



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:14 AM UTC

PDB ID : 4BGI / pdb_00004bgi
Title : Crystal structure of InhA(S94A) mutant in complex with OH-141
Authors : Pojer, F.; Hartkoorn, R.C.; Cole, S.T.
Deposited on : 2013-03-27
Resolution : 2.09 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

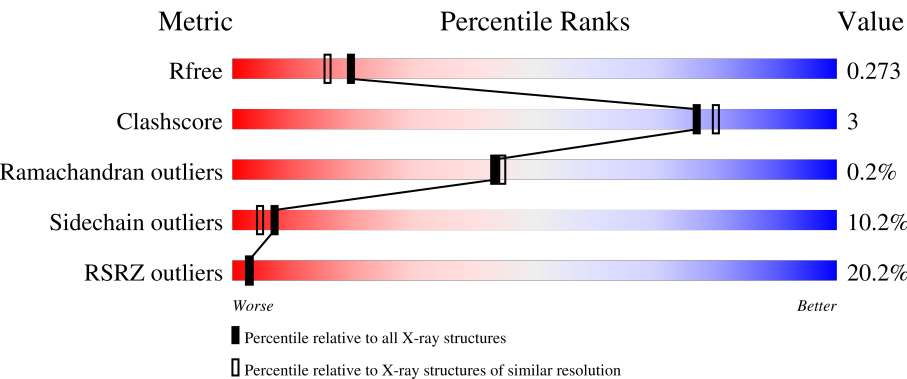
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.09 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	281	7% 80%14%• 5%
1	B	281	9% 85%9%• 5%
1	C	281	24% 76%12%• 10%
1	D	281	18% 77%12%• 10%
1	E	281	25% 75%12%• 11%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	281	29% 81% 12% • 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12366 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 Enoyl-[acyl-carrier-protein] reductase [NADH].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	267	Total	C	N	O	S	0	0	0
			1987	1260	347	370	10			
1	B	267	Total	C	N	O	S	0	1	0
			1992	1265	347	370	10			
1	C	254	Total	C	N	O	S	0	0	0
			1908	1210	334	355	9			
1	D	252	Total	C	N	O	S	0	0	0
			1888	1199	329	351	9			
1	E	251	Total	C	N	O	S	0	0	0
			1888	1199	331	349	9			
1	F	267	Total	C	N	O	S	0	0	0
			1987	1260	347	370	10			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	MET	-	initiating methionine	UNP P9WGR1
A	-2	ASP	-	expression tag	UNP P9WGR1
A	-1	ILE	-	expression tag	UNP P9WGR1
A	0	GLU	-	expression tag	UNP P9WGR1
A	1	PHE	-	expression tag	UNP P9WGR1
A	94	ALA	SER	engineered mutation	UNP P9WGR1
A	270	GLY	-	expression tag	UNP P9WGR1
A	271	SER	-	expression tag	UNP P9WGR1
A	272	HIS	-	expression tag	UNP P9WGR1
A	273	HIS	-	expression tag	UNP P9WGR1
A	274	HIS	-	expression tag	UNP P9WGR1
A	275	HIS	-	expression tag	UNP P9WGR1
A	276	HIS	-	expression tag	UNP P9WGR1
A	277	HIS	-	expression tag	UNP P9WGR1
B	-3	MET	-	initiating methionine	UNP P9WGR1
B	-2	ASP	-	expression tag	UNP P9WGR1
B	-1	ILE	-	expression tag	UNP P9WGR1

Continued on next page...

Continued from previous page...

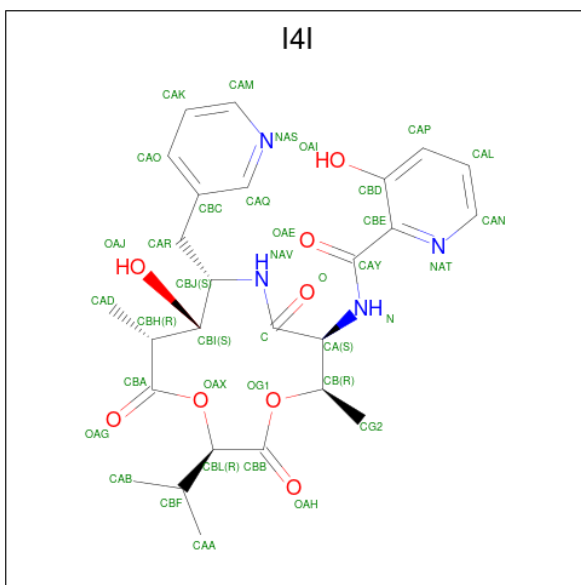
Chain	Residue	Modelled	Actual	Comment	Reference
B	0	GLU	-	expression tag	UNP P9WGR1
B	1	PHE	-	expression tag	UNP P9WGR1
B	94	ALA	SER	engineered mutation	UNP P9WGR1
B	270	GLY	-	expression tag	UNP P9WGR1
B	271	SER	-	expression tag	UNP P9WGR1
B	272	HIS	-	expression tag	UNP P9WGR1
B	273	HIS	-	expression tag	UNP P9WGR1
B	274	HIS	-	expression tag	UNP P9WGR1
B	275	HIS	-	expression tag	UNP P9WGR1
B	276	HIS	-	expression tag	UNP P9WGR1
B	277	HIS	-	expression tag	UNP P9WGR1
C	-3	MET	-	initiating methionine	UNP P9WGR1
C	-2	ASP	-	expression tag	UNP P9WGR1
C	-1	ILE	-	expression tag	UNP P9WGR1
C	0	GLU	-	expression tag	UNP P9WGR1
C	1	PHE	-	expression tag	UNP P9WGR1
C	94	ALA	SER	engineered mutation	UNP P9WGR1
C	270	GLY	-	expression tag	UNP P9WGR1
C	271	SER	-	expression tag	UNP P9WGR1
C	272	HIS	-	expression tag	UNP P9WGR1
C	273	HIS	-	expression tag	UNP P9WGR1
C	274	HIS	-	expression tag	UNP P9WGR1
C	275	HIS	-	expression tag	UNP P9WGR1
C	276	HIS	-	expression tag	UNP P9WGR1
C	277	HIS	-	expression tag	UNP P9WGR1
D	-3	MET	-	initiating methionine	UNP P9WGR1
D	-2	ASP	-	expression tag	UNP P9WGR1
D	-1	ILE	-	expression tag	UNP P9WGR1
D	0	GLU	-	expression tag	UNP P9WGR1
D	1	PHE	-	expression tag	UNP P9WGR1
D	94	ALA	SER	engineered mutation	UNP P9WGR1
D	270	GLY	-	expression tag	UNP P9WGR1
D	271	SER	-	expression tag	UNP P9WGR1
D	272	HIS	-	expression tag	UNP P9WGR1
D	273	HIS	-	expression tag	UNP P9WGR1
D	274	HIS	-	expression tag	UNP P9WGR1
D	275	HIS	-	expression tag	UNP P9WGR1
D	276	HIS	-	expression tag	UNP P9WGR1
D	277	HIS	-	expression tag	UNP P9WGR1
E	-3	MET	-	initiating methionine	UNP P9WGR1
E	-2	ASP	-	expression tag	UNP P9WGR1
E	-1	ILE	-	expression tag	UNP P9WGR1

Continued on next page...

Continued from previous page...

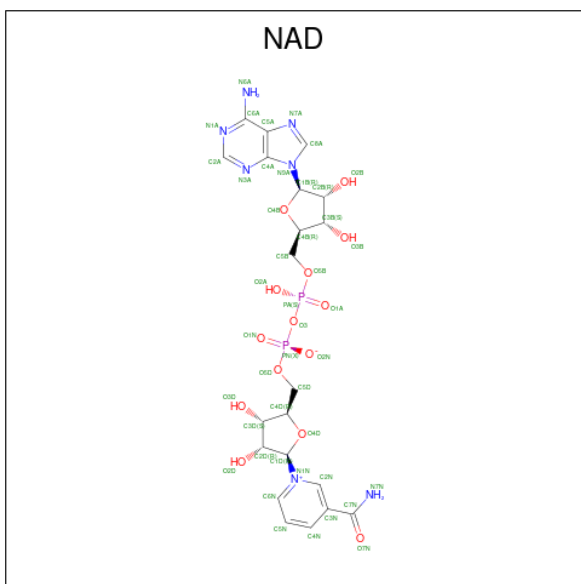
Chain	Residue	Modelled	Actual	Comment	Reference
E	0	GLU	-	expression tag	UNP P9WGR1
E	1	PHE	-	expression tag	UNP P9WGR1
E	94	ALA	SER	engineered mutation	UNP P9WGR1
E	270	GLY	-	expression tag	UNP P9WGR1
E	271	SER	-	expression tag	UNP P9WGR1
E	272	HIS	-	expression tag	UNP P9WGR1
E	273	HIS	-	expression tag	UNP P9WGR1
E	274	HIS	-	expression tag	UNP P9WGR1
E	275	HIS	-	expression tag	UNP P9WGR1
E	276	HIS	-	expression tag	UNP P9WGR1
E	277	HIS	-	expression tag	UNP P9WGR1
F	-3	MET	-	initiating methionine	UNP P9WGR1
F	-2	ASP	-	expression tag	UNP P9WGR1
F	-1	ILE	-	expression tag	UNP P9WGR1
F	0	GLU	-	expression tag	UNP P9WGR1
F	1	PHE	-	expression tag	UNP P9WGR1
F	94	ALA	SER	engineered mutation	UNP P9WGR1
F	270	GLY	-	expression tag	UNP P9WGR1
F	271	SER	-	expression tag	UNP P9WGR1
F	272	HIS	-	expression tag	UNP P9WGR1
F	273	HIS	-	expression tag	UNP P9WGR1
F	274	HIS	-	expression tag	UNP P9WGR1
F	275	HIS	-	expression tag	UNP P9WGR1
F	276	HIS	-	expression tag	UNP P9WGR1
F	277	HIS	-	expression tag	UNP P9WGR1

- Molecule 2 is 3-hydroxy-N-[(2R,5R,6S,9S,10S,11R)-10-hydroxy-5,11-dimethyl-3,7,12-trioxo-2-(propan-2-yl)-9-(pyridin-3-ylmethyl)-1,4-dioxo-8-azacyclododecan-6-yl]pyridine-2-carboxamide (CCD ID: I4I) (formula: C₂₆H₃₂N₄O₈).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 38	C 26	N 4	O 8	0	0
2	B	1	Total 38	C 26	N 4	O 8	0	0
2	F	1	Total 38	C 26	N 4	O 8	0	0

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $\text{C}_{21}\text{H}_{27}\text{N}_7\text{O}_{14}\text{P}_2$).



