



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:05 PM UTC

PDB ID : 1IY8 / pdb_00001iy8
Title : Crystal Structure of Levodione Reductase
Authors : Sogabe, S.; Fukami, T.; Shiratori, Y.; Yoshizumi, A.; Wada, M.
Deposited on : 2002-07-25
Resolution : 1.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

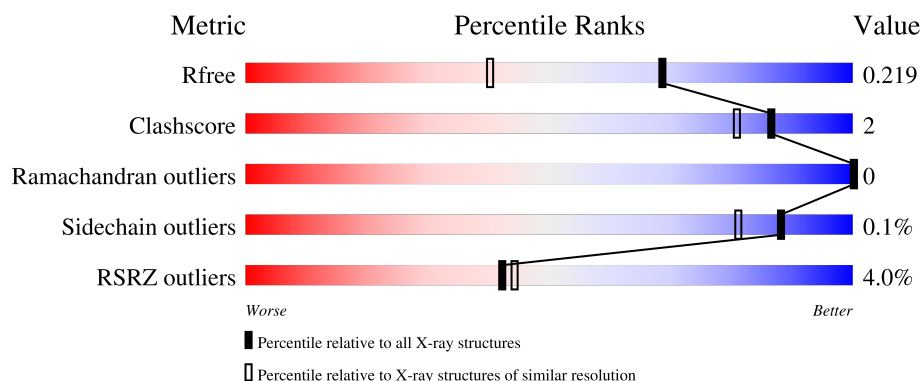
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 Å.

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



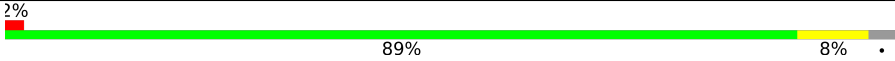
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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

Mol	Chain	Length	Quality of chain
1	A	267	3% 89% 8% .
1	B	267	4% 88% 9% .
1	C	267	4% 88% 8% .
1	D	267	4% 90% 7% .
1	E	267	3% 91% 5% .

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Mol	Chain	Length	Quality of chain
1	F	267	
1	G	267	
1	H	267	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16602 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 LEVODIONE REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	258	Total	C	N	O	S	0	0	0
			1904	1189	332	379	4			
1	B	258	Total	C	N	O	S	0	0	0
			1904	1189	332	379	4			
1	C	258	Total	C	N	O	S	0	0	0
			1904	1189	332	379	4			
1	D	258	Total	C	N	O	S	0	0	0
			1904	1189	332	379	4			
1	E	258	Total	C	N	O	S	0	0	0
			1904	1189	332	379	4			
1	F	258	Total	C	N	O	S	0	0	0
			1904	1189	332	379	4			
1	G	258	Total	C	N	O	S	0	0	0
			1904	1189	332	379	4			
1	H	258	Total	C	N	O	S	0	0	0
			1904	1189	332	379	4			

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



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		
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 (4R)-2-METHYLPENTANE-2,4-DIOL (CCD ID: MRD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 8 6 2	0	0
3	B	1	Total C O 8 6 2	0	0
3	C	1	Total C O 8 6 2	0	0
3	D	1	Total C O 8 6 2	0	0
3	E	1	Total C O 8 6 2	0	0
3	F	1	Total C O 8 6 2	0	0
3	G	1	Total C O 8 6 2	0	0
3	H	1	Total C O 8 6 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	121	Total O 121 121	0	0
4	B	114	Total O 114 114	0	0
4	C	125	Total O 125 125	0	0
4	D	117	Total O 117 117	0	0

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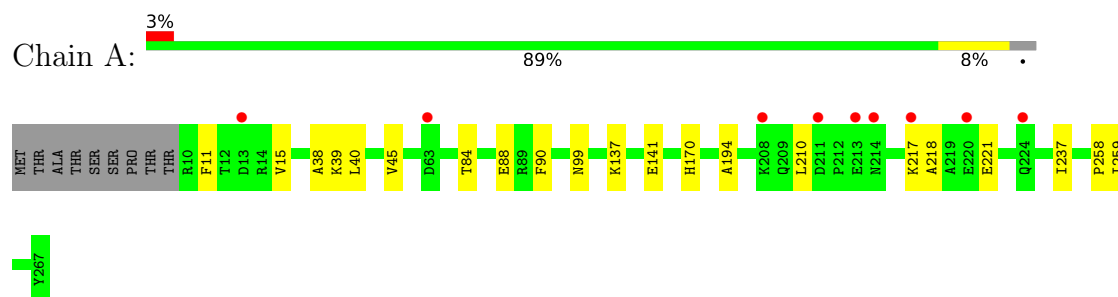
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	130	Total 130	O 130	0	0
4	F	117	Total 117	O 117	0	0
4	G	127	Total 127	O 127	0	0
4	H	103	Total 103	O 103	0	0

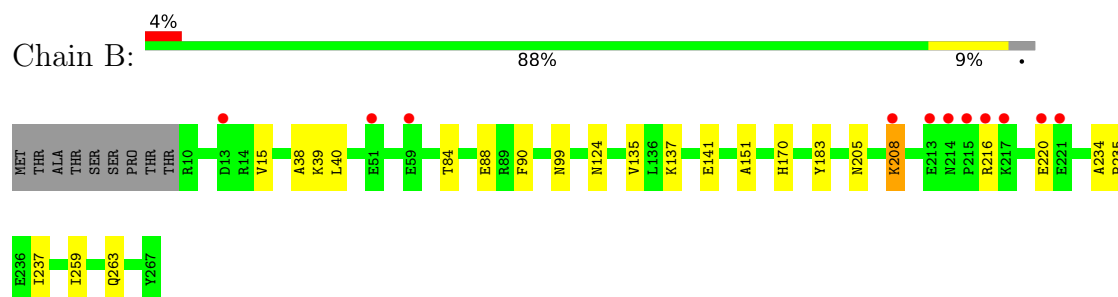
3 Residue-property plots [i](#)

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.

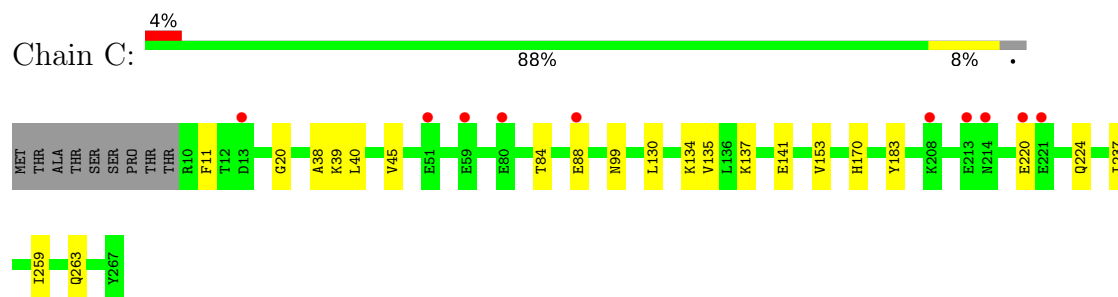
• Molecule 1: LEVODIONE REDUCTASE



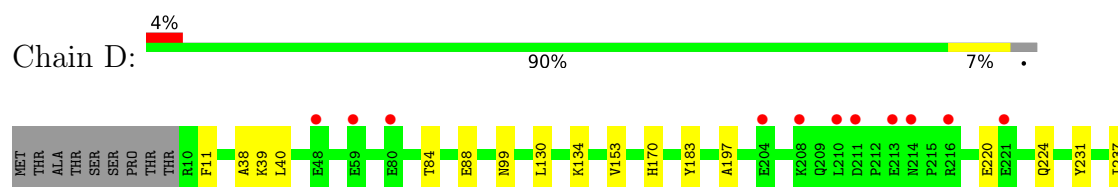
• Molecule 1: LEVODIONE REDUCTASE



• Molecule 1: LEVODIONE REDUCTASE

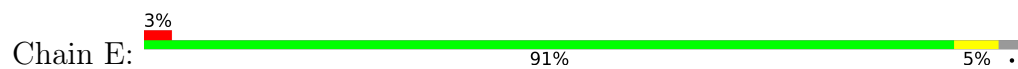


• Molecule 1: LEVODIONE REDUCTASE

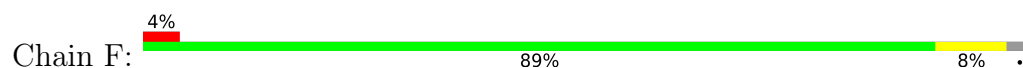




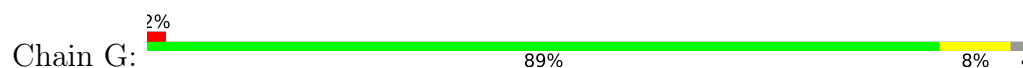
• Molecule 1: LEVODIONE REDUCTASE



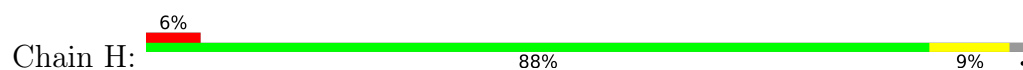
• Molecule 1: LEVODIONE REDUCTASE



• Molecule 1: LEVODIONE REDUCTASE



• Molecule 1: LEVODIONE REDUCTASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	66.67Å 79.18Å 112.67Å 103.87° 91.40° 105.48°	Depositor
Resolution (Å)	40.00 – 1.60 40.00 – 1.60	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-1.60) 92.1 (40.00-1.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.26 (at 1.60Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.199 , 0.219 0.199 , 0.219	Depositor DCC
R_{free} test set	13162 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	14.2	Xtriage
Anisotropy	0.449	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 37.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16602	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.11% 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, MRD

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	0.38	0/1931	0.92	5/2617 (0.2%)
1	B	0.38	0/1931	0.94	10/2617 (0.4%)
1	C	0.38	0/1931	0.92	9/2617 (0.3%)
1	D	0.39	0/1931	0.93	8/2617 (0.3%)
1	E	0.38	0/1931	0.91	6/2617 (0.2%)
1	F	0.37	0/1931	0.92	7/2617 (0.3%)
1	G	0.38	0/1931	0.92	8/2617 (0.3%)
1	H	0.37	0/1931	0.92	7/2617 (0.3%)
All	All	0.38	0/15448	0.92	60/20936 (0.3%)

There are no bond length outliers.

