



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 10:43 PM UTC

PDB ID : 2IZZ / pdb_00002izz
Title : Crystal structure of human pyrroline-5-carboxylate reductase
Authors : Pike, A.C.W.; Guo, K.; Kavanagh, K.; Pilka, E.S.; Berridge, G.; Colebrook, S.; Bray, J.; Salah, E.; Savitsky, P.; Papagrigoriou, E.; Turnbull, A.P.; von Delft, F.; Arrowsmith, C.; Edwards, A.; Weigelt, J.; Sundstrom, M.; Oppermann, U.
Deposited on : 2006-07-31
Resolution : 1.95 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

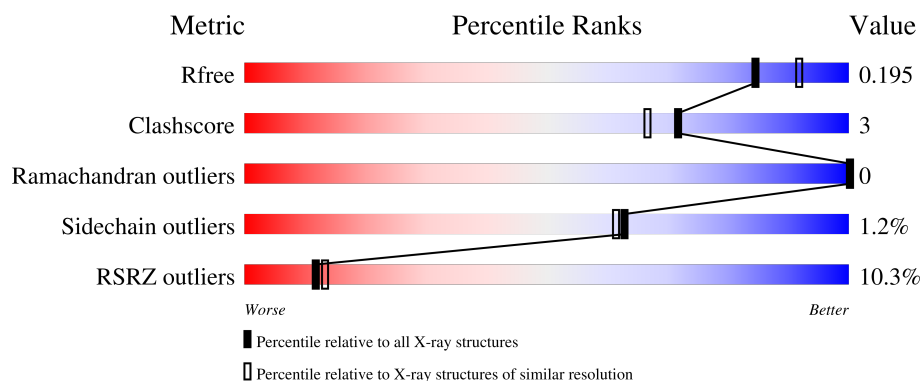
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	322	3% 78% 6% 16%
1	B	322	4% 81% 6% 13%
1	C	322	4% 82% • • 14%
1	D	322	20% 80% 5% 14%

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Mol	Chain	Length	Quality of chain
1	E	322	

2 Entry composition ⓘ

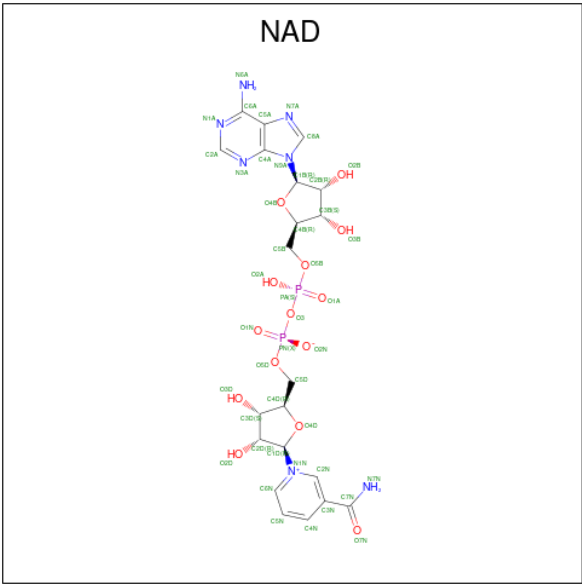
There are 4 unique types of molecules in this entry. The entry contains 10933 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PYRROLINE-5-CARBOXYLATE REDUCTASE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	272	Total	C	N	O	S	0	6	0
			1990	1253	353	370	14			
1	B	279	Total	C	N	O	S	0	1	0
			2042	1290	360	380	12			
1	C	276	Total	C	N	O	S	0	4	0
			1997	1255	351	378	13			
1	D	276	Total	C	N	O	S	0	2	0
			1985	1251	348	374	12			
1	E	272	Total	C	N	O	S	0	2	0
			1976	1245	353	365	13			

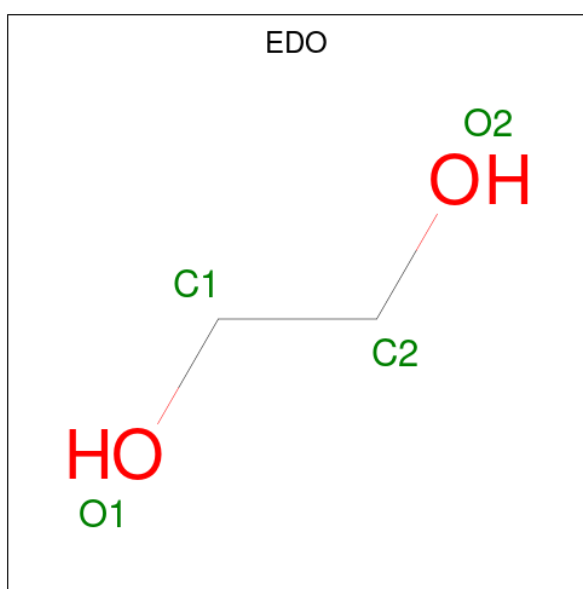
- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	E	1	Total	C	O	0	0
			4	2	2		

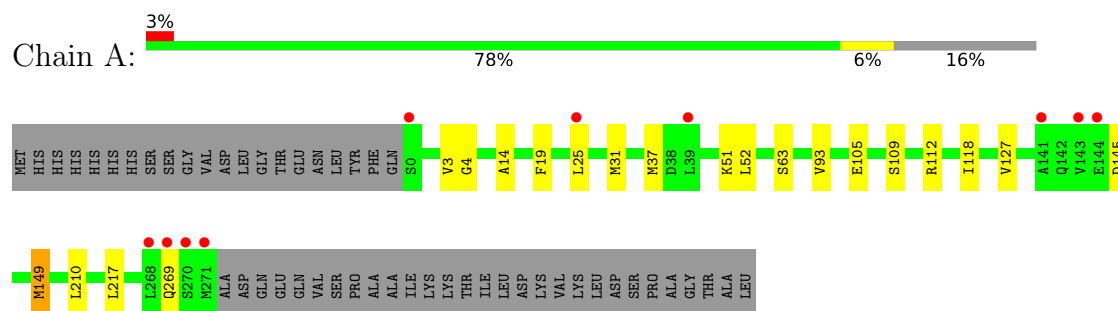
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	154	Total 154	O 154	0	0
4	B	166	Total 166	O 166	0	0
4	C	127	Total 127	O 127	0	0
4	D	127	Total 127	O 127	0	0
4	E	121	Total 121	O 121	0	2

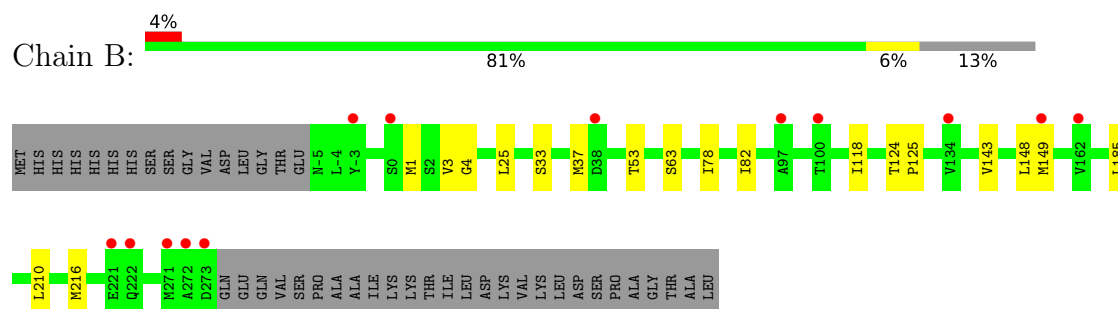
3 Residue-property plots [i](#)

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.