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

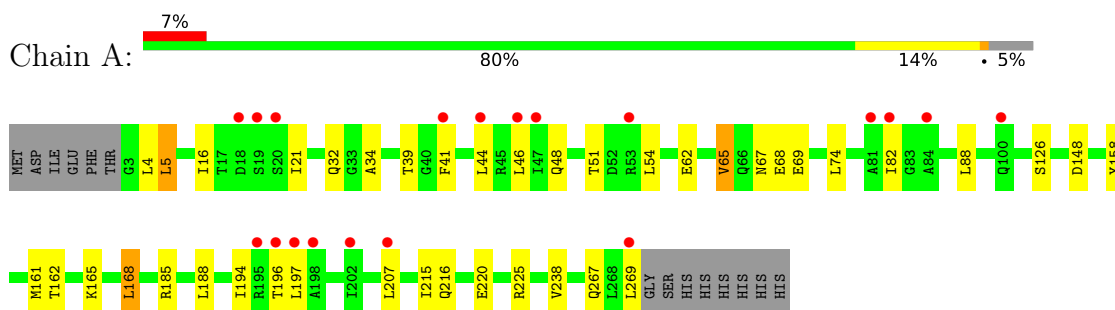
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	119	Total	O	0	0
			119	119		
4	B	78	Total	O	0	0
			78	78		
4	C	67	Total	O	0	0
			67	67		
4	D	60	Total	O	0	0
			60	60		
4	E	46	Total	O	0	0
			46	46		
4	F	100	Total	O	0	0
			100	100		

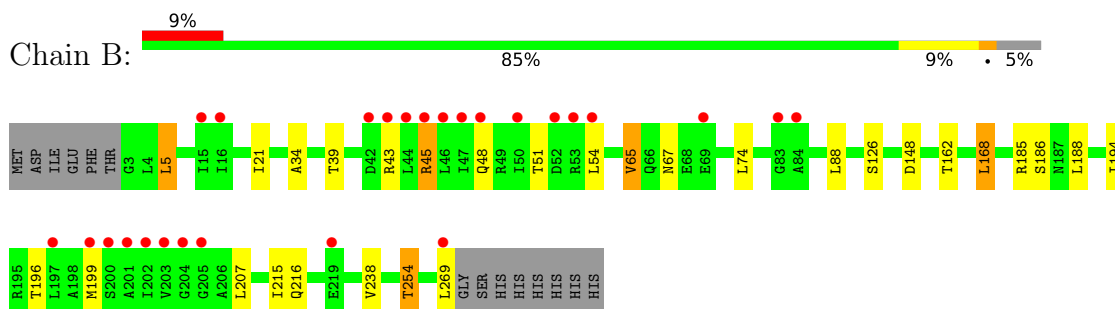
3 Residue-property plots

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.

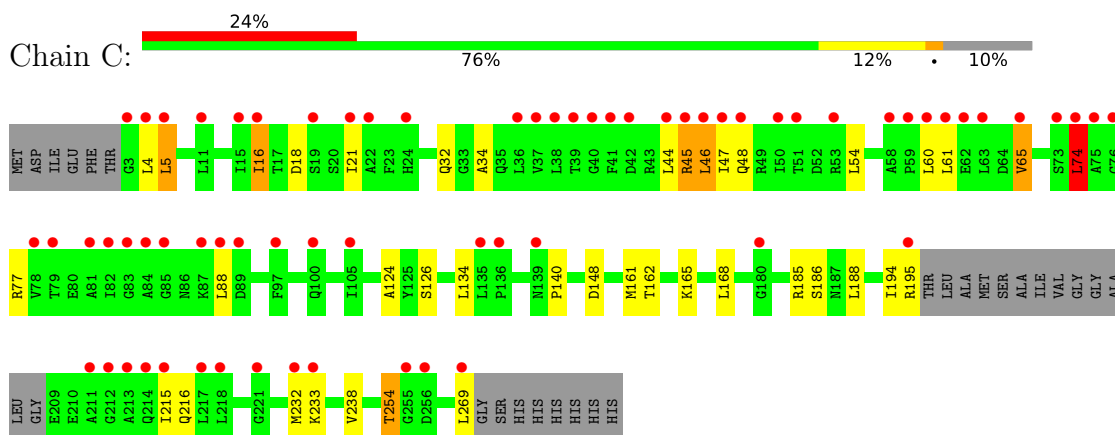
- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]



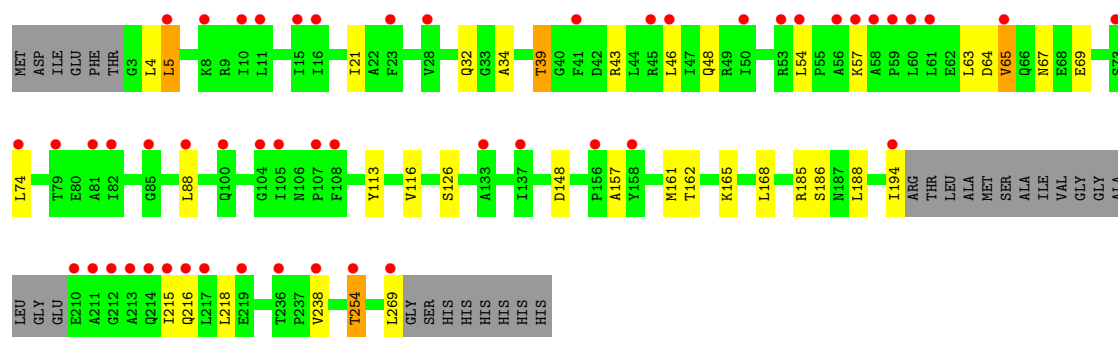
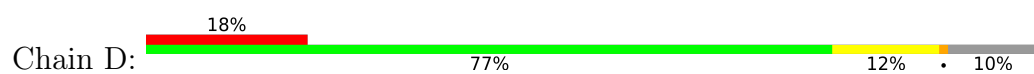
- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]



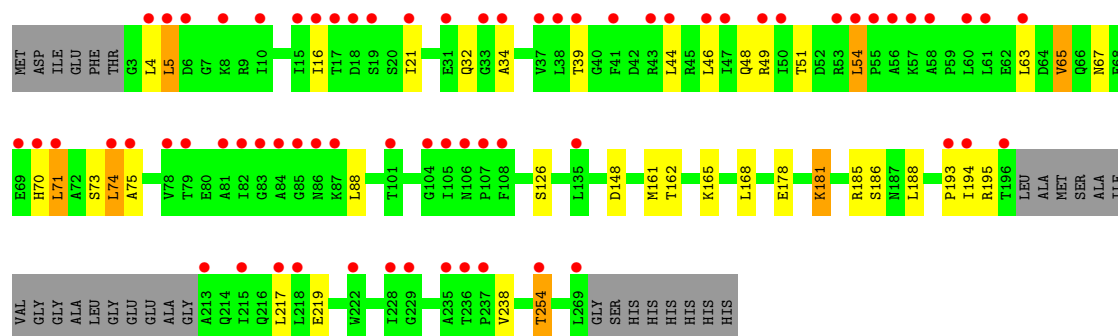
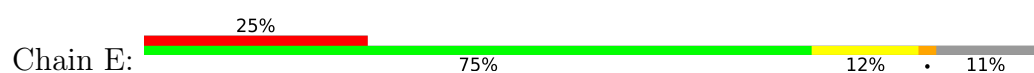
- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]



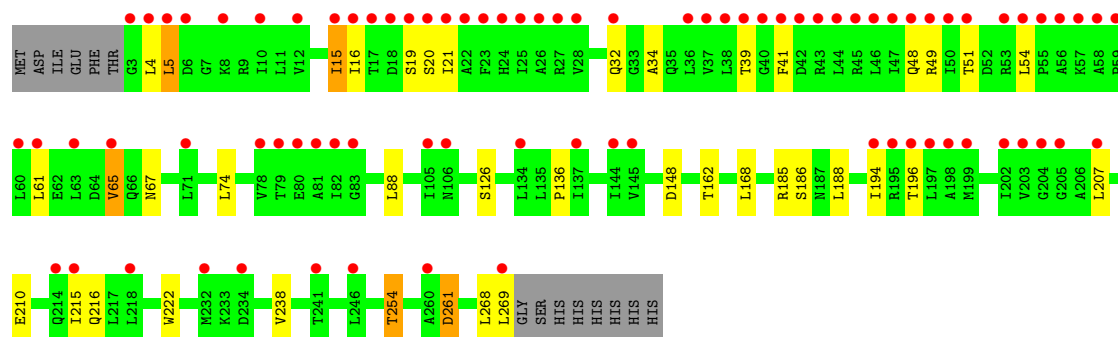
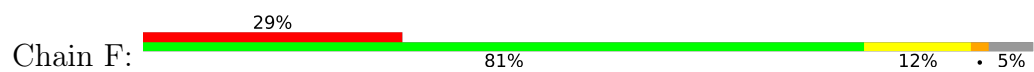
- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]



- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]



- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	100.44Å 82.45Å 189.65Å 90.00° 95.63° 90.00°	Depositor
Resolution (Å)	30.60 – 2.09 30.60 – 2.09	Depositor EDS
% Data completeness (in resolution range)	99.0 (30.60-2.09) 99.4 (30.60-2.09)	Depositor EDS
R_{merge}	0.01	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 2.10Å)	Xtriage
Refinement program	BUSTER 2.11.5	Depositor
R, R_{free}	0.211 , 0.238 0.242 , 0.273	Depositor DCC
R_{free} test set	4530 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	27.5	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 68.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	12366	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% 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: I4I, NAD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.91	0/2025	1.30	2/2750 (0.1%)
1	B	0.91	0/2033	1.29	2/2761 (0.1%)
1	C	0.82	0/1945	1.27	2/2640 (0.1%)
1	D	0.84	0/1925	1.27	2/2614 (0.1%)
1	E	0.83	0/1925	1.29	3/2614 (0.1%)
1	F	0.82	0/2025	1.32	4/2750 (0.1%)
All	All	0.86	0/11878	1.29	15/16129 (0.1%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	148	ASP	CA-CB-CG	6.91	119.51	112.60
1	A	148	ASP	CA-CB-CG	6.84	119.44	112.60
1	F	148	ASP	CA-CB-CG	6.62	119.22	112.60
1	E	148	ASP	CA-CB-CG	6.36	118.95	112.60
1	E	73	SER	N-CA-C	-6.19	104.79	112.90
1	C	148	ASP	CA-CB-CG	6.11	118.71	112.60
1	F	261	ASP	CA-CB-CG	6.08	118.68	112.60
1	E	71	LEU	N-CA-C	-5.92	101.71	110.48
1	D	148	ASP	CA-CB-CG	5.64	118.24	112.60
1	B	168	LEU	CD1-CG-CD2	5.45	122.79	110.80
1	A	168	LEU	CD1-CG-CD2	5.33	122.53	110.80
1	F	41	PHE	CA-CB-CG	5.07	118.87	113.80
1	C	18	ASP	CA-CB-CG	5.06	117.66	112.60
1	D	64	ASP	N-CA-C	-5.04	99.58	108.20
1	F	15	ILE	N-CA-CB	5.03	116.58	110.95

