Full wwPDB X-ray Structure Validation Report (i)

Nov 15, 2023 – 01:23 AM JST

PDB ID	:	6IQM
Title	:	Crystal Structure of Cell Surface Glyceraldehyde-3-Phosphate Dehydrogenase Complexed with NAD+ from Lactobacillus plantarum
Authors	:	Yoneda, K.; Kinoshita, H.
Deposited on	:	2018-11-08
Resolution	:	1.85 Å(reported)

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

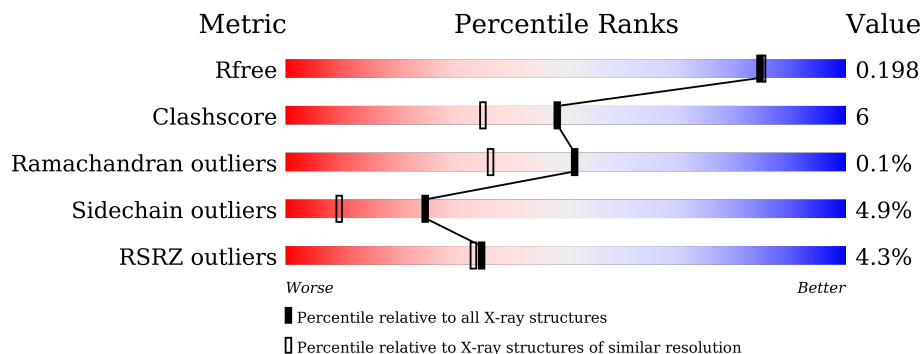|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.85 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	Percentile Ranks	Value
Rfree		0.198
Clashscore		6
Ramachandran outliers		0.1%
Sidechain outliers		4.9%
RSRZ outliers		4.3%

Worse   *Better*

▉ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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 <=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	340	.% / 88% / 9% · ·
1	B	340	6% / 80% / 11% · 5%
1	C	340	9% / 82% / 15% · ·
1	D	340	91% / 8% ·

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

| Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	TRS	B	401	-	X	X	-

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 11450 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 Glyceraldehyde-3-phosphate dehydrogenase, type I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	339	Total	C	N	O	S	0	0	0
			2558	1606	438	506	8			
1	B	323	Total	C	N	O	S	0	0	0
			2424	1520	416	481	7			
1	C	334	Total	C	N	O	S	0	0	0
			2519	1582	432	498	7			
1	D	340	Total	C	N	O	S	0	0	0
			2564	1609	439	508	8			

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).
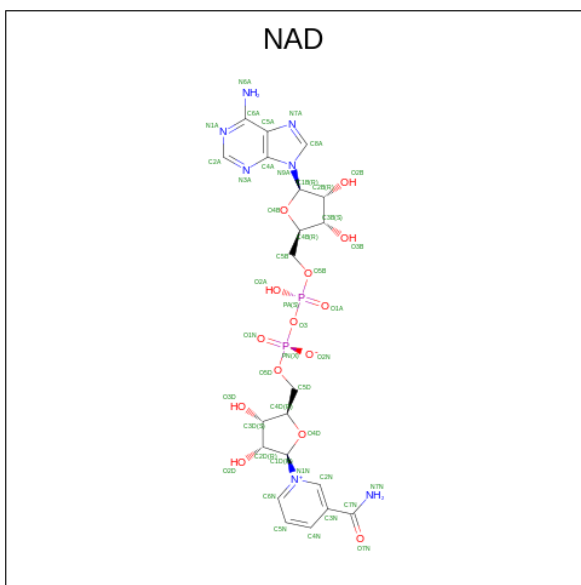
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).
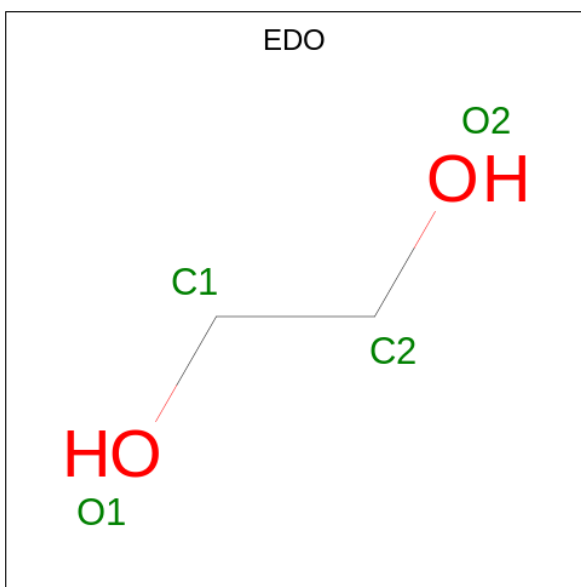
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).
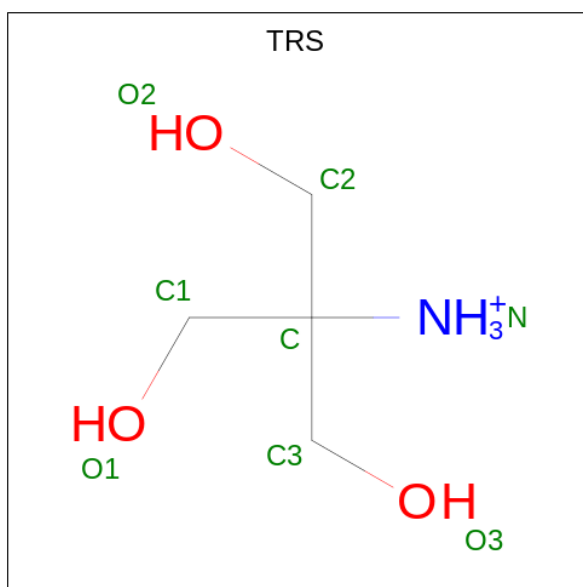
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total C N O				0	0
			8	4	1	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	292	Total O		0	0
			292	292		
5	B	279	Total O		0	0
			279	279		
5	C	278	Total O		0	0
			278	278		
5	D	332	Total O		0	0
			332	332		

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 p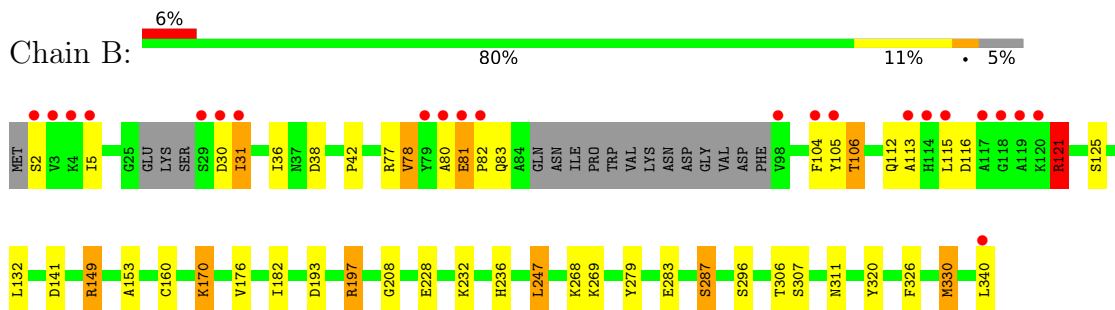roportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 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: Glyceraldehyde-3-phosphate dehydrogenase, type I
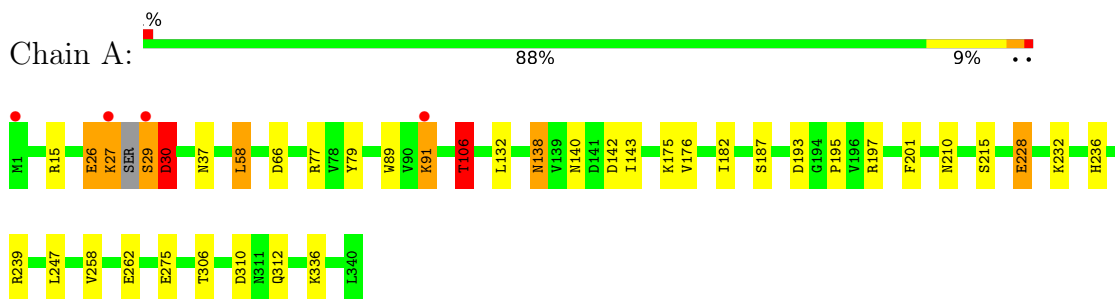
Chain A:

