



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 13, 2020 – 10:35 PM BST

PDB ID : 5VLD
Title : Crystal Structure of Medicago truncatula L-Histidinol Dehydrogenase in Complex with L-Histidine and NAD⁺
Authors : Ruszkowski, M.; Dauter, Z.
Deposited on : 2017-04-25
Resolution : 2.59 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.14.4.dev1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.14.4.dev1

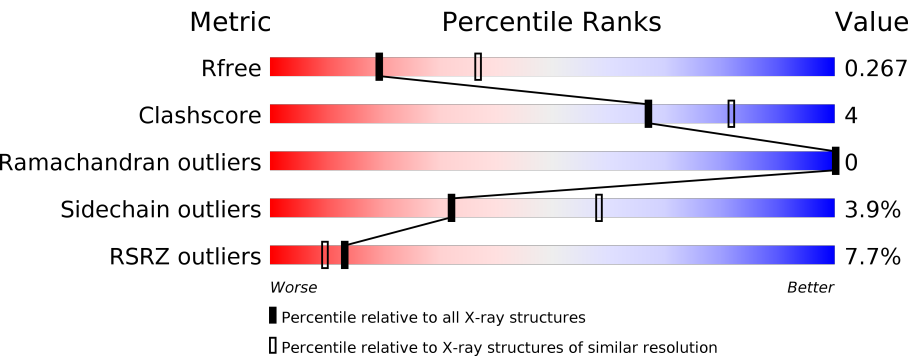
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.59 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}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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	446	<div><div>0%</div><div><div></div><div>87%</div><div>8%</div><div></div><div></div></div><div></div></div>
1	B	446	<div><div>5%</div><div><div></div><div>85%</div><div>10%</div><div></div><div></div></div><div></div></div>
1	C	446	<div><div>17%</div><div><div></div><div>88%</div><div>8%</div><div></div><div></div></div><div></div></div>
1	D	446	<div><div>14%</div><div><div></div><div>89%</div><div>8%</div><div></div><div></div></div><div></div></div>
1	E	446	<div><div>2%</div><div><div></div><div>89%</div><div>7%</div><div></div><div></div></div><div></div></div>
1	F	446	<div><div>5%</div><div><div></div><div>89%</div><div>8%</div><div></div><div></div></div><div></div></div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 20242 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 Histidinol dehydrogenase, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	430	Total	C	N	O	S	0	0	0
			3266	2071	548	631	16			
1	B	429	Total	C	N	O	S	0	1	0
			3261	2069	547	629	16			
1	C	431	Total	C	N	O	S	0	0	0
			3272	2074	549	633	16			
1	D	433	Total	C	N	O	S	0	0	0
			3288	2083	554	635	16			
1	E	432	Total	C	N	O	S	0	0	0
			3277	2077	550	634	16			
1	F	435	Total	C	N	O	S	0	0	0
			3304	2093	557	638	16			

There are 18 discrepancies between the modelled and reference sequences:

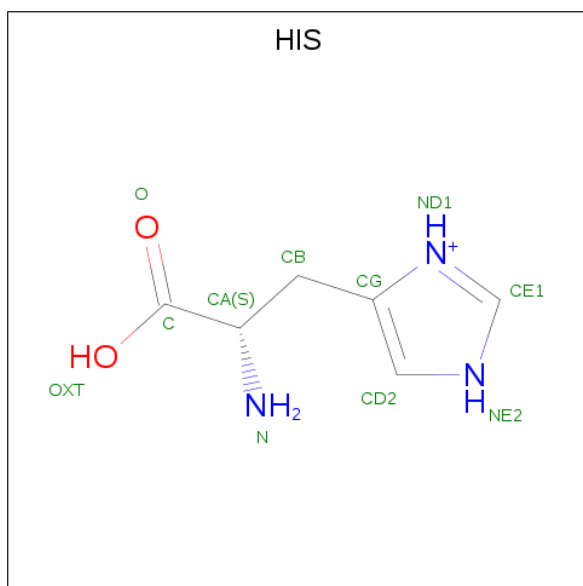
Chain	Residue	Modelled	Actual	Comment	Reference
A	33	SER	-	expression tag	UNP G7IKX3
A	34	ASN	-	expression tag	UNP G7IKX3
A	35	ALA	-	expression tag	UNP G7IKX3
B	33	SER	-	expression tag	UNP G7IKX3
B	34	ASN	-	expression tag	UNP G7IKX3
B	35	ALA	-	expression tag	UNP G7IKX3
C	33	SER	-	expression tag	UNP G7IKX3
C	34	ASN	-	expression tag	UNP G7IKX3
C	35	ALA	-	expression tag	UNP G7IKX3
D	33	SER	-	expression tag	UNP G7IKX3
D	34	ASN	-	expression tag	UNP G7IKX3
D	35	ALA	-	expression tag	UNP G7IKX3
E	33	SER	-	expression tag	UNP G7IKX3
E	34	ASN	-	expression tag	UNP G7IKX3
E	35	ALA	-	expression tag	UNP G7IKX3
F	33	SER	-	expression tag	UNP G7IKX3
F	34	ASN	-	expression tag	UNP G7IKX3

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Chain	Residue	Modelled	Actual	Comment	Reference
F	35	ALA	-	expression tag	UNP G7IKX3

- Molecule 2 is HISTIDINE (three-letter code: HIS) (formula: $C_6H_{10}N_3O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			11	6	3	2		
2	B	1	Total	C	N	O	0	0
			11	6	3	2		
2	C	1	Total	C	N	O	0	0
			11	6	3	2		
2	D	1	Total	C	N	O	0	0
			11	6	3	2		
2	E	1	Total	C	N	O	0	0
			11	6	3	2		
2	F	1	Total	C	N	O	0	0
			11	6	3	2		

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



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		
3	E	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	F	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Zn	0	0
			1	1		
4	A	1	Total	Zn	0	0
			1	1		
4	D	1	Total	Zn	0	0
			1	1		
4	C	1	Total	Zn	0	0
			1	1		
4	E	2	Total	Zn	0	0
			2	2		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		
5	F	1	Total	C	O	0	0
			7	4	3		

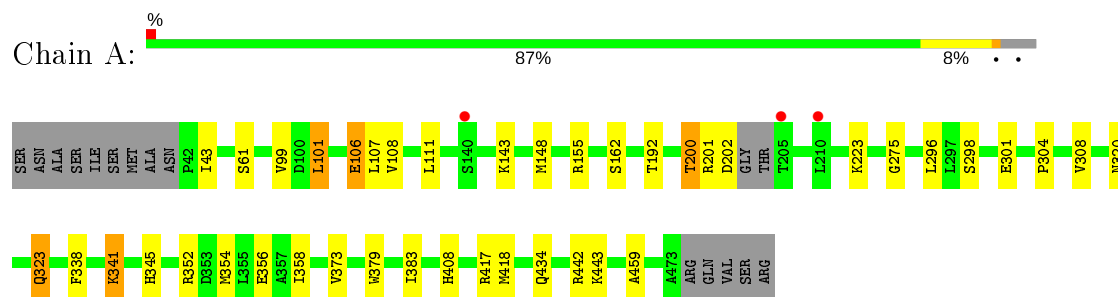
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	51	Total	O	0	0
			51	51		
6	B	55	Total	O	0	0
			55	55		
6	C	22	Total	O	0	0
			22	22		
6	D	25	Total	O	0	0
			25	25		
6	E	37	Total	O	0	0
			37	37		
6	F	34	Total	O	0	0
			34	34		

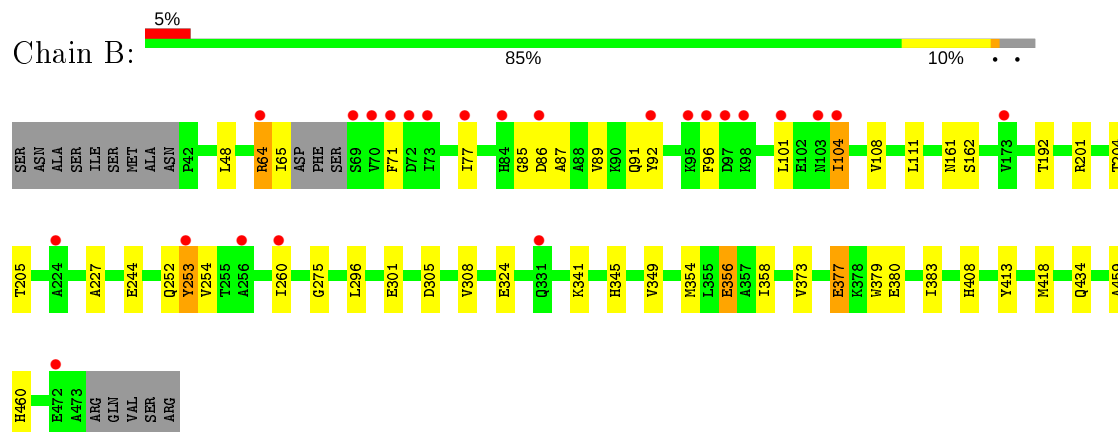
3 Residue-property plots [i](#)

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.

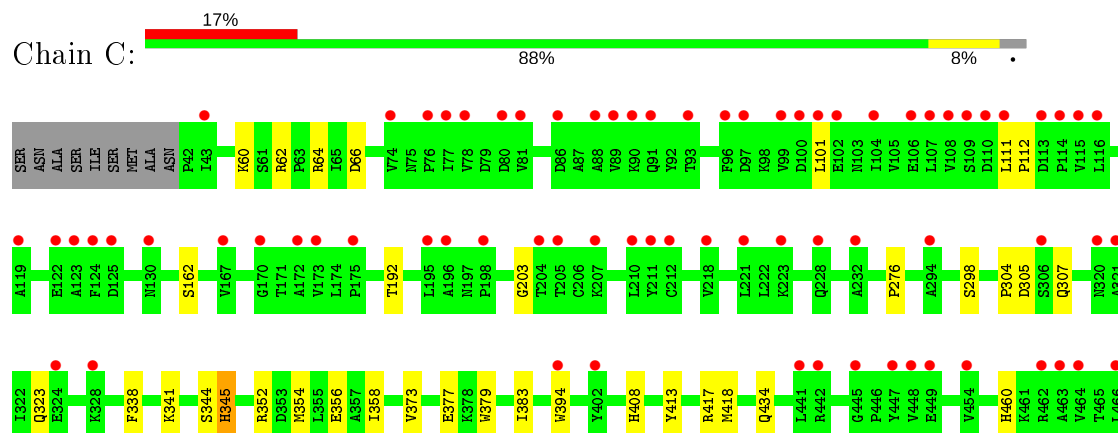
- Molecule 1: Histidinol dehydrogenase, chloroplastic