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	1987	0	2006	11	0
1	B	1992	0	2017	9	0
1	C	1908	0	1918	15	0
1	D	1888	0	1899	12	0
1	E	1888	0	1905	15	0
1	F	1987	0	2006	11	0
2	A	38	0	31	2	0
2	B	38	0	31	0	0
2	F	38	0	31	0	0
3	C	44	0	26	0	0
3	D	44	0	26	0	0
3	E	44	0	26	0	0
4	A	119	0	0	1	0
4	B	78	0	0	1	0
4	C	67	0	0	0	0
4	D	60	0	0	0	0
4	E	46	0	0	1	0
4	F	100	0	0	1	0
All	All	12366	0	11922	69	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 (69) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:254:THR:HG21	4:B:2052:HOH:O	1.61	1.00
1:D:4:LEU:H	1:D:32:GLN:HE21	1.39	0.71
1:A:4:LEU:H	1:A:32:GLN:HE21	1.38	0.71
1:F:4:LEU:H	1:F:32:GLN:HE21	1.38	0.71
1:C:140:PRO:HG2	1:E:195:ARG:HH12	1.57	0.70
1:E:254:THR:HG21	4:E:2037:HOH:O	1.92	0.70
1:C:4:LEU:H	1:C:32:GLN:HE21	1.39	0.69
1:E:4:LEU:H	1:E:32:GLN:HE21	1.39	0.68
1:B:45:ARG:HB3	1:F:136:PRO:HB3	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:21:ILE:HD11	1:F:194:ILE:HG13	1.85	0.58
1:B:21:ILE:HD11	1:B:194:ILE:HG13	1.86	0.57
1:E:161:MET:HE3	1:E:165:LYS:HE2	1.85	0.57
1:C:74:LEU:HD22	1:C:134:LEU:HD21	1.85	0.57
1:E:21:ILE:HD11	1:E:194:ILE:HG13	1.87	0.57
1:C:21:ILE:HD11	1:C:194:ILE:HG13	1.88	0.56
1:A:21:ILE:HD11	1:A:194:ILE:HG13	1.87	0.55
1:D:21:ILE:HD11	1:D:194:ILE:HG13	1.90	0.52
1:F:222:TRP:HE1	1:F:261:ASP:HB2	1.74	0.52
1:D:161:MET:HE3	1:D:165:LYS:HE2	1.92	0.52
1:C:16:ILE:HD12	1:C:47:ILE:HD11	1.92	0.52
1:E:70:HIS:O	1:E:74:LEU:HB2	2.10	0.52
1:A:44:LEU:HD11	1:A:62:GLU:HB2	1.92	0.51
1:D:185:ARG:HA	1:D:254:THR:HG23	1.93	0.51
1:C:185:ARG:HA	1:C:254:THR:HG23	1.92	0.51
1:E:185:ARG:HA	1:E:254:THR:HG23	1.94	0.50
1:B:185:ARG:HA	1:B:254:THR:HG23	1.94	0.50
1:F:185:ARG:HA	1:F:254:THR:HG23	1.94	0.49
1:C:45:ARG:HE	1:C:46:LEU:HG	1.78	0.48
1:A:161:MET:HE3	1:A:165:LYS:HE2	1.96	0.47
1:F:15:ILE:HA	4:F:2002:HOH:O	2.16	0.45
1:B:65:VAL:CG2	1:B:126:SER:HB2	2.47	0.44
1:C:65:VAL:CG2	1:C:126:SER:HB2	2.47	0.44
1:A:5:LEU:HB3	1:A:34:ALA:HB2	2.00	0.44
1:B:186:SER:H	1:B:254:THR:HG23	1.81	0.44
1:A:51:THR:O	1:A:54:LEU:HB2	2.18	0.43
1:A:225:ARG:HD2	1:A:267:GLN:O	2.18	0.43
1:F:5:LEU:HB3	1:F:34:ALA:HB2	2.00	0.43
1:C:195:ARG:HD3	1:C:232:MET:HG3	1.99	0.43
1:E:193:PRO:HB2	1:E:219:GLU:HG2	2.01	0.43
1:C:124:ALA:HA	1:C:168:LEU:HD13	2.01	0.43
1:D:63:LEU:HD13	1:D:74:LEU:HD13	2.00	0.43
1:D:65:VAL:CG2	1:D:126:SER:HB2	2.49	0.43
1:F:186:SER:H	1:F:254:THR:HG23	1.83	0.43
1:B:51:THR:O	1:B:54:LEU:HB2	2.18	0.43
1:E:5:LEU:HB3	1:E:34:ALA:HB2	2.01	0.43
1:E:178:GLU:O	1:E:181:LYS:HG2	2.18	0.43
1:B:5:LEU:HB3	1:B:34:ALA:HB2	2.01	0.43
1:D:5:LEU:HB3	1:D:34:ALA:HB2	2.01	0.43
1:F:51:THR:O	1:F:54:LEU:HB2	2.19	0.43
1:E:65:VAL:CG2	1:E:126:SER:HB2	2.49	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:43:ARG:HB3	1:D:46:LEU:HB3	2.01	0.42
1:C:161:MET:HE3	1:C:165:LYS:HE2	2.02	0.42
1:A:158:TYR:HD1	2:A:1270:I4I:HAB	1.84	0.42
1:C:61:LEU:HD22	1:C:77:ARG:HB3	2.01	0.42
1:F:65:VAL:CG2	1:F:126:SER:HB2	2.50	0.42
1:A:21:ILE:HD12	2:A:1270:I4I:CAK	2.49	0.41
1:E:51:THR:O	1:E:54:LEU:HB2	2.19	0.41
1:C:140:PRO:HG2	1:E:195:ARG:NH1	2.29	0.41
1:D:218:LEU:HD11	1:F:268:LEU:HD23	2.03	0.41
1:D:39:THR:HG23	1:D:63:LEU:HB3	2.03	0.41
1:A:65:VAL:CG2	1:A:126:SER:HB2	2.51	0.41
1:C:5:LEU:HB3	1:C:34:ALA:HB2	2.01	0.41
1:D:113:TYR:HA	1:D:116:VAL:HG22	2.03	0.41
1:E:63:LEU:HD11	1:E:71:LEU:HD12	2.02	0.41
1:E:186:SER:H	1:E:254:THR:HG23	1.86	0.41
1:A:185:ARG:HD2	4:A:2106:HOH:O	2.21	0.40
1:D:186:SER:H	1:D:254:THR:HG23	1.86	0.40
1:B:43:ARG:H	1:B:43:ARG:HG2	1.75	0.40
1:C:186:SER:H	1:C:254:THR:HG23	1.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	265/281 (94%)	252 (95%)	13 (5%)	0	100	100
1	B	266/281 (95%)	257 (97%)	9 (3%)	0	100	100
1	C	250/281 (89%)	238 (95%)	11 (4%)	1 (0%)	30	28
1	D	248/281 (88%)	238 (96%)	9 (4%)	1 (0%)	30	28
1	E	247/281 (88%)	233 (94%)	13 (5%)	1 (0%)	30	28

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	265/281 (94%)	251 (95%)	14 (5%)	0	100	100
All	All	1541/1686 (91%)	1469 (95%)	69 (4%)	3 (0%)	43	44

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	75	ALA
1	C	74	LEU
1	D	157	ALA

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	202/215 (94%)	178 (88%)	24 (12%)	5	3
1	B	203/215 (94%)	184 (91%)	19 (9%)	8	6
1	C	195/215 (91%)	176 (90%)	19 (10%)	8	5
1	D	193/215 (90%)	176 (91%)	17 (9%)	9	7
1	E	194/215 (90%)	175 (90%)	19 (10%)	7	5
1	F	202/215 (94%)	179 (89%)	23 (11%)	5	3
All	All	1189/1290 (92%)	1068 (90%)	121 (10%)	7	4

All (121) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	16	ILE
1	A	39	THR
1	A	41	PHE
1	A	46	LEU
1	A	48	GLN
1	A	65	VAL
1	A	67	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	68	GLU
1	A	69	GLU
1	A	74	LEU
1	A	82	ILE
1	A	88	LEU
1	A	162	THR
1	A	168	LEU
1	A	188	LEU
1	A	196	THR
1	A	197	LEU
1	A	207	LEU
1	A	215	ILE
1	A	216	GLN
1	A	220	GLU
1	A	238	VAL
1	A	269	LEU
1	B	5	LEU
1	B	39	THR
1	B	45	ARG
1	B	48	GLN
1	B	65	VAL
1	B	67	ASN
1	B	74	LEU
1	B	88	LEU
1	B	162	THR
1	B	168	LEU
1	B	188	LEU
1	B	196	THR
1	B	199	MET
1	B	207	LEU
1	B	215	ILE
1	B	216	GLN
1	B	238	VAL
1	B	254	THR
1	B	269	LEU
1	C	5	LEU
1	C	16	ILE
1	C	44	LEU
1	C	45	ARG
1	C	46	LEU
1	C	48	GLN
1	C	54	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	60	LEU
1	C	65	VAL
1	C	74	LEU
1	C	88	LEU
1	C	162	THR
1	C	188	LEU
1	C	215	ILE
1	C	216	GLN
1	C	233	LYS
1	C	238	VAL
1	C	254	THR
1	C	269	LEU
1	D	5	LEU
1	D	39	THR
1	D	48	GLN
1	D	54	LEU
1	D	57	LYS
1	D	65	VAL
1	D	67	ASN
1	D	69	GLU
1	D	88	LEU
1	D	162	THR
1	D	168	LEU
1	D	188	LEU
1	D	215	ILE
1	D	216	GLN
1	D	238	VAL
1	D	254	THR
1	D	269	LEU
1	E	5	LEU
1	E	16	ILE
1	E	39	THR
1	E	44	LEU
1	E	46	LEU
1	E	48	GLN
1	E	49	ARG
1	E	54	LEU
1	E	65	VAL
1	E	67	ASN
1	E	74	LEU
1	E	88	LEU
1	E	162	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	168	LEU
1	E	181	LYS
1	E	188	LEU
1	E	217	LEU
1	E	238	VAL
1	E	254	THR
1	F	5	LEU
1	F	16	ILE
1	F	19	SER
1	F	20	SER
1	F	39	THR
1	F	48	GLN
1	F	49	ARG
1	F	61	LEU
1	F	65	VAL
1	F	67	ASN
1	F	74	LEU
1	F	88	LEU
1	F	162	THR
1	F	168	LEU
1	F	188	LEU
1	F	196	THR
1	F	207	LEU
1	F	210	GLU
1	F	215	ILE
1	F	216	GLN
1	F	238	VAL
1	F	254	THR
1	F	269	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	67	ASN
1	A	86	ASN
1	A	106	ASN
1	A	172	ASN
1	A	216	GLN
1	A	231	ASN
1	B	67	ASN
1	B	86	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	106	ASN
1	B	231	ASN
1	C	32	GLN
1	C	86	ASN
1	C	106	ASN
1	C	231	ASN
1	D	32	GLN
1	D	66	GLN
1	D	67	ASN
1	D	86	ASN
1	D	106	ASN
1	D	121	HIS
1	D	214	GLN
1	D	216	GLN
1	D	231	ASN
1	E	32	GLN
1	E	86	ASN
1	E	106	ASN
1	E	231	ASN
1	F	32	GLN
1	F	48	GLN
1	F	67	ASN
1	F	86	ASN
1	F	106	ASN
1	F	216	GLN
1	F	231	ASN

