



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:50 PM UTC

PDB ID : 6O4H / pdb_00006o4h
Title : Structure of ALDH7A1 mutant A171V complexed with NAD
Authors : Tanner, J.J.; Korasick, D.A.; Laciak, A.R.
Deposited on : 2019-02-28
Resolution : 2.05 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

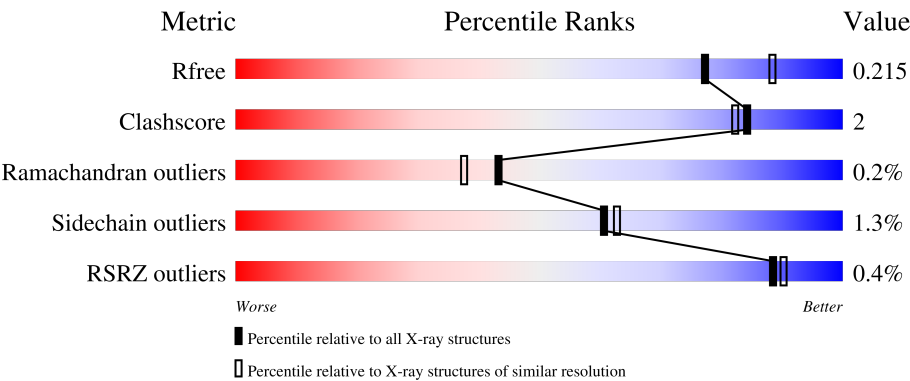
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.05 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	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

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	513	90%6%.
1	B	513	% 90%6%.
1	C	513	% 89%7%.
1	D	513	90%7%.
1	E	513	90%7%.

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Mol	Chain	Length	Quality of chain
1	F	513	 90% 7% .
1	G	513	 91% 5% .
1	H	513	 93% . .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 31649 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 Alpha-aminoadipic semialdehyde dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	497	Total	C	N	O	S	0	1	0
			3745	2376	651	701	17			
1	B	497	Total	C	N	O	S	0	1	0
			3721	2360	645	699	17			
1	C	497	Total	C	N	O	S	0	1	0
			3696	2349	639	691	17			
1	D	497	Total	C	N	O	S	0	1	0
			3725	2368	644	696	17			
1	E	498	Total	C	N	O	S	0	2	0
			3767	2392	652	705	18			
1	F	497	Total	C	N	O	S	0	1	0
			3762	2389	653	703	17			
1	G	497	Total	C	N	O	S	0	0	0
			3763	2389	654	703	17			
1	H	497	Total	C	N	O	S	0	2	0
			3767	2393	653	703	18			

There are 24 discrepancies between the modelled and reference sequences:

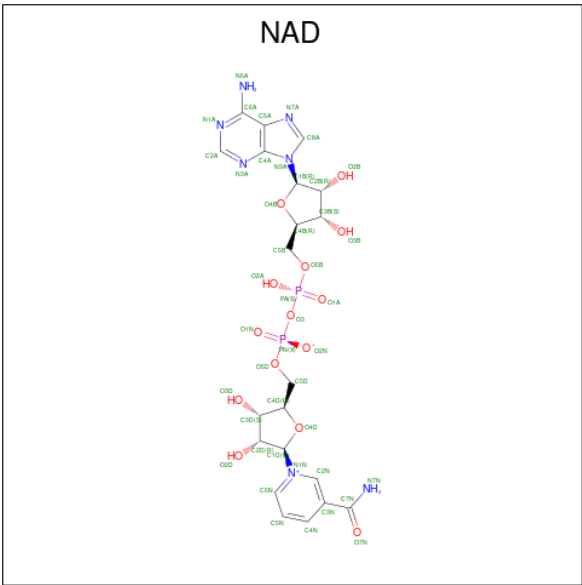
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P49419
A	0	HIS	-	expression tag	UNP P49419
A	171	VAL	ALA	engineered mutation	UNP P49419
B	-1	GLY	-	expression tag	UNP P49419
B	0	HIS	-	expression tag	UNP P49419
B	171	VAL	ALA	engineered mutation	UNP P49419
C	-1	GLY	-	expression tag	UNP P49419
C	0	HIS	-	expression tag	UNP P49419
C	171	VAL	ALA	engineered mutation	UNP P49419
D	-1	GLY	-	expression tag	UNP P49419
D	0	HIS	-	expression tag	UNP P49419
D	171	VAL	ALA	engineered mutation	UNP P49419
E	-1	GLY	-	expression tag	UNP P49419

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Chain	Residue	Modelled	Actual	Comment	Reference
E	0	HIS	-	expression tag	UNP P49419
E	171	VAL	ALA	engineered mutation	UNP P49419
F	-1	GLY	-	expression tag	UNP P49419
F	0	HIS	-	expression tag	UNP P49419
F	171	VAL	ALA	engineered mutation	UNP P49419
G	-1	GLY	-	expression tag	UNP P49419
G	0	HIS	-	expression tag	UNP P49419
G	171	VAL	ALA	engineered mutation	UNP P49419
H	-1	GLY	-	expression tag	UNP P49419
H	0	HIS	-	expression tag	UNP P49419
H	171	VAL	ALA	engineered mutation	UNP P49419

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂) (labeled as "Ligand of Interest" by depositor).



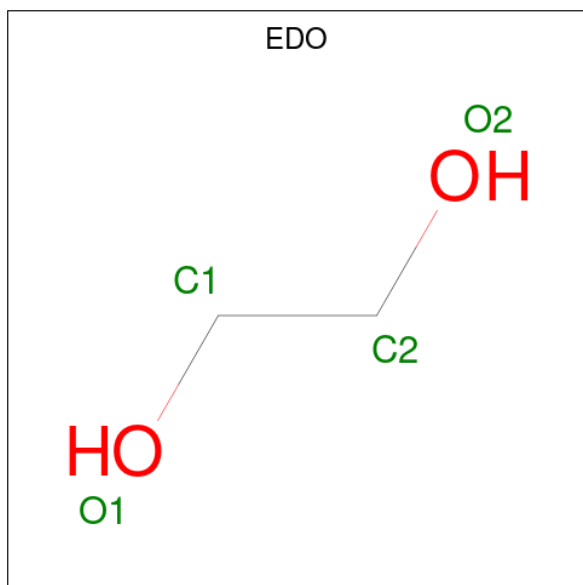
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	E	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	F	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	G	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	H	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			4	2	2		
3	F	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	206	Total	O	0	0
			206	206		
4	B	157	Total	O	0	0
			157	157		
4	C	134	Total	O	0	0
			134	134		
4	D	133	Total	O	0	0
			133	133		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	188	Total 188	O 188	0	0
4	F	175	Total 175	O 175	0	0
4	G	177	Total 177	O 177	0	0
4	H	173	Total 173	O 173	0	0



- Molecule 1: Alpha-aminoadipic semialdehyde dehydrogenase

Chain E: 90% 7% .



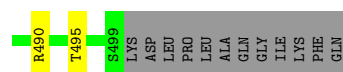
- Molecule 1: Alpha-aminoadipic semialdehyde dehydrogenase

Chain F: 90% 7% .



- Molecule 1: Alpha-aminoadipic semialdehyde dehydrogenase

Chain G: 91% 5% .



- Molecule 1: Alpha-aminoadipic semialdehyde dehydrogenase

Chain H: 93% . .



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	155.98Å 161.36Å 159.16Å 90.00° 95.00° 90.00°	Depositor
Resolution (Å)	56.55 – 2.05 56.55 – 2.05	Depositor EDS
% Data completeness (in resolution range)	97.7 (56.55-2.05) 99.6 (56.55-2.05)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.95 (at 2.05Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.174 , 0.219 0.169 , 0.215	Depositor DCC
R_{free} test set	12115 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	26.8	Xtriage
Anisotropy	0.458	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 39.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	31649	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.42% 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: EDO, 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	0.33	0/3825	0.49	0/5199
1	B	0.32	0/3800	0.47	0/5170
1	C	0.31	0/3775	0.48	0/5139
1	D	0.29	0/3805	0.46	0/5175
1	E	0.32	0/3850	0.50	0/5229
1	F	0.31	0/3842	0.48	0/5218
1	G	0.31	0/3840	0.49	0/5213
1	H	0.32	0/3850	0.49	0/5228
All	All	0.31	0/30587	0.48	0/41571

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	3745	0	3699	25	0
1	B	3721	0	3653	18	0
1	C	3696	0	3617	21	0
1	D	3725	0	3665	21	0
1	E	3767	0	3735	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3762	0	3738	20	0
1	G	3763	0	3746	14	0
1	H	3767	0	3747	13	0
2	A	44	0	24	2	0
2	B	44	0	24	0	0
2	C	44	0	25	2	0
2	D	44	0	24	1	0
2	E	44	0	24	0	0
2	F	44	0	24	2	0
2	G	44	0	24	1	0
2	H	44	0	24	2	0
3	B	4	0	6	0	0
3	F	4	0	6	0	0
4	A	206	0	0	2	0
4	B	157	0	0	1	0
4	C	134	0	0	0	0
4	D	133	0	0	1	0
4	E	188	0	0	2	0
4	F	175	0	0	1	0
4	G	177	0	0	0	0
4	H	173	0	0	1	0
All	All	31649	0	29805	138	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 2.