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	99	ASN	N-CA-C	7.44	123.49	113.97
1	F	99	ASN	N-CA-C	7.42	123.47	113.97
1	A	99	ASN	N-CA-C	7.36	123.39	113.97
1	D	99	ASN	N-CA-C	7.21	123.61	114.31
1	B	99	ASN	N-CA-C	7.05	123.41	114.31
1	C	99	ASN	N-CA-C	7.05	123.00	113.97
1	F	263	GLN	N-CA-C	6.88	118.86	111.36
1	E	170	HIS	N-CA-C	-6.84	103.90	111.36
1	C	263	GLN	N-CA-C	6.83	118.73	111.28
1	E	99	ASN	N-CA-C	6.82	122.70	113.97
1	F	39	LYS	N-CA-C	-6.81	98.60	109.76
1	D	39	LYS	N-CA-C	-6.69	98.78	109.76
1	G	99	ASN	N-CA-C	6.67	122.92	114.31
1	G	39	LYS	N-CA-C	-6.62	98.91	109.76
1	G	263	GLN	N-CA-C	6.58	118.54	111.36
1	C	39	LYS	N-CA-C	-6.57	98.99	109.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	263	GLN	N-CA-C	6.45	119.30	111.82
1	B	39	LYS	N-CA-C	-6.44	99.20	109.76
1	E	39	LYS	N-CA-C	-6.43	99.22	109.76
1	B	170	HIS	N-CA-C	-6.34	104.45	111.36
1	H	170	HIS	N-CA-C	-6.31	104.48	111.36
1	A	40	LEU	N-CA-C	6.24	119.36	109.50
1	G	170	HIS	N-CA-C	-6.15	104.66	111.36
1	A	39	LYS	N-CA-C	-6.14	99.69	109.76
1	A	170	HIS	N-CA-C	-6.09	104.72	111.36
1	F	170	HIS	N-CA-C	-6.08	104.73	111.36
1	E	263	GLN	N-CA-C	6.03	118.82	111.82
1	D	263	GLN	N-CA-C	5.96	117.77	111.28
1	D	170	HIS	N-CA-C	-5.95	104.88	111.36
1	B	263	GLN	N-CA-C	5.93	117.83	111.36
1	H	39	LYS	N-CA-C	-5.89	100.09	109.76
1	H	153	VAL	N-CA-C	-5.87	103.83	112.04
1	C	170	HIS	N-CA-C	-5.86	104.97	111.36
1	B	124	ASN	N-CA-C	5.78	117.67	111.36
1	E	40	LEU	N-CA-C	5.66	118.78	109.72
1	H	40	LEU	N-CA-C	5.64	118.74	109.72
1	B	40	LEU	N-CA-C	5.59	118.67	109.72
1	F	153	VAL	N-CA-C	-5.54	104.28	112.04
1	G	99	ASN	N-CA-CB	-5.49	103.59	110.90
1	D	183	TYR	N-CA-C	5.48	120.08	113.17
1	F	40	LEU	N-CA-C	5.47	118.48	109.72
1	D	99	ASN	N-CA-CB	-5.46	103.64	110.90
1	G	153	VAL	N-CA-C	-5.43	104.43	112.04
1	B	151	ALA	N-CA-C	-5.38	104.37	108.78
1	H	183	TYR	N-CA-C	5.37	119.93	113.17
1	B	38	ALA	N-CA-C	5.31	117.54	110.53
1	G	40	LEU	N-CA-C	5.24	117.78	109.50
1	C	40	LEU	N-CA-C	5.20	118.04	109.72
1	C	135	VAL	N-CA-C	5.19	115.97	110.72
1	D	40	LEU	N-CA-C	5.19	118.03	109.72
1	B	183	TYR	N-CA-C	5.18	119.75	113.38
1	D	153	VAL	N-CA-C	-5.17	104.80	112.04
1	C	153	VAL	N-CA-C	-5.13	104.86	112.04
1	E	135	VAL	N-CA-C	5.10	115.87	110.72
1	G	20	GLY	N-CA-C	-5.10	107.05	114.90
1	C	20	GLY	N-CA-C	-5.07	106.06	114.48
1	C	183	TYR	N-CA-C	5.07	119.56	113.17
1	F	183	TYR	N-CA-C	5.07	119.56	113.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	99	ASN	N-CA-CB	-5.03	103.68	110.67
1	B	135	VAL	N-CA-C	5.01	115.78	110.72

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	1904	0	1894	10	0
1	B	1904	0	1894	8	0
1	C	1904	0	1894	8	0
1	D	1904	0	1894	6	0
1	E	1904	0	1894	4	0
1	F	1904	0	1894	9	0
1	G	1904	0	1894	11	0
1	H	1904	0	1894	10	0
2	A	44	0	26	2	0
2	B	44	0	26	0	0
2	C	44	0	26	2	0
2	D	44	0	26	0	0
2	E	44	0	26	0	0
2	F	44	0	26	0	0
2	G	44	0	26	2	0
2	H	44	0	26	1	0
3	A	8	0	14	0	0
3	B	8	0	14	0	0
3	C	8	0	14	0	0
3	D	8	0	14	0	0
3	E	8	0	14	0	0
3	F	8	0	14	0	0
3	G	8	0	14	0	0
3	H	8	0	14	0	0
4	A	121	0	0	0	0
4	B	114	0	0	0	0
4	C	125	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	117	0	0	0	0
4	E	130	0	0	0	0
4	F	117	0	0	0	0
4	G	127	0	0	0	0
4	H	103	0	0	0	0
All	All	16602	0	15472	66	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 (66) 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:216:ARG:HH12	1:H:220:GLU:HG3	1.58	0.66
1:F:198:ILE:HD12	1:F:237:ILE:HD11	1.78	0.66
1:G:198:ILE:HD12	1:G:237:ILE:HD11	1.84	0.58
1:H:237:ILE:HD13	1:H:259:ILE:HG21	1.86	0.57
1:C:237:ILE:HD13	1:C:259:ILE:HG21	1.86	0.56
1:C:137:LYS:O	1:C:141:GLU:HG3	2.04	0.56
1:E:237:ILE:HD13	1:E:259:ILE:HG21	1.89	0.55
1:E:84:THR:O	1:E:88:GLU:HG3	2.07	0.55
1:B:84:THR:O	1:B:88:GLU:HG3	2.07	0.54
1:G:237:ILE:HD12	1:G:237:ILE:N	2.24	0.53
1:B:208:LYS:HB2	1:B:208:LYS:NZ	2.23	0.53
1:F:84:THR:O	1:F:88:GLU:HG3	2.10	0.52
1:B:237:ILE:HD13	1:B:259:ILE:HG21	1.90	0.52
1:C:84:THR:O	1:C:88:GLU:HG3	2.09	0.52
1:A:217:LYS:O	1:A:221:GLU:HG3	2.10	0.52
1:B:137:LYS:O	1:B:141:GLU:HG3	2.09	0.52
1:D:237:ILE:HD13	1:D:259:ILE:HG21	1.92	0.51
1:H:84:THR:O	1:H:88:GLU:HG3	2.11	0.51
1:B:216:ARG:O	1:B:220:GLU:HG2	2.11	0.50
1:A:84:THR:O	1:A:88:GLU:HG3	2.12	0.49
1:A:137:LYS:O	1:A:141:GLU:HG3	2.12	0.49
1:G:11:PHE:HB3	1:G:38:ALA:HB2	1.95	0.49
1:G:45:VAL:HG13	2:G:7268:NAD:C2A	2.43	0.49
1:D:84:THR:O	1:D:88:GLU:HG3	2.13	0.49
1:H:220:GLU:O	1:H:224:GLN:HG2	2.13	0.48
1:C:220:GLU:O	1:C:224:GLN:HG2	2.12	0.48
1:F:237:ILE:HD12	1:F:237:ILE:N	2.29	0.48
1:F:198:ILE:CD1	1:F:237:ILE:HD11	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:ILE:HD13	1:A:259:ILE:HG21	1.95	0.47
1:G:45:VAL:HG13	2:G:7268:NAD:N1A	2.29	0.47
1:H:194:ALA:HB3	1:H:258:PRO:HA	1.95	0.47
1:H:216:ARG:NH1	1:H:220:GLU:HG3	2.28	0.47
1:G:84:THR:O	1:G:88:GLU:HG3	2.15	0.47
1:B:15:VAL:HG21	1:B:90:PHE:HB3	1.97	0.46
1:F:220:GLU:O	1:F:224:GLN:HG2	2.14	0.46
1:C:11:PHE:HB3	1:C:38:ALA:HB2	1.97	0.46
1:E:220:GLU:O	1:E:224:GLN:HG2	2.16	0.46
1:C:45:VAL:HG13	2:C:3268:NAD:C2A	2.45	0.46
1:D:197:ALA:HB1	1:D:231:TYR:CE1	2.51	0.45
1:D:11:PHE:HB3	1:D:38:ALA:HB2	1.98	0.45
1:A:210:LEU:HD23	1:A:218:ALA:HB1	1.98	0.44
1:H:45:VAL:HG13	2:H:8268:NAD:C2A	2.48	0.44
1:C:45:VAL:HG13	2:C:3268:NAD:N1A	2.33	0.44
1:A:15:VAL:HG21	1:A:90:PHE:HB3	2.00	0.44
1:H:210:LEU:HD23	1:H:218:ALA:HB1	1.99	0.44
1:G:198:ILE:CD1	1:G:237:ILE:HD11	2.48	0.43
1:B:205:ASN:O	1:B:208:LYS:HB3	2.18	0.43
1:G:15:VAL:HG21	1:G:90:PHE:HB3	2.00	0.43
1:D:220:GLU:O	1:D:224:GLN:HG2	2.19	0.43
1:A:11:PHE:HB3	1:A:38:ALA:HB2	2.01	0.43
1:E:234:ALA:HB3	1:E:235:PRO:HD3	2.01	0.42
1:H:15:VAL:HG21	1:H:90:PHE:HB3	2.00	0.42
1:B:234:ALA:HB3	1:B:235:PRO:HD3	2.01	0.42
1:G:130:LEU:O	1:G:134:LYS:HG2	2.20	0.42
1:D:130:LEU:O	1:D:134:LYS:HG2	2.20	0.42
1:F:55:ALA:O	1:F:59:GLU:HG3	2.20	0.41
1:G:208:LYS:HE2	1:G:208:LYS:HB2	1.94	0.41
1:A:45:VAL:HG13	2:A:1268:NAD:C2A	2.51	0.41
1:A:194:ALA:HB3	1:A:258:PRO:HA	2.03	0.41
1:H:197:ALA:HB1	1:H:231:TYR:CE2	2.56	0.41
1:A:45:VAL:HG13	2:A:1268:NAD:N1A	2.36	0.40
1:F:194:ALA:HB3	1:F:258:PRO:HA	2.04	0.40
1:G:226:ASN:HA	1:G:227:PRO:HD3	1.96	0.40
1:C:130:LEU:O	1:C:134:LYS:HG2	2.21	0.40
1:F:210:LEU:HD23	1:F:218:ALA:HB1	2.02	0.40
1:F:234:ALA:HB3	1:F:235:PRO:HD3	2.03	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	256/267 (96%)	248 (97%)	8 (3%)	0	100	100
1	B	256/267 (96%)	248 (97%)	8 (3%)	0	100	100
1	C	256/267 (96%)	248 (97%)	8 (3%)	0	100	100
1	D	256/267 (96%)	248 (97%)	8 (3%)	0	100	100
1	E	256/267 (96%)	247 (96%)	9 (4%)	0	100	100
1	F	256/267 (96%)	248 (97%)	8 (3%)	0	100	100
1	G	256/267 (96%)	247 (96%)	9 (4%)	0	100	100
1	H	256/267 (96%)	247 (96%)	9 (4%)	0	100	100
All	All	2048/2136 (96%)	1981 (97%)	67 (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	195/203 (96%)	195 (100%)	0	100	100
1	B	195/203 (96%)	194 (100%)	1 (0%)	81	70
1	C	195/203 (96%)	195 (100%)	0	100	100
1	D	195/203 (96%)	195 (100%)	0	100	100
1	E	195/203 (96%)	195 (100%)	0	100	100
1	F	195/203 (96%)	195 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	195/203 (96%)	195 (100%)	0	100	100
1	H	195/203 (96%)	194 (100%)	1 (0%)	81	70
All	All	1560/1624 (96%)	1558 (100%)	2 (0%)	88	81

