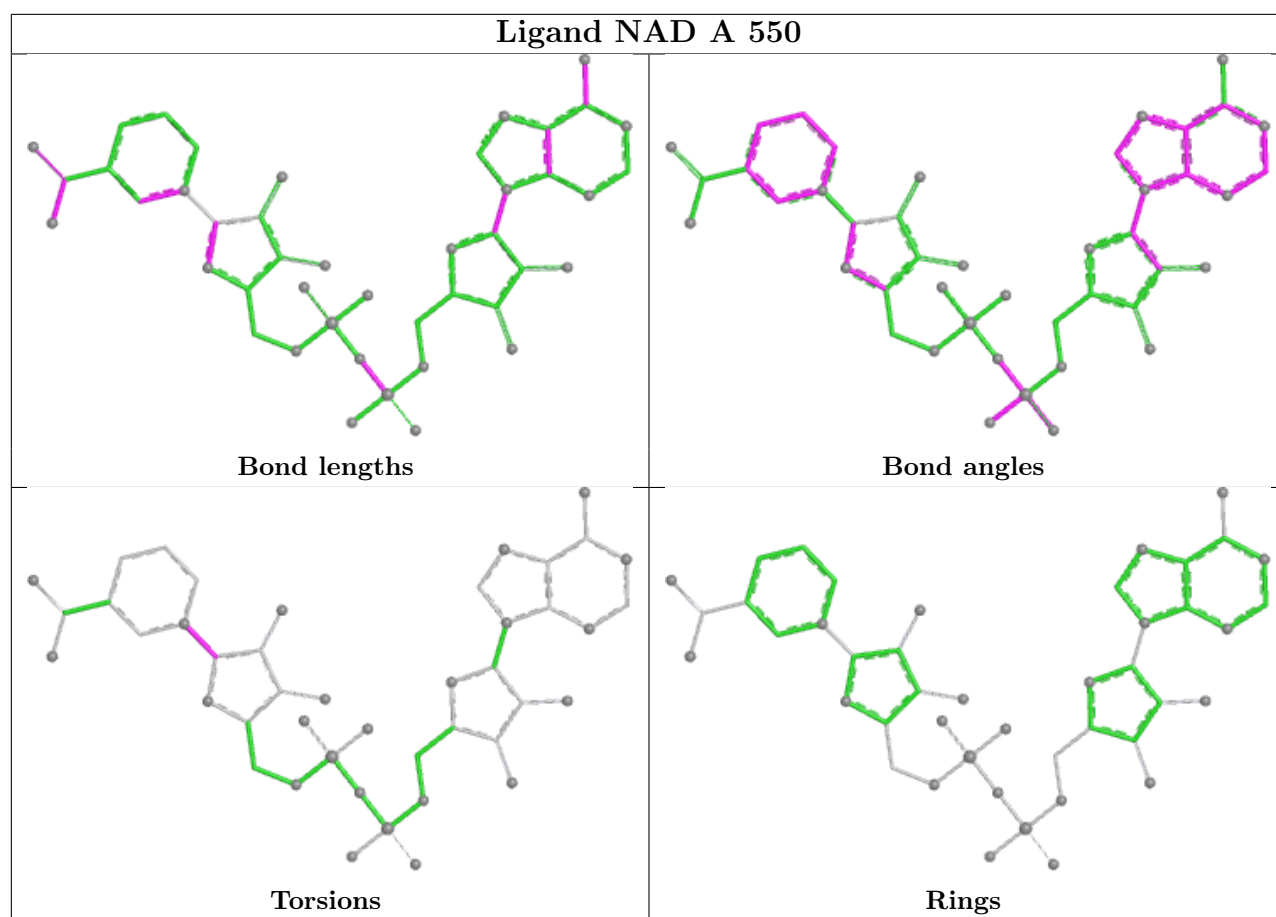
8 monomers are involved in 9 short contacts:

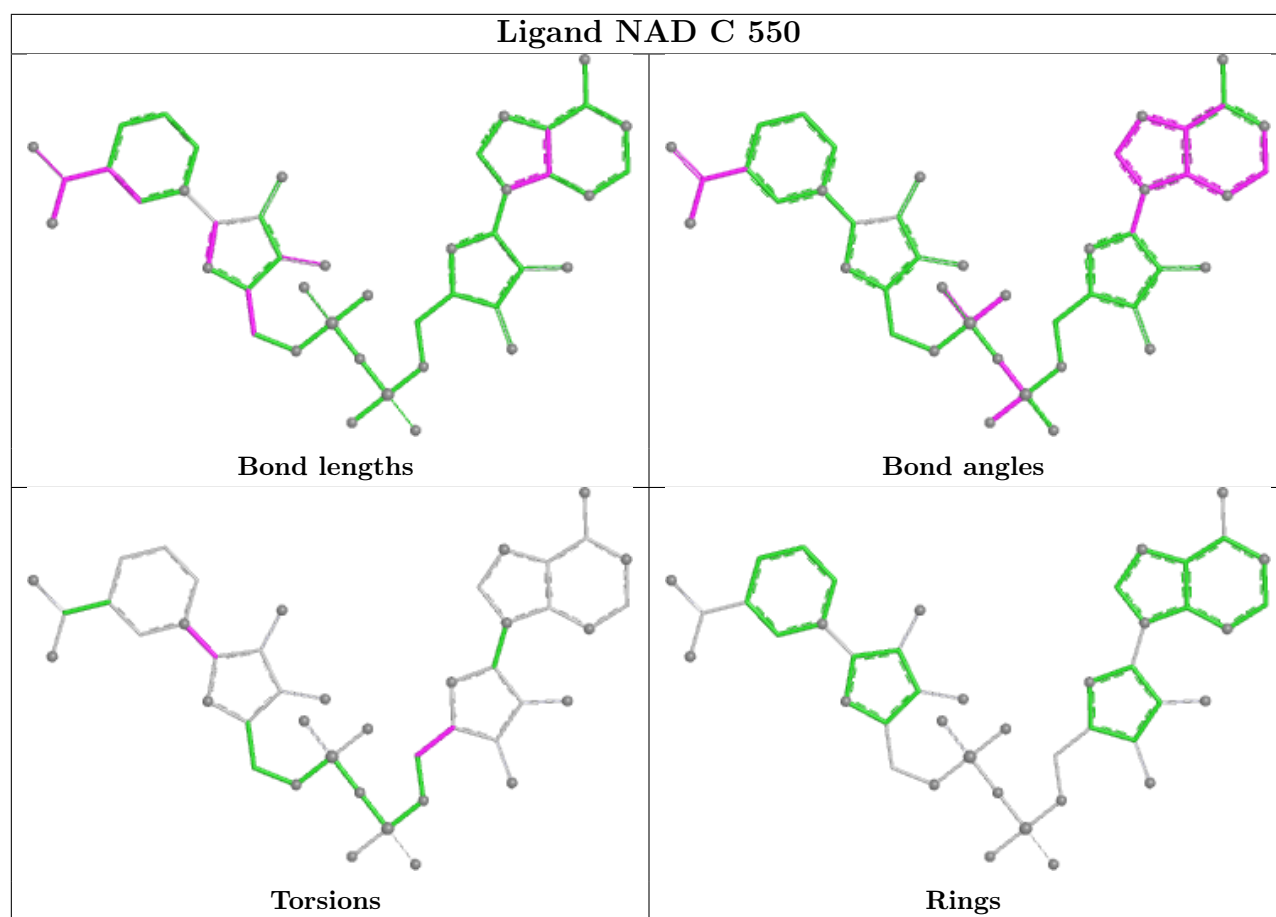
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	AD3	3	0
3	A	550	NAD	2	0
3	C	550	NAD	1	0
3	B	550	NAD	2	0
2	B	500	AD3	1	0
3	D	550	NAD	2	0
2	D	500	AD3	1	0
2	C	500	AD3	1	0