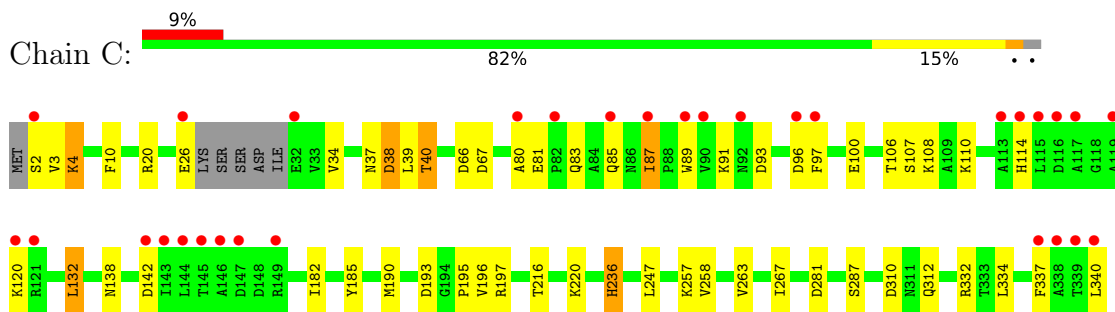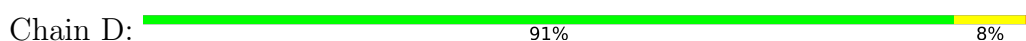• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase, type I

Chain B:

• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase, type I

Chain C:

• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase, type I

Chain D:

M1 E26 T40 S41 L44 D67 K74 R77 Q83 W89 V90 K91 D116 D131 L132 M179 I182 D193 R202 E228 H236 L247 D255 K256 K257 V258 E275 Q312 Y320 R332 T333 L334 L340

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	126.21Å　　171.95Å　　149.75Å 90.00°　　　90.00°　　　90.00°	Depositor
Resolution (Å)	101.74　–　1.85 49.28　–　1.85	Depositor EDS
% Data completeness (in resolution range)	99.0 (101.74-1.85) 99.0 (49.28-1.85)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.14 (at 1.84Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.159　,　0.190 0.170　,　0.198	Depositor DCC
R_{free} test set	6891 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	18.3	Xtriage
Anisotropy	0.019	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 51.1	EDS
L-test for twinning [2]	$< |L| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	11450	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.91% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: TRS, 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	1.04	3/2598 (0.1%)	1.05	12/3525 (0.3%)
1	B	1.09	0/2459	1.08	7/3335 (0.2%)
1	C	1.07	3/2559 (0.1%)	1.10	13/3474 (0.4%)
1	D	1.03	3/2605 (0.1%)	1.04	9/3536 (0.3%)
All	All	1.06	9/10221 (0.1%)	1.07	41/13870 (0.3%)

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	A	0	2
1	B	0	1
All	All	0	3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	275	GLU	CD-OE1	7.85	1.34	1.25
1	D	228	GLU	CD-OE2	6.83	1.33	1.25
1	D	275	GLU	CD-OE2	5.60	1.31	1.25
1	A	262	GLU	CD-OE2	5.58	1.31	1.25
1	A	228	GLU	CD-OE1	5.24	1.31	1.25
1	C	287	SER	CA-CB	5.14	1.60	1.52
1	D	228	GLU	CD-OE1	5.14	1.31	1.25
1	C	185	TYR	CG-CD2	5.08	1.45	1.39
1	C	38	ASP	CB-CG	5.00	1.62	1.51

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	77	ARG	NE-CZ-NH2	-9.16	115.72	120.30
1	A	193	ASP	CB-CG-OD1	8.31	125.78	118.30
1	C	193	ASP	CB-CG-OD1	7.81	125.33	118.30
1	D	193	ASP	CB-CG-OD1	7.63	125.17	118.30
1	B	197	ARG	NE-CZ-NH1	7.58	124.09	120.30
1	A	30	ASP	CB-CG-OD2	7.36	124.93	118.30
1	C	20	ARG	NE-CZ-NH1	7.20	123.90	120.30
1	A	15	ARG	NE-CZ-NH1	7.06	123.83	120.30
1	A	58	LEU	CB-CG-CD2	6.48	122.02	111.00
1	C	281	ASP	CB-CG-OD2	-6.44	112.51	118.30
1	A	201	PHE	CB-CG-CD2	-6.43	116.30	120.80
1	A	30	ASP	CB-CA-C	6.41	123.22	110.40
1	C	66	ASP	CB-CG-OD1	-6.39	112.55	118.30
1	B	287	SER	CA-CB-OG	-6.26	94.29	111.20
1	C	287	SER	CA-CB-OG	-6.22	94.41	111.20
1	C	66	ASP	CB-CG-OD2	6.21	123.89	118.30
1	A	66	ASP	CB-CG-OD2	-6.11	112.80	118.30
1	D	332	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	B	121	ARG	NE-CZ-NH1	5.95	123.28	120.30
1	D	131	ASP	CB-CG-OD1	5.91	123.61	118.30
1	B	193	ASP	CB-CG-OD1	5.83	123.54	118.30
1	D	116	ASP	CB-CG-OD2	-5.82	113.06	118.30
1	B	330	MET	CG-SD-CE	-5.82	90.89	100.20
1	C	281	ASP	CB-CG-OD1	5.80	123.52	118.30
1	C	193	ASP	CB-CG-OD2	-5.75	113.12	118.30
1	D	255	ASP	CB-CG-OD2	-5.69	113.18	118.30
1	C	190	MET	CA-CB-CG	5.67	122.95	113.30
1	A	106	THR	N-CA-CB	-5.58	99.70	110.30
1	B	141	ASP	CB-CG-OD1	5.50	123.25	118.30
1	B	170	LYS	CD-CE-NZ	5.49	124.34	111.70
1	C	93	ASP	CB-CG-OD2	5.45	123.21	118.30
1	C	38	ASP	CB-CG-OD1	5.41	123.17	118.30
1	A	239	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	A	193	ASP	CB-CG-OD2	-5.30	113.53	118.30
1	A	30	ASP	CB-CG-OD1	-5.28	113.55	118.30
1	D	202	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	C	332	ARG	NE-CZ-NH2	-5.25	117.68	120.30
1	A	187	SER	CA-CB-OG	-5.23	97.08	111.20
1	D	179	MET	CG-SD-CE	-5.22	91.85	100.20
1	D	67	ASP	CB-CG-OD1	5.16	122.94	118.30
1	C	67	ASP	CB-CG-OD1	5.15	122.93	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	26	GLU	Peptide
1	A	29	SER	Peptide
1	B	30	ASP	Peptide

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	2558	0	2544	32	0
1	B	2424	0	2413	38	0
1	C	2519	0	2499	33	0
1	D	2564	0	2550	13	0
2	A	44	0	26	6	0
2	B	44	0	26	0	0
2	C	44	0	26	0	0
2	D	44	0	26	0	0
3	A	8	0	12	0	0
3	B	4	0	6	0	0
3	C	4	0	6	0	0
3	D	4	0	6	0	0
4	B	8	0	11	9	0
5	A	292	0	0	19	0
5	B	279	0	0	11	0
5	C	278	0	0	11	0
5	D	332	0	0	5	0
All	All	11450	0	10151	122	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 6.