All (138) 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:291:LEU:HD11	1:D:329:ILE:HD11	1.77	0.66
1:E:295:VAL:HG11	1:E:329:ILE:HD13	1.78	0.65
1:E:94:ARG:NH1	1:E:127:ASP:OD2	2.30	0.64
1:A:68:ARG:HD2	1:A:238:ARG:HB3	1.81	0.63
1:H:228:ASP:HB2	4:H:854:HOH:O	2.00	0.61
1:C:323:LYS:HE2	1:C:368:VAL:HB	1.82	0.60
1:F:118:GLU:HG2	1:F:171:VAL:HB	1.83	0.60
1:A:291:LEU:HD11	1:A:329:ILE:HD11	1.85	0.59
1:D:94:ARG:NH1	1:D:127:ASP:OD2	2.33	0.59
1:C:478:ARG:O	1:C:487:GLN:NE2	2.30	0.59
1:E:293:ALA:HB2	1:E:458:PRO:HB3	1.83	0.59
1:G:430:SER:HB3	1:G:454:ASN:HB2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:165:ALA:HB1	2:H:601:NAD:H52N	1.87	0.57
1:D:374:MET:HE3	1:D:382:GLU:HA	1.87	0.57
1:C:68:ARG:HD2	1:C:238:ARG:HB3	1.88	0.56
1:B:140:ILE:HG22	1:C:138:GLY:O	2.05	0.56
1:F:138:GLY:O	1:G:140:ILE:HG22	2.05	0.56
1:C:365:GLY:HA3	1:C:389:LEU:HD12	1.87	0.55
1:F:61:GLU:OE1	1:F:65:LYS:NZ	2.39	0.55
1:E:68:ARG:HD2	1:E:238:ARG:HB3	1.89	0.55
1:F:427:LEU:HD13	1:F:474:THR:HG21	1.89	0.54
1:A:293:ALA:HB2	1:A:458:PRO:HB3	1.90	0.54
4:A:883:HOH:O	1:F:38:ILE:HD11	2.05	0.54
1:B:68:ARG:HD2	1:B:238:ARG:HB3	1.88	0.54
1:A:68:ARG:NH1	1:A:238:ARG:O	2.41	0.53
1:E:291:LEU:HD11	1:E:329:ILE:HD11	1.89	0.53
1:E:442:TRP:CH2	1:E:448:SER:HB2	2.44	0.53
1:A:94:ARG:NH1	1:A:127:ASP:OD2	2.40	0.53
1:F:276:ILE:HB	1:F:431:ILE:HG22	1.90	0.53
1:H:94:ARG:NH1	1:H:127:ASP:OD2	2.39	0.53
1:E:138:GLY:O	1:H:140:ILE:HG22	2.09	0.52
1:E:331:VAL:HG21	1:E:374:MET:HE1	1.91	0.52
1:C:454:ASN:HB3	1:C:457:ILE:HG13	1.91	0.52
1:C:108:MET:HE3	1:C:167:ASN:HA	1.93	0.51
1:F:331:VAL:HG22	1:F:341:TYR:HB3	1.91	0.51
1:D:104:VAL:HA	1:D:198:ILE:HD11	1.92	0.51
1:F:330:ARG:HD3	1:F:338:ASN:O	2.11	0.50
1:C:344:LEU:HD21	1:C:403:PRO:HD3	1.93	0.50
1:C:94:ARG:NH1	1:C:127:ASP:OD2	2.35	0.50
1:D:3:THR:N	4:D:704:HOH:O	2.45	0.50
1:A:136:ILE:O	1:D:142:PRO:HD3	2.11	0.50
1:B:108:MET:HE3	1:B:167:ASN:HA	1.94	0.50
1:F:145:ARG:NH2	4:F:704:HOH:O	2.46	0.49
1:G:68:ARG:HD2	1:G:238:ARG:HB3	1.95	0.49
1:D:22:GLU:HG2	1:D:53:ARG:HE	1.78	0.48
1:F:140:ILE:CD1	1:G:151:ILE:HG23	2.44	0.48
1:A:142:PRO:HD3	1:D:136:ILE:O	2.14	0.47
1:E:51:ARG:HD3	4:E:724:HOH:O	2.13	0.47
1:A:138:GLY:O	1:D:140:ILE:HG22	2.14	0.47
1:D:37:VAL:HG22	1:D:53:ARG:HG2	1.95	0.47
1:D:269:LEU:O	2:D:601:NAD:H2N	2.14	0.47
1:E:145:ARG:NH2	4:E:701:HOH:O	2.36	0.47
1:C:427:LEU:HD13	1:C:474:THR:HG21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:344:LEU:HD21	1:E:403:PRO:HD3	1.97	0.47
1:B:138:GLY:O	1:C:140:ILE:HG22	2.15	0.47
1:G:495:THR:HB	1:H:457:ILE:HD11	1.97	0.47
1:G:442:TRP:CH2	1:G:448:SER:HB2	2.50	0.47
1:G:114:GLU:OE2	1:G:301:ARG:NH2	2.48	0.46
1:C:268:GLU:HB3	2:C:601:NAD:C7N	2.45	0.46
1:D:68:ARG:HD2	1:D:238:ARG:HB3	1.97	0.46
1:A:495:THR:HB	1:B:457:ILE:HD11	1.97	0.46
1:B:291:LEU:O	1:B:295:VAL:HG22	2.16	0.46
1:F:108:MET:HE3	1:F:167:ASN:HA	1.99	0.45
1:A:457:ILE:HG12	1:A:458:PRO:HD2	1.98	0.45
1:D:276:ILE:HB	1:D:431:ILE:HG22	1.99	0.45
1:D:469:GLY:HA3	1:D:478:ARG:HD3	1.99	0.45
1:D:315:HIS:CD2	1:D:409:LYS:HG2	2.52	0.45
1:C:457:ILE:HG23	1:D:497:ASN:HB2	1.99	0.44
1:D:295:VAL:HG11	1:D:329:ILE:HD13	1.99	0.44
1:E:126:CYS:O	1:E:130:VAL:HG23	2.18	0.44
1:B:144:GLU:O	1:C:81:LYS:NZ	2.45	0.44
1:D:341:TYR:OH	1:D:403:PRO:HG3	2.18	0.44
1:F:140:ILE:HD13	1:G:151:ILE:HG23	1.97	0.44
1:A:118:GLU:HG2	1:A:171:VAL:HB	2.00	0.44
1:G:20:ARG:NH2	1:G:24:GLU:OE2	2.50	0.44
1:A:269:LEU:O	2:A:601:NAD:H2N	2.18	0.44
1:B:442:TRP:CZ2	1:B:448:SER:HB2	2.53	0.44
1:F:268:GLU:HB3	2:F:602:NAD:C7N	2.48	0.44
1:F:126:CYS:O	1:F:130:VAL:HG23	2.18	0.44
2:G:601:NAD:H8A	2:G:601:NAD:H2B	1.87	0.44
1:E:104:VAL:HA	1:E:198:ILE:HD11	1.99	0.44
1:A:113:VAL:HG13	4:A:849:HOH:O	2.16	0.43
1:C:291:LEU:HD11	1:C:329:ILE:HD11	2.00	0.43
1:A:431:ILE:HG23	1:A:442:TRP:CE2	2.53	0.43
1:B:104:VAL:HA	1:B:198:ILE:HD11	2.01	0.43
1:D:419:TRP:O	1:D:422:GLU:HG2	2.19	0.43
1:A:246:GLY:HA3	2:A:601:NAD:H51A	2.00	0.43
1:F:142:PRO:HD3	1:G:136:ILE:O	2.18	0.43
1:F:254:VAL:HA	1:F:257:MET:HE3	2.01	0.43
1:H:374:MET:HE3	1:H:381:VAL:O	2.18	0.43
1:H:454:ASN:HB3	1:H:457:ILE:HG13	1.99	0.43
1:E:310:ILE:HG22	1:E:314:ILE:HG13	1.99	0.43
1:C:312:GLU:HG3	1:C:410:PHE:O	2.19	0.43
1:E:289:SER:HB3	1:E:458:PRO:HD3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:LEU:HD12	1:A:322:LEU:HA	1.87	0.42
1:A:430[A]:SER:HB3	1:A:454:ASN:HB2	2.00	0.42
1:F:145:ARG:HE	1:F:145:ARG:HB2	1.49	0.42
1:B:111:ILE:HB	4:B:730:HOH:O	2.19	0.42
1:G:293:ALA:HB2	1:G:458:PRO:CB	2.50	0.42
1:B:310:ILE:HG22	1:B:314:ILE:HG13	2.00	0.42
1:F:122:TYR:O	1:F:125:ILE:HG22	2.19	0.42
1:A:291:LEU:O	1:A:295:VAL:HG22	2.20	0.42
1:E:136:ILE:O	1:H:142:PRO:HD3	2.19	0.42
1:G:457:ILE:HG23	1:H:497:ASN:HB2	2.00	0.42
1:G:264:ARG:HH22	1:G:490:ARG:HA	1.85	0.42
1:H:276:ILE:HB	1:H:431:ILE:HG22	2.01	0.42
1:A:140:ILE:HG22	1:D:138:GLY:O	2.20	0.42
1:C:365:GLY:HA3	1:C:389:LEU:CD1	2.50	0.41
1:E:392:ASP:HA	1:E:397:HIS:NE2	2.36	0.41
1:A:108:MET:HE3	1:A:167:ASN:HA	2.02	0.41
1:B:427:LEU:HD13	1:B:474:THR:HG21	2.02	0.41
1:A:391:HIS:HA	1:A:408:PHE:CE1	2.55	0.41
1:B:142:PRO:HD3	1:C:136:ILE:O	2.20	0.41
1:B:344:LEU:HD21	1:B:403:PRO:HD3	2.02	0.41
1:E:118:GLU:HG2	1:E:171:VAL:HB	2.01	0.41
1:B:432:PHE:CD2	1:B:456:ASN:HA	2.56	0.41
1:A:431:ILE:HG12	1:A:442:TRP:CD1	2.55	0.41
1:C:468:PHE:O	1:C:478:ARG:HA	2.21	0.41
1:F:104:VAL:HA	1:F:198:ILE:HD11	2.01	0.41
1:C:293:ALA:HB2	1:C:458:PRO:HB3	2.02	0.41
1:F:310:ILE:HG22	1:F:314:ILE:HG13	2.02	0.41
1:A:293:ALA:HB2	1:A:458:PRO:CB	2.51	0.41
1:D:454:ASN:HB3	1:D:457:ILE:HD12	2.03	0.41
1:H:104:VAL:HA	1:H:198:ILE:HD11	2.03	0.41
1:B:118:GLU:HG2	1:B:171:VAL:HB	2.03	0.41
1:G:126:CYS:O	1:G:130:VAL:HG23	2.20	0.41
1:H:126:CYS:O	1:H:130:VAL:HG23	2.21	0.41
1:B:431:ILE:HG23	1:B:442:TRP:CE2	2.56	0.40
2:C:601:NAD:H8A	2:C:601:NAD:H2B	1.89	0.40
1:A:442:TRP:CH2	1:A:448:SER:HB2	2.56	0.40
1:C:4:LEU:CD1	1:C:21:GLU:HG3	2.52	0.40
1:E:182:ILE:HG13	1:E:183:CYS:N	2.36	0.40
1:H:165:ALA:CB	2:H:601:NAD:H52N	2.51	0.40
1:A:188:LEU:HD22	1:A:233:MET:HE3	2.04	0.40
1:B:248:THR:HA	1:B:269:LEU:HD13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:108:MET:HE3	1:E:167:ASN:HA	2.03	0.40
1:E:293:ALA:HB2	1:E:458:PRO:CB	2.50	0.40
2:F:602:NAD:H8A	2:F:602:NAD:H2B	1.89	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	496/513 (97%)	481 (97%)	14 (3%)	1 (0%)	43	37
1	B	496/513 (97%)	481 (97%)	14 (3%)	1 (0%)	43	37
1	C	496/513 (97%)	480 (97%)	15 (3%)	1 (0%)	43	37
1	D	496/513 (97%)	480 (97%)	15 (3%)	1 (0%)	43	37
1	E	498/513 (97%)	482 (97%)	15 (3%)	1 (0%)	43	37
1	F	496/513 (97%)	482 (97%)	13 (3%)	1 (0%)	43	37
1	G	495/513 (96%)	480 (97%)	14 (3%)	1 (0%)	43	37
1	H	497/513 (97%)	482 (97%)	14 (3%)	1 (0%)	43	37
All	All	3970/4104 (97%)	3848 (97%)	114 (3%)	8 (0%)	43	37

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	480	SER
1	E	480	SER
1	F	480	SER
1	G	480	SER
1	H	480	SER
1	B	480	SER
1	C	480	SER

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Mol	Chain	Res	Type
1	D	480	SER

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	387/411 (94%)	385 (100%)	2 (0%)	81	85
1	B	381/411 (93%)	376 (99%)	5 (1%)	61	63
1	C	374/411 (91%)	366 (98%)	8 (2%)	47	46
1	D	381/411 (93%)	377 (99%)	4 (1%)	68	72
1	E	391/411 (95%)	387 (99%)	4 (1%)	68	72
1	F	391/411 (95%)	384 (98%)	7 (2%)	51	51
1	G	392/411 (95%)	385 (98%)	7 (2%)	51	51
1	H	392/411 (95%)	390 (100%)	2 (0%)	81	85
All	All	3089/3288 (94%)	3050 (99%)	39 (1%)	61	63

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	94	ARG
1	A	297	THR
1	B	94	ARG
1	B	146	SER
1	B	291	LEU
1	B	295	VAL
1	B	401	PHE
1	C	24	GLU
1	C	94	ARG
1	C	291	LEU
1	C	297	THR
1	C	352	MET
1	C	400	THR
1	C	401	PHE

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Mol	Chain	Res	Type
1	C	430	SER
1	D	121	GLU
1	D	297	THR
1	D	352	MET
1	D	457	ILE
1	E	10	GLN
1	E	145	ARG
1	E	372	LYS
1	E	457	ILE
1	F	20	ARG
1	F	38	ILE
1	F	65	LYS
1	F	94	ARG
1	F	401	PHE
1	F	457	ILE
1	F	460	SER
1	G	6	ILE
1	G	94	ARG
1	G	145	ARG
1	G	297	THR
1	G	372	LYS
1	G	401	PHE
1	G	430	SER
1	H	297	THR
1	H	401	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	98	GLN
1	A	155	ASN
1	A	259	GLN
1	A	338	ASN
1	B	46	ASN
1	B	155	ASN
1	B	348	GLN
1	B	379	ASN
1	B	420	ASN
1	C	120	GLN
1	C	155	ASN
1	D	8	GLN
1	E	155	ASN