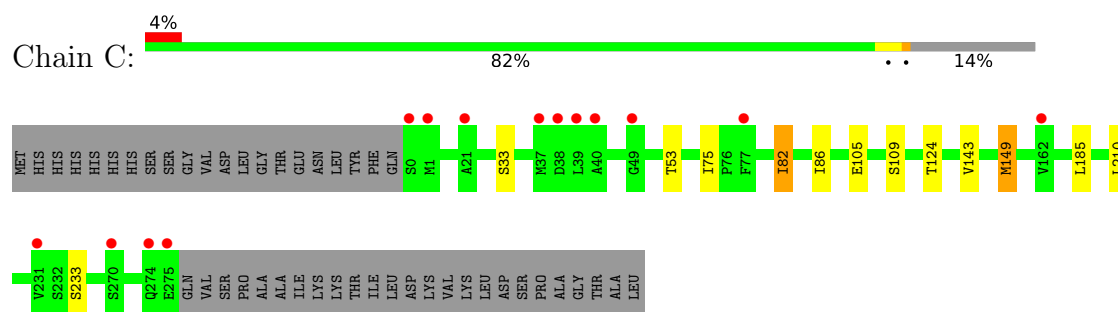
• Molecule 1: PYRROLINE-5-CARBOXYLATE REDUCTASE 1



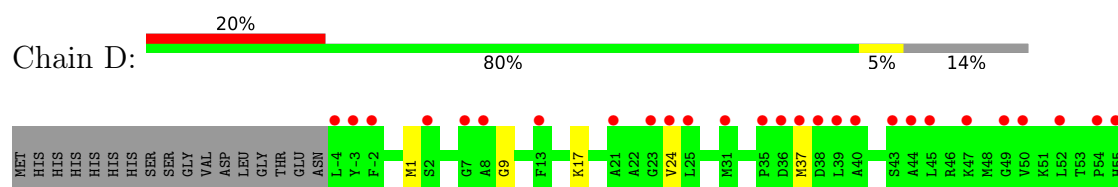
• Molecule 1: PYRROLINE-5-CARBOXYLATE REDUCTASE 1

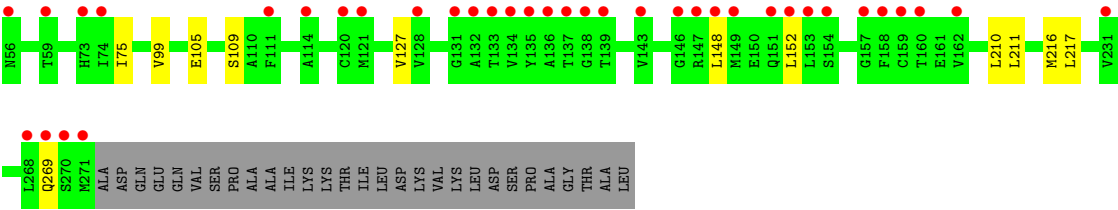


• Molecule 1: PYRROLINE-5-CARBOXYLATE REDUCTASE 1

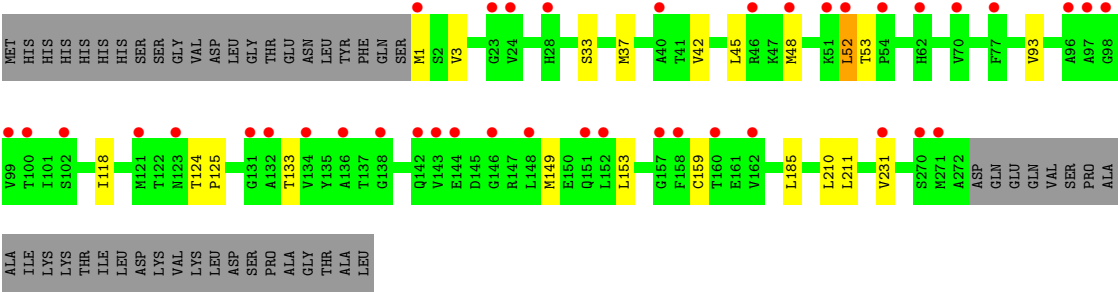
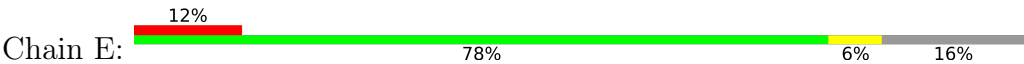


• Molecule 1: PYRROLINE-5-CARBOXYLATE REDUCTASE 1





● Molecule 1: PYRROLINE-5-CARBOXYLATE REDUCTASE 1



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	110.45Å 177.94Å 87.92Å 90.00° 106.70° 90.00°	Depositor
Resolution (Å)	40.00 – 1.95 40.00 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.9 (40.00-1.95) 99.9 (40.00-1.95)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.07 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.166 , 0.190 0.170 , 0.195	Depositor DCC
R_{free} test set	1835 reflections (1.56%)	wwPDB-VP
Wilson B-factor (Å ²)	27.5	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 42.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10933	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 4.27% 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, EDO

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	0.69	0/2050	0.89	0/2776
1	B	0.68	0/2080	0.84	0/2820
1	C	0.69	1/2048 (0.0%)	0.87	0/2781
1	D	0.66	0/2027	0.84	0/2754
1	E	0.70	0/2017	0.86	0/2733
All	All	0.68	1/10222 (0.0%)	0.86	0/13864

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	2	0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	75	ILE	CA-CB	5.21	1.56	1.54

There are no bond angle outliers.

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	124[A]	THR	CB
1	C	124[B]	THR	CB

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	1990	0	2038	17	0
1	B	2042	0	2070	10	0
1	C	1997	0	2002	13	0
1	D	1985	0	1976	11	0
1	E	1976	0	2011	22	0
2	A	44	0	26	0	0
2	B	44	0	26	0	0
2	C	44	0	26	0	0
2	D	44	0	26	1	0
2	E	44	0	26	0	0
3	A	12	0	18	0	0
3	C	8	0	12	0	0
3	D	4	0	6	0	0
3	E	4	0	6	0	0
4	A	154	0	0	0	0
4	B	166	0	0	0	0
4	C	127	0	0	0	0
4	D	127	0	0	1	0
4	E	121	0	0	0	0
All	All	10933	0	10269	67	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 (67) 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:A:210:LEU:HD11	1:B:210:LEU:HD13	1.45	0.98
1:C:124[B]:THR:HG23	1:D:216:MET:SD	2.23	0.79
1:E:149[B]:MET:HE3	1:E:153:LEU:CD1	2.16	0.76
1:C:124[B]:THR:HG21	4:D:2092:HOH:O	1.89	0.72
1:E:185:LEU:HD21	1:E:210:LEU:HD22	1.71	0.71
1:C:185:LEU:HD21	1:C:210:LEU:HD12	1.73	0.69
1:A:118:ILE:HD12	1:A:149[B]:MET:HG3	1.78	0.66
1:E:185:LEU:CD2	1:E:210:LEU:HD22	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:37:MET:HE1	1:E:52:LEU:HB3	1.80	0.62
1:E:149[B]:MET:HE3	1:E:153:LEU:HD13	1.82	0.61
1:C:185:LEU:HD13	1:D:217:LEU:HD23	1.84	0.60
1:E:93:VAL:HG21	1:E:149[A]:MET:HE2	1.83	0.60
1:A:14:ALA:HA	1:A:127:VAL:HG12	1.84	0.59
1:C:185:LEU:CD2	1:C:210:LEU:HD12	2.32	0.59
1:C:82:ILE:C	1:C:82:ILE:HD12	2.28	0.59
1:A:118:ILE:CD1	1:A:149[B]:MET:HG3	2.36	0.56
1:E:149[B]:MET:CE	1:E:153:LEU:CD1	2.83	0.56
1:C:185:LEU:HD21	1:C:210:LEU:CD1	2.36	0.56
1:A:105:GLU:O	1:A:109[A]:SER:HB3	2.06	0.55
1:A:37:MET:HE1	1:A:52:LEU:HB3	1.89	0.55
1:E:118:ILE:HD13	1:E:149[A]:MET:HG3	1.88	0.54
1:A:3:VAL:HG21	1:A:25:LEU:HD11	1.88	0.54
1:A:217:LEU:HD23	1:B:185:LEU:HD13	1.89	0.54
1:D:105:GLU:O	1:D:109[A]:SER:HB3	2.08	0.53
1:E:211:LEU:C	1:E:211:LEU:HD23	2.33	0.52
1:A:269:GLN:HA	1:A:269:GLN:OE1	2.10	0.52
1:E:231:VAL:HG12	1:E:231:VAL:O	2.10	0.52
1:D:269:GLN:OE1	1:D:269:GLN:HA	2.10	0.51
1:A:4:GLY:HA3	1:A:63[A]:SER:OG	2.11	0.51
1:D:9:GLY:HA3	2:D:350:NAD:O1A	2.12	0.50
1:E:42:VAL:O	1:E:52:LEU:HD21	2.12	0.50
1:C:210:LEU:HD13	1:D:210:LEU:HD11	1.93	0.49
1:E:45:LEU:HD23	1:E:48:MET:HE2	1.96	0.48
1:C:33:SER:HA	1:C:53:THR:O	2.14	0.48
1:B:78:ILE:O	1:B:82:ILE:HG13	2.13	0.48
1:B:1:MET:HE2	1:B:148:LEU:HD21	1.97	0.47
1:E:93:VAL:HG21	1:E:149[A]:MET:CE	2.44	0.47
1:C:185:LEU:CD2	1:C:210:LEU:CD1	2.92	0.46
1:C:82:ILE:C	1:C:82:ILE:CD1	2.89	0.46
1:D:17:LYS:HB3	1:D:127:VAL:HG23	1.98	0.45
1:C:105:GLU:O	1:C:109[A]:SER:HB3	2.17	0.45
1:E:211:LEU:HD23	1:E:211:LEU:O	2.16	0.45
1:E:33:SER:HA	1:E:53:THR:O	2.16	0.45
1:A:93:VAL:HG21	1:A:149[B]:MET:HE2	1.99	0.44
1:E:133:THR:O	1:E:159:CYS:HA	2.17	0.44
1:A:14:ALA:HA	1:A:127:VAL:CG1	2.46	0.44
1:A:93:VAL:HG21	1:A:149[B]:MET:CE	2.48	0.44
1:E:118:ILE:CD1	1:E:149[A]:MET:HG3	2.47	0.43
1:E:1:MET:HE3	1:E:3:VAL:CG2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:231:VAL:O	1:E:231:VAL:CG1	2.66	0.43
1:A:127:VAL:HG21	1:B:216:MET:HE3	2.00	0.43
1:E:45:LEU:HA	1:E:48:MET:HE2	2.01	0.43
1:A:145:ASP:O	1:A:149[B]:MET:HG2	2.19	0.42
1:D:1:MET:HE1	1:D:152:LEU:HD13	2.00	0.42
1:D:75:ILE:HG21	1:D:99:VAL:HG11	2.01	0.42
1:E:45:LEU:HD23	1:E:48:MET:CE	2.49	0.42
1:B:118:ILE:HD12	1:B:149:MET:HG3	2.01	0.42
1:A:31:MET:HA	1:A:51:LYS:O	2.20	0.42
1:E:124:THR:N	1:E:125:PRO:CD	2.83	0.41
1:A:19:PHE:HB3	1:A:25:LEU:HD12	2.01	0.41
1:D:148:LEU:C	1:D:148:LEU:HD23	2.45	0.41
1:B:4:GLY:HA3	1:B:63:SER:OG	2.21	0.41
1:B:124:THR:N	1:B:125:PRO:CD	2.84	0.41
1:D:211:LEU:HD23	1:D:211:LEU:C	2.46	0.41
1:B:33:SER:HA	1:B:53:THR:O	2.21	0.41
1:B:3:VAL:HG21	1:B:25:LEU:HD11	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	276/322 (86%)	272 (99%)	4 (1%)	0	100	100
1	B	278/322 (86%)	274 (99%)	4 (1%)	0	100	100
1	C	278/322 (86%)	273 (98%)	5 (2%)	0	100	100
1	D	276/322 (86%)	271 (98%)	5 (2%)	0	100	100
1	E	272/322 (84%)	267 (98%)	5 (2%)	0	100	100
All	All	1380/1610 (86%)	1357 (98%)	23 (2%)	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	209/254 (82%)	206 (99%)	3 (1%)	59	56
1	B	211/254 (83%)	209 (99%)	2 (1%)	70	70
1	C	206/254 (81%)	200 (97%)	6 (3%)	37	29
1	D	201/254 (79%)	199 (99%)	2 (1%)	68	67
1	E	203/254 (80%)	202 (100%)	1 (0%)	81	82
All	All	1030/1270 (81%)	1016 (99%)	14 (1%)	63	56

