



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 03:23 PM UTC

PDB ID : 4ZUK / pdb_00004zuk
Title : Structure ALDH7A1 complexed with NAD+
Authors : Luo, M.; Tanner, J.J.
Deposited on : 2015-05-16
Resolution : 2.00 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

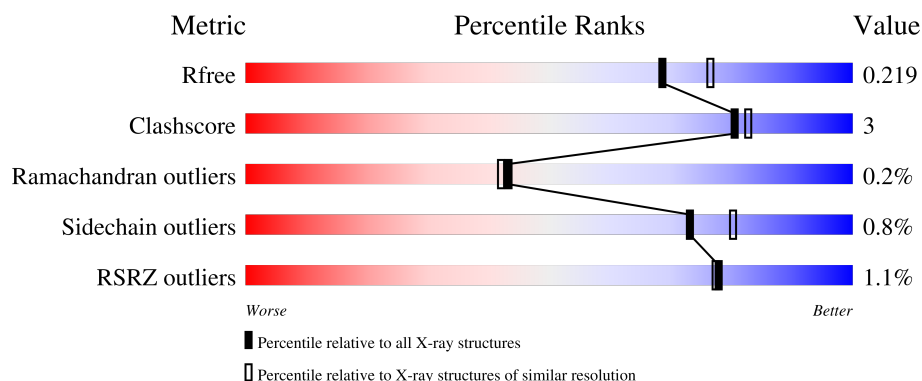
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	% 93% 6% .
1	B	513	2% 91% 8% .
1	C	513	% 92% 7% .
1	D	513	% 94% 6% .
1	E	513	% 94% 6% .

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Mol	Chain	Length	Quality of chain
1	F	513	2% 92% 8%
1	G	513	% 90% 7%
1	H	513	% 92% 7%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 32089 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	509	Total	C	N	O	S	0	0	0
			3811	2423	661	710	17			
1	B	509	Total	C	N	O	S	0	0	0
			3818	2429	660	712	17			
1	C	509	Total	C	N	O	S	0	0	0
			3809	2422	659	711	17			
1	D	509	Total	C	N	O	S	0	0	0
			3788	2410	656	705	17			
1	E	509	Total	C	N	O	S	0	2	0
			3826	2434	662	712	18			
1	F	509	Total	C	N	O	S	0	0	0
			3819	2424	663	715	17			
1	G	499	Total	C	N	O	S	0	0	0
			3745	2377	650	701	17			
1	H	509	Total	C	N	O	S	0	0	0
			3824	2429	663	715	17			

There are 16 discrepancies between the modelled and reference sequences:

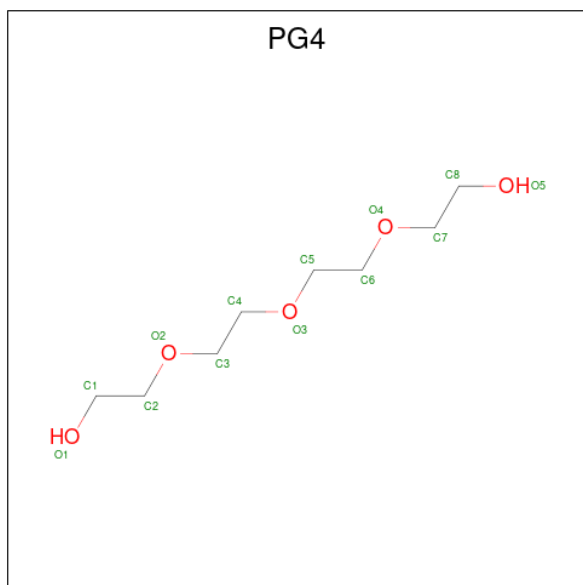
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P49419
A	0	HIS	-	expression tag	UNP P49419
B	-1	GLY	-	expression tag	UNP P49419
B	0	HIS	-	expression tag	UNP P49419
C	-1	GLY	-	expression tag	UNP P49419
C	0	HIS	-	expression tag	UNP P49419
D	-1	GLY	-	expression tag	UNP P49419
D	0	HIS	-	expression tag	UNP P49419
E	-1	GLY	-	expression tag	UNP P49419
E	0	HIS	-	expression tag	UNP P49419
F	-1	GLY	-	expression tag	UNP P49419
F	0	HIS	-	expression tag	UNP P49419
G	-1	GLY	-	expression tag	UNP P49419

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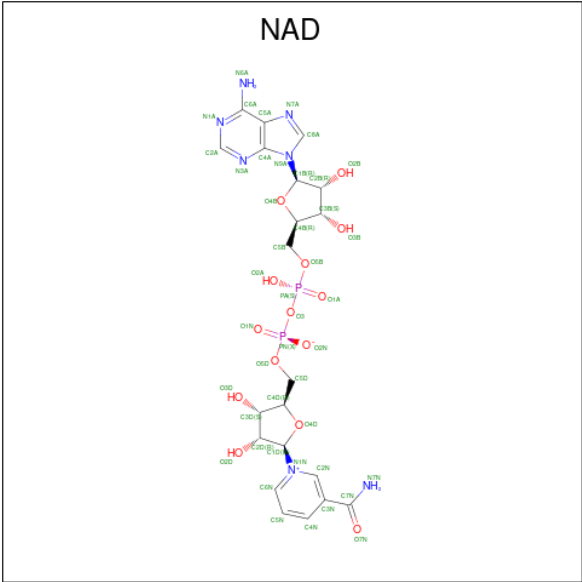
Chain	Residue	Modelled	Actual	Comment	Reference
G	0	HIS	-	expression tag	UNP P49419
H	-1	GLY	-	expression tag	UNP P49419
H	0	HIS	-	expression tag	UNP P49419

- Molecule 2 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	8	5		
2	B	1	Total	C	O	0	0
			13	8	5		
2	C	1	Total	C	O	0	0
			13	8	5		
2	D	1	Total	C	O	0	0
			13	8	5		
2	E	1	Total	C	O	0	0
			13	8	5		
2	F	1	Total	C	O	0	0
			13	8	5		
2	G	1	Total	C	O	0	0
			13	8	5		
2	H	1	Total	C	O	0	0
			13	8	5		

- 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	C	N	O	P	0	0
			27	10	5	10	2		
3	B	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	F	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	G	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	H	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	188	Total	O	0	0
			188	188		
4	B	170	Total	O	0	0
			170	170		
4	C	171	Total	O	0	0
			171	171		
4	D	139	Total	O	0	0
			139	139		

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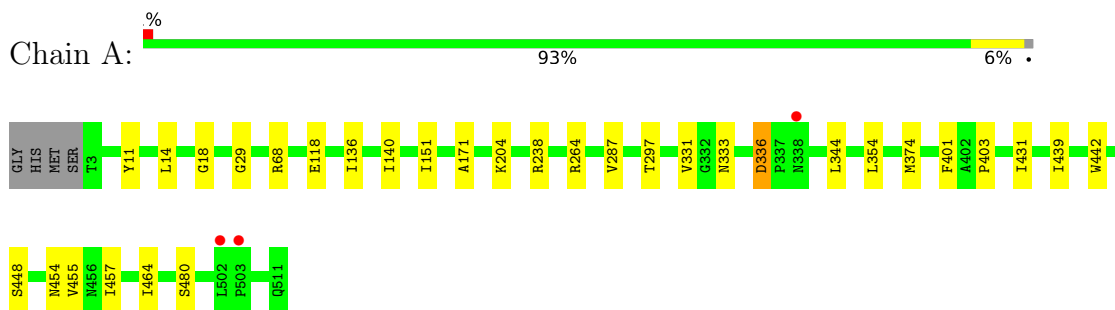
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	173	Total 173	O 173	0	0
4	F	165	Total 165	O 165	0	0
4	G	165	Total 165	O 165	0	0
4	H	174	Total 174	O 174	0	0

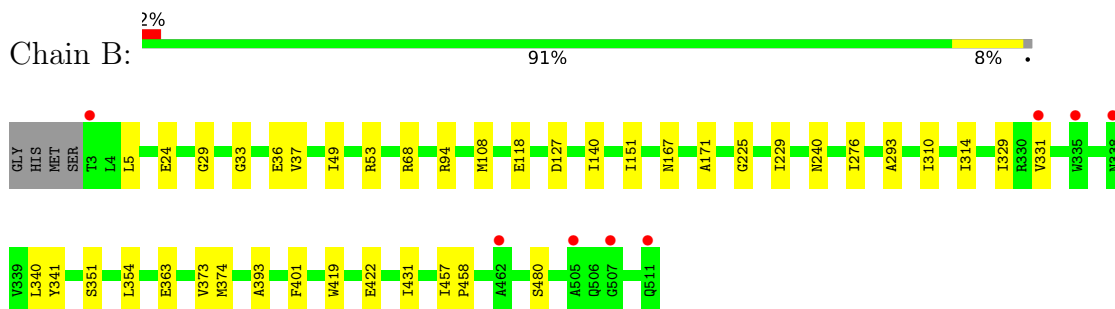
3 Residue-property plots [i](#)

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.

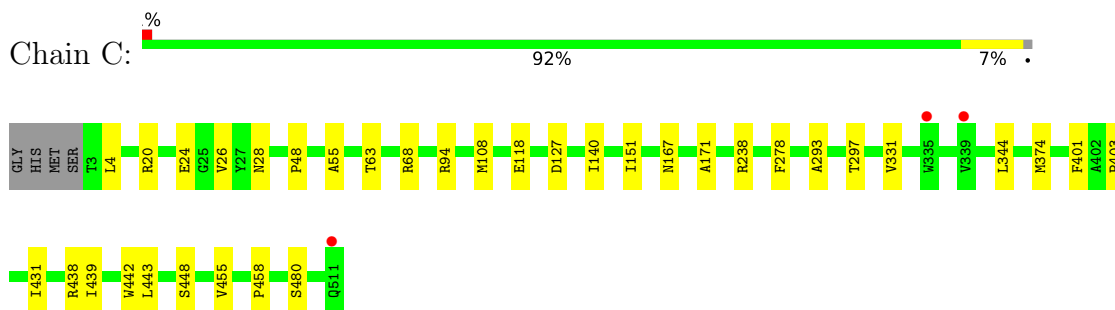
- Molecule 1: Alpha-aminoadipic semialdehyde dehydrogenase



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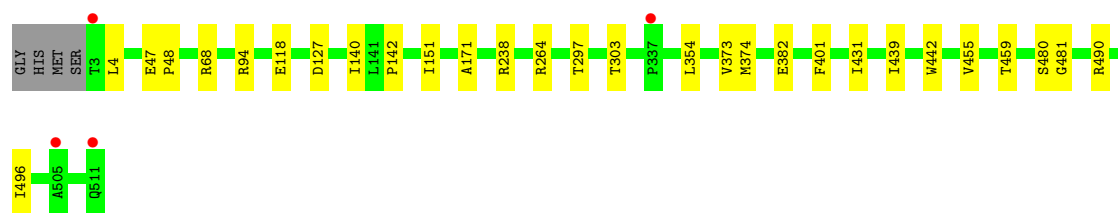