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Mol	Chain	Res	Type
1	E	338	ASN
1	F	46	ASN
1	F	88	GLN
1	F	120	GLN
1	F	155	ASN
1	F	213	ASN
1	F	379	ASN
1	G	8	GLN
1	G	46	ASN
1	G	120	GLN
1	G	155	ASN
1	G	213	ASN
1	G	348	GLN
1	G	379	ASN
1	H	46	ASN
1	H	88	GLN
1	H	213	ASN

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](#)

10 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	B	601	-	3,3,3	0.43	0	2,2,2	0.20	0
2	NAD	A	601	-	46,48,48	3.52	15 (32%)	64,73,73	1.59	9 (14%)
2	NAD	D	601	-	46,48,48	3.60	15 (32%)	64,73,73	1.55	11 (17%)
2	NAD	C	601	-	46,48,48	3.63	17 (36%)	64,73,73	1.59	11 (17%)
2	NAD	G	601	-	46,48,48	3.57	15 (32%)	64,73,73	1.62	11 (17%)
2	NAD	F	602	-	46,48,48	3.58	14 (30%)	64,73,73	1.69	11 (17%)
2	NAD	H	601	-	46,48,48	3.58	16 (34%)	64,73,73	1.55	12 (18%)
3	EDO	F	601	-	3,3,3	0.41	0	2,2,2	0.35	0
2	NAD	B	602	-	46,48,48	3.51	14 (30%)	64,73,73	1.64	13 (20%)
2	NAD	E	601	-	46,48,48	3.57	15 (32%)	64,73,73	1.56	11 (17%)

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
3	EDO	B	601	-	-	0/1/1/1	-
2	NAD	A	601	-	-	6/30/62/62	0/5/5/5
2	NAD	D	601	-	-	7/30/62/62	0/5/5/5
2	NAD	C	601	-	-	8/30/62/62	0/5/5/5
2	NAD	G	601	-	-	6/30/62/62	0/5/5/5
2	NAD	F	602	-	-	6/30/62/62	0/5/5/5
2	NAD	H	601	-	-	9/30/62/62	0/5/5/5
3	EDO	F	601	-	-	0/1/1/1	-
2	NAD	B	602	-	-	7/30/62/62	0/5/5/5
2	NAD	E	601	-	-	7/30/62/62	0/5/5/5

All (121) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	NAD	O4D-C1D	15.63	1.61	1.40
2	D	601	NAD	O4D-C1D	15.47	1.61	1.40
2	F	602	NAD	O4D-C1D	15.42	1.61	1.40
2	H	601	NAD	O4D-C1D	15.34	1.61	1.40
2	G	601	NAD	O4D-C1D	15.27	1.60	1.40
2	E	601	NAD	O4D-C1D	15.26	1.60	1.40
2	A	601	NAD	O4D-C1D	15.23	1.60	1.40
2	B	602	NAD	O4D-C1D	15.17	1.60	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	602	NAD	O4B-C1B	8.43	1.61	1.42
2	H	601	NAD	O4B-C1B	8.41	1.61	1.42
2	D	601	NAD	O4B-C1B	8.41	1.61	1.42
2	C	601	NAD	O4B-C1B	8.38	1.61	1.42
2	A	601	NAD	O4B-C1B	8.33	1.61	1.42
2	F	602	NAD	O4B-C1B	8.10	1.60	1.42
2	E	601	NAD	O4B-C1B	8.03	1.60	1.42
2	G	601	NAD	O4B-C1B	8.00	1.60	1.42
2	D	601	NAD	C2B-C1B	-7.89	1.28	1.53
2	H	601	NAD	C2B-C1B	-7.71	1.29	1.53
2	C	601	NAD	C2B-C1B	-7.66	1.29	1.53
2	G	601	NAD	C2B-C1B	-7.63	1.29	1.53
2	E	601	NAD	C2B-C1B	-7.54	1.29	1.53
2	B	602	NAD	C2B-C1B	-7.44	1.30	1.53
2	E	601	NAD	C7N-N7N	7.34	1.46	1.33
2	A	601	NAD	C2B-C1B	-7.32	1.30	1.53
2	F	602	NAD	C2B-C1B	-7.28	1.30	1.53
2	G	601	NAD	C7N-N7N	6.98	1.45	1.33
2	F	602	NAD	C7N-N7N	6.98	1.45	1.33
2	H	601	NAD	C7N-N7N	6.88	1.45	1.33
2	C	601	NAD	C7N-N7N	6.76	1.45	1.33
2	D	601	NAD	C7N-N7N	6.72	1.45	1.33
2	C	601	NAD	O4B-C4B	-6.66	1.30	1.45
2	A	601	NAD	C7N-N7N	6.63	1.45	1.33
2	B	602	NAD	C7N-N7N	6.52	1.45	1.33
2	D	601	NAD	O4B-C4B	-6.34	1.30	1.45
2	G	601	NAD	O4D-C4D	-6.28	1.31	1.45
2	B	602	NAD	O4D-C4D	-6.27	1.31	1.45
2	A	601	NAD	O4D-C4D	-6.26	1.31	1.45
2	H	601	NAD	O4B-C4B	-6.25	1.31	1.45
2	H	601	NAD	O4D-C4D	-6.23	1.31	1.45
2	D	601	NAD	O4D-C4D	-6.23	1.31	1.45
2	G	601	NAD	O4B-C4B	-6.23	1.31	1.45
2	E	601	NAD	O4D-C4D	-6.15	1.31	1.45
2	C	601	NAD	O4D-C4D	-6.14	1.31	1.45
2	E	601	NAD	O4B-C4B	-6.05	1.31	1.45
2	F	602	NAD	O4D-C4D	-6.02	1.31	1.45
2	B	602	NAD	O4B-C4B	-5.85	1.32	1.45
2	F	602	NAD	O4B-C4B	-5.83	1.32	1.45
2	A	601	NAD	O4B-C4B	-5.72	1.32	1.45
2	F	602	NAD	C6A-N6A	3.94	1.44	1.34
2	D	601	NAD	C6A-N6A	3.76	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	602	NAD	C6A-N6A	3.65	1.43	1.34
2	F	602	NAD	C2N-N1N	3.62	1.39	1.35
2	G	601	NAD	C6A-N6A	3.59	1.43	1.34
2	C	601	NAD	C6A-N6A	3.59	1.43	1.34
2	H	601	NAD	C6A-N6A	3.55	1.43	1.34
2	F	602	NAD	C3N-C7N	3.51	1.55	1.50
2	E	601	NAD	C6A-N6A	3.49	1.43	1.34
2	A	601	NAD	C6A-N6A	3.38	1.42	1.34
2	B	602	NAD	O2B-C2B	3.34	1.51	1.43
2	E	601	NAD	C3N-C7N	3.31	1.55	1.50
2	A	601	NAD	C3N-C7N	3.27	1.55	1.50
2	C	601	NAD	C3N-C7N	3.27	1.55	1.50
2	H	601	NAD	C3N-C7N	3.15	1.55	1.50
2	G	601	NAD	O2B-C2B	3.12	1.50	1.43
2	E	601	NAD	C2N-N1N	3.10	1.38	1.35
2	C	601	NAD	O2B-C2B	3.07	1.50	1.43
2	G	601	NAD	C3N-C7N	3.06	1.55	1.50
2	B	602	NAD	O3B-C3B	-3.06	1.35	1.43
2	F	602	NAD	O2B-C2B	3.05	1.50	1.43
2	C	601	NAD	O3D-C3D	-2.98	1.35	1.43
2	E	601	NAD	O2B-C2B	2.98	1.50	1.43
2	H	601	NAD	O2B-C2B	2.97	1.50	1.43
2	G	601	NAD	C2N-N1N	2.97	1.38	1.35
2	G	601	NAD	O3D-C3D	-2.97	1.35	1.43
2	A	601	NAD	O3D-C3D	-2.94	1.35	1.43
2	B	602	NAD	O3D-C3D	-2.93	1.35	1.43
2	A	601	NAD	O3B-C3B	-2.89	1.35	1.43
2	F	602	NAD	O3D-C3D	-2.86	1.35	1.43
2	D	601	NAD	C2N-N1N	2.86	1.38	1.35
2	H	601	NAD	C2N-N1N	2.85	1.38	1.35
2	D	601	NAD	O3D-C3D	-2.85	1.35	1.43
2	E	601	NAD	O3D-C3D	-2.84	1.35	1.43
2	D	601	NAD	O2B-C2B	2.82	1.49	1.43
2	F	602	NAD	O3B-C3B	-2.81	1.36	1.43
2	D	601	NAD	C3N-C7N	2.79	1.54	1.50
2	A	601	NAD	O2B-C2B	2.74	1.49	1.43
2	C	601	NAD	C2N-N1N	2.73	1.38	1.35
2	A	601	NAD	C2N-N1N	2.69	1.37	1.35
2	G	601	NAD	O3B-C3B	-2.64	1.36	1.43
2	H	601	NAD	O3D-C3D	-2.57	1.36	1.43
2	B	602	NAD	C2N-N1N	2.56	1.37	1.35
2	E	601	NAD	O3B-C3B	-2.52	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	601	NAD	O3B-C3B	-2.52	1.36	1.43
2	H	601	NAD	O3B-C3B	-2.52	1.36	1.43
2	B	602	NAD	C3N-C7N	2.51	1.54	1.50
2	F	602	NAD	O2D-C2D	2.45	1.49	1.43
2	D	601	NAD	O2D-C2D	2.40	1.48	1.43
2	C	601	NAD	O2D-C2D	2.40	1.48	1.43
2	B	602	NAD	O2D-C2D	2.36	1.48	1.43
2	C	601	NAD	C2A-N1A	2.32	1.38	1.33
2	B	602	NAD	C8A-N7A	2.32	1.36	1.31
2	E	601	NAD	C8A-N7A	2.31	1.36	1.31
2	C	601	NAD	O3B-C3B	-2.31	1.37	1.43
2	G	601	NAD	C8A-N7A	2.30	1.36	1.31
2	A	601	NAD	C8A-N7A	2.29	1.36	1.31
2	D	601	NAD	C8A-N7A	2.27	1.36	1.31
2	A	601	NAD	O2D-C2D	2.24	1.48	1.43
2	E	601	NAD	O2D-C2D	2.20	1.48	1.43
2	G	601	NAD	O2D-C2D	2.20	1.48	1.43
2	C	601	NAD	C8A-N7A	2.16	1.35	1.31
2	H	601	NAD	C8A-N7A	2.16	1.35	1.31
2	H	601	NAD	PA-O3	2.15	1.61	1.59
2	D	601	NAD	C5A-C4A	-2.15	1.35	1.39
2	G	601	NAD	C5A-C4A	-2.14	1.35	1.39
2	H	601	NAD	O2D-C2D	2.14	1.48	1.43
2	F	602	NAD	C5A-C4A	-2.13	1.35	1.39
2	E	601	NAD	C5A-C4A	-2.12	1.35	1.39
2	C	601	NAD	C2A-N3A	2.12	1.37	1.33
2	A	601	NAD	C2A-N1A	2.06	1.37	1.33
2	C	601	NAD	PN-O3	2.05	1.61	1.59
2	H	601	NAD	PN-O3	2.03	1.61	1.59