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	112	ARG
1	A	149[A]	MET
1	A	149[B]	MET
1	B	37	MET
1	B	143	VAL
1	C	82	ILE
1	C	86	ILE
1	C	143	VAL
1	C	149[A]	MET
1	C	149[B]	MET
1	C	233	SER
1	D	24	VAL
1	D	37	MET
1	E	52	LEU

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

Mol	Chain	Res	Type
1	B	-5	ASN

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Mol	Chain	Res	Type
1	B	10	GLN
1	B	62	HIS
1	B	219	HIS
1	C	55	HIS
1	C	140	HIS
1	C	151	GLN
1	D	142	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

12 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	D	350	-	46,48,48	1.92	7 (15%)	64,73,73	2.07	17 (26%)
3	EDO	E	1273	-	3,3,3	0.43	0	2,2,2	0.13	0
3	EDO	D	1272	-	3,3,3	0.36	0	2,2,2	0.37	0
3	EDO	A	1273	-	3,3,3	0.47	0	2,2,2	0.11	0
3	EDO	C	1276	-	3,3,3	0.67	0	2,2,2	0.16	0
3	EDO	A	1272	-	3,3,3	0.40	0	2,2,2	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAD	C	350	-	46,48,48	1.45	7 (15%)	64,73,73	1.77	12 (18%)
3	EDO	A	1274	-	3,3,3	0.43	0	2,2,2	0.08	0
2	NAD	A	350	-	46,48,48	1.55	8 (17%)	64,73,73	1.86	15 (23%)
3	EDO	C	1277	-	3,3,3	0.40	0	2,2,2	0.48	0
2	NAD	E	350	-	46,48,48	1.69	7 (15%)	64,73,73	1.89	14 (21%)
2	NAD	B	350	-	46,48,48	1.54	6 (13%)	64,73,73	1.75	15 (23%)

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	D	350	-	-	5/30/62/62	0/5/5/5
3	EDO	E	1273	-	-	0/1/1/1	-
3	EDO	D	1272	-	-	1/1/1/1	-
3	EDO	A	1273	-	-	1/1/1/1	-
3	EDO	C	1276	-	-	0/1/1/1	-
3	EDO	A	1272	-	-	1/1/1/1	-
2	NAD	C	350	-	-	4/30/62/62	0/5/5/5
3	EDO	A	1274	-	-	1/1/1/1	-
2	NAD	A	350	-	-	4/30/62/62	0/5/5/5
3	EDO	C	1277	-	-	0/1/1/1	-
2	NAD	E	350	-	-	5/30/62/62	0/5/5/5
2	NAD	B	350	-	-	3/30/62/62	0/5/5/5

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	350	NAD	C2N-N1N	6.99	1.42	1.35
2	E	350	NAD	C2N-N1N	6.79	1.42	1.35
2	D	350	NAD	C2N-N1N	5.99	1.41	1.35
2	D	350	NAD	PN-O3	5.97	1.65	1.59
2	D	350	NAD	PA-O3	5.85	1.65	1.59
2	A	350	NAD	C2N-N1N	5.61	1.41	1.35
2	C	350	NAD	C2N-N1N	5.50	1.41	1.35
2	E	350	NAD	O4D-C1D	4.38	1.46	1.40
2	A	350	NAD	O4D-C1D	4.25	1.46	1.40
2	E	350	NAD	C3N-C7N	3.43	1.55	1.50
2	B	350	NAD	C3N-C7N	3.22	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	350	NAD	O4D-C1D	3.20	1.45	1.40
2	E	350	NAD	PA-O3	3.14	1.62	1.59
2	A	350	NAD	C3N-C7N	3.00	1.55	1.50
2	D	350	NAD	C5A-N7A	-2.82	1.33	1.39
2	C	350	NAD	C5A-N7A	-2.82	1.33	1.39
2	D	350	NAD	C3N-C7N	2.80	1.54	1.50
2	A	350	NAD	PN-O3	2.77	1.62	1.59
2	D	350	NAD	C6N-N1N	2.70	1.41	1.35
2	C	350	NAD	C3N-C7N	2.64	1.54	1.50
2	A	350	NAD	C5A-N7A	-2.63	1.34	1.39
2	E	350	NAD	C5A-N7A	-2.58	1.34	1.39
2	B	350	NAD	C5A-N7A	-2.48	1.34	1.39
2	E	350	NAD	C6N-N1N	2.47	1.41	1.35
2	B	350	NAD	C4A-N9A	-2.47	1.32	1.37
2	C	350	NAD	C4A-N9A	-2.32	1.32	1.37
2	B	350	NAD	C6N-N1N	2.30	1.40	1.35
2	C	350	NAD	C6N-N1N	2.28	1.40	1.35
2	B	350	NAD	PA-O3	2.24	1.61	1.59
2	A	350	NAD	C6N-N1N	2.17	1.40	1.35
2	C	350	NAD	PN-O3	2.11	1.61	1.59
2	D	350	NAD	O4D-C1D	2.07	1.43	1.40
2	A	350	NAD	PA-O3	2.06	1.61	1.59
2	E	350	NAD	C4A-N9A	-2.02	1.33	1.37
2	A	350	NAD	C4A-N9A	-2.01	1.33	1.37