- Molecule 1: Alpha-aminoadipic semialdehyde dehydrogenase

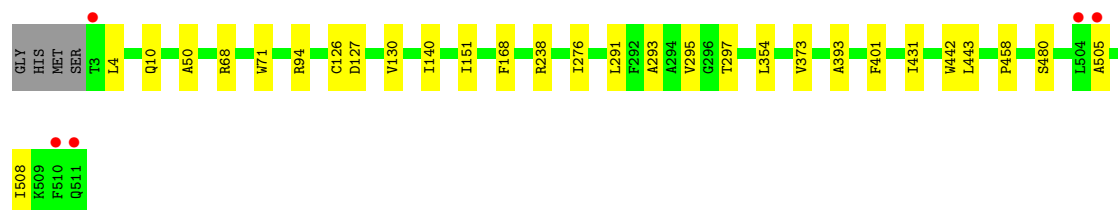
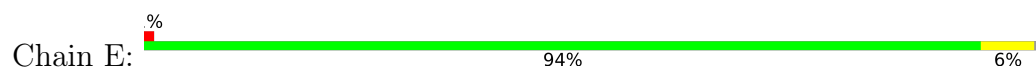


- Molecule 1: Alpha-aminoadipic semialdehyde dehydrogenase

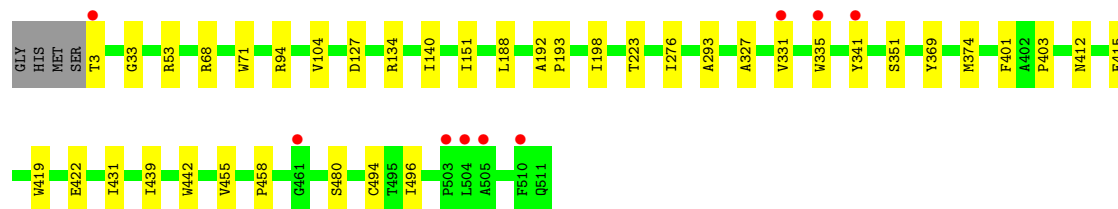
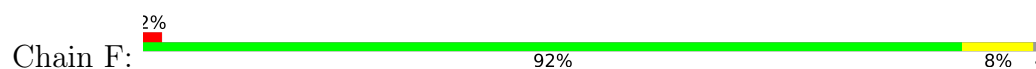




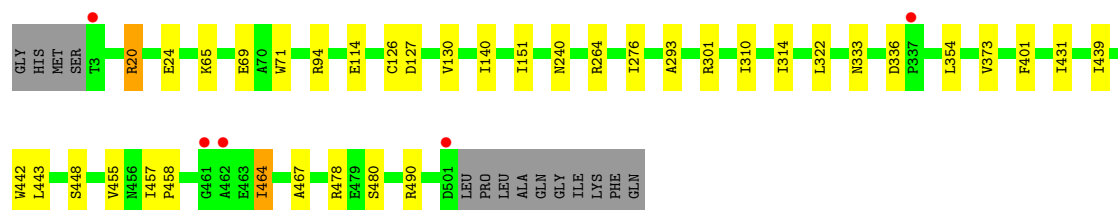
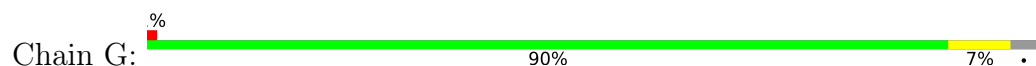
- Molecule 1: Alpha-aminoadipic semialdehyde dehydrogenase



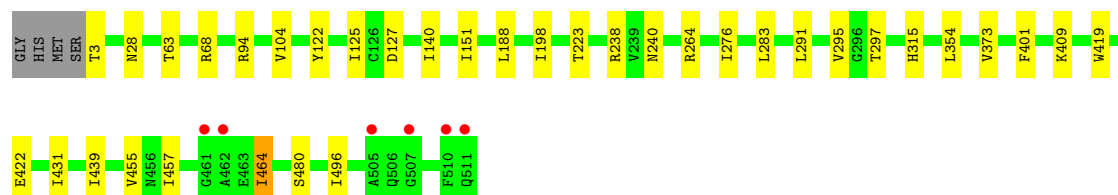
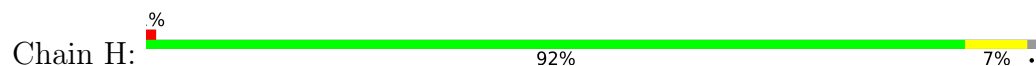
- Molecule 1: Alpha-aminoadipic semialdehyde dehydrogenase



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4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	155.67Å 161.58Å 158.93Å 90.00° 94.76° 90.00°	Depositor
Resolution (Å)	62.89 – 2.00 62.89 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.4 (62.89-2.00) 99.4 (62.89-2.00)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.171 , 0.218 0.173 , 0.219	Depositor DCC
R_{free} test set	12918 reflections (2.99%)	wwPDB-VP
Wilson B-factor (Å ²)	24.9	Xtriage
Anisotropy	0.582	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 40.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	32089	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.86% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAD, PG4

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	0.49	0/3890	0.79	3/5287 (0.1%)
1	B	0.48	0/3897	0.79	1/5294 (0.0%)
1	C	0.48	0/3888	0.78	0/5285
1	D	0.45	0/3867	0.77	1/5260 (0.0%)
1	E	0.47	0/3911	0.78	2/5314 (0.0%)
1	F	0.48	0/3897	0.76	0/5296
1	G	0.48	0/3822	0.77	0/5195
1	H	0.47	0/3903	0.76	1/5304 (0.0%)
All	All	0.47	0/31075	0.78	8/42235 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	457	ILE	N-CA-C	-6.00	104.27	109.19
1	B	29	GLY	N-CA-C	-5.77	107.04	113.79
1	A	29	GLY	N-CA-C	-5.66	107.17	113.79
1	A	287	VAL	CA-C-N	-5.31	113.56	119.19
1	A	287	VAL	C-N-CA	-5.31	113.56	119.19
1	E	168	PHE	CA-C-N	5.14	125.22	119.87
1	E	168	PHE	C-N-CA	5.14	125.22	119.87
1	D	481	GLY	N-CA-C	5.11	119.91	112.60

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	3811	0	3752	18	0
1	B	3818	0	3769	25	0
1	C	3809	0	3744	21	0
1	D	3788	0	3714	17	0
1	E	3826	0	3781	18	0
1	F	3819	0	3766	25	0
1	G	3745	0	3684	26	0
1	H	3824	0	3767	24	0
2	A	13	0	18	0	0
2	B	13	0	18	4	0
2	C	13	0	18	0	0
2	D	13	0	18	2	0
2	E	13	0	18	2	0
2	F	13	0	18	4	0
2	G	13	0	18	3	0
2	H	13	0	18	5	0
3	A	27	0	12	0	0
3	B	23	0	12	0	0
3	C	27	0	12	0	0
3	D	27	0	12	0	0
3	E	27	0	12	0	0
3	F	23	0	12	0	0
3	G	23	0	12	0	0
3	H	23	0	12	0	0
4	A	188	0	0	1	0
4	B	170	0	0	0	0
4	C	171	0	0	0	0
4	D	139	0	0	0	0
4	E	173	0	0	0	0
4	F	165	0	0	0	0
4	G	165	0	0	1	0
4	H	174	0	0	2	0
All	All	32089	0	30217	157	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 3.