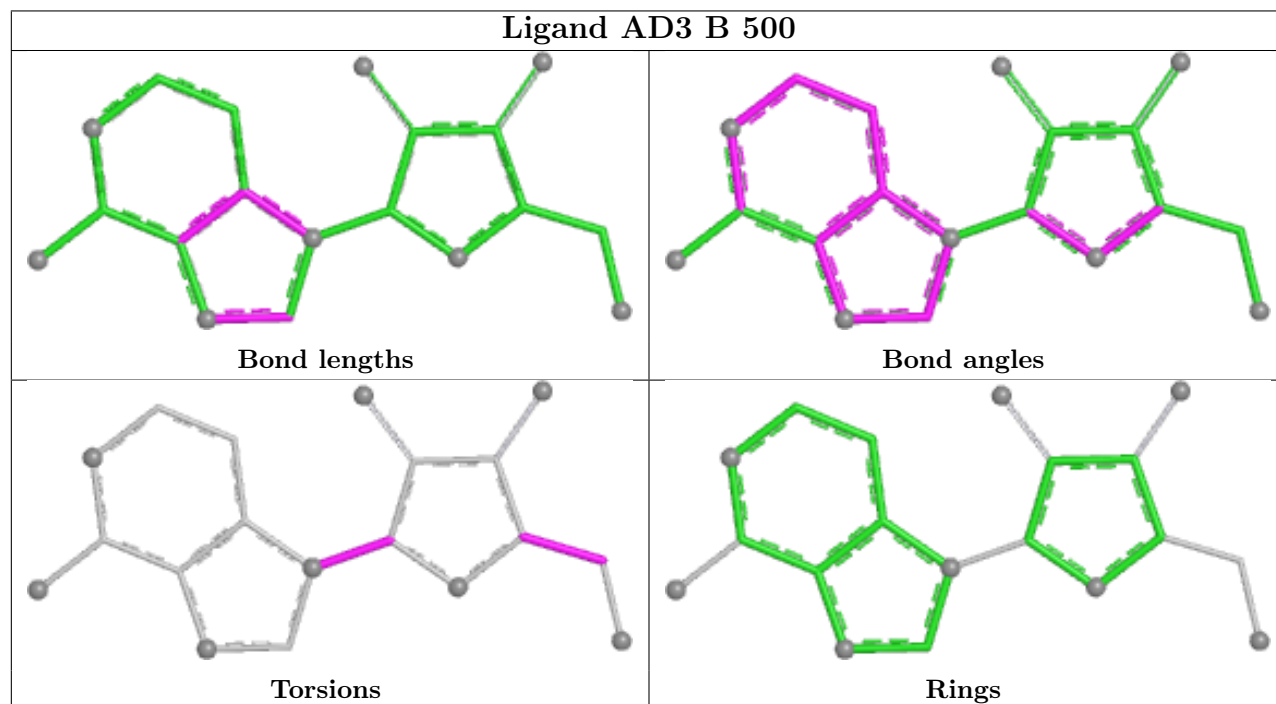
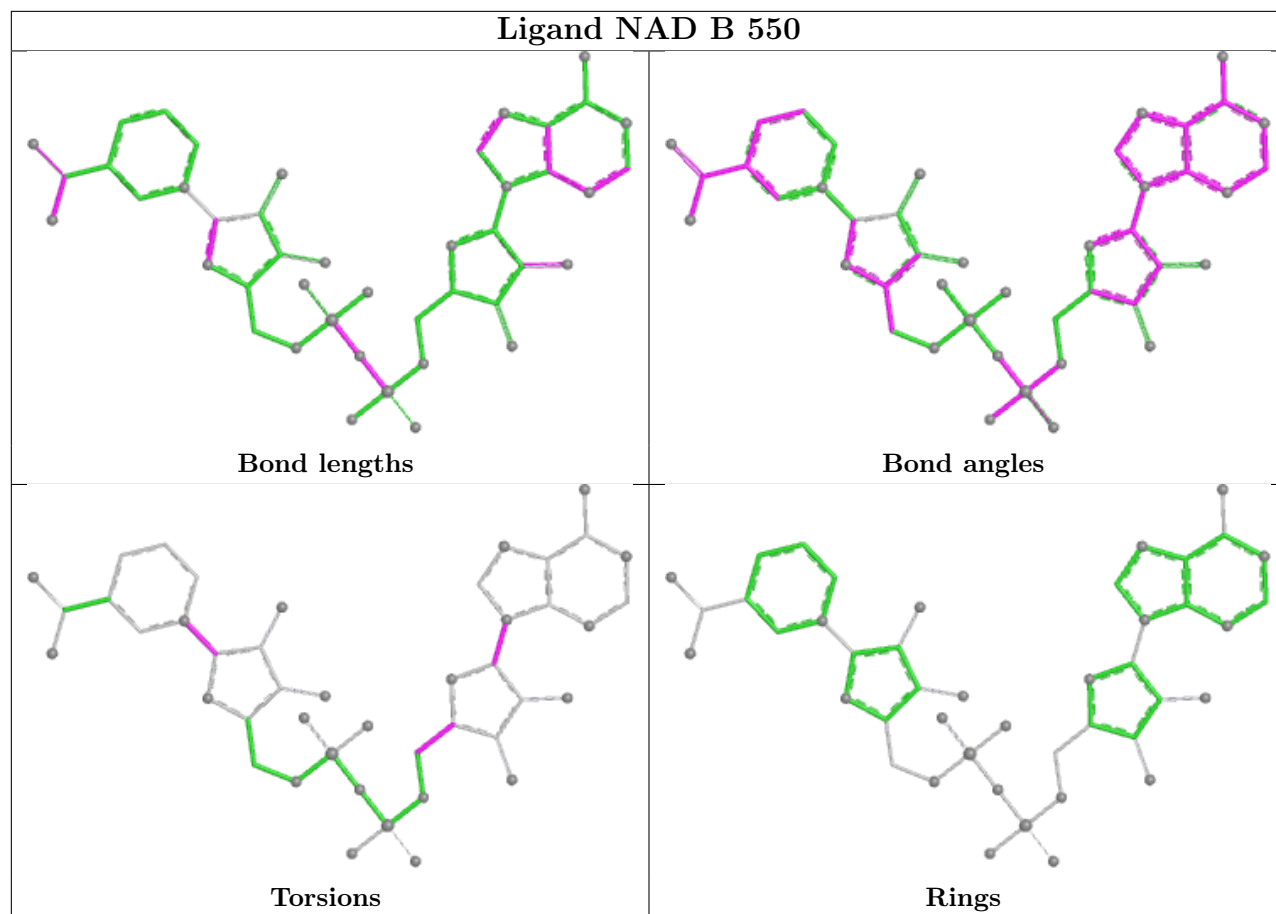
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