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	350	NAD	O5B-PA-O1A	-5.96	85.33	108.94
2	E	350	NAD	O5B-PA-O1A	-5.66	86.51	108.94
2	D	350	NAD	O2A-PA-O5B	-5.22	83.91	107.57
2	A	350	NAD	C5A-C4A-N3A	-5.14	119.64	126.72
2	A	350	NAD	O5B-PA-O1A	-5.11	88.67	108.94
2	D	350	NAD	C5A-C4A-N3A	-5.06	119.75	126.72
2	E	350	NAD	N3A-C2A-N1A	-4.98	121.05	128.58
2	C	350	NAD	O2A-PA-O3	4.94	120.61	107.27
2	A	350	NAD	O2A-PA-O5B	-4.90	85.37	107.57
2	E	350	NAD	C5A-C4A-N3A	-4.88	119.99	126.72
2	C	350	NAD	C5A-C4A-N3A	-4.82	120.08	126.72
2	B	350	NAD	N3A-C2A-N1A	-4.77	121.36	128.58
2	D	350	NAD	N3A-C2A-N1A	-4.54	121.70	128.58
2	A	350	NAD	N3A-C2A-N1A	-4.44	121.86	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	350	NAD	N3A-C2A-N1A	-4.32	122.04	128.58
2	B	350	NAD	C5A-C4A-N3A	-4.31	120.79	126.72
2	C	350	NAD	O5B-PA-O1A	-4.03	92.96	108.94
2	B	350	NAD	O5B-PA-O1A	-4.02	92.98	108.94
2	C	350	NAD	O2A-PA-O5B	-3.83	90.19	107.57
2	E	350	NAD	N9A-C8A-N7A	-3.81	108.53	113.94
2	B	350	NAD	O2A-PA-O5B	-3.71	90.76	107.57
2	E	350	NAD	C2A-N3A-C4A	3.65	120.76	111.83
2	D	350	NAD	O4B-C1B-N9A	3.64	115.07	108.09
2	B	350	NAD	O2A-PA-O3	3.60	117.02	107.27
2	D	350	NAD	O2A-PA-O3	3.59	116.99	107.27
2	A	350	NAD	N3A-C4A-N9A	3.54	133.19	127.17
2	D	350	NAD	N3A-C4A-N9A	3.51	133.14	127.17
2	D	350	NAD	N9A-C8A-N7A	-3.45	109.03	113.94
2	A	350	NAD	C2A-N3A-C4A	3.44	120.24	111.83
2	D	350	NAD	C2A-N3A-C4A	3.41	120.17	111.83
2	E	350	NAD	N3A-C4A-N9A	3.40	132.96	127.17
2	D	350	NAD	C4B-O4B-C1B	-3.40	101.96	109.47
2	C	350	NAD	C2A-N3A-C4A	3.39	120.11	111.83
2	D	350	NAD	O4B-C1B-C2B	-3.36	99.43	106.62
2	D	350	NAD	O2A-PA-O1A	3.36	128.06	112.44
2	B	350	NAD	C2A-N3A-C4A	3.36	120.03	111.83
2	E	350	NAD	O4B-C1B-N9A	3.27	114.36	108.09
2	A	350	NAD	O2A-PA-O3	3.26	116.10	107.27
2	E	350	NAD	O2A-PA-O3	3.22	115.98	107.27
2	E	350	NAD	O2A-PA-O5B	-3.07	93.65	107.57
2	B	350	NAD	N9A-C8A-N7A	-3.04	109.62	113.94
2	C	350	NAD	N3A-C4A-N9A	3.04	132.33	127.17
2	C	350	NAD	N9A-C8A-N7A	-3.02	109.66	113.94
2	E	350	NAD	C5A-N7A-C8A	2.98	108.14	103.45
2	D	350	NAD	C5A-N7A-C8A	2.97	108.12	103.45
2	E	350	NAD	O3-PA-O1A	2.95	119.57	110.70
2	A	350	NAD	N9A-C8A-N7A	-2.91	109.81	113.94
2	E	350	NAD	C4A-N9A-C8A	2.86	108.74	105.74
2	D	350	NAD	C4A-C5A-N7A	-2.85	107.32	110.58
2	B	350	NAD	O2A-PA-O1A	2.83	125.62	112.44
2	C	350	NAD	C4A-C5A-N7A	-2.77	107.41	110.58
2	A	350	NAD	O2A-PA-O1A	2.77	125.33	112.44
2	B	350	NAD	N3A-C4A-N9A	2.75	131.85	127.17
2	E	350	NAD	C4A-C5A-N7A	-2.66	107.54	110.58
2	D	350	NAD	C6N-N1N-C2N	-2.63	119.64	121.88
2	A	350	NAD	O4B-C1B-C2B	-2.61	101.04	106.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	350	NAD	C6N-N1N-C2N	-2.59	119.68	121.88
2	D	350	NAD	C4A-N9A-C8A	2.54	108.41	105.74
2	C	350	NAD	C5A-N7A-C8A	2.54	107.44	103.45
2	B	350	NAD	C6N-N1N-C2N	-2.54	119.72	121.88
2	E	350	NAD	O2A-PA-O1A	2.49	124.04	112.44
2	C	350	NAD	O2A-PA-O1A	2.43	123.76	112.44
2	A	350	NAD	O3-PA-O1A	2.42	117.99	110.70
2	A	350	NAD	C5A-N7A-C8A	2.39	107.21	103.45
2	A	350	NAD	C4A-C5A-N7A	-2.33	107.92	110.58
2	B	350	NAD	C4A-C5A-N7A	-2.27	107.98	110.58
2	B	350	NAD	C5A-N7A-C8A	2.26	107.01	103.45
2	B	350	NAD	O4B-C1B-N9A	2.25	112.40	108.09
2	B	350	NAD	C4A-N9A-C8A	2.17	108.02	105.74
2	B	350	NAD	O3-PA-O1A	2.14	117.16	110.70
2	D	350	NAD	O2N-PN-O3	2.07	112.87	107.27
2	C	350	NAD	C4A-N9A-C8A	2.07	107.91	105.74
2	A	350	NAD	C4A-N9A-C8A	2.06	107.90	105.74

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	350	NAD	O4D-C1D-N1N-C2N
2	A	350	NAD	O4D-C1D-N1N-C6N
2	B	350	NAD	O4D-C1D-N1N-C2N
2	C	350	NAD	O4D-C1D-N1N-C2N
2	C	350	NAD	O4D-C1D-N1N-C6N
2	D	350	NAD	O4D-C1D-N1N-C2N
2	D	350	NAD	O4D-C1D-N1N-C6N
2	D	350	NAD	C2D-C1D-N1N-C6N
2	E	350	NAD	O4D-C1D-N1N-C2N
2	E	350	NAD	O4D-C1D-N1N-C6N
2	E	350	NAD	C2D-C1D-N1N-C6N
2	C	350	NAD	C2B-C1B-N9A-C8A
2	D	350	NAD	O4B-C4B-C5B-O5B
2	B	350	NAD	C2B-C1B-N9A-C8A
2	A	350	NAD	C2D-C1D-N1N-C6N
2	D	350	NAD	C2D-C1D-N1N-C2N
2	E	350	NAD	C2D-C1D-N1N-C2N
3	A	1274	EDO	O1-C1-C2-O2
2	B	350	NAD	O4D-C1D-N1N-C6N
3	A	1273	EDO	O1-C1-C2-O2