All (122) 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:C:196:VAL:HG12	5:C:675:HOH:O	1.38	1.19
1:A:215:SER:HB2	5:A:519:HOH:O	1.51	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:GLU:O	1:A:27:LYS:HB2	1.45	1.04
1:A:106:THR:HG21	5:A:764:HOH:O	1.59	0.99
1:C:40:THR:HB	5:C:510:HOH:O	1.63	0.98
1:B:113:ALA:HA	1:B:116:ASP:HB2	1.53	0.89
1:C:258:VAL:H	1:C:312:GLN:HE22	1.23	0.87
1:A:142:ASP:HB2	5:A:715:HOH:O	1.75	0.85
1:C:40:THR:CB	5:C:510:HOH:O	2.22	0.83
1:A:26:GLU:O	1:A:27:LYS:CB	2.28	0.82
1:B:5:ILE:HD11	1:B:31:ILE:HD11	1.63	0.80
4:B:401:TRS:H12	5:B:744:HOH:O	1.80	0.80
1:C:263:VAL:O	1:C:267:ILE:HD13	1.86	0.75
1:A:258:VAL:H	1:A:312:GLN:HE22	1.31	0.75
1:D:40:THR:HG22	5:D:783:HOH:O	1.86	0.75
4:B:401:TRS:H32	5:C:583:HOH:O	1.86	0.75
4:B:401:TRS:H31	5:B:744:HOH:O	1.89	0.71
1:A:336:LYS:HE3	5:A:569:HOH:O	1.89	0.71
1:C:247:LEU:O	1:C:247:LEU:HD12	1.91	0.70
1:D:182:ILE:HD13	1:D:247:LEU:HD11	1.74	0.70
1:A:336:LYS:CE	5:A:569:HOH:O	2.38	0.70
1:A:215:SER:CB	5:A:519:HOH:O	2.20	0.69
2:A:401:NAD:H3B	5:A:745:HOH:O	1.92	0.69
4:B:401:TRS:C3	5:B:744:HOH:O	2.40	0.68
1:C:142:ASP:HB2	5:C:750:HOH:O	1.93	0.68
1:A:37:ASN:ND2	2:A:401:NAD:H2A	2.09	0.67
1:D:258:VAL:H	1:D:312:GLN:HE22	1.41	0.67
4:B:401:TRS:H11	5:C:583:HOH:O	1.95	0.64
1:D:40:THR:HG21	1:D:44:LEU:HD23	1.79	0.64
1:B:283:GLU:CD	5:B:545:HOH:O	2.36	0.63
1:A:306:THR:HG22	1:B:176:VAL:CG2	2.28	0.63
1:B:36:ILE:HB	1:B:78:VAL:HG23	1.81	0.63
2:A:401:NAD:O1N	2:A:401:NAD:N7N	2.30	0.63
1:C:216:THR:HG22	1:C:236:HIS:HA	1.82	0.62
1:D:40:THR:HG22	1:D:41:SER:H	1.65	0.62
1:A:176:VAL:CG2	1:B:306:THR:HG22	2.30	0.62
1:B:104:PHE:HD1	1:B:105:TYR:CE2	2.18	0.62
1:A:37:ASN:HD22	2:A:401:NAD:H2A	1.65	0.61
1:B:104:PHE:HB2	5:B:761:HOH:O	2.01	0.60
1:C:197:ARG:HD3	5:C:668:HOH:O	2.01	0.60
1:B:121:ARG:NH2	1:B:340:LEU:HB2	2.17	0.60
1:C:247:LEU:HD12	1:C:247:LEU:C	2.24	0.58
1:C:96:ASP:HB2	1:C:120:LYS:HD3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:247:LEU:HD12	1:B:247:LEU:O	2.06	0.56
1:A:91:LYS:HE3	5:A:501:HOH:O	2.04	0.56
1:C:258:VAL:H	1:C:312:GLN:NE2	2.00	0.55
1:C:85:GLN:CG	5:C:501:HOH:O	2.53	0.55
2:A:401:NAD:H8A	5:A:751:HOH:O	2.07	0.55
5:B:501:HOH:O	1:D:40:THR:HG23	2.06	0.55
1:B:228:GLU:O	1:B:232:LYS:HE2	2.06	0.54
1:C:3:VAL:HG13	1:C:96:ASP:OD1	2.07	0.54
1:A:247:LEU:HD12	1:A:247:LEU:O	2.08	0.54
1:B:106:THR:HB	5:B:671:HOH:O	2.08	0.53
1:C:81:GLU:HB3	1:C:87:ILE:HG23	1.91	0.53
1:B:182:ILE:HD13	1:B:247:LEU:HD11	1.90	0.52
4:B:401:TRS:C1	5:C:583:HOH:O	2.54	0.52
1:A:182:ILE:CD1	1:A:247:LEU:HD11	2.40	0.52
1:C:258:VAL:N	1:C:312:GLN:HE22	2.02	0.51
1:B:104:PHE:HB2	5:B:734:HOH:O	2.11	0.51
1:A:138:ASN:CG	5:A:517:HOH:O	2.48	0.51
1:C:85:GLN:HG3	5:C:501:HOH:O	2.10	0.50
1:D:40:THR:CG2	5:D:783:HOH:O	2.52	0.50
1:C:138:ASN:CG	5:C:603:HOH:O	2.50	0.50
1:C:38:ASP:O	1:C:80:ALA:HA	2.12	0.50
1:C:39:LEU:C	1:C:40:THR:HG22	2.32	0.49
1:B:115:LEU:HD21	1:B:149:ARG:HB3	1.93	0.49
1:D:275:GLU:HG2	5:D:669:HOH:O	2.11	0.49
1:B:121:ARG:HH21	1:B:340:LEU:HB2	1.76	0.49
1:A:77:ARG:HG2	1:A:79:TYR:CZ	2.47	0.49
1:D:258:VAL:H	1:D:312:GLN:NE2	2.11	0.48
1:A:210:ASN:OD1	1:B:287:SER:HB2	2.14	0.48
1:A:106:THR:HG22	5:A:727:HOH:O	2.13	0.47
1:C:37:ASN:ND2	1:C:87:ILE:HD13	2.29	0.47
1:A:195:PRO:HB3	1:C:40:THR:HG21	1.97	0.47
2:A:401:NAD:C6N	5:A:680:HOH:O	2.62	0.47
1:B:42:PRO:HG3	1:B:78:VAL:CG1	2.45	0.47
4:B:401:TRS:H22	5:B:744:HOH:O	2.15	0.46
1:C:2:SER:OG	1:C:4:LYS:CE	2.64	0.46
1:B:160:CYS:HA	1:B:296:SER:HB2	1.97	0.46
1:A:182:ILE:HD13	1:A:247:LEU:HD11	1.97	0.45
5:A:545:HOH:O	4:B:401:TRS:H11	2.16	0.45
1:B:330:MET:HE3	1:B:330:MET:HB2	1.52	0.45
1:B:104:PHE:HD2	5:B:761:HOH:O	1.99	0.45
1:B:113:ALA:CA	1:B:116:ASP:HB2	2.36	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:74:LYS:HG3	5:D:593:HOH:O	2.17	0.45
1:B:106:THR:HG23	1:B:106:THR:O	2.17	0.45
1:C:3:VAL:CG1	1:C:96:ASP:OD1	2.65	0.44
1:B:153:ALA:HB3	1:B:330:MET:HE2	2.00	0.44
1:B:247:LEU:HD12	1:B:247:LEU:C	2.37	0.44
1:A:215:SER:C	5:A:519:HOH:O	2.56	0.44
1:A:247:LEU:HD12	1:A:247:LEU:C	2.37	0.44
1:B:326:PHE:CE2	1:B:330:MET:HE1	2.52	0.44
1:B:81:GLU:OE1	1:B:83:GLN:O	2.36	0.44
1:A:195:PRO:CG	1:C:40:THR:HG21	2.48	0.44
1:B:38:ASP:O	1:B:80:ALA:HA	2.18	0.43
1:B:112:GLN:OE1	1:B:115:LEU:HD12	2.18	0.43
1:D:83:GLN:NE2	5:D:511:HOH:O	2.50	0.43
1:B:125:SER:HA	1:B:330:MET:CE	2.48	0.43
1:C:263:VAL:O	1:C:267:ILE:CD1	2.60	0.43
1:B:106:THR:HG22	5:B:724:HOH:O	2.16	0.43
1:A:138:ASN:ND2	5:A:517:HOH:O	2.50	0.43
1:A:140:ASN:O	1:A:143:ILE:HG12	2.19	0.43
1:C:107:SER:HB2	1:C:110:LYS:H	1.84	0.43
1:D:258:VAL:N	1:D:312:GLN:HE22	2.12	0.43
1:B:106:THR:O	1:B:106:THR:CG2	2.68	0.42
1:C:38:ASP:OD2	1:C:40:THR:CG2	2.68	0.42
1:C:100:GLU:OE1	1:C:114:HIS:HE1	2.02	0.42
1:B:268:LYS:HE3	1:B:279:TYR:CZ	2.55	0.41
1:A:175:LYS:HD3	1:B:311:ASN:ND2	2.35	0.41
1:C:108:LYS:HE3	1:C:132:LEU:HB3	2.02	0.41
1:B:182:ILE:CD1	1:B:247:LEU:HD11	2.50	0.41
1:A:228:GLU:HG3	5:A:714:HOH:O	2.20	0.41
1:B:208:GLY:O	4:B:401:TRS:O2	2.39	0.41
1:A:142:ASP:CB	5:A:715:HOH:O	2.49	0.41
1:B:81:GLU:OE2	1:B:82:PRO:HD2	2.21	0.41
1:C:182:ILE:CD1	1:C:247:LEU:HD11	2.51	0.41
1:D:257:LYS:HA	1:D:312:GLN:HE22	1.85	0.41
1:A:228:GLU:O	1:A:232:LYS:HE2	2.21	0.41
5:A:541:HOH:O	1:C:195:PRO:CG	2.69	0.40
1:A:197:ARG:NH1	5:A:508:HOH:O	2.42	0.40
1:C:97:PHE:HZ	1:C:337:PHE:CD1	2.39	0.40
1:B:104:PHE:HD1	1:B:105:TYR:CZ	2.38	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	335/340 (98%)	324 (97%)	10 (3%)	1 (0%)	41	26
1	B	317/340 (93%)	302 (95%)	15 (5%)	0	100	100
1	C	330/340 (97%)	317 (96%)	13 (4%)	0	100	100
1	D	338/340 (99%)	326 (96%)	12 (4%)	0	100	100
All	All	1320/1360 (97%)	1269 (96%)	50 (4%)	1 (0%)	51	36