All (157) 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:H:240:ASN:HD21	2:H:601:PG4:H11	1.42	0.85
1:F:140:ILE:HD11	1:G:151:ILE:HB	1.62	0.80
1:B:240:ASN:HD21	2:B:601:PG4:H81	1.48	0.78
1:A:151:ILE:HB	1:D:140:ILE:HD11	1.64	0.77
1:H:68:ARG:HH22	2:H:601:PG4:H12	1.49	0.76
1:B:151:ILE:HB	1:C:140:ILE:HD11	1.65	0.76
1:B:68:ARG:HH22	2:B:601:PG4:H61	1.51	0.75
1:E:151:ILE:HB	1:H:140:ILE:HD11	1.67	0.75
1:A:140:ILE:HD11	1:D:151:ILE:HB	1.69	0.74
1:B:331:VAL:HG21	1:B:374:MET:HE1	1.74	0.70
1:E:94:ARG:NH2	1:E:127:ASP:OD2	2.24	0.70
1:F:331:VAL:HG21	1:F:374:MET:HE1	1.74	0.69
1:E:140:ILE:HD11	1:H:151:ILE:HB	1.75	0.67
1:F:151:ILE:HB	1:G:140:ILE:HD11	1.76	0.67
1:F:331:VAL:HG13	1:F:341:TYR:HD2	1.61	0.65
1:H:68:ARG:NH2	2:H:601:PG4:H12	2.10	0.65
1:B:140:ILE:HD11	1:C:151:ILE:HB	1.77	0.64
1:G:443:LEU:HD11	1:H:496:ILE:HD11	1.81	0.62
1:C:94:ARG:NH2	1:C:127:ASP:OD2	2.28	0.62
1:D:94:ARG:NH2	1:D:127:ASP:OD2	2.33	0.60
1:G:240:ASN:HD21	2:G:601:PG4:H81	1.65	0.60
1:E:354:LEU:HD21	1:E:373:VAL:HG23	1.82	0.60
1:H:240:ASN:ND2	2:H:601:PG4:H11	2.14	0.60
1:B:118:GLU:HG3	1:B:171:ALA:HB2	1.83	0.59
1:D:118:GLU:HG3	1:D:171:ALA:HB2	1.85	0.58
1:C:20:ARG:NH2	1:C:24:GLU:OE1	2.35	0.58
1:G:443:LEU:HD13	1:H:151:ILE:HD11	1.85	0.57
1:D:140:ILE:HG23	1:D:151:ILE:HG22	1.86	0.57
1:H:94:ARG:NH2	1:H:127:ASP:OD2	2.34	0.56
1:C:293:ALA:HB2	1:C:458:PRO:HB2	1.87	0.56
1:F:134:ARG:HD2	1:H:464:ILE:HD11	1.87	0.56
1:B:94:ARG:NH2	1:B:127:ASP:OD2	2.35	0.55
1:A:354:LEU:HD12	1:F:351:SER:HB2	1.89	0.55
1:G:293:ALA:HB2	1:G:458:PRO:HB2	1.88	0.55
1:C:140:ILE:HG23	1:C:151:ILE:HG22	1.89	0.54
1:H:28:ASN:HB3	1:H:63:THR:HG23	1.89	0.54
1:E:293:ALA:HB2	1:E:458:PRO:HB2	1.89	0.54
1:F:33:GLY:O	1:F:53:ARG:HG2	2.07	0.54
1:A:140:ILE:HG23	1:A:151:ILE:HG22	1.88	0.54
1:F:104:VAL:HA	1:F:198:ILE:HD11	1.90	0.54
1:B:293:ALA:HB2	1:B:458:PRO:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:457:ILE:HG12	1:G:458:PRO:HD2	1.91	0.53
1:C:331:VAL:HG21	1:C:374:MET:HE1	1.90	0.53
1:A:344:LEU:HD21	1:A:403:PRO:HD3	1.90	0.53
1:E:71:TRP:CE3	2:E:601:PG4:H52	2.43	0.52
1:B:24:GLU:HG3	1:B:53:ARG:NH1	2.24	0.52
1:G:71:TRP:CE3	2:G:601:PG4:H42	2.45	0.52
1:C:443:LEU:HD11	1:D:496:ILE:HD11	1.90	0.52
1:E:68:ARG:HB3	2:E:601:PG4:H62	1.91	0.52
1:G:94:ARG:NH2	1:G:127:ASP:OD2	2.43	0.52
1:B:68:ARG:NH2	2:B:601:PG4:H61	2.20	0.52
1:C:442:TRP:CH2	1:C:448:SER:HB2	2.45	0.51
1:H:354:LEU:HD21	1:H:373:VAL:HG23	1.93	0.51
1:A:68:ARG:HD2	1:A:238:ARG:HB3	1.92	0.51
1:A:118:GLU:HG2	1:A:171:ALA:HB2	1.93	0.51
1:F:94:ARG:NH2	1:F:127:ASP:OD2	2.38	0.51
1:C:108:MET:HE3	1:C:167:ASN:HA	1.92	0.50
1:B:276:ILE:HB	1:B:431:ILE:HG22	1.93	0.50
1:G:20:ARG:NH2	1:G:24:GLU:OE1	2.44	0.49
1:A:264:ARG:NH2	4:A:703:HOH:O	2.42	0.49
1:C:118:GLU:HG3	1:C:171:ALA:HB2	1.94	0.49
1:D:264:ARG:HH22	1:D:490:ARG:HA	1.78	0.49
1:F:68:ARG:NH2	2:F:601:PG4:H52	2.27	0.49
1:C:4:LEU:HD23	1:C:48:PRO:HB2	1.94	0.49
1:D:68:ARG:CZ	2:D:601:PG4:H41	2.43	0.49
1:F:293:ALA:HB2	1:F:458:PRO:HB2	1.95	0.49
1:G:126:CYS:O	1:G:130:VAL:HG23	2.11	0.49
1:F:341:TYR:OH	1:F:403:PRO:HG3	2.13	0.49
1:E:443:LEU:HD11	1:F:496:ILE:HD11	1.95	0.48
1:G:439:ILE:HG23	1:G:455:VAL:HG21	1.95	0.48
1:C:28:ASN:HB3	1:C:63:THR:HG23	1.96	0.48
1:B:310:ILE:HG22	1:B:314:ILE:HG13	1.96	0.48
1:H:276:ILE:HB	1:H:431:ILE:HG22	1.94	0.47
1:G:442:TRP:CH2	1:G:448:SER:HB2	2.49	0.47
1:F:68:ARG:CZ	2:F:601:PG4:H52	2.44	0.47
1:C:439:ILE:HG23	1:C:455:VAL:HG21	1.96	0.47
1:A:431:ILE:HG23	1:A:442:TRP:CE2	2.50	0.47
1:G:264:ARG:HH22	1:G:490:ARG:HA	1.79	0.47
1:B:37:VAL:HG22	1:B:53:ARG:HG2	1.96	0.47
1:H:439:ILE:HG23	1:H:455:VAL:HG21	1.96	0.46
1:B:363:GLU:OE1	1:B:393:ALA:HB1	2.16	0.46
1:E:126:CYS:O	1:E:130:VAL:HG23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:354:LEU:HD21	1:D:373:VAL:HG23	1.97	0.46
1:A:442:TRP:CH2	1:A:448:SER:HB2	2.51	0.46
1:E:431:ILE:HG23	1:E:442:TRP:CE2	2.50	0.46
1:H:291:LEU:O	1:H:295:VAL:HG22	2.16	0.45
1:B:329:ILE:HG23	1:B:340:LEU:HD23	1.98	0.45
1:B:5:LEU:HB2	1:B:49:ILE:HA	1.97	0.45
1:G:310:ILE:HG22	1:G:314:ILE:HG13	1.99	0.45
1:H:315:HIS:CD2	1:H:409:LYS:HG2	2.51	0.45
1:D:374:MET:HE3	1:D:382:GLU:HA	1.99	0.45
1:F:71:TRP:CE3	2:F:601:PG4:H62	2.52	0.45
1:B:33:GLY:O	1:B:53:ARG:NH2	2.49	0.45
1:G:464:ILE:HG23	4:H:763:HOH:O	2.16	0.45
1:G:467:ALA:HB1	1:G:478:ARG:HB3	1.98	0.44
1:A:333:ASN:O	1:A:336:ASP:HB2	2.18	0.44
1:H:419:TRP:O	1:H:422:GLU:HG2	2.18	0.44
1:G:114:GLU:OE2	1:G:301:ARG:NH1	2.51	0.44
1:B:351:SER:HB2	1:E:354:LEU:HD12	1.99	0.44
1:D:439:ILE:HG23	1:D:455:VAL:HG21	2.00	0.44
1:F:419:TRP:O	1:F:422:GLU:HG2	2.18	0.44
1:F:188:LEU:HD11	1:F:223:THR:HG23	2.00	0.44
1:F:431:ILE:HG23	1:F:442:TRP:CE2	2.53	0.44
1:C:68:ARG:HD2	1:C:238:ARG:HB3	1.99	0.44
1:C:278:PHE:CE2	1:C:438:ARG:HD3	2.53	0.43
1:A:354:LEU:HD23	1:A:354:LEU:HA	1.84	0.43
1:B:225:GLY:HA3	1:B:229:ILE:HG13	2.00	0.43
1:D:68:ARG:HD2	1:D:238:ARG:HB3	2.00	0.43
1:D:431:ILE:HG23	1:D:442:TRP:CE2	2.53	0.43
1:F:151:ILE:HG12	1:F:494:CYS:HB2	2.01	0.43
1:B:151:ILE:HB	1:C:140:ILE:CD1	2.43	0.43
1:H:104:VAL:HA	1:H:198:ILE:HD11	2.00	0.43
1:E:4:LEU:HD22	1:E:50:ALA:HA	2.01	0.43
1:A:439:ILE:HG23	1:A:455:VAL:HG21	2.00	0.43
1:E:68:ARG:HD2	1:E:238:ARG:HB3	2.01	0.42
1:E:276:ILE:HB	1:E:431:ILE:HG22	2.00	0.42
1:B:108:MET:HE3	1:B:167:ASN:HA	2.01	0.42
1:H:188:LEU:HD11	1:H:223:THR:HG23	2.00	0.42
1:A:454:ASN:HB3	1:A:457:ILE:HG23	2.01	0.42
1:B:419:TRP:O	1:B:422:GLU:HG2	2.19	0.42
1:C:431:ILE:HG23	1:C:442:TRP:CE2	2.54	0.42
1:E:291:LEU:O	1:E:295:VAL:HG22	2.20	0.42
1:E:505:ALA:HB1	1:E:508:ILE:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:431:ILE:HG23	1:E:442:TRP:CZ2	2.54	0.42
1:D:4:LEU:HD23	1:D:48:PRO:HB2	2.01	0.42
1:G:354:LEU:HD21	1:G:373:VAL:HG23	2.02	0.42
1:B:331:VAL:HG22	1:B:341:TYR:CD2	2.54	0.42
1:D:303:THR:HB	1:D:459:THR:O	2.20	0.42
2:D:601:PG4:H32	2:D:601:PG4:H52	1.83	0.42
1:G:65:LYS:O	1:G:69:GLU:HG2	2.19	0.42
1:C:344:LEU:HD21	1:C:403:PRO:HD3	2.01	0.41
1:G:240:ASN:ND2	2:G:601:PG4:H81	2.34	0.41
1:G:276:ILE:HB	1:G:431:ILE:HG22	2.02	0.41
1:G:322:LEU:HD12	1:G:322:LEU:HA	1.93	0.41
1:B:36:GLU:OE2	1:E:393:ALA:HA	2.20	0.41
1:H:264:ARG:NH2	4:H:710:HOH:O	2.52	0.41
1:A:11:TYR:HB3	1:A:14:LEU:HD12	2.02	0.41
2:B:601:PG4:H42	2:B:601:PG4:H22	1.86	0.41
1:A:136:ILE:O	1:D:142:PRO:HD3	2.20	0.41
1:F:276:ILE:HB	1:F:431:ILE:HG22	2.03	0.41
1:G:333:ASN:O	1:G:336:ASP:HB2	2.21	0.41
1:A:18:GLY:O	1:A:204:LYS:HE3	2.21	0.41
1:A:331:VAL:HG21	1:A:374:MET:HE1	2.03	0.41
1:B:354:LEU:HD21	1:B:373:VAL:HG23	2.03	0.41
1:C:443:LEU:HD13	1:D:151:ILE:HD11	2.03	0.41
1:F:327:ALA:HA	1:F:369:TYR:OH	2.21	0.41
1:H:68:ARG:HD2	1:H:238:ARG:HB3	2.03	0.41
1:H:122:TYR:O	1:H:125:ILE:HG22	2.21	0.41
1:G:293:ALA:HB2	1:G:458:PRO:CB	2.51	0.40
1:H:240:ASN:HD21	2:H:601:PG4:C1	2.22	0.40
1:F:68:ARG:HH22	2:F:601:PG4:H31	1.86	0.40
1:H:283:LEU:HD23	1:H:283:LEU:HA	1.85	0.40
1:F:439:ILE:HG23	1:F:455:VAL:HG21	2.03	0.40
1:F:412:ASN:O	1:F:415:GLU:HG2	2.21	0.40
1:G:264:ARG:NH2	4:G:706:HOH:O	2.53	0.40
1:C:26:VAL:HG22	1:C:55:ALA:HB2	2.04	0.40
1:F:192:ALA:HA	1:F:193:PRO:HD3	1.92	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	507/513 (99%)	493 (97%)	13 (3%)	1 (0%)	43	42
1	B	507/513 (99%)	493 (97%)	13 (3%)	1 (0%)	43	42
1	C	507/513 (99%)	490 (97%)	16 (3%)	1 (0%)	43	42
1	D	507/513 (99%)	492 (97%)	14 (3%)	1 (0%)	43	42
1	E	509/513 (99%)	490 (96%)	18 (4%)	1 (0%)	43	42
1	F	507/513 (99%)	495 (98%)	11 (2%)	1 (0%)	43	42
1	G	497/513 (97%)	480 (97%)	16 (3%)	1 (0%)	43	42
1	H	507/513 (99%)	490 (97%)	16 (3%)	1 (0%)	43	42
All	All	4048/4104 (99%)	3923 (97%)	117 (3%)	8 (0%)	43	42

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	480	SER
1	C	480	SER
1	B	480	SER
1	E	480	SER
1	F	480	SER
1	D	480	SER
1	G	480	SER
1	H	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	388/410 (95%)	384 (99%)	4 (1%)	68	75
1	B	390/410 (95%)	388 (100%)	2 (0%)	81	87
1	C	387/410 (94%)	385 (100%)	2 (0%)	81	87
1	D	383/410 (93%)	380 (99%)	3 (1%)	73	80
1	E	392/410 (96%)	389 (99%)	3 (1%)	73	80
1	F	391/410 (95%)	388 (99%)	3 (1%)	73	80
1	G	383/410 (93%)	380 (99%)	3 (1%)	73	80
1	H	391/410 (95%)	387 (99%)	4 (1%)	68	75
All	All	3105/3280 (95%)	3081 (99%)	24 (1%)	73	80

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	297	THR
1	A	336	ASP
1	A	401	PHE
1	A	464	ILE
1	B	401	PHE
1	B	457	ILE
1	C	297	THR
1	C	401	PHE
1	D	47	GLU
1	D	297	THR
1	D	401	PHE
1	E	10	GLN
1	E	297	THR
1	E	401	PHE
1	F	3	THR
1	F	335	TRP
1	F	401	PHE
1	G	20	ARG
1	G	401	PHE
1	G	464	ILE
1	H	3	THR
1	H	297	THR
1	H	401	PHE
1	H	464	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	153	GLN
1	A	155	ASN
1	B	46	ASN
1	B	54	GLN
1	B	153	GLN
1	B	155	ASN
1	B	412	ASN
1	C	54	GLN
1	C	120	GLN
1	C	153	GLN
1	C	155	ASN
1	C	338	ASN
1	D	155	ASN
1	E	88	GLN
1	E	153	GLN
1	E	155	ASN
1	E	213	ASN
1	F	155	ASN
1	G	8	GLN
1	G	153	GLN
1	G	155	ASN
1	H	120	GLN
1	H	155	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](#)