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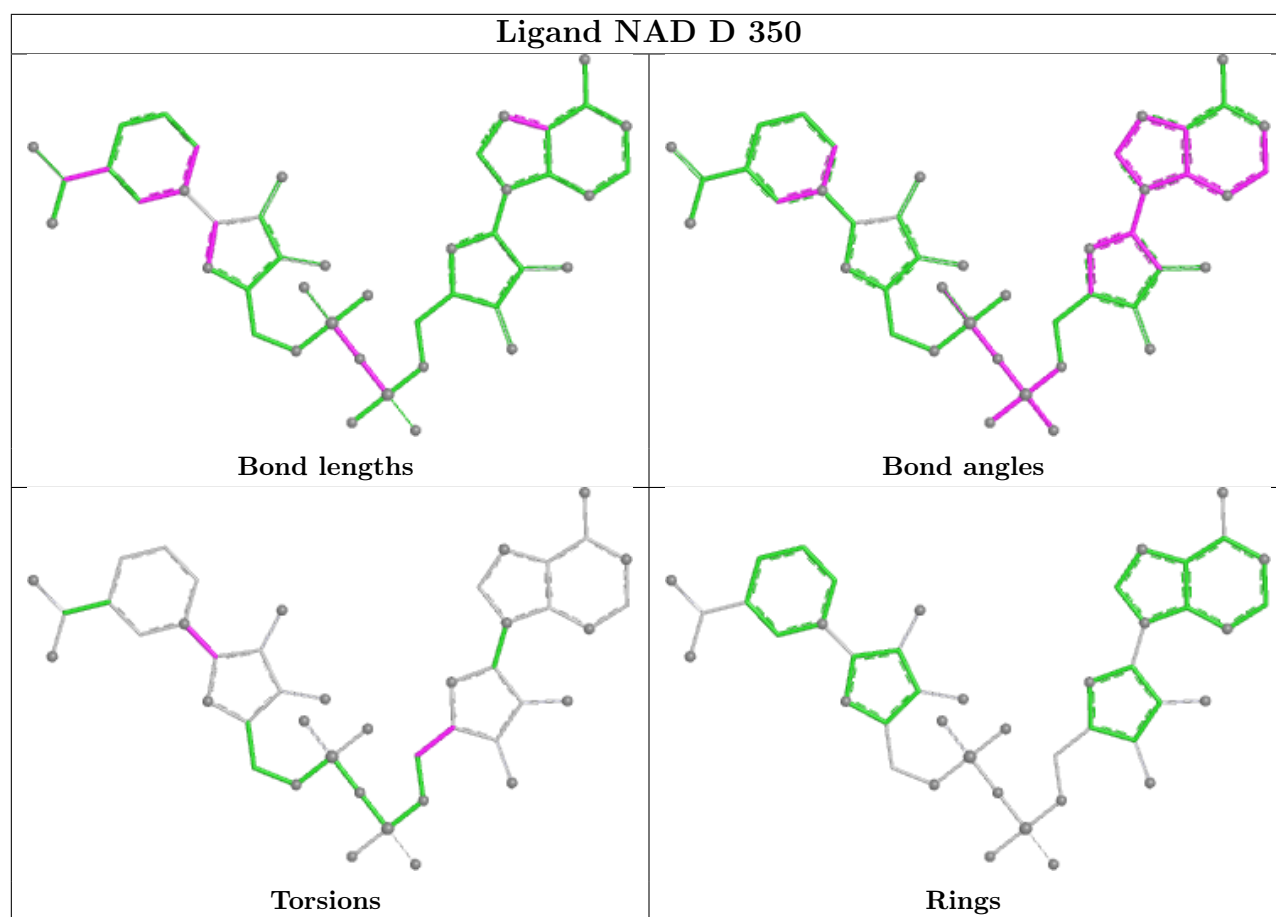
Mol	Chain	Res	Type	Atoms
3	D	1272	EDO	O1-C1-C2-O2
3	A	1272	EDO	O1-C1-C2-O2
2	A	350	NAD	C2B-C1B-N9A-C8A
2	E	350	NAD	C2B-C1B-N9A-C8A
2	C	350	NAD	O4B-C4B-C5B-O5B

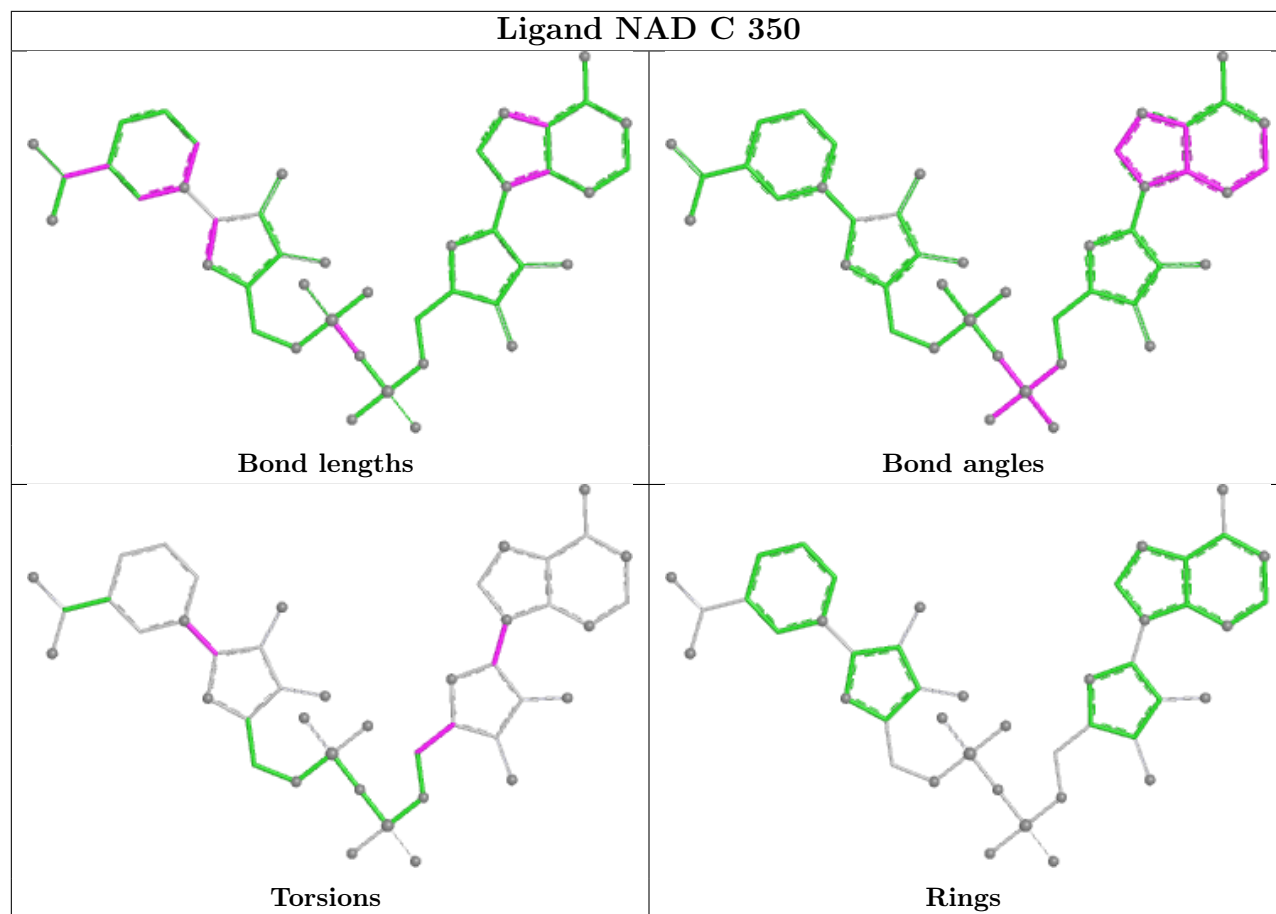
There are no ring outliers.