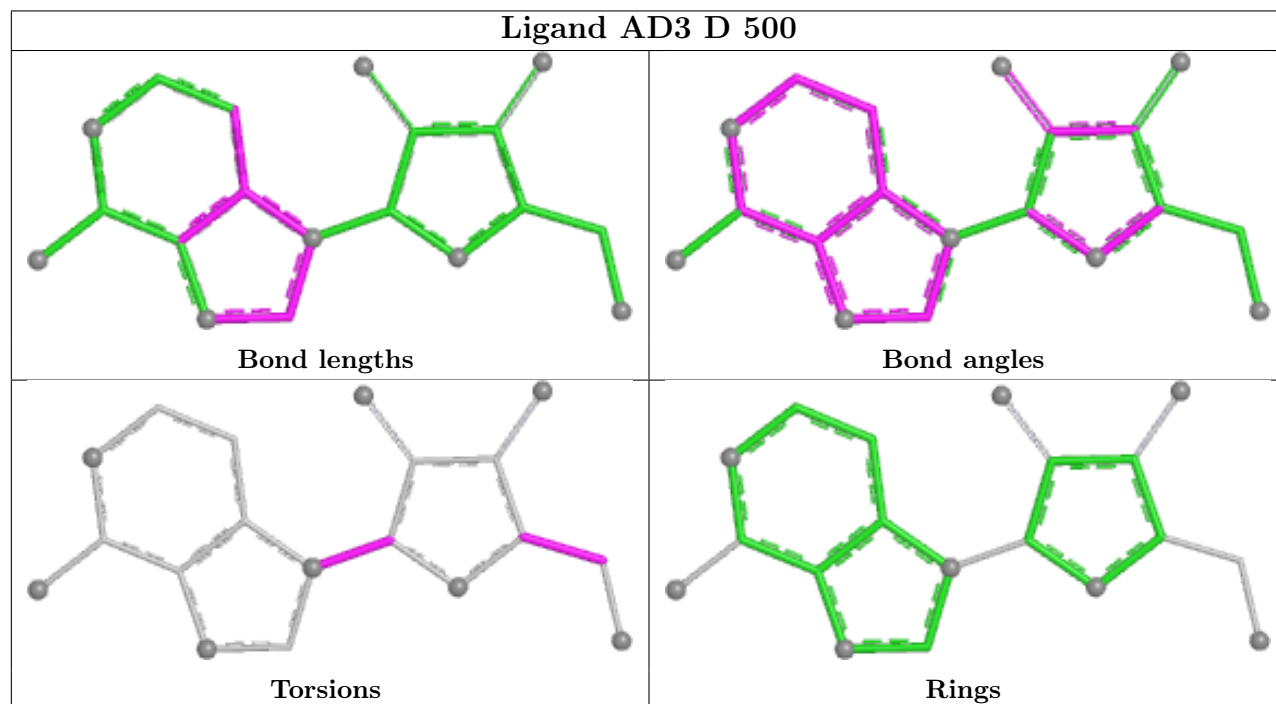
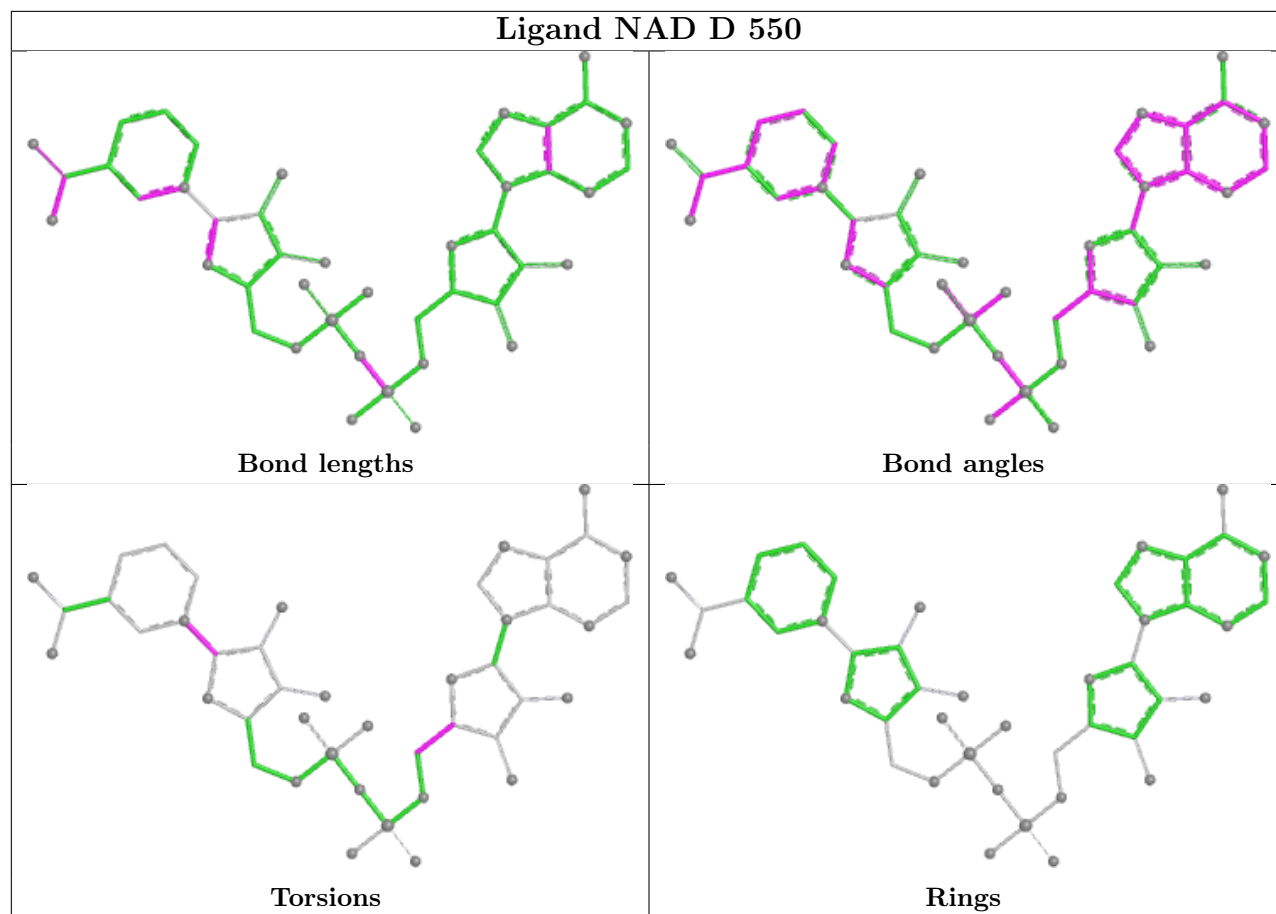
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question 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.

