



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 21, 2026 – 12:42 PM EDT

PDB ID : 9Q6G / pdb_00009q6g
Title : PYCR2 complexed with NAD⁺ and (2S)-2-hydroxy-3,3-dimethylbutanoic acid
Authors : Tanner, J.J.; Meeks, K.R.
Deposited on : 2025-08-22
Resolution : 2.65 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	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

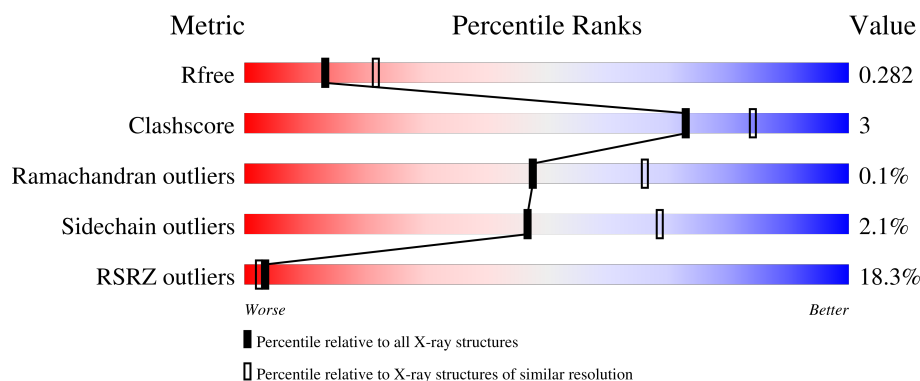
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	316	6% 79% 8% 14%
1	B	316	3% 78% 9% 14%
1	C	316	27% 76% 9% 15%
1	D	316	36% 71% 8% 22%
1	E	316	5% 82% • 14%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9079 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 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	273	Total	C	N	O	S	0	0	0
			1858	1158	329	356	15			
1	B	273	Total	C	N	O	S	0	0	0
			1853	1150	331	357	15			
1	C	269	Total	C	N	O	S	0	0	0
			1711	1053	309	336	13			
1	D	248	Total	C	N	O	S	0	0	0
			1565	966	282	306	11			
1	E	273	Total	C	N	O	S	0	0	0
			1860	1156	330	360	14			

There are 115 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	initiating methionine	UNP Q96C36
A	-20	HIS	-	expression tag	UNP Q96C36
A	-19	HIS	-	expression tag	UNP Q96C36
A	-18	HIS	-	expression tag	UNP Q96C36
A	-17	HIS	-	expression tag	UNP Q96C36
A	-16	HIS	-	expression tag	UNP Q96C36
A	-15	HIS	-	expression tag	UNP Q96C36
A	-14	SER	-	expression tag	UNP Q96C36
A	-13	SER	-	expression tag	UNP Q96C36
A	-12	GLY	-	expression tag	UNP Q96C36
A	-11	VAL	-	expression tag	UNP Q96C36
A	-10	ASP	-	expression tag	UNP Q96C36
A	-9	LEU	-	expression tag	UNP Q96C36
A	-8	GLY	-	expression tag	UNP Q96C36
A	-7	THR	-	expression tag	UNP Q96C36
A	-6	GLU	-	expression tag	UNP Q96C36
A	-5	ASN	-	expression tag	UNP Q96C36
A	-4	LEU	-	expression tag	UNP Q96C36
A	-3	TYR	-	expression tag	UNP Q96C36

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	PHE	-	expression tag	UNP Q96C36
A	-1	GLN	-	expression tag	UNP Q96C36
A	0	SER	-	expression tag	UNP Q96C36
A	276	GLN	LYS	engineered mutation	UNP Q96C36
B	-21	MET	-	initiating methionine	UNP Q96C36
B	-20	HIS	-	expression tag	UNP Q96C36
B	-19	HIS	-	expression tag	UNP Q96C36
B	-18	HIS	-	expression tag	UNP Q96C36
B	-17	HIS	-	expression tag	UNP Q96C36
B	-16	HIS	-	expression tag	UNP Q96C36
B	-15	HIS	-	expression tag	UNP Q96C36
B	-14	SER	-	expression tag	UNP Q96C36
B	-13	SER	-	expression tag	UNP Q96C36
B	-12	GLY	-	expression tag	UNP Q96C36
B	-11	VAL	-	expression tag	UNP Q96C36
B	-10	ASP	-	expression tag	UNP Q96C36
B	-9	LEU	-	expression tag	UNP Q96C36
B	-8	GLY	-	expression tag	UNP Q96C36
B	-7	THR	-	expression tag	UNP Q96C36
B	-6	GLU	-	expression tag	UNP Q96C36
B	-5	ASN	-	expression tag	UNP Q96C36
B	-4	LEU	-	expression tag	UNP Q96C36
B	-3	TYR	-	expression tag	UNP Q96C36
B	-2	PHE	-	expression tag	UNP Q96C36
B	-1	GLN	-	expression tag	UNP Q96C36
B	0	SER	-	expression tag	UNP Q96C36
B	276	GLN	LYS	engineered mutation	UNP Q96C36
C	-21	MET	-	initiating methionine	UNP Q96C36
C	-20	HIS	-	expression tag	UNP Q96C36
C	-19	HIS	-	expression tag	UNP Q96C36
C	-18	HIS	-	expression tag	UNP Q96C36
C	-17	HIS	-	expression tag	UNP Q96C36
C	-16	HIS	-	expression tag	UNP Q96C36
C	-15	HIS	-	expression tag	UNP Q96C36
C	-14	SER	-	expression tag	UNP Q96C36
C	-13	SER	-	expression tag	UNP Q96C36
C	-12	GLY	-	expression tag	UNP Q96C36
C	-11	VAL	-	expression tag	UNP Q96C36
C	-10	ASP	-	expression tag	UNP Q96C36
C	-9	LEU	-	expression tag	UNP Q96C36
C	-8	GLY	-	expression tag	UNP Q96C36
C	-7	THR	-	expression tag	UNP Q96C36

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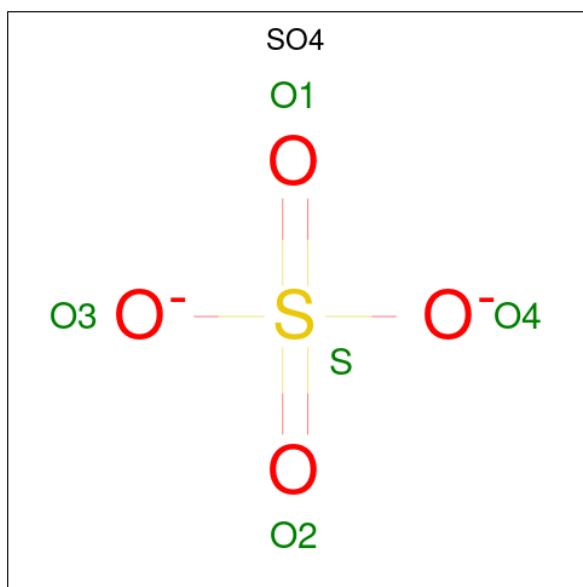
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C	-6	GLU	-	expression tag	UNP Q96C36
C	-5	ASN	-	expression tag	UNP Q96C36
C	-4	LEU	-	expression tag	UNP Q96C36
C	-3	TYR	-	expression tag	UNP Q96C36
C	-2	PHE	-	expression tag	UNP Q96C36
C	-1	GLN	-	expression tag	UNP Q96C36
C	0	SER	-	expression tag	UNP Q96C36
C	276	GLN	LYS	engineered mutation	UNP Q96C36
D	-21	MET	-	initiating methionine	UNP Q96C36
D	-20	HIS	-	expression tag	UNP Q96C36
D	-19	HIS	-	expression tag	UNP Q96C36
D	-18	HIS	-	expression tag	UNP Q96C36
D	-17	HIS	-	expression tag	UNP Q96C36
D	-16	HIS	-	expression tag	UNP Q96C36
D	-15	HIS	-	expression tag	UNP Q96C36
D	-14	SER	-	expression tag	UNP Q96C36
D	-13	SER	-	expression tag	UNP Q96C36
D	-12	GLY	-	expression tag	UNP Q96C36
D	-11	VAL	-	expression tag	UNP Q96C36
D	-10	ASP	-	expression tag	UNP Q96C36
D	-9	LEU	-	expression tag	UNP Q96C36
D	-8	GLY	-	expression tag	UNP Q96C36
D	-7	THR	-	expression tag	UNP Q96C36
D	-6	GLU	-	expression tag	UNP Q96C36
D	-5	ASN	-	expression tag	UNP Q96C36
D	-4	LEU	-	expression tag	UNP Q96C36
D	-3	TYR	-	expression tag	UNP Q96C36
D	-2	PHE	-	expression tag	UNP Q96C36
D	-1	GLN	-	expression tag	UNP Q96C36
D	0	SER	-	expression tag	UNP Q96C36
D	276	GLN	LYS	engineered mutation	UNP Q96C36
E	-21	MET	-	initiating methionine	UNP Q96C36
E	-20	HIS	-	expression tag	UNP Q96C36
E	-19	HIS	-	expression tag	UNP Q96C36
E	-18	HIS	-	expression tag	UNP Q96C36
E	-17	HIS	-	expression tag	UNP Q96C36
E	-16	HIS	-	expression tag	UNP Q96C36
E	-15	HIS	-	expression tag	UNP Q96C36
E	-14	SER	-	expression tag	UNP Q96C36
E	-13	SER	-	expression tag	UNP Q96C36
E	-12	GLY	-	expression tag	UNP Q96C36
E	-11	VAL	-	expression tag	UNP Q96C36