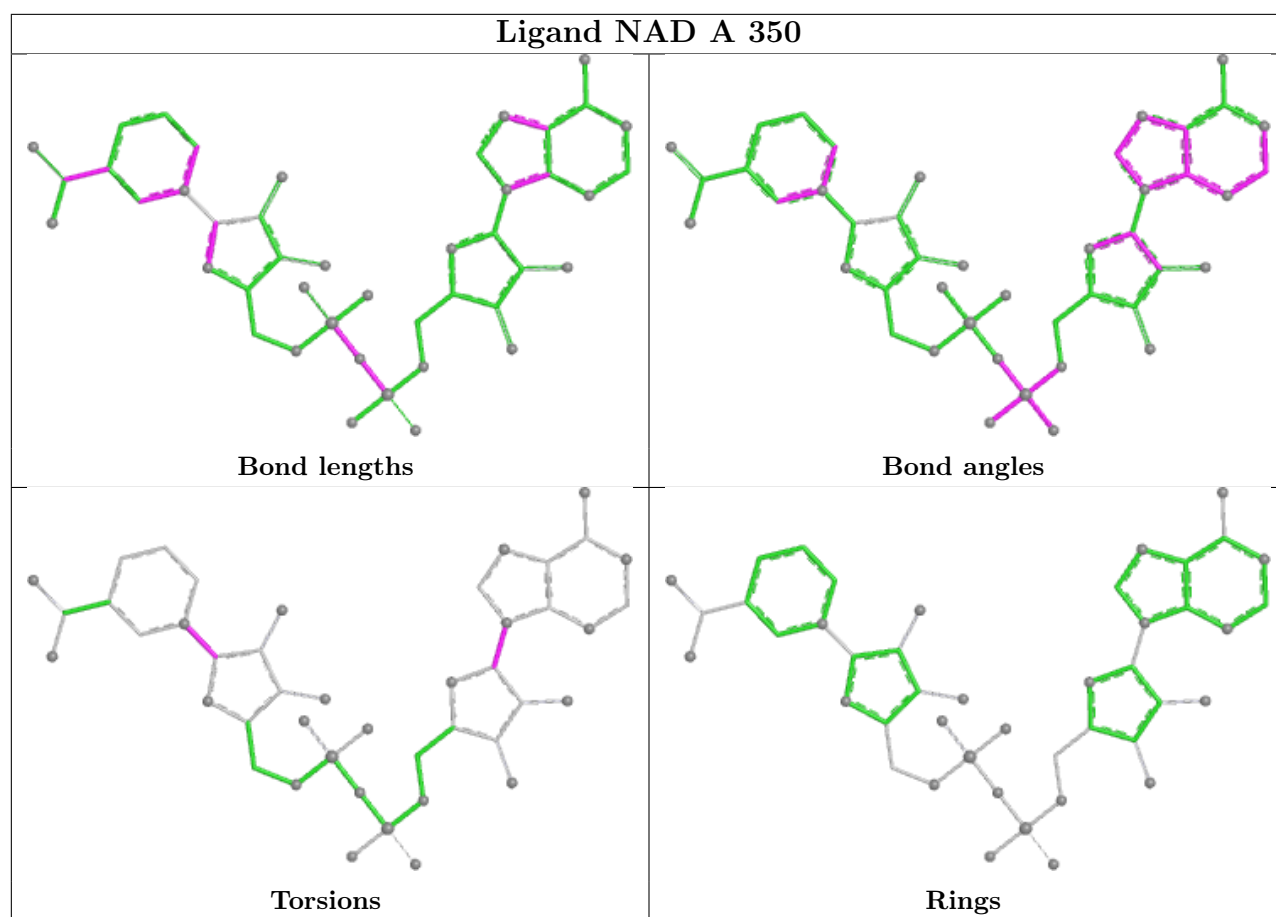
1 monomer is involved in 1 short contact:

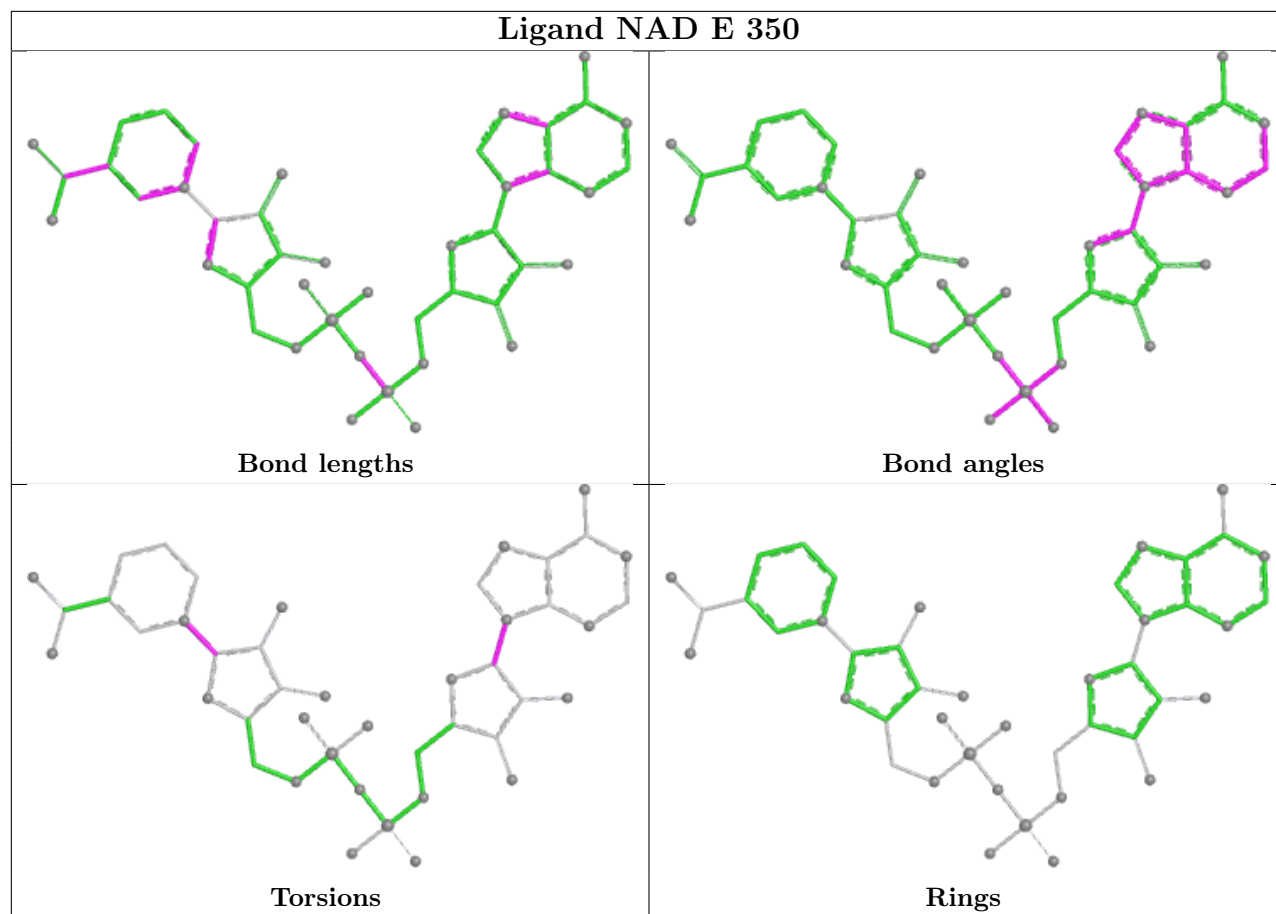
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	350	NAD	1	0

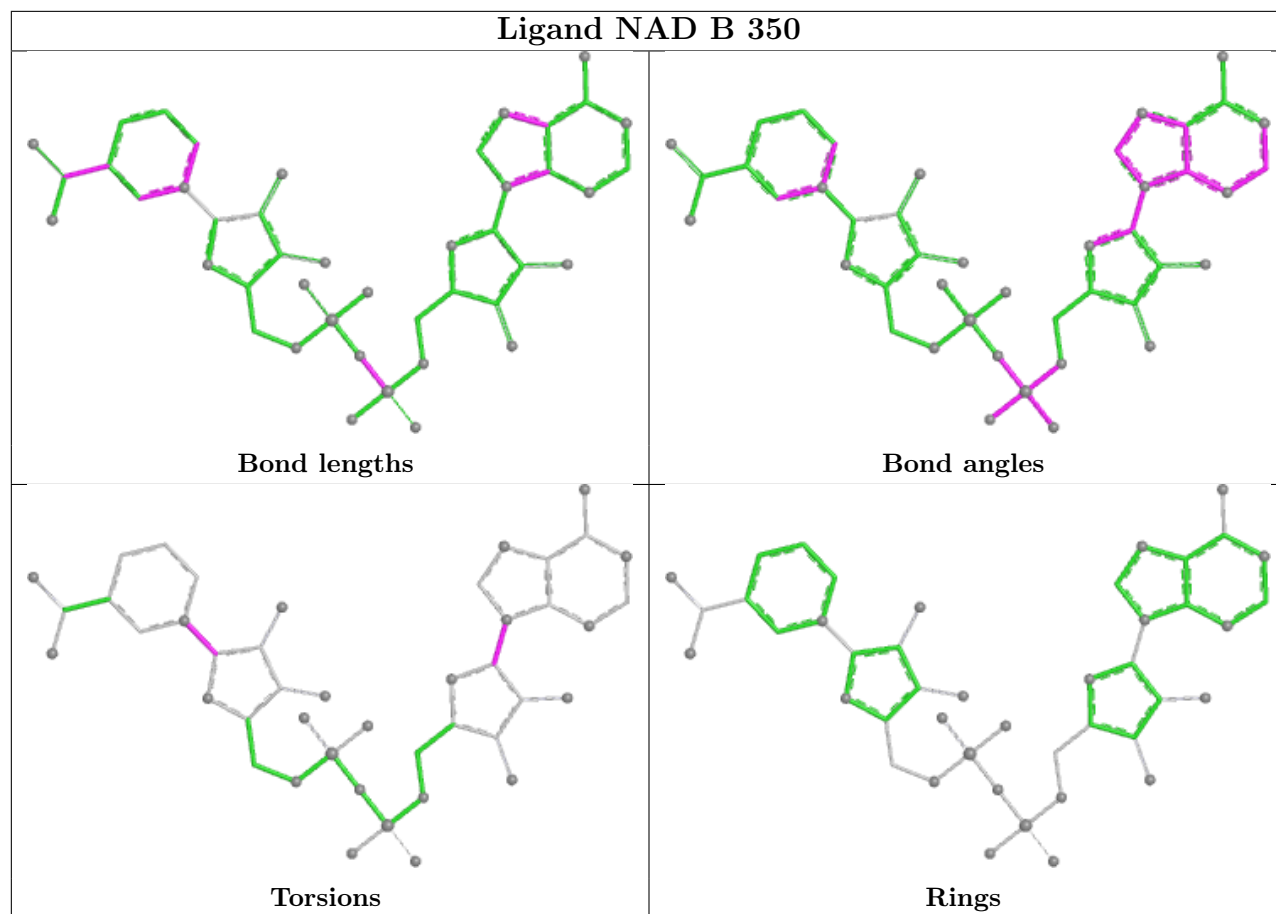
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