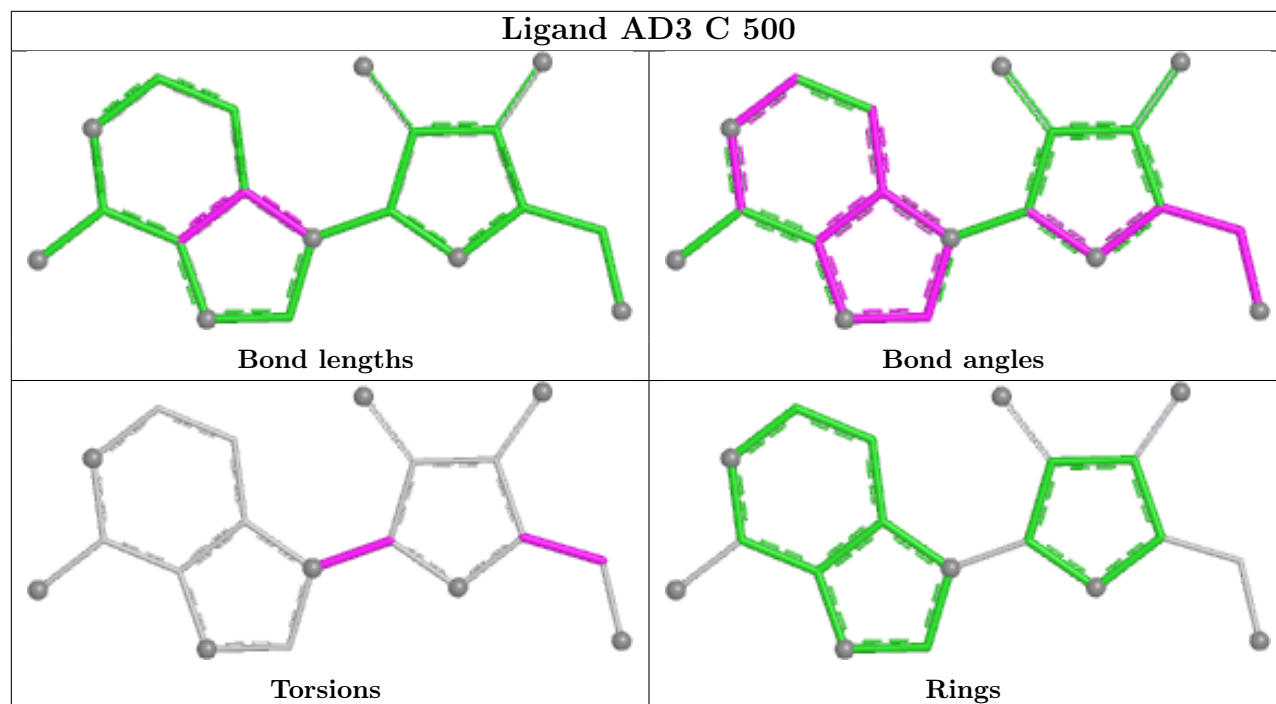












5.7 Other polymers [i](#)

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	485/495 (97%)	-0.15	1 (0%) 91 90	19, 33, 58, 81	0
1	B	485/495 (97%)	0.35	13 (2%) 56 53	22, 43, 82, 103	0
1	C	485/495 (97%)	-0.05	3 (0%) 85 83	21, 37, 65, 98	0
1	D	485/495 (97%)	0.32	20 (4%) 41 38	19, 46, 86, 116	0
All	All	1940/1980 (97%)	0.12	37 (1%) 66 63	19, 39, 76, 116	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	182	ASP	4.0
1	D	175	VAL	3.3
1	D	147	ASP	3.2
1	D	363	HIS	3.0
1	B	54	ALA	3.0
1	D	54	ALA	3.0
1	B	175	VAL	2.9
1	D	165	LEU	2.8
1	D	176	VAL	2.7
1	D	117	PRO	2.7
1	B	150	ALA	2.7
1	D	130	LEU	2.6
1	B	176	VAL	2.6
1	D	236	ALA	2.6
1	D	149	PRO	2.5
1	C	363	HIS	2.5
1	B	185	ALA	2.5
1	B	186	GLU	2.4
1	B	153	ILE	2.4
1	B	83	ALA	2.3
1	B	56	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	56	VAL	2.3
1	D	146	PRO	2.2
1	D	174	GLY	2.2
1	B	371	ALA	2.2
1	D	231	ALA	2.2
1	B	179	ALA	2.2
1	C	11	LEU	2.1
1	C	54	ALA	2.1
1	B	227	TYR	2.1
1	D	439	ASN	2.1
1	D	364	PHE	2.1
1	D	209	ALA	2.1
1	D	108	VAL	2.1
1	D	225	ARG	2.1
1	D	53	TYR	2.0
1	B	59	LEU	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
2	AD3	C	500	19/19	0.93	0.08	18,26,36,45	0
2	AD3	D	500	19/19	0.93	0.08	21,27,35,46	0
3	NAD	B	550	44/44	0.94	0.07	30,36,41,46	0
2	AD3	B	500	19/19	0.95	0.07	21,33,53,59	0
2	AD3	A	500	19/19	0.95	0.07	15,24,33,44	0
3	NAD	A	550	44/44	0.96	0.06	20,29,33,36	0
3	NAD	C	550	44/44	0.96	0.06	24,31,36,39	0