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	601	NAD	N3A-C2A-N1A	-5.43	120.36	128.58
2	B	602	NAD	C5A-C4A-N3A	-5.38	119.31	126.72
2	F	602	NAD	N3A-C2A-N1A	-5.36	120.47	128.58
2	H	601	NAD	C5A-C4A-N3A	-5.18	119.59	126.72
2	G	601	NAD	C5A-C4A-N3A	-5.15	119.62	126.72
2	C	601	NAD	N3A-C2A-N1A	-5.04	120.95	128.58
2	C	601	NAD	C5A-C4A-N3A	-5.01	119.81	126.72
2	E	601	NAD	N3A-C2A-N1A	-4.95	121.09	128.58
2	F	602	NAD	C5A-C4A-N3A	-4.95	119.91	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	601	NAD	N3A-C2A-N1A	-4.93	121.12	128.58
2	D	601	NAD	N9A-C8A-N7A	-4.88	107.02	113.94
2	A	601	NAD	N3A-C2A-N1A	-4.86	121.22	128.58
2	G	601	NAD	N9A-C8A-N7A	-4.85	107.05	113.94
2	A	601	NAD	C5A-C4A-N3A	-4.80	120.11	126.72
2	H	601	NAD	N3A-C2A-N1A	-4.68	121.50	128.58
2	E	601	NAD	C5A-C4A-N3A	-4.63	120.34	126.72
2	A	601	NAD	N9A-C8A-N7A	-4.61	107.40	113.94
2	C	601	NAD	N9A-C8A-N7A	-4.56	107.47	113.94
2	F	602	NAD	N9A-C8A-N7A	-4.52	107.53	113.94
2	E	601	NAD	N9A-C8A-N7A	-4.51	107.53	113.94
2	D	601	NAD	C5A-C4A-N3A	-4.46	120.58	126.72
2	B	602	NAD	N3A-C2A-N1A	-4.37	121.96	128.58
2	B	602	NAD	N9A-C8A-N7A	-4.31	107.81	113.94
2	H	601	NAD	N9A-C8A-N7A	-4.29	107.85	113.94
2	F	602	NAD	C4D-O4D-C1D	-3.92	106.34	109.92
2	F	602	NAD	C3N-C7N-N7N	3.88	122.51	117.74
2	B	602	NAD	C4D-O4D-C1D	-3.59	106.64	109.92
2	A	601	NAD	C3N-C7N-N7N	3.51	122.07	117.74
2	G	601	NAD	C5A-N7A-C8A	3.37	108.75	103.45
2	G	601	NAD	C2A-N3A-C4A	3.35	120.02	111.83
2	A	601	NAD	N3A-C4A-N9A	3.32	132.82	127.17
2	C	601	NAD	N3A-C4A-N9A	3.31	132.79	127.17
2	F	602	NAD	N3A-C4A-N9A	3.26	132.71	127.17
2	B	602	NAD	C5A-N7A-C8A	3.25	108.56	103.45
2	F	602	NAD	C2A-N3A-C4A	3.24	119.74	111.83
2	D	601	NAD	C5A-N7A-C8A	3.19	108.47	103.45
2	G	601	NAD	N3A-C4A-N9A	3.17	132.56	127.17
2	C	601	NAD	C5A-N7A-C8A	3.15	108.41	103.45
2	B	602	NAD	C2A-N3A-C4A	3.15	119.51	111.83
2	H	601	NAD	C2A-N3A-C4A	3.12	119.44	111.83
2	C	601	NAD	C2A-N3A-C4A	3.11	119.43	111.83
2	F	602	NAD	C5A-N7A-C8A	3.08	108.29	103.45
2	D	601	NAD	C4A-N9A-C8A	3.06	108.95	105.74
2	B	602	NAD	N3A-C4A-N9A	3.06	132.36	127.17
2	H	601	NAD	N3A-C4A-N9A	3.03	132.32	127.17
2	A	601	NAD	C5A-N7A-C8A	3.03	108.21	103.45
2	E	601	NAD	C5A-N7A-C8A	2.99	108.15	103.45
2	B	602	NAD	C2N-C3N-C4N	2.97	121.72	118.26
2	E	601	NAD	C2A-N3A-C4A	2.97	119.09	111.83
2	H	601	NAD	C5A-N7A-C8A	2.97	108.12	103.45
2	B	602	NAD	C4A-C5A-N7A	-2.95	107.21	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	NAD	C4A-N9A-C8A	2.94	108.82	105.74
2	C	601	NAD	C4A-N9A-C8A	2.93	108.82	105.74
2	D	601	NAD	C2A-N3A-C4A	2.90	118.92	111.83
2	F	602	NAD	C4A-N9A-C8A	2.86	108.74	105.74
2	E	601	NAD	N3A-C4A-N9A	2.86	132.03	127.17
2	A	601	NAD	C2A-N3A-C4A	2.84	118.77	111.83
2	G	601	NAD	C4A-N9A-C8A	2.83	108.71	105.74
2	D	601	NAD	N3A-C4A-N9A	2.68	131.72	127.17
2	E	601	NAD	C4A-N9A-C8A	2.59	108.45	105.74
2	G	601	NAD	C4A-C5A-N7A	-2.54	107.67	110.58
2	B	602	NAD	N6A-C6A-N1A	-2.49	112.84	118.38
2	H	601	NAD	C4A-C5A-N7A	-2.47	107.76	110.58
2	D	601	NAD	C3N-C7N-N7N	2.41	120.70	117.74
2	C	601	NAD	C3N-C7N-N7N	2.40	120.70	117.74
2	D	601	NAD	C4A-C5A-N7A	-2.37	107.87	110.58
2	G	601	NAD	C6A-C5A-C4A	2.36	120.39	117.18
2	C	601	NAD	C4A-C5A-N7A	-2.34	107.91	110.58
2	H	601	NAD	C4A-N9A-C8A	2.33	108.19	105.74
2	B	602	NAD	C5A-C4A-N9A	2.31	108.33	105.81
2	G	601	NAD	C2N-C3N-C4N	2.30	120.94	118.26
2	D	601	NAD	C2N-C3N-C4N	2.27	120.90	118.26
2	A	601	NAD	C6A-C5A-C4A	2.25	120.26	117.18
2	H	601	NAD	C6A-C5A-C4A	2.25	120.25	117.18
2	F	602	NAD	C6A-C5A-C4A	2.24	120.24	117.18
2	B	602	NAD	C4A-N9A-C8A	2.24	108.09	105.74
2	B	602	NAD	C6A-C5A-C4A	2.24	120.23	117.18
2	E	601	NAD	C4D-O4D-C1D	-2.22	107.89	109.92
2	F	602	NAD	C4A-C5A-N7A	-2.20	108.06	110.58
2	C	601	NAD	C6A-C5A-C4A	2.20	120.18	117.18
2	G	601	NAD	C3N-C7N-N7N	2.17	120.41	117.74
2	E	601	NAD	C6A-C5A-C4A	2.15	120.11	117.18
2	E	601	NAD	C3N-C7N-N7N	2.14	120.38	117.74
2	H	601	NAD	C2N-C3N-C4N	2.12	120.72	118.26
2	H	601	NAD	C5A-C4A-N9A	2.09	108.08	105.81
2	D	601	NAD	C6A-C5A-C4A	2.08	120.02	117.18
2	H	601	NAD	N6A-C6A-N1A	-2.05	113.81	118.38
2	E	601	NAD	C4A-C5A-N7A	-2.05	108.24	110.58
2	C	601	NAD	C2N-C3N-C4N	2.03	120.62	118.26

There are no chirality outliers.

All (56) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	601	NAD	O4D-C1D-N1N-C6N
2	A	601	NAD	O4D-C4D-C5D-O5D
2	C	601	NAD	O4D-C4D-C5D-O5D
2	D	601	NAD	O4D-C4D-C5D-O5D
2	E	601	NAD	O4D-C4D-C5D-O5D
2	E	601	NAD	C3D-C4D-C5D-O5D
2	F	602	NAD	O4D-C4D-C5D-O5D
2	G	601	NAD	O4D-C4D-C5D-O5D
2	A	601	NAD	C3D-C4D-C5D-O5D
2	B	602	NAD	C3D-C4D-C5D-O5D
2	G	601	NAD	C3D-C4D-C5D-O5D
2	H	601	NAD	C3D-C4D-C5D-O5D
2	B	602	NAD	O4D-C4D-C5D-O5D
2	C	601	NAD	C3D-C4D-C5D-O5D
2	D	601	NAD	C3D-C4D-C5D-O5D
2	F	602	NAD	C3D-C4D-C5D-O5D
2	H	601	NAD	O4D-C4D-C5D-O5D
2	F	602	NAD	C2B-C1B-N9A-C8A
2	A	601	NAD	C4D-C5D-O5D-PN
2	G	601	NAD	C2B-C1B-N9A-C8A
2	G	601	NAD	C4D-C5D-O5D-PN
2	H	601	NAD	C4D-C5D-O5D-PN
2	A	601	NAD	C2B-C1B-N9A-C8A
2	C	601	NAD	C2B-C1B-N9A-C8A
2	E	601	NAD	C2B-C1B-N9A-C8A
2	B	602	NAD	C2B-C1B-N9A-C8A
2	D	601	NAD	C2B-C1B-N9A-C8A
2	H	601	NAD	C2B-C1B-N9A-C8A
2	B	602	NAD	C5B-O5B-PA-O1A
2	D	601	NAD	C5B-O5B-PA-O1A
2	E	601	NAD	C5B-O5B-PA-O1A
2	H	601	NAD	C5B-O5B-PA-O1A
2	C	601	NAD	C4D-C5D-O5D-PN
2	D	601	NAD	C4D-C5D-O5D-PN
2	E	601	NAD	C4D-C5D-O5D-PN
2	F	602	NAD	C4D-C5D-O5D-PN
2	B	602	NAD	C4D-C5D-O5D-PN
2	A	601	NAD	C2B-C1B-N9A-C4A
2	C	601	NAD	C2B-C1B-N9A-C4A
2	E	601	NAD	C2B-C1B-N9A-C4A
2	F	602	NAD	C2B-C1B-N9A-C4A
2	G	601	NAD	C2B-C1B-N9A-C4A
2	H	601	NAD	C2B-C1B-N9A-C4A