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	30	ASP

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	276/277 (100%)	265 (96%)	11 (4%)	31	14
1	B	261/277 (94%)	245 (94%)	16 (6%)	18	5
1	C	271/277 (98%)	254 (94%)	17 (6%)	18	4
1	D	277/277 (100%)	268 (97%)	9 (3%)	39	22
All	All	1085/1108 (98%)	1032 (95%)	53 (5%)	25	9

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	LYS
1	A	29	SER
1	A	30	ASP
1	A	58	LEU
1	A	89	TRP
1	A	91	LYS
1	A	106	THR
1	A	132	LEU
1	A	138	ASN
1	A	236	HIS
1	A	310	ASP
1	B	2	SER
1	B	31	ILE
1	B	77	ARG
1	B	78	VAL
1	B	81	GLU
1	B	106	THR
1	B	121	ARG
1	B	132	LEU
1	B	149	ARG
1	B	170	LYS
1	B	197	ARG
1	B	236	HIS
1	B	247	LEU
1	B	269	LYS
1	B	307	SER
1	B	320	TYR
1	C	4	LYS
1	C	10	PHE
1	C	26	GLU
1	C	34	VAL
1	C	40	THR
1	C	83	GLN
1	C	87	ILE
1	C	89	TRP
1	C	91	LYS
1	C	106	THR
1	C	132	LEU
1	C	220	LYS
1	C	236	HIS
1	C	257	LYS
1	C	310	ASP
1	C	334	LEU

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Mol	Chain	Res	Type
1	C	340	LEU
1	D	1	MET
1	D	26	GLU
1	D	40	THR
1	D	89	TRP
1	D	91	LYS
1	D	132	LEU
1	D	236	HIS
1	D	320	TYR
1	D	334	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	234	GLN
1	A	312	GLN
1	B	311	ASN
1	C	75	ASN
1	C	83	GLN
1	C	114	HIS
1	C	312	GLN
1	D	83	GLN
1	D	86	ASN
1	D	312	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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

10 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	C	401	-	42,48,48	1.29	6 (14%)	50,73,73	1.34	7 (14%)
3	EDO	A	403	-	3,3,3	0.47	0	2,2,2	0.32	0
4	TRS	B	401	-	7,7,7	1.73	2 (28%)	9,9,9	3.17	7 (77%)
3	EDO	A	402	-	3,3,3	0.79	0	2,2,2	0.67	0
3	EDO	C	402	-	3,3,3	0.47	0	2,2,2	0.27	0
2	NAD	A	401	-	42,48,48	1.66	7 (16%)	50,73,73	2.09	14 (28%)
3	EDO	D	402	-	3,3,3	0.36	0	2,2,2	0.28	0
3	EDO	B	403	-	3,3,3	0.55	0	2,2,2	0.12	0
2	NAD	B	402	-	42,48,48	1.21	4 (9%)	50,73,73	1.34	7 (14%)
2	NAD	D	401	-	42,48,48	1.44	9 (21%)	50,73,73	1.45	8 (16%)

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	C	401	-	-	6/26/62/62	0/5/5/5
3	EDO	A	403	-	-	0/1/1/1	-
4	TRS	B	401	-	-	8/9/9/9	-
3	EDO	A	402	-	-	0/1/1/1	-
3	EDO	C	402	-	-	0/1/1/1	-
2	NAD	A	401	-	-	6/26/62/62	0/5/5/5
3	EDO	D	402	-	-	0/1/1/1	-
3	EDO	B	403	-	-	1/1/1/1	-
2	NAD	B	402	-	-	6/26/62/62	0/5/5/5
2	NAD	D	401	-	-	5/26/62/62	0/5/5/5

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	NAD	O4B-C1B	5.51	1.48	1.41
2	A	401	NAD	C5A-C4A	3.69	1.50	1.40
2	A	401	NAD	O4D-C1D	3.49	1.45	1.41
2	D	401	NAD	PN-O2N	-3.21	1.40	1.55
2	D	401	NAD	PA-O2A	-3.07	1.40	1.55
2	A	401	NAD	PN-O5D	2.96	1.71	1.59
2	B	402	NAD	C4A-N3A	-2.94	1.31	1.35
4	B	401	TRS	O2-C2	-2.88	1.32	1.42
2	C	401	NAD	O7N-C7N	-2.82	1.18	1.24
2	B	402	NAD	PN-O2N	-2.82	1.42	1.55
2	C	401	NAD	PA-O2A	-2.72	1.42	1.55
2	C	401	NAD	PA-O1A	-2.64	1.41	1.50
2	C	401	NAD	PN-O2N	-2.61	1.43	1.55
2	D	401	NAD	PA-O1A	-2.53	1.41	1.50
2	B	402	NAD	PA-O2A	-2.50	1.43	1.55
2	D	401	NAD	C6N-N1N	-2.43	1.29	1.35
2	A	401	NAD	O2B-C2B	2.39	1.48	1.43
2	B	402	NAD	O7N-C7N	-2.38	1.19	1.24
2	D	401	NAD	O4B-C4B	-2.37	1.39	1.45
4	B	401	TRS	C-N	2.35	1.57	1.49
2	A	401	NAD	C3B-C4B	2.25	1.58	1.53
2	A	401	NAD	C4A-N3A	2.18	1.38	1.35
2	C	401	NAD	C5A-C4A	2.16	1.46	1.40
2	D	401	NAD	O7N-C7N	-2.12	1.20	1.24
2	D	401	NAD	C4A-N3A	-2.09	1.32	1.35
2	D	401	NAD	C5A-N7A	-2.05	1.32	1.39
2	C	401	NAD	C6N-N1N	-2.03	1.30	1.35
2	D	401	NAD	O5B-C5B	-2.00	1.37	1.44