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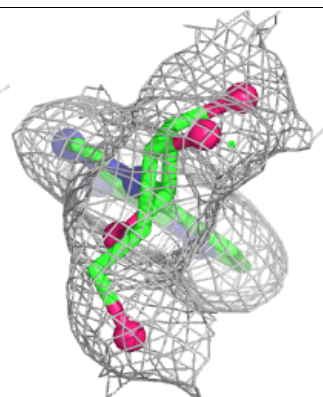
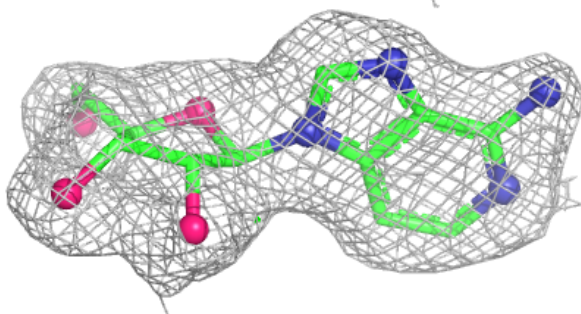
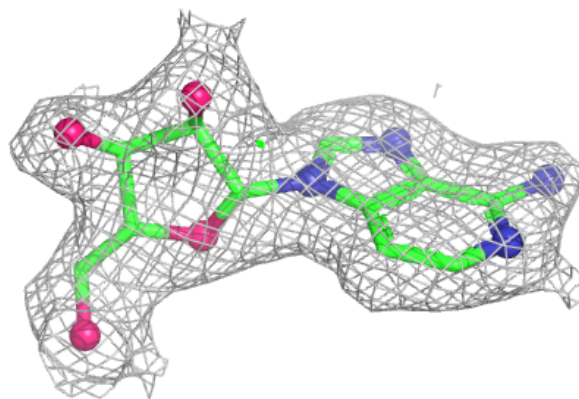
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAD	D	550	44/44	0.96	0.07	24,33,40,41	0

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.

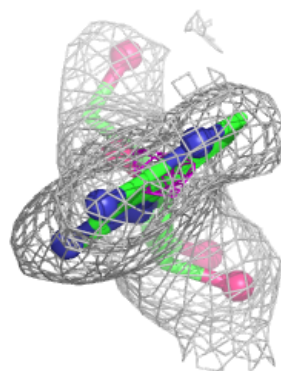
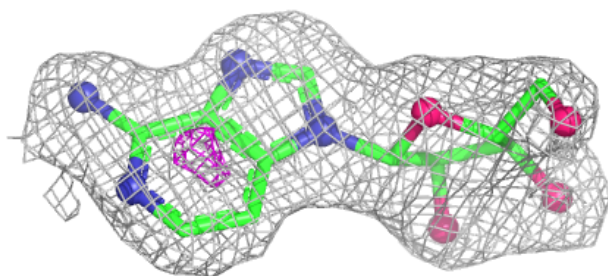
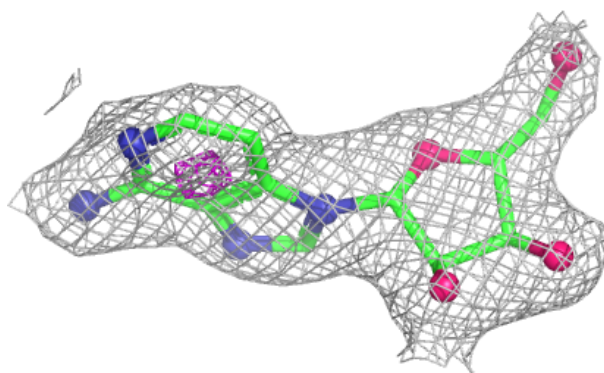
Electron density around AD3 C 500:

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

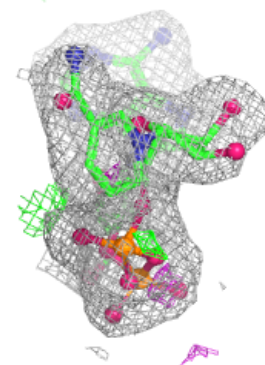
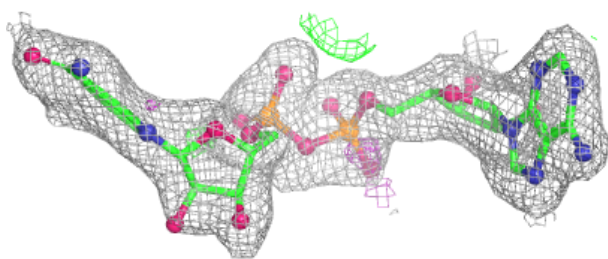
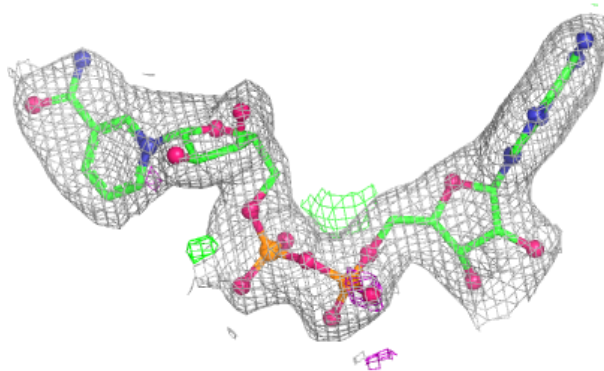


Electron density around AD3 D 500:

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

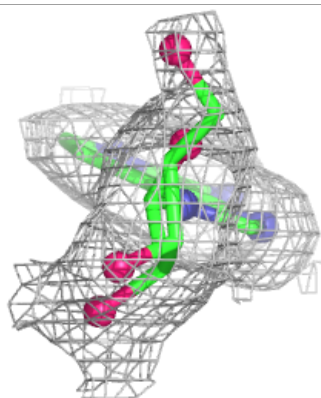
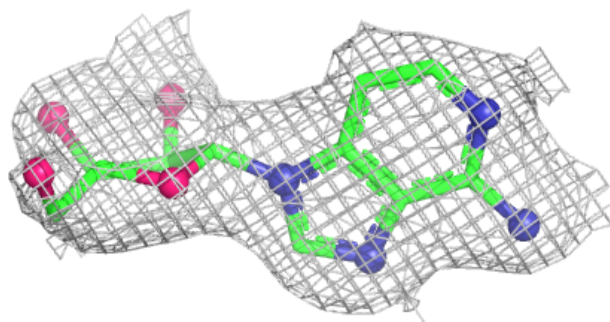
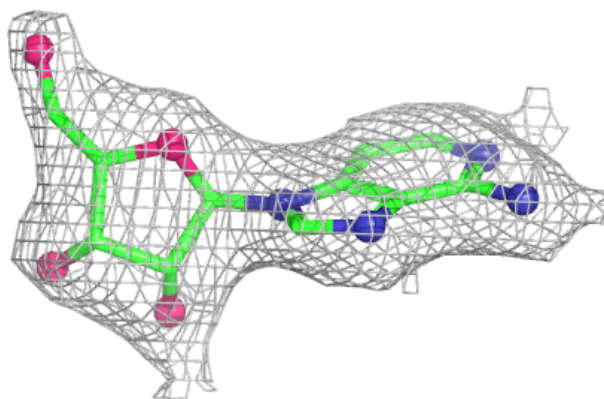
**Electron density around NAD B 550:**

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

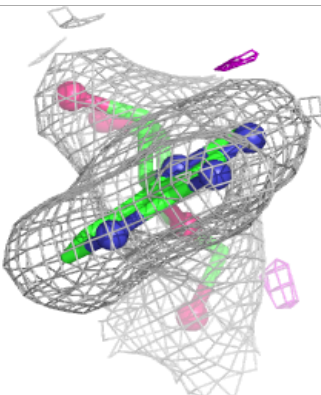
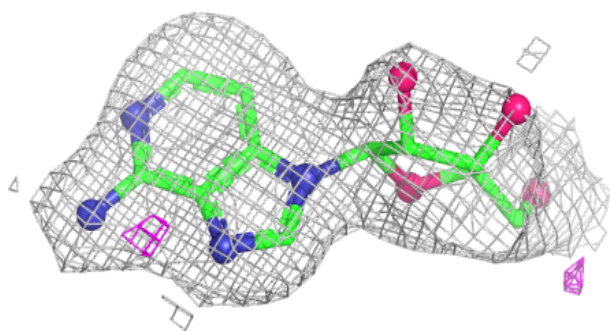
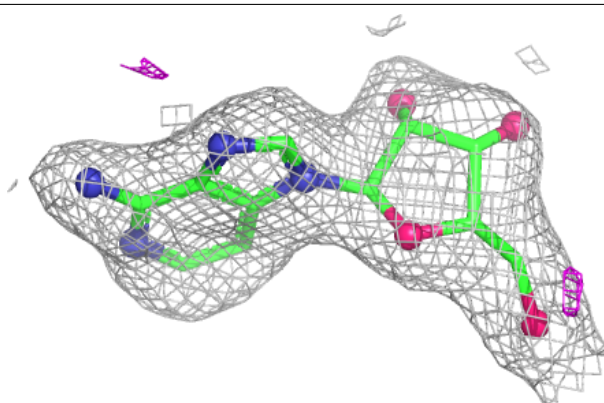