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	208	LYS
1	H	48	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	162	GLN
1	A	224	GLN
1	B	162	GLN
1	C	162	GLN
1	D	162	GLN
1	E	162	GLN
1	F	162	GLN
1	H	162	GLN
1	H	224	GLN

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	NAD	F	6268	-	46,48,48	2.57	12 (26%)	64,73,73	1.35	10 (15%)
3	MRD	E	5269	-	7,7,7	0.42	0	9,10,10	0.43	0
2	NAD	B	2268	-	46,48,48	2.66	12 (26%)	64,73,73	1.25	6 (9%)
3	MRD	G	7269	-	7,7,7	0.52	0	9,10,10	0.44	0
2	NAD	D	4268	-	46,48,48	2.55	12 (26%)	64,73,73	1.34	9 (14%)
3	MRD	A	1269	-	7,7,7	0.62	0	9,10,10	0.38	0
3	MRD	D	4269	-	7,7,7	0.56	0	9,10,10	0.38	0
3	MRD	C	3269	-	7,7,7	0.54	0	9,10,10	0.41	0
3	MRD	F	6269	-	7,7,7	0.56	0	9,10,10	0.35	0
2	NAD	G	7268	-	46,48,48	2.59	12 (26%)	64,73,73	1.33	6 (9%)
2	NAD	A	1268	-	46,48,48	2.70	11 (23%)	64,73,73	1.44	7 (10%)
2	NAD	C	3268	-	46,48,48	2.62	12 (26%)	64,73,73	1.47	8 (12%)
2	NAD	H	8268	-	46,48,48	2.68	13 (28%)	64,73,73	1.44	7 (10%)
3	MRD	B	2269	-	7,7,7	0.52	0	9,10,10	0.32	0
2	NAD	E	5268	-	46,48,48	2.70	14 (30%)	64,73,73	1.24	5 (7%)
3	MRD	H	8269	-	7,7,7	0.46	0	9,10,10	0.41	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	NAD	F	6268	-	-	6/30/62/62	0/5/5/5
3	MRD	E	5269	-	-	0/5/5/5	-
2	NAD	B	2268	-	-	4/30/62/62	0/5/5/5
3	MRD	G	7269	-	-	0/5/5/5	-
2	NAD	D	4268	-	-	7/30/62/62	0/5/5/5
3	MRD	A	1269	-	-	0/5/5/5	-
3	MRD	D	4269	-	-	0/5/5/5	-
3	MRD	C	3269	-	-	0/5/5/5	-
3	MRD	F	6269	-	-	0/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	G	7268	-	-	5/30/62/62	0/5/5/5
2	NAD	A	1268	-	-	7/30/62/62	0/5/5/5
2	NAD	C	3268	-	-	5/30/62/62	0/5/5/5
2	NAD	H	8268	-	-	6/30/62/62	0/5/5/5
3	MRD	B	2269	-	-	0/5/5/5	-
2	NAD	E	5268	-	-	6/30/62/62	0/5/5/5
3	MRD	H	8269	-	-	0/5/5/5	-

All (98) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	8268	NAD	C2N-C3N	9.35	1.53	1.39
2	A	1268	NAD	C4N-C3N	9.21	1.53	1.39
2	B	2268	NAD	C2N-C3N	9.17	1.53	1.39
2	A	1268	NAD	C2N-C3N	8.68	1.52	1.39
2	E	5268	NAD	C2N-C3N	8.59	1.52	1.39
2	F	6268	NAD	C2N-C3N	8.53	1.52	1.39
2	C	3268	NAD	C2N-C3N	8.46	1.52	1.39
2	B	2268	NAD	C4N-C3N	8.24	1.51	1.39
2	D	4268	NAD	C2N-C3N	8.23	1.52	1.39
2	G	7268	NAD	C4N-C3N	8.05	1.51	1.39
2	G	7268	NAD	C2N-C3N	8.02	1.51	1.39
2	H	8268	NAD	C4N-C3N	8.00	1.51	1.39
2	E	5268	NAD	C4N-C3N	7.97	1.51	1.39
2	C	3268	NAD	C4N-C3N	7.84	1.51	1.39
2	E	5268	NAD	C5N-C4N	7.71	1.52	1.38
2	D	4268	NAD	C4N-C3N	7.69	1.51	1.39
2	C	3268	NAD	C5N-C4N	7.65	1.52	1.38
2	F	6268	NAD	C4N-C3N	7.64	1.51	1.39
2	H	8268	NAD	C5N-C4N	7.64	1.52	1.38
2	B	2268	NAD	C5N-C4N	7.57	1.51	1.38
2	A	1268	NAD	C5N-C4N	7.52	1.51	1.38
2	F	6268	NAD	C5N-C4N	7.41	1.51	1.38
2	G	7268	NAD	C5N-C4N	7.13	1.51	1.38
2	D	4268	NAD	C5N-C4N	6.92	1.50	1.38
2	D	4268	NAD	C5A-C4A	5.06	1.48	1.39
2	F	6268	NAD	C5A-C4A	4.97	1.48	1.39
2	E	5268	NAD	C5A-C4A	4.92	1.47	1.39
2	C	3268	NAD	C5A-C4A	4.81	1.47	1.39
2	A	1268	NAD	C5A-C4A	4.77	1.47	1.39
2	G	7268	NAD	C5A-C4A	4.74	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	5268	NAD	C5A-N7A	-4.55	1.30	1.39
2	B	2268	NAD	C5A-C4A	4.53	1.47	1.39
2	H	8268	NAD	C5A-C4A	4.40	1.46	1.39
2	C	3268	NAD	C5A-N7A	-4.27	1.31	1.39
2	G	7268	NAD	C5A-N7A	-4.14	1.31	1.39
2	H	8268	NAD	C5A-N7A	-4.13	1.31	1.39
2	A	1268	NAD	C5A-N7A	-4.02	1.31	1.39
2	F	6268	NAD	C5A-N7A	-3.99	1.31	1.39
2	D	4268	NAD	C5A-N7A	-3.96	1.31	1.39
2	B	2268	NAD	C5A-N7A	-3.92	1.31	1.39
2	C	3268	NAD	C8A-N7A	3.67	1.38	1.31
2	E	5268	NAD	PA-O3	3.63	1.63	1.59
2	A	1268	NAD	C8A-N7A	3.59	1.38	1.31
2	C	3268	NAD	C2N-N1N	3.48	1.38	1.35
2	F	6268	NAD	C3N-C7N	-3.48	1.45	1.50
2	G	7268	NAD	C2A-N3A	3.46	1.40	1.33
2	D	4268	NAD	C8A-N7A	3.46	1.38	1.31
2	E	5268	NAD	C8A-N7A	3.42	1.38	1.31
2	G	7268	NAD	C8A-N7A	3.37	1.38	1.31
2	H	8268	NAD	C3N-C7N	-3.17	1.45	1.50
2	F	6268	NAD	C8A-N7A	3.14	1.37	1.31
2	B	2268	NAD	C8A-N7A	3.07	1.37	1.31
2	D	4268	NAD	C3N-C7N	-3.01	1.46	1.50
2	B	2268	NAD	C4A-N3A	-2.97	1.28	1.34
2	H	8268	NAD	C8A-N7A	2.96	1.37	1.31
2	E	5268	NAD	C2A-N3A	2.94	1.39	1.33
2	H	8268	NAD	C2A-N3A	2.93	1.39	1.33
2	B	2268	NAD	C2A-N3A	2.88	1.39	1.33
2	A	1268	NAD	C2N-N1N	2.87	1.38	1.35
2	F	6268	NAD	C2A-N3A	2.83	1.39	1.33
2	B	2268	NAD	PA-O3	2.80	1.62	1.59
2	A	1268	NAD	C2A-N3A	2.76	1.38	1.33
2	C	3268	NAD	C4A-N3A	-2.74	1.29	1.34
2	C	3268	NAD	C2A-N3A	2.73	1.38	1.33
2	E	5268	NAD	C4A-N3A	-2.69	1.29	1.34
2	D	4268	NAD	C2A-N3A	2.68	1.38	1.33
2	G	7268	NAD	C3N-C7N	-2.67	1.46	1.50
2	D	4268	NAD	C4A-N3A	-2.67	1.29	1.34
2	G	7268	NAD	C2N-N1N	2.67	1.37	1.35
2	H	8268	NAD	C2N-N1N	2.66	1.37	1.35
2	B	2268	NAD	C3N-C7N	-2.66	1.46	1.50
2	A	1268	NAD	C3N-C7N	-2.66	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	6268	NAD	C4A-N3A	-2.54	1.29	1.34
2	E	5268	NAD	C3N-C7N	-2.49	1.46	1.50
2	G	7268	NAD	PN-O3	2.48	1.62	1.59
2	G	7268	NAD	C4A-N3A	-2.44	1.29	1.34
2	C	3268	NAD	C3N-C7N	-2.44	1.47	1.50
2	H	8268	NAD	C4A-N3A	-2.42	1.29	1.34
2	E	5268	NAD	C4A-N9A	2.38	1.42	1.37
2	D	4268	NAD	PN-O3	2.37	1.62	1.59
2	H	8268	NAD	O4D-C1D	2.33	1.43	1.40
2	D	4268	NAD	C2N-N1N	2.31	1.37	1.35
2	E	5268	NAD	C2N-N1N	2.27	1.37	1.35
2	A	1268	NAD	C4A-N3A	-2.27	1.30	1.34
2	B	2268	NAD	C4A-N9A	2.23	1.42	1.37
2	B	2268	NAD	C2N-N1N	2.20	1.37	1.35
2	F	6268	NAD	PN-O3	2.18	1.61	1.59
2	E	5268	NAD	O4D-C1D	2.17	1.43	1.40
2	H	8268	NAD	C4A-N9A	2.16	1.42	1.37
2	A	1268	NAD	C6N-N1N	2.14	1.40	1.35
2	C	3268	NAD	C4A-N9A	2.12	1.42	1.37
2	F	6268	NAD	C2N-N1N	2.12	1.37	1.35
2	G	7268	NAD	C4A-N9A	2.11	1.42	1.37
2	H	8268	NAD	PN-O3	2.06	1.61	1.59
2	C	3268	NAD	O4D-C1D	2.03	1.43	1.40
2	F	6268	NAD	C4A-N9A	2.01	1.41	1.37
2	D	4268	NAD	C4A-N9A	2.01	1.41	1.37
2	E	5268	NAD	C6N-N1N	2.00	1.39	1.35