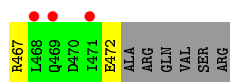


- Molecule 1: Histidinol dehydrogenase, chloroplastic

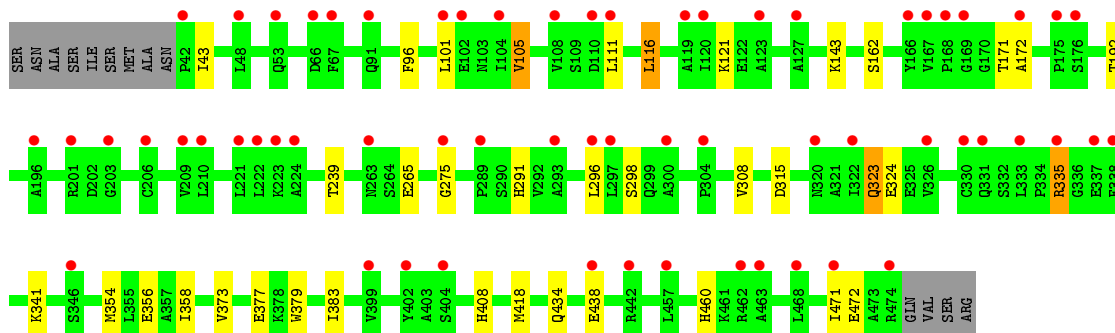
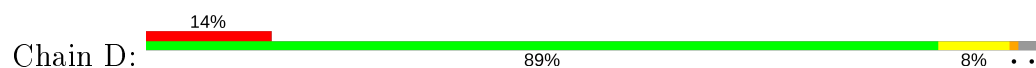


- Molecule 1: Histidinol dehydrogenase, chloroplastic

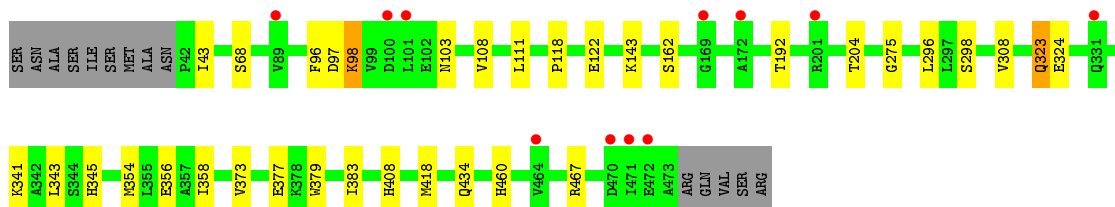
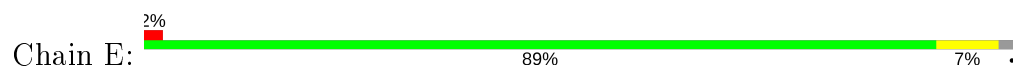




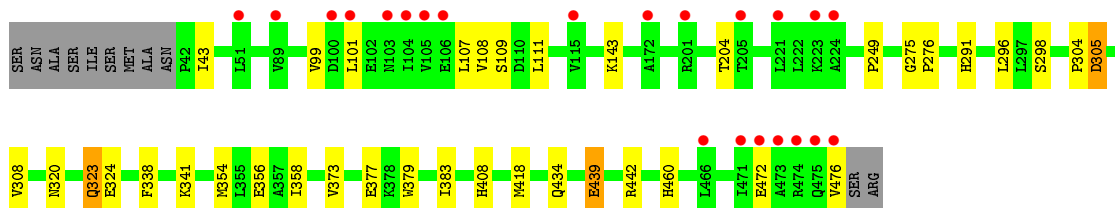
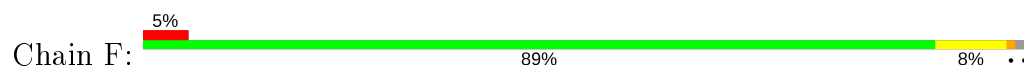
- Molecule 1: Histidinol dehydrogenase, chloroplastic



- Molecule 1: Histidinol dehydrogenase, chloroplastic



- Molecule 1: Histidinol dehydrogenase, chloroplastic



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	103.65Å 139.09Å 103.56Å 90.00° 119.47° 90.00°	Depositor
Resolution (Å)	48.89 – 2.59 48.89 – 2.59	Depositor EDS
% Data completeness (in resolution range)	96.7 (48.89-2.59) 96.7 (48.89-2.59)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.221 , 0.264 0.224 , 0.267	Depositor DCC
R_{free} test set	1152 reflections (1.50%)	wwPDB-VP
Wilson B-factor (Å ²)	40.6	Xtriage
Anisotropy	0.282	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 45.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.027 for l,k,-h-l 0.027 for -h-l,k,h 0.036 for -h-l,-k,l 0.038 for h,-k,-h-l 0.046 for l,-k,h	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	20242	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% 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: ZN, PEG, 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	0.75	0/3332	0.80	0/4529
1	B	0.76	0/3330	0.83	0/4527
1	C	0.63	0/3339	0.77	0/4540
1	D	0.60	0/3355	0.77	0/4561
1	E	0.68	0/3344	0.80	0/4547
1	F	0.65	0/3371	0.80	0/4583
All	All	0.68	0/20071	0.80	0/27287

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3266	0	3263	27	0
1	B	3261	0	3264	44	0
1	C	3272	0	3269	29	0
1	D	3288	0	3287	29	0
1	E	3277	0	3274	19	0
1	F	3304	0	3304	23	0
2	A	11	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	11	0	6	0	0
2	C	11	0	6	0	0
2	D	11	0	6	0	0
2	E	11	0	6	0	0
2	F	11	0	6	0	0
3	A	44	0	26	1	0
3	B	44	0	26	4	0
3	C	44	0	26	0	0
3	D	44	0	26	2	0
3	E	44	0	26	2	0
3	F	44	0	26	2	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	2	0	0	0	0
5	A	7	0	10	0	0
5	F	7	0	10	0	0
6	A	51	0	0	0	0
6	B	55	0	0	3	0
6	C	22	0	0	2	0
6	D	25	0	0	0	0
6	E	37	0	0	0	0
6	F	34	0	0	0	0
All	All	20242	0	19873	154	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 4.