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	NAD	C3N-C7N-N7N	6.06	125.02	117.75
2	A	401	NAD	O7N-C7N-C3N	-5.16	113.46	119.63
2	A	401	NAD	C6N-N1N-C2N	-5.14	117.29	121.97
4	B	401	TRS	O3-C3-C	5.12	127.23	111.00
2	A	401	NAD	O2B-C2B-C3B	4.22	125.46	111.82
4	B	401	TRS	C2-C-N	4.15	120.38	107.98
4	B	401	TRS	O2-C2-C	4.15	124.15	111.00
2	A	401	NAD	O3D-C3D-C4D	-4.15	99.05	111.05
4	B	401	TRS	C2-C-C1	-3.84	98.91	110.81
2	D	401	NAD	C3N-C7N-N7N	3.83	122.34	117.75
2	D	401	NAD	N3A-C2A-N1A	-3.59	123.07	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	402	NAD	N3A-C2A-N1A	-3.44	123.31	128.68
2	C	401	NAD	C4A-C5A-N7A	-3.40	105.85	109.40
2	C	401	NAD	N3A-C2A-N1A	-3.38	123.39	128.68
2	A	401	NAD	O5B-PA-O1A	3.16	121.43	109.07
2	A	401	NAD	C2A-N1A-C6A	2.97	123.83	118.75
2	B	402	NAD	C4A-C5A-N7A	-2.87	106.41	109.40
2	B	402	NAD	C2A-N1A-C6A	2.82	123.58	118.75
2	D	401	NAD	C3N-C2N-N1N	2.78	123.15	120.43
2	B	402	NAD	C1B-N9A-C4A	-2.78	121.76	126.64
2	A	401	NAD	C5N-C4N-C3N	-2.58	117.29	120.34
2	A	401	NAD	N6A-C6A-N1A	2.57	123.92	118.57
2	A	401	NAD	N3A-C2A-N1A	-2.47	124.81	128.68
2	C	401	NAD	C3N-C7N-N7N	2.41	120.65	117.75
2	D	401	NAD	C4A-C5A-N7A	-2.39	106.91	109.40
2	D	401	NAD	C2A-N1A-C6A	2.35	122.78	118.75
2	C	401	NAD	C2N-N1N-C1D	2.33	124.33	119.14
2	A	401	NAD	C2B-C3B-C4B	2.31	107.14	102.64
4	B	401	TRS	O1-C1-C	2.29	118.27	111.00
2	A	401	NAD	O3D-C3D-C2D	2.29	119.24	111.82
2	A	401	NAD	C3N-C2N-N1N	2.29	122.67	120.43
2	D	401	NAD	O7N-C7N-N7N	-2.27	119.35	122.58
2	B	402	NAD	C6N-N1N-C2N	-2.26	119.92	121.97
2	D	401	NAD	C2N-C3N-C4N	-2.25	115.71	118.26
2	D	401	NAD	C2N-C3N-C7N	2.22	125.91	119.46
2	B	402	NAD	C2N-N1N-C1D	2.21	124.05	119.14
2	B	402	NAD	O7N-C7N-C3N	2.15	122.20	119.63
2	C	401	NAD	O2A-PA-O1A	2.12	122.73	112.24
4	B	401	TRS	C3-C-C2	-2.09	104.34	110.81
2	C	401	NAD	C5B-C4B-C3B	-2.04	107.52	115.18
2	A	401	NAD	O5D-PN-O1N	-2.02	101.16	109.07
2	C	401	NAD	C6N-N1N-C2N	-2.02	120.13	121.97
4	B	401	TRS	C3-C-N	2.01	113.99	107.98

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	NAD	O4D-C4D-C5D-O5D
2	A	401	NAD	O4D-C1D-N1N-C2N
2	A	401	NAD	O4D-C1D-N1N-C6N
2	B	402	NAD	O4D-C1D-N1N-C2N
2	B	402	NAD	O4D-C1D-N1N-C6N

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Mol	Chain	Res	Type	Atoms
2	B	402	NAD	C2D-C1D-N1N-C6N
2	C	401	NAD	O4D-C1D-N1N-C2N
2	C	401	NAD	O4D-C1D-N1N-C6N
2	C	401	NAD	C2D-C1D-N1N-C2N
2	C	401	NAD	C2D-C1D-N1N-C6N
2	D	401	NAD	O4D-C1D-N1N-C2N
2	D	401	NAD	O4D-C1D-N1N-C6N
2	D	401	NAD	C2D-C1D-N1N-C2N
2	D	401	NAD	C2D-C1D-N1N-C6N
4	B	401	TRS	N-C-C1-O1
4	B	401	TRS	C2-C-C3-O3
2	A	401	NAD	C3D-C4D-C5D-O5D
2	B	402	NAD	O4B-C4B-C5B-O5B
2	C	401	NAD	O4B-C4B-C5B-O5B
2	C	401	NAD	C3B-C4B-C5B-O5B
4	B	401	TRS	C1-C-C2-O2
4	B	401	TRS	N-C-C2-O2
4	B	401	TRS	C1-C-C3-O3
2	D	401	NAD	O4B-C4B-C5B-O5B
4	B	401	TRS	C3-C-C1-O1
4	B	401	TRS	C3-C-C2-O2
2	A	401	NAD	PN-O3-PA-O1A
3	B	403	EDO	O1-C1-C2-O2
2	B	402	NAD	C2D-C1D-N1N-C2N
4	B	401	TRS	N-C-C3-O3
2	A	401	NAD	O4B-C4B-C5B-O5B
2	B	402	NAD	C3B-C4B-C5B-O5B

There are no ring outliers.