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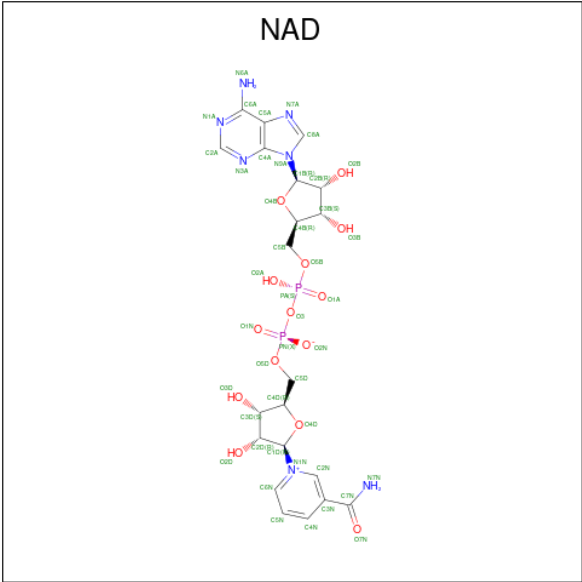
Chain	Residue	Modelled	Actual	Comment	Reference
E	-10	ASP	-	expression tag	UNP Q96C36
E	-9	LEU	-	expression tag	UNP Q96C36
E	-8	GLY	-	expression tag	UNP Q96C36
E	-7	THR	-	expression tag	UNP Q96C36
E	-6	GLU	-	expression tag	UNP Q96C36
E	-5	ASN	-	expression tag	UNP Q96C36
E	-4	LEU	-	expression tag	UNP Q96C36
E	-3	TYR	-	expression tag	UNP Q96C36
E	-2	PHE	-	expression tag	UNP Q96C36
E	-1	GLN	-	expression tag	UNP Q96C36
E	0	SER	-	expression tag	UNP Q96C36
E	276	GLN	LYS	engineered mutation	UNP Q96C36

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



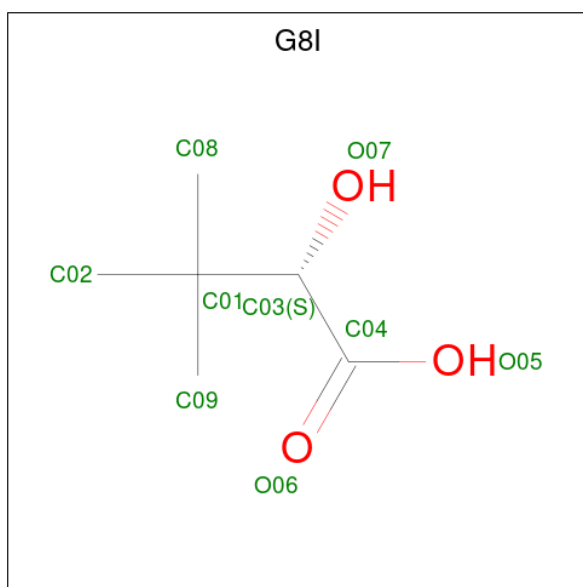
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	D	1	Total	C	N	O	P	0	0
			36	15	6	13	2		
3	E	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 4 is (2S)-2-hydroxy-3,3-dimethylbutanoic acid (CCD ID: G8I) (formula: C₆H₁₂O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			9	6	3		
4	E	1	Total	C	O	0	0
			9	6	3		

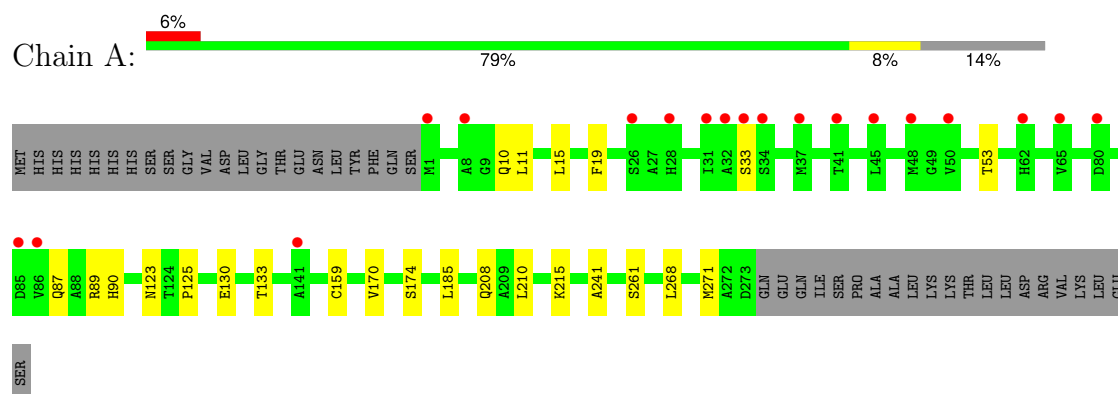
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	4	Total	O	0	0
			4	4		
5	B	4	Total	O	0	0
			4	4		
5	E	1	Total	O	0	0
			1	1		

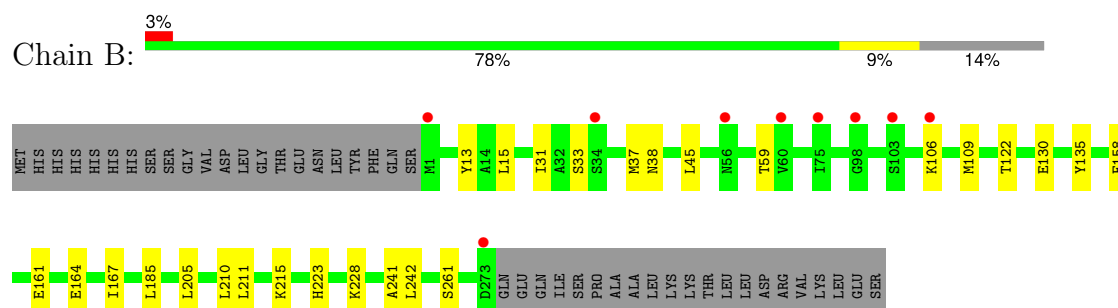
3 Residue-property plots [i](#)

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.

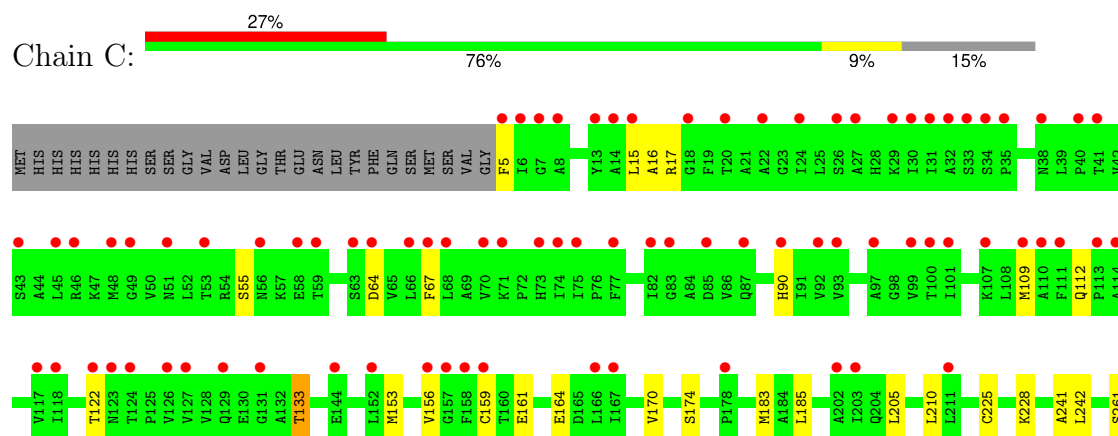
• Molecule 1: Pyrroline-5-carboxylate reductase 2

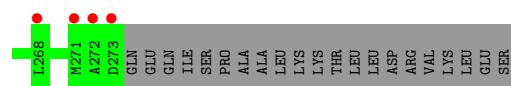


• Molecule 1: Pyrroline-5-carboxylate reductase 2

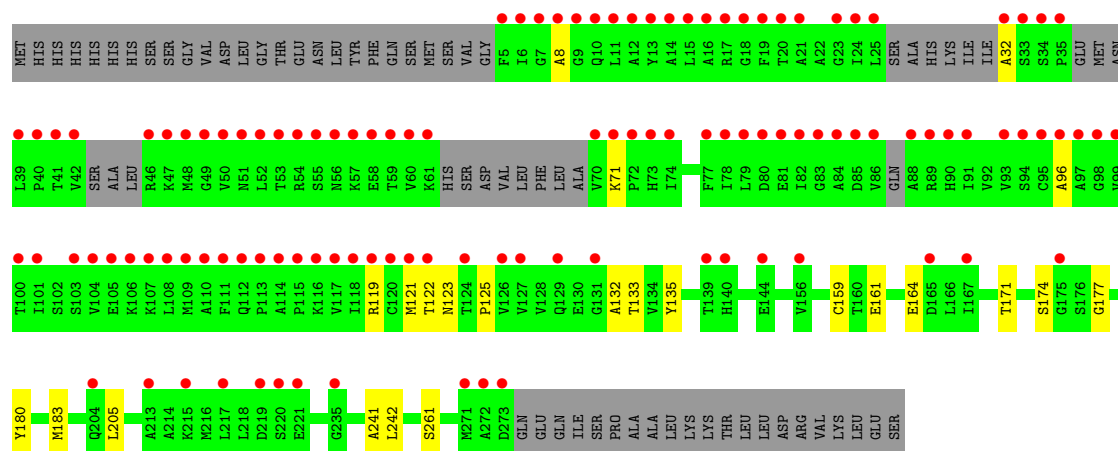


• Molecule 1: Pyrroline-5-carboxylate reductase 2

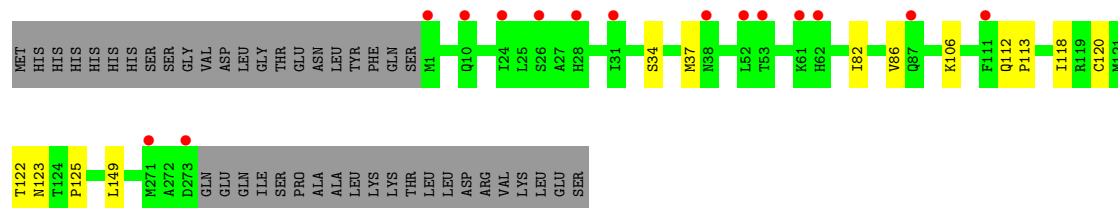
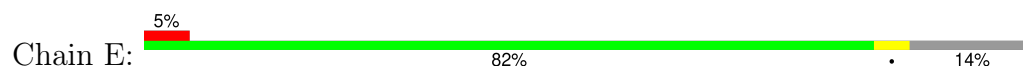




• Molecule 1: Pyrroline-5-carboxylate reductase 2



• Molecule 1: Pyrroline-5-carboxylate reductase 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 2 21	Depositor
Cell constants a, b, c, α , β , γ	104.34Å 109.94Å 154.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.63 – 2.65 48.63 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.63-2.65) 99.9 (48.63-2.65)	Depositor EDS
R_{merge}	0.30	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 2.65Å)	Xtriage
Refinement program	PHENIX (1.21.2_5419: ???)	Depositor
R, R_{free}	0.268 , 0.284 0.264 , 0.282	Depositor DCC
R_{free} test set	939 reflections (1.80%)	wwPDB-VP
Wilson B-factor (Å ²)	41.7	Xtriage
Anisotropy	0.574	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 85.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.026 for k,h,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	9079	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.26% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: G8I, SO4, 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	0.12	0/1884	0.31	0/2566
1	B	0.12	0/1881	0.31	0/2560
1	C	0.13	0/1736	0.34	0/2375
1	D	0.12	0/1581	0.34	0/2155
1	E	0.12	0/1886	0.31	0/2567
All	All	0.12	0/8968	0.32	0/12223