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

6 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	I4I	A	1270	-	40,40,40	1.21	5 (12%)	48,56,56	1.38	6 (12%)
3	NAD	D	1270	-	46,48,48	0.50	0	64,73,73	0.61	0
3	NAD	E	1270	-	46,48,48	0.48	0	64,73,73	0.52	0
2	I4I	B	1270	-	40,40,40	1.32	6 (15%)	48,56,56	1.44	6 (12%)
2	I4I	F	1270	-	40,40,40	1.38	7 (17%)	48,56,56	1.35	6 (12%)
3	NAD	C	1270	-	46,48,48	0.58	0	64,73,73	0.50	1 (1%)

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	I4I	A	1270	-	-	7/52/52/52	0/2/3/3
3	NAD	D	1270	-	-	10/30/62/62	0/5/5/5
3	NAD	E	1270	-	-	12/30/62/62	0/5/5/5
2	I4I	B	1270	-	-	6/52/52/52	0/2/3/3
2	I4I	F	1270	-	-	8/52/52/52	0/2/3/3
3	NAD	C	1270	-	-	7/30/62/62	0/5/5/5

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1270	I4I	CBL-CBB	3.35	1.58	1.52
2	B	1270	I4I	CBE-NAT	3.14	1.40	1.34
2	A	1270	I4I	CBE-NAT	2.96	1.39	1.34
2	F	1270	I4I	CBL-CBB	2.96	1.57	1.52
2	F	1270	I4I	CBI-CBJ	2.75	1.58	1.53
2	F	1270	I4I	CAY-N	2.71	1.40	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1270	I4I	CBD-CBE	2.70	1.44	1.40
2	B	1270	I4I	CBI-CBJ	2.60	1.58	1.53
2	A	1270	I4I	CBI-CBJ	2.48	1.57	1.53
2	A	1270	I4I	CBD-CBE	2.39	1.43	1.40
2	A	1270	I4I	OAX-CBA	2.38	1.39	1.34
2	F	1270	I4I	CBE-NAT	2.28	1.38	1.34
2	F	1270	I4I	CAQ-CBC	2.18	1.43	1.38
2	A	1270	I4I	C-NAV	2.16	1.38	1.34
2	B	1270	I4I	CAQ-CBC	2.16	1.43	1.38
2	B	1270	I4I	CBD-CBE	2.10	1.43	1.40
2	B	1270	I4I	CAQ-NAS	2.02	1.38	1.34
2	F	1270	I4I	C-NAV	2.00	1.38	1.34

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1270	I4I	CB-OG1-CBB	5.00	124.95	117.55
2	F	1270	I4I	CB-OG1-CBB	4.96	124.89	117.55
2	A	1270	I4I	C-CA-N	-4.21	98.88	110.32
2	B	1270	I4I	C-CA-N	-3.95	99.59	110.32
2	A	1270	I4I	CA-N-CAY	3.82	129.24	121.53
2	F	1270	I4I	CA-N-CAY	3.49	128.57	121.53
2	F	1270	I4I	C-CA-N	-3.36	101.20	110.32
2	B	1270	I4I	CA-N-CAY	3.30	128.18	121.53
2	A	1270	I4I	CB-OG1-CBB	3.26	122.37	117.55
2	F	1270	I4I	CB-CA-C	2.95	116.94	110.73
2	B	1270	I4I	CB-CA-C	2.95	116.93	110.73
2	A	1270	I4I	OAX-CBA-OAG	-2.61	119.24	123.95
2	A	1270	I4I	CB-CA-C	2.55	116.10	110.73
2	B	1270	I4I	OG1-CB-CA	-2.34	100.66	105.77
2	F	1270	I4I	OAX-CBA-OAG	-2.23	119.92	123.95
2	B	1270	I4I	CAY-CBE-NAT	-2.20	111.89	115.81
3	C	1270	NAD	C4D-O4D-C1D	-2.18	107.93	109.92
2	F	1270	I4I	CAY-CBE-NAT	-2.10	112.06	115.81
2	A	1270	I4I	CAY-CBE-NAT	-2.06	112.13	115.81

There are no chirality outliers.

All (50) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1270	NAD	O4D-C1D-N1N-C2N
3	D	1270	NAD	PA-O3-PN-O5D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	D	1270	NAD	C5D-O5D-PN-O3
3	D	1270	NAD	C5D-O5D-PN-O1N
3	D	1270	NAD	C5D-O5D-PN-O2N
3	D	1270	NAD	O4D-C1D-N1N-C2N
3	E	1270	NAD	C5B-O5B-PA-O1A
3	E	1270	NAD	C5B-O5B-PA-O2A
3	E	1270	NAD	C5B-O5B-PA-O3
3	E	1270	NAD	O4D-C1D-N1N-C2N
3	C	1270	NAD	O4B-C4B-C5B-O5B
3	C	1270	NAD	C3B-C4B-C5B-O5B
2	A	1270	I4I	OAE-CAY-CBE-NAT
2	B	1270	I4I	OAE-CAY-CBE-NAT
2	F	1270	I4I	OAE-CAY-CBE-NAT
2	A	1270	I4I	N-CAY-CBE-NAT
2	B	1270	I4I	N-CAY-CBE-NAT
2	F	1270	I4I	N-CAY-CBE-NAT
3	E	1270	NAD	O4B-C4B-C5B-O5B
3	C	1270	NAD	O4D-C4D-C5D-O5D
3	E	1270	NAD	C3B-C4B-C5B-O5B
3	C	1270	NAD	C3D-C4D-C5D-O5D
3	D	1270	NAD	PN-O3-PA-O5B
2	A	1270	I4I	OAG-CBA-CBH-CBI
2	B	1270	I4I	OAG-CBA-CBH-CBI
2	F	1270	I4I	OAG-CBA-CBH-CBI
2	A	1270	I4I	N-CAY-CBE-CBD
2	B	1270	I4I	N-CAY-CBE-CBD
2	F	1270	I4I	N-CAY-CBE-CBD
3	E	1270	NAD	O4D-C4D-C5D-O5D
2	A	1270	I4I	OAE-CAY-CBE-CBD
2	B	1270	I4I	OAE-CAY-CBE-CBD
2	F	1270	I4I	OAE-CAY-CBE-CBD
3	D	1270	NAD	C5B-O5B-PA-O2A
3	D	1270	NAD	C5B-O5B-PA-O3
2	B	1270	I4I	OAX-CBA-CBH-CBI
2	F	1270	I4I	OAX-CBA-CBH-CBI
3	C	1270	NAD	C4D-C5D-O5D-PN
2	A	1270	I4I	OAX-CBA-CBH-CBI
3	C	1270	NAD	O4D-C1D-N1N-C6N
3	D	1270	NAD	O4D-C1D-N1N-C6N
3	E	1270	NAD	C3D-C4D-C5D-O5D
3	E	1270	NAD	O4D-C1D-N1N-C6N
3	E	1270	NAD	PA-O3-PN-O1N

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	E	1270	NAD	C4B-C5B-O5B-PA
3	E	1270	NAD	PA-O3-PN-O2N
3	D	1270	NAD	O4B-C4B-C5B-O5B
2	A	1270	I4I	OAH-CBB-CBL-OAX
2	F	1270	I4I	OAH-CBB-CBL-OAX
2	F	1270	I4I	CBA-CBH-CBI-CBJ

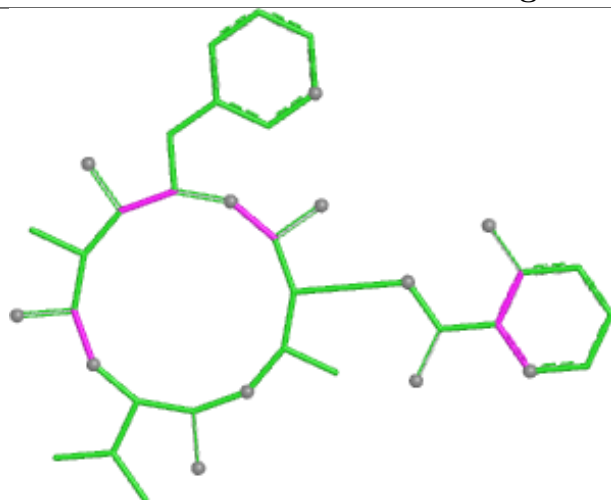
There are no ring outliers.

1 monomer is involved in 2 short contacts:

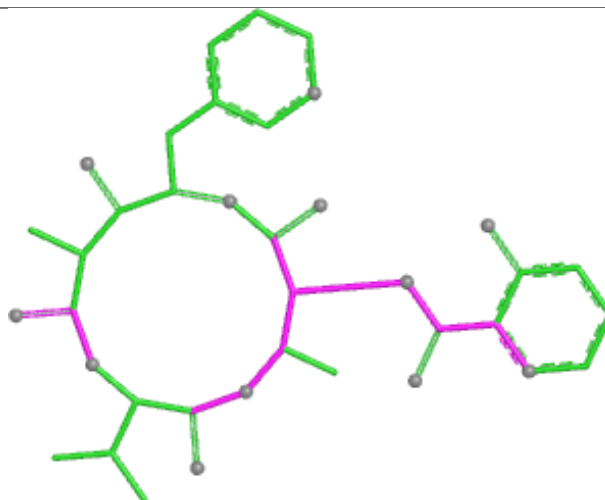
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1270	I4I	2	0

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.