2 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	401	TRS	9	0
2	A	401	NAD	6	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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring
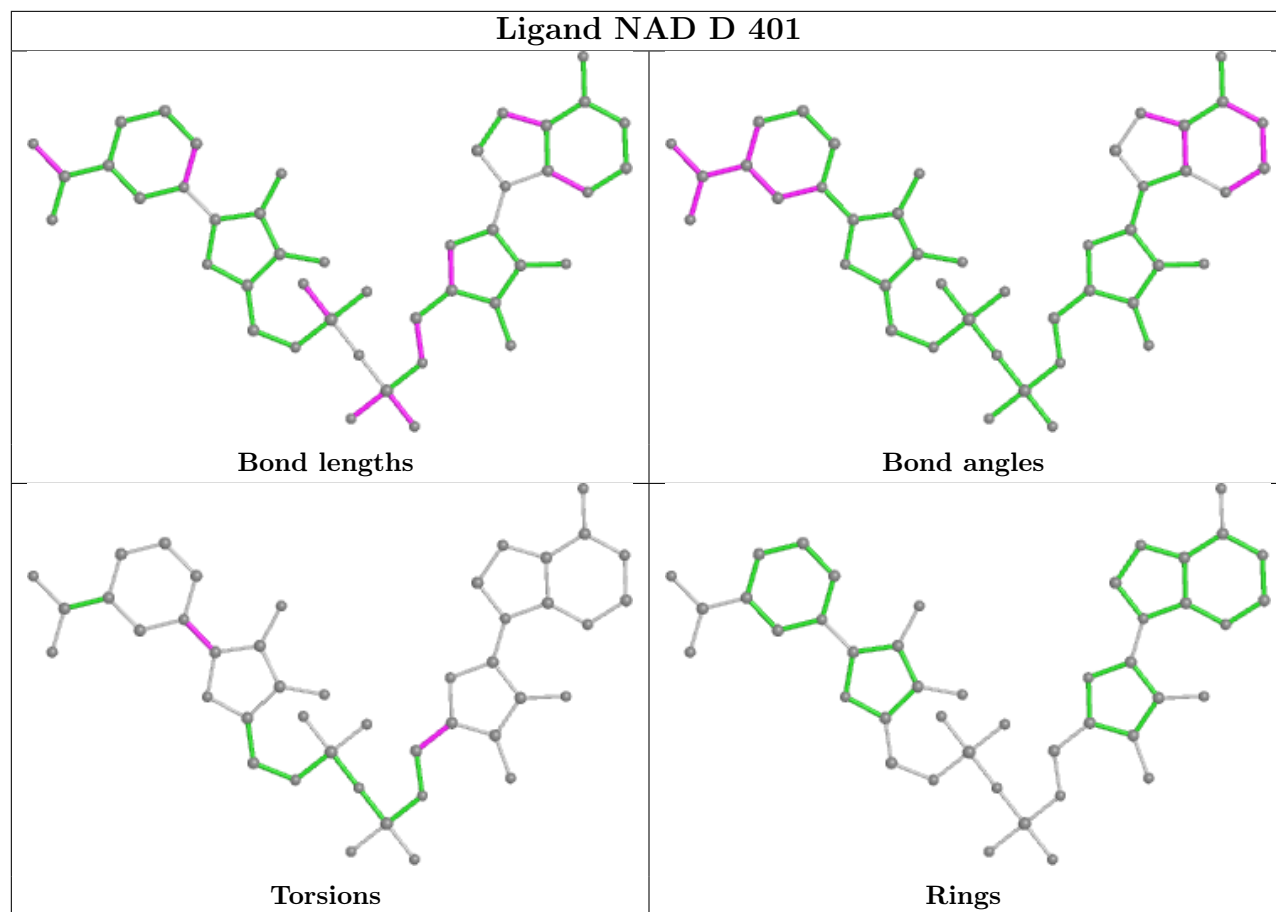
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand NAD C 401