16 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	PG4	B	601	-	12,12,12	0.64	0	11,11,11	0.32	0
2	PG4	G	601	-	12,12,12	0.71	0	11,11,11	0.28	0
2	PG4	A	601	-	12,12,12	0.68	0	11,11,11	0.31	0
3	NAD	B	602	-	25,25,48	1.66	6 (24%)	37,38,73	2.41	12 (32%)
2	PG4	D	601	-	12,12,12	0.66	0	11,11,11	0.22	0
3	NAD	C	602	-	28,29,48	2.52	6 (21%)	43,45,73	2.14	10 (23%)
3	NAD	G	602	-	25,25,48	1.58	3 (12%)	37,38,73	2.34	14 (37%)
3	NAD	D	602	-	28,29,48	2.67	7 (25%)	43,45,73	2.24	13 (30%)
2	PG4	H	601	-	12,12,12	0.68	0	11,11,11	0.29	0
2	PG4	C	601	-	12,12,12	0.69	0	11,11,11	0.37	0
3	NAD	H	602	-	25,25,48	1.62	3 (12%)	37,38,73	2.21	12 (32%)
3	NAD	F	602	-	25,25,48	1.56	3 (12%)	37,38,73	2.39	13 (35%)
3	NAD	E	602	-	28,29,48	2.54	3 (10%)	43,45,73	2.00	10 (23%)
2	PG4	F	601	-	12,12,12	0.64	0	11,11,11	0.21	0
3	NAD	A	602	-	28,29,48	2.64	8 (28%)	43,45,73	2.07	12 (27%)
2	PG4	E	601	-	12,12,12	0.68	0	11,11,11	0.29	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PG4	B	601	-	-	7/10/10/10	-
2	PG4	G	601	-	-	2/10/10/10	-
2	PG4	A	601	-	-	6/10/10/10	-
3	NAD	B	602	-	-	3/10/26/62	0/3/3/5
2	PG4	D	601	-	-	7/10/10/10	-
3	NAD	C	602	-	-	3/16/32/62	0/3/3/5
3	NAD	G	602	-	-	6/10/26/62	0/3/3/5
3	NAD	D	602	-	-	3/16/32/62	0/3/3/5
2	PG4	H	601	-	-	6/10/10/10	-
2	PG4	C	601	-	-	1/10/10/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAD	H	602	-	-	3/10/26/62	0/3/3/5
3	NAD	F	602	-	-	3/10/26/62	0/3/3/5
3	NAD	E	602	-	-	3/16/32/62	0/3/3/5
2	PG4	F	601	-	-	7/10/10/10	-
3	NAD	A	602	-	-	3/16/32/62	0/3/3/5
2	PG4	E	601	-	-	3/10/10/10	-

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	602	NAD	PA-O3	-11.61	1.47	1.59
3	A	602	NAD	PA-O3	-11.27	1.47	1.59
3	E	602	NAD	PA-O3	-10.92	1.47	1.59
3	C	602	NAD	PA-O3	-10.84	1.47	1.59
3	A	602	NAD	C6A-N6A	3.94	1.44	1.34
3	B	602	NAD	C6A-N6A	3.94	1.44	1.34
3	E	602	NAD	C6A-N6A	3.93	1.44	1.34
3	D	602	NAD	C6A-N6A	3.88	1.44	1.34
3	F	602	NAD	C6A-N6A	3.85	1.44	1.34
3	H	602	NAD	C6A-N6A	3.72	1.43	1.34
3	G	602	NAD	C6A-N6A	3.71	1.43	1.34
3	C	602	NAD	C6A-N6A	3.71	1.43	1.34
3	H	602	NAD	PA-O5B	-3.69	1.48	1.60
3	F	602	NAD	PA-O5B	-3.50	1.49	1.60
3	G	602	NAD	PA-O5B	-3.38	1.49	1.60
3	B	602	NAD	PA-O5B	-3.36	1.49	1.60
3	B	602	NAD	C4A-N9A	2.61	1.43	1.37
3	E	602	NAD	PA-O5B	-2.58	1.49	1.59
3	C	602	NAD	PA-O5B	-2.51	1.49	1.59
3	A	602	NAD	C4A-N9A	2.49	1.42	1.37
3	G	602	NAD	PA-O2A	-2.48	1.45	1.54
3	D	602	NAD	PA-O5B	-2.46	1.49	1.59
3	A	602	NAD	PA-O5B	-2.40	1.50	1.59
3	D	602	NAD	PN-O1N	2.36	1.57	1.50
3	A	602	NAD	C5A-C4A	2.35	1.43	1.39
3	H	602	NAD	C5A-C4A	2.30	1.43	1.39
3	C	602	NAD	C5A-C4A	2.24	1.43	1.39
3	D	602	NAD	O3B-C3B	-2.24	1.37	1.43
3	B	602	NAD	C5A-C4A	2.21	1.43	1.39
3	C	602	NAD	C4A-N9A	2.17	1.42	1.37
3	D	602	NAD	C5A-C4A	2.14	1.42	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	NAD	O3B-C3B	-2.13	1.37	1.43
3	D	602	NAD	C4A-N9A	2.13	1.42	1.37
3	A	602	NAD	C2B-C3B	-2.10	1.47	1.53
3	C	602	NAD	PA-O2A	-2.08	1.45	1.55
3	A	602	NAD	PA-O2A	-2.07	1.45	1.55
3	F	602	NAD	C4A-N9A	2.06	1.42	1.37
3	A	602	NAD	O3B-C3B	-2.05	1.37	1.43
3	B	602	NAD	PA-O3	-2.02	1.47	1.54

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	602	NAD	N3A-C2A-N1A	-6.05	119.43	128.58
3	B	602	NAD	C5A-C4A-N3A	-5.75	118.79	126.72
3	C	602	NAD	C5A-C4A-N3A	-5.53	119.10	126.72
3	D	602	NAD	C5A-C4A-N3A	-5.44	119.22	126.72
3	F	602	NAD	C5A-C4A-N3A	-5.35	119.35	126.72
3	B	602	NAD	N3A-C2A-N1A	-5.29	120.58	128.58
3	D	602	NAD	O3-PA-O1A	-5.25	94.91	110.70
3	F	602	NAD	N3A-C2A-N1A	-5.23	120.67	128.58
3	D	602	NAD	N3A-C2A-N1A	-5.20	120.71	128.58
3	C	602	NAD	O2A-PA-O3	-5.19	93.23	107.27
3	A	602	NAD	C5A-C4A-N3A	-5.04	119.78	126.72
3	E	602	NAD	N3A-C2A-N1A	-5.03	120.96	128.58
3	H	602	NAD	C5A-C4A-N3A	-5.02	119.80	126.72
3	F	602	NAD	N3A-C4A-N9A	5.01	135.69	127.17
3	A	602	NAD	N3A-C2A-N1A	-5.00	121.01	128.58
3	C	602	NAD	N3A-C2A-N1A	-4.93	121.12	128.58
3	H	602	NAD	N3A-C2A-N1A	-4.90	121.17	128.58
3	E	602	NAD	C5A-C4A-N3A	-4.88	120.00	126.72
3	A	602	NAD	O2A-PA-O3	-4.54	95.01	107.27
3	D	602	NAD	O2A-PA-O3	4.52	119.50	107.27
3	B	602	NAD	N3A-C4A-N9A	4.48	134.79	127.17
3	C	602	NAD	N3A-C4A-N9A	4.46	134.75	127.17
3	B	602	NAD	O2A-PA-O5B	4.45	118.26	106.67
3	G	602	NAD	C5A-C4A-N3A	-4.43	120.61	126.72
3	E	602	NAD	O2A-PA-O3	-4.41	95.34	107.27
3	D	602	NAD	N3A-C4A-N9A	4.37	134.60	127.17
3	A	602	NAD	N3A-C4A-N9A	4.26	134.42	127.17
3	F	602	NAD	C5A-N7A-C8A	4.25	110.14	103.45
3	B	602	NAD	C5A-N7A-C8A	4.25	110.12	103.45
3	G	602	NAD	N3A-C4A-N9A	4.20	134.32	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	602	NAD	C5A-N7A-C8A	4.06	109.84	103.45
3	A	602	NAD	C5A-N7A-C8A	4.03	109.79	103.45
3	H	602	NAD	N3A-C4A-N9A	4.02	134.00	127.17
3	H	602	NAD	C5A-N7A-C8A	3.95	109.66	103.45
3	G	602	NAD	O3-PA-O5B	3.94	116.95	106.67
3	E	602	NAD	N3A-C4A-N9A	3.94	133.87	127.17
3	E	602	NAD	C5A-N7A-C8A	3.84	109.49	103.45
3	F	602	NAD	O2A-PA-O5B	3.80	116.57	106.67
3	F	602	NAD	O3-PA-O1A	-3.76	96.18	110.83
3	C	602	NAD	O3-PA-O1A	3.76	122.00	110.70
3	B	602	NAD	C2A-N3A-C4A	3.73	120.94	111.83
3	G	602	NAD	O2A-PA-O1A	-3.72	96.34	110.83
3	D	602	NAD	C5A-N7A-C8A	3.68	109.24	103.45
3	F	602	NAD	N9A-C8A-N7A	-3.62	108.81	113.94
3	G	602	NAD	C5A-N7A-C8A	3.55	109.03	103.45
3	D	602	NAD	C2A-N3A-C4A	3.46	120.29	111.83
3	H	602	NAD	O3-PA-O1A	-3.42	97.50	110.83
3	C	602	NAD	C2A-N3A-C4A	3.41	120.17	111.83
3	F	602	NAD	C2A-N3A-C4A	3.36	120.04	111.83
3	G	602	NAD	C2A-N3A-C4A	3.35	120.02	111.83
3	B	602	NAD	C4A-C5A-N7A	-3.35	106.75	110.58
3	B	602	NAD	N9A-C8A-N7A	-3.32	109.23	113.94
3	G	602	NAD	N9A-C8A-N7A	-3.29	109.27	113.94
3	E	602	NAD	C2A-N3A-C4A	3.28	119.85	111.83
3	H	602	NAD	O2A-PA-O5B	3.27	115.20	106.67
3	H	602	NAD	O3-PA-O2A	3.27	120.06	107.80
3	B	602	NAD	O3-PA-O1A	-3.27	98.10	110.83
3	B	602	NAD	O5B-PA-O1A	-3.25	97.66	106.44
3	C	602	NAD	C4A-C5A-N7A	-3.24	106.88	110.58
3	A	602	NAD	N9A-C8A-N7A	-3.24	109.34	113.94
3	E	602	NAD	O3-PA-O1A	3.24	120.44	110.70
3	A	602	NAD	O3-PA-O1A	3.22	120.38	110.70
3	A	602	NAD	C2A-N3A-C4A	3.20	119.64	111.83
3	H	602	NAD	C2A-N3A-C4A	3.15	119.53	111.83
3	H	602	NAD	N9A-C8A-N7A	-3.14	109.48	113.94
3	G	602	NAD	O3-PA-O2A	3.13	119.52	107.80
3	H	602	NAD	C4A-C5A-N7A	-3.12	107.01	110.58
3	C	602	NAD	N9A-C8A-N7A	-3.12	109.52	113.94
3	E	602	NAD	N9A-C8A-N7A	-3.08	109.56	113.94
3	F	602	NAD	O3-PA-O2A	3.00	119.06	107.80
3	E	602	NAD	C4A-C5A-N7A	-2.98	107.17	110.58
3	A	602	NAD	C4A-C5A-N7A	-2.96	107.19	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	602	NAD	O3-PA-O2A	2.92	118.73	107.80
3	D	602	NAD	O5B-PA-O1A	-2.91	97.40	108.94
3	H	602	NAD	O5B-PA-O1A	-2.85	98.74	106.44
3	G	602	NAD	O2A-PA-O5B	-2.82	99.31	106.67
3	D	602	NAD	C4A-C5A-N7A	-2.76	107.43	110.58
3	D	602	NAD	N9A-C8A-N7A	-2.75	110.04	113.94
3	G	602	NAD	C4A-N9A-C8A	2.72	108.59	105.74
3	F	602	NAD	C4A-N9A-C8A	2.68	108.55	105.74
3	F	602	NAD	C4A-C5A-N7A	-2.65	107.55	110.58
3	F	602	NAD	O5B-PA-O1A	-2.59	99.45	106.44
3	D	602	NAD	O2A-PA-O5B	2.49	118.87	107.57
3	F	602	NAD	O2A-PA-O1A	2.30	119.79	110.83
3	C	602	NAD	O5B-PA-O1A	2.27	117.94	108.94
3	E	602	NAD	O5B-PA-O1A	2.25	117.86	108.94
3	G	602	NAD	O3-PA-O1A	2.23	119.54	110.83
3	G	602	NAD	C4A-C5A-N7A	-2.22	108.04	110.58
3	D	602	NAD	O2N-PN-O3	2.21	112.05	104.64
3	H	602	NAD	O2A-PA-O1A	2.21	119.43	110.83
3	D	602	NAD	O4B-C1B-N9A	2.15	112.22	108.09
3	G	602	NAD	C2A-N1A-C6A	2.13	122.23	118.73
3	A	602	NAD	C4A-N9A-C8A	2.03	107.87	105.74
3	A	602	NAD	O5B-PA-O1A	2.03	116.98	108.94
3	B	602	NAD	O3-PA-O5B	-2.02	101.40	106.67
3	A	602	NAD	O2A-PA-O5B	-2.02	98.42	107.57