All (154) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:ARG:CB	1:B:252:GLN:HE22	1.55	1.19
1:B:64:ARG:HB3	1:B:252:GLN:NE2	1.61	1.15
1:B:64:ARG:HB3	1:B:252:GLN:HE22	0.93	1.07
1:D:438:GLU:HG2	1:D:471:ILE:HD11	1.39	1.03
1:B:87:ALA:O	1:B:91:GLN:HG3	1.59	1.01
1:E:118:PRO:O	1:E:122:GLU:HG3	1.63	0.98
1:C:394:TRP:CZ3	1:D:471:ILE:HG13	2.10	0.86
1:B:65:ILE:HD12	1:B:65:ILE:H	1.39	0.86
1:C:66:ASP:HB2	1:D:265:GLU:OE1	1.77	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:438:GLU:HG2	1:D:471:ILE:CD1	2.07	0.83
1:B:161:ASN:HB2	6:B:629:HOH:O	1.79	0.83
1:B:64:ARG:CB	1:B:252:GLN:NE2	2.28	0.81
1:C:276:PRO:HB3	1:C:305:ASP:HB3	1.62	0.81
1:F:107:LEU:HD23	1:F:109:SER:OG	1.81	0.80
1:A:148:MET:HE1	1:A:443:LYS:HG3	1.65	0.78
1:B:77:ILE:HG12	1:B:92:TYR:CE2	2.20	0.76
1:B:64:ARG:HG2	1:B:305:ASP:OD1	1.85	0.75
1:F:320:ASN:O	1:F:324:GLU:HG3	1.86	0.75
1:B:64:ARG:CG	1:B:252:GLN:HE22	2.02	0.72
1:A:148:MET:CE	1:A:443:LYS:HG3	2.19	0.72
1:B:96:PHE:CE1	3:B:503:NAD:C2A	2.74	0.70
1:C:323:GLN:HG3	1:C:323:GLN:O	1.92	0.70
1:F:99:VAL:HG12	1:F:101:LEU:HD23	1.73	0.70
1:E:118:PRO:O	1:E:122:GLU:CG	2.40	0.70
1:A:148:MET:CE	1:A:443:LYS:CG	2.71	0.69
1:B:227:ALA:N	6:B:601:HOH:O	2.27	0.68
1:C:394:TRP:CH2	1:D:471:ILE:CG1	2.79	0.65
1:C:60:LYS:HE3	1:C:417:ARG:NH2	2.13	0.64
1:F:107:LEU:CD2	1:F:109:SER:OG	2.44	0.64
1:F:439:GLU:OE2	1:F:442:ARG:NH2	2.32	0.63
1:C:394:TRP:CH2	1:D:471:ILE:HG12	2.35	0.62
1:D:171:THR:O	1:D:335:ARG:NH1	2.33	0.61
1:C:394:TRP:CZ3	1:D:471:ILE:CG1	2.83	0.60
1:A:148:MET:HE3	1:A:443:LYS:HG2	1.85	0.59
1:F:99:VAL:CG1	1:F:101:LEU:HD23	2.33	0.58
1:B:48:LEU:HD23	1:B:356:GLU:OE1	2.04	0.57
1:C:64:ARG:NH2	1:C:66:ASP:HA	2.19	0.57
1:B:65:ILE:HD12	1:B:65:ILE:N	2.17	0.57
1:C:276:PRO:CB	1:C:305:ASP:HB3	2.32	0.57
1:F:354:MET:HE1	1:F:373:VAL:HG11	1.86	0.56
1:D:438:GLU:CG	1:D:471:ILE:CD1	2.82	0.56
1:B:275:GLY:O	3:B:503:NAD:H2N	2.05	0.56
1:A:148:MET:HE3	1:A:443:LYS:CG	2.35	0.55
1:A:106:GLU:OE1	1:A:223:LYS:HE2	2.06	0.55
1:A:304:PRO:HD3	1:A:338:PHE:CD1	2.41	0.55
1:E:275:GLY:O	3:E:503:NAD:H2N	2.06	0.55
1:B:253:TYR:N	1:B:253:TYR:CD1	2.75	0.55
1:E:354:MET:CE	1:E:373:VAL:HG11	2.37	0.55
1:A:148:MET:CE	1:A:443:LYS:HG2	2.38	0.54
1:C:354:MET:CE	1:C:373:VAL:HG11	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:254:VAL:HA	6:B:601:HOH:O	2.07	0.54
1:F:354:MET:CE	1:F:373:VAL:HG11	2.38	0.54
1:B:354:MET:CE	1:B:373:VAL:HG11	2.37	0.53
1:A:354:MET:CE	1:A:373:VAL:HG11	2.38	0.53
1:B:253:TYR:N	1:B:253:TYR:HD1	2.05	0.53
1:E:43:ILE:N	1:E:323:GLN:OE1	2.42	0.52
1:D:354:MET:CE	1:D:373:VAL:HG11	2.39	0.51
1:C:298:SER:O	1:D:460:HIS:CE1	2.63	0.51
1:B:85:GLY:O	1:B:89:VAL:HG23	2.10	0.51
1:A:43:ILE:N	1:A:323:GLN:OE1	2.43	0.50
1:C:341:LYS:O	1:C:345:HIS:CE1	2.65	0.50
1:C:111:LEU:HD12	1:C:111:LEU:N	2.28	0.49
1:D:111:LEU:N	1:D:111:LEU:HD12	2.27	0.49
1:F:275:GLY:O	3:F:502:NAD:H2N	2.12	0.49
1:A:459:ALA:HB3	1:B:301:GLU:CD	2.33	0.49
1:B:48:LEU:HD13	1:B:349:VAL:HG13	1.94	0.49
1:D:43:ILE:N	1:D:323:GLN:OE1	2.43	0.49
1:B:380:GLU:HA	1:B:383:ILE:HD12	1.95	0.48
1:E:354:MET:HE1	1:E:373:VAL:HG11	1.95	0.48
1:B:358:ILE:HD11	1:B:383:ILE:HG12	1.95	0.48
1:C:394:TRP:CH2	1:D:471:ILE:HG13	2.42	0.48
1:C:304:PRO:HD3	1:C:338:PHE:CD1	2.49	0.47
1:F:43:ILE:N	1:F:323:GLN:OE1	2.45	0.47
1:C:467:ARG:HG2	1:D:291:HIS:CD2	2.49	0.47
1:E:460:HIS:CE1	1:F:298:SER:O	2.67	0.47
1:A:296:LEU:HD22	1:A:308:VAL:CG1	2.45	0.47
1:B:108:VAL:HA	1:B:111:LEU:HD12	1.96	0.47
1:C:62:ARG:HG3	1:C:307:GLN:OE1	2.14	0.46
1:B:96:PHE:CZ	3:B:503:NAD:H2A	2.51	0.46
1:A:296:LEU:HD22	1:A:308:VAL:HG13	1.97	0.46
1:E:108:VAL:HA	1:E:111:LEU:HD12	1.98	0.46
1:D:354:MET:HE1	1:D:373:VAL:HG11	1.97	0.46
1:C:64:ARG:HG2	1:C:413:TYR:CD1	2.51	0.45
1:D:111:LEU:N	1:D:111:LEU:CD1	2.78	0.45
1:F:108:VAL:HA	1:F:111:LEU:HD12	1.97	0.45
1:C:111:LEU:CD1	1:C:111:LEU:N	2.79	0.45
1:B:96:PHE:CE1	3:B:503:NAD:H2A	2.51	0.45
1:F:296:LEU:HD22	1:F:308:VAL:CG1	2.46	0.45
1:E:296:LEU:HD22	1:E:308:VAL:CG1	2.47	0.45
1:B:48:LEU:HD13	1:B:349:VAL:CG1	2.47	0.45
1:D:296:LEU:HD22	1:D:308:VAL:CG1	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:298:SER:O	1:F:460:HIS:CE1	2.69	0.45
1:F:296:LEU:HD22	1:F:308:VAL:HG13	1.97	0.45
1:A:108:VAL:HA	1:A:111:LEU:HD12	1.99	0.44
1:A:162:SER:CB	1:A:192:THR:HB	2.47	0.44
1:A:200:THR:HB	1:A:202:ASP:OD1	2.17	0.44
1:B:296:LEU:HD22	1:B:308:VAL:CG1	2.47	0.44
1:F:358:ILE:HD11	1:F:383:ILE:HG12	1.99	0.44
1:E:96:PHE:HB3	3:E:503:NAD:H2B	1.98	0.44
1:D:275:GLY:O	3:D:503:NAD:H2N	2.17	0.44
1:F:354:MET:HG2	1:F:379:TRP:CE2	2.53	0.44
1:D:116:LEU:HD23	1:D:121:LYS:N	2.32	0.44
1:A:101:LEU:HD21	1:A:223:LYS:HE3	2.00	0.44
1:C:417:ARG:NE	6:C:603:HOH:O	2.49	0.44
1:A:275:GLY:O	3:A:502:NAD:H2N	2.17	0.44
1:B:87:ALA:O	1:B:91:GLN:CG	2.49	0.44
1:A:298:SER:O	1:B:460:HIS:CE1	2.71	0.43
1:B:296:LEU:HD22	1:B:308:VAL:HG13	2.00	0.43
1:F:276:PRO:HB3	1:F:305:ASP:HB3	1.99	0.43
1:C:112:PRO:HA	1:F:476:VAL:HG11	1.99	0.43
1:C:358:ILE:HD11	1:C:383:ILE:HG12	1.99	0.43
1:D:296:LEU:HD22	1:D:308:VAL:HG13	1.99	0.43
1:A:354:MET:HG2	1:A:379:TRP:CE2	2.53	0.43
1:B:71:PHE:CD2	1:B:260:ILE:HG13	2.54	0.43
1:E:296:LEU:HD22	1:E:308:VAL:HG13	1.99	0.43
1:C:460:HIS:CE1	1:D:298:SER:O	2.72	0.43
1:D:162:SER:CB	1:D:192:THR:HB	2.49	0.43
1:E:97:ASP:O	1:E:98:LYS:HB2	2.18	0.43
1:A:358:ILE:HD11	1:A:383:ILE:HG12	2.01	0.42
1:B:162:SER:CB	1:B:192:THR:HB	2.49	0.42
1:B:354:MET:HE1	1:B:373:VAL:HG11	2.00	0.42
1:E:98:LYS:HD2	1:E:98:LYS:HA	1.53	0.42
1:D:354:MET:HG2	1:D:379:TRP:CE2	2.54	0.42
1:A:341:LYS:HD3	1:A:341:LYS:HA	1.36	0.42
1:D:105:VAL:HG13	1:D:239:THR:HB	2.02	0.42
1:A:301:GLU:CD	1:B:459:ALA:HB3	2.39	0.42
1:C:354:MET:HE1	1:C:373:VAL:HG11	2.00	0.42
1:A:354:MET:HE1	1:A:373:VAL:HG11	2.02	0.42
1:B:71:PHE:CD2	1:B:260:ILE:CG1	3.03	0.42
1:C:162:SER:CB	1:C:192:THR:HB	2.50	0.42
1:C:417:ARG:HD3	6:C:603:HOH:O	2.20	0.42
1:D:358:ILE:HD11	1:D:383:ILE:HG12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:358:ILE:HD11	1:E:383:ILE:HG12	2.02	0.41
1:B:65:ILE:CD1	1:B:65:ILE:H	2.19	0.41
1:E:354:MET:HG2	1:E:379:TRP:CE2	2.55	0.41
1:D:438:GLU:CG	1:D:471:ILE:HD13	2.49	0.41
1:B:354:MET:HG2	1:B:379:TRP:CE2	2.55	0.41
1:A:99:VAL:CG1	1:A:101:LEU:HD13	2.51	0.41
1:B:377:GLU:CD	1:B:377:GLU:H	2.22	0.41
1:B:86:ASP:CG	1:B:104:ILE:HD11	2.41	0.41
1:E:162:SER:CB	1:E:192:THR:HB	2.50	0.41
1:F:323:GLN:CA	1:F:323:GLN:HE21	2.34	0.41
1:C:354:MET:HG2	1:C:379:TRP:CE2	2.55	0.41
1:A:417:ARG:NH1	1:B:244:GLU:OE2	2.51	0.41
1:E:467:ARG:HG2	1:F:291:HIS:CD2	2.56	0.41
1:F:249:PRO:HB2	3:F:502:NAD:C2N	2.51	0.41
1:A:107:LEU:HD12	1:A:107:LEU:HA	1.93	0.40
1:D:172:ALA:HB2	1:D:335:ARG:NH1	2.36	0.40
1:B:65:ILE:O	1:B:65:ILE:CG2	2.69	0.40
1:C:101:LEU:HD11	1:C:203:GLY:O	2.20	0.40
1:D:96:PHE:HB3	3:D:503:NAD:H2B	2.03	0.40
1:F:304:PRO:HD3	1:F:338:PHE:CD1	2.57	0.40
1:B:64:ARG:CG	1:B:252:GLN:NE2	2.76	0.40
1:E:98:LYS:N	1:E:98:LYS:CD	2.83	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	426/446 (96%)	415 (97%)	11 (3%)	0	100	100
1	B	426/446 (96%)	414 (97%)	12 (3%)	0	100	100
1	C	429/446 (96%)	416 (97%)	13 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	431/446 (97%)	419 (97%)	12 (3%)	0	100	100
1	E	430/446 (96%)	419 (97%)	11 (3%)	0	100	100
1	F	433/446 (97%)	421 (97%)	12 (3%)	0	100	100
All	All	2575/2676 (96%)	2504 (97%)	71 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	356/369 (96%)	339 (95%)	17 (5%)	25	49
1	B	355/369 (96%)	338 (95%)	17 (5%)	25	49
1	C	357/369 (97%)	348 (98%)	9 (2%)	47	73
1	D	358/369 (97%)	343 (96%)	15 (4%)	30	55
1	E	357/369 (97%)	342 (96%)	15 (4%)	30	55
1	F	360/369 (98%)	348 (97%)	12 (3%)	38	64
All	All	2143/2214 (97%)	2058 (96%)	85 (4%)	32	57

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	SER
1	A	101	LEU
1	A	106	GLU
1	A	143	LYS
1	A	155	ARG
1	A	200	THR
1	A	201	ARG
1	A	320	ASN
1	A	323	GLN
1	A	341	LYS

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Mol	Chain	Res	Type
1	A	345	HIS
1	A	352	ARG
1	A	356	GLU
1	A	408	HIS
1	A	418	MET
1	A	434	GLN
1	A	442	ARG
1	B	64	ARG
1	B	101	LEU
1	B	104	ILE
1	B	201	ARG
1	B	204	THR
1	B	205	THR
1	B	253	TYR
1	B	324	GLU
1	B	341	LYS
1	B	345	HIS
1	B	356	GLU
1	B	377	GLU
1	B	408	HIS
1	B	413[A]	TYR
1	B	413[B]	TYR
1	B	418	MET
1	B	434	GLN
1	C	344	SER
1	C	345	HIS
1	C	352	ARG
1	C	356	GLU
1	C	377	GLU
1	C	408	HIS
1	C	418	MET
1	C	434	GLN
1	C	472	GLU
1	D	101	LEU
1	D	105	VAL
1	D	116	LEU
1	D	143	LYS
1	D	315	ASP
1	D	323	GLN
1	D	324	GLU
1	D	335	ARG
1	D	341	LYS

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Mol	Chain	Res	Type
1	D	356	GLU
1	D	377	GLU
1	D	408	HIS
1	D	418	MET
1	D	434	GLN
1	D	472	GLU
1	E	68	SER
1	E	98	LYS
1	E	103	ASN
1	E	143	LYS
1	E	204	THR
1	E	323	GLN
1	E	324	GLU
1	E	341	LYS
1	E	343	LEU
1	E	345	HIS
1	E	356	GLU
1	E	377	GLU
1	E	408	HIS
1	E	418	MET
1	E	434	GLN
1	F	143	LYS
1	F	204	THR
1	F	305	ASP
1	F	323	GLN
1	F	341	LYS
1	F	356	GLU
1	F	377	GLU
1	F	408	HIS
1	F	418	MET
1	F	434	GLN
1	F	439	GLU
1	F	472	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	82	HIS
1	B	82	HIS
1	B	252	GLN
1	D	82	HIS
1	E	82	HIS

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Mol	Chain	Res	Type
1	E	161	ASN
1	F	82	HIS
1	F	345	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 6 are monoatomic - leaving 14 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HIS	E	502	4	4,11,11	0.45	0	3,14,14	1.40	1 (33%)
2	HIS	A	501	4	4,11,11	1.08	1 (25%)	3,14,14	1.18	0
2	HIS	C	502	4	4,11,11	0.41	0	3,14,14	1.38	1 (33%)
5	PEG	A	504	-	6,6,6	0.70	0	5,5,5	0.74	0
3	NAD	F	502	-	42,48,48	1.12	3 (7%)	50,73,73	1.90	10 (20%)
3	NAD	A	502	-	42,48,48	0.93	0	50,73,73	1.57	7 (14%)
3	NAD	C	503	-	42,48,48	0.88	2 (4%)	50,73,73	1.88	12 (24%)
3	NAD	E	503	-	42,48,48	1.44	4 (9%)	50,73,73	1.74	12 (24%)
5	PEG	F	503	-	6,6,6	0.67	0	5,5,5	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HIS	D	502	4	4,11,11	0.53	0	3,14,14	1.36	1 (33%)
3	NAD	D	503	-	42,48,48	1.09	4 (9%)	50,73,73	1.63	9 (18%)
2	HIS	F	501	4	4,11,11	0.50	0	3,14,14	1.43	0
2	HIS	B	502	4	4,11,11	0.58	0	3,14,14	1.63	1 (33%)
3	NAD	B	503	-	42,48,48	0.97	3 (7%)	50,73,73	1.79	12 (24%)