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	272/322 (84%)	0.36	10 (3%)	45	52	18, 28, 38, 64	6 (2%)
1	B	279/322 (86%)	0.66	13 (4%)	36	42	18, 28, 40, 52	1 (0%)
1	C	276/322 (85%)	0.57	14 (5%)	33	39	18, 29, 40, 53	4 (1%)
1	D	276/322 (85%)	1.17	64 (23%)	2	2	18, 29, 39, 56	2 (0%)
1	E	272/322 (84%)	0.96	40 (14%)	6	6	18, 29, 40, 49	2 (0%)
All	All	1375/1610 (85%)	0.75	141 (10%)	12	13	18, 29, 40, 64	15 (1%)

All (141) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	-4	LEU	5.5
1	D	271	MET	5.2
1	E	98	GLY	4.8
1	D	162	VAL	4.3
1	D	158	PHE	4.2
1	D	143	VAL	4.2
1	D	160	THR	4.0
1	B	273	ASP	3.9
1	D	154	SER	3.7
1	D	269	GLN	3.7
1	D	35	PRO	3.7
1	C	39	LEU	3.6
1	E	148	LEU	3.6
1	D	268	LEU	3.6
1	D	135	TYR	3.6
1	D	25	LEU	3.6
1	A	271	MET	3.5
1	D	134	VAL	3.5
1	E	162	VAL	3.5
1	D	159	CYS	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	38	ASP	3.4
1	D	36	ASP	3.3
1	D	-3	TYR	3.3
1	E	158	PHE	3.3
1	D	47	LYS	3.3
1	B	162	VAL	3.3
1	D	132	ALA	3.3
1	E	97	ALA	3.3
1	E	134	VAL	3.3
1	A	25	LEU	3.2
1	D	8	ALA	3.1
1	D	39	LEU	3.1
1	D	128	VAL	3.1
1	E	52	LEU	3.1
1	A	144	GLU	3.1
1	D	52	LEU	3.0
1	D	24	VAL	3.0
1	E	160	THR	3.0
1	D	136	ALA	3.0
1	E	99	VAL	3.0
1	C	270	SER	3.0
1	D	43	SER	3.0
1	D	131	GLY	2.9
1	E	144	GLU	2.9
1	E	136	ALA	2.9
1	D	-2	PHE	2.8
1	E	23	GLY	2.8
1	E	100	THR	2.8
1	D	157	GLY	2.8
1	B	271	MET	2.8
1	D	50	VAL	2.8
1	C	274	GLN	2.7
1	D	146	GLY	2.7
1	D	139	THR	2.7
1	D	149	MET	2.7
1	A	143	VAL	2.7
1	D	7	GLY	2.7
1	D	151	GLN	2.7
1	E	143	VAL	2.7
1	B	-3	TYR	2.7
1	B	272	ALA	2.6
1	E	231	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	1	MET	2.6
1	D	121	MET	2.6
1	E	151	GLN	2.6
1	E	102	SER	2.6
1	A	269	GLN	2.6
1	E	132	ALA	2.6
1	D	55	HIS	2.5
1	D	231	VAL	2.5
1	D	137	THR	2.5
1	D	120	CYS	2.5
1	D	138	GLY	2.5
1	D	44	ALA	2.5
1	E	24	VAL	2.5
1	C	38	ASP	2.5
1	C	77	PHE	2.5
1	D	147	ARG	2.5
1	E	51	LYS	2.5
1	D	13	PHE	2.4
1	D	152	LEU	2.4
1	B	221	GLU	2.4
1	C	0	SER	2.4
1	A	141	ALA	2.4
1	D	40	ALA	2.4
1	D	133	THR	2.4
1	C	275	GLU	2.4
1	A	0	SER	2.4
1	D	111	PHE	2.4
1	C	231	VAL	2.4
1	D	73	HIS	2.3
1	E	28	HIS	2.3
1	E	270	SER	2.3
1	B	38	ASP	2.3
1	E	1	MET	2.3
1	E	62	HIS	2.3
1	E	46	ARG	2.3
1	D	148	LEU	2.3
1	E	40	ALA	2.2
1	D	56	ASN	2.2
1	B	149	MET	2.2
1	D	31	MET	2.2
1	D	45	LEU	2.2
1	D	153	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	222	GLN	2.2
1	D	49	GLY	2.2
1	D	114	ALA	2.2
1	C	37	MET	2.2
1	B	134	VAL	2.2
1	E	142	GLN	2.2
1	E	152	LEU	2.2
1	A	270	SER	2.2
1	B	0	SER	2.2
1	D	2	SER	2.2
1	D	270	SER	2.2
1	C	40	ALA	2.2
1	E	121	MET	2.2
1	E	271	MET	2.2
1	E	70	VAL	2.2
1	A	268	LEU	2.2
1	E	131	GLY	2.2
1	E	54	PRO	2.2
1	C	21	ALA	2.2
1	D	54	PRO	2.1
1	D	21	ALA	2.1
1	C	49	GLY	2.1
1	C	162	VAL	2.1
1	E	157	GLY	2.1
1	E	146	GLY	2.1
1	B	97	ALA	2.1
1	E	77	PHE	2.0
1	B	100	THR	2.0
1	E	138	GLY	2.0
1	E	123	ASN	2.0
1	A	39	LEU	2.0
1	E	96	ALA	2.0
1	D	37	MET	2.0
1	E	48	MET	2.0
1	D	74	ILE	2.0
1	D	23	GLY	2.0
1	D	59	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

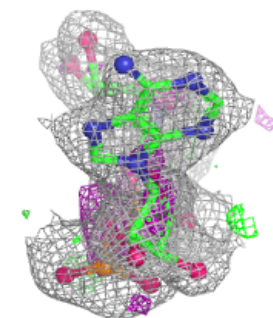
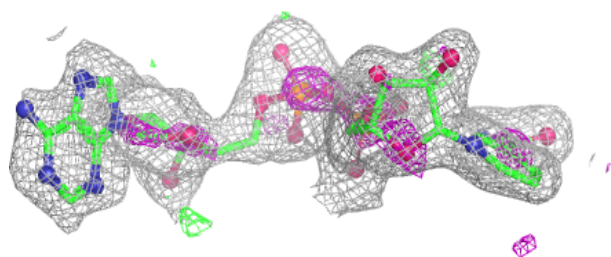
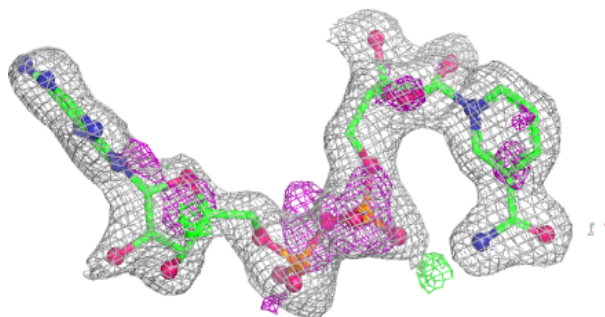
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
3	EDO	C	1276	4/4	0.75	0.23	44,45,46,47	0
3	EDO	D	1272	4/4	0.75	0.24	46,47,47,50	0
3	EDO	E	1273	4/4	0.87	0.20	54,55,55,55	0
2	NAD	D	350	44/44	0.89	0.13	33,49,56,57	0
3	EDO	C	1277	4/4	0.89	0.18	42,43,43,45	0
3	EDO	A	1272	4/4	0.91	0.15	36,37,37,38	0
3	EDO	A	1274	4/4	0.92	0.18	39,39,39,40	0
2	NAD	E	350	44/44	0.93	0.10	34,38,40,41	0
3	EDO	A	1273	4/4	0.94	0.13	39,39,39,40	0
2	NAD	C	350	44/44	0.94	0.10	32,36,41,42	0
2	NAD	A	350	44/44	0.94	0.10	28,34,39,39	0
2	NAD	B	350	44/44	0.95	0.10	24,28,32,32	0