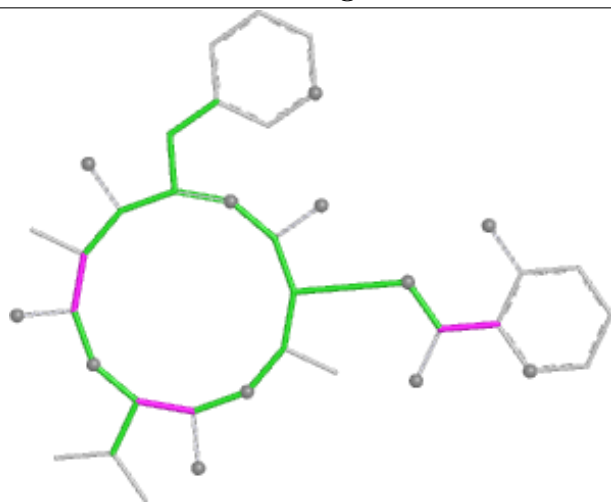
Ligand I4I A 1270



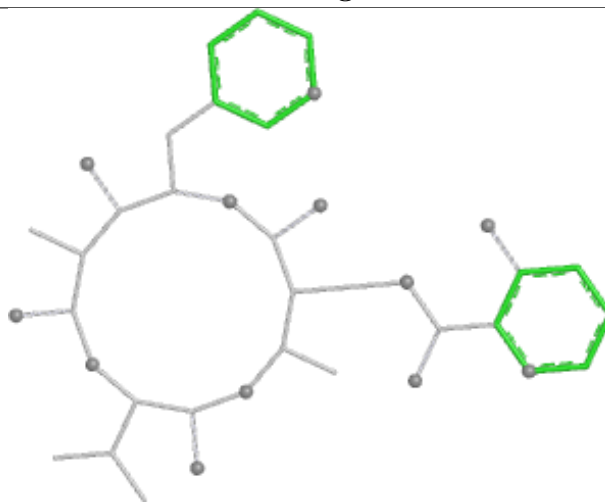
Bond lengths



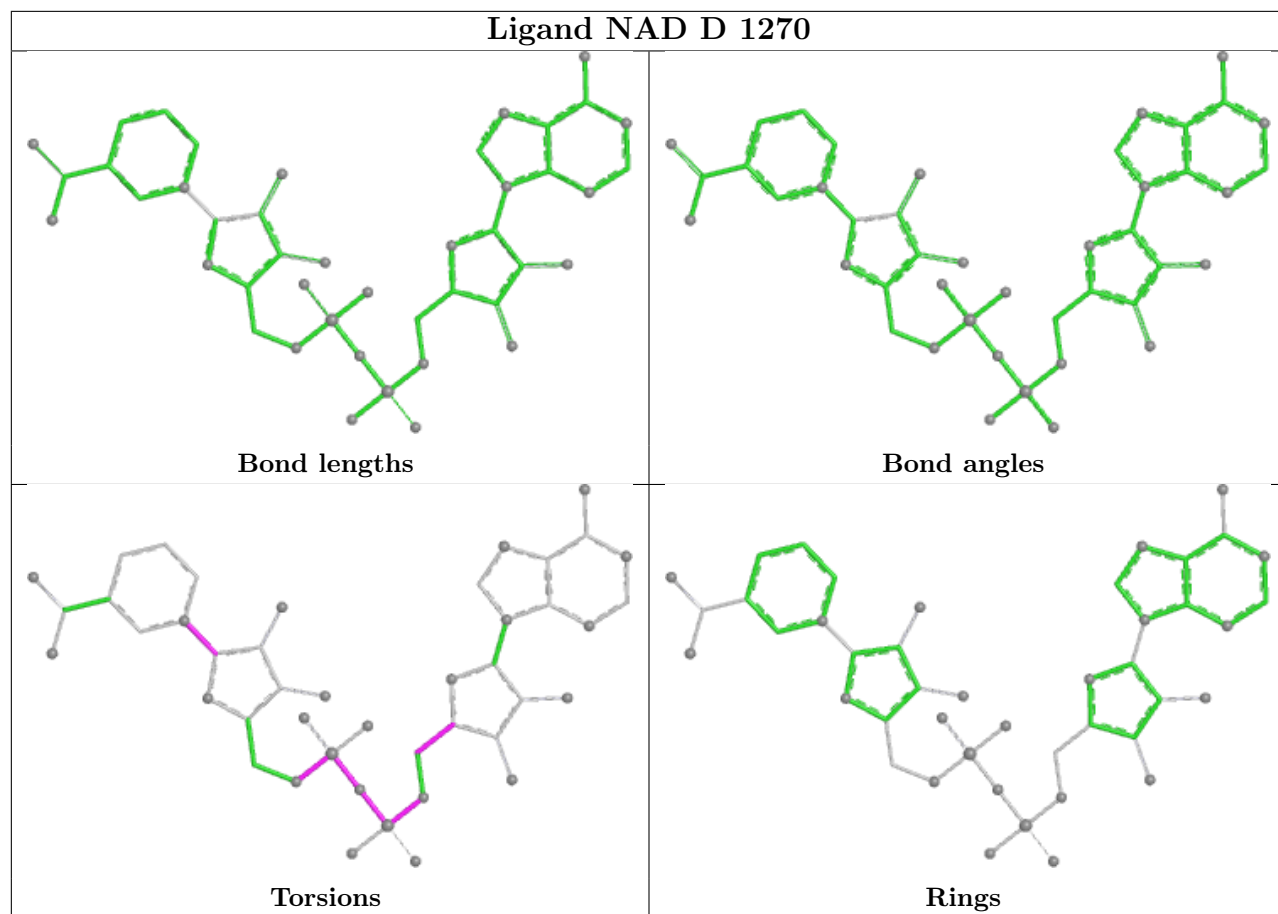
Bond angles

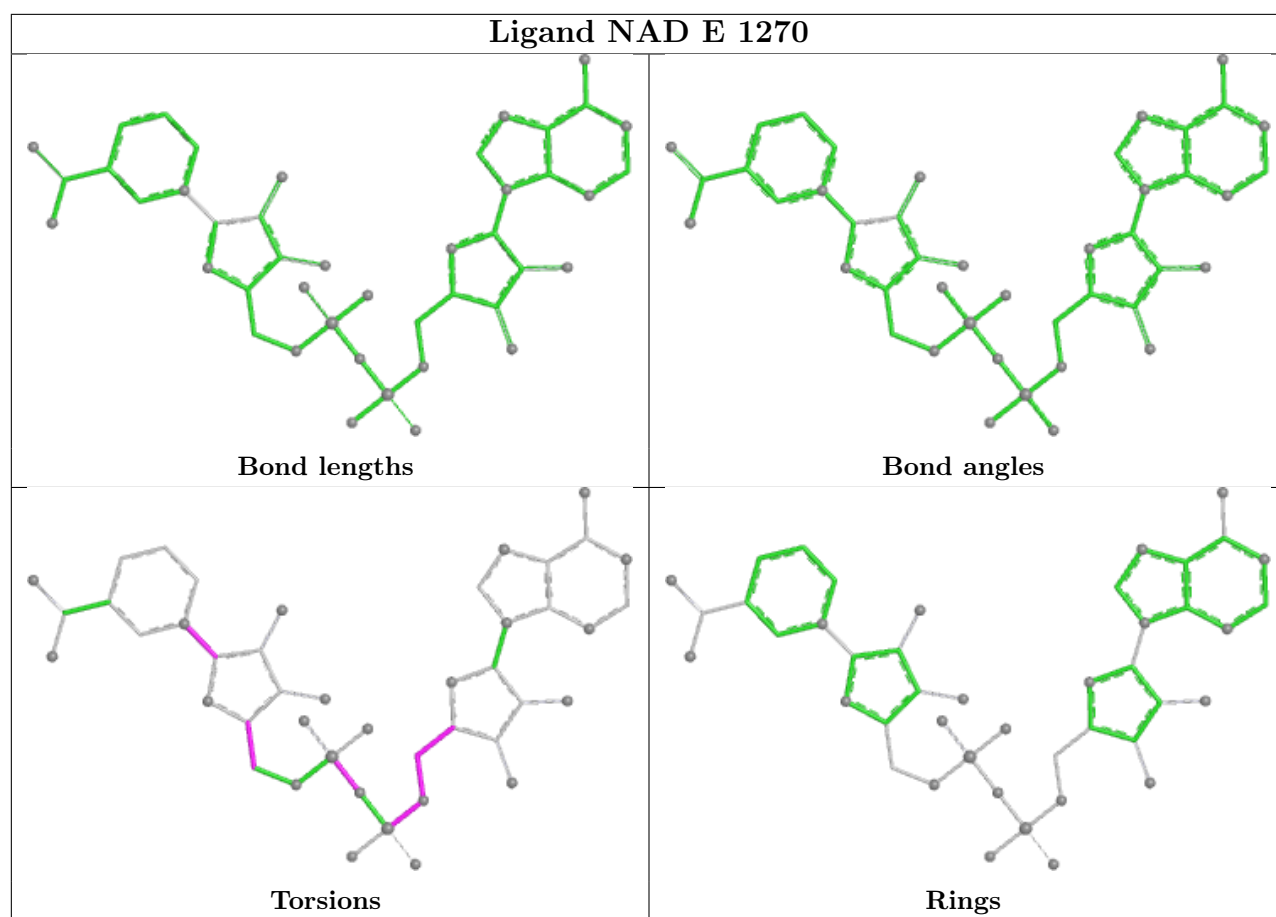


Torsions

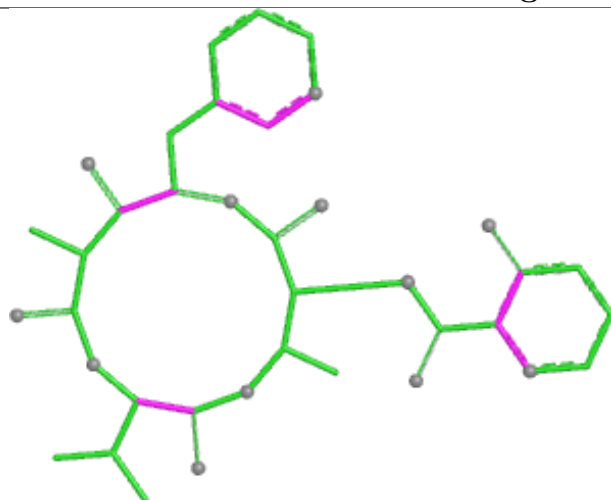


Rings

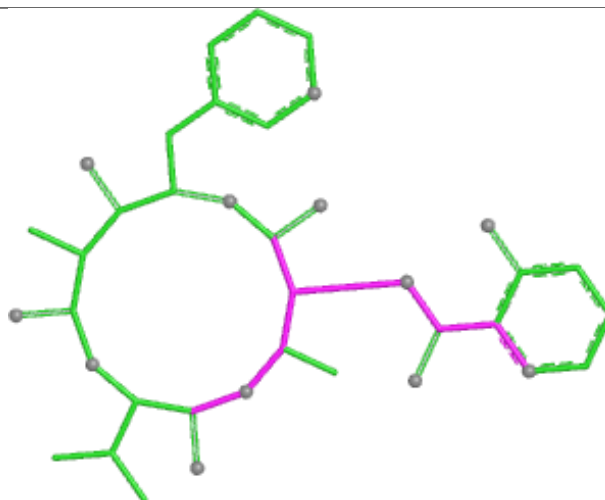




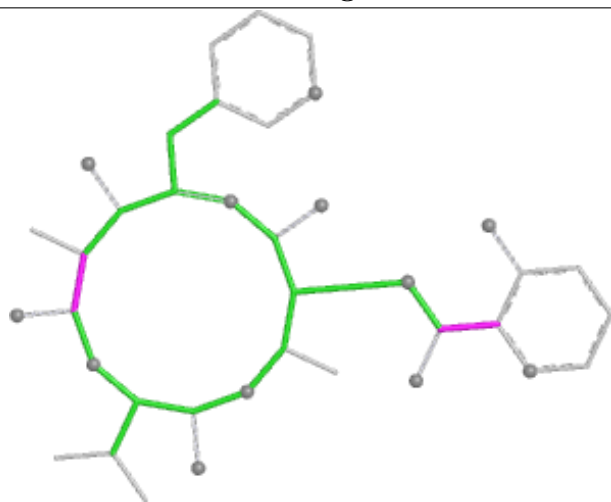
Ligand I4I B 1270



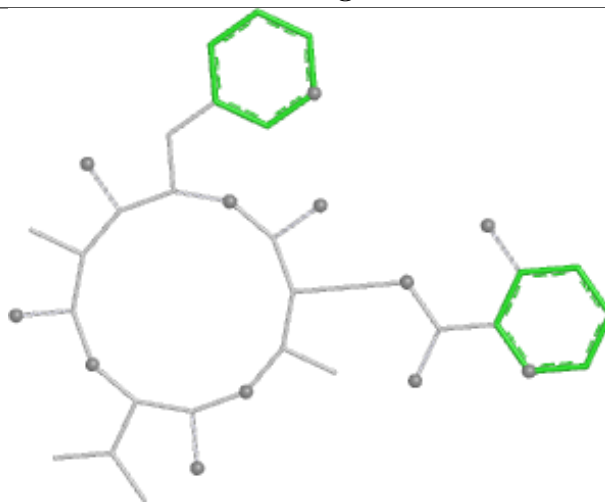
Bond lengths



Bond angles

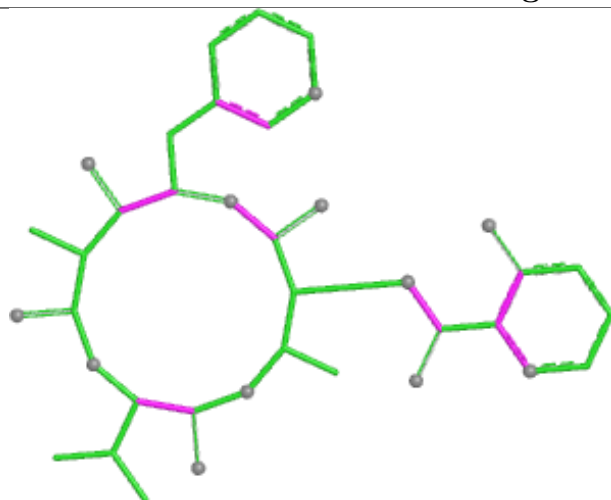


Torsions

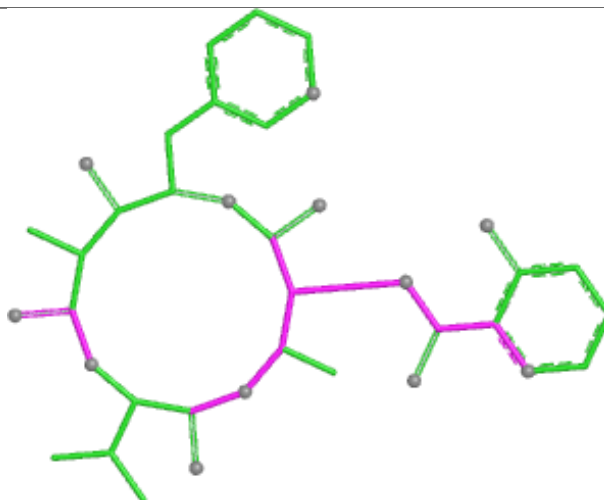


Rings

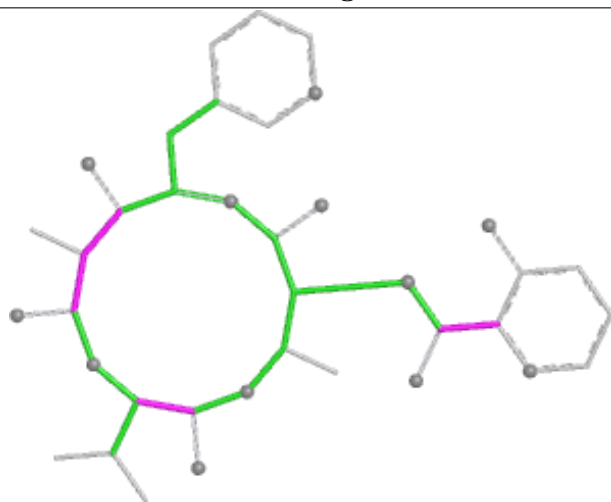