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	HIS	E	502	4	-	1/4/8/8	0/1/1/1
2	HIS	A	501	4	-	0/4/8/8	0/1/1/1
2	HIS	C	502	4	-	0/4/8/8	0/1/1/1
5	PEG	A	504	-	-	2/4/4/4	-
3	NAD	F	502	-	-	5/26/62/62	0/5/5/5
3	NAD	A	502	-	-	6/26/62/62	0/5/5/5
3	NAD	C	503	-	-	9/26/62/62	0/5/5/5
3	NAD	E	503	-	-	7/26/62/62	0/5/5/5
5	PEG	F	503	-	-	0/4/4/4	-
2	HIS	D	502	4	-	0/4/8/8	0/1/1/1
3	NAD	D	503	-	-	12/26/62/62	0/5/5/5
2	HIS	F	501	4	-	0/4/8/8	0/1/1/1
2	HIS	B	502	4	-	1/4/8/8	0/1/1/1
3	NAD	B	503	-	-	10/26/62/62	0/5/5/5

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	503	NAD	O4D-C1D	4.81	1.47	1.41
3	D	503	NAD	O4B-C1B	3.89	1.46	1.41
3	E	503	NAD	O4B-C1B	3.70	1.46	1.41
3	E	503	NAD	C2A-N3A	3.38	1.37	1.32
3	F	502	NAD	O4D-C1D	3.21	1.45	1.41
3	F	502	NAD	C5A-C4A	3.13	1.49	1.40
3	B	503	NAD	C5A-C4A	2.79	1.48	1.40
3	B	503	NAD	O4D-C1D	2.43	1.44	1.41
3	D	503	NAD	C5A-C4A	2.43	1.47	1.40
3	C	503	NAD	O7N-C7N	-2.20	1.19	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	502	NAD	C8A-N7A	2.19	1.38	1.34
3	D	503	NAD	C2A-N3A	2.17	1.35	1.32
3	E	503	NAD	C2B-C1B	-2.15	1.50	1.53
3	B	503	NAD	O4B-C1B	2.13	1.44	1.41
2	A	501	HIS	CA-N	2.11	1.51	1.47
3	D	503	NAD	O7N-C7N	-2.08	1.20	1.24
3	C	503	NAD	C5A-C4A	2.02	1.46	1.40

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	503	NAD	C3N-C7N-N7N	7.58	126.84	117.75
3	F	502	NAD	C3N-C7N-N7N	6.91	126.04	117.75
3	E	503	NAD	C3N-C7N-N7N	6.23	125.22	117.75
3	A	502	NAD	C3N-C7N-N7N	4.99	123.74	117.75
3	B	503	NAD	C3N-C7N-N7N	4.56	123.22	117.75
3	C	503	NAD	N3A-C2A-N1A	-4.54	121.58	128.68
3	F	502	NAD	O7N-C7N-N7N	-4.27	116.50	122.58
3	F	502	NAD	N3A-C2A-N1A	-4.22	122.09	128.68
3	D	503	NAD	C3B-C2B-C1B	4.18	107.27	100.98
3	B	503	NAD	O7N-C7N-C3N	-4.15	114.67	119.63
3	A	502	NAD	N3A-C2A-N1A	-4.03	122.37	128.68
3	D	503	NAD	O7N-C7N-C3N	4.00	124.42	119.63
3	A	502	NAD	C3B-C2B-C1B	3.99	106.98	100.98
3	D	503	NAD	C4A-C5A-N7A	-3.83	105.40	109.40
3	D	503	NAD	N3A-C2A-N1A	-3.80	122.74	128.68
3	C	503	NAD	O7N-C7N-C3N	-3.65	115.27	119.63
3	B	503	NAD	N3A-C2A-N1A	-3.61	123.03	128.68
3	E	503	NAD	C4A-C5A-N7A	-3.61	105.64	109.40
3	F	502	NAD	C3B-C2B-C1B	3.56	106.33	100.98
3	B	503	NAD	C6N-N1N-C2N	-3.55	118.74	121.97
3	C	503	NAD	O7N-C7N-N7N	-3.30	117.89	122.58
3	B	503	NAD	C5N-C4N-C3N	-3.28	116.46	120.34
3	A	502	NAD	O7N-C7N-N7N	-3.20	118.03	122.58
3	E	503	NAD	C6N-N1N-C2N	-3.12	119.13	121.97
3	E	503	NAD	N3A-C2A-N1A	-3.04	123.93	128.68
3	E	503	NAD	C3B-C2B-C1B	2.99	105.49	100.98
3	B	503	NAD	C3B-C2B-C1B	2.99	105.48	100.98
3	E	503	NAD	O3D-C3D-C4D	-2.92	102.60	111.05
3	B	503	NAD	C4A-C5A-N7A	-2.89	106.39	109.40
3	E	503	NAD	O7N-C7N-C3N	-2.86	116.21	119.63
3	E	503	NAD	O7N-C7N-N7N	-2.82	118.57	122.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	503	NAD	C4A-C5A-N7A	-2.76	106.52	109.40
3	F	502	NAD	C4A-C5A-N7A	-2.74	106.54	109.40
3	B	503	NAD	C2A-N1A-C6A	2.74	123.44	118.75
3	F	502	NAD	O2N-PN-O1N	2.72	125.68	112.24
3	F	502	NAD	C2A-N1A-C6A	2.70	123.38	118.75
3	C	503	NAD	C1B-N9A-C4A	-2.60	122.07	126.64
3	D	503	NAD	O5D-PN-O1N	-2.50	99.29	109.07
3	D	503	NAD	C5N-C4N-C3N	-2.47	117.42	120.34
3	C	503	NAD	C2A-N1A-C6A	2.45	122.95	118.75
3	F	502	NAD	C2N-C3N-C4N	-2.39	115.55	118.26
3	C	503	NAD	O2B-C2B-C3B	2.38	119.52	111.82
3	A	502	NAD	N6A-C6A-N1A	2.36	123.48	118.57
3	D	503	NAD	O2N-PN-O1N	2.36	123.91	112.24
3	B	503	NAD	C3N-C2N-N1N	2.35	122.73	120.43
3	B	503	NAD	C5A-C6A-N6A	2.33	123.90	120.35
3	E	503	NAD	O4D-C1D-C2D	-2.30	103.56	106.93
3	E	503	NAD	C3N-C2N-N1N	2.30	122.68	120.43
3	C	503	NAD	O5D-PN-O1N	-2.28	100.16	109.07
3	A	502	NAD	O2A-PA-O1A	2.27	123.44	112.24
3	C	503	NAD	O2N-PN-O1N	2.26	123.41	112.24
2	B	502	HIS	CD2-NE2-CE1	2.21	109.23	105.78
3	D	503	NAD	C2N-C3N-C4N	2.19	120.74	118.26
3	C	503	NAD	C2B-C3B-C4B	2.18	106.89	102.64
3	F	502	NAD	PN-O3-PA	-2.16	125.41	132.83
3	E	503	NAD	O2N-PN-O1N	2.15	122.88	112.24
3	F	502	NAD	C3N-C2N-N1N	2.15	122.53	120.43
3	E	503	NAD	C2D-C3D-C4D	2.14	106.79	102.64
2	D	502	HIS	CD2-NE2-CE1	2.14	109.11	105.78
3	A	502	NAD	C3D-C2D-C1D	-2.13	97.76	100.98
3	B	503	NAD	O2N-PN-O1N	2.11	122.68	112.24
2	E	502	HIS	CD2-NE2-CE1	2.08	109.02	105.78
3	C	503	NAD	O4D-C4D-C3D	2.07	109.20	105.11
3	D	503	NAD	C3D-C2D-C1D	2.05	104.07	100.98
2	C	502	HIS	CD2-NE2-CE1	2.02	108.93	105.78
3	B	503	NAD	O4B-C4B-C3B	2.02	109.11	105.11

There are no chirality outliers.

All (53) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	502	NAD	PN-O3-PA-O5B
3	F	502	NAD	O4D-C4D-C5D-O5D

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Mol	Chain	Res	Type	Atoms
3	F	502	NAD	O4D-C1D-N1N-C2N
3	F	502	NAD	O4D-C1D-N1N-C6N
3	A	502	NAD	O4D-C1D-N1N-C2N
3	A	502	NAD	O4D-C1D-N1N-C6N
3	C	503	NAD	PN-O3-PA-O5B
3	C	503	NAD	C5D-O5D-PN-O3
3	C	503	NAD	O4D-C1D-N1N-C2N
3	C	503	NAD	O4D-C1D-N1N-C6N
3	C	503	NAD	C2D-C1D-N1N-C2N
3	E	503	NAD	O4D-C4D-C5D-O5D
3	E	503	NAD	O4D-C1D-N1N-C2N
3	E	503	NAD	O4D-C1D-N1N-C6N
3	E	503	NAD	C2D-C1D-N1N-C2N
3	E	503	NAD	C2D-C1D-N1N-C6N
3	D	503	NAD	C5D-O5D-PN-O2N
3	D	503	NAD	O4D-C4D-C5D-O5D
3	D	503	NAD	O4D-C1D-N1N-C2N
3	D	503	NAD	O4D-C1D-N1N-C6N
3	D	503	NAD	C2D-C1D-N1N-C2N
3	D	503	NAD	C2D-C1D-N1N-C6N
3	B	503	NAD	O4D-C1D-N1N-C2N
3	B	503	NAD	O4D-C1D-N1N-C6N
3	B	503	NAD	C2D-C1D-N1N-C2N
3	A	502	NAD	O4D-C4D-C5D-O5D
3	F	502	NAD	C3D-C4D-C5D-O5D
3	A	502	NAD	C3D-C4D-C5D-O5D
3	E	503	NAD	C3D-C4D-C5D-O5D
3	D	503	NAD	C3D-C4D-C5D-O5D
5	A	504	PEG	O1-C1-C2-O2
5	A	504	PEG	O2-C3-C4-O4
3	A	502	NAD	PA-O3-PN-O5D
3	E	503	NAD	PA-O3-PN-O5D
3	D	503	NAD	PA-O3-PN-O5D
3	B	503	NAD	PN-O3-PA-O5B
3	D	503	NAD	C5D-O5D-PN-O3
3	B	503	NAD	O4D-C4D-C5D-O5D
3	D	503	NAD	C5D-O5D-PN-O1N
2	E	502	HIS	CA-CB-CG-ND1
2	B	502	HIS	CA-CB-CG-ND1
3	D	503	NAD	PA-O3-PN-O1N
3	C	503	NAD	C4B-C5B-O5B-PA
3	D	503	NAD	C3B-C4B-C5B-O5B