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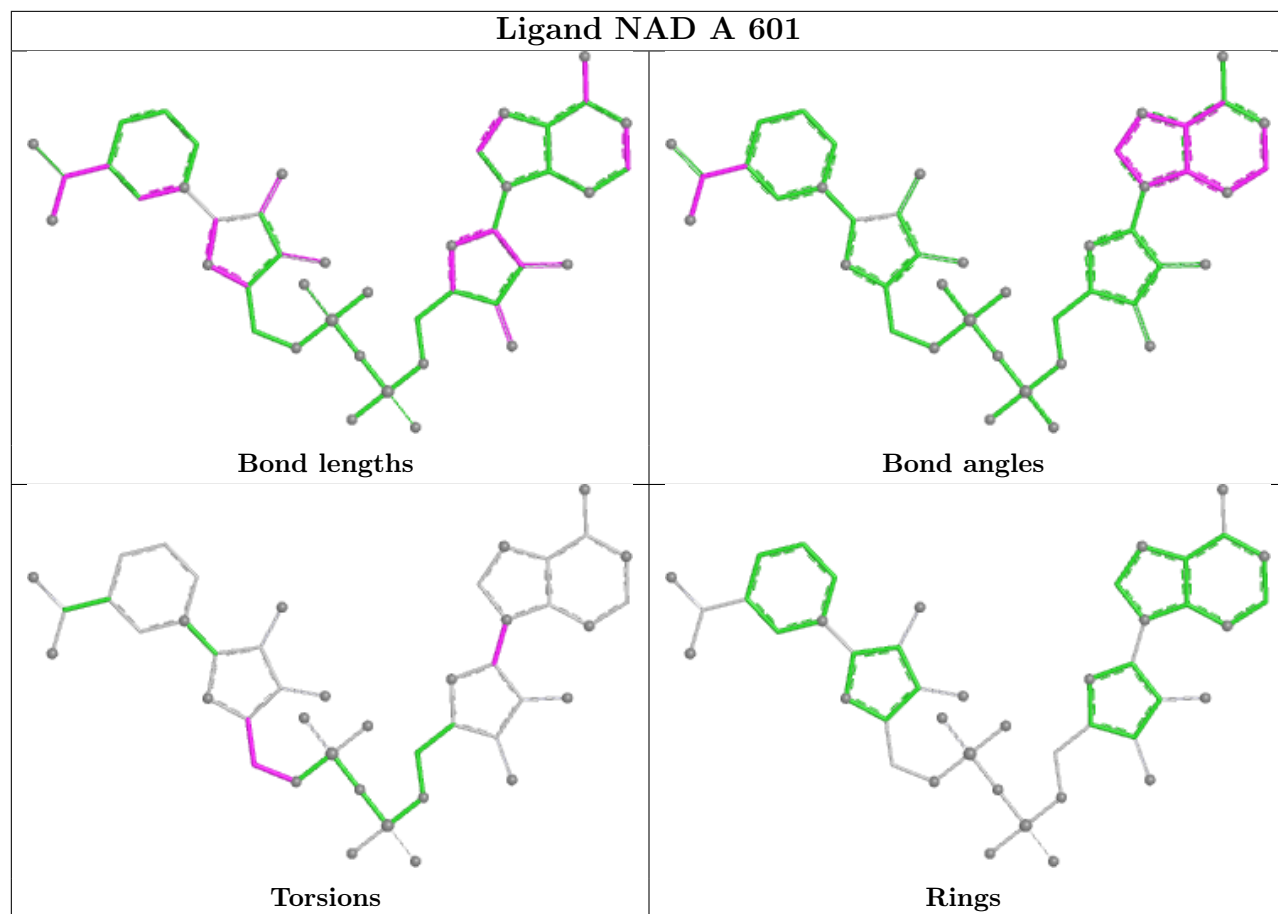
Mol	Chain	Res	Type	Atoms
2	D	601	NAD	C2B-C1B-N9A-C4A
2	C	601	NAD	O4D-C1D-N1N-C2N
2	C	601	NAD	O4D-C1D-N1N-C6N
2	H	601	NAD	O4D-C1D-N1N-C2N
2	A	601	NAD	O4B-C1B-N9A-C8A
2	E	601	NAD	O4B-C1B-N9A-C8A
2	G	601	NAD	O4B-C1B-N9A-C8A
2	B	602	NAD	C2B-C1B-N9A-C4A
2	B	602	NAD	O4B-C1B-N9A-C8A
2	C	601	NAD	O4B-C1B-N9A-C8A
2	D	601	NAD	O4B-C1B-N9A-C8A
2	F	602	NAD	O4B-C1B-N9A-C8A
2	H	601	NAD	O4B-C1B-N9A-C8A

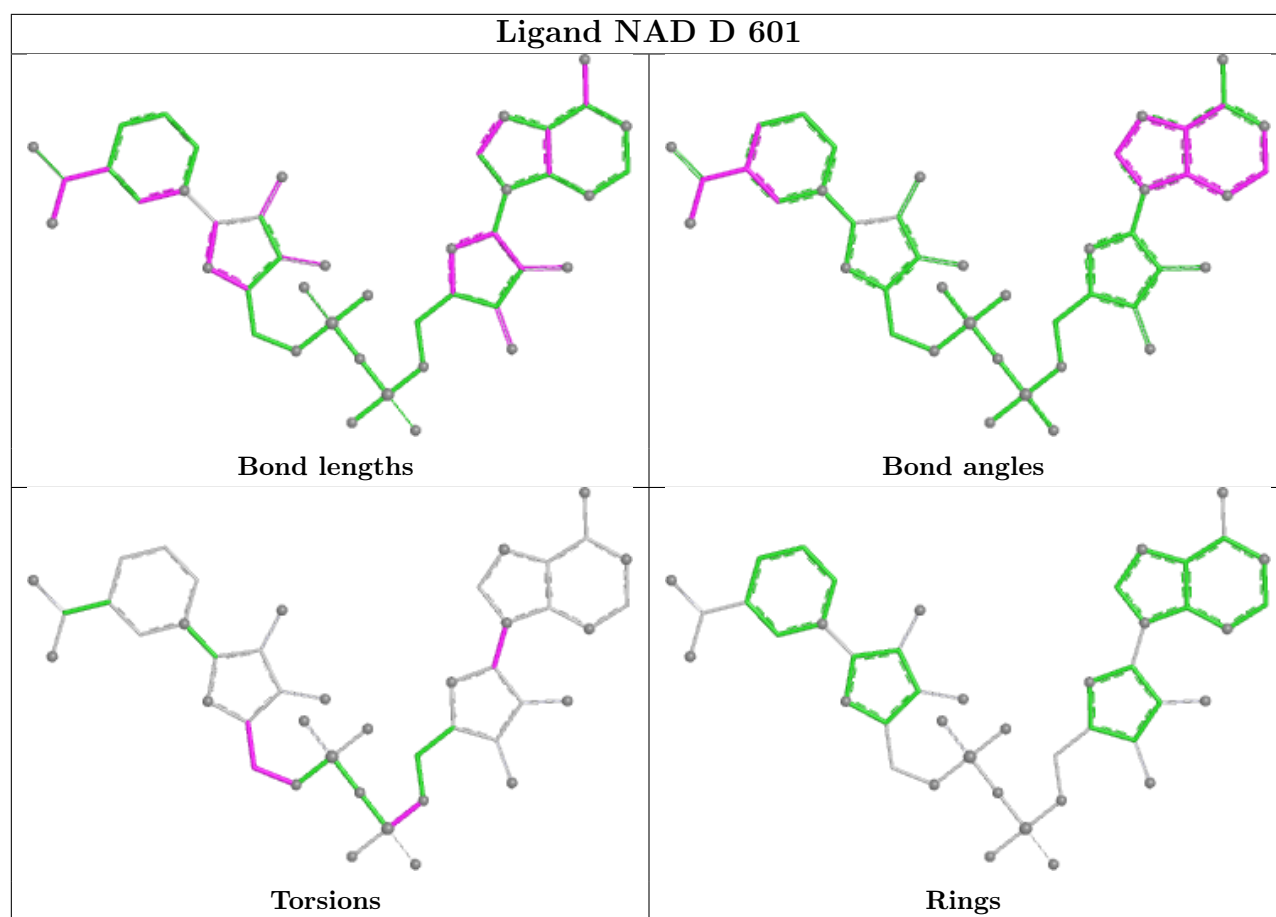
There are no ring outliers.

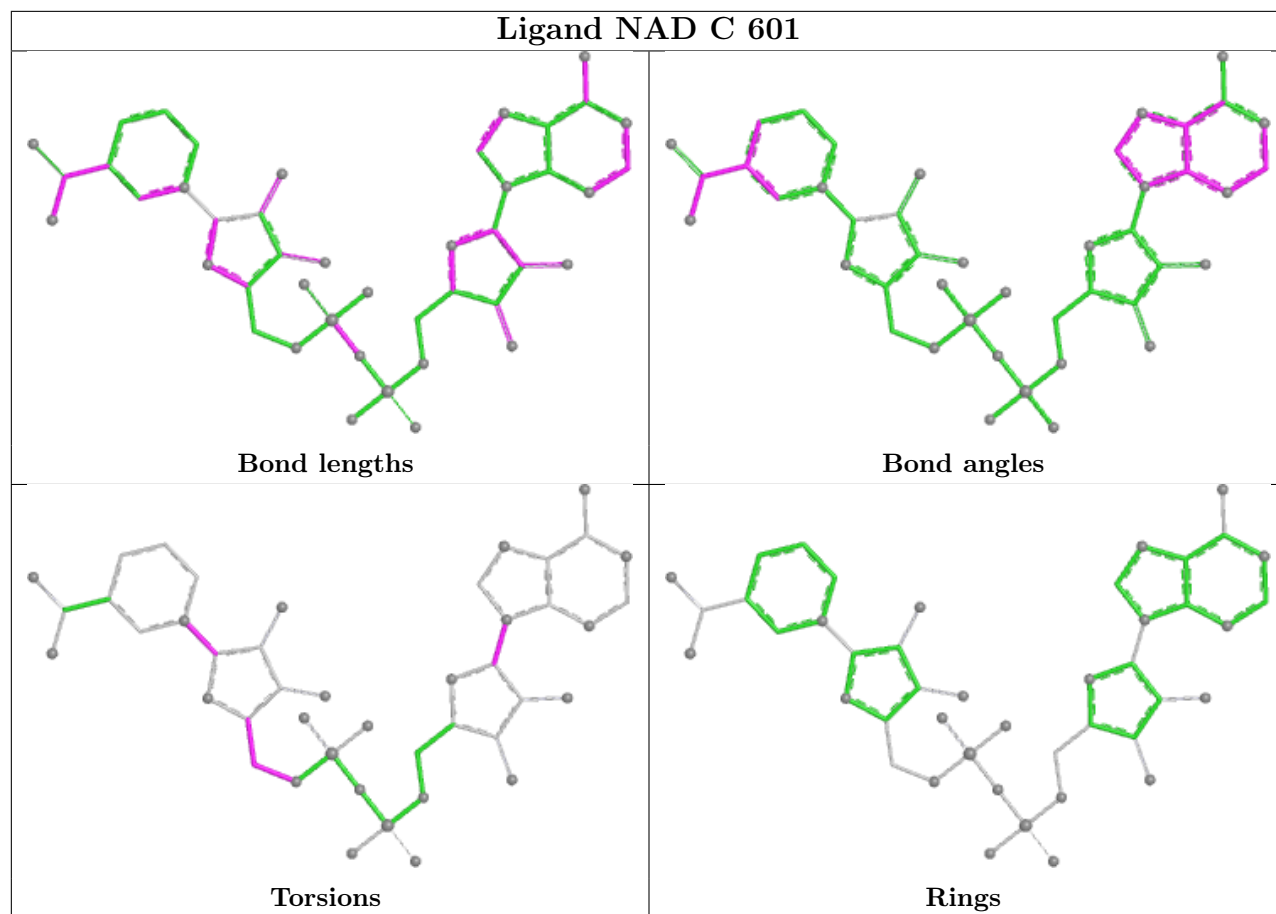
6 monomers are involved in 10 short contacts:

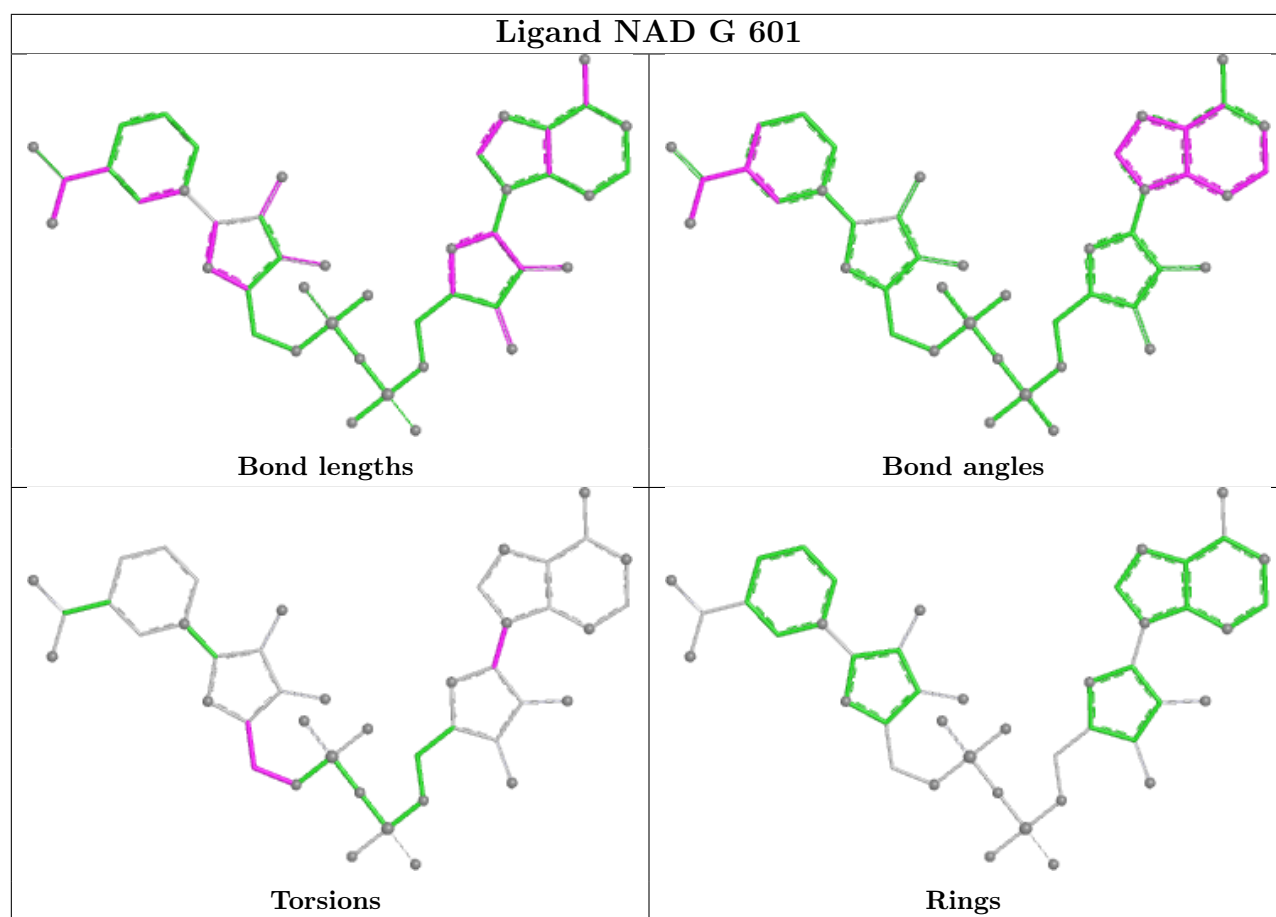
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	NAD	2	0
2	D	601	NAD	1	0
2	C	601	NAD	2	0
2	G	601	NAD	1	0
2	F	602	NAD	2	0
2	H	601	NAD	2	0

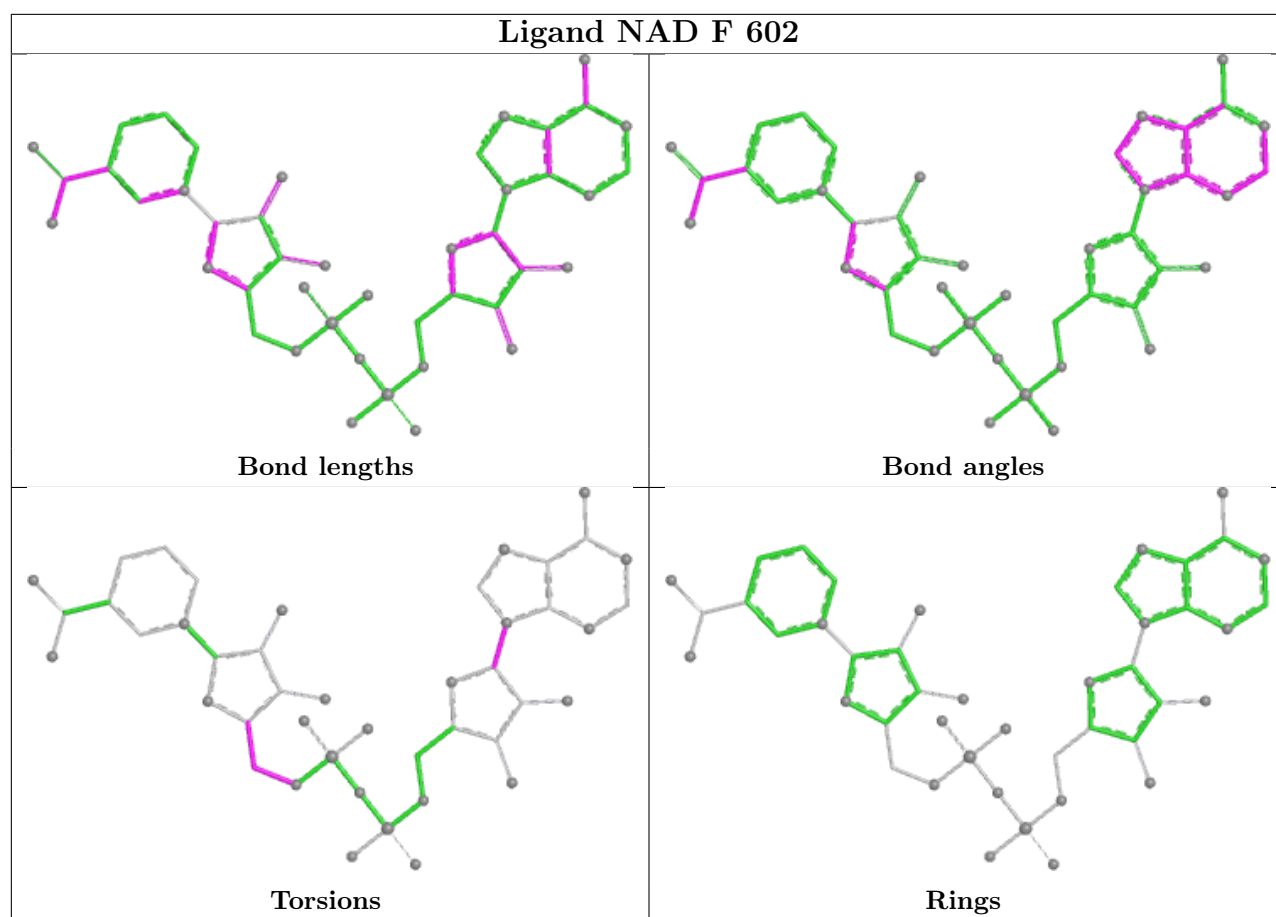
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