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1858	0	1726	15	0
1	B	1853	0	1697	17	0
1	C	1711	0	1408	16	0
1	D	1565	0	1296	16	0
1	E	1860	0	1718	6	0
2	A	5	0	0	0	0
2	E	5	0	0	0	0
3	A	44	0	26	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	44	0	26	1	0
3	C	27	0	12	0	0
3	D	36	0	20	1	0
3	E	44	0	26	1	0
4	B	9	0	0	0	0
4	E	9	0	0	0	0
5	A	4	0	0	0	0
5	B	4	0	0	0	0
5	E	1	0	0	0	0
All	All	9079	0	7955	55	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 (55) 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:130:GLU:HG3	1:B:215:LYS:HD3	1.71	0.72
1:B:106:LYS:HA	1:B:109:MET:HE2	1.73	0.70
1:B:228:LYS:HE2	1:B:242:LEU:HD13	1.77	0.67
1:B:31:ILE:HG23	1:B:59:THR:HG23	1.78	0.64
1:C:170:VAL:HG13	1:D:205:LEU:HD13	1.79	0.64
1:C:205:LEU:HB3	1:D:174:SER:HB3	1.82	0.61
1:E:112:GLN:HG2	1:E:113:PRO:HD2	1.85	0.56
1:B:164:GLU:HA	1:B:167:ILE:HD13	1.89	0.54
1:D:122:THR:HA	1:D:132:ALA:O	2.08	0.53
1:A:133:THR:O	1:A:159:CYS:HA	2.09	0.52
1:A:170:VAL:HG13	1:B:205:LEU:HD13	1.93	0.51
1:D:135:TYR:CZ	1:D:161:GLU:HB2	2.45	0.51
1:E:123:ASN:CG	1:E:125:PRO:HD2	2.36	0.50
1:C:183:MET:HE3	1:D:242:LEU:HD22	1.94	0.50
1:E:118:ILE:HG21	1:E:149:LEU:HD22	1.95	0.48
1:A:174:SER:HB3	1:B:205:LEU:HB3	1.96	0.48
1:A:241:ALA:HB2	1:B:261:SER:HB2	1.96	0.48
1:B:13:TYR:HA	1:B:45:LEU:HD21	1.96	0.47
1:C:122:THR:HB	1:C:133:THR:HG23	1.96	0.47
1:A:261:SER:HB2	1:B:241:ALA:HB2	1.96	0.47
1:A:268:LEU:HA	1:A:271:MET:HE2	1.96	0.46
1:C:261:SER:HB2	1:D:241:ALA:HB2	1.96	0.46
1:B:223:HIS:CE1	1:C:225:CYS:HB3	2.51	0.46
1:C:153:MET:HA	1:C:156:VAL:HG22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:LEU:HB2	3:A:302:NAD:H2N	1.98	0.45
1:E:82:ILE:O	1:E:86:VAL:HG23	2.17	0.45
1:A:87:GLN:H	1:A:90:HIS:HD1	1.65	0.44
1:E:122:THR:O	3:E:303:NAD:H5N	2.18	0.44
1:B:185:LEU:HD21	1:B:210:LEU:HD22	1.99	0.44
1:A:33:SER:HA	1:A:53:THR:HG23	2.00	0.43
1:C:15:LEU:HD12	1:C:16:ALA:N	2.33	0.43
1:C:64:ASP:O	1:C:90:HIS:HA	2.18	0.43
1:D:8:ALA:HB2	1:D:32:ALA:HB1	2.00	0.43
1:C:174:SER:HB3	1:D:205:LEU:HB3	2.00	0.43
1:D:123:ASN:CG	1:D:125:PRO:HD2	2.43	0.43
1:C:133:THR:O	1:C:159:CYS:HA	2.18	0.43
1:D:133:THR:O	1:D:159:CYS:HA	2.19	0.43
1:E:34:SER:HB3	1:E:37:MET:HE3	2.01	0.43
1:C:109:MET:HA	1:C:112:GLN:O	2.19	0.43
1:D:177:GLY:HA2	1:D:180:TYR:CD2	2.54	0.43
1:C:241:ALA:HB2	1:D:261:SER:HB2	2.00	0.42
1:C:242:LEU:HD22	1:D:183:MET:HE3	2.01	0.42
1:A:215:LYS:HD3	1:B:130:GLU:HG3	2.00	0.42
1:A:208:GLN:HG3	1:B:158:PHE:CB	2.49	0.42
1:A:185:LEU:HD21	1:A:210:LEU:HD22	2.01	0.42
1:B:122:THR:O	3:B:302:NAD:H5N	2.20	0.42
1:A:123:ASN:CG	1:A:125:PRO:HD2	2.45	0.41
1:D:96:ALA:HA	3:D:301:NAD:O3D	2.20	0.41
1:B:33:SER:HB3	1:B:59:THR:OG1	2.21	0.41
1:D:121:MET:HE3	1:D:171:THR:OG1	2.21	0.41
1:B:135:TYR:CZ	1:B:161:GLU:HB2	2.56	0.41
1:D:119:ARG:O	1:D:135:TYR:HA	2.20	0.40
1:A:15:LEU:HG	1:A:19:PHE:CZ	2.57	0.40
1:C:5:PHE:HA	1:C:67:PHE:HB2	2.03	0.40
1:C:185:LEU:HD21	1:C:210:LEU:HD22	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	271/316 (86%)	259 (96%)	12 (4%)	0	100	100
1	B	271/316 (86%)	262 (97%)	9 (3%)	0	100	100
1	C	267/316 (84%)	256 (96%)	10 (4%)	1 (0%)	30	45
1	D	236/316 (75%)	228 (97%)	8 (3%)	0	100	100
1	E	271/316 (86%)	262 (97%)	9 (3%)	0	100	100
All	All	1316/1580 (83%)	1267 (96%)	48 (4%)	1 (0%)	48	66

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	55	SER

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	166/253 (66%)	164 (99%)	2 (1%)	63	79
1	B	164/253 (65%)	160 (98%)	4 (2%)	43	65
1	C	124/253 (49%)	119 (96%)	5 (4%)	28	47
1	D	110/253 (44%)	108 (98%)	2 (2%)	51	72
1	E	166/253 (66%)	164 (99%)	2 (1%)	63	79
All	All	730/1265 (58%)	715 (98%)	15 (2%)	47	69

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	89	ARG
1	B	15	LEU
1	B	37	MET

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Mol	Chain	Res	Type
1	B	38	ASN
1	B	211	LEU
1	C	17	ARG
1	C	133	THR
1	C	161	GLU
1	C	164	GLU
1	C	228	LYS
1	D	71	LYS
1	D	164	GLU
1	E	106	LYS
1	E	120	CYS

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	129	GLN
1	A	226	GLN
1	B	87	GLN
1	B	112	GLN
1	B	240	HIS
1	C	256	ASN
1	E	129	GLN
1	E	140	HIS
1	E	226	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

9 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAD	D	301	-	38,39,48	1.43	2 (5%)	55,60,73	0.77	1 (1%)
4	G8I	E	301	-	8,8,8	1.32	1 (12%)	11,12,12	1.03	2 (18%)
2	SO4	E	302	-	4,4,4	0.66	0	6,6,6	0.08	0
3	NAD	E	303	-	46,48,48	1.24	3 (6%)	64,73,73	0.98	4 (6%)
3	NAD	B	302	-	46,48,48	1.22	3 (6%)	64,73,73	0.89	3 (4%)
2	SO4	A	301	-	4,4,4	0.65	0	6,6,6	0.08	0
4	G8I	B	301	-	8,8,8	1.40	1 (12%)	11,12,12	0.92	0
3	NAD	A	302	-	46,48,48	1.21	3 (6%)	64,73,73	0.84	2 (3%)
3	NAD	C	301	-	28,29,48	1.38	2 (7%)	43,45,73	1.01	5 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAD	D	301	-	-	12/22/54/62	0/4/4/5
4	G8I	E	301	-	-	2/10/10/10	-
3	NAD	E	303	-	-	6/30/62/62	0/5/5/5
3	NAD	B	302	-	-	2/30/62/62	0/5/5/5
4	G8I	B	301	-	-	6/10/10/10	-
3	NAD	A	302	-	-	9/30/62/62	0/5/5/5
3	NAD	C	301	-	-	6/16/32/62	0/3/3/5

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	301	NAD	PA-O3	6.09	1.66	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	301	NAD	PA-O3	5.96	1.65	1.59
3	E	303	NAD	PA-O3	5.64	1.65	1.59
3	B	302	NAD	PA-O3	5.63	1.65	1.59
3	A	302	NAD	PA-O3	5.55	1.65	1.59
3	D	301	NAD	PN-O3	4.54	1.64	1.59
3	B	302	NAD	PN-O3	3.94	1.63	1.59
3	A	302	NAD	PN-O3	3.82	1.63	1.59
3	E	303	NAD	PN-O3	3.80	1.63	1.59
4	B	301	G8I	C01-C03	-3.05	1.53	1.55
4	E	301	G8I	C01-C03	-2.88	1.53	1.55
3	E	303	NAD	O4D-C1D	-2.58	1.37	1.40
3	C	301	NAD	PN-O5D	2.50	1.64	1.54
3	B	302	NAD	O4D-C1D	-2.21	1.38	1.40
3	A	302	NAD	O4D-C1D	-2.21	1.38	1.40