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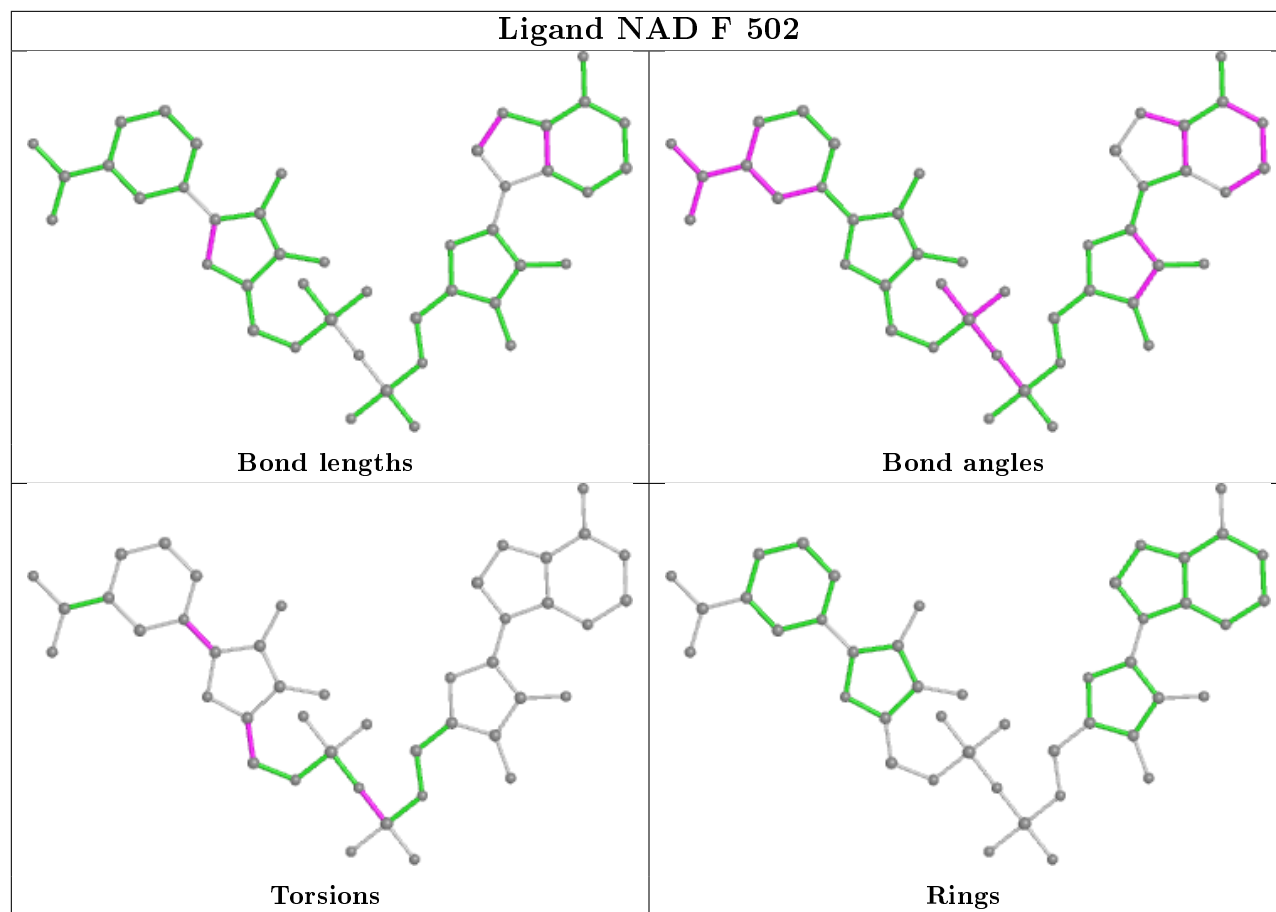
Mol	Chain	Res	Type	Atoms
3	A	502	NAD	C2D-C1D-N1N-C2N
3	C	503	NAD	C2D-C1D-N1N-C6N
3	B	503	NAD	C5B-O5B-PA-O3
3	B	503	NAD	C2D-C1D-N1N-C6N
3	B	503	NAD	C3B-C4B-C5B-O5B
3	C	503	NAD	C5D-O5D-PN-O1N
3	C	503	NAD	O4D-C4D-C5D-O5D
3	B	503	NAD	O4B-C4B-C5B-O5B
3	B	503	NAD	C4B-C5B-O5B-PA

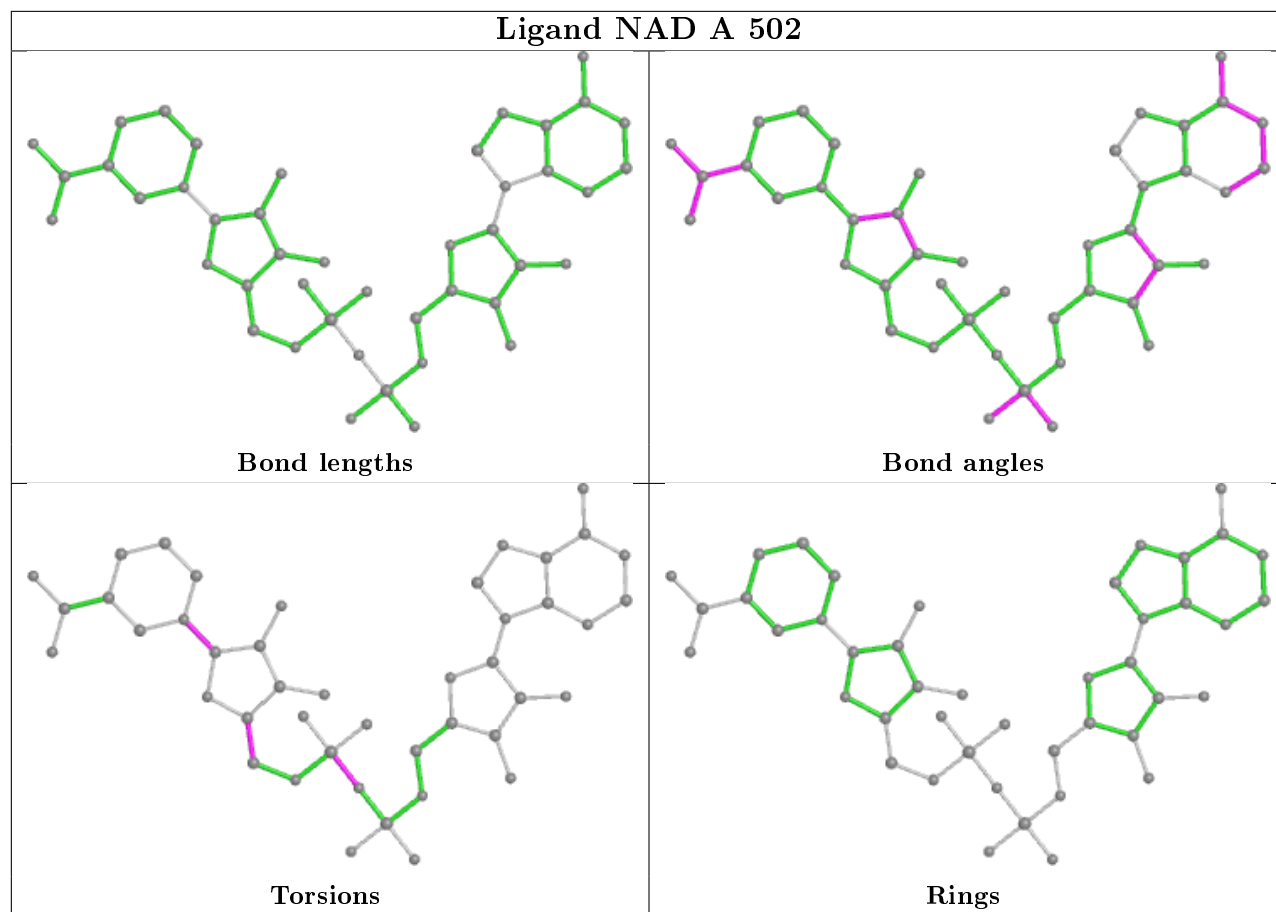
There are no ring outliers.

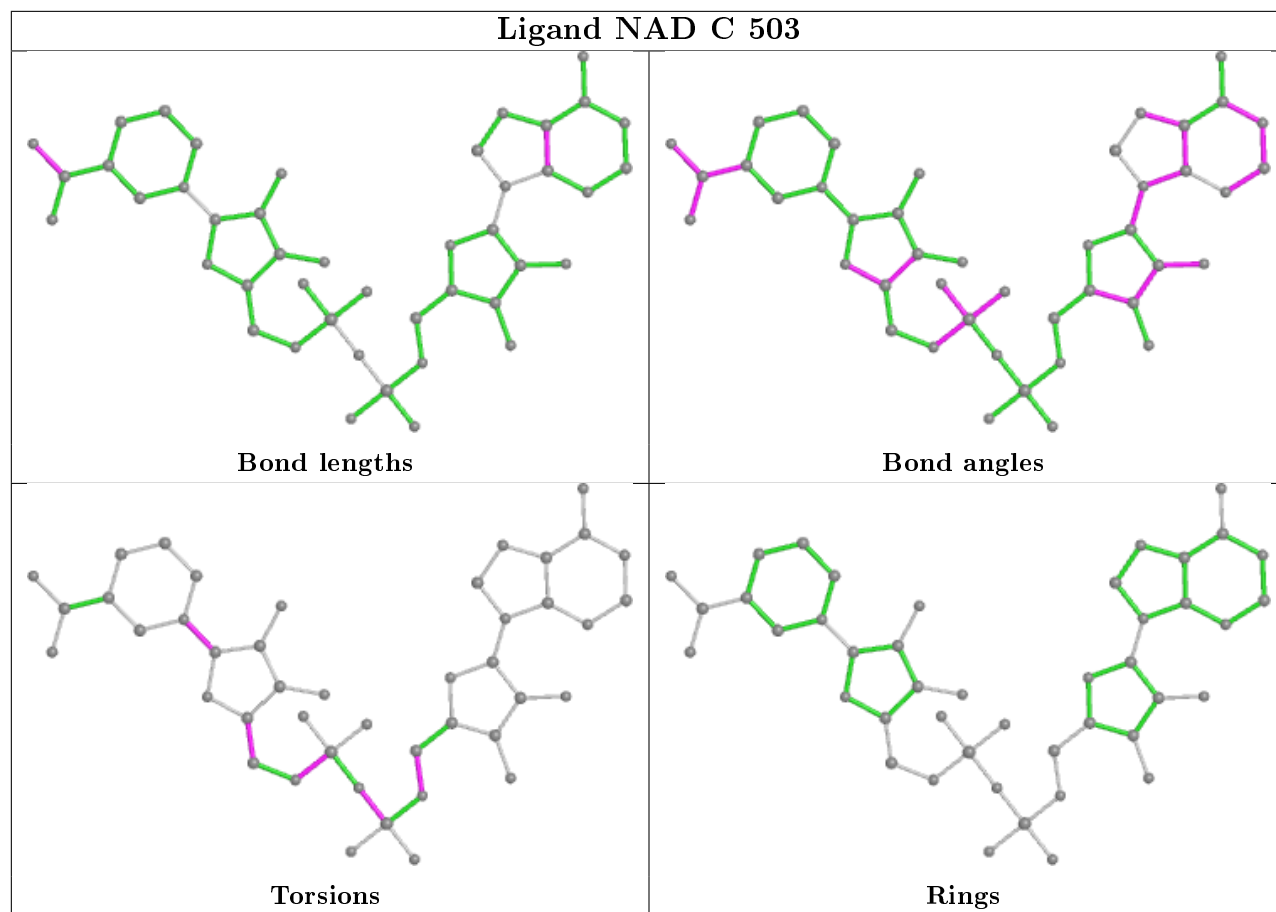
5 monomers are involved in 11 short contacts:

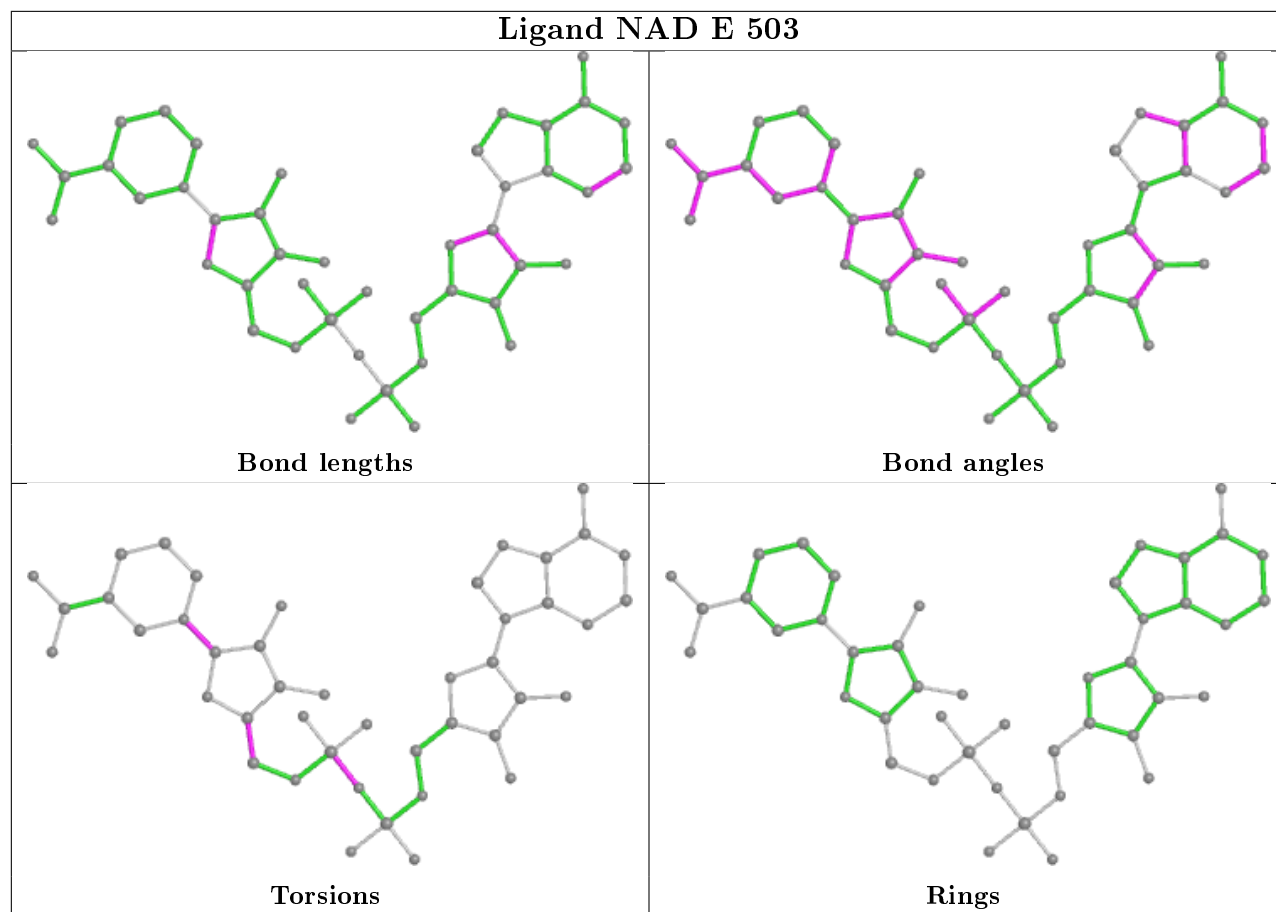
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	502	NAD	2	0
3	A	502	NAD	1	0
3	E	503	NAD	2	0
3	D	503	NAD	2	0
3	B	503	NAD	4	0

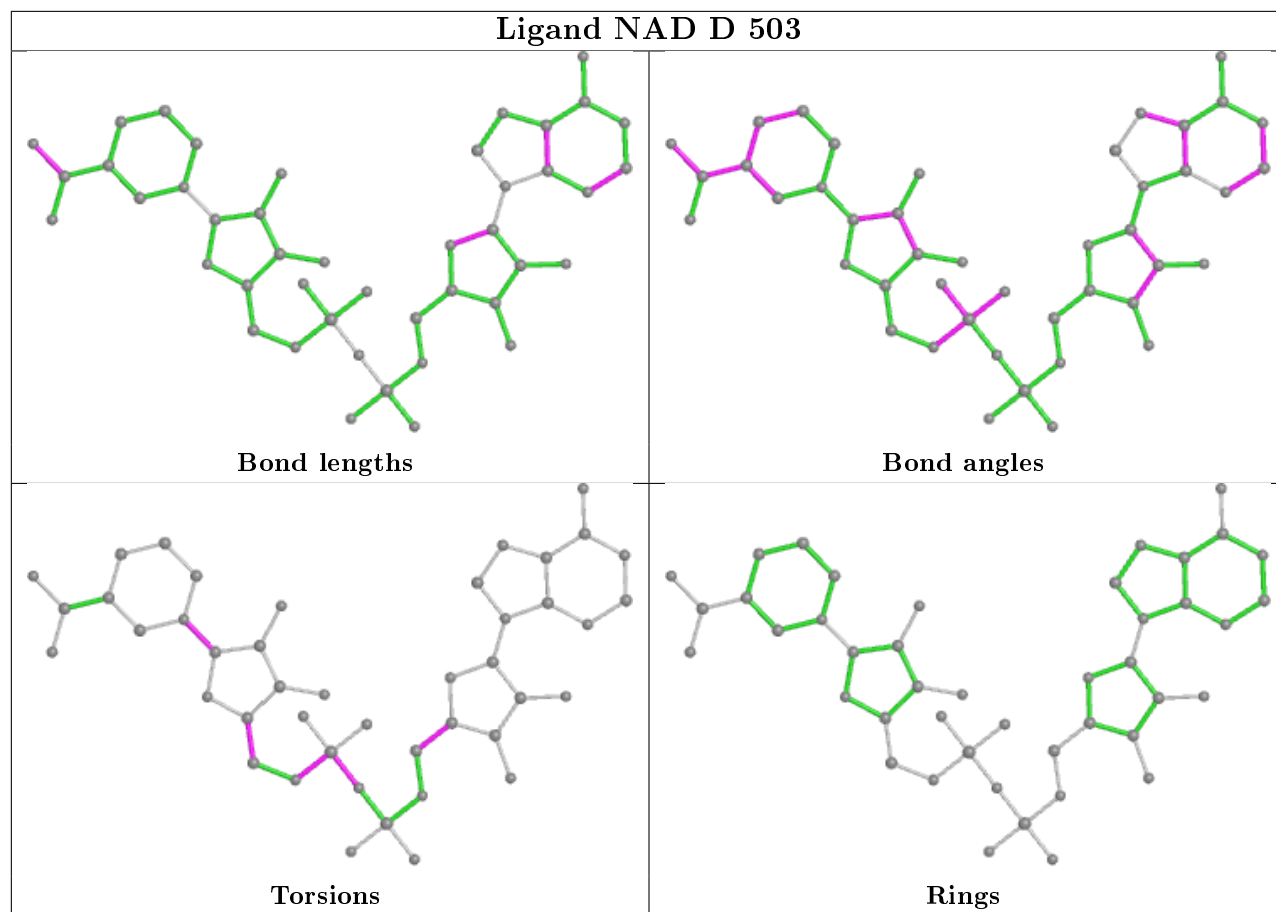
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

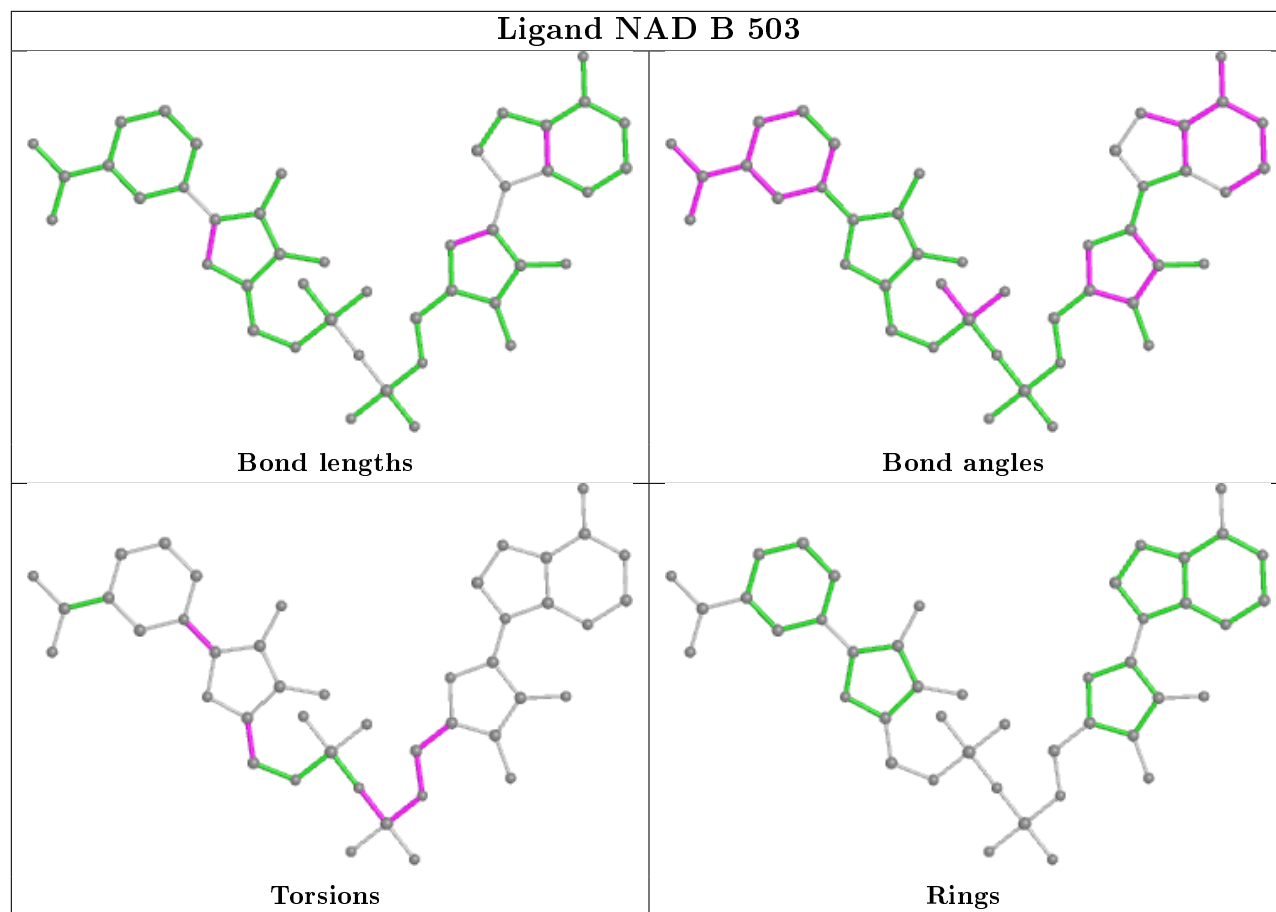












5.7 Other polymers [i](#)

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	430/446 (96%)	-0.11	3 (0%) 87 86	19, 38, 66, 92	0
1	B	429/446 (96%)	0.12	24 (5%) 24 19	18, 37, 91, 112	0
1	C	431/446 (96%)	1.05	77 (17%) 1 0	43, 83, 134, 171	0
1	D	433/446 (97%)	0.92	62 (14%) 2 1	29, 75, 112, 136	0
1	E	432/446 (96%)	0.13	11 (2%) 57 51	26, 44, 77, 120	0
1	F	435/446 (97%)	0.28	22 (5%) 28 22	26, 49, 87, 129	0
All	All	2590/2676 (96%)	0.40	199 (7%) 13 10	18, 51, 110, 171	0