Ligand I4I F 1270



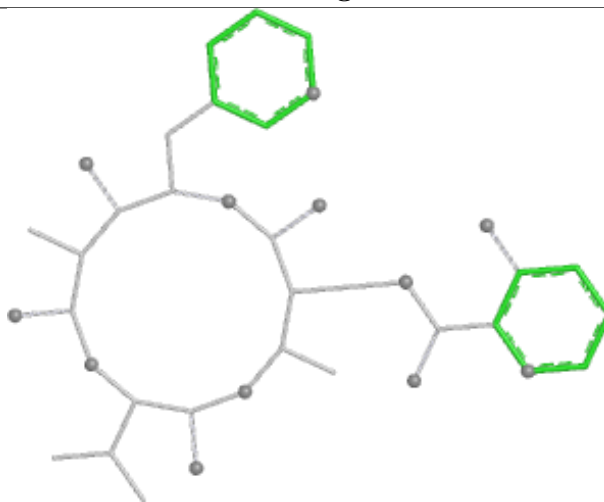
Bond lengths



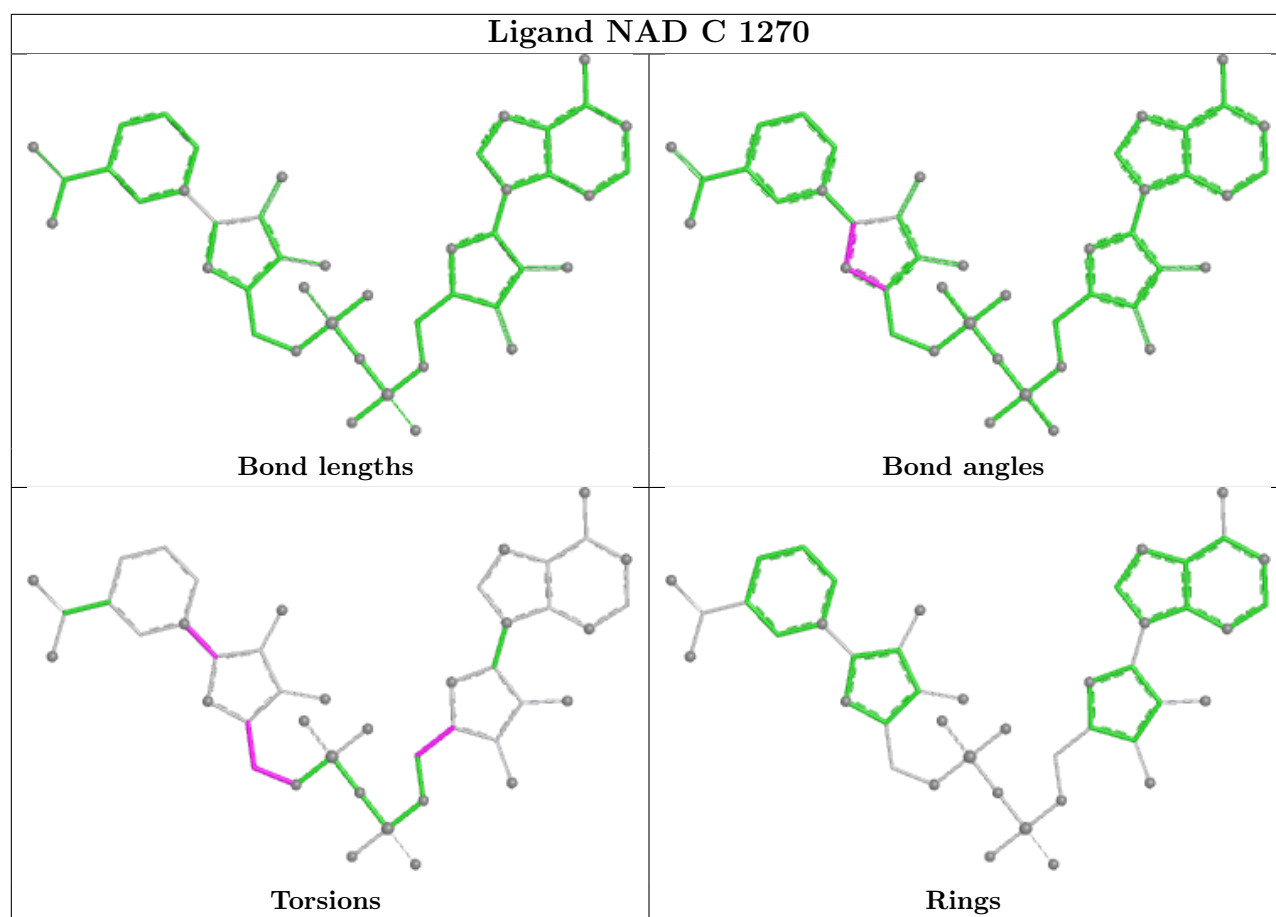
Bond angles



Torsions



Rings



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	267/281 (95%)	0.34	19 (7%)	22 23	7, 22, 52, 65	0
1	B	267/281 (95%)	0.35	26 (9%)	13 14	7, 21, 53, 82	1 (0%)
1	C	254/281 (90%)	1.37	67 (26%)	1 1	21, 40, 65, 85	0
1	D	252/281 (89%)	1.22	51 (20%)	3 3	21, 39, 63, 89	0
1	E	251/281 (89%)	1.41	69 (27%)	1 1	21, 40, 65, 85	0
1	F	267/281 (95%)	1.52	82 (30%)	1 1	24, 43, 74, 92	0
All	All	1558/1686 (92%)	1.03	314 (20%)	3 3	7, 35, 64, 92	1 (0%)