There are no chirality outliers.

All (66) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602	NAD	C5B-O5B-PA-O3
3	G	602	NAD	C5B-O5B-PA-O1A
3	G	602	NAD	C5B-O5B-PA-O2A
3	G	602	NAD	C5B-O5B-PA-O3
2	H	601	PG4	O3-C5-C6-O4
2	A	601	PG4	O1-C1-C2-O2
2	A	601	PG4	O4-C7-C8-O5
2	B	601	PG4	O3-C5-C6-O4
2	H	601	PG4	O1-C1-C2-O2
2	D	601	PG4	C3-C4-O3-C5
2	B	601	PG4	O1-C1-C2-O2
2	B	601	PG4	C4-C3-O2-C2
2	B	601	PG4	O4-C7-C8-O5

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Mol	Chain	Res	Type	Atoms
2	F	601	PG4	O3-C5-C6-O4
2	H	601	PG4	C5-C6-O4-C7
2	D	601	PG4	O1-C1-C2-O2
2	F	601	PG4	O4-C7-C8-O5
2	H	601	PG4	O4-C7-C8-O5
2	A	601	PG4	C5-C6-O4-C7
2	A	601	PG4	C3-C4-O3-C5
2	A	601	PG4	C8-C7-O4-C6
2	D	601	PG4	C6-C5-O3-C4
2	B	601	PG4	C1-C2-O2-C3
2	H	601	PG4	C8-C7-O4-C6
2	G	601	PG4	C4-C3-O2-C2
2	D	601	PG4	C4-C3-O2-C2
2	F	601	PG4	C1-C2-O2-C3
2	F	601	PG4	C5-C6-O4-C7
2	C	601	PG4	O1-C1-C2-O2
2	D	601	PG4	C5-C6-O4-C7
2	H	601	PG4	C3-C4-O3-C5
3	A	602	NAD	C2B-C1B-N9A-C8A
3	B	602	NAD	C2B-C1B-N9A-C8A
3	C	602	NAD	C2B-C1B-N9A-C8A
3	D	602	NAD	C2B-C1B-N9A-C8A
3	E	602	NAD	C2B-C1B-N9A-C8A
3	F	602	NAD	C2B-C1B-N9A-C8A
3	G	602	NAD	C2B-C1B-N9A-C8A
3	H	602	NAD	C2B-C1B-N9A-C8A
2	D	601	PG4	O4-C7-C8-O5
2	B	601	PG4	C5-C6-O4-C7
2	E	601	PG4	C1-C2-O2-C3
3	C	602	NAD	C2B-C1B-N9A-C4A
2	G	601	PG4	C3-C4-O3-C5
2	F	601	PG4	O2-C3-C4-O3
2	F	601	PG4	C6-C5-O3-C4
3	B	602	NAD	C2B-C1B-N9A-C4A
3	D	602	NAD	C2B-C1B-N9A-C4A
3	H	602	NAD	C2B-C1B-N9A-C4A
3	H	602	NAD	O4B-C1B-N9A-C8A
2	E	601	PG4	C3-C4-O3-C5
2	A	601	PG4	O3-C5-C6-O4
3	A	602	NAD	O4B-C1B-N9A-C8A
3	E	602	NAD	O4B-C1B-N9A-C8A
3	G	602	NAD	O4B-C1B-N9A-C8A

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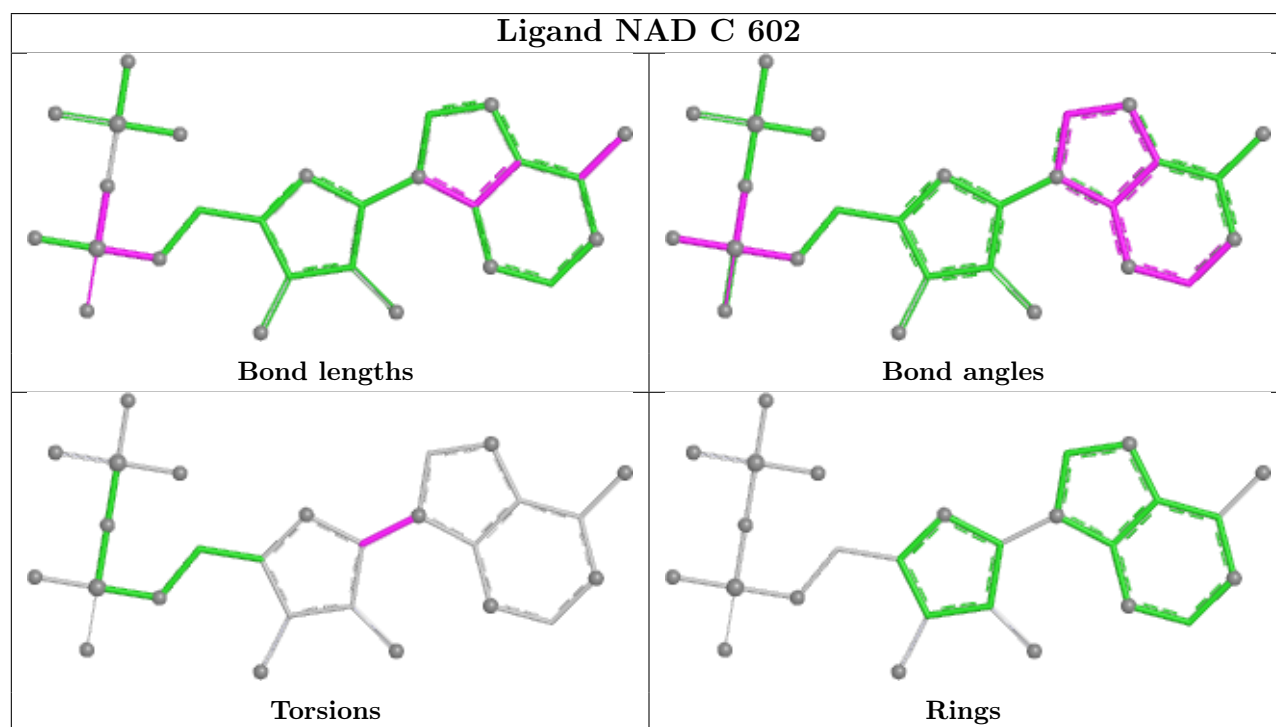
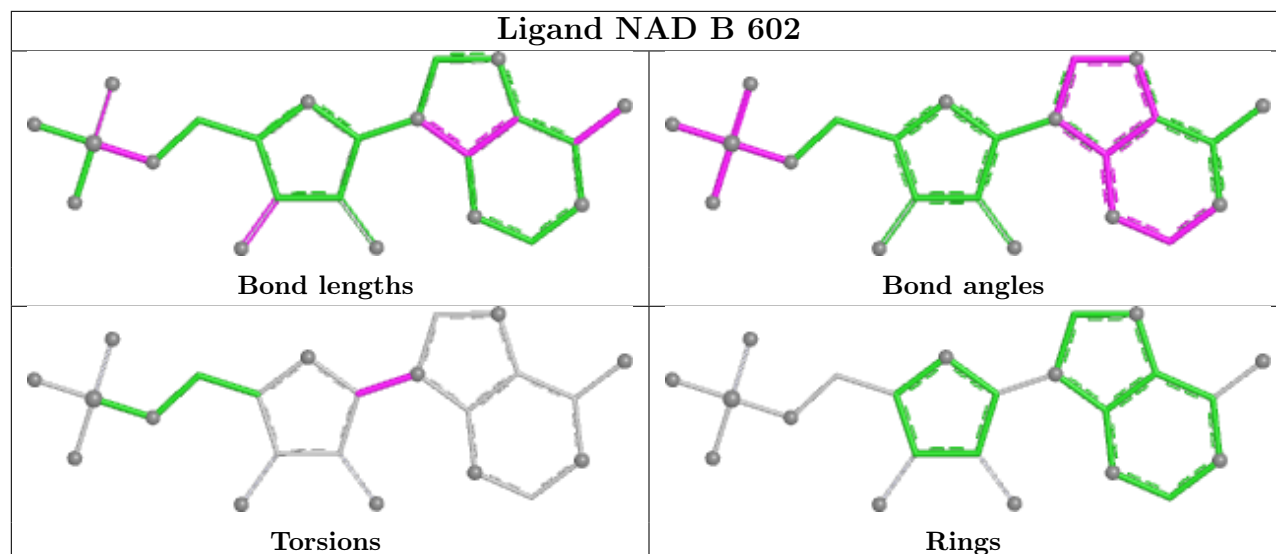
Mol	Chain	Res	Type	Atoms
2	E	601	PG4	C8-C7-O4-C6
3	B	602	NAD	O4B-C1B-N9A-C8A
3	D	602	NAD	O4B-C1B-N9A-C8A
3	F	602	NAD	C2B-C1B-N9A-C4A
3	C	602	NAD	O4B-C1B-N9A-C8A
2	D	601	PG4	O2-C3-C4-O3
3	F	602	NAD	O4B-C1B-N9A-C8A
2	F	601	PG4	C4-C3-O2-C2
3	E	602	NAD	C2B-C1B-N9A-C4A
3	G	602	NAD	C2B-C1B-N9A-C4A
2	B	601	PG4	O2-C3-C4-O3