All (199) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	338	PHE	9.1
1	D	320	ASN	6.4
1	E	471	ILE	6.3
1	A	205	THR	6.1
1	D	293	ALA	6.0
1	C	106	GLU	5.3
1	D	166	TYR	5.3
1	D	322	ILE	5.2
1	C	97	ASP	5.1
1	D	471	ILE	5.0
1	C	223	LYS	4.9
1	F	471	ILE	4.8
1	C	89	VAL	4.8
1	C	101	LEU	4.8
1	D	222	LEU	4.7
1	D	333	LEU	4.7
1	C	104	ILE	4.6
1	D	223	LYS	4.5
1	C	204	THR	4.5

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Mol	Chain	Res	Type	RSRZ
1	D	196	ALA	4.5
1	C	468	LEU	4.5
1	C	205	THR	4.4
1	B	97	ASP	4.4
1	F	473	ALA	4.3
1	D	172	ALA	4.2
1	F	201	ARG	4.2
1	D	326	VAL	4.2
1	C	119	ALA	4.1
1	D	474	ARG	4.1
1	C	221	LEU	4.1
1	D	48	LEU	4.1
1	E	101	LEU	4.1
1	D	104	ILE	4.0
1	C	114	PRO	4.0
1	D	210	LEU	4.0
1	E	201	ARG	3.9
1	D	468	LEU	3.9
1	C	115	VAL	3.8
1	D	101	LEU	3.8
1	B	96	PHE	3.8
1	C	320	ASN	3.8
1	F	475	GLN	3.8
1	B	69	SER	3.8
1	D	296	LEU	3.7
1	C	207	LYS	3.6
1	C	107	LEU	3.6
1	C	91	GLN	3.6
1	C	76	PRO	3.5
1	C	210	LEU	3.5
1	C	328	LYS	3.5
1	C	172	ALA	3.5
1	C	116	LEU	3.5
1	B	72	ASP	3.4
1	D	442	ARG	3.4
1	B	92	TYR	3.4
1	F	101	LEU	3.4
1	B	224	ALA	3.4
1	C	464	VAL	3.4
1	F	115	VAL	3.4
1	C	469	GLN	3.3
1	E	169	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	201	ARG	3.3
1	C	466	LEU	3.3
1	C	88	ALA	3.3
1	D	66	ASP	3.3
1	D	304	PRO	3.3
1	D	297	LEU	3.3
1	E	472	GLU	3.2
1	D	330	CYS	3.2
1	C	111	LEU	3.2
1	B	98	LYS	3.2
1	C	212	CYS	3.2
1	C	462	ARG	3.2
1	D	402	TYR	3.1
1	C	175	PRO	3.1
1	B	71	PHE	3.1
1	B	77	ILE	3.0
1	F	103	ASN	3.0
1	C	195	LEU	3.0
1	C	109	SER	3.0
1	D	457	LEU	3.0
1	F	221	LEU	3.0
1	C	90	LYS	3.0
1	D	123	ALA	3.0
1	F	172	ALA	2.9
1	C	445	GLY	2.9
1	D	300	ALA	2.9
1	D	110	ASP	2.9
1	F	474	ARG	2.9
1	B	95	LYS	2.9
1	D	203	GLY	2.9
1	B	70	VAL	2.8
1	C	173	VAL	2.8
1	D	111	LEU	2.8
1	D	176	SER	2.8
1	D	275	GLY	2.8
1	C	86	ASP	2.8
1	C	96	PHE	2.8
1	C	78	VAL	2.8
1	C	449	GLU	2.8
1	D	108	VAL	2.7
1	F	223	LYS	2.7
1	D	399	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	F	51	LEU	2.7
1	B	472	GLU	2.7
1	D	67	PHE	2.7
1	C	80	ASP	2.7
1	F	476	VAL	2.7
1	B	101	LEU	2.7
1	B	253	TYR	2.7
1	C	170	GLY	2.7
1	C	123	ALA	2.7
1	E	464	VAL	2.6
1	D	289	PRO	2.6
1	D	221	LEU	2.6
1	E	89	VAL	2.6
1	D	91	GLN	2.6
1	D	119	ALA	2.6
1	C	99	VAL	2.6
1	C	198	PRO	2.6
1	B	73	ILE	2.6
1	D	127	ALA	2.5
1	C	74	VAL	2.5
1	D	175	PRO	2.5
1	D	209	VAL	2.5
1	F	205	THR	2.5
1	C	454	VAL	2.5
1	D	167	VAL	2.5
1	E	470	ASP	2.5
1	D	331	GLN	2.5
1	C	108	VAL	2.5
1	C	471	ILE	2.5
1	C	394	TRP	2.5
1	D	438	GLU	2.5
1	D	337	GLU	2.5
1	D	462	ARG	2.4
1	D	346	SER	2.4
1	F	105	VAL	2.4
1	E	100	ASP	2.4
1	C	77	ILE	2.4
1	E	172	ALA	2.4
1	F	466	LEU	2.4
1	F	100	ASP	2.4
1	D	404	SER	2.4
1	C	130	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	102	GLU	2.4
1	D	169	GLY	2.3
1	B	86	ASP	2.3
1	C	441	LEU	2.3
1	C	110	ASP	2.3
1	F	89	VAL	2.3
1	C	232	ALA	2.3
1	C	294	ALA	2.3
1	C	402	TYR	2.3
1	C	125	ASP	2.3
1	D	120	ILE	2.3
1	C	211	TYR	2.3
1	C	218	VAL	2.2
1	C	306	SER	2.2
1	A	140	SER	2.2
1	B	256	ALA	2.2
1	C	463	ALA	2.2
1	D	224	ALA	2.2
1	B	331	GLN	2.2
1	D	263	ASN	2.2
1	F	106	GLU	2.2
1	C	113	ASP	2.2
1	C	122	GLU	2.2
1	C	196	ALA	2.2
1	C	228	GLN	2.2
1	B	104	ILE	2.2
1	B	260	ILE	2.2
1	C	93	THR	2.2
1	C	448	VAL	2.1
1	C	447	TYR	2.1
1	C	167	VAL	2.1
1	D	53	GLN	2.1
1	A	210	LEU	2.1
1	B	103	ASN	2.1
1	E	331	GLN	2.1
1	D	206	CYS	2.1
1	C	102	GLU	2.1
1	C	100	ASP	2.1
1	C	324	GLU	2.1
1	F	472	GLU	2.1
1	B	64	ARG	2.1
1	C	442	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	168	PRO	2.1
1	F	104	ILE	2.1
1	F	224	ALA	2.0
1	C	81	VAL	2.0
1	C	321	ALA	2.0
1	D	42	PRO	2.0
1	D	463	ALA	2.0
1	B	84	HIS	2.0
1	B	173	VAL	2.0
1	D	335	ARG	2.0
1	C	43	ILE	2.0
1	C	124	PHE	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

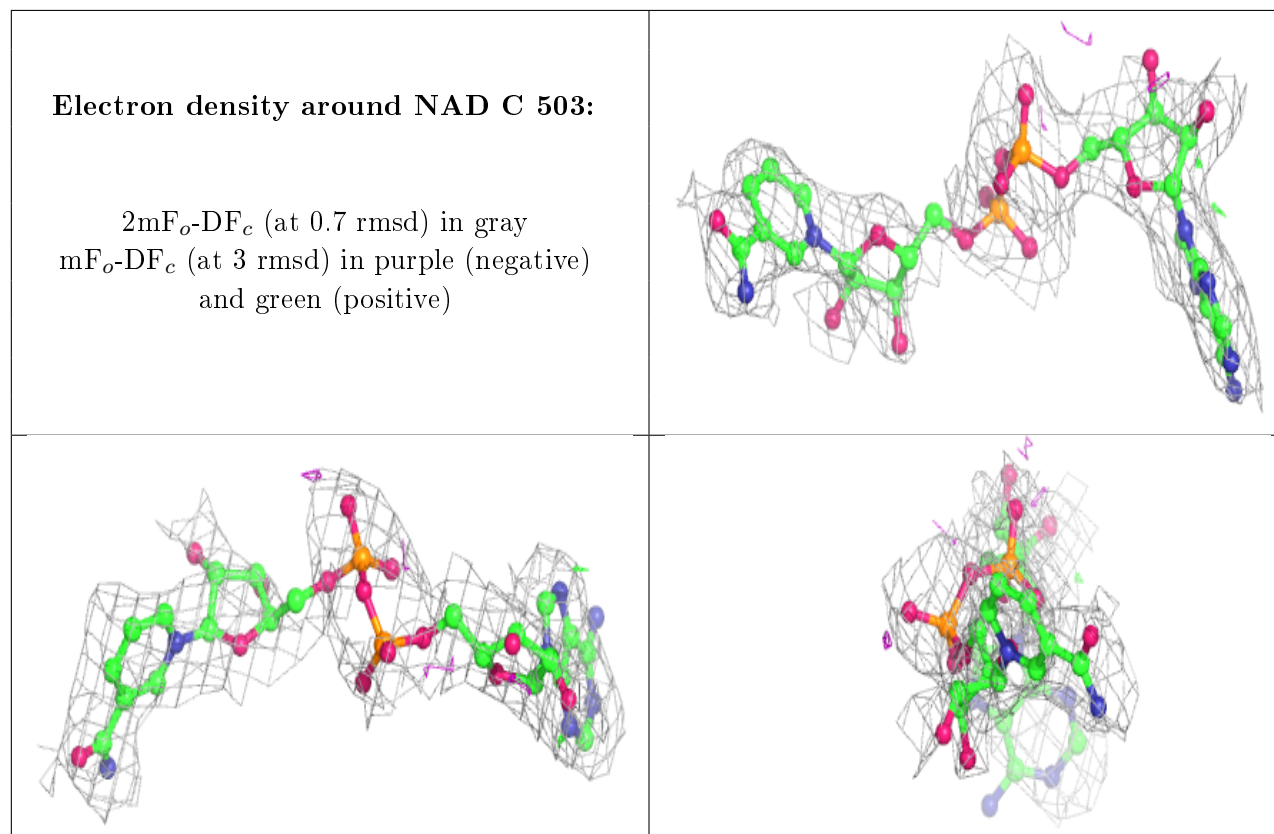
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	PEG	F	503	7/7	0.77	0.17	52,65,72,72	0
5	PEG	A	504	7/7	0.78	0.21	51,56,61,63	0
3	NAD	C	503	44/44	0.89	0.19	65,93,118,123	0
2	HIS	C	502	11/11	0.91	0.22	70,75,81,82	0
3	NAD	B	503	44/44	0.91	0.19	46,60,99,101	0
3	NAD	D	503	44/44	0.92	0.19	62,77,101,106	0
4	ZN	D	501	1/1	0.93	0.05	68,68,68,68	0
2	HIS	D	502	11/11	0.94	0.28	68,70,75,75	0
4	ZN	C	501	1/1	0.95	0.09	79,79,79,79	0
3	NAD	E	503	44/44	0.95	0.14	29,37,51,53	0
2	HIS	F	501	11/11	0.96	0.14	40,43,46,47	0