All (314) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	215	ILE	7.0
1	C	213	ALA	6.3
1	E	50	ILE	5.2
1	F	202	ILE	4.9
1	F	204	GLY	4.9
1	E	82	ILE	4.9
1	E	56	ALA	4.8
1	E	217	LEU	4.7
1	F	44	LEU	4.7
1	E	196	THR	4.6
1	B	197[A]	LEU	4.6
1	E	105	ILE	4.6
1	A	198	ALA	4.6
1	C	73	SER	4.5
1	D	211	ALA	4.5
1	C	83	GLY	4.4
1	F	197	LEU	4.3
1	C	44	LEU	4.3
1	B	84	ALA	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	47	ILE	4.2
1	F	50	ILE	4.2
1	E	71	LEU	4.1
1	C	50	ILE	4.1
1	F	82	ILE	4.0
1	C	195	ARG	4.0
1	D	213	ALA	3.9
1	F	58	ALA	3.9
1	A	196	THR	3.9
1	F	37	VAL	3.8
1	C	82	ILE	3.8
1	F	203	VAL	3.8
1	D	82	ILE	3.7
1	D	158	TYR	3.7
1	B	219	GLU	3.7
1	F	196	THR	3.7
1	C	41	PHE	3.7
1	F	16	ILE	3.6
1	D	11	LEU	3.6
1	F	46	LEU	3.6
1	C	218	LEU	3.6
1	E	106	ASN	3.6
1	C	40	GLY	3.6
1	C	39	THR	3.5
1	E	63	LEU	3.5
1	C	76	GLY	3.5
1	F	63	LEU	3.4
1	C	21	ILE	3.4
1	F	21	ILE	3.4
1	D	65	VAL	3.4
1	E	19	SER	3.4
1	C	211	ALA	3.4
1	F	198	ALA	3.4
1	F	61	LEU	3.4
1	F	269	LEU	3.4
1	D	16	ILE	3.3
1	A	207	LEU	3.3
1	F	41	PHE	3.3
1	F	5	LEU	3.3
1	F	22	ALA	3.3
1	D	214	GLN	3.3
1	C	19	SER	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	106	ASN	3.2
1	F	40	GLY	3.2
1	F	83	GLY	3.2
1	F	49	ARG	3.2
1	F	199	MET	3.2
1	A	197	LEU	3.2
1	B	47	ILE	3.2
1	E	46	LEU	3.2
1	F	218	LEU	3.2
1	B	48	GLN	3.2
1	B	43	ARG	3.2
1	E	21	ILE	3.2
1	B	44	LEU	3.1
1	F	194	ILE	3.1
1	F	65	VAL	3.1
1	F	20	SER	3.1
1	D	105	ILE	3.1
1	A	41	PHE	3.1
1	F	53	ARG	3.1
1	E	60	LEU	3.1
1	F	54	LEU	3.1
1	B	16	ILE	3.1
1	C	214	GLN	3.1
1	F	79	THR	3.0
1	C	42	ASP	3.0
1	C	78	VAL	3.0
1	D	137	ILE	3.0
1	C	135	LEU	3.0
1	E	135	LEU	3.0
1	F	19	SER	3.0
1	B	83	GLY	3.0
1	C	22	ALA	3.0
1	F	56	ALA	3.0
1	C	11	LEU	3.0
1	B	50	ILE	3.0
1	E	41	PHE	3.0
1	E	34	ALA	2.9
1	C	61	LEU	2.9
1	E	229	GLY	2.9
1	C	15	ILE	2.9
1	F	25	ILE	2.9
1	F	51	THR	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	46	LEU	2.9
1	C	88	LEU	2.9
1	F	36	LEU	2.9
1	F	195	ARG	2.9
1	D	74	LEU	2.8
1	B	202	ILE	2.8
1	E	57	LYS	2.8
1	F	23	PHE	2.8
1	F	205	GLY	2.8
1	E	54	LEU	2.8
1	C	105	ILE	2.8
1	E	70	HIS	2.8
1	C	84	ALA	2.8
1	E	78	VAL	2.8
1	F	105	ILE	2.8
1	F	137	ILE	2.8
1	F	48	GLN	2.8
1	F	232	MET	2.8
1	C	74	LEU	2.8
1	C	269	LEU	2.8
1	E	44	LEU	2.8
1	C	45	ARG	2.7
1	F	214	GLN	2.7
1	D	210	GLU	2.7
1	F	43	ARG	2.7
1	A	202	ILE	2.7
1	D	57	LYS	2.7
1	F	10	ILE	2.7
1	D	73	SER	2.7
1	F	42	ASP	2.7
1	D	8	LYS	2.7
1	E	58	ALA	2.6
1	E	84	ALA	2.6
1	E	108	PHE	2.6
1	D	88	LEU	2.6
1	F	24	HIS	2.6
1	F	57	LYS	2.6
1	A	82	ILE	2.6
1	D	194	ILE	2.6
1	F	15	ILE	2.6
1	C	212	GLY	2.6
1	D	133	ALA	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	79	THR	2.6
1	A	44	LEU	2.6
1	B	203	VAL	2.6
1	F	12	VAL	2.6
1	C	48	GLN	2.6
1	E	69	GLU	2.6
1	A	84	ALA	2.6
1	B	46	LEU	2.6
1	E	218	LEU	2.6
1	E	43	ARG	2.6
1	C	16	ILE	2.6
1	E	10	ILE	2.6
1	C	58	ALA	2.6
1	C	37	VAL	2.5
1	E	194	ILE	2.5
1	D	53	ARG	2.5
1	E	269	LEU	2.5
1	D	41	PHE	2.5
1	B	204	GLY	2.5
1	D	212	GLY	2.5
1	E	18	ASP	2.5
1	C	5	LEU	2.5
1	C	38	LEU	2.5
1	D	61	LEU	2.5
1	D	269	LEU	2.5
1	F	207	LEU	2.5
1	C	53	ARG	2.5
1	B	52	ASP	2.5
1	E	6	ASP	2.5
1	B	200	SER	2.5
1	D	54	LEU	2.5
1	C	47	ILE	2.5
1	C	65	VAL	2.4
1	F	234	ASP	2.4
1	D	46	LEU	2.4
1	D	60	LEU	2.4
1	E	74	LEU	2.4
1	E	16	ILE	2.4
1	E	228	ILE	2.4
1	E	222	TRP	2.4
1	E	236	THR	2.4
1	F	241	THR	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	55	PRO	2.4
1	F	81	ALA	2.4
1	C	256	ASP	2.4
1	F	6	ASP	2.4
1	D	254	THR	2.4
1	F	39	THR	2.4
1	B	201	ALA	2.4
1	C	4	LEU	2.4
1	E	5	LEU	2.4
1	F	134	LEU	2.4
1	E	86	ASN	2.4
1	F	32	GLN	2.4
1	D	10	ILE	2.4
1	D	15	ILE	2.4
1	B	53	ARG	2.4
1	D	28	VAL	2.4
1	F	26	ALA	2.3
1	C	63	LEU	2.3
1	C	100	GLN	2.3
1	C	3	GLY	2.3
1	C	87	LYS	2.3
1	F	45	ARG	2.3
1	A	47	ILE	2.3
1	D	215	ILE	2.3
1	E	15	ILE	2.3
1	C	59	PRO	2.3
1	D	236	THR	2.3
1	E	17	THR	2.3
1	C	62	GLU	2.3
1	D	100	GLN	2.3
1	C	255	GLY	2.3
1	E	61	LEU	2.3
1	A	19	SER	2.3
1	D	219	GLU	2.3
1	F	78	VAL	2.3
1	E	101	THR	2.3
1	F	55	PRO	2.3
1	C	139	ASN	2.3
1	F	260	ALA	2.3
1	A	46	LEU	2.3
1	B	45	ARG	2.3
1	F	4	LEU	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	87	LYS	2.3
1	F	80	GLU	2.3
1	D	216	GLN	2.3
1	E	47	ILE	2.3
1	D	79	THR	2.3
1	C	85	GLY	2.3
1	B	199	MET	2.3
1	D	5	LEU	2.3
1	E	107	PRO	2.2
1	D	85	GLY	2.2
1	E	83	GLY	2.2
1	E	104	GLY	2.2
1	A	269	LEU	2.2
1	C	217	LEU	2.2
1	F	246	LEU	2.2
1	C	51	THR	2.2
1	E	39	THR	2.2
1	E	254	THR	2.2
1	E	37	VAL	2.2
1	F	59	PRO	2.2
1	C	81	ALA	2.2
1	D	56	ALA	2.2
1	C	60	LEU	2.2
1	F	60	LEU	2.2
1	F	8	LYS	2.2
1	B	15	ILE	2.2
1	C	136	PRO	2.2
1	D	59	PRO	2.2
1	D	108	PHE	2.2
1	D	58	ALA	2.2
1	E	213	ALA	2.2
1	B	54	LEU	2.2
1	D	217	LEU	2.2
1	F	27	ARG	2.2
1	F	144	ILE	2.1
1	E	81	ALA	2.1
1	E	49	ARG	2.1
1	E	53	ARG	2.1
1	F	38	LEU	2.1
1	B	42	ASP	2.1
1	B	69	GLU	2.1
1	A	100	GLN	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	205	GLY	2.1
1	D	104	GLY	2.1
1	F	3	GLY	2.1
1	A	81	ALA	2.1
1	E	75	ALA	2.1
1	C	36	LEU	2.1
1	C	233	LYS	2.1
1	E	38	LEU	2.1
1	C	232	MET	2.1
1	F	18	ASP	2.1
1	D	156	PRO	2.1
1	A	53	ARG	2.1
1	C	180	GLY	2.1
1	E	8	LYS	2.1
1	E	235	ALA	2.1
1	A	20	SER	2.1
1	A	18	ASP	2.1
1	A	195	ARG	2.1
1	D	45	ARG	2.1
1	F	17	THR	2.1
1	C	221	GLY	2.1
1	D	50	ILE	2.1
1	F	215	ILE	2.1
1	C	97	PHE	2.1
1	D	23	PHE	2.1
1	D	238	VAL	2.1
1	D	81	ALA	2.1
1	C	89	ASP	2.0
1	E	237	PRO	2.0
1	E	33	GLY	2.0
1	E	85	GLY	2.0
1	C	215	ILE	2.0
1	E	31	GLU	2.0
1	F	28	VAL	2.0
1	F	145	VAL	2.0
1	C	75	ALA	2.0
1	B	269	LEU	2.0
1	E	4	LEU	2.0
1	F	71	LEU	2.0
1	C	24	HIS	2.0
1	D	107	PRO	2.0
1	E	79	THR	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	193	PRO	2.0