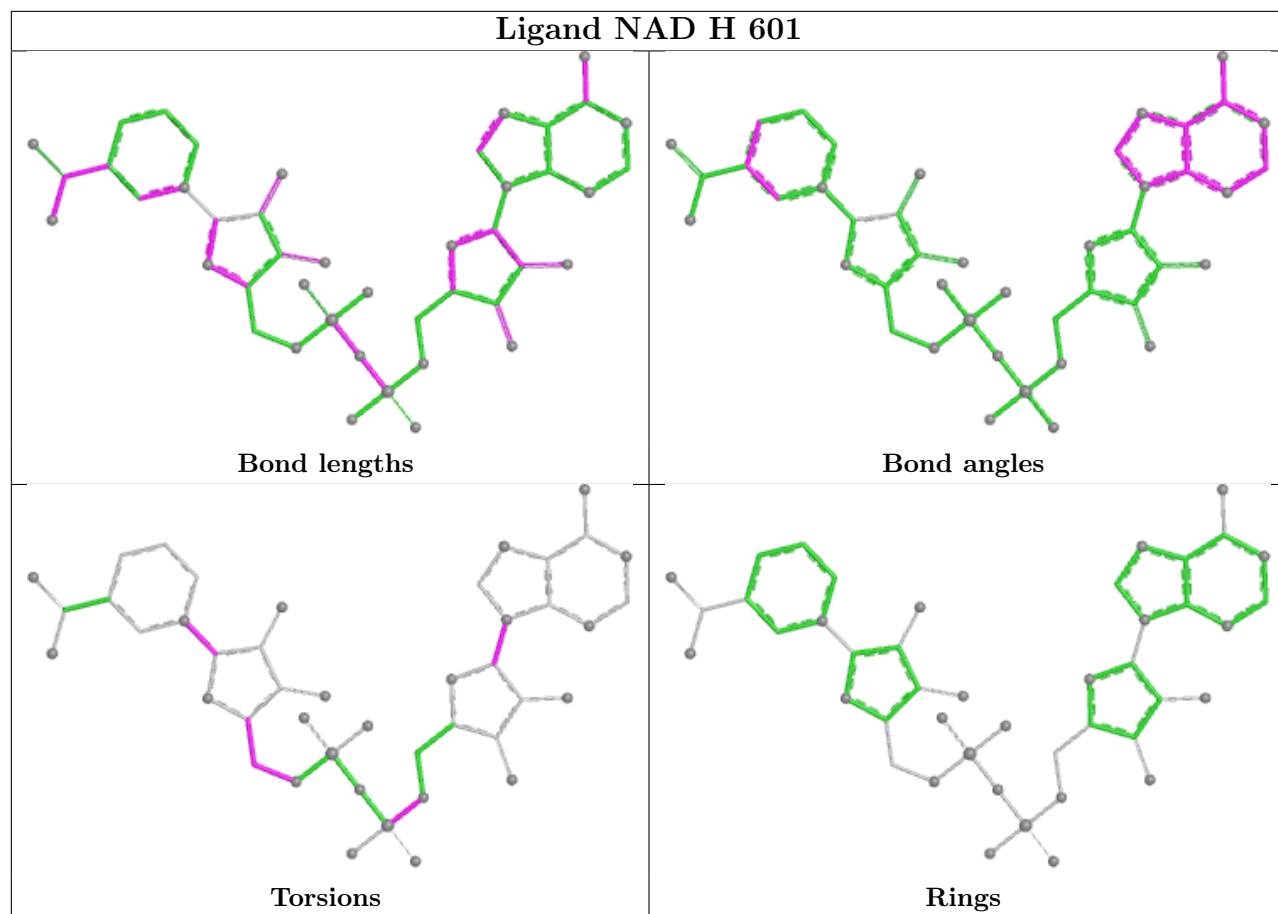


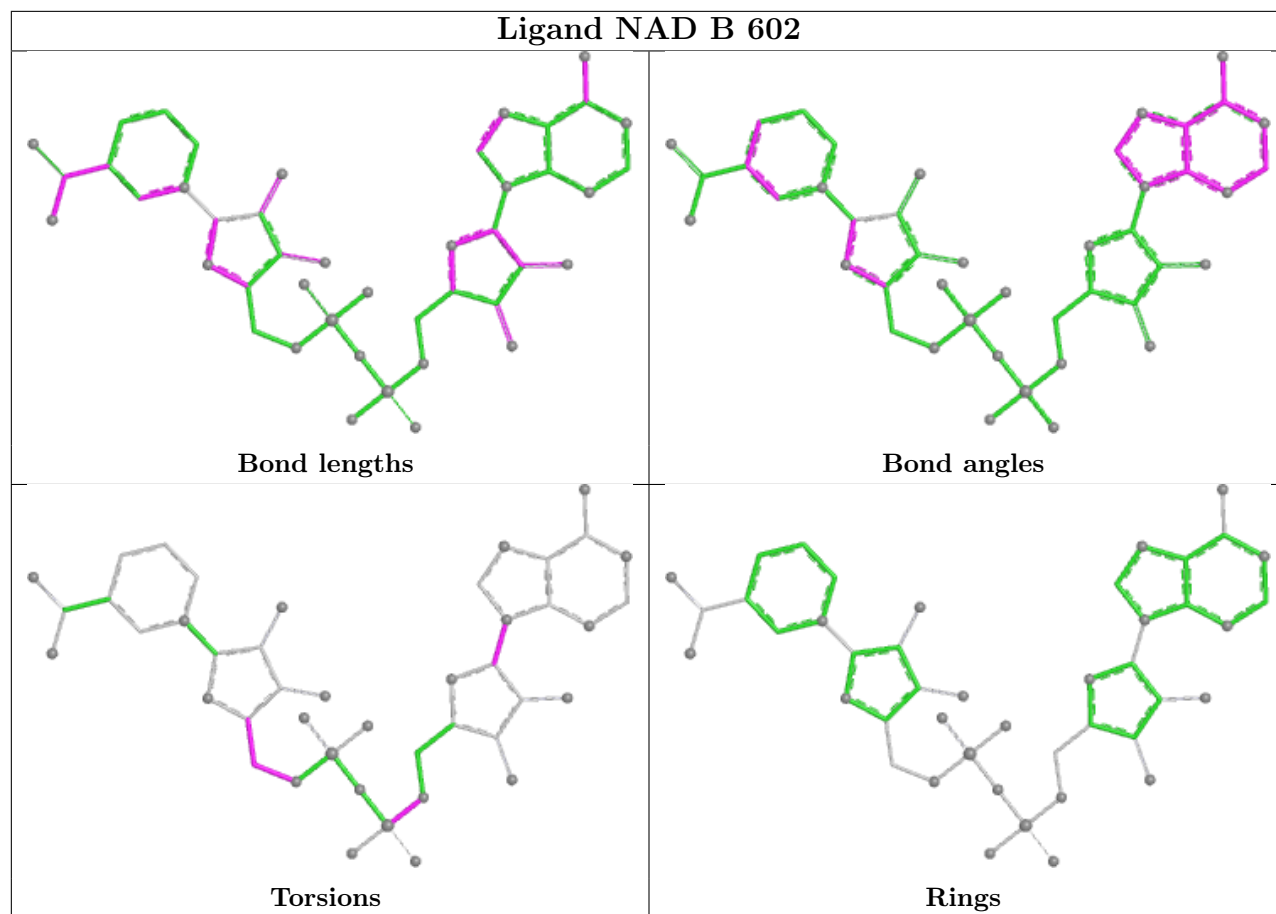


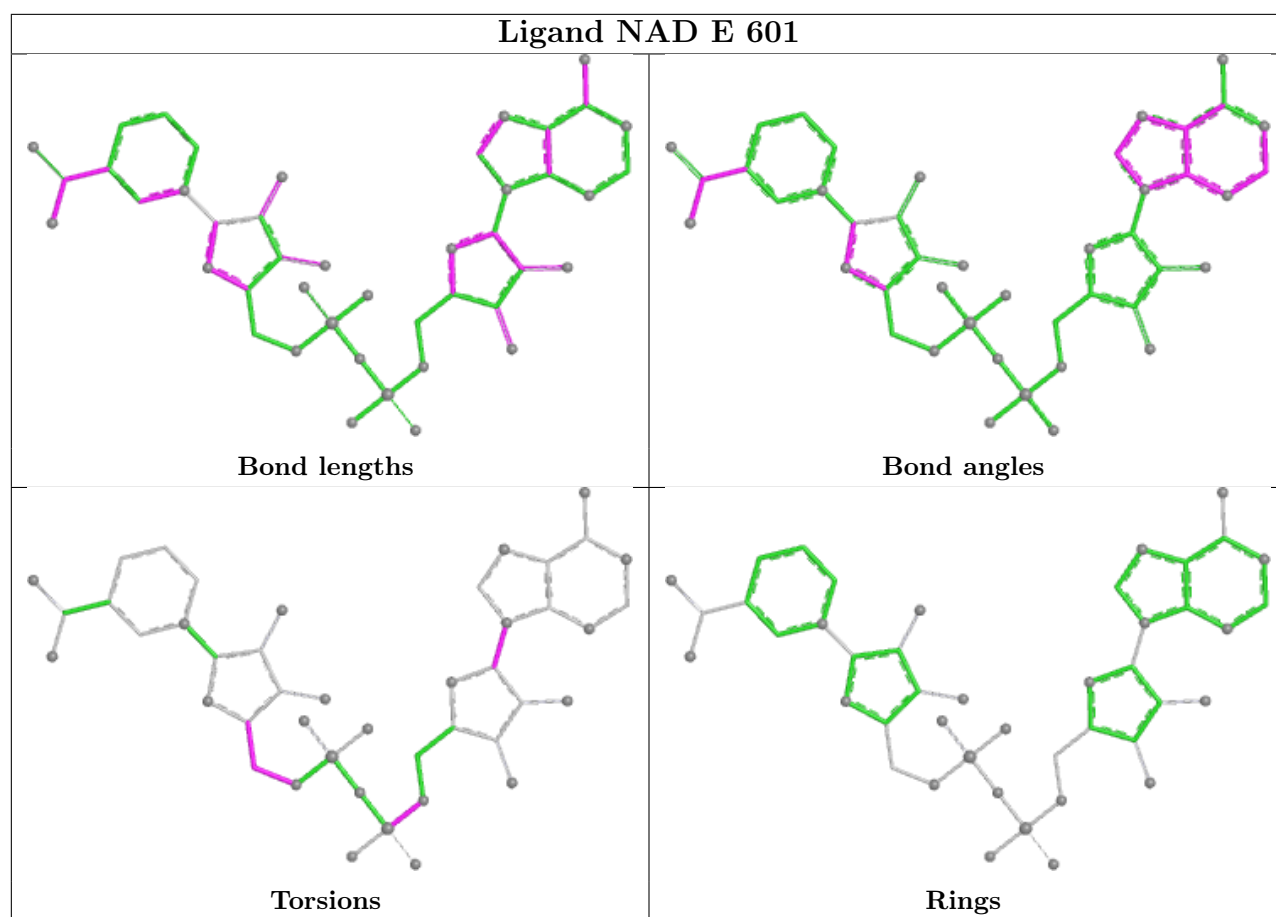












5.7 Other polymers [i](#)

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	497/513 (96%)	-0.56	0 100 100	15, 24, 38, 52	1 (0%)
1	B	497/513 (96%)	-0.45	4 (0%) 82 84	16, 26, 42, 63	1 (0%)
1	C	497/513 (96%)	-0.28	5 (1%) 79 81	16, 29, 56, 67	1 (0%)
1	D	497/513 (96%)	-0.34	2 (0%) 88 90	17, 29, 48, 64	1 (0%)
1	E	498/513 (97%)	-0.57	0 100 100	11, 24, 38, 54	2 (0%)
1	F	497/513 (96%)	-0.45	2 (0%) 88 90	17, 25, 42, 72	1 (0%)
1	G	497/513 (96%)	-0.47	2 (0%) 88 90	18, 26, 40, 58	0
1	H	497/513 (96%)	-0.51	1 (0%) 91 93	10, 26, 42, 63	2 (0%)
All	All	3977/4104 (96%)	-0.45	16 (0%) 88 90	10, 26, 44, 72	9 (0%)

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	337	PRO	3.0
1	B	462	ALA	2.8
1	B	398	THR	2.8
1	D	461	GLY	2.7
1	F	461	GLY	2.6
1	C	330	ARG	2.6
1	D	3	THR	2.5
1	C	337	PRO	2.4
1	C	338	ASN	2.4
1	G	461	GLY	2.2
1	H	461	GLY	2.2
1	C	461	GLY	2.1
1	C	331	VAL	2.1
1	F	292	PHE	2.1
1	B	329	ILE	2.0
1	B	3	THR	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 oligosaccharides in this entry.

6.4 Ligands ⓘ

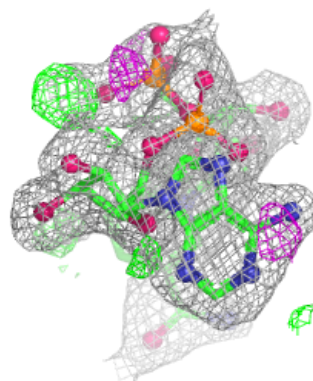
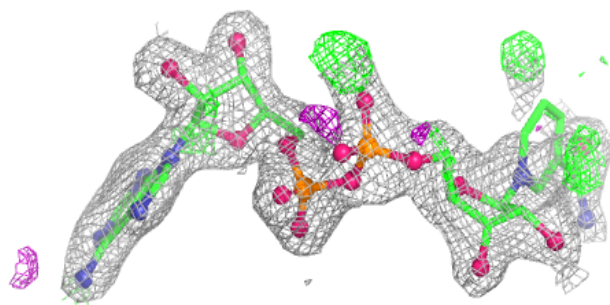
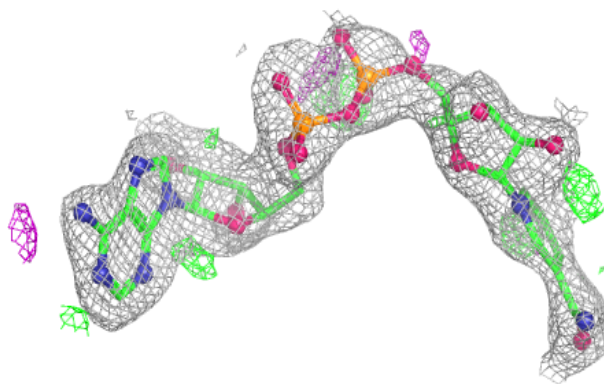
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAD	G	601	44/44	0.89	0.12	20,32,56,58	44
2	NAD	E	601	44/44	0.90	0.10	18,27,43,48	44
2	NAD	C	601	44/44	0.90	0.12	15,33,54,56	44
2	NAD	D	601	44/44	0.92	0.10	17,33,46,49	44
2	NAD	B	602	44/44	0.92	0.11	15,33,51,52	44
2	NAD	F	602	44/44	0.92	0.10	15,33,46,52	44
2	NAD	A	601	44/44	0.92	0.11	15,28,47,49	44
2	NAD	H	601	44/44	0.92	0.10	20,32,46,49	44
3	EDO	F	601	4/4	0.94	0.09	27,32,33,37	0
3	EDO	B	601	4/4	0.95	0.09	27,33,35,35	0

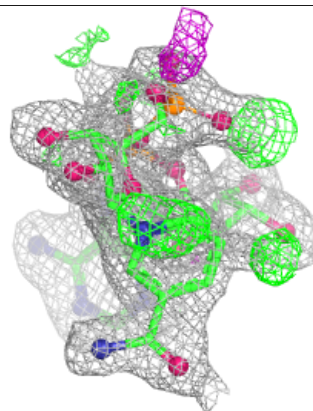
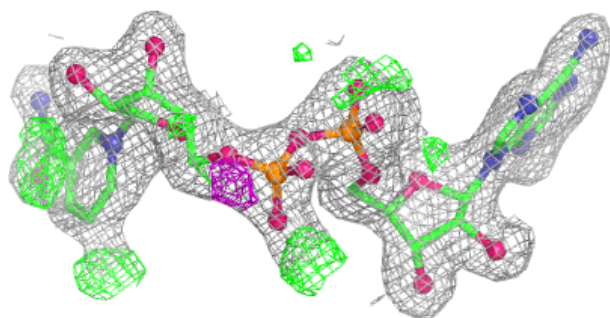
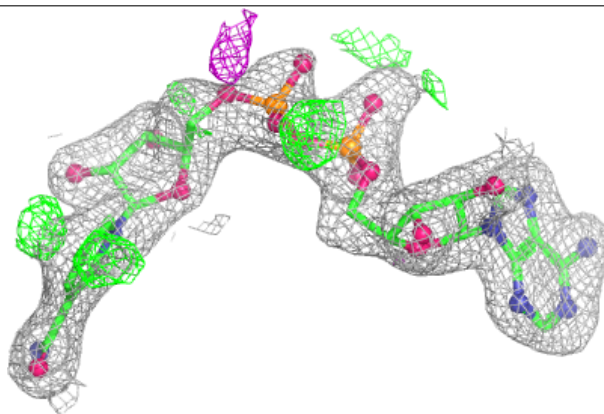
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAD G 601:

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

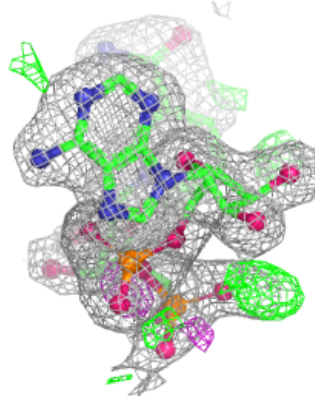
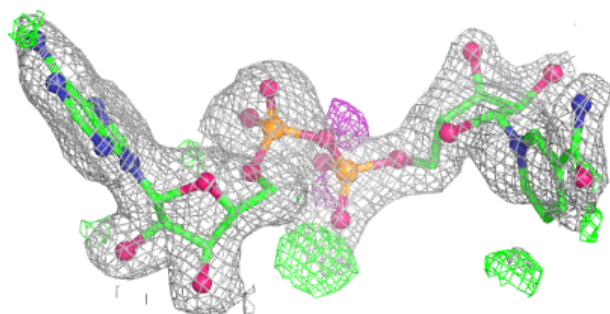
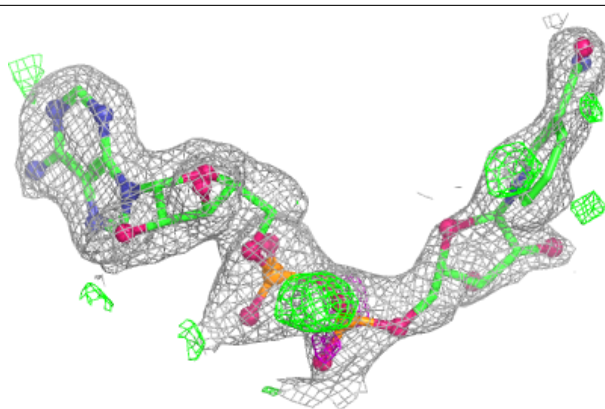
**Electron density around NAD E 601:**

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

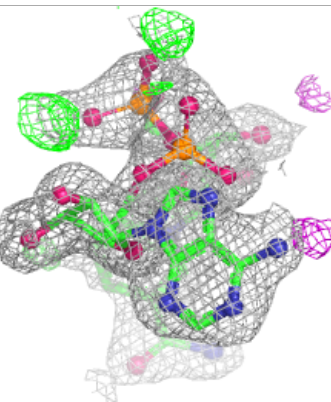
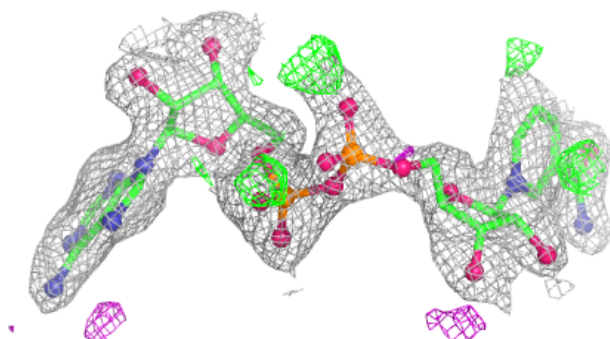
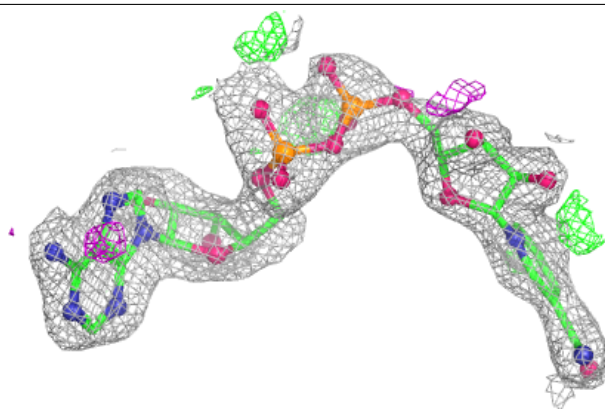


Electron density around NAD C 601:

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

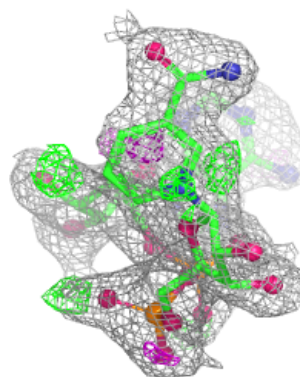
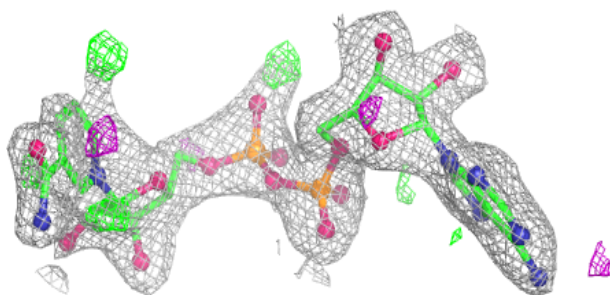
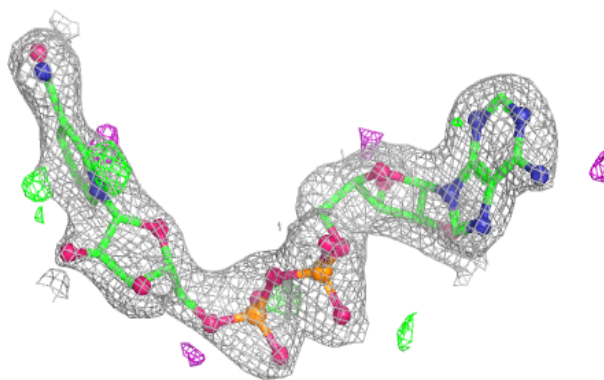
**Electron density around NAD D 601:**

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

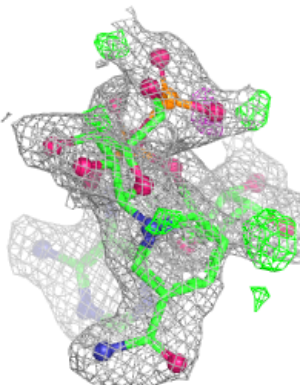
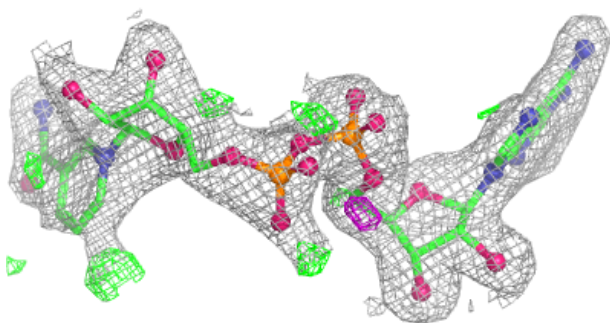
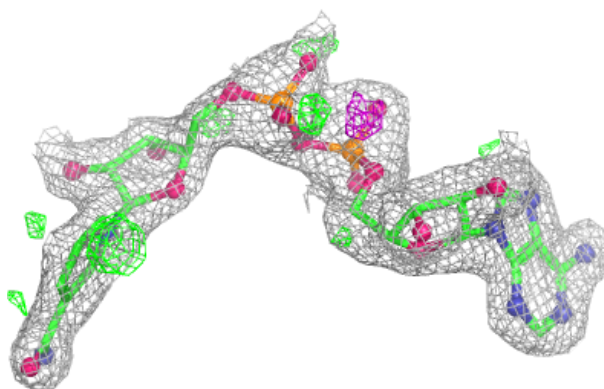


Electron density around NAD B 602:

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

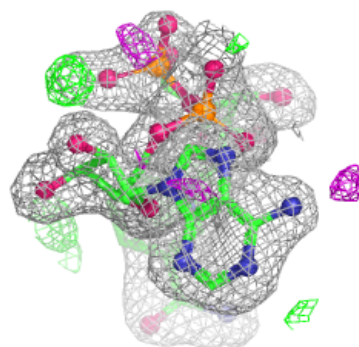
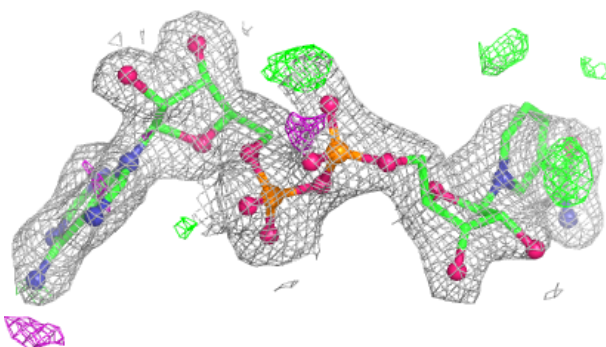
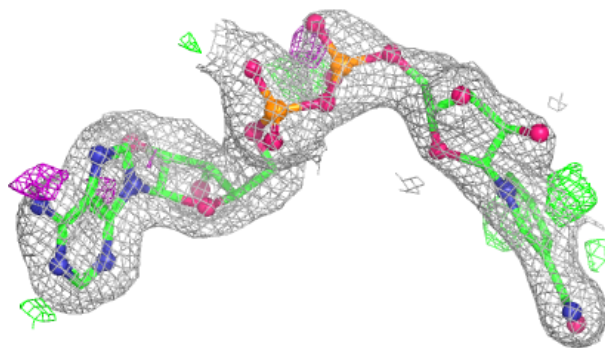
**Electron density around NAD F 602:**

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

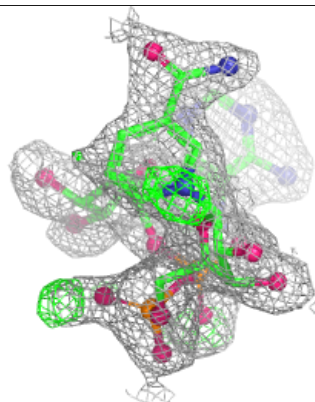
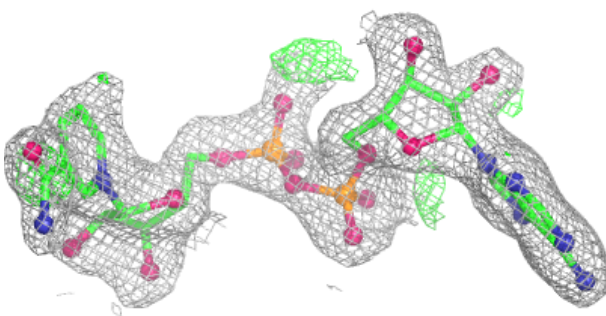
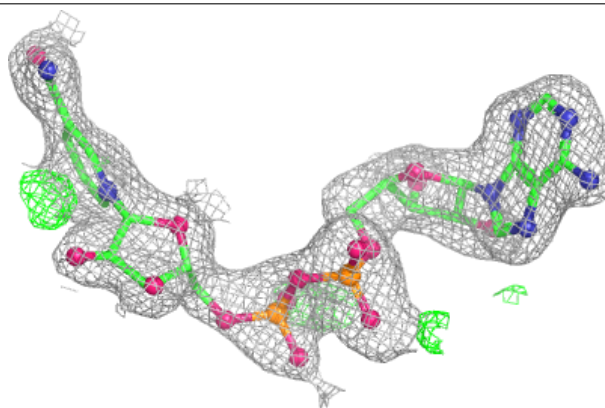


Electron density around NAD A 601:

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

**Electron density around NAD H 601:**

$2mF_o-DF_c$ (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.