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1268	NAD	C5N-C4N-C3N	-4.79	115.65	120.36
2	H	8268	NAD	C5N-C4N-C3N	-4.77	115.67	120.36
2	B	2268	NAD	C5N-C4N-C3N	-4.51	115.93	120.36
2	H	8268	NAD	C5A-C4A-N9A	-4.18	101.25	105.81
2	A	1268	NAD	C5A-C4A-N9A	-4.18	101.25	105.81
2	F	6268	NAD	C5N-C4N-C3N	-4.17	116.27	120.36
2	G	7268	NAD	C5A-C4A-N9A	-4.16	101.28	105.81
2	G	7268	NAD	C5N-C4N-C3N	-4.10	116.33	120.36
2	C	3268	NAD	C5N-C4N-C3N	-4.04	116.39	120.36
2	F	6268	NAD	C5A-C4A-N9A	-3.90	101.56	105.81
2	E	5268	NAD	C5N-C4N-C3N	-3.88	116.55	120.36
2	D	4268	NAD	C5A-C4A-N9A	-3.88	101.59	105.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	3268	NAD	O7N-C7N-C3N	-3.86	114.88	119.60
2	C	3268	NAD	C5A-C4A-N9A	-3.61	101.88	105.81
2	E	5268	NAD	C5A-C4A-N9A	-3.43	102.07	105.81
2	C	3268	NAD	C3N-C7N-N7N	3.36	121.88	117.74
2	C	3268	NAD	C2A-N1A-C6A	3.35	124.23	118.73
2	B	2268	NAD	C5A-C4A-N9A	-3.31	102.20	105.81
2	E	5268	NAD	C2A-N1A-C6A	3.28	124.11	118.73
2	A	1268	NAD	C6A-C5A-C4A	-3.27	112.71	117.18
2	F	6268	NAD	O7N-C7N-C3N	-3.21	115.67	119.60
2	D	4268	NAD	C5N-C4N-C3N	-3.20	117.22	120.36
2	A	1268	NAD	C4A-N9A-C8A	3.08	108.97	105.74
2	A	1268	NAD	C2A-N1A-C6A	3.04	123.72	118.73
2	H	8268	NAD	C6A-C5A-C4A	-2.92	113.19	117.18
2	C	3268	NAD	C6A-C5A-C4A	-2.89	113.23	117.18
2	C	3268	NAD	N3A-C2A-N1A	-2.87	124.23	128.58
2	H	8268	NAD	C2A-N1A-C6A	2.84	123.40	118.73
2	D	4268	NAD	O7N-C7N-C3N	-2.82	116.15	119.60
2	G	7268	NAD	C4A-N9A-C8A	2.82	108.70	105.74
2	G	7268	NAD	C2A-N1A-C6A	2.79	123.32	118.73
2	H	8268	NAD	C4A-N9A-C8A	2.76	108.64	105.74
2	H	8268	NAD	N3A-C2A-N1A	-2.72	124.46	128.58
2	A	1268	NAD	N3A-C2A-N1A	-2.69	124.51	128.58
2	D	4268	NAD	C6N-N1N-C2N	2.67	124.15	121.88
2	D	4268	NAD	C4A-N9A-C8A	2.63	108.50	105.74
2	F	6268	NAD	C3N-C7N-N7N	2.62	120.96	117.74
2	B	2268	NAD	C2A-N1A-C6A	2.61	123.02	118.73
2	D	4268	NAD	C6A-C5A-C4A	-2.58	113.65	117.18
2	E	5268	NAD	C6A-C5A-C4A	-2.58	113.65	117.18
2	F	6268	NAD	C6A-C5A-C4A	-2.56	113.68	117.18
2	F	6268	NAD	C4A-N9A-C8A	2.56	108.42	105.74
2	E	5268	NAD	N3A-C2A-N1A	-2.54	124.74	128.58
2	H	8268	NAD	O7N-C7N-C3N	-2.52	116.51	119.60
2	G	7268	NAD	N3A-C2A-N1A	-2.41	124.94	128.58
2	G	7268	NAD	C6A-C5A-C4A	-2.41	113.89	117.18
2	D	4268	NAD	C2A-N1A-C6A	2.35	122.59	118.73
2	A	1268	NAD	C4A-N9A-C1B	-2.30	121.26	126.63
2	F	6268	NAD	C6N-N1N-C2N	2.21	123.76	121.88
2	F	6268	NAD	N3A-C4A-N9A	2.15	130.82	127.17
2	B	2268	NAD	O7N-C7N-C3N	-2.14	116.98	119.60
2	F	6268	NAD	C2A-N1A-C6A	2.13	122.22	118.73
2	D	4268	NAD	C3N-C7N-N7N	2.11	120.33	117.74
2	C	3268	NAD	C4D-O4D-C1D	2.08	111.83	109.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	6268	NAD	N3A-C2A-N1A	-2.08	125.43	128.58
2	D	4268	NAD	C4D-O4D-C1D	2.05	111.80	109.92
2	B	2268	NAD	C4A-N9A-C8A	2.05	107.89	105.74
2	B	2268	NAD	C6A-C5A-C4A	-2.02	114.42	117.18

There are no chirality outliers.

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1268	NAD	PN-O3-PA-O5B
2	A	1268	NAD	C5D-O5D-PN-O3
2	A	1268	NAD	C5D-O5D-PN-O1N
2	A	1268	NAD	C5D-O5D-PN-O2N
2	B	2268	NAD	C5D-O5D-PN-O3
2	B	2268	NAD	C5D-O5D-PN-O1N
2	C	3268	NAD	C5D-O5D-PN-O3
2	C	3268	NAD	C5D-O5D-PN-O1N
2	D	4268	NAD	C5D-O5D-PN-O3
2	D	4268	NAD	C5D-O5D-PN-O1N
2	D	4268	NAD	C5D-O5D-PN-O2N
2	E	5268	NAD	C5D-O5D-PN-O3
2	E	5268	NAD	C5D-O5D-PN-O1N
2	F	6268	NAD	C5D-O5D-PN-O3
2	F	6268	NAD	C5D-O5D-PN-O1N
2	G	7268	NAD	C5D-O5D-PN-O3
2	G	7268	NAD	C5D-O5D-PN-O1N
2	G	7268	NAD	C5D-O5D-PN-O2N
2	H	8268	NAD	C5D-O5D-PN-O3
2	H	8268	NAD	C5D-O5D-PN-O1N
2	D	4268	NAD	PN-O3-PA-O5B
2	E	5268	NAD	PN-O3-PA-O5B
2	F	6268	NAD	PN-O3-PA-O5B
2	G	7268	NAD	PN-O3-PA-O5B
2	H	8268	NAD	PN-O3-PA-O5B
2	A	1268	NAD	PA-O3-PN-O1N
2	G	7268	NAD	PA-O3-PN-O1N
2	B	2268	NAD	C5D-O5D-PN-O2N
2	C	3268	NAD	C5D-O5D-PN-O2N
2	E	5268	NAD	C5D-O5D-PN-O2N
2	F	6268	NAD	C5D-O5D-PN-O2N
2	H	8268	NAD	C5D-O5D-PN-O2N
2	D	4268	NAD	PA-O3-PN-O1N

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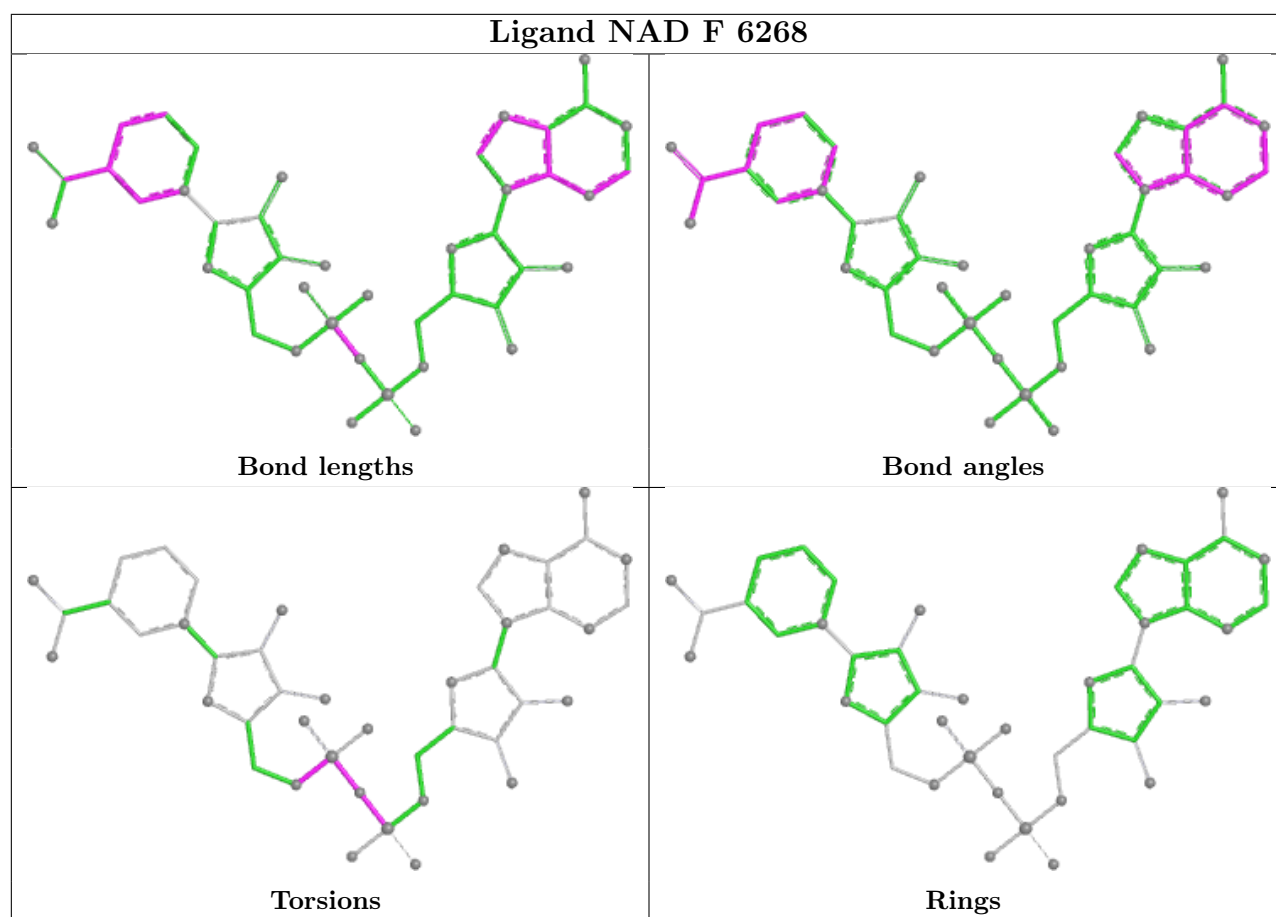
Mol	Chain	Res	Type	Atoms
2	F	6268	NAD	PA-O3-PN-O1N
2	H	8268	NAD	PA-O3-PN-O1N
2	A	1268	NAD	PA-O3-PN-O2N
2	E	5268	NAD	PA-O3-PN-O1N
2	A	1268	NAD	O4B-C4B-C5B-O5B
2	D	4268	NAD	O4B-C4B-C5B-O5B
2	C	3268	NAD	O4B-C4B-C5B-O5B
2	B	2268	NAD	PA-O3-PN-O2N
2	C	3268	NAD	PA-O3-PN-O2N
2	D	4268	NAD	PA-O3-PN-O2N
2	E	5268	NAD	PA-O3-PN-O2N
2	F	6268	NAD	PA-O3-PN-O2N
2	H	8268	NAD	PA-O3-PN-O2N