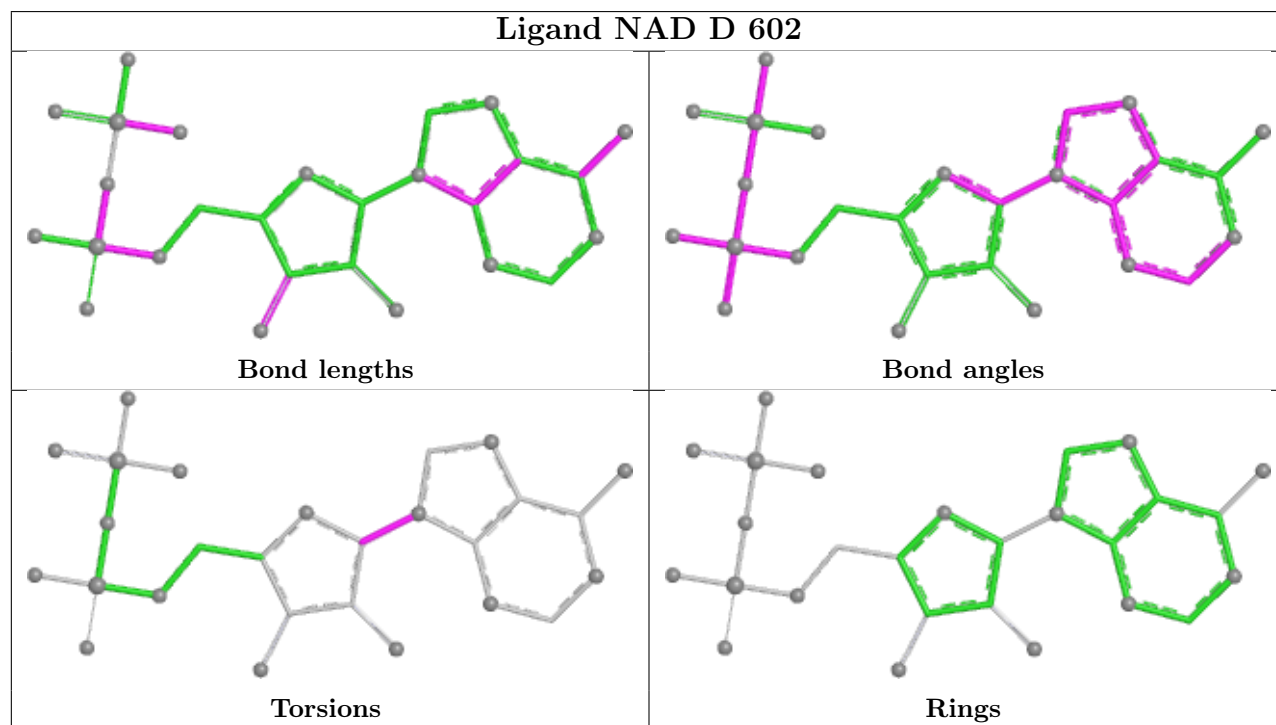
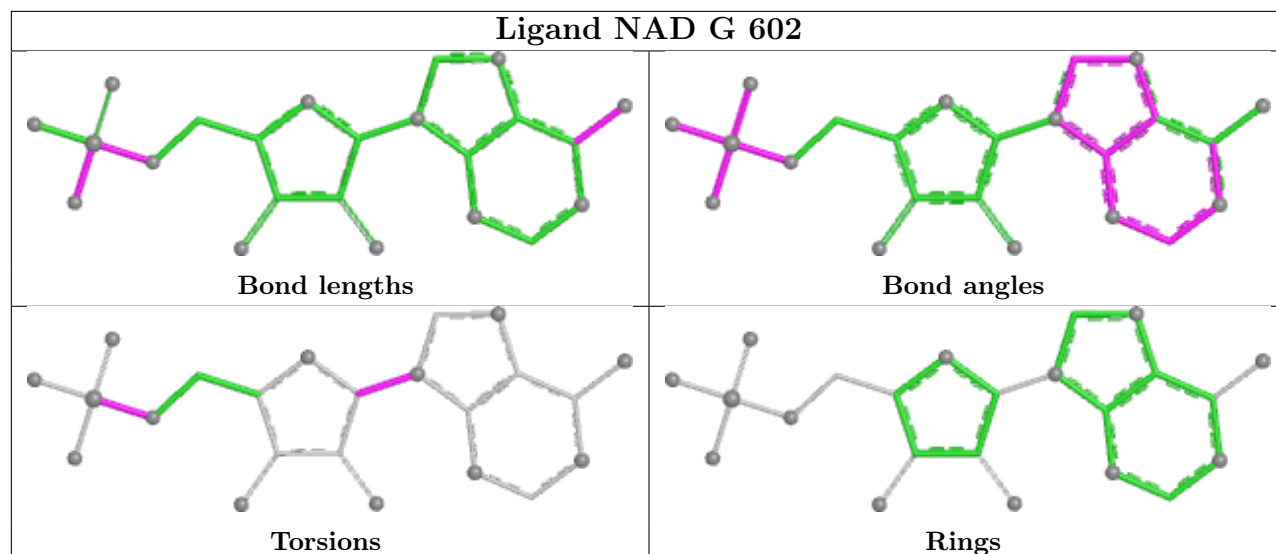
There are no ring outliers.

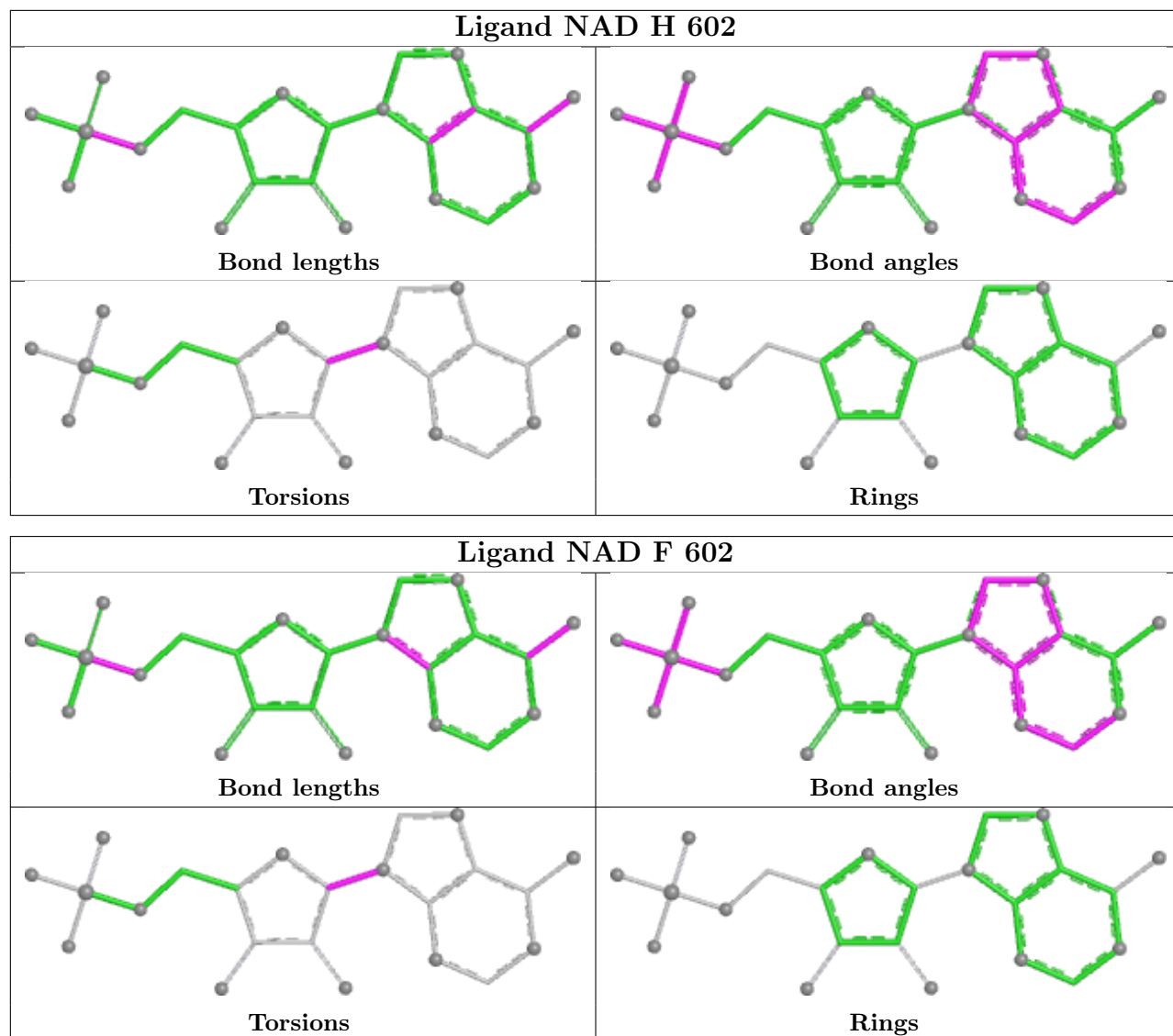
6 monomers are involved in 20 short contacts:

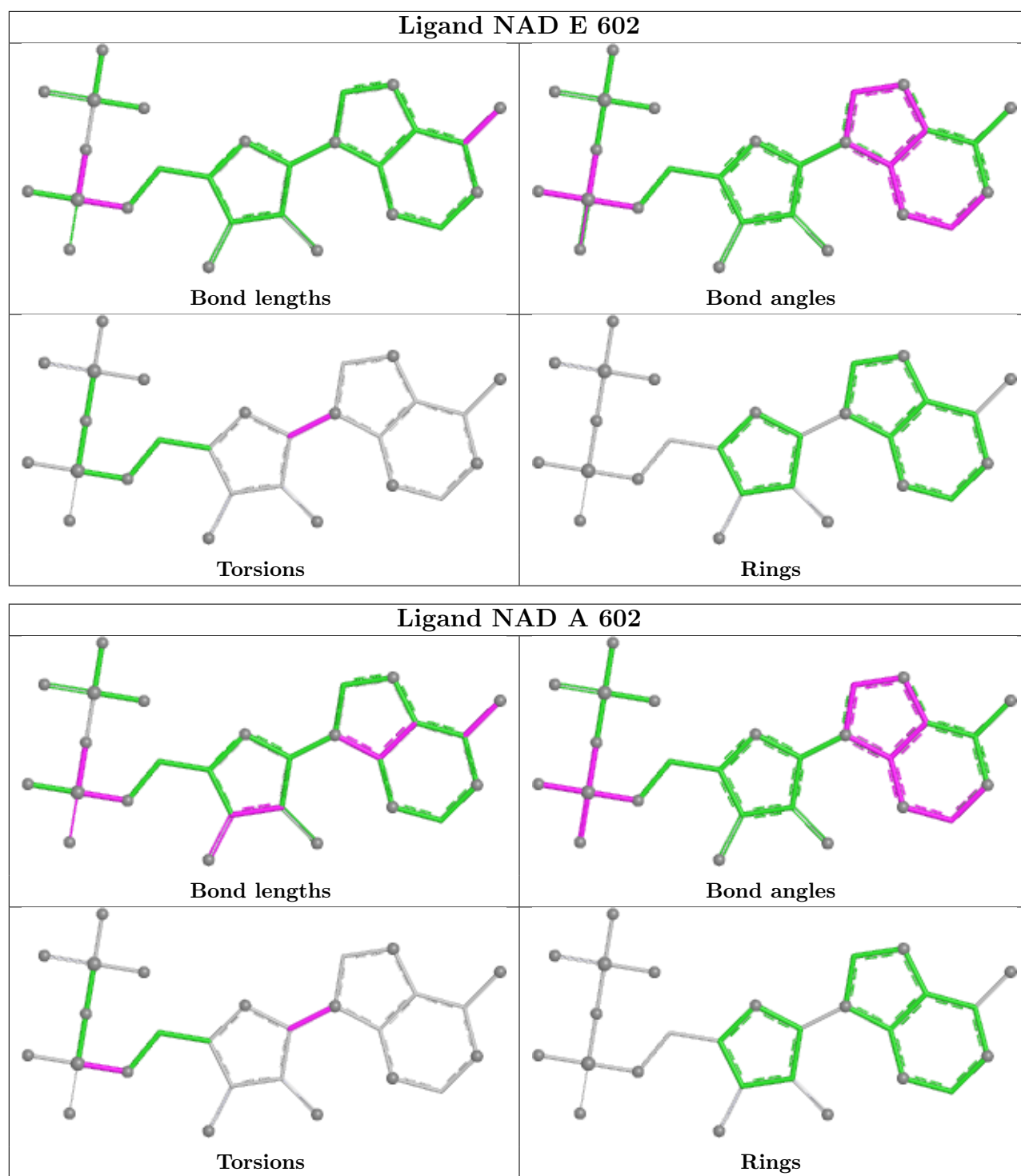
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	PG4	4	0
2	G	601	PG4	3	0
2	D	601	PG4	2	0
2	H	601	PG4	5	0
2	F	601	PG4	4	0
2	E	601	PG4	2	0