Electron density around AD3 B 500:

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

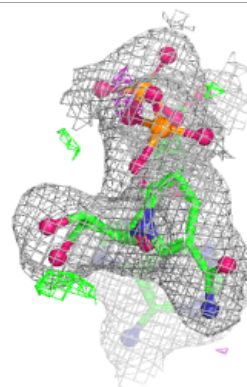
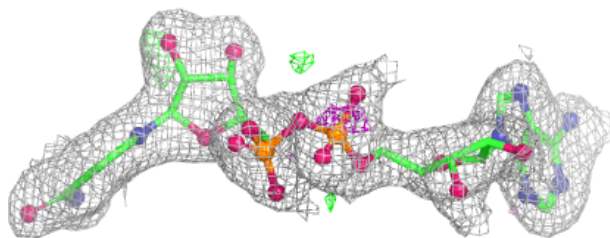
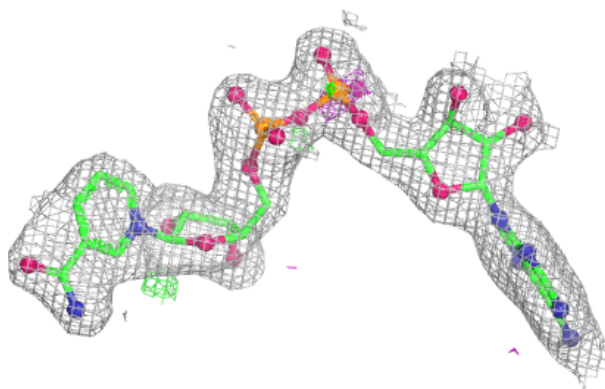
**Electron density around AD3 A 500:**

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

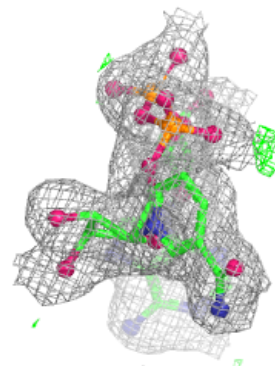
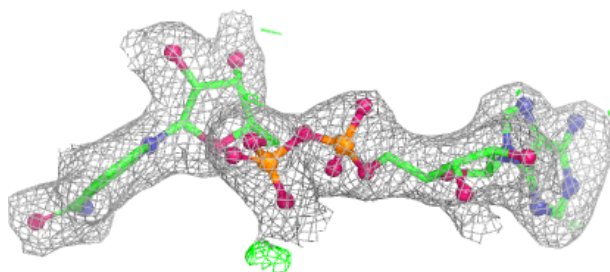
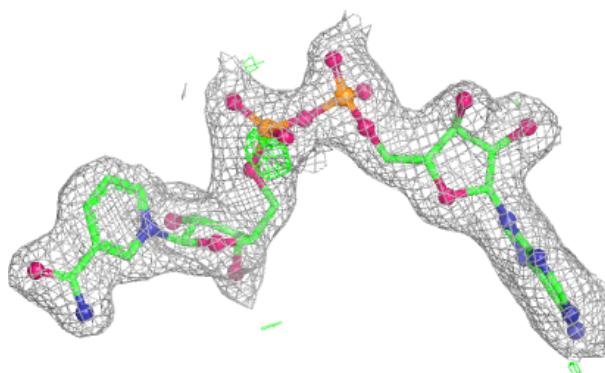


Electron density around NAD A 550:

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

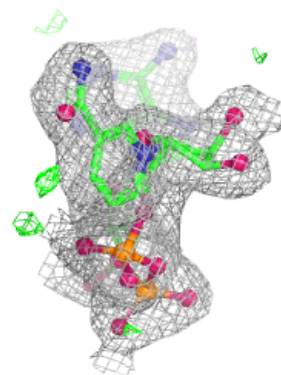
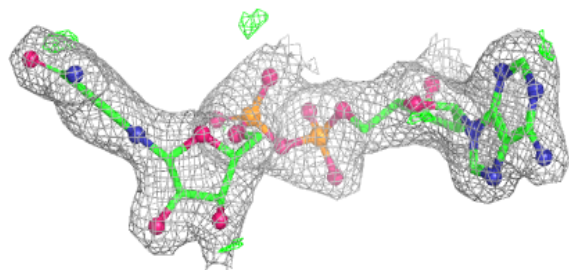
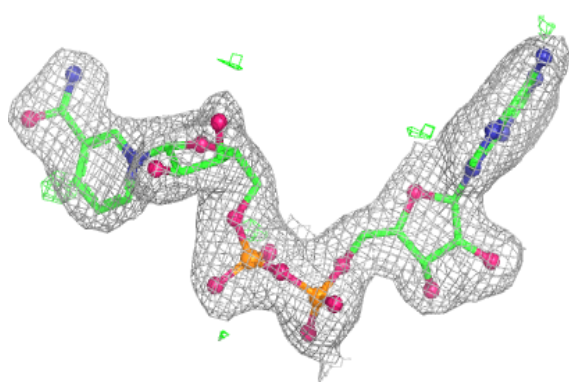
**Electron density around NAD C 550:**

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



Electron density around 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.