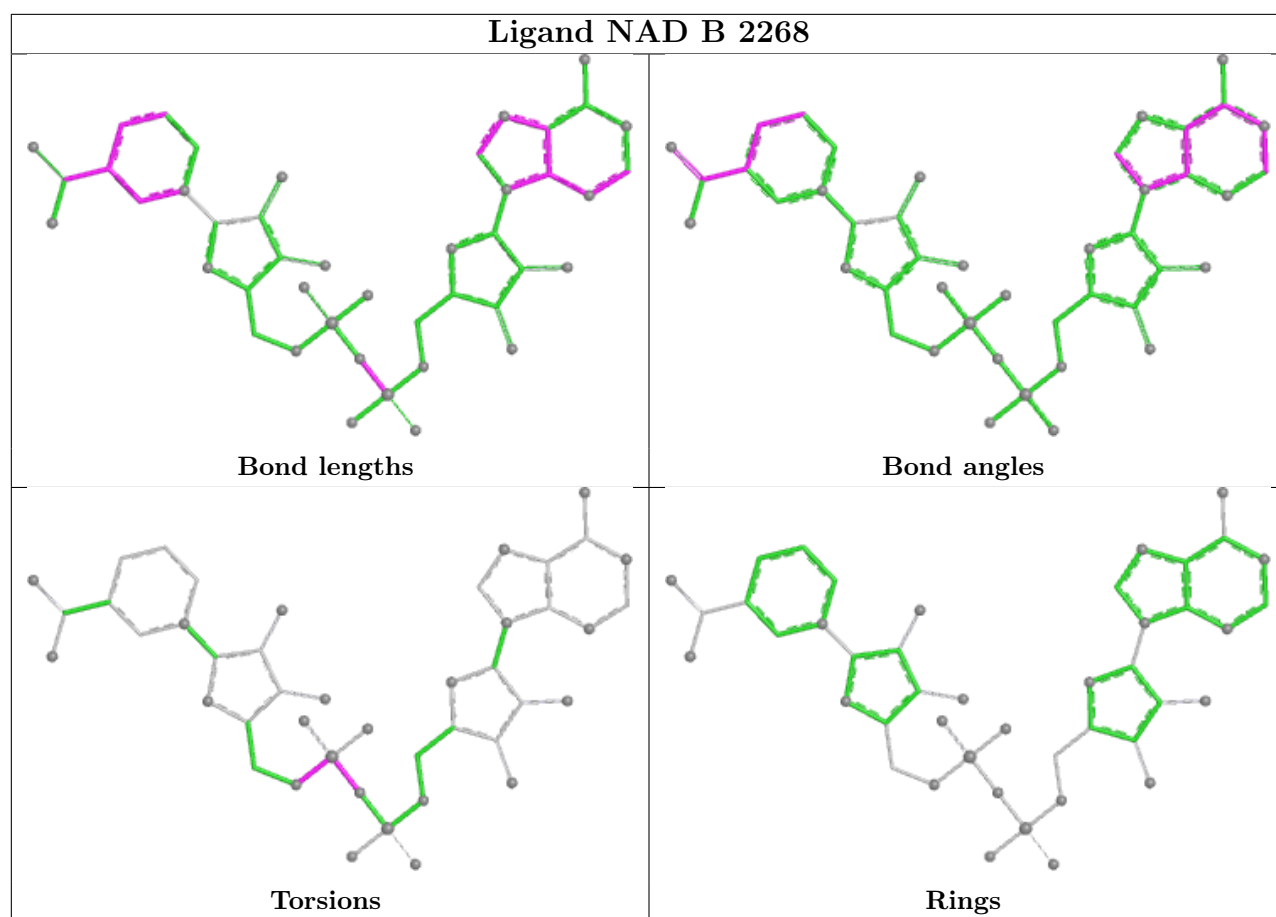
There are no ring outliers.

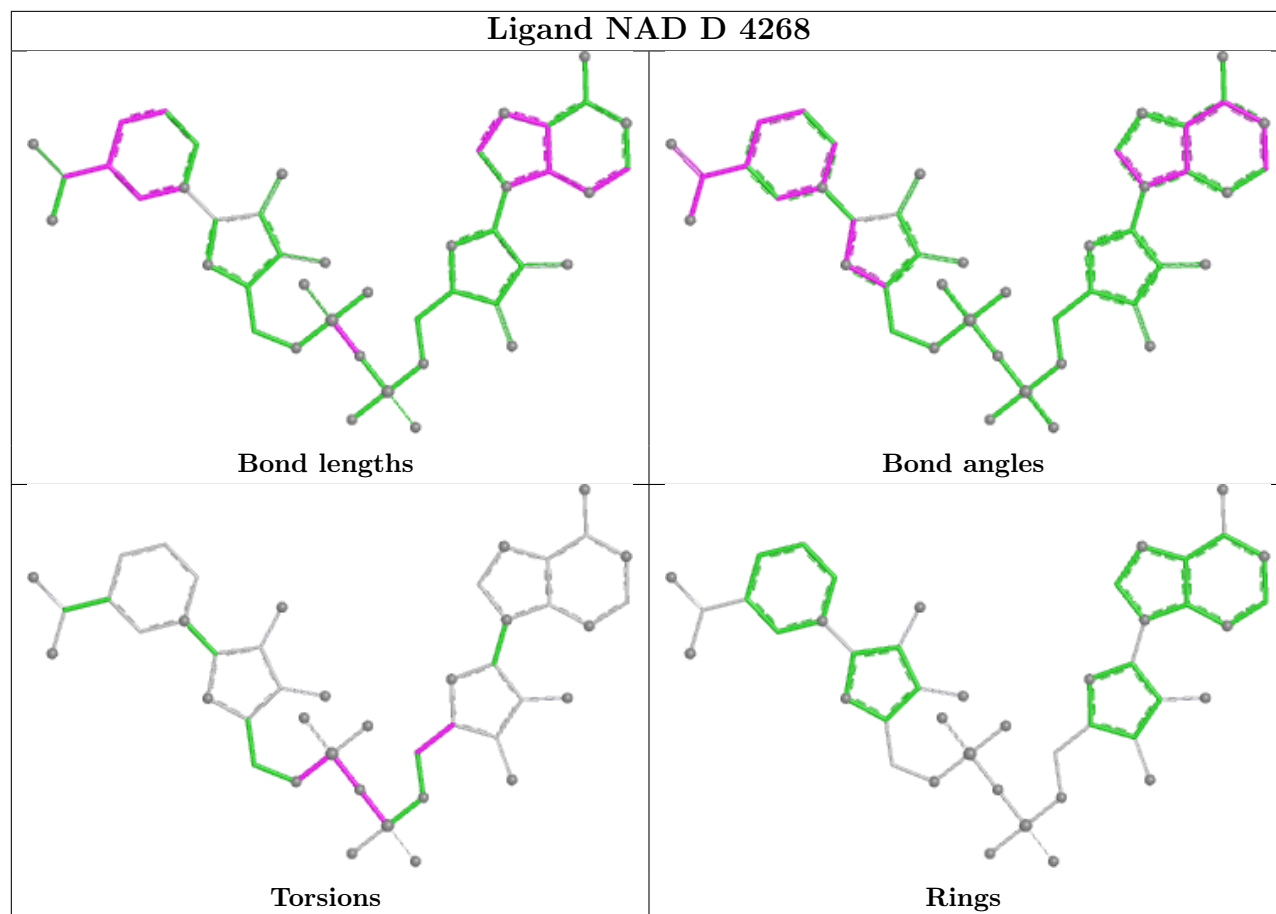
4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	7268	NAD	2	0
2	A	1268	NAD	2	0
2	C	3268	NAD	2	0
2	H	8268	NAD	1	0

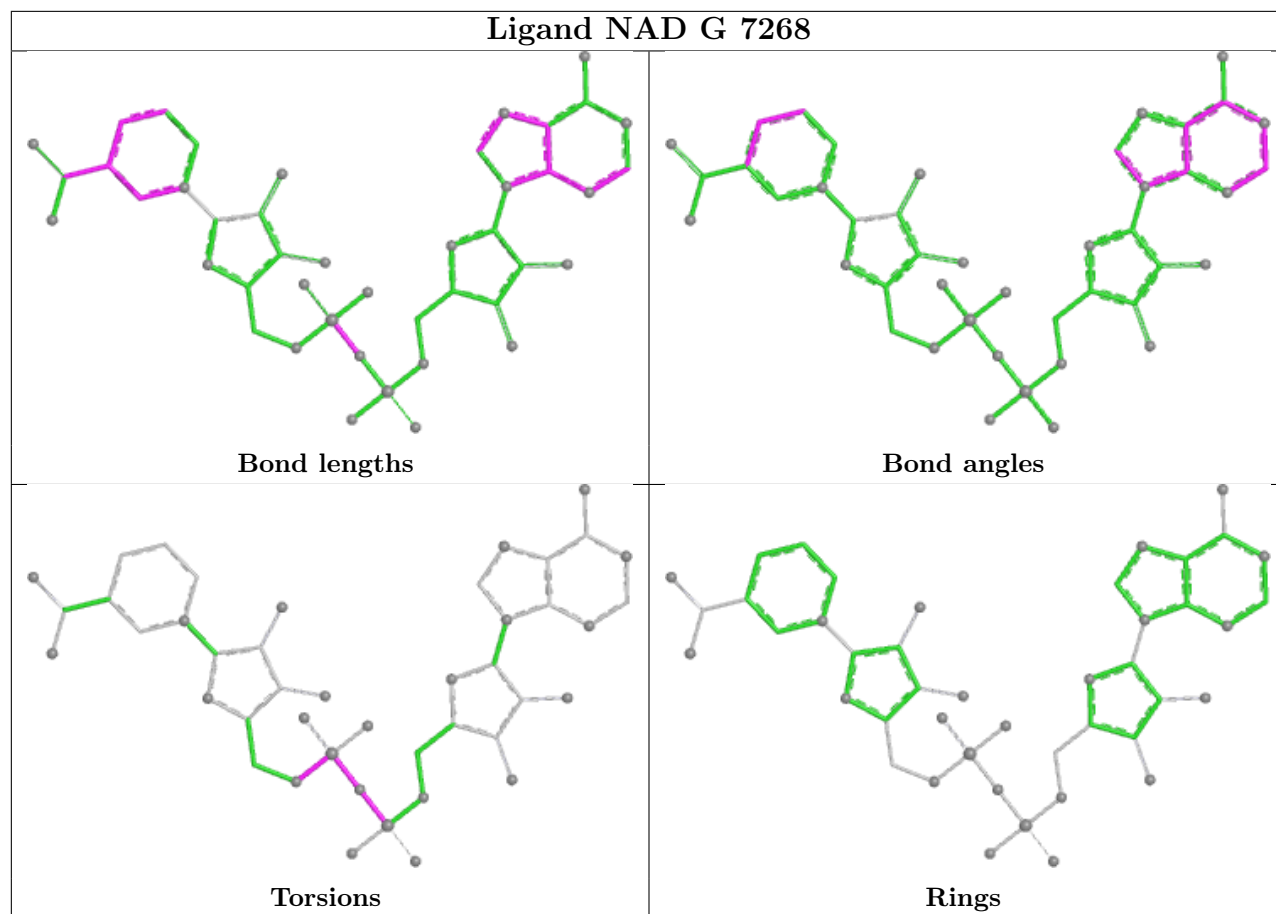
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