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](#)

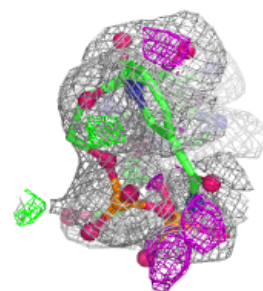
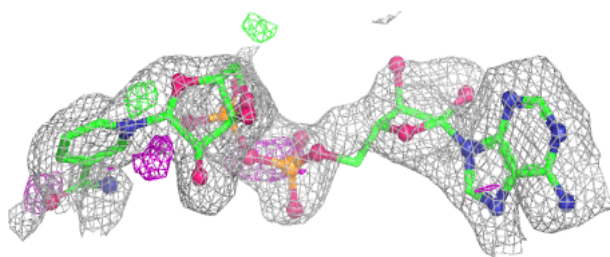
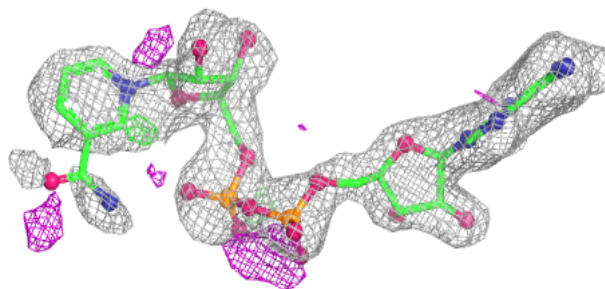
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAD	C	1270	44/44	0.73	0.16	42,53,64,68	0
2	I4I	F	1270	38/38	0.78	0.15	44,51,56,57	0
3	NAD	E	1270	44/44	0.83	0.13	27,48,62,66	0
3	NAD	D	1270	44/44	0.84	0.12	30,39,47,50	0
2	I4I	A	1270	38/38	0.91	0.08	14,23,30,33	0
2	I4I	B	1270	38/38	0.92	0.08	18,23,33,36	0

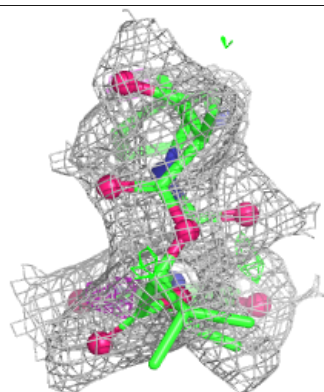
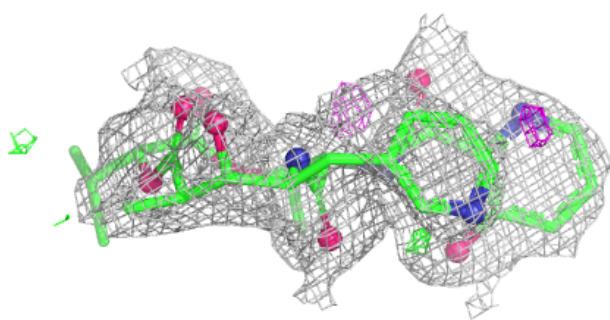
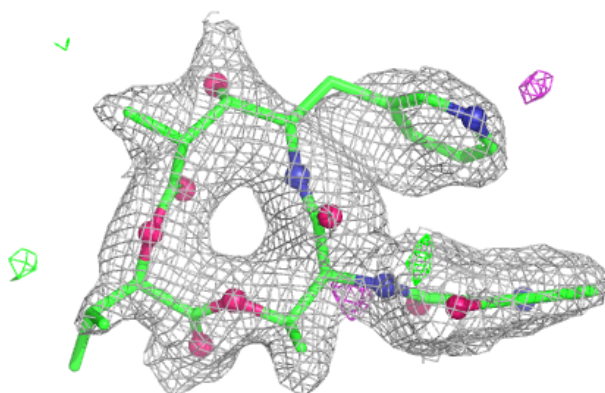
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAD C 1270:

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

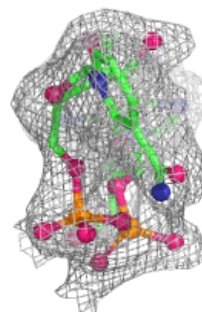
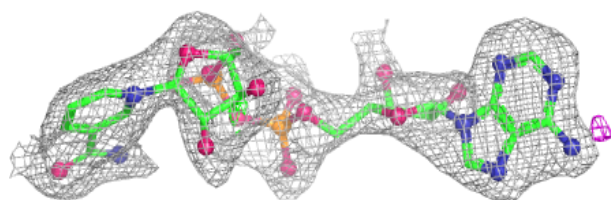
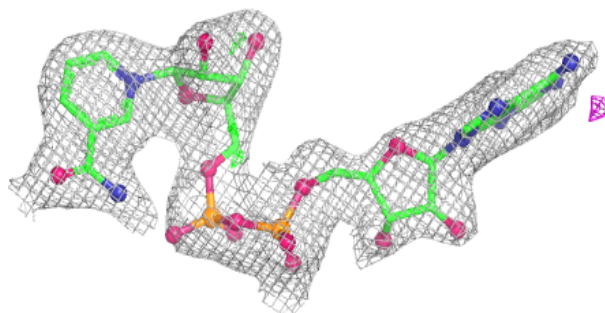
**Electron density around I4I F 1270:**

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

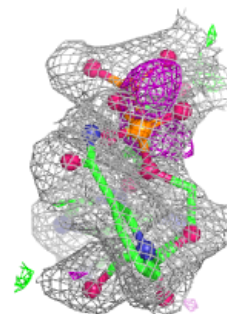
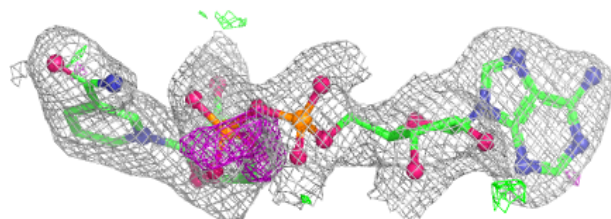
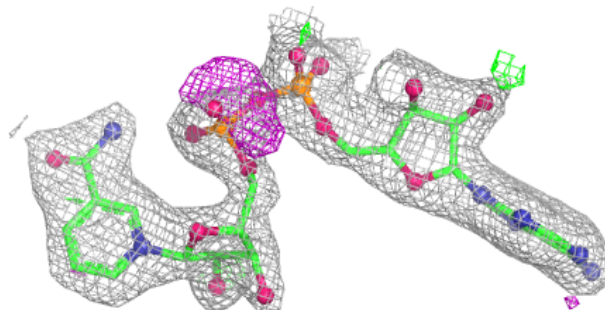


Electron density around NAD E 1270:

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

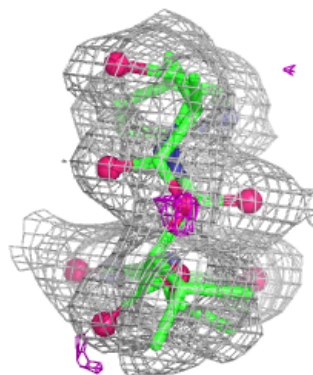
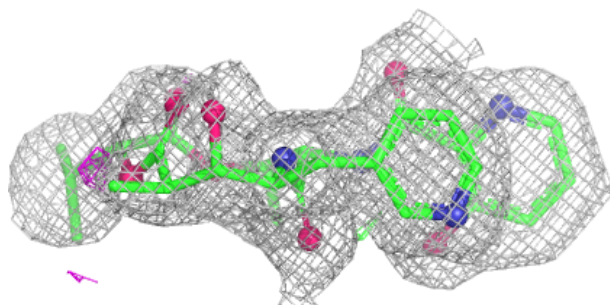
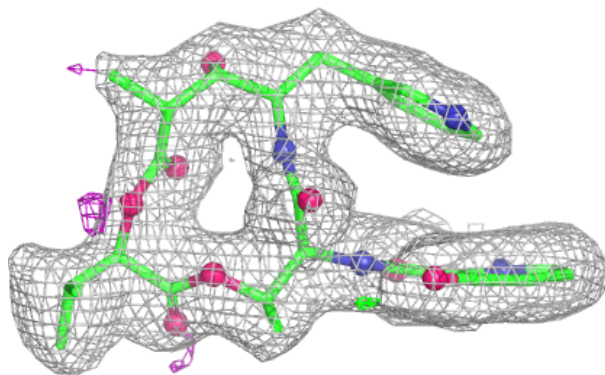
**Electron density around NAD D 1270:**

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

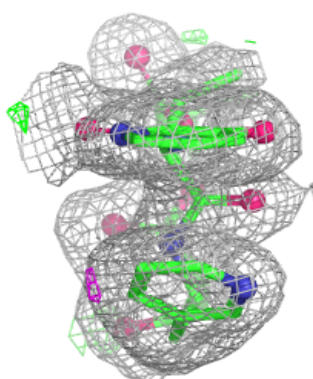
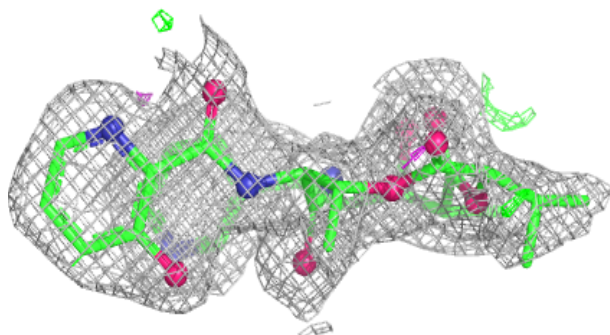
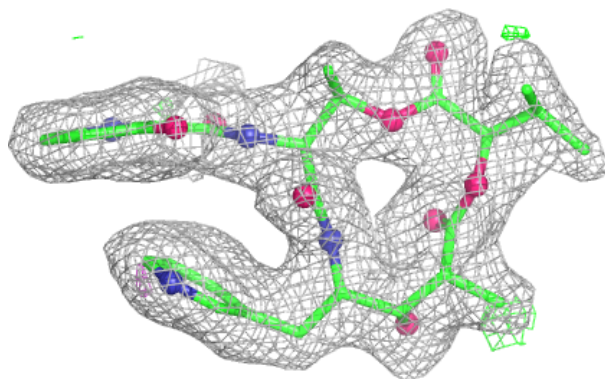


Electron density around I4I A 1270:

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

**Electron density around I4I B 1270:**

$2mF_o-DF_c$ (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.