Bond lengths

Bond angles

Torsions

Rings

Ligand NAD A 401

Bond lengths

Bond angles

Torsions

Rings

Ligand NAD B 402

Bond lengths

Bond angles

Torsions

Rings

Ligand NAD D 401

Bond lengths

Bond angles

Torsions

Rings
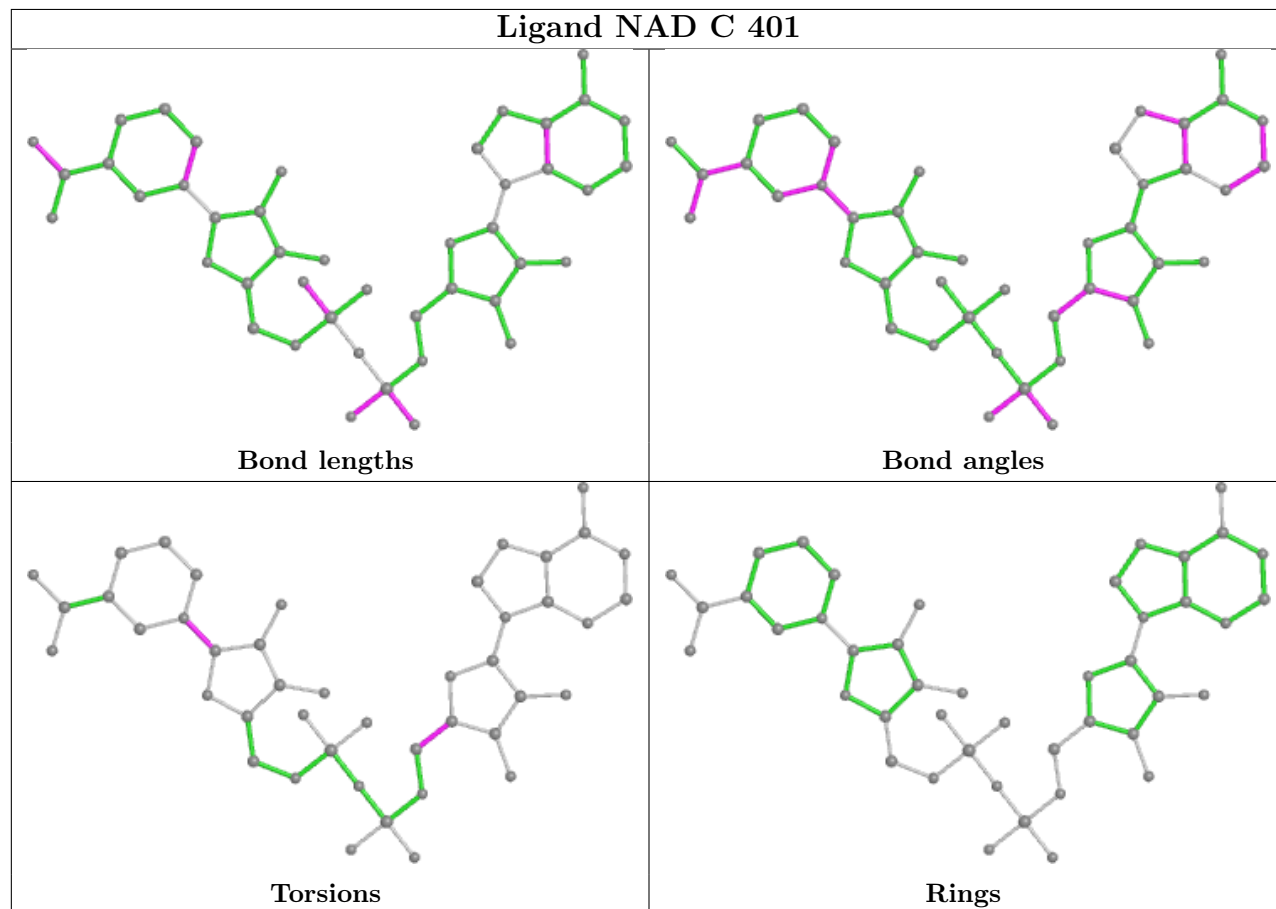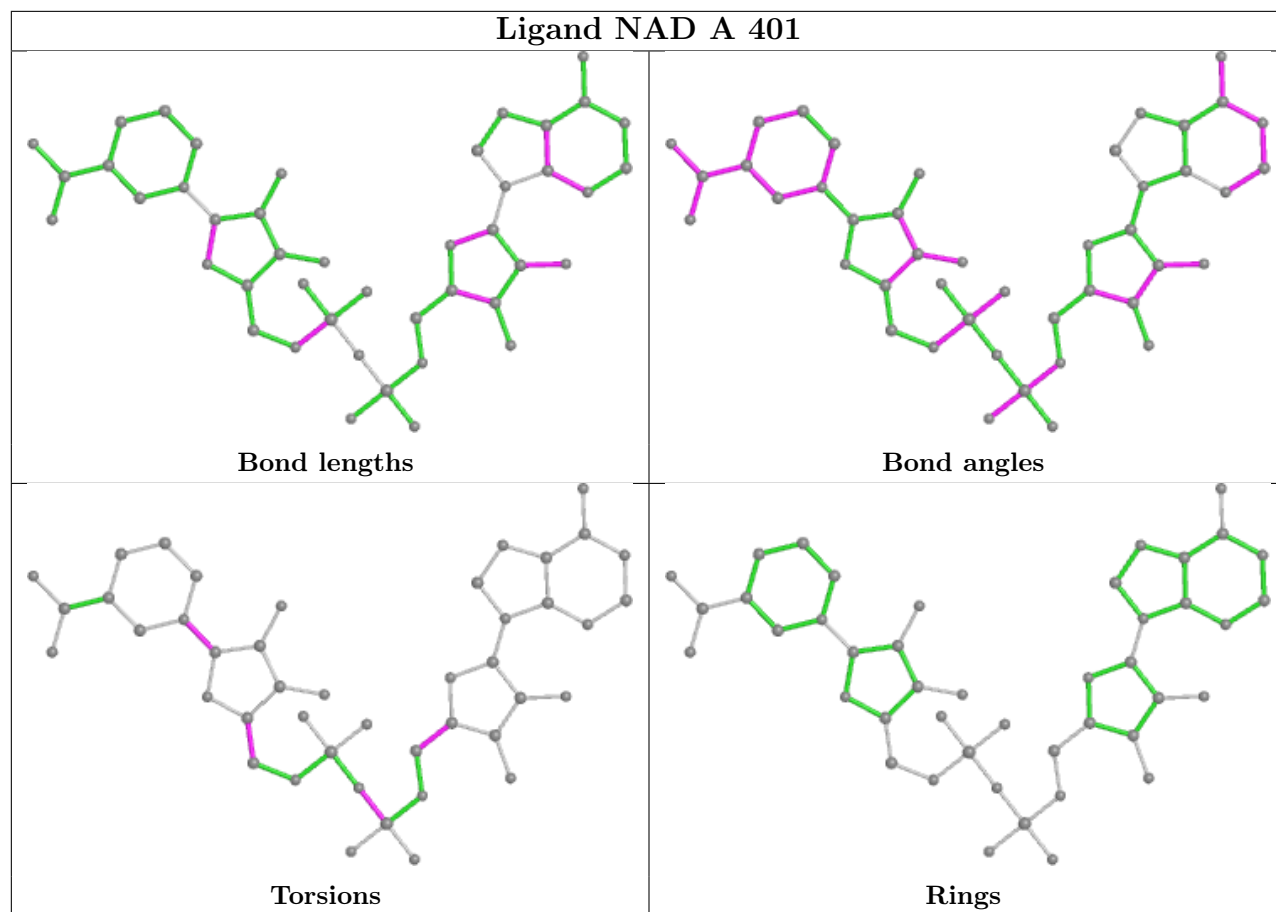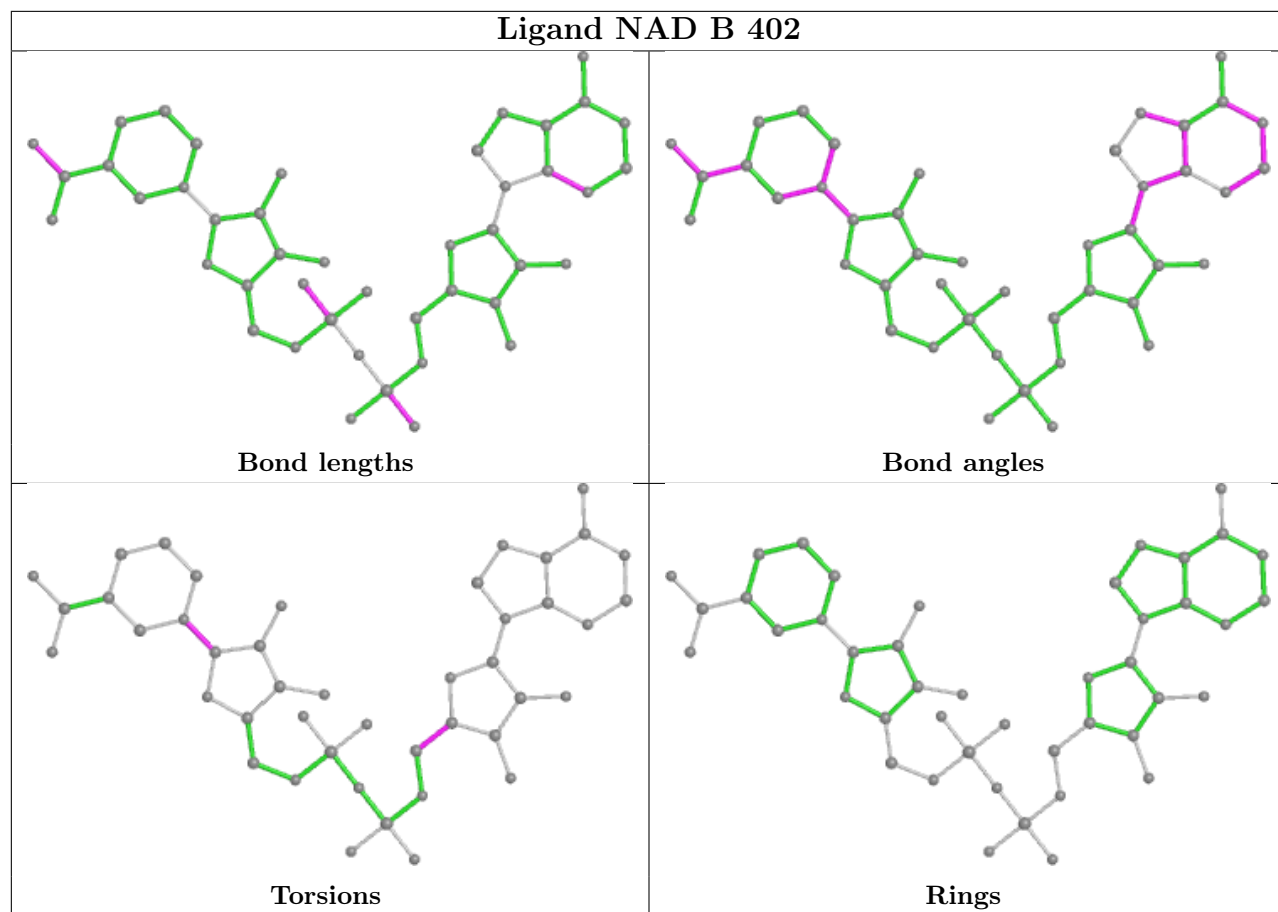
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	339/340 (99%)	-0.19	4 (1%)	79	79	11, 18, 38, 61	0
1	B	323/340 (95%)	-0.04	22 (6%)	17	16	11, 19, 52, 74	0
1	C	334/340 (98%)	0.27	31 (9%)	8	8	11, 21, 45, 64	0
1	D	340/340 (100%)	-0.38	1 (0%)	94	93	11, 17, 31, 54	0
All	All	1336/1360 (98%)	-0.09	58 (4%)	35	33	11, 18, 43, 74	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	29	SER	6.3
1	A	1	MET	5.6
1	B	104	PHE	4.8
1	B	3	VAL	4.4
1	C	149	ARG	4.4
1	B	2	SER	4.3
1	C	338	ALA	4.2
1	B	82	PRO	4.0
1	B	31	ILE	4.0
1	B	118	GLY	4.0
1	C	97	PHE	3.9
1	A	27	LYS	3.8
1	C	87	ILE	3.6
1	C	80	ALA	3.6
1	C	89	TRP	3.5
1	D	1	MET	3.5
1	B	113	ALA	3.5
1	C	340	LEU	3.5
1	B	4	LYS	3.4
1	C	145	THR	3.4
1	B	81	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	146	ALA	3.3
1	B	340	LEU	3.2
1	C	339	THR	3.1
1	C	337	PHE	3.1
1	C	147	ASP	3.1
1	C	114	HIS	3.1
1	B	105	TYR	2.9
1	C	119	ALA	2.9
1	C	143	ILE	2.9
1	C	32	GLU	2.9
1	B	30	ASP	2.8
1	C	90	VAL	2.8
1	B	29	SER	2.8
1	C	144	LEU	2.7
1	B	120	LYS	2.7
1	B	119	ALA	2.6
1	B	114	HIS	2.6
1	C	82	PRO	2.6
1	C	115	LEU	2.6
1	B	117	ALA	2.6
1	C	120	LYS	2.5
1	C	113	ALA	2.5
1	B	80	ALA	2.5
1	B	5	ILE	2.5
1	B	115	LEU	2.4
1	C	142	ASP	2.4
1	C	2	SER	2.3
1	A	91	LYS	2.3
1	B	98	VAL	2.3
1	B	79	TYR	2.3
1	C	121	ARG	2.2
1	C	26	GLU	2.2
1	C	92	ASN	2.1
1	C	116	ASP	2.1
1	C	85	GLN	2.1
1	C	96	ASP	2.0
1	C	117	ALA	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 (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
2	NAD	A	401	44/44	0.76	0.27	32,52,72,78	0
4	TRS	B	401	8/8	0.87	0.22	11,15,24,24	0
3	EDO	B	403	4/4	0.93	0.08	24,25,27,28	0
3	EDO	A	403	4/4	0.95	0.15	20,20,20,20	0
2	NAD	B	402	44/44	0.95	0.13	19,25,28,31	0
2	NAD	C	401	44/44	0.95	0.10	18,23,27,29	0
3	EDO	C	402	4/4	0.96	0.07	18,18,19,21	0
3	EDO	D	402	4/4	0.97	0.08	18,19,21,21	0
3	EDO	A	402	4/4	0.97	0.08	20,22,22,25	0
2	NAD	D	401	44/44	0.98	0.06	13,16,17,18	0