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	509/513 (99%)	-0.43	3 (0%) 85 85	15, 26, 44, 59	0
1	B	509/513 (99%)	-0.34	8 (1%) 70 70	17, 27, 46, 63	0
1	C	509/513 (99%)	-0.29	3 (0%) 85 85	17, 28, 50, 73	0
1	D	509/513 (99%)	-0.27	4 (0%) 82 82	15, 31, 50, 66	0
1	E	509/513 (99%)	-0.42	5 (0%) 79 79	15, 27, 44, 62	2 (0%)
1	F	509/513 (99%)	-0.37	9 (1%) 67 67	19, 27, 44, 67	0
1	G	499/513 (97%)	-0.40	5 (1%) 79 79	18, 28, 42, 60	0
1	H	509/513 (99%)	-0.39	6 (1%) 76 76	17, 28, 46, 65	0
All	All	4062/4104 (98%)	-0.36	43 (1%) 78 77	15, 28, 47, 73	2 (0%)

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	335	TRP	3.7
1	D	3	THR	3.7
1	F	335	TRP	3.6
1	F	331	VAL	3.5
1	B	335	TRP	3.5
1	G	501	ASP	3.1
1	B	507	GLY	3.0
1	F	504	LEU	3.0
1	G	462	ALA	2.9
1	D	511	GLN	2.9
1	E	3	THR	2.9
1	B	338	ASN	2.8
1	B	505	ALA	2.8
1	B	331	VAL	2.8
1	E	511	GLN	2.8
1	H	461	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	502	LEU	2.7
1	B	3	THR	2.7
1	H	462	ALA	2.6
1	H	507	GLY	2.6
1	E	505	ALA	2.6
1	F	3	THR	2.5
1	F	510	PHE	2.5
1	G	461	GLY	2.5
1	G	337	PRO	2.5
1	G	3	THR	2.4
1	F	461	GLY	2.4
1	H	505	ALA	2.4
1	E	504	LEU	2.4
1	F	503	PRO	2.3
1	C	511	GLN	2.3
1	H	511	GLN	2.3
1	F	341	TYR	2.3
1	A	338	ASN	2.3
1	H	510	PHE	2.2
1	F	505	ALA	2.2
1	C	339	VAL	2.2
1	B	462	ALA	2.2
1	B	511	GLN	2.2
1	D	505	ALA	2.2
1	A	503	PRO	2.1
1	D	337	PRO	2.1
1	E	510	PHE	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

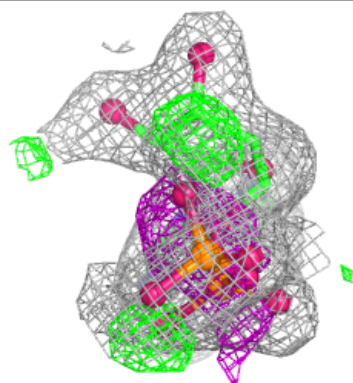
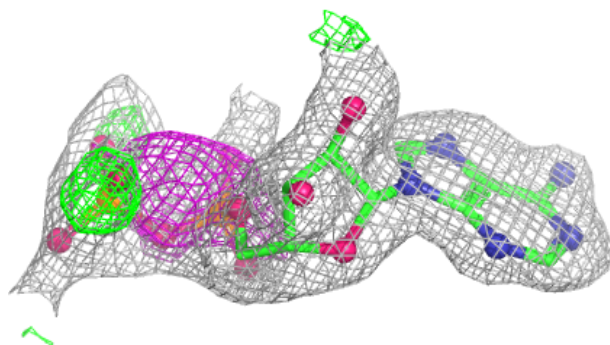
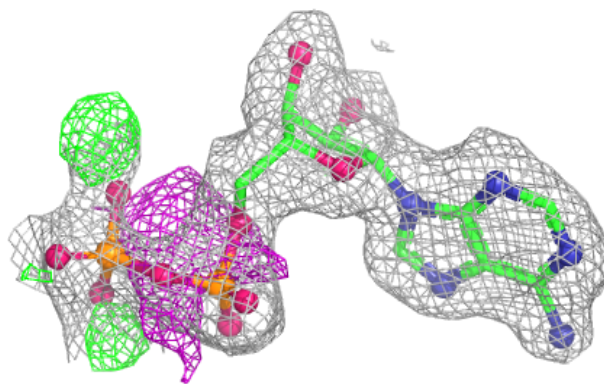
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAD	E	602	27/44	0.83	0.12	24,36,104,107	0
2	PG4	E	601	13/13	0.86	0.15	43,47,56,56	0
3	NAD	A	602	27/44	0.86	0.11	28,33,84,90	0
2	PG4	A	601	13/13	0.86	0.15	34,47,51,53	0
3	NAD	C	602	27/44	0.87	0.10	26,33,81,83	0
2	PG4	G	601	13/13	0.87	0.13	40,45,57,58	0
3	NAD	D	602	27/44	0.88	0.11	26,35,107,118	0
3	NAD	B	602	23/44	0.88	0.10	24,34,48,86	0
3	NAD	G	602	23/44	0.88	0.09	24,33,46,56	0
3	NAD	F	602	23/44	0.89	0.09	21,32,47,58	0
2	PG4	D	601	13/13	0.89	0.13	36,43,56,58	0
2	PG4	B	601	13/13	0.90	0.12	33,39,46,48	0
2	PG4	H	601	13/13	0.90	0.12	33,43,50,51	0
2	PG4	F	601	13/13	0.90	0.12	31,43,55,56	0
3	NAD	H	602	23/44	0.90	0.09	21,27,37,42	23
2	PG4	C	601	13/13	0.91	0.10	30,39,46,46	0

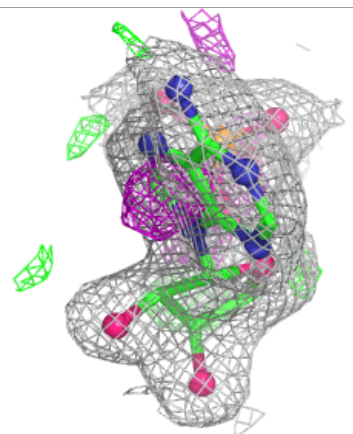
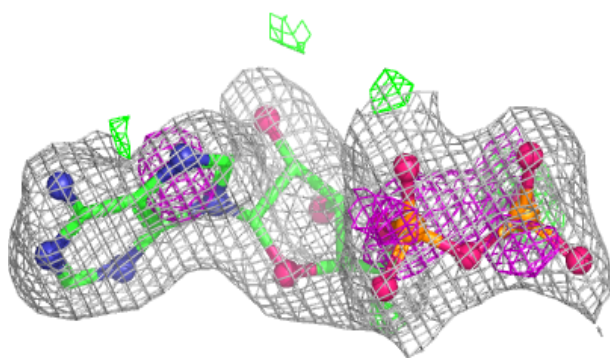
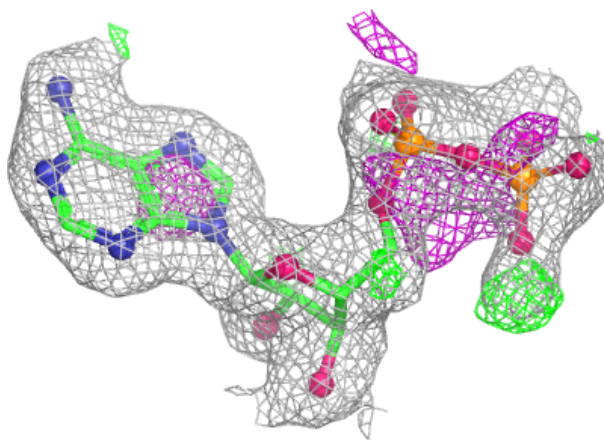
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAD E 602:

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

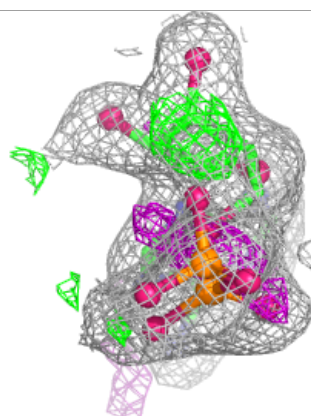
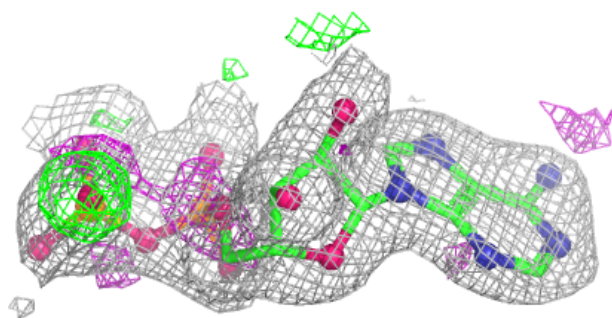
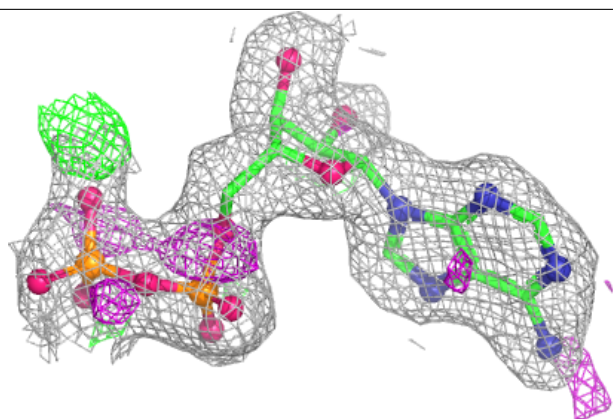
**Electron density around NAD A 602:**