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	303	NAD	C6N-N1N-C1D	-2.77	114.30	119.73
3	E	303	NAD	O7N-C7N-N7N	2.39	126.06	122.62
4	E	301	G8I	O05-C04-O06	-2.37	118.71	124.08
3	C	301	NAD	O2N-PN-O1N	2.32	119.86	110.83
3	B	302	NAD	O2A-PA-O1A	2.28	123.07	112.44
3	C	301	NAD	C3B-C2B-C1B	2.28	105.77	101.46
3	B	302	NAD	O4B-C1B-N9A	2.25	112.40	108.09
3	E	303	NAD	O4B-C1B-N9A	2.20	112.31	108.09
3	A	302	NAD	O2A-PA-O1A	2.20	122.67	112.44
3	E	303	NAD	O2A-PA-O1A	2.17	122.52	112.44
3	C	301	NAD	O2A-PA-O1A	2.12	122.31	112.44
3	D	301	NAD	O2A-PA-O1A	2.10	122.19	112.44
4	E	301	G8I	O05-C04-C03	2.07	121.01	112.80
3	B	302	NAD	O7N-C7N-N7N	2.07	125.60	122.62
3	A	302	NAD	O3-PA-O1A	-2.05	104.54	110.70
3	C	301	NAD	O5D-PN-O3	-2.03	97.82	104.64
3	C	301	NAD	O2N-PN-O3	2.02	111.42	104.64

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	302	NAD	C5D-O5D-PN-O2N
3	C	301	NAD	C5B-O5B-PA-O1A

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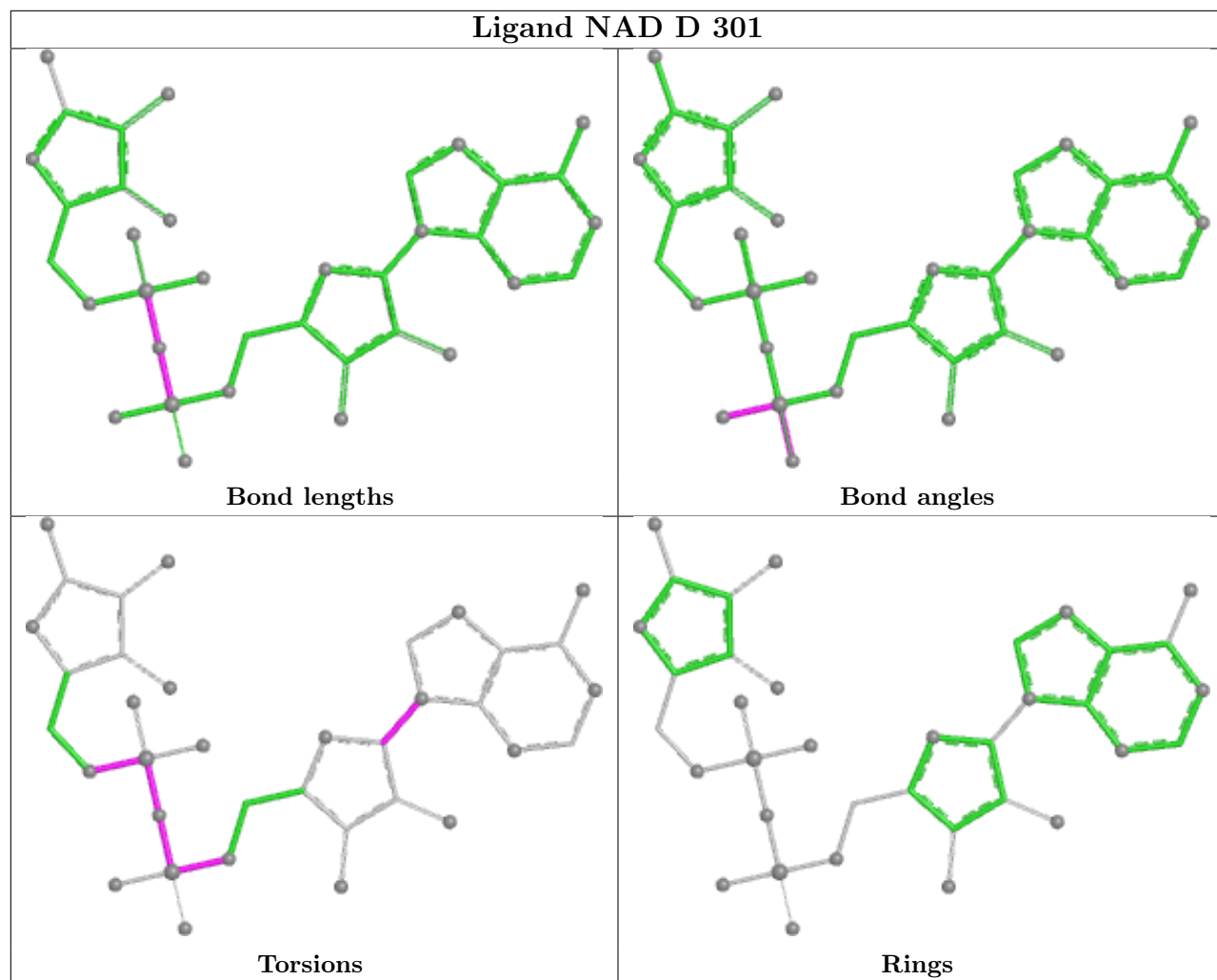
Mol	Chain	Res	Type	Atoms
3	C	301	NAD	O4B-C4B-C5B-O5B
3	D	301	NAD	C5B-O5B-PA-O1A
3	D	301	NAD	C5B-O5B-PA-O3
3	D	301	NAD	C5D-O5D-PN-O3
3	D	301	NAD	C5D-O5D-PN-O1N
3	D	301	NAD	C5D-O5D-PN-O2N
3	E	303	NAD	C2N-C3N-C7N-O7N
3	E	303	NAD	C2N-C3N-C7N-N7N
4	B	301	G8I	C02-C01-C03-C04
4	B	301	G8I	C02-C01-C03-O07
4	B	301	G8I	C08-C01-C03-C04
4	B	301	G8I	C08-C01-C03-O07
4	B	301	G8I	C09-C01-C03-C04
4	B	301	G8I	C09-C01-C03-O07
3	E	303	NAD	C4N-C3N-C7N-O7N
3	E	303	NAD	C4N-C3N-C7N-N7N
3	C	301	NAD	C3B-C4B-C5B-O5B
4	E	301	G8I	O07-C03-C04-O05
3	C	301	NAD	PA-O3-PN-O1N
3	C	301	NAD	PN-O3-PA-O5B
3	D	301	NAD	PN-O3-PA-O5B
3	D	301	NAD	C2B-C1B-N9A-C8A
3	D	301	NAD	PA-O3-PN-O2N
3	A	302	NAD	C5B-O5B-PA-O1A
3	A	302	NAD	C5D-O5D-PN-O3
3	D	301	NAD	C5B-O5B-PA-O2A
4	E	301	G8I	O07-C03-C04-O06
3	A	302	NAD	C4N-C3N-C7N-O7N
3	A	302	NAD	C4N-C3N-C7N-N7N
3	D	301	NAD	PA-O3-PN-O1N
3	C	301	NAD	C4B-C5B-O5B-PA
3	A	302	NAD	C2N-C3N-C7N-N7N
3	B	302	NAD	C2B-C1B-N9A-C8A
3	A	302	NAD	C2N-C3N-C7N-O7N
3	D	301	NAD	C2B-C1B-N9A-C4A
3	D	301	NAD	O4B-C1B-N9A-C8A
3	A	302	NAD	O4B-C4B-C5B-O5B
3	B	302	NAD	O4B-C4B-C5B-O5B
3	E	303	NAD	O4B-C4B-C5B-O5B
3	E	303	NAD	C2B-C1B-N9A-C8A
3	A	302	NAD	C2B-C1B-N9A-C8A

There are no ring outliers.

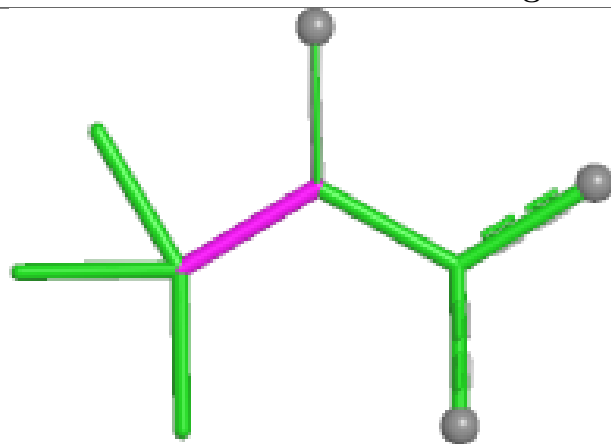
4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	301	NAD	1	0
3	E	303	NAD	1	0
3	B	302	NAD	1	0
3	A	302	NAD	1	0

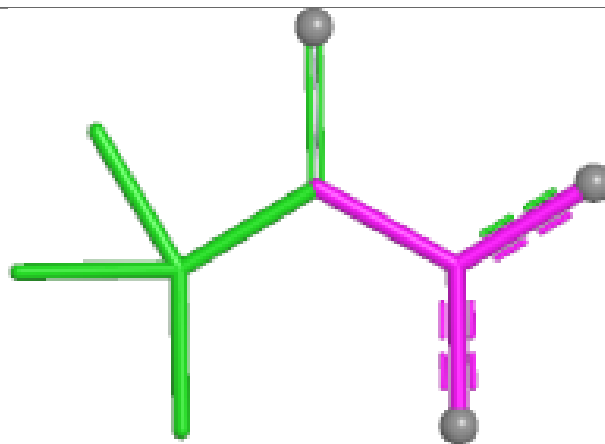
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