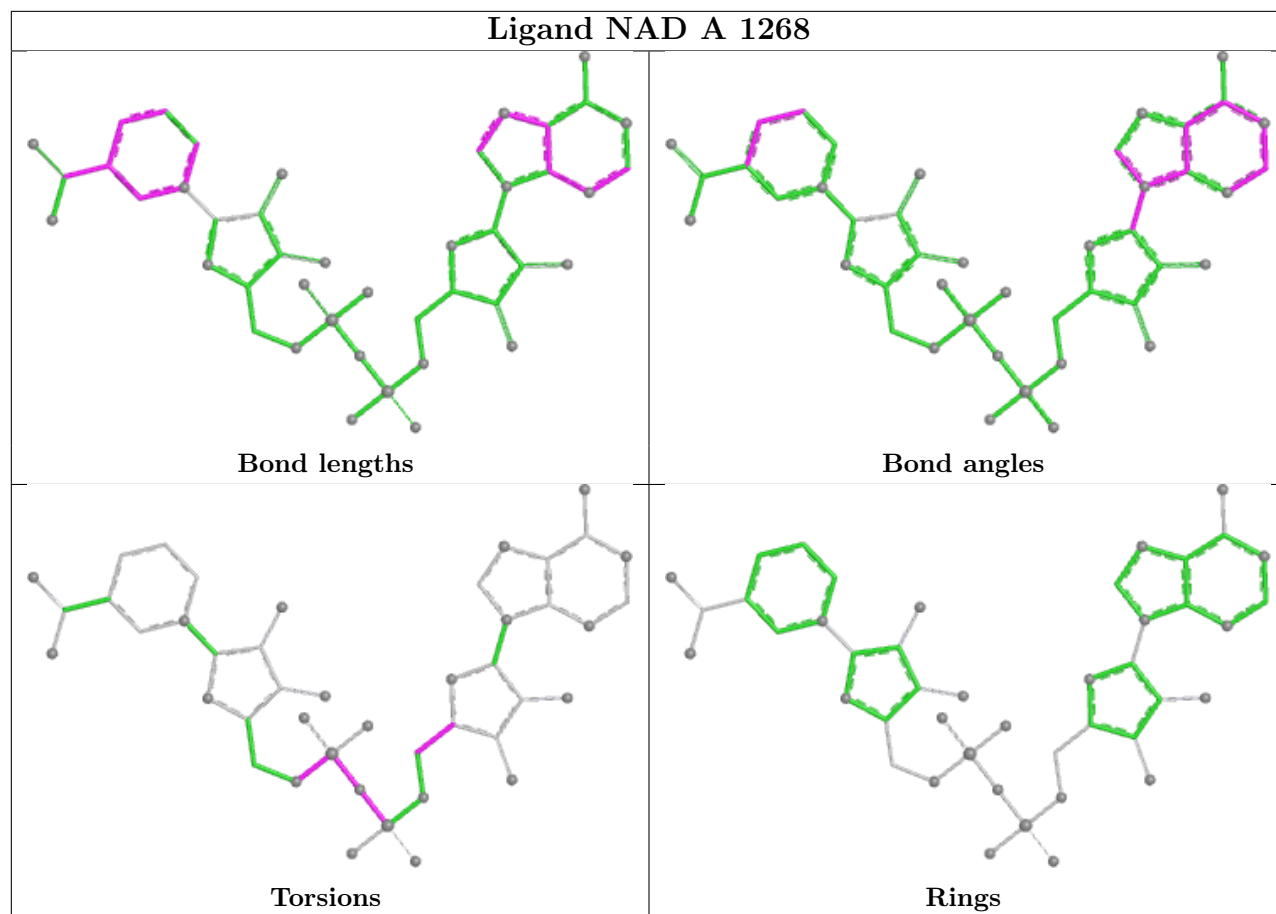


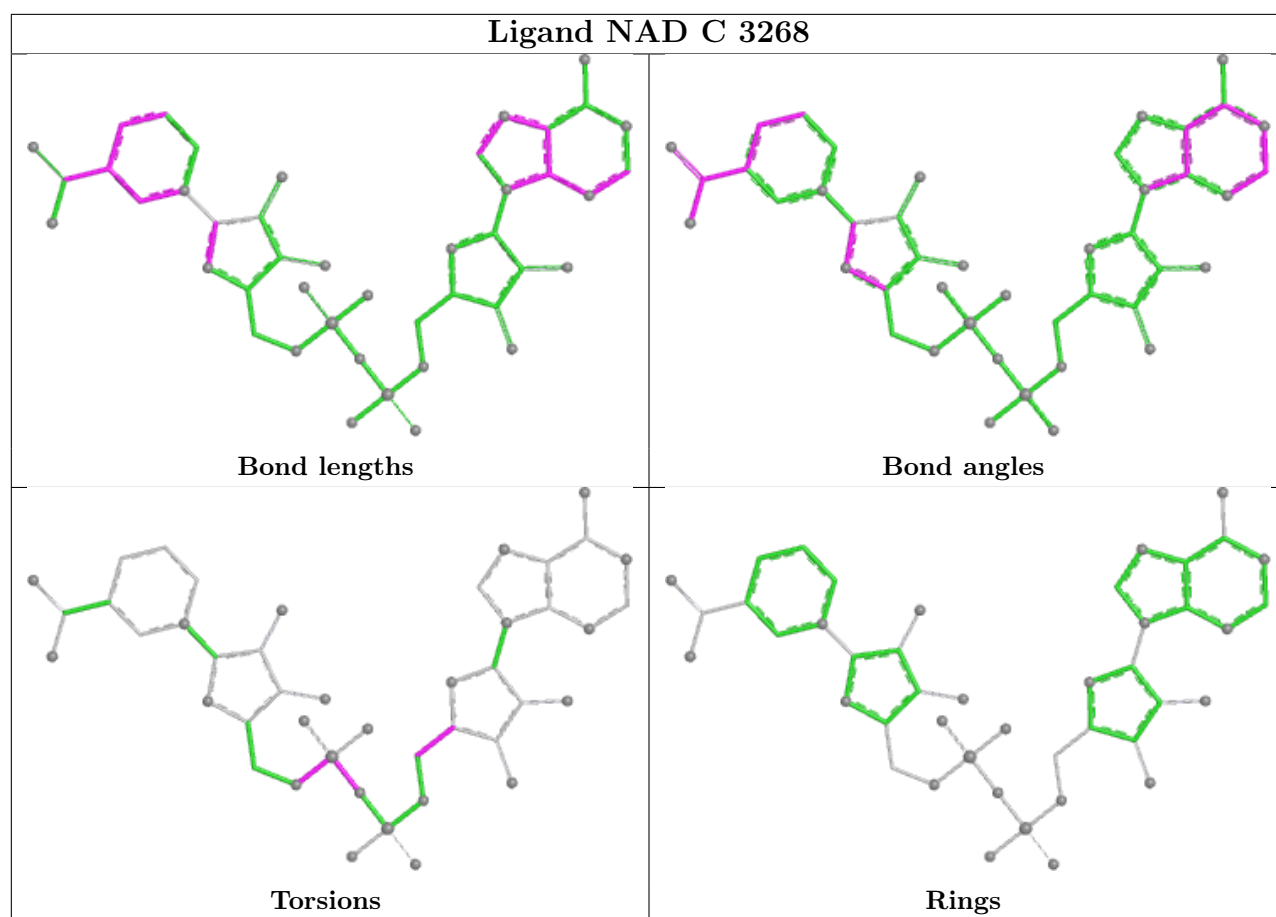


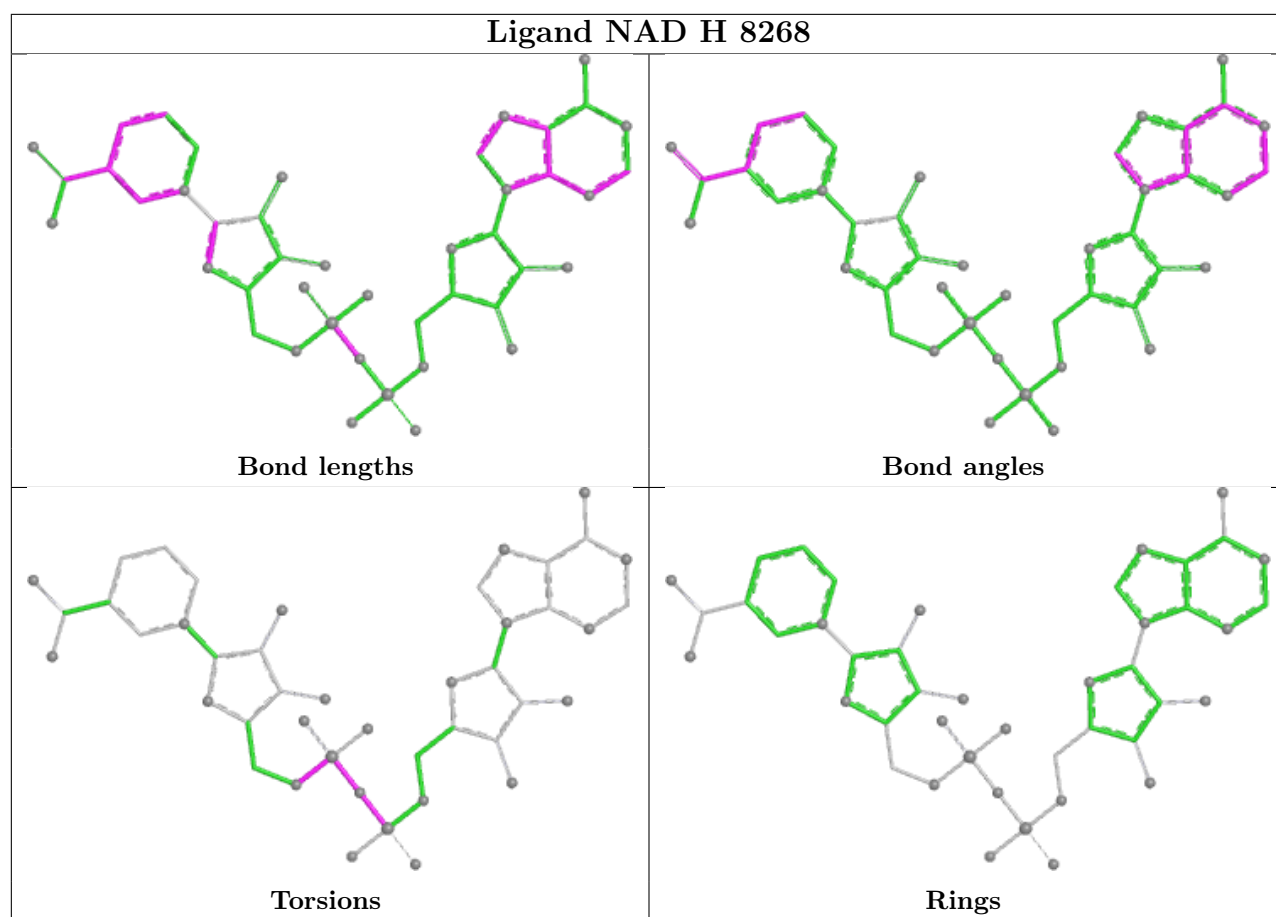
Ligand NAD G 7268

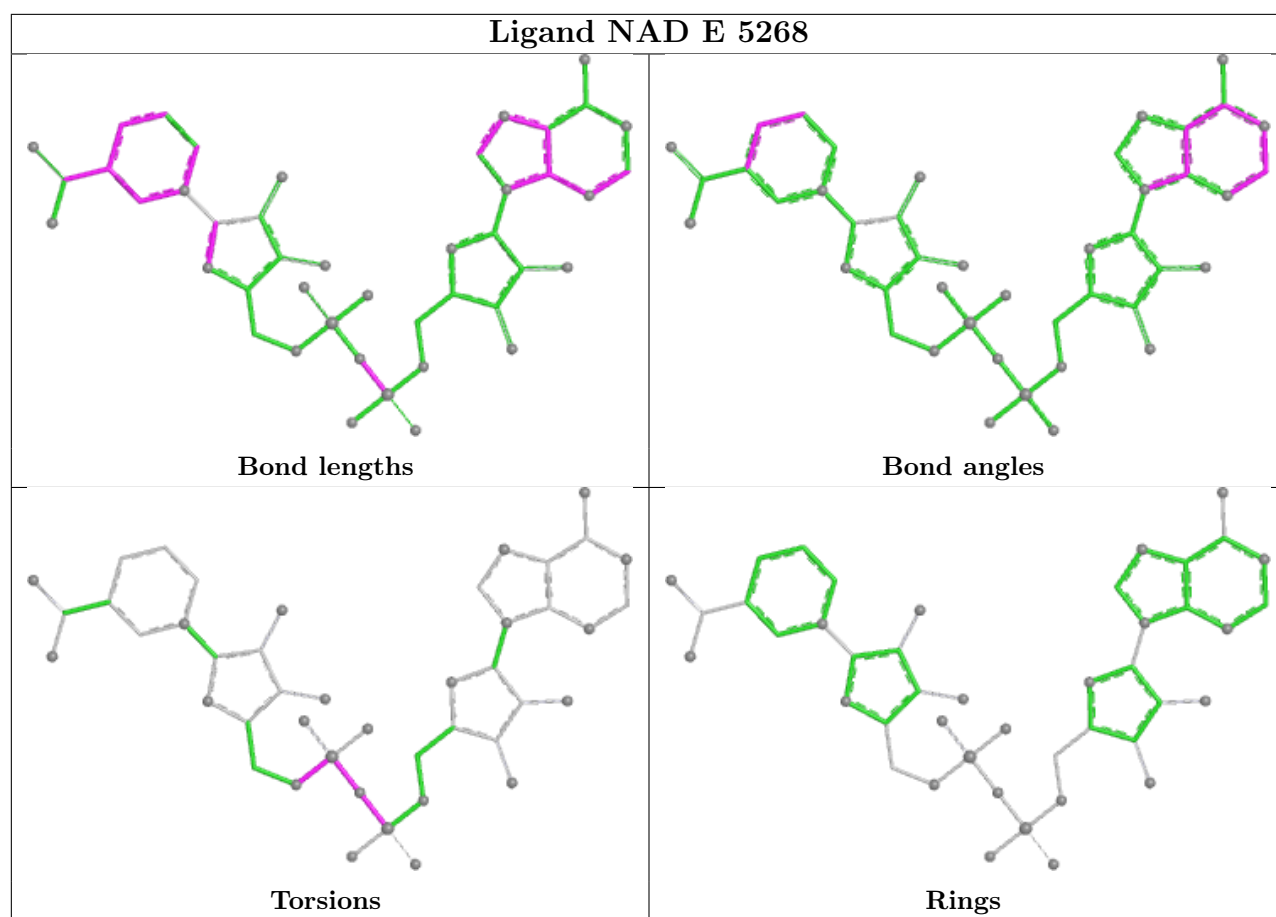


Ligand NAD A 1268









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	258/267 (96%)	0.14	9 (3%) 47 49	9, 14, 21, 27	0
1	B	258/267 (96%)	0.22	11 (4%) 40 41	9, 15, 22, 26	0
1	C	258/267 (96%)	0.15	10 (3%) 43 45	9, 15, 21, 26	0
1	D	258/267 (96%)	0.19	11 (4%) 40 41	8, 14, 22, 27	0
1	E	258/267 (96%)	0.17	9 (3%) 47 49	9, 14, 22, 27	0
1	F	258/267 (96%)	0.25	12 (4%) 36 38	9, 15, 23, 27	0
1	G	258/267 (96%)	0.10	6 (2%) 61 64	9, 14, 21, 27	0
1	H	258/267 (96%)	0.31	15 (5%) 29 29	10, 15, 23, 27	0
All	All	2064/2136 (96%)	0.19	83 (4%) 42 44	8, 15, 22, 27	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	213	GLU	4.7
1	H	213	GLU	4.5
1	G	213	GLU	4.4
1	C	214	ASN	4.2
1	F	214	ASN	4.0
1	E	214	ASN	3.9
1	H	216	ARG	3.9
1	D	214	ASN	3.9
1	E	213	GLU	3.9
1	A	213	GLU	3.8
1	F	213	GLU	3.8
1	C	51	GLU	3.7
1	H	48	GLU	3.6
1	H	212	PRO	3.5
1	G	214	ASN	3.5
1	C	213	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	221	GLU	3.4
1	F	221	GLU	3.3
1	F	217	LYS	3.3
1	E	220	GLU	3.2
1	B	13	ASP	3.2
1	H	220	GLU	3.2
1	G	13	ASP	3.1
1	A	214	ASN	3.1
1	F	216	ARG	3.1
1	F	212	PRO	3.0
1	E	51	GLU	3.0
1	E	211	ASP	3.0
1	A	13	ASP	2.9
1	B	215	PRO	2.8
1	C	220	GLU	2.8
1	F	220	GLU	2.8
1	D	216	ARG	2.7
1	H	224	GLN	2.7
1	F	211	ASP	2.7
1	B	59	GLU	2.7
1	C	59	GLU	2.7
1	H	214	ASN	2.7
1	A	211	ASP	2.7
1	B	216	ARG	2.7
1	A	220	GLU	2.7
1	B	213	GLU	2.7
1	D	59	GLU	2.6
1	F	51	GLU	2.6
1	C	13	ASP	2.6
1	D	80	GLU	2.6
1	D	48	GLU	2.6