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

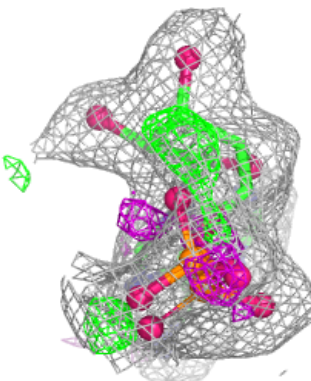
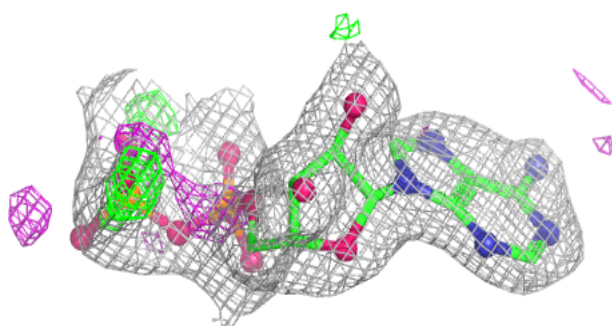
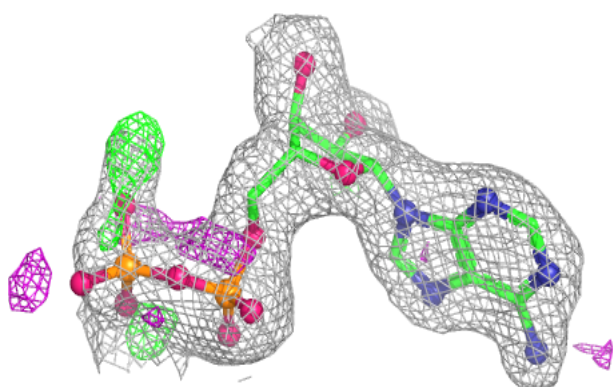


Electron density around NAD C 602:

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

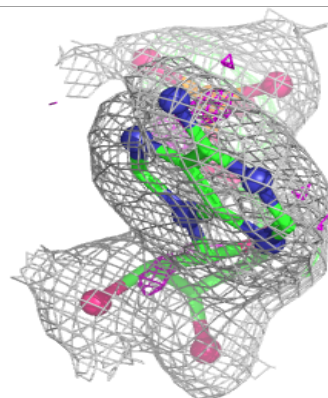
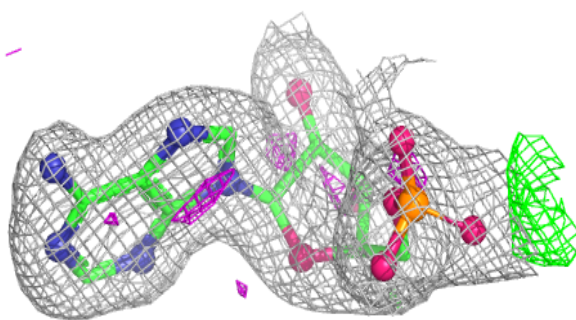
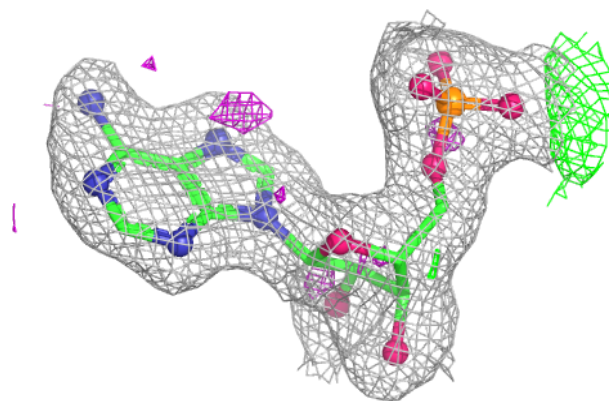
**Electron density around NAD D 602:**

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

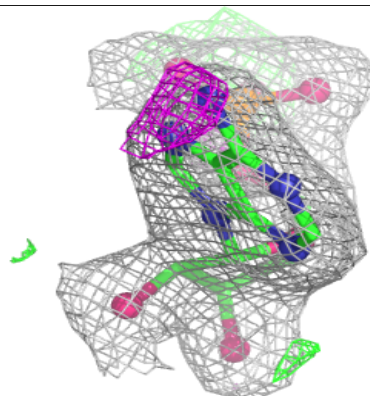
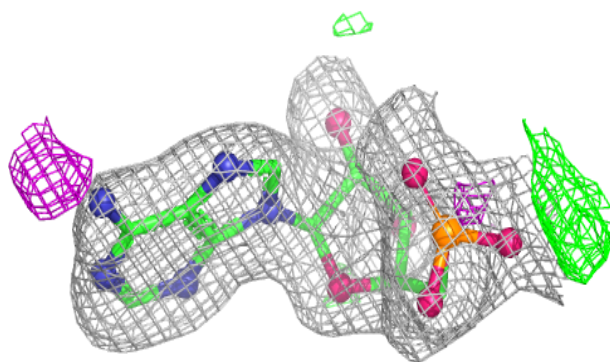
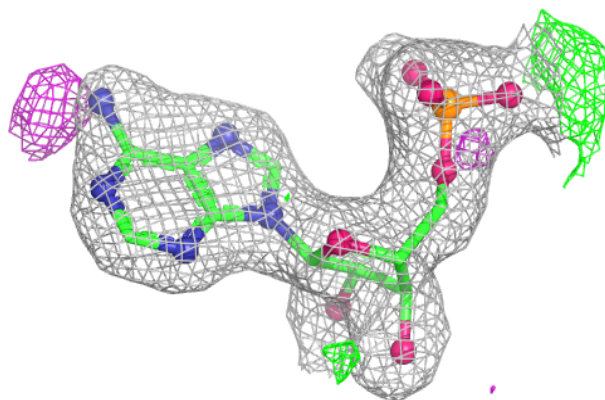


Electron density around NAD B 602:

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

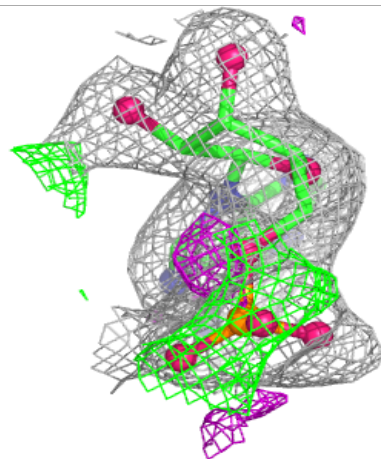
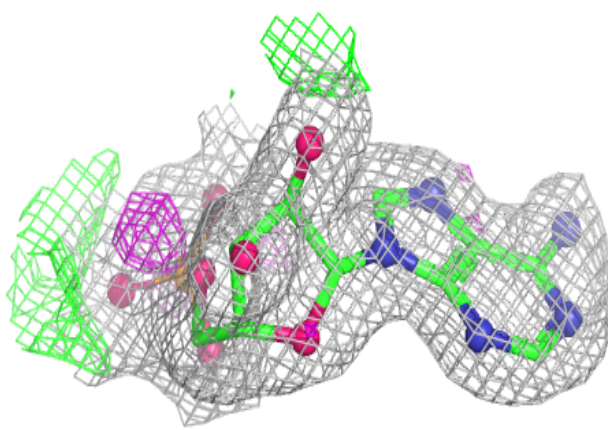
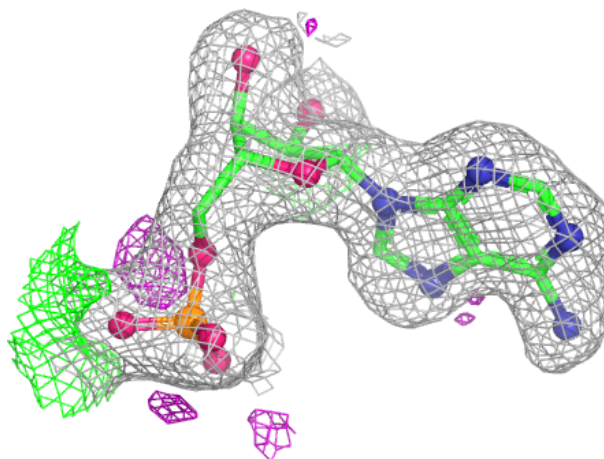
**Electron density around NAD G 602:**

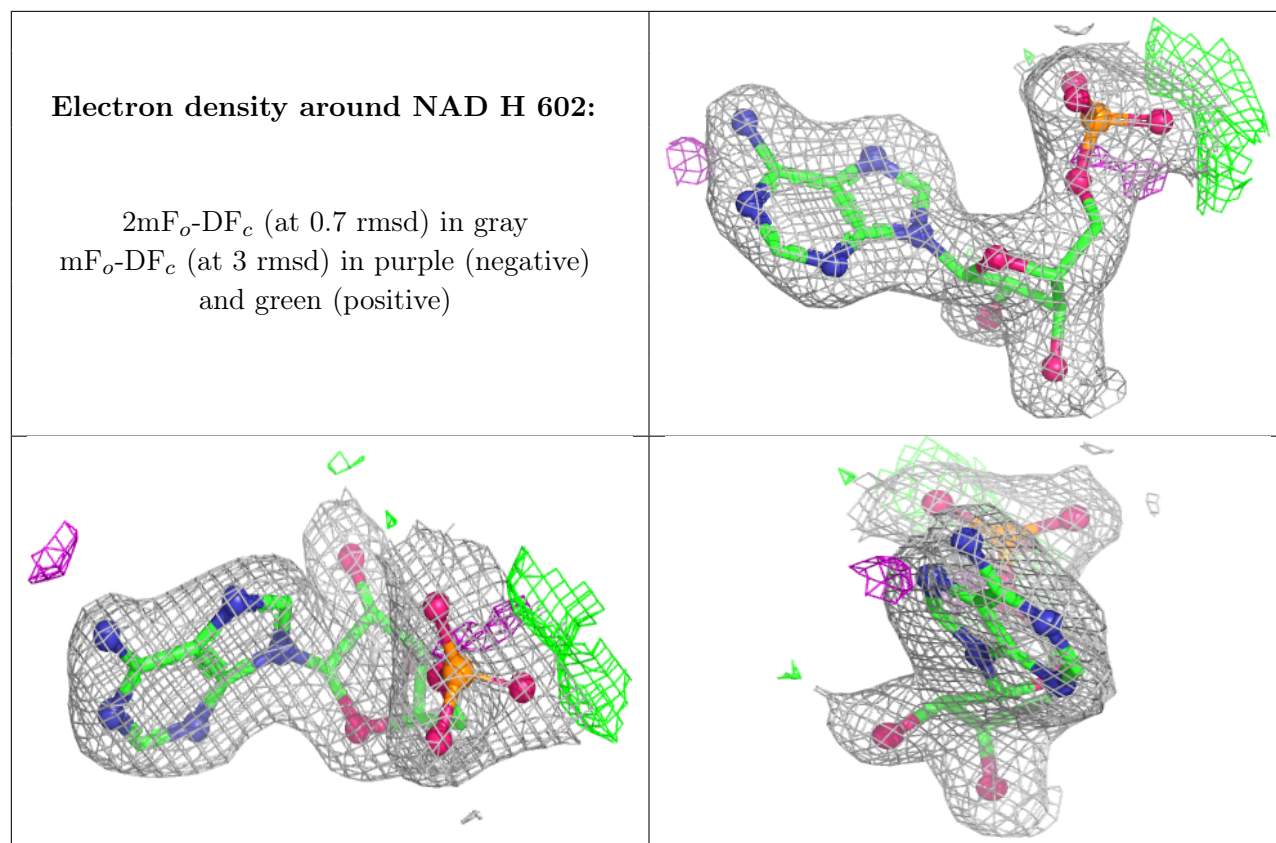
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.5 Other polymers [i](#)

There are no such residues in this entry.