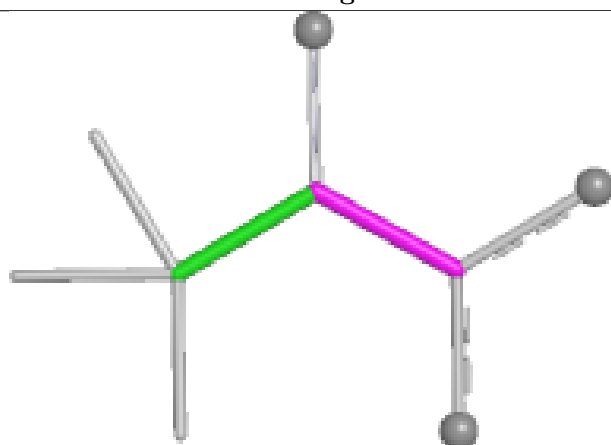
Ligand G8I E 301



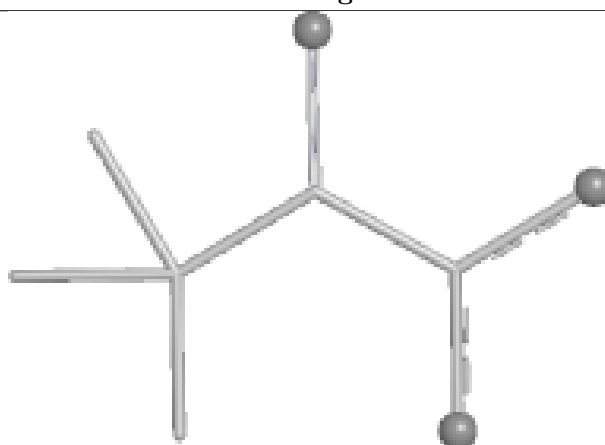
Bond lengths



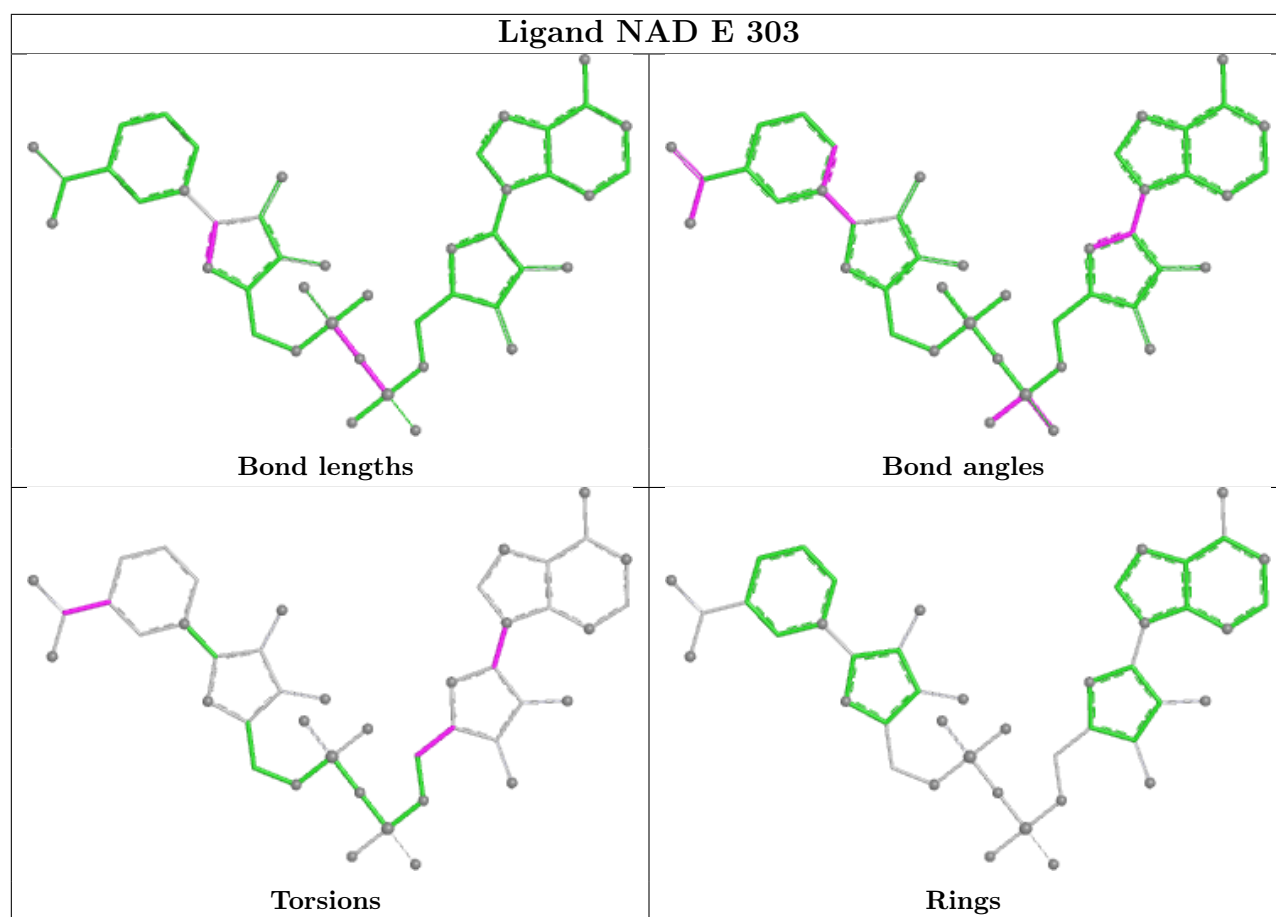
Bond angles

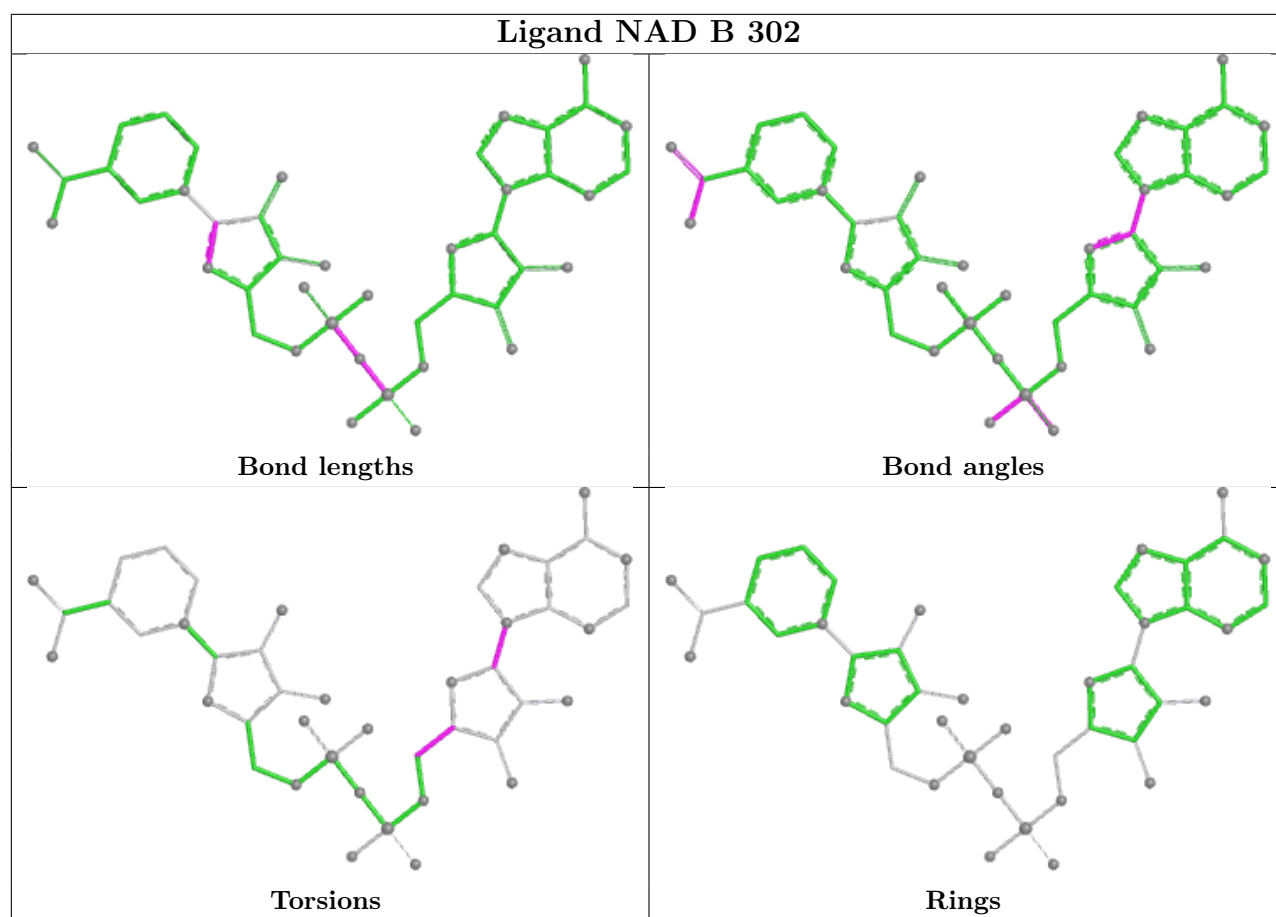


Torsions

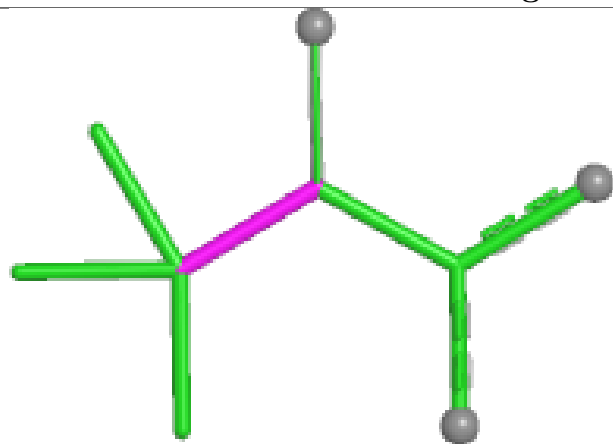


Rings

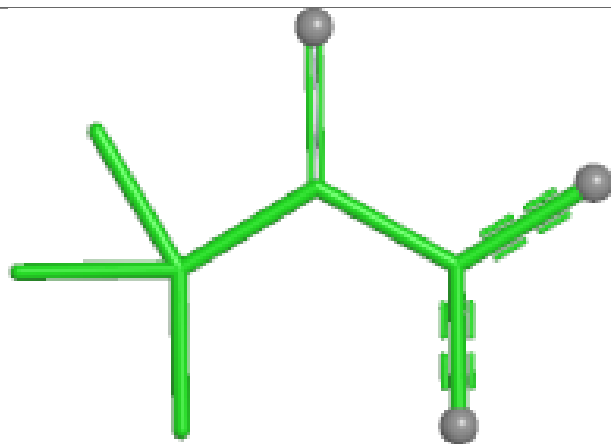




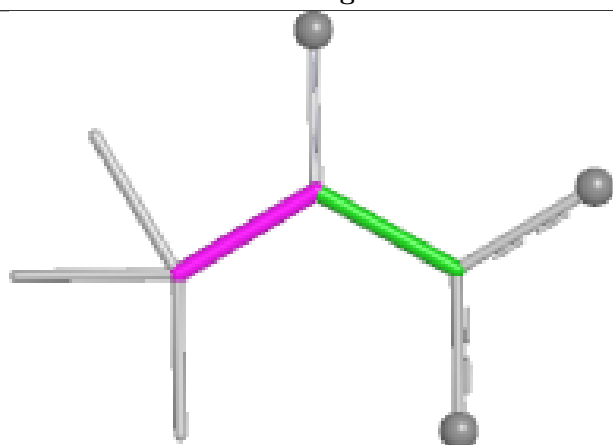
Ligand G8I B 301



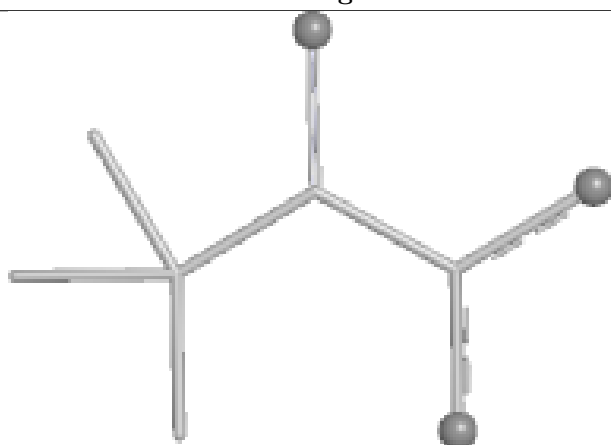
Bond lengths



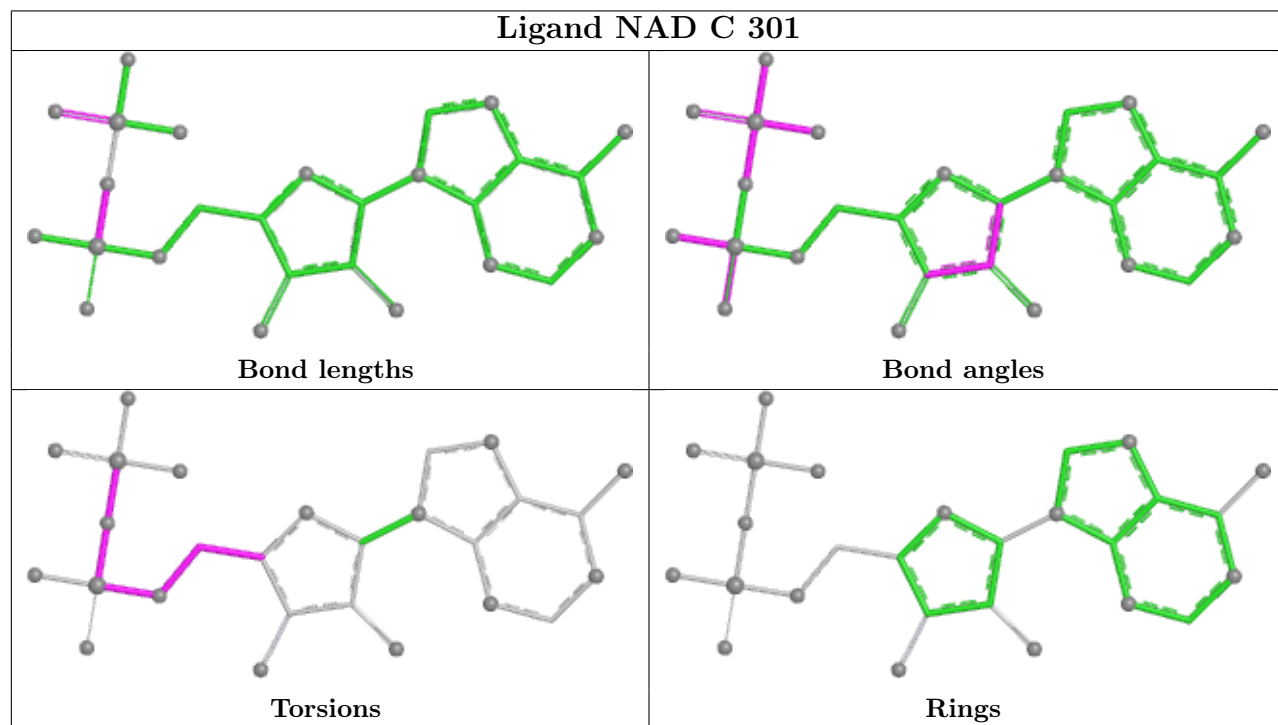
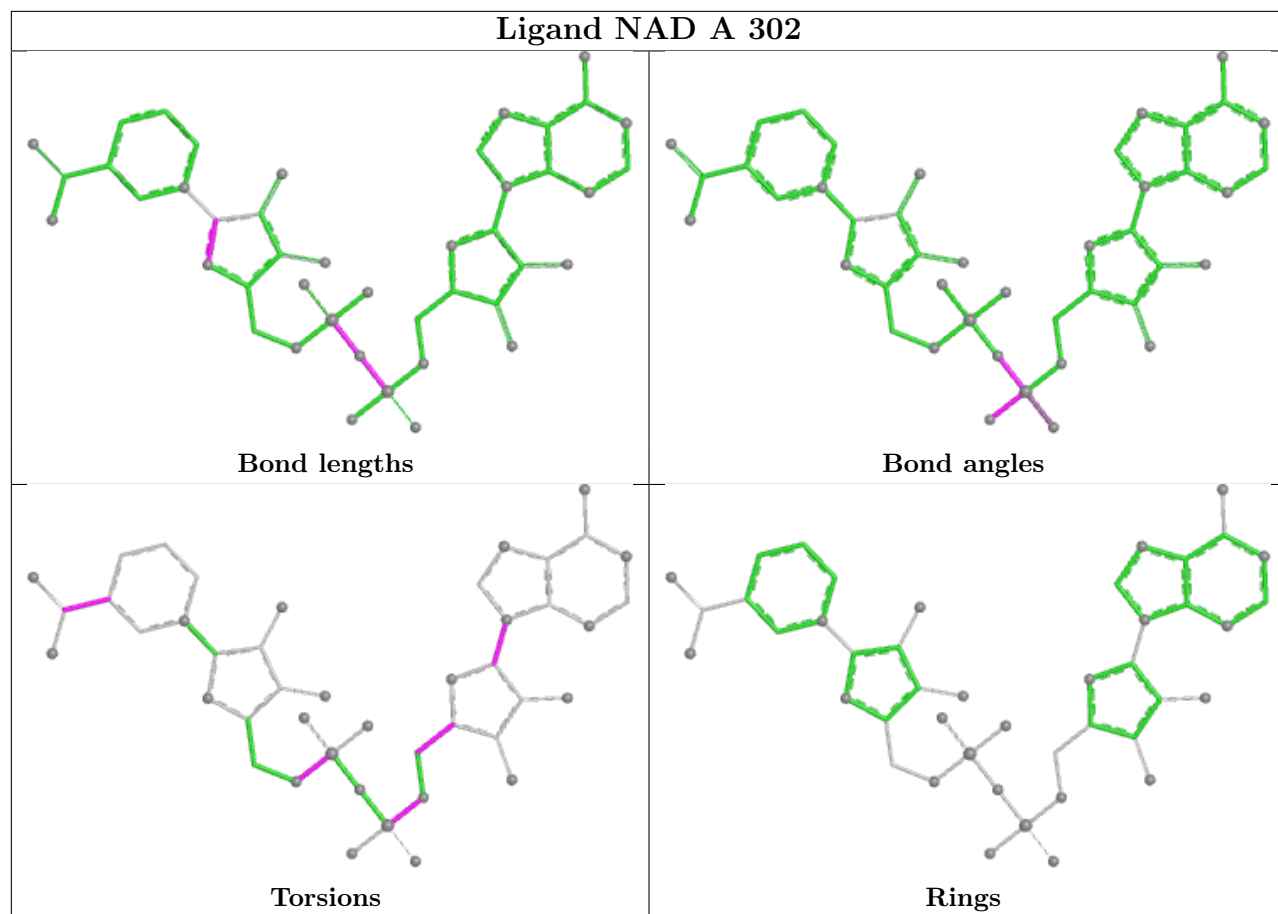
Bond angles



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	273/316 (86%)	0.52	19 (6%)	22 17	26, 49, 103, 141	0
1	B	273/316 (86%)	0.41	9 (3%)	49 40	22, 52, 91, 115	0
1	C	269/316 (85%)	1.58	86 (31%)	1 0	44, 83, 120, 135	0
1	D	248/316 (78%)	2.16	115 (46%)	0 0	48, 82, 149, 186	0
1	E	273/316 (86%)	0.31	15 (5%)	30 24	19, 47, 82, 117	0
All	All	1336/1580 (84%)	0.97	244 (18%)	3 2	19, 62, 119, 186	0

All (244) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	90	HIS	9.1
1	D	60	VAL	6.6
1	D	6	ILE	6.5
1	D	42	VAL	6.2
1	D	52	LEU	6.2
1	D	14	ALA	6.1
1	D	115	PRO	6.0
1	D	15	LEU	5.8
1	D	85	ASP	5.8
1	D	70	VAL	5.7
1	D	91	ILE	5.7
1	D	11	LEU	5.7
1	D	86	VAL	5.5
1	C	34	SER	5.5
1	D	108	LEU	5.4
1	D	117	VAL	5.1
1	D	51	ASN	5.1
1	D	116	LYS	5.1
1	D	32	ALA	5.1
1	D	8	ALA	5.0