1	H	211	ASP	2.6
1	H	217	LYS	2.6
1	G	220	GLU	2.6
1	E	59	GLU	2.5
1	B	221	GLU	2.5
1	F	224	GLN	2.5
1	D	210	LEU	2.5
1	E	63	ASP	2.4
1	B	214	ASN	2.4
1	D	204	GLU	2.4
1	A	208	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	221	GLU	2.3
1	G	221	GLU	2.3
1	C	80	GLU	2.2
1	H	51	GLU	2.2
1	H	59	GLU	2.2
1	B	51	GLU	2.2
1	B	217	LYS	2.2
1	E	105	LYS	2.2
1	D	211	ASP	2.1
1	C	208	LYS	2.1
1	H	208	LYS	2.1
1	A	63	ASP	2.1
1	H	13	ASP	2.1
1	H	63	ASP	2.1
1	B	220	GLU	2.1
1	H	45	VAL	2.1
1	B	208	LYS	2.1
1	D	208	LYS	2.1
1	A	224	GLN	2.1
1	G	211	ASP	2.1
1	E	216	ARG	2.1
1	F	215	PRO	2.1
1	C	88	GLU	2.0
1	F	13	ASP	2.0
1	A	217	LYS	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 ⓘ

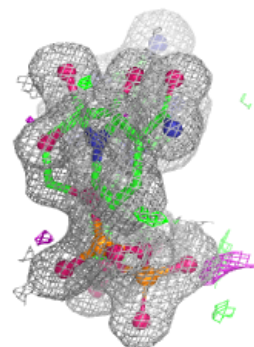
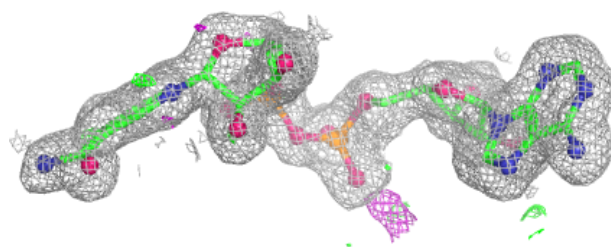
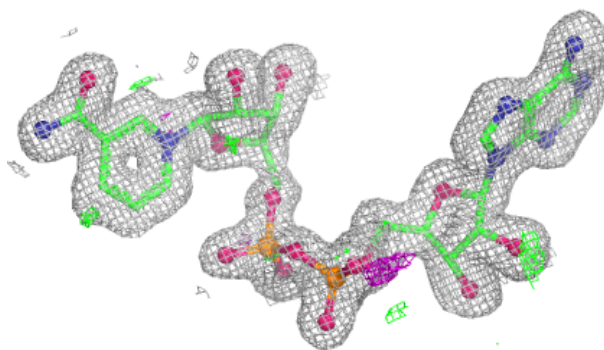
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
3	MRD	B	2269	8/8	0.87	0.10	19,20,21,22	0
3	MRD	G	7269	8/8	0.89	0.10	17,19,21,21	0
3	MRD	H	8269	8/8	0.90	0.10	20,20,21,22	0
3	MRD	F	6269	8/8	0.91	0.09	19,20,21,22	0
3	MRD	C	3269	8/8	0.92	0.08	19,20,21,21	0
3	MRD	D	4269	8/8	0.92	0.08	18,19,21,21	0
3	MRD	E	5269	8/8	0.92	0.07	17,19,21,21	0
3	MRD	A	1269	8/8	0.94	0.07	18,20,21,21	0
2	NAD	A	1268	44/44	0.96	0.07	11,14,16,17	0
2	NAD	B	2268	44/44	0.96	0.07	13,16,18,19	0
2	NAD	C	3268	44/44	0.96	0.07	12,15,17,19	0
2	NAD	D	4268	44/44	0.96	0.07	12,15,17,18	0
2	NAD	E	5268	44/44	0.96	0.07	11,15,17,19	0
2	NAD	F	6268	44/44	0.96	0.07	14,16,17,18	0
2	NAD	G	7268	44/44	0.96	0.07	10,14,16,17	0
2	NAD	H	8268	44/44	0.96	0.07	14,16,18,20	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.