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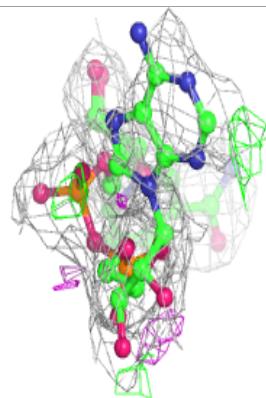
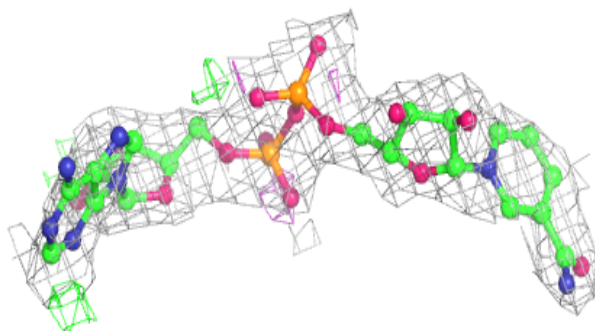
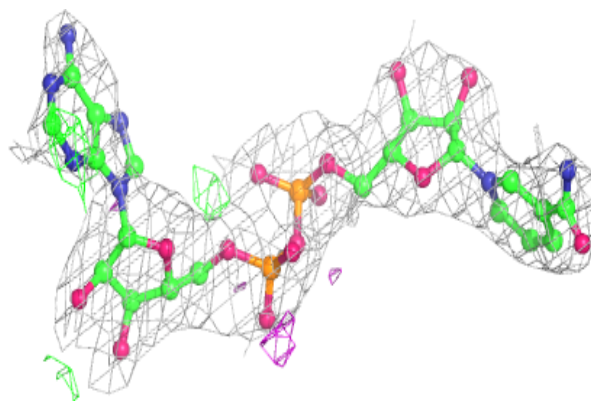
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NAD	F	502	44/44	0.97	0.12	34,44,54,55	0
3	NAD	A	502	44/44	0.98	0.14	27,31,42,44	0
2	HIS	B	502	11/11	0.98	0.13	25,25,26,27	0
2	HIS	A	501	11/11	0.99	0.09	26,27,28,28	0
4	ZN	A	503	1/1	0.99	0.11	25,25,25,25	0
2	HIS	E	502	11/11	0.99	0.10	32,34,36,36	0
4	ZN	B	501	1/1	0.99	0.07	30,30,30,30	0
4	ZN	E	501	1/1	1.00	0.07	37,37,37,37	0
4	ZN	E	504	1/1	1.00	0.07	48,48,48,48	0

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

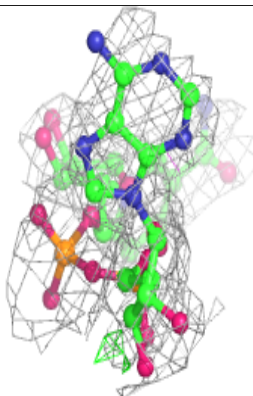
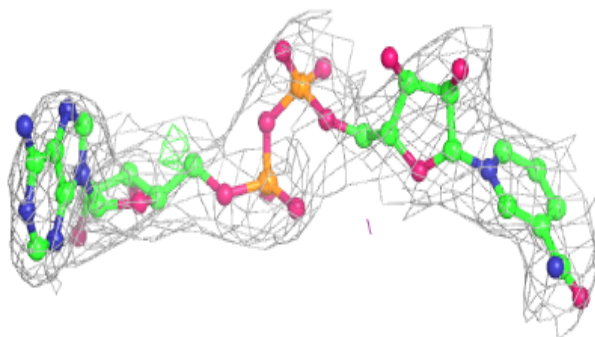
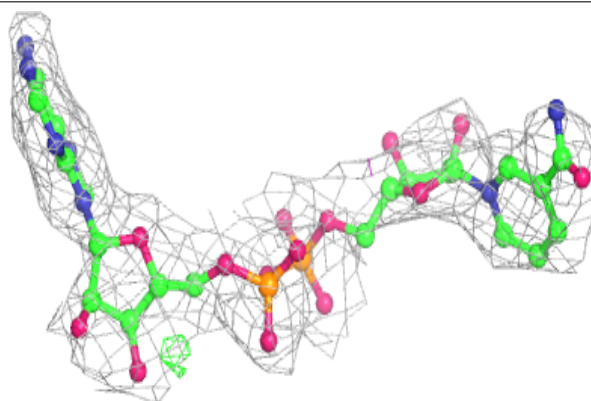


Electron density around NAD B 503:

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

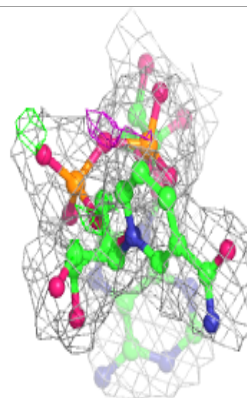
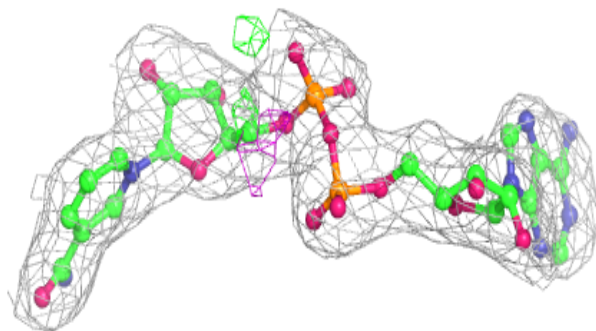
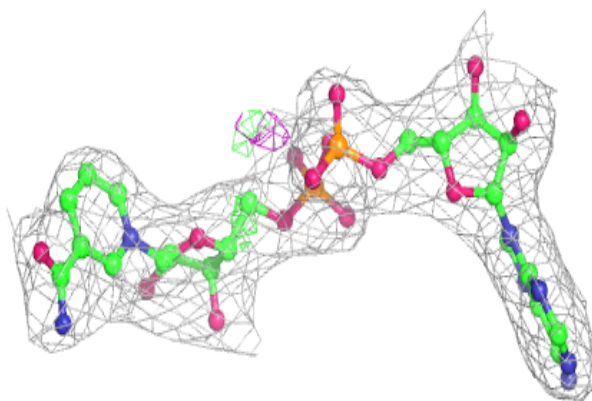
**Electron density around NAD D 503:**

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

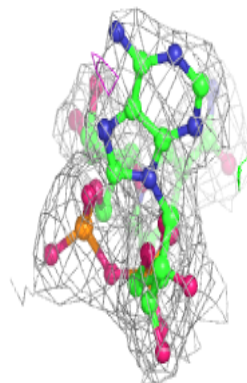
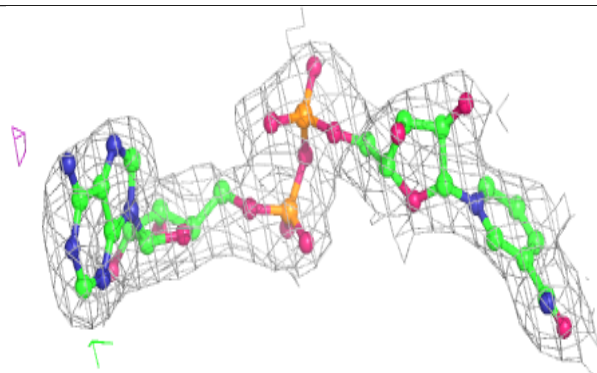
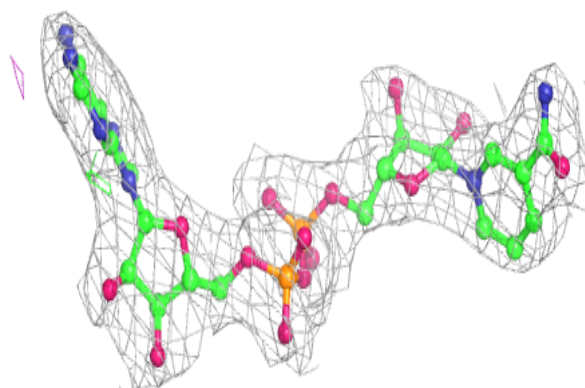


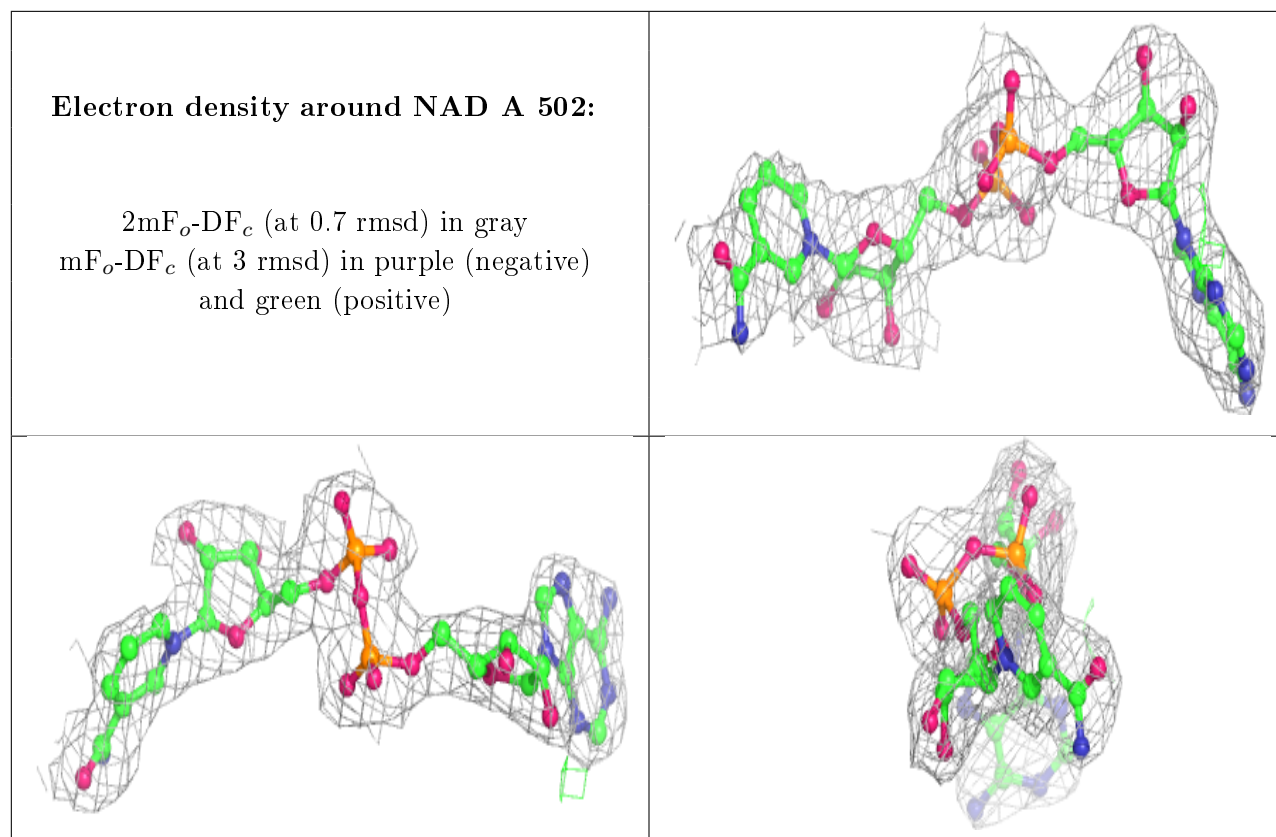
Electron density around NAD E 503:

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

**Electron density around NAD F 502:**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.