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Mol	Chain	Res	Type	RSRZ
1	D	10	GLN	4.9
1	D	41	THR	4.9
1	D	5	PHE	4.9
1	D	46	ARG	4.9
1	D	95	CYS	4.8
1	D	121	MET	4.7
1	D	17	ARG	4.7
1	D	113	PRO	4.7
1	D	7	GLY	4.6
1	D	98	GLY	4.5
1	D	35	PRO	4.5
1	D	54	ARG	4.5
1	D	47	LYS	4.4
1	D	19	PHE	4.4
1	D	74	ILE	4.4
1	D	59	THR	4.3
1	D	18	GLY	4.3
1	D	50	VAL	4.3
1	B	273	ASP	4.2
1	D	39	LEU	4.1
1	C	51	ASN	4.1
1	C	118	ILE	4.1
1	D	99	VAL	4.1
1	D	77	PHE	4.1
1	C	5	PHE	4.0
1	C	41	THR	4.0
1	D	13	TYR	4.0
1	C	85	ASP	4.0
1	D	221	GLU	4.0
1	D	78	ILE	3.9
1	D	12	ALA	3.9
1	E	62	HIS	3.9
1	D	120	CYS	3.9
1	C	63	SER	3.9
1	D	105	GLU	3.9
1	D	104	VAL	3.9
1	D	71	LYS	3.8
1	E	26	SER	3.8
1	D	49	GLY	3.8
1	C	127	VAL	3.8
1	C	117	VAL	3.7
1	D	55	SER	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	48	MET	3.7
1	C	66	LEU	3.7
1	D	96	ALA	3.6
1	D	81	GLU	3.6
1	C	124	THR	3.6
1	D	273	ASP	3.6
1	D	101	ILE	3.5
1	C	99	VAL	3.5
1	C	152	LEU	3.5
1	C	24	ILE	3.5
1	C	87	GLN	3.5
1	C	15	LEU	3.5
1	B	34	SER	3.5
1	D	88	ALA	3.5
1	C	74	ILE	3.5
1	D	103	SER	3.5
1	D	118	ILE	3.5
1	B	98	GLY	3.5
1	C	157	GLY	3.5
1	D	114	ALA	3.5
1	D	109	MET	3.4
1	C	59	THR	3.4
1	C	67	PHE	3.4
1	D	73	HIS	3.4
1	C	156	VAL	3.4
1	C	18	GLY	3.4
1	D	72	PRO	3.4
1	C	158	PHE	3.4
1	D	131	GLY	3.4
1	D	175	GLY	3.4
1	C	48	MET	3.4
1	C	271	MET	3.4
1	A	31	ILE	3.3
1	E	28	HIS	3.3
1	A	45	LEU	3.3
1	C	272	ALA	3.3
1	C	71	LYS	3.3
1	C	38	ASN	3.3
1	C	70	VAL	3.3
1	C	107	LYS	3.3
1	D	83	GLY	3.3
1	D	219	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	26	SER	3.2
1	C	8	ALA	3.2
1	C	31	ILE	3.2
1	C	40	PRO	3.2
1	D	126	VAL	3.2
1	B	56	ASN	3.2
1	C	64	ASP	3.2
1	D	53	THR	3.2
1	D	25	LEU	3.1
1	C	30	ILE	3.1
1	C	75	ILE	3.1
1	D	127	VAL	3.1
1	E	1	MET	3.1
1	A	32	ALA	3.0
1	D	110	ALA	3.0
1	C	111	PHE	3.0
1	D	111	PHE	3.0
1	A	80	ASP	3.0
1	C	20	THR	3.0
1	D	97	ALA	3.0
1	B	60	VAL	3.0
1	C	113	PRO	2.9
1	E	38	ASN	2.9
1	D	220	SER	2.9
1	A	28	HIS	2.9
1	A	26	SER	2.9
1	C	100	THR	2.9
1	D	57	LYS	2.9
1	D	112	GLN	2.8
1	D	82	ILE	2.8
1	D	93	VAL	2.8
1	A	34	SER	2.8
1	C	6	ILE	2.8
1	D	84	ALA	2.8
1	D	89	ARG	2.8
1	D	34	SER	2.8
1	D	94	SER	2.8
1	B	1	MET	2.8
1	C	49	GLY	2.8
1	C	110	ALA	2.8
1	D	40	PRO	2.7
1	D	24	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	43	SER	2.7
1	D	271	MET	2.7
1	C	22	ALA	2.7
1	D	80	ASP	2.7
1	C	211	LEU	2.7
1	A	33	SER	2.7
1	C	53	THR	2.7
1	D	21	ALA	2.7
1	D	122	THR	2.7
1	D	156	VAL	2.7
1	D	106	LYS	2.7
1	E	273	ASP	2.7
1	A	8	ALA	2.6
1	D	56	ASN	2.6
1	D	139	THR	2.6
1	C	32	ALA	2.6
1	C	77	PHE	2.6
1	B	106	LYS	2.6
1	C	7	GLY	2.6
1	C	97	ALA	2.6
1	C	203	ILE	2.5
1	C	33	SER	2.5
1	D	165	ASP	2.5
1	D	204	GLN	2.5
1	C	90	HIS	2.5
1	D	9	GLY	2.5
1	D	129	GLN	2.5
1	C	56	ASN	2.5
1	C	45	LEU	2.5
1	D	33	SER	2.5
1	C	46	ARG	2.4
1	C	73	HIS	2.4
1	C	273	ASP	2.4
1	D	23	GLY	2.4
1	D	235	GLY	2.4
1	D	16	ALA	2.4
1	C	68	LEU	2.4
1	E	24	ILE	2.4
1	C	159	CYS	2.4
1	D	61	LYS	2.4
1	D	217	LEU	2.4
1	D	215	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	129	GLN	2.4
1	D	79	LEU	2.3
1	D	20	THR	2.3
1	C	178	PRO	2.3
1	D	167	ILE	2.3
1	D	124	THR	2.3
1	C	114	ALA	2.3
1	C	268	LEU	2.3
1	E	53	THR	2.3
1	D	119	ARG	2.3
1	C	131	GLY	2.3
1	C	126	VAL	2.3
1	C	13	TYR	2.2
1	A	86	VAL	2.2
1	A	37	MET	2.2
1	D	140	HIS	2.2
1	D	272	ALA	2.2
1	E	10	GLN	2.2
1	C	109	MET	2.2
1	C	167	ILE	2.2
1	D	213	ALA	2.2
1	A	85	ASP	2.2
1	A	65	VAL	2.2
1	C	14	ALA	2.2
1	C	27	ALA	2.2
1	E	61	LYS	2.2
1	C	202	ALA	2.1
1	C	144	GLU	2.1
1	D	58	GLU	2.1
1	E	111	PHE	2.1
1	A	41	THR	2.1
1	D	100	THR	2.1
1	A	1	MET	2.1
1	C	83	GLY	2.1
1	A	62	HIS	2.1
1	A	141	ALA	2.1
1	D	144	GLU	2.1
1	C	29	LYS	2.1
1	C	101	ILE	2.1
1	C	35	PRO	2.1
1	E	271	MET	2.1
1	C	166	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	50	VAL	2.1
1	D	107	LYS	2.0
1	E	52	LEU	2.0
1	B	75	ILE	2.0
1	E	31	ILE	2.0
1	C	92	VAL	2.0
1	C	58	GLU	2.0
1	B	103	SER	2.0
1	A	48	MET	2.0
1	C	122	THR	2.0
1	E	87	GLN	2.0
1	C	82	ILE	2.0
1	C	123	ASN	2.0
1	C	93	VAL	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](#)

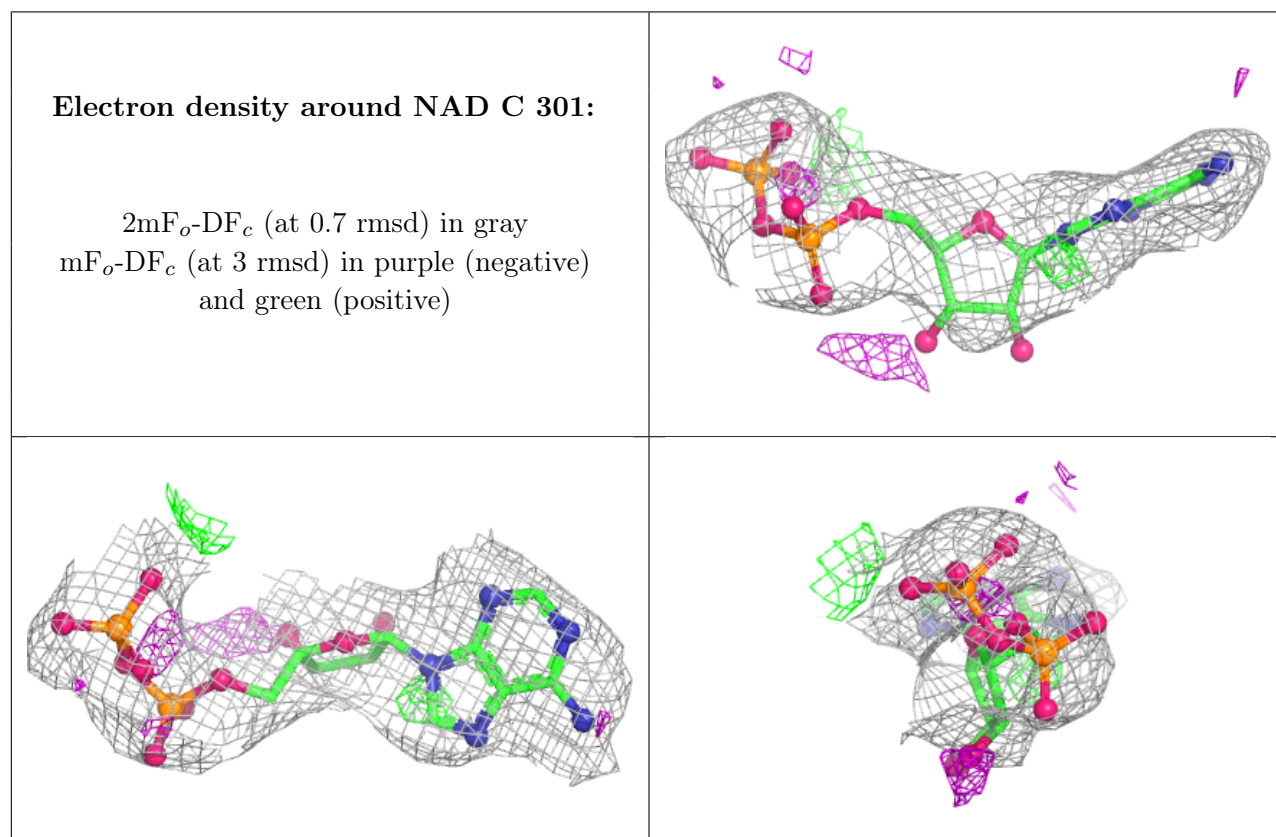
There are no oligosaccharides in this entry.

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.