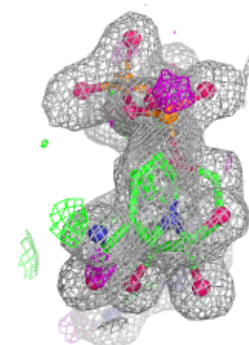
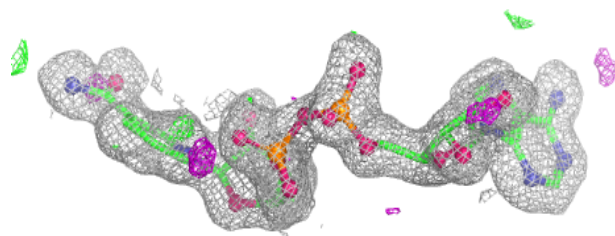
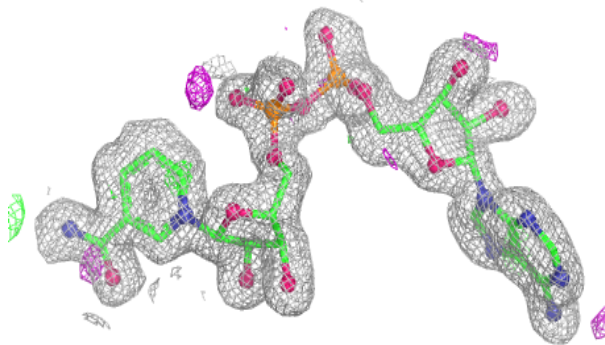
Electron density around NAD A 1268:

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

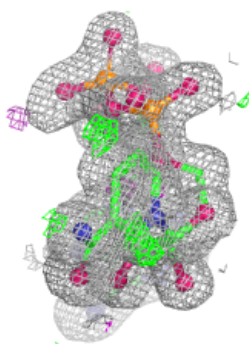
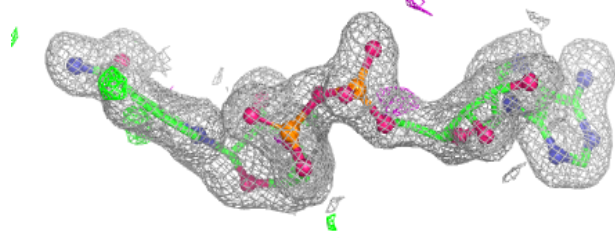
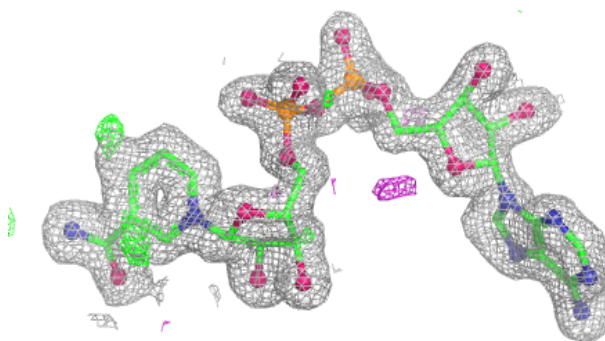


Electron density around NAD B 2268:

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

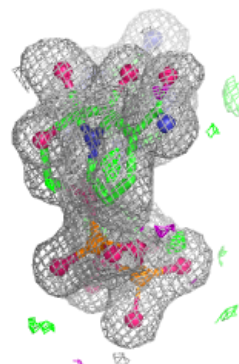
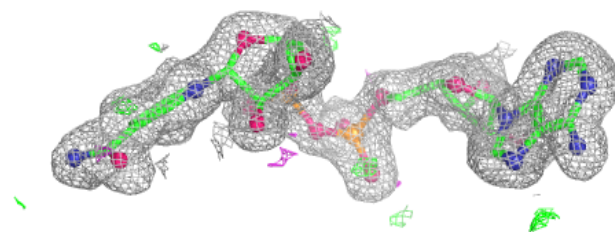
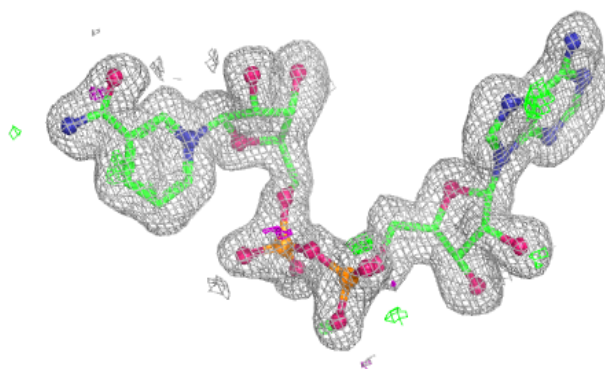
**Electron density around NAD C 3268:**

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

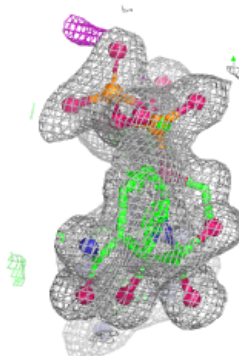
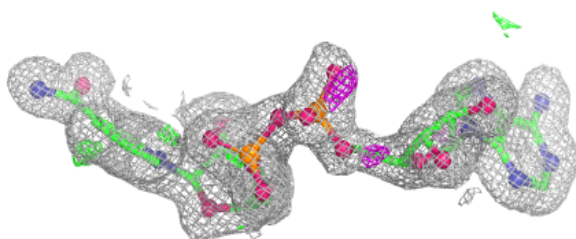
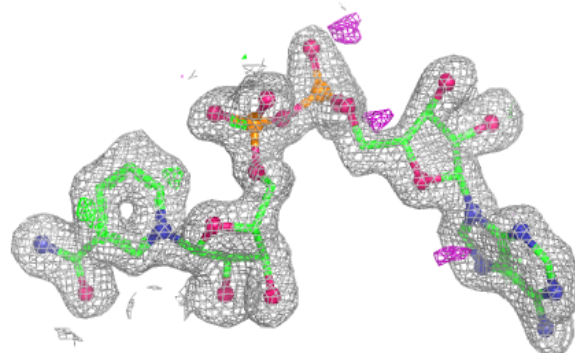


Electron density around NAD D 4268:

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

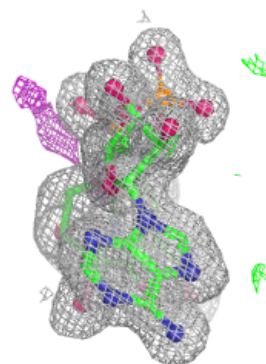
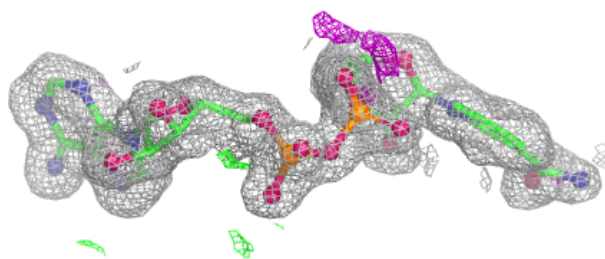
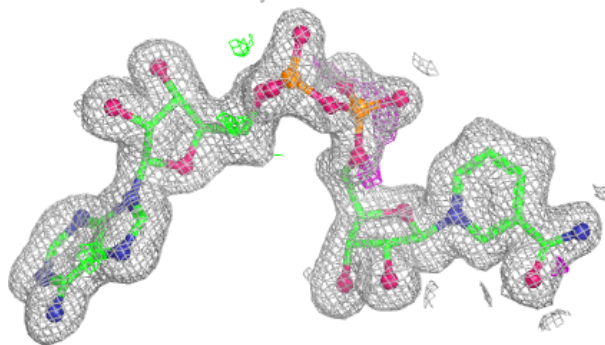
**Electron density around NAD E 5268:**

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

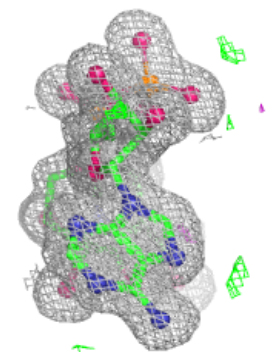
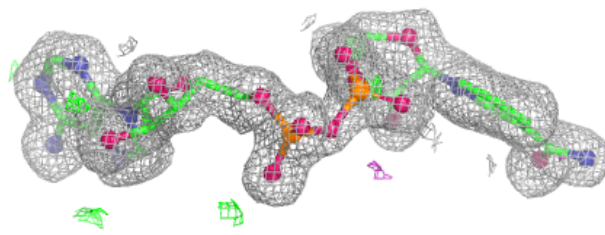
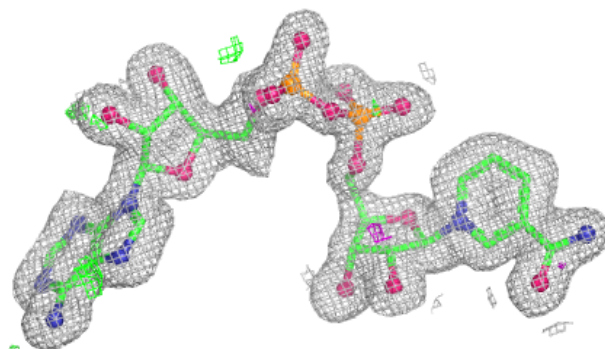


Electron density around NAD F 6268:

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

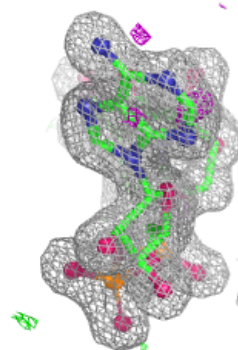
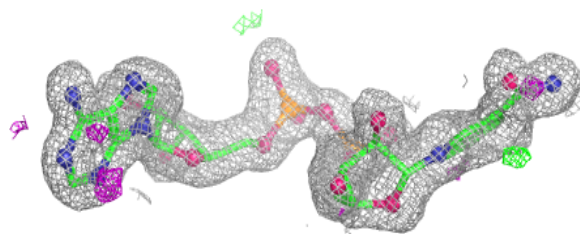
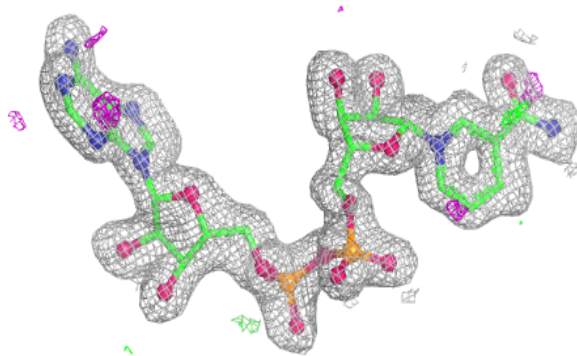
**Electron density around NAD G 7268:**

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



Electron density around NAD H 8268:

$2mF_o-DF_c$ (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.