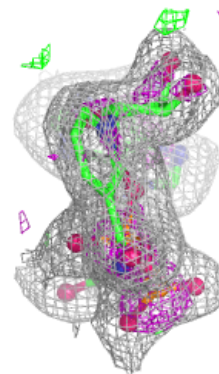
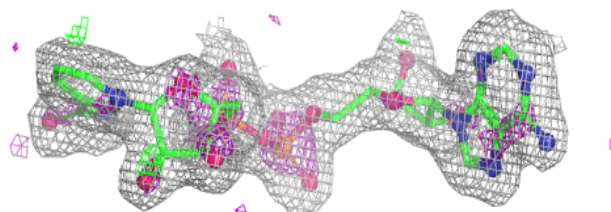
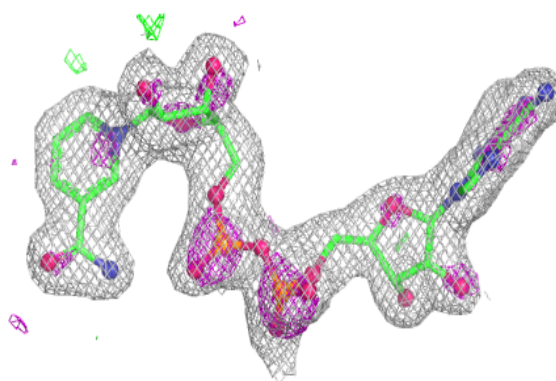
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAD D 350:

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

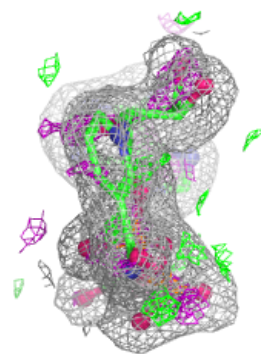
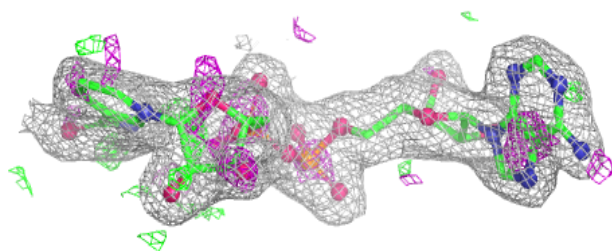
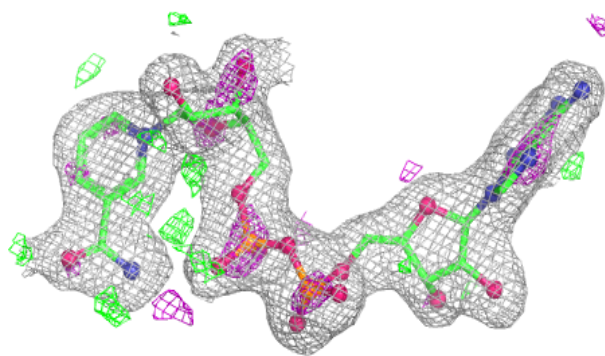
**Electron density around NAD E 350:**

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

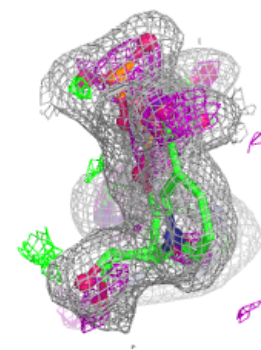
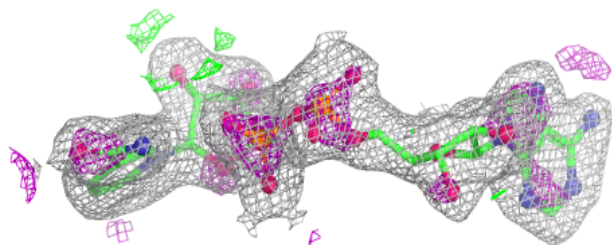
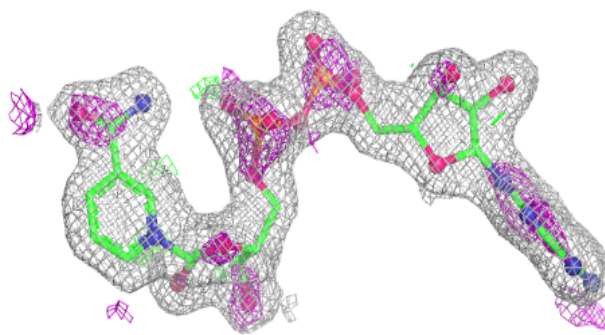


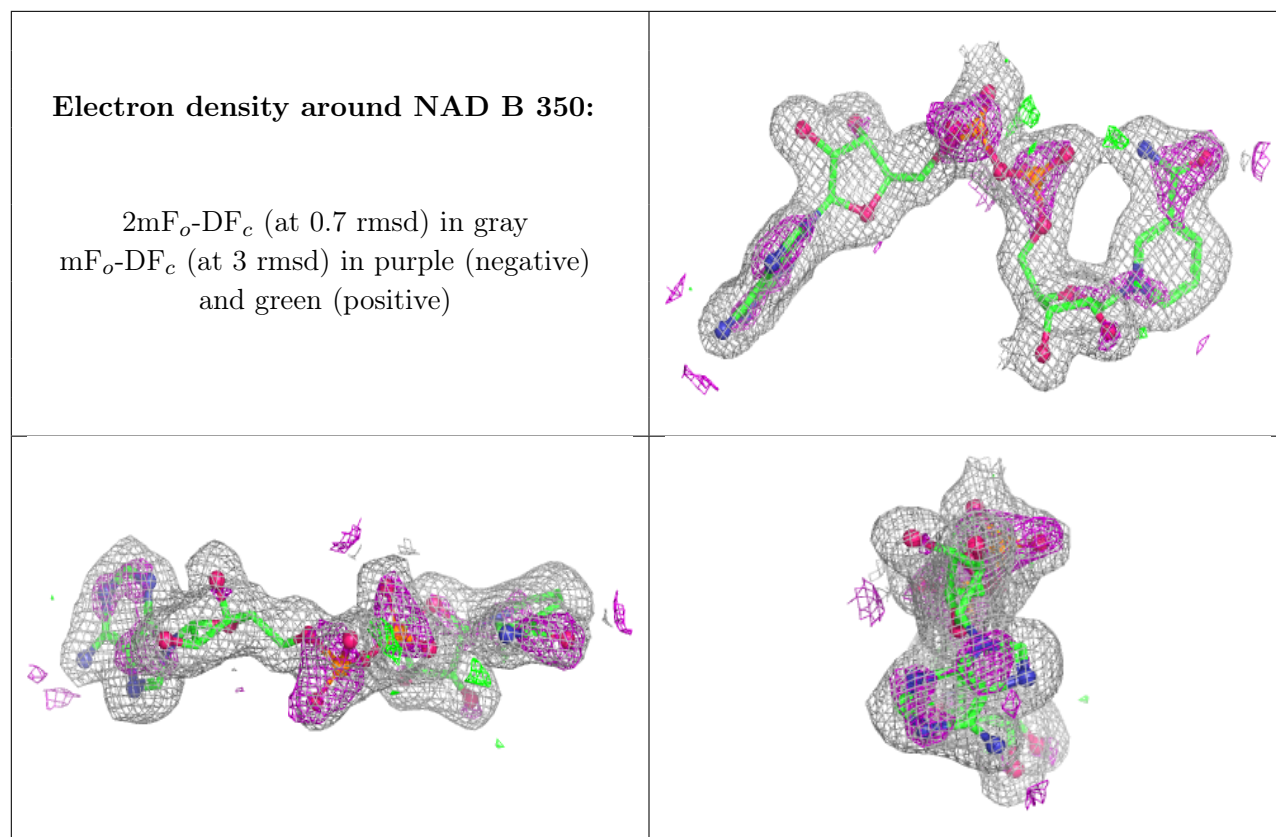
Electron density around NAD C 350:

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

**Electron density around NAD A 350:**

$2mF_o-DF_c$ (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.