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

Electron density around NAD A 401:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
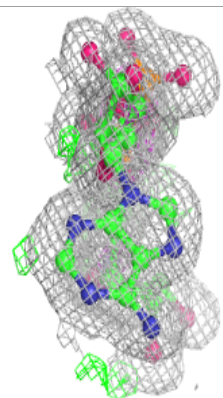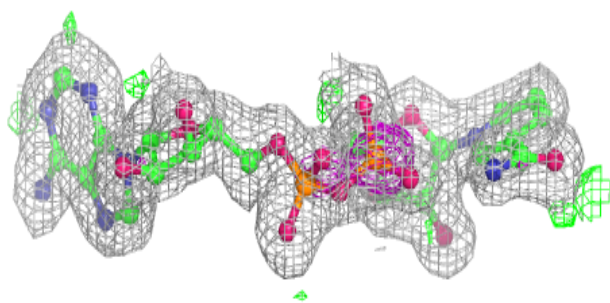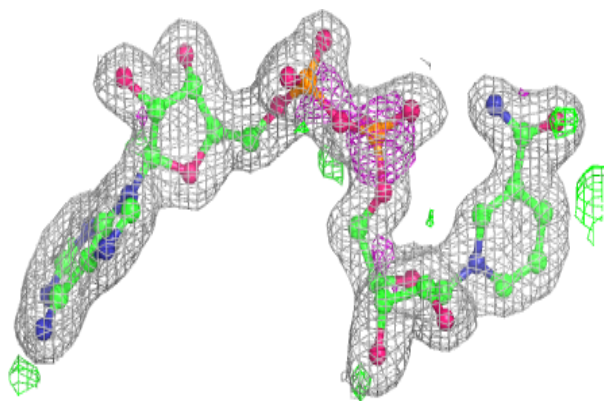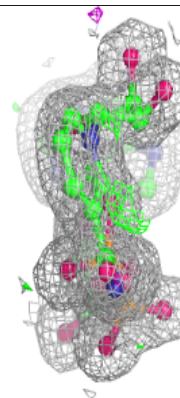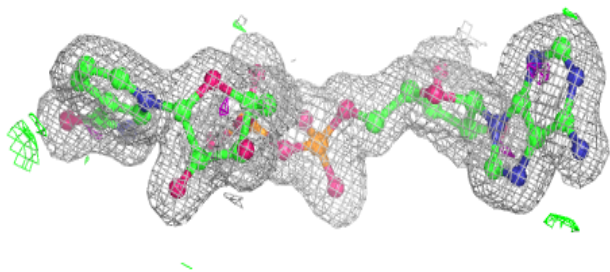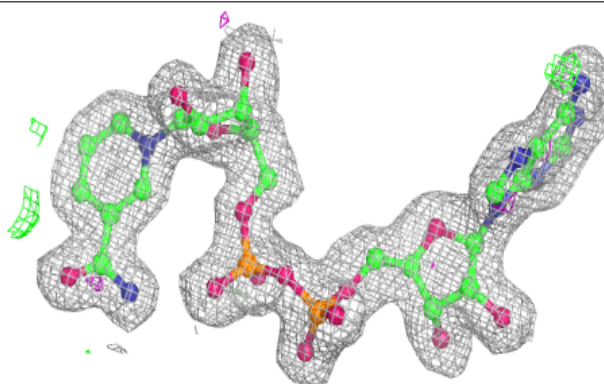and green (positive)
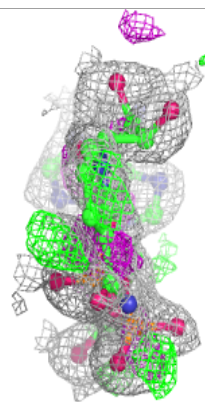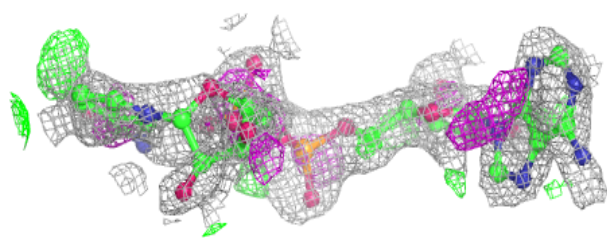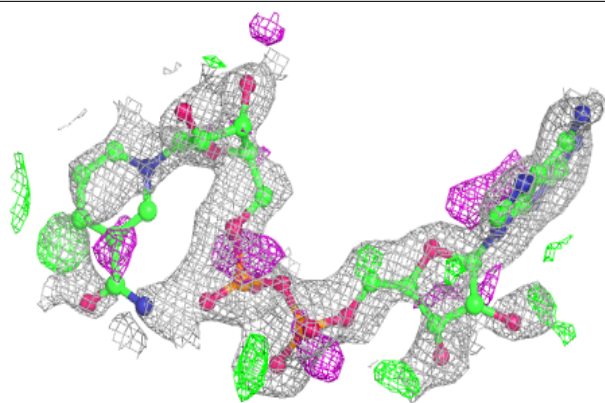
Electron density around NAD B 402:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
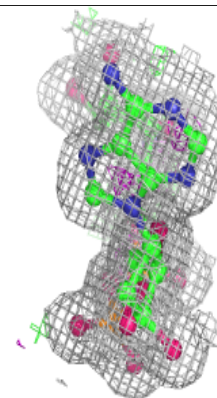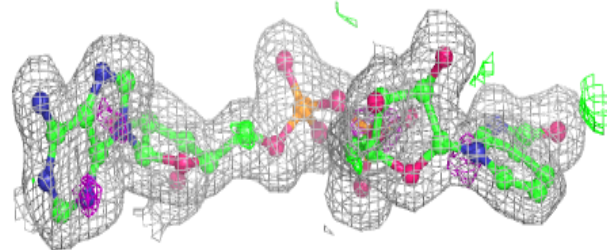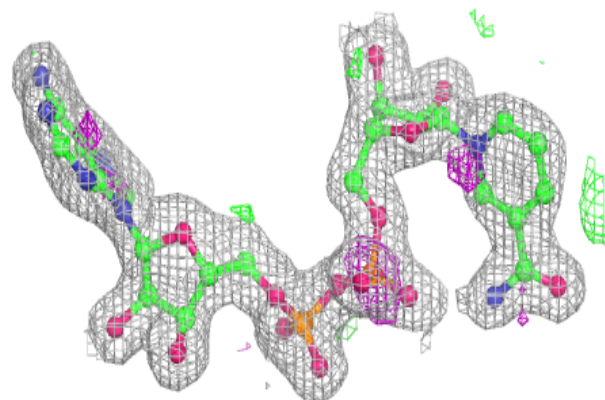
Electron density around NAD C 401:

$2mF_o$-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 401:

$2mF_o$-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.