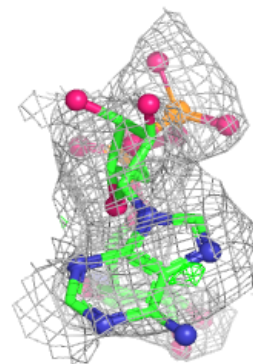
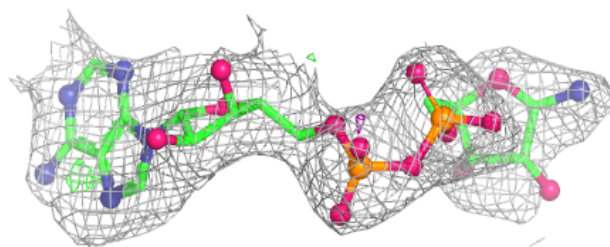
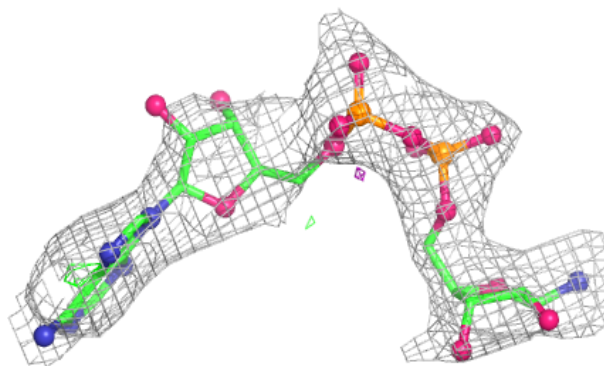
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAD	C	301	27/44	0.73	0.16	73,91,106,106	0
3	NAD	D	301	36/44	0.75	0.18	76,104,115,117	36
2	SO4	E	302	5/5	0.82	0.12	78,83,92,94	5
3	NAD	B	302	44/44	0.84	0.13	44,59,72,76	44
3	NAD	A	302	44/44	0.86	0.15	44,65,78,87	44
2	SO4	A	301	5/5	0.90	0.12	35,36,41,45	5
3	NAD	E	303	44/44	0.90	0.11	41,55,64,66	44
4	G8I	B	301	9/9	0.91	0.12	38,41,48,49	0
4	G8I	E	301	9/9	0.91	0.13	33,36,39,42	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.

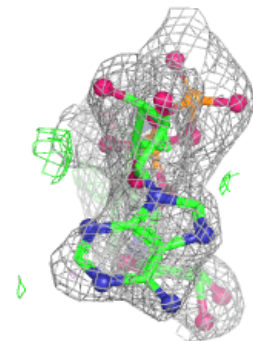
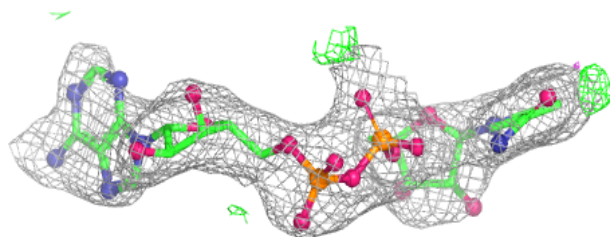
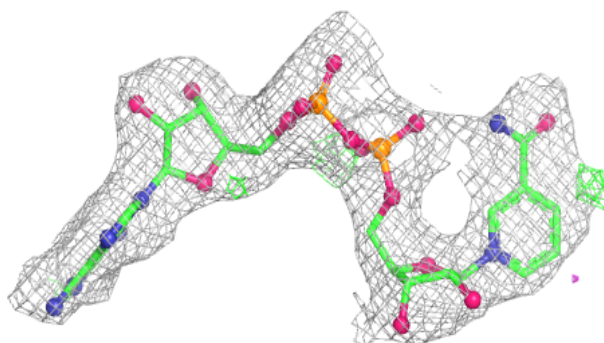


Electron density around NAD D 301:

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

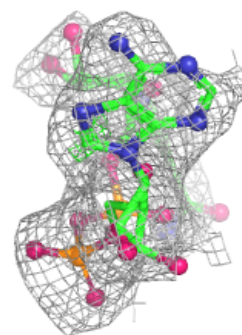
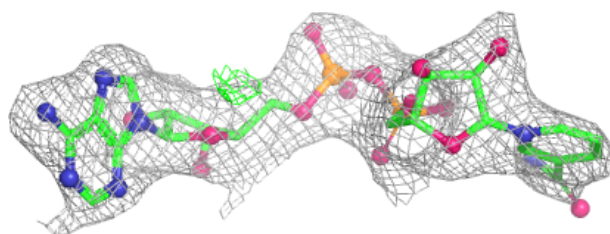
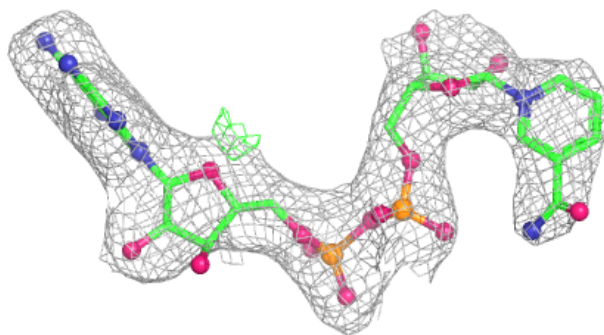
**Electron density around NAD B 302:**

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

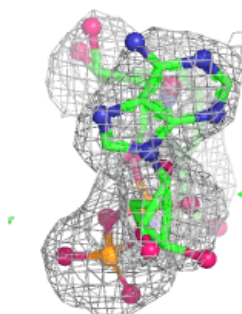
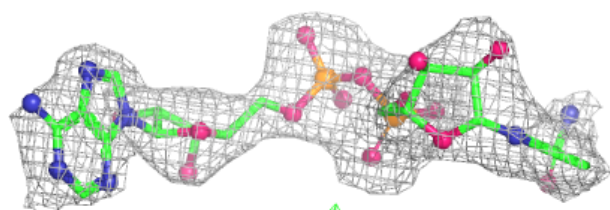
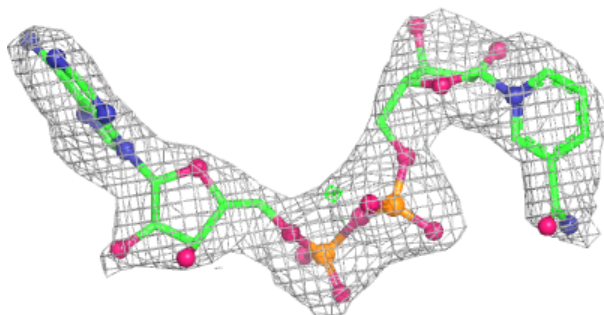


Electron density around NAD A 302:

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

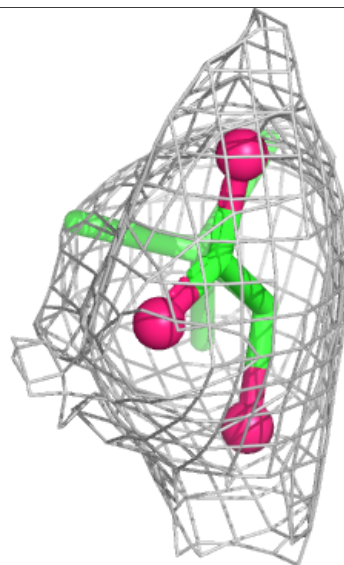
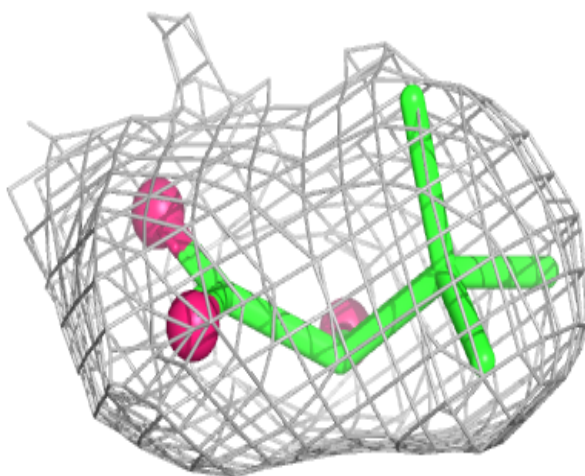
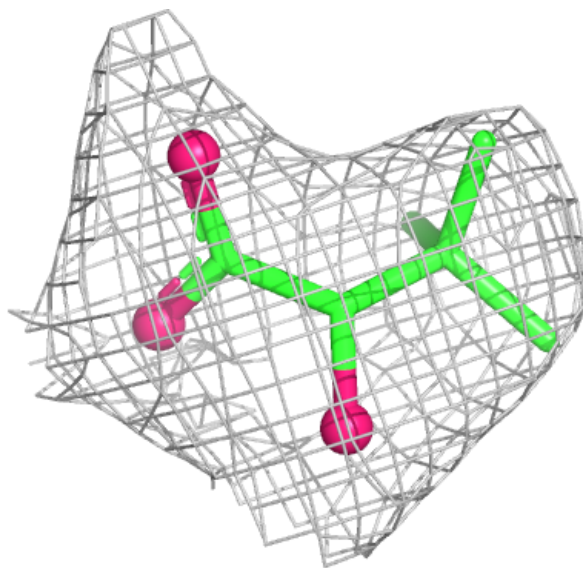
**Electron density around NAD E 303:**

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



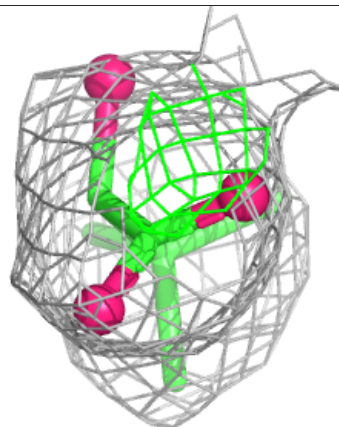
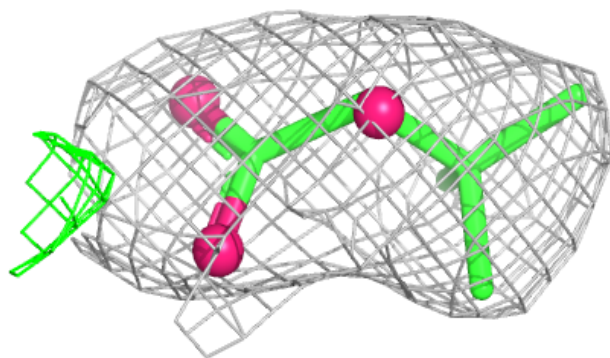
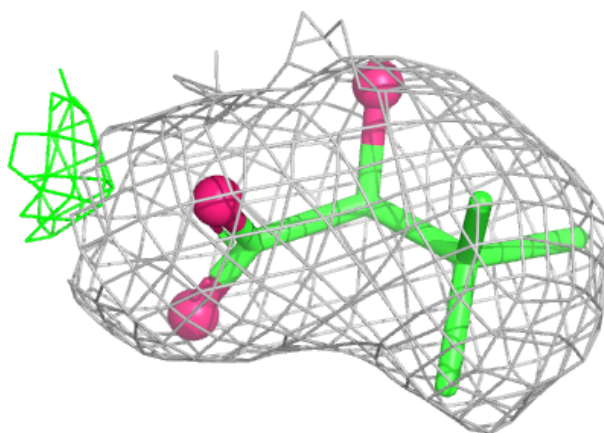
Electron density around G8I B 301:

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



Electron density around G8I E 301:

$2mF_o-DF_c$ (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.